

# Regression Methods

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**Dictionary**

- ☐ **Regression:** (statistics) a measure of the relation between the mean value of
  - one variable (e.g., output), denoted  $y$  (the **response variable**) and
  - corresponding values of other variables (e.g., time and cost), denoted  $x$  (**explanatory variables**).
- ☐ The explanatory variables are also called **covariates** or **features** (ML).
- ☐ We avoid the terms **dependent variable** ( $Y$ ) and **independent variable** ( $x$ ) used in older books.
- ☐ Questions we try and answer:
  - (**description/explanation**) how does  $y$  depend on  $x$ ? How much of the variation of  $y$  is due to  $x$ ? Do I need all of  $x$  to explain the variation in  $y$ ?
  - (**prediction**) what will  $y$  be if  $x = x_+$ ?
  - (**causation**) if I change  $x$ , what will happen to  $y$ ?
- ☐ The causation question presupposes that we can change (some of)  $x$ , which is not always true.

**Linear model**

- ☐ Simplest explanation of  $y$  in terms of  $x$  is **linear model**:

$$y = g(x) = x_1\beta_1 + \dots + x_p\beta_p = x^T\beta,$$

where

$$y \in \mathbb{R}, \quad x^T = (x_1, \dots, x_p) \in \mathbb{R}^p, \quad \beta^T = (\beta_1, \dots, \beta_p) \in \mathbb{R}^p.$$

- ☐ The data consist of  $n$  **instances/examples/cases**  $(x_j, y_j)$  for  $j = 1, \dots, n$ , so

$$y_{n \times 1} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \quad X_{n \times p} = \begin{pmatrix} x_{11} & \dots & x_{1p} \\ \vdots & \vdots & \vdots \\ x_{n1} & \dots & x_{np} \end{pmatrix}, \quad \beta_{p \times 1} = \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_p \end{pmatrix}$$

and we write

$$y = X\beta.$$

- ☐ **Key point:** linearity refers to linearity in  $\beta$ , not in terms of elements of  $X$ , which might be polynomials, or basis functions, or ...
- ☐ Sometimes we can transform to a linear model. For example, the multiplicative expression  $y = \gamma x_1^{\beta_1} x_2^{\beta_2}$  becomes

$$\log y = \log \gamma + \beta_1 \log x_1 + \beta_2 \log x_2.$$

## Notation

- ☐ Vectors are column vectors
- ☐ We write  $X_{n \times p}$  to give the dimensions of a matrix or vector
- ☐  $a^T$  (row vector) is the transpose of  $a$  (column vector)
- ☐  $j \in \{1, \dots, n\}$  (or sometimes  $i$ ) indexes the rows of  $y$  (cases/examples)
- ☐  $x_j^T$  is the  $j$ th row of  $X$
- ☐  $r, s, t, \dots \in \{1, \dots, p\}$  indexes the columns of  $X$  (covariates/features)
- ☐ Roman letters ( $y, X, z, \dots$ ) denote observed quantities, and may be the realisations of random variables
- ☐ Greek letters ( $\beta, \gamma, \theta, \sigma, \dots$ ) denote unknown (often vector) parameters of models
- ☐  $\hat{\beta}$  denotes an estimate of  $\beta$
- ☐  $\alpha$  denotes the level of significance tests and confidence intervals
- ☐ If  $Q$  is scalar (or a row vector) and  $\beta$  is a vector, then  $\partial Q / \partial \beta$  denotes the vector (or matrix) the same shape as  $\beta$  with elements  $\partial Q / \partial \beta_r$ .
- ☐ If  $Q$  is scalar and  $\beta, \gamma$  are vectors, then  $\partial^2 Q / \partial \beta \partial \gamma^T$  denotes the matrix with  $(r, s)$  element  $\partial^2 Q / \partial \beta_r \partial \gamma_s$ .
- ☐  $u \perp v$  means that the vectors  $u$  and  $v$  are orthogonal (i.e.,  $u^T v = 0$ ); ditto for matrices.
- ☐  $Y \perp\!\!\!\perp Z$  means that the random variables  $Y$  and  $Z$  are independent.

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## Useful matrix decompositions

- ☐ **Singular value decomposition (SVD)**: any real matrix  $X$  can be written in the form

$$X_{n \times p} = U_{n \times n} D_{n \times p} V_{p \times p}^T$$

where

- $U = (u_1, \dots, u_n)$  and  $V = (v_1, \dots, v_p)$  are orthogonal (i.e.,  $U^T U = U U^T = I_n$ ,  $V^T V = V V^T = I_p$ ) and  $D$  is  $n \times p$  rectangular diagonal with real diagonal entries (**singular values**)  $d_1 \geq \dots \geq d_m \geq 0$ , where  $m = \min(n, p)$ ,
  - if one or more  $d_j = 0$ , then  $X$  is singular, and
  - the  $u_j$  and  $v_r$  respectively span the column and row spaces of  $X$ .
- ☐ The SVD implies that the ranks of  $X$ ,  $X^T X$  and  $X X^T$  are equal and at most  $m$ .
  - ☐ **Spectral theorem**: any real symmetric matrix  $H$  can be written as

$$H_{n \times n} = U_{n \times n} D_{n \times n} U_{n \times n}^T,$$

where

- $D = \text{diag}(d_1, \dots, d_n)$  contains the eigenvalues of  $H$ ;
- $U$  is an orthogonal matrix whose columns are the corresponding eigenvectors; and
- if  $H$  is positive semi-definite then  $d_1 \geq \dots \geq d_n \geq 0$ .

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## Least squares fit

- Assume that

$$y = X\beta$$

and find the 'best fit' by choosing  $\beta$  to minimise the (squared) Euclidean distance between  $y$  and  $X\beta$ , i.e., the sum of squares

$$\|y - X\beta\|^2 = (y - X\beta)^T(y - X\beta) = \sum_{j=1}^n (y_j - x_j^T \beta)^2.$$

- In vector space terms,  $y \in \mathbb{R}^n$  and  $X\beta \in \text{span}(X) \subset \mathbb{R}^n$ .
- The 'best fit' vector  $\hat{y}$  is the vector in  $\text{span}(X)$  closest to  $y$ ; Pythagoras' theorem (sketch) gives  $\hat{y} \perp (y - \hat{y})$  (but see below).
- We call  $\hat{y} \in \mathbb{R}^n$  the **fitted value(s)** and  $e = y - \hat{y} \in \mathbb{R}^n$  the **residual (vector)**.

**Lemma 1** When  $X$  has rank  $p$  and  $n \geq p$  then  $\hat{y} = X\hat{\beta} = Hy$ , where

$$\hat{\beta} = (X^T X)^{-1} X^T y, \quad H = X(X^T X)^{-1} X^T.$$

The 'hat matrix'  $H$  has rank  $p$ , is symmetric and idempotent, and satisfies  $HX = X$ : it gives the orthogonal projection of  $\mathbb{R}^n$  onto  $\text{span}(X)$ .

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## Note to Lemma 1

- If  $X$  has rank  $p$ , so too does the  $p \times p$  matrix  $X^T X$ , which is therefore invertible.
- The sum of squares

$$Q = (y - X\beta)^T(y - X\beta) = y^T y - \beta^T X^T y - y^T X\beta + \beta^T X^T X\beta = y^T y - 2y^T X\beta + \beta^T X^T X\beta$$

has first and second derivatives (respectively a  $p \times 1$  vector and  $p \times p$  matrix)

$$\frac{\partial Q}{\partial \beta} = -2X^T y + 2X^T X\beta, \quad \frac{\partial^2 Q}{\partial \beta \partial \beta^T} = 2X^T X$$

with respect to  $\beta$ . Setting  $\partial Q / \partial \beta = 0$  implies that  $(X^T X)\beta = X^T y$ , and as  $X^T X$  is invertible we can write

$$\hat{\beta} = (X^T X)^{-1} X^T y, \quad \hat{y} = X\hat{\beta} = X(X^T X)^{-1} X^T y = Hy,$$

say. The matrix  $X^T X$  is positive definite, so  $(y - X\beta)^T(y - X\beta)$  is minimised at  $\hat{\beta}$ .

- The  $n \times n$  'hat matrix'  $H$  (which 'puts a hat' on  $y$ ) satisfies  $H^T = H$ ,  $H^2 = H$ , so it is symmetric and idempotent, i.e., its eigenvalues equal 0 or 1, and their multiplicities must be  $n - p$  and  $p$ , as its rank is  $p$ .  $H$  is the matrix that projects  $\mathbb{R}^n$  orthogonally onto the span of the columns of  $X$ ,  $\text{span}(X)$ .
- The inner product between  $\hat{y}$  and  $y - \hat{y}$  equals zero, because  $\hat{y} = Hy$ ,  $y - \hat{y} = (I - H)y$ , and  $\hat{y}^T(y - \hat{y}) = y^T H^T(I - H)y = y^T(H - H)y = 0$ . Hence  $\hat{y}$  and  $y - \hat{y}$  are orthogonal.
- Clearly  $HX = X(X^T X)^{-1} X^T X = X$ , so  $H(X\beta) = X\beta$  for any  $\beta \in \mathbb{R}^p$ , i.e., a vector in  $\text{span}(X)$  is left unchanged by multiplication by  $H$ .

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## Analysis of variance I

**Lemma 2** Let  $X_{n \times p} = (X_0, X_1, \dots, X_R)$  have rank  $p$ , where  $p \leq n$ , and let  $H_r$  denote the projection matrices formed using  $(X_0, \dots, X_r)$ , for  $r = 0, \dots, R$ ; hence  $H_R = H$ . Define  $P_r = H_r - H_{r-1}$  for  $r = 1, \dots, R$  and  $P_{R+1} = I - H$ . Then (i)  $H_r H_s = H_r$  whenever  $r \leq s$ , (ii)  $H_0 P_r = 0$  for any  $r$ , and (iii) the matrices  $P_r$  are symmetric and idempotent, with  $P_r P_s = 0$  when  $r \neq s$ .

- In the setup of Lemma 2 suppose we fit the models with projection matrices  $H_0, \dots, H_R = H$  and corresponding fitted values  $\hat{y}_r = H_r y$ . Then

$$\begin{aligned} y &= \hat{y}_0 + (\hat{y}_1 - \hat{y}_0) + \dots + (\hat{y}_R - \hat{y}_{R-1}) + (y - \hat{y}_R) \\ &= H_0 y + (H_1 - H_0)y + \dots + (H_R - H_{R-1})y + (I - H)y \\ &= H_0 y + P_1 y + \dots + P_R y + P_{R+1} y, \end{aligned}$$

and Lemma 2 implies that the terms on the RHS are orthogonal, i.e.,

$$(H_0 y)^T (P_r y) = 0, \quad (P_s y)^T (P_r y) = 0, \quad r \neq s.$$

- Hence Pythagoras' theorem gives the **analysis of variance (ANOVA)** decomposition

$$\|y\|^2 = \|\hat{y}_0\|^2 + \sum_{r=1}^R \|\hat{y}_r - \hat{y}_{r-1}\|^2 + \|y - \hat{y}\|^2.$$

## Note to Lemma 2

- (i) Let  $\mathcal{V}_0 \subset \dots \subset \mathcal{V}_R$  denote the linear spaces onto which  $\mathbb{R}^n$  is projected by  $H_0, \dots, H_R = H$ , and suppose that  $r \leq s$ . Now  $H_r y \in \mathcal{V}_r$  for any  $y \in \mathbb{R}^n$ , so as  $\mathcal{V}_r \subset \mathcal{V}_s$ ,  $H_r y \in \mathcal{V}_s$ . Hence  $H_s H_r y = H_r y$  for any  $y \in \mathbb{R}^n$ , so  $H_s H_r = H_r$ . This implies that

$$H_s H_r = H_r = H_r^T = (H_s H_r)^T = H_r^T H_s^T = H_r H_s, \quad s \geq r.$$

- (ii) For  $r = 1, \dots, R$ , (i) yields  $H_0 P_r = H_0 H_r - H_0 H_{r-1} = H_0 - H_0 = 0$ , and  $H_0 P_{R+1} = H_0(I - H_R) = 0$ .
- (iii) The matrices  $P_1, \dots, P_R$  are symmetric because

$$P_r^T = (H_r - H_{r-1})^T = H_r^T - H_{r-1}^T = H_r - H_{r-1} = P_r,$$

and idempotent because (i) gives

$$\begin{aligned} P_r^2 &= (H_r - H_{r-1})(H_r - H_{r-1}) \\ &= H_r^2 - H_r H_{r-1} - H_{r-1} H_r + H_{r-1}^2 \\ &= H_r - H_{r-1} - H_{r-1} + H_{r-1} \\ &= H_r - H_{r-1} = P_r. \end{aligned}$$

Moreover if  $r < s \leq R$ , then

$$\begin{aligned} P_r P_s &= (H_r - H_{r-1})(H_s - H_{s-1}) \\ &= H_r H_s - H_r H_{s-1} - H_{s-1} H_r + H_{s-1} H_{r-1} \\ &= H_r - H_r - H_{r-1} + H_{r-1} \\ &= 0. \end{aligned}$$

The corresponding results for  $P_{R+1}$  are equally easy to check.

## Analysis of variance II

- Usually  $X_0 = 1_n$ ; then  $\hat{y}_0 = 1_n(1_n^T 1_n)^{-1} 1_n^T y = \bar{y} 1_n$  and

$$\|y\|^2 - \|\hat{y}_0\|^2 = \sum_{j=1}^n y_j^2 - \sum_{j=1}^n \bar{y}^2 = \sum_{j=1}^n (y_j - \bar{y})^2,$$

equals  $n$  times the empirical variance of  $y_1, \dots, y_n$ . Hence

$$\sum_{j=1}^n (y_j - \bar{y})^2 = \|y\|^2 - \|\hat{y}_0\|^2 = \sum_{r=1}^R \|\hat{y}_r - \hat{y}_{r-1}\|^2 + \|y - \hat{y}\|^2$$

decomposes ('analyses') the variability of  $y$  around its average  $\bar{y}$  into

- the contributions  $\|\hat{y}_r - \hat{y}_{r-1}\|^2$  due to adding the columns of  $X_r$  to  $X_0, \dots, X_{r-1}$ ,
  - the **residual sum of squares**  $\|y - \hat{y}\|^2$  left after fitting  $X = (X_0, \dots, X_R)$ .
- Large  $\|\hat{y}_r - \hat{y}_{r-1}\|^2$  implies that  $X_r$  explains a lot of the variation of  $y$  even after allowing for that explained by  $X_0, \dots, X_{r-1}$ .
- The
- **degrees of freedom** of a fit is the rank  $\nu_r$  of the corresponding  $H_r$ , and the
  - **residual degrees of freedom** is  $n - \nu_R = n - p$ .

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## Terms

- A constant column  $X_0 = 1_n$  is almost always present in the design matrix, so

$$X\beta = (1_n \quad X_1 \quad \cdots \quad X_R) \begin{pmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_R \end{pmatrix} = 1_n \beta_0 + X_1 \beta_1 + \cdots + X_R \beta_R,$$

where the matrices  $X_1, \dots, X_R$ , the **terms**, are successively included.

- The baseline model with only  $1_n$  has fitted value and residual vector

$$\hat{y}_0 = \bar{y} 1_n, \quad y - \hat{y}_0 = y - \bar{y} 1_n.$$

- Starting from the baseline we ask which terms lead to large reductions in the residual sum of squares, i.e., best explain the variation of  $y$ .
- The successive residual degrees of freedom, i.e., the ranks of the matrices  $I - H_r$ , are

$$n - 1 = n - \nu_0 \geq n - \nu_1 \geq \cdots \geq n - \nu_R.$$

- When the columns of  $X_{r+1}$  depend linearly on those of  $1_n, X_1, \dots, X_r$ , we have  $\nu_{r+1} = \nu_r$ , so inclusion of  $X_{r+1}$  does not change the fitted value or improve the fit.

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## Model formulae

- A mean vector such as  $1_n\beta_0 + X_1\beta_1 + X_2\beta_2$  is often written as the right-hand side of

$$y \sim X1 + X2$$

where

- the columns of 1s is (silently) included first by default,
  - $X1$  and  $X2$  represent the vector subspaces of  $\mathbb{R}^n$  generated by the corresponding terms, and
  - $+$  represents addition of vector subspaces.
- Software generally drops any column of a design matrix that is linearly dependent on previous columns, and this affects which elements of  $\beta$  can be estimated and the meaning of estimates corresponding to later columns.
- Carefully choosing the order of terms in a model can give easily interpreted estimates of the parameters of interest — for example, if  $X_2$  is full-rank and a column of 1s lies in  $\text{span}(X_1) + \text{span}(X_2)$  then

$$y \sim X1 + X2, \quad y \sim X2 + X1 - 1,$$

span the same linear space but the second estimates the parameters of  $\beta_2$  (unadjusted for the mean) and the parameters of  $\beta_1$ , adjusted for the presence of  $X_2$ .

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## ANOVA

Terms	Residual df	Residual SS	Term added	Reduction in residual df	Reduction in SS	Mean square
$1_n$	$n - \nu_0 = n - 1$	$SS_0$				
$1_n, X_1$	$n - \nu_1$	$SS_1$	$X_1$	$\nu_1 - \nu_0$	$SS_0 - SS_1$	$\frac{SS_0 - SS_1}{\nu_1 - \nu_0}$
$1_n, X_1, X_2$	$n - \nu_2$	$SS_2$	$X_2$	$\nu_2 - \nu_1$	$SS_1 - SS_2$	$\frac{SS_1 - SS_2}{\nu_2 - \nu_1}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$1_n, X_1, \dots, X_R$	$n - \nu_R = n - p$	$SS_R$	$X_R$	$\nu_R - \nu_{R-1}$	$SS_{R-1} - SS_R$	$\frac{SS_{R-1} - SS_R}{\nu_R - \nu_{R-1}}$

- The sum of squares when including terms  $1_n, X_1, \dots, X_r$  is

$$SS_r = \|y - \hat{y}_r\|^2.$$

- The ‘mean square’ for term  $X_r$ ,

$$MS_r = \frac{SS_{r-1} - SS_r}{\nu_r - \nu_{r-1}}$$

is the average reduction in  $SS_r$  per degree of freedom when  $X_r$  is added to the model.

- Usually show only the RHS of the table and the bottom line of its LHS (next slide).

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## ANOVA table

Term added	df	Reduction in SS	Mean square
$X_1$	$\nu_1 - \nu_0$	$SS_0 - SS_1$	$MS_1 = (SS_0 - SS_1)/(\nu_1 - \nu_0)$
$X_2$	$\nu_2 - \nu_1$	$SS_1 - SS_2$	$MS_2 = (SS_1 - SS_2)/(\nu_2 - \nu_1)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$X_R$	$\nu_R - \nu_{R-1}$	$SS_{R-1} - SS_R$	$MS_R = (SS_{R-1} - SS_R)/(\nu_R - \nu_{R-1})$
Residual	$n - \nu_R$	$SS_R$	$MS_{\text{Res}} = SS_R/(n - \nu_R)$

- ☐ Used to screen which terms give the largest reductions, comparing  $MS_r$  with the residual mean square  $MS_{\text{Res}}$ .
- ☐ Judge 'significance' of reductions relative to residual using  $F$ -tests (later).
- ☐ Problem: the order of adding terms matters, so there is no unique reduction in general.

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## Coefficient of determination

- ☐ **Coefficient of determination  $R^2$**  measures reduction in variance of  $y$  as

$$R^2 = \frac{\|\hat{y} - \bar{y}1_n\|^2}{\|y - \bar{y}1_n\|^2} = \frac{\{(I - H_0)\hat{y}\}^T(I - H_0)\hat{y}}{\{(I - H_0)y\}^T(I - H_0)y} = \frac{y^T(H - H_0)y}{y^T(I - H_0)y},$$

where  $H_0$  and  $H$  are the hat matrices for regression on  $1_n$  and  $X$ , and  $1_n \in \text{span}(X)$ .

- ☐  $R^2 \in [0, 1]$  is the squared empirical correlation between  $y$  and  $\hat{y}$ , so  $R^2 \approx 1$  implies that most of the variation in  $y$  is explained by  $\hat{y}$ .
- ☐ There is a geometric interpretation, as the terms on the right of

$$(I_n - H_0)y = (I_n - H)y + (H - H_0)y$$

are orthogonal.

- ☐ Adding columns to  $X$  must increase  $R^2$ , unlike the **adjusted  $R^2$** ,

$$R_a^2 = R^2 + (1 - R^2)\frac{n - 1}{n - p}.$$

- ☐ If  $1_n \notin \text{span}(X)$ , use

$$R_0^2 = \frac{\hat{y}^T \hat{y}}{y^T y}, \quad R_{0,a}^2 = R_0^2 + (1 - R_0^2)\frac{n}{n - p}.$$

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## Comments

- ☐ We have supposed that  $X_{n \times p}$  has rank  $p$ :
  - if  $X$  is rank-deficient, then a least squares algorithm usually drops columns that lie in the span of preceding ones, but care is needed to construct  $X$  so that the resulting  $\hat{\beta}$  is easy to interpret;
  - if  $X$  is nearly rank-deficient, then some form of regularisation may be needed. More later ...
- ☐ Everything so far as purely numerical:
  - least squares estimation is a numerical technique for using  $X$  to approximate  $y$ ;
  - $\hat{y} = X\hat{\beta}$  is the resulting approximation, which lies in  $\text{span}(X)$ ;
  - $\hat{\beta}$  gives the coefficients of the columns of  $X$  for the best approximation;
  - the coefficient of determination  $R^2$  measures how much of the overall variation of  $y$  was explained by  $X$ ; and
  - the ANOVA decomposition summarises how much of the variation in  $y$  is explained by different subsets of columns of  $X$  (terms).
- ☐ For statistics we need to add some distributional assumptions ... shortly ...
- ☐ First some reminders ...

## 1.2 Inference

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### Reminder: Moment-generating function

**Definition 3** The **moment-generating function (MGF)** of a random vector  $Y_{n \times 1}$  is

$$M_Y(t) = E(e^{t^T Y}) = E(e^{\sum_{j=1}^n t_j Y_j}), \quad t \in \mathcal{T} = \{t \in \mathbb{R}^n : M_Y(t) < \infty\},$$

and the **cumulant-generating function** of  $Y$  is  $K_Y(t) = \log M_Y(t)$ ,  $t \in \mathcal{T}$ .

Then

- ☐  $0 \in \mathcal{T}$ , so  $M_Y(0) = 1$  and  $K_Y(0) = 0$ ;
- ☐ if  $\mathcal{T}$  contains an open set, then

$$\mu = E(Y) = K'_Y(0) = \left. \frac{\partial K_Y(t)}{\partial t} \right|_{t=0}, \quad \Omega = \text{var}(Y) = \left. \frac{\partial^2 K_Y(t)}{\partial t \partial t^T} \right|_{t=0};$$

- ☐ if  $\mathcal{A}, \mathcal{B}$  are disjoint subsets of  $\{1, \dots, n\}$  and  $Y_{\mathcal{A}}$  denotes the sub-vector of  $Y$  containing  $\{Y_j : j \in \mathcal{A}\}$ , etc., then  $Y_{\mathcal{A}} \perp\!\!\!\perp Y_{\mathcal{B}}$  if and only if

$$M_Y(t) = E(e^{t_{\mathcal{A}}^T Y_{\mathcal{A}} + t_{\mathcal{B}}^T Y_{\mathcal{B}}}) = M_{Y_{\mathcal{A}}}(t_{\mathcal{A}}) M_{Y_{\mathcal{B}}}(t_{\mathcal{B}}), \quad t \in \mathcal{T};$$

- ☐ the MGF of  $Y_{\mathcal{A}}$  equals  $M_Y(t)$  evaluated with  $t_{\mathcal{B}} = 0$ ;
- ☐ if we recognise an MGF, then we know the probability distribution that gave it.

## Reminder: Multivariate normal distribution

A random variable  $Y_{n \times 1}$  with real components has the **multivariate normal distribution**,  $Y \sim \mathcal{N}_n(\mu, \Omega)$ , if  $a^T Y \sim \mathcal{N}(a^T \mu, a^T \Omega a)$  for every constant vector  $a_{n \times 1}$ , and then

(a)  $\Omega$  is symmetric semi-positive definite with real components and

$$E(Y) = \mu_{n \times 1}, \quad \text{var}(Y) = \Omega_{n \times n}, \quad M_Y(t) = \exp(t^T \mu + \frac{1}{2} t^T \Omega t), \quad t \in \mathbb{R}^n,$$

where we call  $\mu$  the **mean vector** and  $\Omega$  the **(co)variance matrix** of  $X$ ;

(b) for any constants  $a_{m \times 1}$  and  $B_{m \times n}$ ,  $a + BY \sim \mathcal{N}_m(a + B\mu, B\Omega B^T)$ ;

(c) if  $Y^T = (Y_1^T, Y_2^T)$ , where  $Y_1$  is  $m \times 1$ , and  $\mu$  and  $\Omega$  are partitioned correspondingly, then the marginal and conditional distributions of  $Y_1$  are also multivariate normal:

$$Y_1 \sim \mathcal{N}_m(\mu_1, \Omega_{11}), \quad Y_1 | Y_2 = y_2 \sim \mathcal{N}_m \{ \mu_1 + \Omega_{12} \Omega_{22}^{-1} (y_2 - \mu_2), \Omega_{11} - \Omega_{12} \Omega_{22}^{-1} \Omega_{21} \};$$

(d)  $Y_1 \perp\!\!\!\perp Y_2$  iff  $\Omega_{12} = 0$ , and  $a + BY \perp\!\!\!\perp c + DY$  iff  $B\Omega D^T = 0$ ;

(e) if  $Y_1, \dots, Y_n \stackrel{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)$ , then  $Y_{n \times 1} \sim \mathcal{N}_n(\mu 1_n, \sigma^2 I_n)$ ; and finally,

(f)  $Y$  has a density on  $\mathbb{R}^n$  iff  $\Omega$  is positive definite (i.e., has rank  $n$ ), and then

$$f(y; \mu, \Omega) = \frac{1}{(2\pi)^{n/2} |\Omega|^{1/2}} \exp \left\{ -\frac{1}{2} (y - \mu)^T \Omega^{-1} (y - \mu) \right\}, \quad y \in \mathbb{R}^n. \quad (1)$$

### Note: Multivariate normal distribution

(a) Let  $e_j$  denote the  $n$ -vector with 1 in the  $j$ th place and zeros everywhere else.

□ Then  $Y_j = e_j^T Y \sim N(\mu_j, \omega_{jj})$ , giving the mean and variance of  $Y_j$ .

□ Now  $\text{var}(Y_j + Y_k) = \text{var}(Y_j) + \text{var}(Y_k) + 2\text{cov}(Y_j, Y_k)$ , and

$$Y_j + Y_k = (e_j + e_k)^T Y \sim \mathcal{N}(\mu_j + \mu_k, \omega_{jj} + \omega_{kk} + 2\omega_{jk}),$$

which implies that  $\text{cov}(Y_j, Y_k) = \omega_{jk} = \omega_{kj}$ . This gives the mean and covariance matrix of  $Y$ .

□ Since  $u^T Y \sim \mathcal{N}(u^T \mu, u^T \Omega u)$ , its MGF is  $M_{u^T Y}(t) = E(e^{tu^T Y}) = \exp(tu^T \mu + \frac{1}{2}t^2 u^T \Omega u)$ . The MGF of  $Y$  is  $M_Y(u) = E(e^{u^T Y}) = M_{u^T Y}(1) = \exp(u^T \mu + \frac{1}{2}u^T \Omega u)$ , for any  $u \in \mathbb{R}^p$ , as stated.

(b) The MGF of  $a + BY$  equals

$$\begin{aligned} E[\exp\{t^T(a + BY)\}] &= E[\exp\{t^T a + (B^T t)^T Y\}] \\ &= e^{t^T a} M_Y(B^T t) \\ &= \exp\{t^T a + (B^T t)^T \mu + \frac{1}{2}(B^T t)^T \Omega (B^T t)\} \\ &= \exp\{t^T(a + B\mu) + \frac{1}{2}t^T(B\Omega B^T)t\}, \end{aligned}$$

which is the MGF of the  $\mathcal{N}_m(a + B\mu, B\Omega B^T)$  distribution. Hence linear combinations of normal variables are themselves normal.

(c) Write  $Y^T = (Y_1^T, Y_2^T)$  and partition  $\mu$  and  $\Omega$  conformally. Then

$$M_Y(t) = \exp\{t_1^T \mu_1 + t_2^T \mu_2 + \frac{1}{2}(t_1^T \Omega_{11} t_1 + 2t_1^T \Omega_{12} t_2 + t_2^T \Omega_{22} t_2)\}$$

and by setting  $t_2 = 0$  and  $t_1 = 0$  we see that  $M_{Y_1}(t_1) = \exp(t_1^T \mu_1 + \frac{1}{2}t_1^T \Omega_{11} t_1)$  and

$M_{Y_2}(t_2) = \exp(t_2^T \mu_2 + \frac{1}{2}t_2^T \Omega_{22} t_2)$ . Hence the marginal distribution of  $Y_1$  is  $\mathcal{N}_m(\mu_1, \Omega_{11})$ .

For the conditional distribution, note that  $W = Y_1 - \Omega_{12}\Omega_{22}^{-1}Y_2$  is a linear combination of  $Y$  and

$$E(W) = \mu_1 - \Omega_{12}\Omega_{22}^{-1}\mu_2, \quad \text{var}(W) = \Omega_{11} - \Omega_{12}\Omega_{22}^{-1}\Omega_{21}, \quad \text{cov}(W, Y_2) = \Omega_{12} - \Omega_{12}\Omega_{22}^{-1}\Omega_{22} = 0.$$

Hence  $W \perp\!\!\!\perp Y_2$ . As  $Y_1 = W + \Omega_{12}\Omega_{22}^{-1}Y_2$  and conditioning on  $Y_2$  does not change the distribution of  $W$ ,

$$E(Y_1 | Y_2 = y_2) = E(W) + \Omega_{12}\Omega_{22}^{-1}y_2, \quad \text{var}(Y_1 | Y_2 = y_2) = \text{var}(W + \Omega_{12}\Omega_{22}^{-1}y_2) = \text{var}(W).$$

Putting the pieces together gives the stated conditional distribution.

(d) The joint MGF given in (c) factorises iff the variables are independent, and on inspecting it we see that

$$M_Y(t) = M_{Y_1}(t_1)M_{Y_2}(t_2) \iff \Omega_{12} = 0.$$

The variance matrix of

$$\begin{pmatrix} a \\ c \end{pmatrix} + \begin{pmatrix} B \\ D \end{pmatrix} Y$$

is

$$\begin{pmatrix} B\Omega B^T & B\Omega D^T \\ D\Omega B^T & D\Omega D^T \end{pmatrix},$$

so  $a + BY \perp\!\!\!\perp c + DY$  iff  $B\Omega D^T = 0$ .

## Note: Multivariate normal distribution II

(e) Each  $Y_j$  has mean  $\mu$  and variance  $\sigma^2$ , and since they are independent,  $\text{cov}(Y_j, Y_k) = 0$  for  $j \neq k$ . If  $u \in \mathbb{R}^n$ , then  $u^T Y$  is a linear combination of normal variables, with mean  $\sum_{j=1}^n u_j \mu = u^T \mu 1_n$  and variance  $\sum_{j=1}^n u_j^2 \sigma^2 = u^T \sigma^2 I_n u$ , so  $Y \sim \mathcal{N}_n(\mu 1_n, \sigma^2 I_n)$ , as required.

(f) Since  $\Omega$  is symmetric and positive semi-definite, the spectral theorem tells us that we may write  $\Omega = ADA^T$ , where  $D = \text{diag}(d_1, \dots, d_n)$  contains the (real) eigenvalues of  $\Omega$ , with  $d_1 \geq \dots \geq d_n \geq 0$ , and  $A$  is a  $n \times n$  orthogonal matrix, i.e.,  $A^T A = AA^T = I_n$  and  $|A| = 1$ . The columns  $A_1, \dots, A_n$  of  $A$  are the eigenvectors corresponding to the respective eigenvalues,

$$\Omega = ADA^T = \sum_{j=1}^n d_j a_j a_j^T,$$

with  $|\Omega| = |ADA^T| = |A| \times |D| \times |A^T| = |D|$  and  $\Omega^{-1} = AD^{-1}A^T$  if the inverse exists.

□ Now let  $Z_1, \dots, Z_n \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$   $Z = (Z_1, \dots, Z_n)^T$ , and  $u \in \mathbb{R}^n$ , set and consider

$$u^T(\mu + AD^{1/2}Z) = u^T \mu + \sum_{j=1}^n Z_j u^T a_j d_j^{1/2}.$$

This is a linear combination of normal variables, so it has a normal distribution, with mean  $u^T \mu$  and variance

$$\text{var} \left( u^T \mu + \sum_{j=1}^n Z_j u^T a_j d_j^{1/2} \right) = \sum_{j=1}^n d_j (u^T a_j)^2 \text{var}(Z_j) = u^T \left( \sum_{j=1}^n d_j a_j a_j^T \right) u = u^T \Omega u,$$

so we can write  $X = \mu + AD^{1/2}Z \sim N_n(\mu, \Omega)$ .

□ If  $\Omega$  has rank  $n$ , then  $d_n > 0$ . The change of variables  $z \mapsto x = \mu + AD^{1/2}z$  has Jacobian

$$\left| \frac{\partial x}{\partial z} \right| = |AD^{1/2}| = |A| |D|^{1/2} = 1 \times |D|^{1/2} = |\Omega|^{1/2} > 0.$$

Moreover  $z = D^{-1/2}A^T(x - \mu)$ , and therefore  $z^T z = (x - \mu)^T \Omega^{-1}(x - \mu)$ . Hence using the joint density of  $Z$ ,  $f_Z(z) = (2\pi)^{-n/2} \exp(-\sum_{j=1}^n z_j^2/2)$ ,

$$f_X(x) = f_Z(z)|_{z=D^{-1/2}A^T(x-\mu)} \left| \frac{\partial z}{\partial x} \right| = (2\pi)^{-n/2} \exp\left(-\frac{z^T z}{2}\right) \Big|_{z=D^{-1/2}A^T(x-\mu)} |\Omega|^{-1/2},$$

which reduces to (1). If  $d_n = 0$ , then the Jacobian is zero, so the transformation  $z \mapsto x$  is singular and  $X$  does not have a density on  $\mathbb{R}^n$ .

□ Now suppose that  $d_m > d_{m+1} = 0$ , so just  $m$  eigenvalues of  $\Omega$  are positive. Then

$$X = \mu + \sum_{j=1}^m Z_j a_j d_j^{1/2} \in \mathcal{S} = \mu + \text{span}(a_1, \dots, a_m),$$

where  $\mathcal{S}$  is a hyperplane of dimension  $m$  passing through  $\mu$  and generated by the vectors  $a_1, \dots, a_m$ . In this case the previous argument shows that  $X$  has an  $m$ -dimensional Gaussian density on  $\mathcal{S}$ , but places no probability elsewhere.

## Reminder: $\chi^2$ distribution

**Definition 4** If  $Y_j \stackrel{\text{ind}}{\sim} \mathcal{N}(\mu_j, \sigma^2)$ , then  $W = Y_1^2 + \dots + Y_\nu^2$  has the **non-central chi-square distribution with  $\nu$  degrees of freedom (df) and non-centrality parameter  $\delta^2 = (\mu_1^2 + \dots + \mu_\nu^2)/\sigma^2$** ; we write  $W \sim \sigma^2 \chi_\nu^2(\delta^2)$ . Then

$$M_W(t) = \exp\left(\frac{t\sigma^2\delta^2}{1-2t\sigma^2}\right) (1-2t\sigma^2)^{-\nu/2}, \quad t < 1/(2\sigma^2).$$

If  $\delta^2 = 0$  and  $\sigma^2 = 1$  then  $W$  has the (central) **chi-square distribution with  $\nu$  df**, we write  $W \sim \chi_\nu^2$ , its MGF is  $M_W(t) = (1-2t)^{-\nu/2}$ , and its  $p$ -quantile is  $c_\nu(p)$ .

Chi-square variables satisfy

- $E(W) = \sigma^2(\nu + \delta^2)$ ,  $\text{var}(W) = 2\sigma^4(\nu + 2\delta^2)$ ;
- if  $W_1 \sim \chi_{\nu_1}^2 \perp\!\!\!\perp W_2 \sim \chi_{\nu_2}^2$ , then  $W_1 + W_2 \sim \chi_{\nu_1+\nu_2}^2$ ;
- $W \sim \chi_\nu^2$  implies that  $W$  has the gamma density

$$f(w) = \frac{\beta^\alpha w^{\alpha-1}}{\Gamma(\alpha)} e^{-\beta w}, \quad w > 0, \quad \alpha, \beta > 0,$$

with  $\alpha = \nu/2$  and  $\beta = 1/2$ .

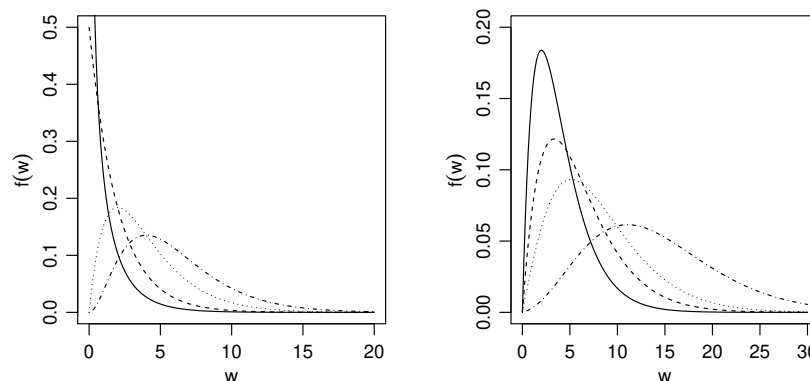
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## Reminder: $\chi_\nu^2$ densities

Left: central densities with  $\nu = 1, 2, 4, 6$  (solid, large dashes, small dashes, dot-dash).

Right: non-central densities with  $\nu = 4$  and  $\delta = 0, 2, 4, 10$  (solid, large dashes, small dashes, dot-dash).



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### Reminder: Student $t$ distribution

**Definition 5** If  $Z \sim \mathcal{N}(0, 1) \perp\!\!\!\perp W \sim \chi^2_\nu$ , then  $T = Z/(W/\nu)^{1/2}$  has the **Student  $t$  distribution with  $\nu$  df**,  $T \sim t_\nu$ , and we write  $t_\nu(p)$  for the corresponding  $p$ -quantile. The density function of  $T$  is

$$f_T(t) = \frac{\Gamma\{(\nu+1)/2\}}{\sqrt{\nu\pi}\Gamma(\nu/2)} \frac{1}{(1+t^2/\nu)^{(\nu+1)/2}}, \quad -\infty < t < \infty, \nu = 1, 2, \dots$$

Properties:

- the mean and variance exist only for  $\nu \geq 2$  and  $\nu \geq 3$  respectively, and then

$$E(T) = 0, \quad \text{var}(T) = \frac{\nu}{\nu-2};$$

- with  $\nu = 1$  we have the **Cauchy density**,

$$\frac{1}{\pi(1+t^2)}, \quad -\infty < t < \infty,$$

and then  $T$  has no moments;

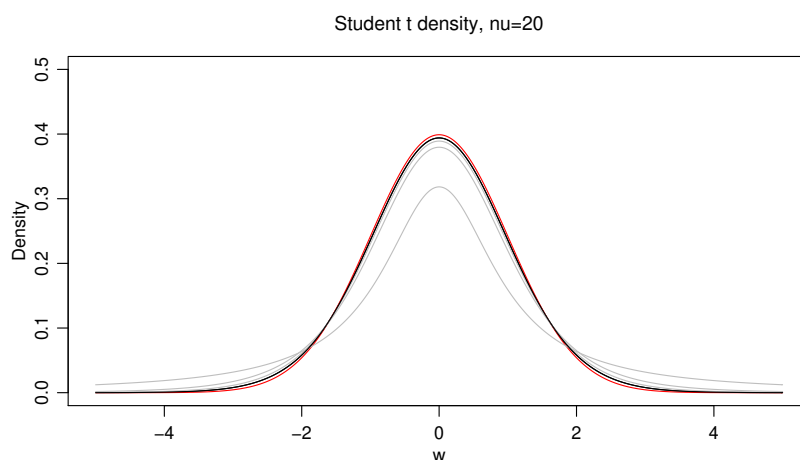
- as  $\nu \rightarrow \infty$ , the limiting distribution of  $T$  is  $\mathcal{N}(0, 1)$ ; usually the approximation is 'good enough' for  $\nu > 25$  (say).

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### Reminder: Student $t$ densities

Student  $t$  density functions with  $\nu = 1, 5, 10, 20$  (black,  $\nu = 20$ ), and the standard normal density (red):



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### Reminder: $F$ distribution

**Definition 6** If  $W_1, W_2 \stackrel{\text{ind}}{\sim} \chi_{\nu_1}^2, \chi_{\nu_2}^2$ , then

$$F = \frac{W_1/\nu_1}{W_2/\nu_2}$$

has the  **$F$  distribution with  $\nu_1$  and  $\nu_2$  df**: we write  $F \sim F_{\nu_1, \nu_2}$ .

The density function is

$$f_F(u) = \frac{\Gamma(\frac{1}{2}\nu_1 + \frac{1}{2}\nu_2) \nu_1^{\nu_1/2} \nu_2^{\nu_2/2}}{\Gamma(\frac{1}{2}\nu_1) \Gamma(\frac{1}{2}\nu_2)} \frac{u^{\frac{1}{2}\nu_1-1}}{(\nu_2 + \nu_1 u)^{(\nu_1+\nu_2)/2}}, \quad u > 0, \nu_1, \nu_2 = 1, 2, \dots,$$

and the  $p$ -quantile is written  $F_{\nu_1, \nu_2}(p)$ .

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### Reminder: Computation

- ☐ Quantiles of the  $\mathcal{N}(\mu, \sigma^2)$ ,  $\chi_{\nu}^2$ ,  $t_{\nu}$ ,  $F_{\nu_1, \nu_2}$  distributions can be found in tables, or in environments such as R (see <http://www.r-project.org/>), where they can also be simulated.
- ☐ Examples:

R : Copyright 2005, The R Foundation for Statistical Computing

Version 2.2.1 (2005-12-20 r36812)

...

```
> qnorm(0.025)      # this is a comment; access normal quantiles
[1] -1.959964        # the [1] means this is the first element of a vector
> ?qnorm            # help on use of function qnorm()
> qchisq(0.025, df=3) # chi-squared quantiles, nu=3
[1] 0.2157953
> qt(0.025, df=3)    # t quantiles, nu=3
[1] -3.182446
> qf(0.025, df1=3, df2=4) # F quantiles, nu1=3, nu2=4
[1] 0.06622087
```

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### Statistical models

- ☐ Least squares fitting gives a deterministic description of the variation in some numbers  $y$  in terms of other numbers  $X$ .
- ☐ A **statistical model** is a description of data  $y$  in terms of a collection of probability distributions on the sample space for  $y$ .
- ☐ We distinguish
  - **primary** aspects of a model, which specify what questions we aim to answer, from
  - **secondary** aspects, which complete the model, indicate what analysis might be suitable, and determine the precision of conclusions.
- ☐ Often the primary aspects are embodied in one or more **parameters** of the model.
- ☐ (Almost) all models are **tentative**, and we must check that they are reasonable.



### Second-order and normal assumptions

- Two distributional assumptions are in general use for the linear model:

- **second-order assumptions**,

$$E(y) = X\beta, \quad \text{var}(y) = \sigma^2 V_{n \times n};$$

- **normal assumptions**,

$$y \sim \mathcal{N}_n(X\beta, \sigma^2 V),$$

i.e.,  $y$  has a multivariate normal distribution with mean vector  $X\beta$  and positive definite (co)variance matrix  $\sigma^2 V$ .

- $X$  is called the **design matrix**: more later.
- $V$  is assumed known. Unless stated otherwise we set  $V = I_n$ , so the  $y_j$  are uncorrelated; if normal they are therefore independent.
- If  $V \neq I_n$ , then we can perform **weighted least squares (WLS)** estimation, minimising

$$\|y - X\beta\|_V^2 = (y - X\beta)^T W (y - X\beta),$$

where  $W = V^{-1}$  is the **weight matrix**.

- Above the **linearity** is (usually) primary, whereas the **distributional assumption**, use of weights, ..., are (usually) secondary.

### Interpretation of coefficients

- Care is needed.
- For economy of notation we may write

$$y = \beta_0 + \varepsilon, \quad y = \beta_0 + x_1\beta_1 + \varepsilon,$$

but the  $\beta_0$ s have different meanings:

- in the first,  $E(y) = \beta_0$  is the mean of  $y$ , regardless of the value of  $x_1$ ;
- in the second,  $E(y) = \beta_0$  only when  $x_1 = 0$ , so  $\beta_0$  is the mean for a specific value of  $x_1$ .

- Likewise the  $\beta_1$ s in the models

$$y = \beta_0 + x_1\beta_1 + \varepsilon, \quad y = \beta_0 + x_1\beta_1 + x_2\beta_2 + \varepsilon,$$

have different interpretations, as

- the change in  $E(y)$  for a unit increase in  $x_1$ , or
- the change in  $E(y)$  for a unit increase in  $x_1$ , allowing for any effect of  $x_2$ .

- It would be preferable to write (for example)

$$y = \beta_0^0 + \varepsilon, \quad y = \beta_0^1 + x_1\beta_1^1 + \varepsilon, \quad \dots,$$

but the notation would then be far too heavy, so we don't — but we should!

## Consequences of second-order assumptions

**Lemma 7** Under the second-order assumptions,  $\hat{\beta}$  is an unbiased estimator of  $\beta$ ,

$$E(\hat{\beta}) = \beta, \quad \text{var}(\hat{\beta}) = \sigma^2(X^T X)^{-1}.$$

and  $S^2 = (n - p)^{-1} \|y - \hat{y}\|^2$  is an unbiased estimator of  $\sigma^2$ .

**Theorem 8 (Gauss–Markov)** The least squares estimator  $\hat{\beta}$  has the smallest variance among all estimators  $\tilde{\beta} = A_{p \times n} y$ ; it is the **best linear unbiased estimator (BLUE)** of  $\beta$ .

- Obviously these results hold under the (stronger) normal assumptions.
- The Gauss–Markov theorem only concerns linear estimators. Nonlinear estimators of  $\beta$  might have smaller variance than  $\sigma^2(X^T X)^{-1}$  (and in fact the optimal maximum likelihood estimators of  $\beta$  for non-normal models will be nonlinear in  $y$ ).

## Note to Lemma 7

- Recall that expectation is linear, and that  $\text{var}(A_{p \times n} y) = A \text{var}(y) A^T$ .
- Set  $A_{p \times n} = (X^T X)^{-1} X^T$  and note that
$$E(\hat{\beta}) = E(Ay) = AE(y) = (X^T X)^{-1} X^T X \beta = \beta,$$
$$\text{var}(\hat{\beta}) = A \text{var}(y) A^T = (X^T X)^{-1} X^T I_n \sigma^2 \{ (X^T X)^{-1} X^T \}^T = \sigma^2 (X^T X)^{-1}.$$
- Recall that  $\text{var}(y) = E(yy^T) - E(y)E(y)^T = \sigma^2 I_n - X\beta\beta^T X^T$ , and note that

$$\|y - \hat{y}\|^2 = (y - \hat{y})^T (y - \hat{y}) = y^T (I_n - H)^T (I_n - H) y = y^T (I_n - H) y = \text{tr}\{(I_n - H)yy^T\}.$$

Hence  $E(\|y - \hat{y}\|^2)$  equals

$$E[\text{tr}\{(I_n - H)yy^T\}] = \text{tr}\{(I_n - H)E(yy^T)\} = \text{tr}\{(I_n - H)(\sigma^2 I_n + X\beta\beta^T X^T)\} = \sigma^2 \text{tr}(I_n - H),$$

because  $(I_n - H)X = 0$ . Moreover  $\text{tr}(I_n) = n$  and

$$\text{tr}(H) = \text{tr}\{X(X^T X)^{-1} X^T\} = \text{tr}\{(X^T X)^{-1} X^T X\} = \text{tr}(I_p) = p,$$

so  $E(S^2) = \sigma^2$ , because

$$E(\|y - \hat{y}\|^2) = \sigma^2 \text{tr}(I_n - H) = \sigma^2(n - p).$$

### Note to Theorem 8

- Let  $\tilde{\beta}$  denote any unbiased estimator of  $\beta$  that is linear in  $y$ . Then a  $p \times n$  matrix  $A$  exists such that  $\tilde{\beta} = Ay$ , and unbiasedness implies that  $E(\tilde{\beta}) = AX\beta = \beta$  for any parameter vector  $\beta$ ; this entails  $AX = I_p$ . Now

$$\begin{aligned}\text{var}(\tilde{\beta}) - \text{var}(\hat{\beta}) &= A\sigma^2 I_n A^T - \sigma^2 (X^T X)^{-1} \\ &= \sigma^2 \{AA^T - AX(X^T X)^{-1} X^T A^T\} \\ &= \sigma^2 A(I_n - H)A^T \\ &= \sigma^2 A(I_n - H)(I_n - H)^T A^T\end{aligned}$$

and this  $p \times p$  matrix is positive semidefinite. Thus  $\hat{\beta}$  has smallest variance in finite samples among all linear unbiased estimators of  $\beta$ .

- This is a finite-sample result that holds for all  $n$  and  $X$  (of rank  $p$ , with  $n \geq p$ ).

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### Second-order assumptions and large samples

- We can write  $y_j = x_j^T \beta + \sigma \varepsilon_j$ , where  $\varepsilon_j \stackrel{\text{ind}}{\sim} (0, 1)$ , so

$$\hat{\beta} = (X^T X)^{-1} X^T y = \sum_{j=1}^n (X^T X)^{-1} x_j y_j = \beta + \sigma n^{-1} \sum_{j=1}^n a_j \varepsilon_j,$$

say, where  $a_1, \dots, a_n$  are  $p \times 1$  vectors. We have  $E(\hat{\beta}) = \beta$  and  $\text{var}(\hat{\beta}) = (X^T X)^{-1}$ , but is  $\hat{\beta}$  approximately normal for large  $n$ ?

- The  $a_j$ , or equivalently  $X$ , must be such that no single  $y_j$  can dominate in  $n^{-1} \sum a_j \varepsilon_j$ .

**Theorem 9 (no proof)** Let  $\{X_n\}$  be a sequence of  $n \times p$  design matrices each of rank  $p$ , let  $h_{11}^n, \dots, h_{nn}^n$  be the diagonal elements of the hat matrices  $X_n(X_n^T X_n)^{-1} X_n^T$  and let  $y_n \sim (X_n \beta, \sigma^2 I_n)$  for each  $n$ . If

$$\lim_{n \rightarrow \infty} \max_{j=1, \dots, n} h_{jj} = 0,$$

then the corresponding sequence of least squares estimators  $\hat{\beta}_n$  satisfies

$$(X_n^T X_n)^{1/2} (\hat{\beta}_n - \beta) \xrightarrow{D} \mathcal{N}_p(0, \sigma^2 I_p), \quad n \rightarrow \infty,$$

i.e., if  $H$  has a ‘well-behaved’ diagonal, then  $\hat{\beta} \sim \mathcal{N}_p\{\beta, \sigma^2 (X^T X)^{-1}\}$  in large samples.

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## Normal-theory linear model

The following results allow exact inferences for  $\beta$  and  $\sigma^2$ , and in analysis of variance.

**Theorem 10** Under the normal-theory linear model,

$$\hat{\beta} \sim \mathcal{N}_p\{\beta, \sigma^2(X^T X)^{-1}\} \quad \perp\!\!\!\perp \quad \frac{(n-p)S^2}{\sigma^2} \sim \chi_{n-p}^2.$$

**Lemma 11** If  $y \sim \mathcal{N}_n(\mu, \sigma^2 I_n)$  and  $H$  is symmetric and idempotent with rank  $p$ , then  $y^T H y \sim \sigma^2 \chi_p^2(\delta^2)$ , where  $\sigma^2 \delta^2 = \mu^T H \mu$ .

**Theorem 12** If  $y \sim \mathcal{N}_n(\mu, \sigma^2 I_n)$  and a linear model is fitted whose design matrix  $X$  is structured as in Lemma 2, then the sums of squares in the ANOVA decomposition

$$\sum_{j=1}^n (y_j - \bar{y})^2 = \sum_{r=1}^R \|\hat{y}_r - \hat{y}_{r-1}\|^2 + \|y - \hat{y}\|^2 = \sum_{r=1}^{R+1} \|P_r y\|^2$$

are independent and  $\|P_r y\|^2 \sim \sigma^2 \chi_{\nu_{r-1} - \nu_r}^2(\delta_r^2/\sigma^2)$ , where  $\sigma^2 \delta_r^2 = \mu^T P_r \mu$ . If  $X_r$  does not explain any variation in  $\mu$  after allowing for  $X_0, \dots, X_{r-1}$ , then  $P_r \mu = 0$ , so  $\delta_r^2 = 0$ .

Theorem 12 implies that the sums of squares for terms that explain variation in  $y$  will tend to be larger than sums of squares for other terms, which can be used to estimate  $\sigma^2$ .

### Note to Theorem 10

- The first part is easy, because  $\hat{\beta}$  is a linear combination of normal variables so it is normal, and its mean and variance matrix were given by Lemma 7.
- Likewise the residual  $e = y - \hat{y} = (I - H)y$  is a linear combination of  $y$  with mean  $0_n$  and variance  $(I - H)\sigma^2$ , so  $e \sim \mathcal{N}_n\{0_p, (I - H)\sigma^2\}$ .
- As  $\text{cov}(\hat{\beta}, e)$  equals

$$\text{cov}\{(X^T X)^{-1} X^T y, (I - H)y\} = (X^T X)^{-1} X^T \text{cov}(y)(I - H)^T = \sigma^2 (X^T X)^{-1} \{(I - H)X\}^T = 0,$$

we see that  $\hat{\beta}$  is independent of (any function of)  $e$ , and therefore in particular of

$$(n-p)S^2/\sigma^2 = \|y - \hat{y}\|^2/\sigma^2 = e^T e/\sigma^2.$$

- The eigenvalues of  $H$  are  $p$  1's and  $n-p$  0's, so those of  $I - H$  are  $n-p$  1's and  $p$  0's. The spectral decomposition implies that there exists an  $n \times n$  orthogonal matrix  $U$  such that  $I - H = U D U^T$ , where  $D = \text{diag}(1, \dots, 1, 0, \dots, 0)$  and  $U U^T = U^T U = I_n$ . Thus  $Z = U^T e/\sigma$  has mean vector  $0_n$  and variance matrix

$$\text{var}(Z) = U^T \text{var}(e) U / \sigma^2 = U^T (I - H) \sigma^2 U / \sigma^2 = U^T U D U^T U = D,$$

i.e. the  $Z_1, \dots, Z_n$  are independent normal variables,  $n-p$  of them have variance 1 and  $p$  of them have variance 0 and therefore equal 0 with probability one. Hence, as required,

$$(n-p)S^2/\sigma^2 = e^T e/\sigma^2 = (U Z)^T (U Z) = Z^T U^T U Z = \sum_{j=1}^{n-p} Z_j^2 \sim \chi_{n-p}^2.$$

### Note to Lemma 11

The spectral decomposition of  $H$  is  $UDU^T$ , where  $D$  is diagonal with  $p$  1's and  $n - p$  0's, and  $Z = U^T y \sim \mathcal{N}_n(U^T \mu, \sigma^2 I_n)$ ; note that the  $Z_j$  are independent. Now

$$y^T H y = (U^T y)^T D (U^T y) = \sum_{j=1}^n d_j Z_j^2 = \sum_{j:d_j=1} Z_j^2,$$

which has a (possibly non-central)  $\chi^2$  distribution with  $p = \text{tr}(H)$  degrees of freedom, scale parameter  $\sigma^2$  and

$$\sigma^2 \delta^2 = \sum_{j:d_j=1} E(Z_j)^2 = \sum_{j=1}^n d_j E(Z_j)^2 = (U^T \mu)^T D (U^T \mu) = \mu^T H \mu.$$

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### Note to Theorem 12

- As  $P_r P_s = 0$  for  $r \neq s$ , we have  $\text{cov}(P_r y, P_s y) = P_r \text{var}(y) P_s^T = \sigma^2 P_r P_s = 0$ , i.e.,  $P_r y$  and  $P_s y$  are independent. Hence the terms in the ANOVA decomposition are independent.
- $P_r$  is a symmetric idempotent matrix, so Lemma 11 gives

$$\|P_r y\|^2 \sim \sigma^2 \chi_{\nu}^2(\delta_r^2 / \sigma^2), \quad \delta_r^2 = \mu^T P_r \mu,$$

where  $\nu = \text{rank}(P_r)$ . These ranks are  $\nu_{r-1} - \nu_r$  for  $r = 1, \dots, R$ , and  $\nu_{R+1} = n - p$  for  $P_{R+1} = I_n - H$ .

- If  $X_r$  does not explain any variation in  $\mu$  after allowing for  $X_0, \dots, X_{r-1}$ , then  $H_r \mu = H_{r-1} \mu \in \mathcal{V}_{r-1}$ , i.e.,  $P_r \mu = 0$ , and thus  $\delta_r^2 = 0$ .

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### Inference on $\beta$

- Theorem 10 implies that for any constant  $c_{p \times 1}$ ,  $c^T \hat{\beta} \sim \mathcal{N}\{c^T \beta, \sigma^2 c^T (X^T X)^{-1} c\}$ , so

$$Z = \frac{c^T \hat{\beta} - c^T \beta}{\sigma \sqrt{c^T (X^T X)^{-1} c}} \sim \mathcal{N}(0, 1) \quad \perp \quad (n - p) S^2 / \sigma^2 = W \sim \chi_{n-p}^2,$$

and thus

$$\frac{c^T \hat{\beta}_r - c^T \beta_r}{S \sqrt{c^T (X^T X)^{-1} c}} = \frac{Z}{\sqrt{W/(n-p)}} \sim t_{n-p}.$$

- Let  $v_{rs}$  denote the  $(r, s)$  element of  $(X^T X)^{-1}$ , so  $v_{rr}$  denotes its  $r$ th diagonal element.
- Different choices of  $c$  allow inferences on the elements of  $\beta$ .
- For example, if  $c^T = (c_1, \dots, c_p)$ ,  $c_r = 1$  and  $c_s = 0$  for  $s \neq r$ , then  $c^T \beta = \beta_r$ , and we
  - test the hypothesis that  $\beta_r = \beta_r^0$  by comparing  $(\hat{\beta}_r - \beta_r^0) / (S v_{rr}^{1/2})$  to the  $t_{n-p}$  distribution, and
  - a  $(1 - \alpha)$  confidence interval for  $\beta_r$  has limits

$$\hat{\beta}_r \pm S v_{rr}^{1/2} t_{n-p}(1 - \alpha/2), \quad 0 < \alpha < 1.$$

- Likewise we can compare  $\beta_r$  and  $\beta_s$  by setting  $c_r = 1$ ,  $c_s = -1$  and all other  $c_t = 0$ .

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## Prediction

- Inference for the value of a further random variable  $Y_+$  with known  $p \times 1$  covariate vector  $x_+$  and satisfying the linear model, so  $Y_+ \sim \mathcal{N}(x_+^T \beta, \sigma^2)$  independent of the other variables, is performed by noting that  $Y_+ \perp\!\!\!\perp \hat{\beta}, S^2$  and

$$Y_+ - x_+^T \hat{\beta} \sim \mathcal{N} [0, \sigma^2 \{1 + x_+^T (X^T X)^{-1} x_+\}] ,$$

so

$$\frac{Y_+ - x_+^T \hat{\beta}}{S \{1 + x_+^T (X^T X)^{-1} x_+\}^{1/2}} \sim t_{n-p},$$

which leads to prediction intervals for  $Y_+$  once  $\hat{\beta}$  and  $S$  have been observed.

- Although we expect inferences for  $\beta$  and  $\sigma^2$  to hold as approximations under second-order assumptions, this is not the case for inference on  $Y_+$ . (Why not?)

## 1.3 Analysis of Variance

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### Analysis of variance

- We previously saw that

$$\sum_{j=1}^n (y_j - \bar{y})^2 = \|y\|^2 - \|\hat{y}_0\|^2 = \sum_{r=1}^R \|\hat{y}_r - \hat{y}_{r-1}\|^2 + \|y - \hat{y}\|^2$$

decomposes ('analyses') the variability of  $y$  around its average  $\bar{y}$  into

- the contributions  $\|\hat{y}_r - \hat{y}_{r-1}\|^2$  due to adding the columns of  $X_r$  to  $X_0, \dots, X_{r-1}$ ,
- the **residual sum of squares**  $\|y - \hat{y}\|^2$  left after fitting  $X = (X_0, \dots, X_R)$ .

- Large  $\|\hat{y}_r - \hat{y}_{r-1}\|^2$  implies that  $X_r$  explains a lot of the variation of  $y$  even after allowing for that explained by  $X_0, \dots, X_{r-1}$ .
- Theorem 12 implies that under the normal assumptions, and if  $E(y) = \mu$  lies in the column space of  $X$ , the sums of squares on the RHS above are independent and satisfy

$$\|\hat{y}_r - \hat{y}_{r-1}\|^2 = \|P_r y\|^2 \sim \sigma^2 \chi_{\nu_{r-1} - \nu_r}^2 (\delta_r^2 / \sigma^2) \quad \perp\!\!\!\perp \quad \|y - \hat{y}\|^2 \sim \sigma^2 \chi_{n-p}^2.$$

Hence if  $\delta_r^2 = 0$ , i.e.,  $\mu \in \text{span}(X_0, \dots, X_{r-1})$ , then

$$\frac{\|\hat{y}_r - \hat{y}_{r-1}\|^2 / (\nu_{r-1} - \nu_r)}{\|y - \hat{y}\|^2 / (n - p)} \sim F_{\nu_{r-1} - \nu_r, n-p}.$$

## ANOVA table

Term added	df	Reduction in SS	Mean square
$X_1$	$n - 1 - \nu_1$	$SS_0 - SS_1$	$MS_1 = (SS_0 - SS_1)/(n - 1 - \nu_1)$
$X_2$	$\nu_1 - \nu_2$	$SS_1 - SS_2$	$MS_2 = (SS_1 - SS_2)/(\nu_1 - \nu_2)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$X_R$	$\nu_{R-1} - \nu_R$	$SS_{R-1} - SS_R$	$MS_R = (SS_{R-1} - SS_R)/(\nu_{R-1} - \nu_R)$
Residual	$\nu_R = n - p$	$SS_R$	$MS_{Res} = SS_R/\nu_R$

□ If  $\mu \in \text{span}(X)$  then the residual mean square  $MS_{Res}$  gives an estimate of  $\sigma^2$ .

□ We test for an effect of term  $X_r$  by noting that

– if  $X_r$  explains no more than  $(X_0, \dots, X_{r-1})$ , then

$$F_r = \frac{MS_r}{MS_{Res}} \sim F_{\nu_{r-1} - \nu_r, \nu_R},$$

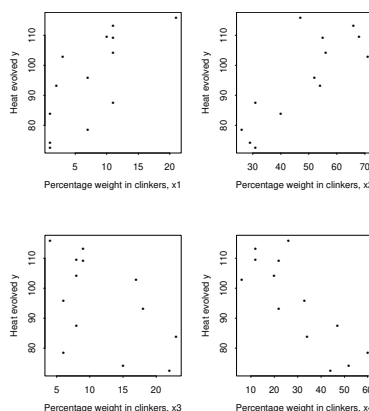
– if  $X_r$  does have additional explanatory power, then the distribution of  $MS_r$  is shifted to the right, and we expect  $F_r$  to be large relative to its null distribution.

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## Example: Cement data

Percentage weights in clinkers of 4 constituents of cement  $(x_1, \dots, x_4)$  and heat evolved  $y$  in calories, in  $n = 13$  samples.



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### Example: Cement data

```
> cement
```

```
  x1 x2 x3 x4    y
1   7 26  6 60  78.5
2   1 29 15 52  74.3
3  11 56  8 20 104.3
4  11 31  8 47  87.6
5   7 52  6 33  95.9
6  11 55  9 22 109.2
7   3 71 17  6 102.7
8   1 31 22 44  72.5
9   2 54 18 22  93.1
10 21 47  4 26 115.9
11  1 40 23 34  83.8
12 11 66  9 12 113.3
13 10 68  8 12 109.4
```

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### Example: Cement data

- ☐ Reductions in overall sum of squares when terms entered in the order given.
- ☐ Clearly  $x_1$  and  $x_2$  should be included, maybe not the others.

Term	df	Reduction in sum of squares	Mean square	$F$
$x_1$	1	1450.1	1450.1	242.5
$x_2$	1	1207.8	1207.8	202.0
$x_3$	1	9.79	9.79	1.64
$x_4$	1	0.25	0.25	0.04
Residual	8	47.86	5.98	

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### Example: Cement data

- ☐ What if we change the order of the terms?

Term	df	Reduction in sum of squares	Mean square	$F$
$x_4$	1	1831.9	1831.9	306.2
$x_3$	1	708.1	708.1	118.4
$x_2$	1	101.9	101.9	17.04
$x_1$	1	26.0	26.0	4.34
Residual	8	47.86	5.98	

- ☐ Should  $x_1$  and  $x_2$  be included or not?

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## Orthogonality

- ☐ In general, the ANOVA and ANOVA table depend on the order of inclusion of terms.
- ☐ Its interpretation is unclear if  $X_r$  is significant when included early, but not when it is included late. Is the term important or not?
- ☐ In a model with orthogonal terms,

$$X\beta = 1_n\beta_0 + X_1\beta_1 + X_2\beta_2, \quad X_r^T X_s = X_r^T 1_n = 0, \quad r \neq s.$$

we obtain

$$\begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \hat{\beta}_2 \end{pmatrix} = \begin{pmatrix} 1^T 1 & 0 & 0 \\ 0 & X_1^T X_1 & 0 \\ 0 & 0 & X_2^T X_2 \end{pmatrix}^{-1} \begin{pmatrix} 1 & X_1 & X_2 \end{pmatrix}^T y$$

so since  $\hat{y} = X\hat{\beta}$ , we have

$$y^T y - \hat{y}^T \hat{y} = y^T y - n\bar{y}^2 - \hat{\beta}_1^T X_1^T X_1 \hat{\beta}_1 - \hat{\beta}_2^T X_2^T X_2 \hat{\beta}_2,$$

and the residual sums of squares for the sub-models  $1_n\beta_0$ ,  $1_n\beta_0 + X_1\beta_1$ ,  $1_n\beta_0 + X_2\beta_2$  are

$$y^T y - n\bar{y}^2, \quad y^T y - n\bar{y}^2 - \hat{\beta}_1^T X_1^T X_1 \hat{\beta}_1, \quad y^T y - n\bar{y}^2 - \hat{\beta}_2^T X_2^T X_2 \hat{\beta}_2,$$

so the reductions do not depend on the order of inclusion. Hooray!

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## Balance

- ☐ Balanced design matrices induce orthogonality after fitting  $1_n$  (or a more complex design  $X_0$ ).
- ☐ Gram–Schmidt orthogonalisation with respect to early terms makes later terms mutually orthogonal, leading to a clear interpretation of the ANOVA for the later terms.
- ☐ If we write  $H_0 = X_0(X_0^T X_0)^{-1} X_0$  and let

$$Z_r = P_0 X_r = (I_n - H_0) X_r, \quad r = 1, 2,$$

denote the versions of  $X_1$  and  $X_2$  after adjusting for  $X_0$ , then

$$\begin{aligned} X_0\beta_0 + X_1\beta_1 + X_2\beta_2 &= (X_0\beta_0 + H_0 X_1\beta_1 + H_0 X_2\beta_2) + P_0 X_1\beta_1 + P_0 X_2\beta_2 \\ &= Z_0\gamma_0 + Z_1\beta_1 + Z_2\beta_2, \end{aligned}$$

say, and  $Z_1^T Z_0 = Z_2^T Z_0 = 0$ , because  $P_0 X_0 = P_0 H_0 = 0$ .

- ☐ If the design satisfies  $Z_1^T Z_2 = 0$ , then the order of inclusion of  $X_1$ ,  $X_2$  is irrelevant, provided  $X_0$  is already present in the fit.

**Example 13 ( $3 \times 2$  layout)** *Observations and their means written as*

$y_{11}$	$y_{12}$	$\mu + \alpha_1 + \delta_1$	$\mu + \alpha_2 + \delta_1$
$y_{21}$	$y_{22}$	$\mu + \alpha_1 + \delta_2$	$\mu + \alpha_2 + \delta_2$
$y_{31}$	$y_{32}$	$\mu + \alpha_1 + \delta_3$	$\mu + \alpha_2 + \delta_3$

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### Note to Example 13

- In terms of the parameter vector  $(\mu, \alpha_1, \alpha_2, \delta_1, \delta_2, \delta_3)^T$ , the design matrix is

$$X_{6 \times 6}^* = \begin{pmatrix} 1 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}, \quad \text{with responses } y = \begin{pmatrix} y_{11} \\ y_{12} \\ y_{21} \\ y_{22} \\ y_{31} \\ y_{32} \end{pmatrix},$$

with  $X_0 \equiv 1_6$  the first column of  $X^*$ , columns 2–3 the term  $X_1^*$  for columns, and columns 4–6 the term  $X_2^*$  for rows.

- This model has six parameters, but they cannot all be estimated, because  $X_0$  lies in the column spaces of  $X_1^*$  and  $X_2^*$ , and it is easy to check that  $X^*$  has rank 4. The usual way to deal with this is to set  $\alpha_1 = \delta_1 = 0$ , corresponding to dropping columns 2 and 4 of  $X^*$ , giving the so-called *corner-point parametrization* in which the means are

$$\begin{array}{cc} y_{11} & y_{12} & \mu & \mu + \alpha_2 \\ y_{21} & y_{22} & \mu + \delta_2 & \mu + \alpha_2 + \delta_2, \\ y_{31} & y_{32} & \mu + \delta_3 & \mu + \alpha_2 + \delta_3 \end{array}$$

i.e.,

- the 'grand mean'  $\mu$  corresponds to the mean of observations with the first level of every factor,
- $\alpha_2$  corresponds to the mean difference between column 2 and column 1,
- $\delta_2$  corresponds to the mean difference between row 2 and row 1, and
- $\delta_3$  corresponds to the mean difference between row 3 and row 1.

This is the default in R. More rarely we might set  $\sum_c \alpha_c = \sum_r \delta_r = 0$ .

- Even after these columns are dropped to give

$$X = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 \end{pmatrix},$$

the terms  $X_1$  for columns and  $X_2$  for rows are not orthogonal, and they are not orthogonal to  $1_n$ . On the other hand  $Z_1$  and  $Z_2$  in the corresponding centred matrix,

$$\begin{pmatrix} 1 & -\frac{1}{2} & -\frac{1}{3} & -\frac{1}{3} \\ 1 & \frac{1}{2} & -\frac{1}{3} & -\frac{1}{3} \\ 1 & -\frac{1}{2} & \frac{2}{3} & -\frac{1}{3} \\ 1 & \frac{1}{2} & \frac{2}{3} & -\frac{1}{3} \\ 1 & -\frac{1}{2} & -\frac{1}{3} & \frac{2}{3} \\ 1 & \frac{1}{2} & -\frac{1}{3} & \frac{2}{3} \end{pmatrix}$$

are orthogonal to the constant by construction and to each other because the design is balanced:  $\delta_2$  and  $\delta_3$  each occur equally often with  $\alpha_2$  and without  $\alpha_2$ . This balance implies that if  $\mu$  is fitted first, the reductions in sums of squares due to  $X_1$  and  $X_2$ , or equivalently  $Z_1$  and  $Z_2$ , are unique.

**Assumptions and model checking**

- ☐ How heavily do our conclusions depend on our assumptions?
- ☐ In any given context,
  - **primary** aspects relate to the questions our analysis will address,
  - **secondary** aspects relate to how we go about finding answers to them.
- ☐ Concerns about primary aspects suggest that we should start again.
- ☐ Concerns about secondary aspects suggest that we modify the analysis.
- ☐ **Regression diagnostics** check that a fitted model is adequate:
  - Does  $y$  depend linearly on the columns of  $X$ ?
  - Does  $y$  depend systematically on variables omitted from  $X$ ?
  - Are the variances constant?
  - Are the responses uncorrelated/independent?
  - Are there outliers or otherwise unusual data?
  - Are the responses normally distributed?
- ☐ Usually these involve plots, sometimes tests — **beware over-interpretation!**
- ☐ Key question: ‘how would the failure I see/suspect change my conclusions?’

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**Residuals**

- ☐ The **raw residuals**

$$e = y - \hat{y} = y - X\hat{\beta} = (I_n - H)y$$

have  $E(e) = 0$ ,  $\text{var}(e) = \sigma^2(I_n - H)$  if model correct, so

$$\text{var}(e_j) = \sigma^2(1 - h_{jj}) \quad \text{cov}(e_j, e_k) = -\sigma^2 h_{jk}, \quad j \neq k.$$

In a good model  $e$  and  $\hat{y}$  should be unrelated, because  $e^T \hat{y} = 0$ .

- ☐ We estimate  $\sigma$  by the residual standard deviation  $s$  and define **standardized residuals**

$$r_j = \frac{e_j}{s(1 - h_{jj})^{1/2}} = \frac{y_j - x_j^T \hat{\beta}}{s(1 - h_{jj})^{1/2}}, \quad j = 1, \dots, n,$$

which have  $E(r_j) = 0$  and  $\text{var}(r_j) \doteq 1$ .

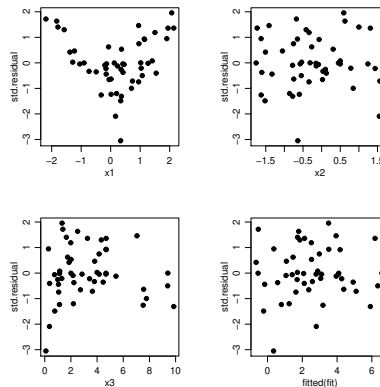
- ☐ We check
  - linearity by plotting  $r_j$  against the covariates (those in  $X$  and those not in  $X$ );
  - constant variance by plotting  $r_j$  (or  $|r_j|$ ) against fitted values  $\hat{y}_j$ ;
  - independence by ACF of residuals (if data time-ordered);
  - for outliers, which are visible as unusual residuals; and
  - normality using a normal QQ-plot of  $r_j$ .

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## Checking linearity

- ☐ Plot  $r$  against each covariate, included or not in the model, and against  $\hat{y}$ , which is uncorrelated with  $e$  (as  $\hat{y}^T e = 0$ ):

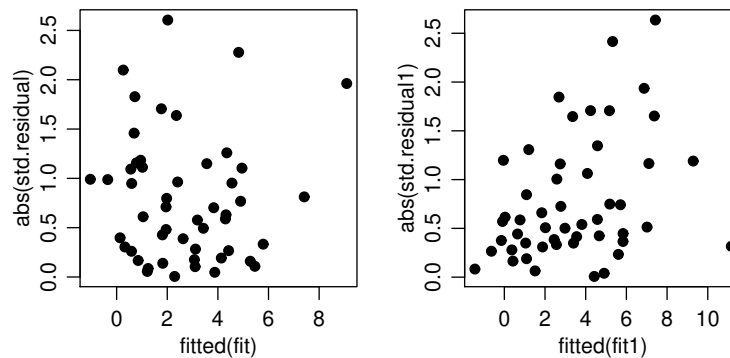


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## Checking the variance

- ☐ Does  $\text{var}(y)$  depend on  $E(y)$ ?
- ☐ Variance function shows how  $\text{var}(y)$  depends on  $\mu = E(y)$ . For normal linear model should have  $\text{var}(y) = \sigma^2$ , so variance is constant function of  $\mu$
- ☐ Plot  $r$  or  $|r|$  against  $\hat{y}$ :



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## Checking independence

- ☐ Dependence can greatly increase uncertainty of final conclusions.
- ☐ Substantive knowledge is helpful in suggesting whether it might be present:
  - were the data gathered in temporal/spatial/... order?
  - were the data sampled/gathered in groups (e.g., spatial, several observations on different individuals, ...)?
  - was randomisation used? If so, how?
- ☐ If observations are time-ordered, try using correlogram (ACF) and partial correlogram (PACF) to estimate serial correlations and partial correlations

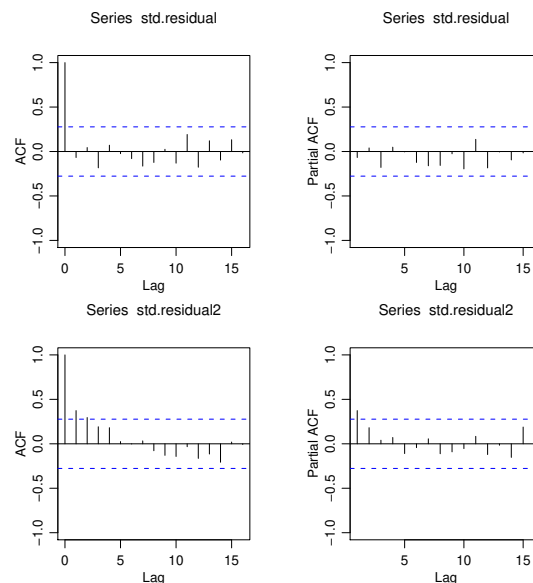
$$\text{corr}(r_j, r_{j+t}), \quad \text{corr}(r_j, r_{j+t} \mid r_{j+1}, \dots, r_{j+t-1}), \quad t = 1, \dots$$

- ☐ On next page, top panels show uncorrelated residuals, lower ones show evidence of correlation, suggesting use of a time series model.

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## Checking independence



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## Checking for outliers and normality

- Normal Q-Q plot for  $Y_1, \dots, Y_n \stackrel{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)$  graphs ordered values

$$Y_{(1)} \leq Y_{(2)} \leq \dots \leq Y_{(n)}$$

against (approximate) expected normal order statistics

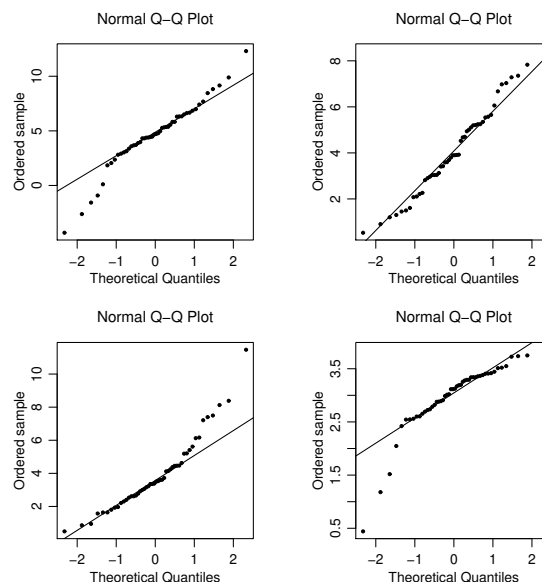
$$\Phi^{-1}\{1/(n+1)\}, \Phi^{-1}\{2/(n+1)\}, \dots, \Phi^{-1}\{n/(n+1)\}.$$

- Normality — roughly straight line, slope  $\sigma$ , intercept  $\mu$ .
- Outliers, skewness, heavy tails (easily) seen.
- Beware over-interpretation of such plots when  $n$  is small — often useful to add simulation envelope.
- Apply to standardized residuals  $r_j$  from regression model.

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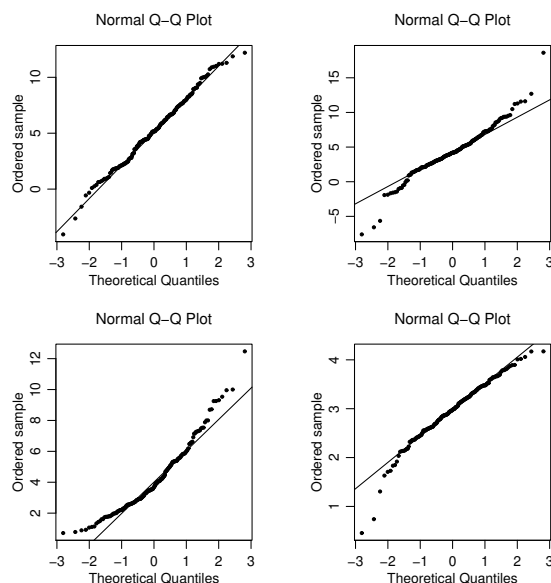
## Checking normality, $n = 50$



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## Checking normality, $n = 200$



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## Leverage and influence

- ☐ Does **case**  $(x_j, y_j)$  strongly influence the fitted model (picture)?

- ☐ As

$$\text{var}(y_j - \hat{y}_j) = \text{var}(y_j - x_j^T \beta) = \sigma^2(1 - h_{jj}),$$

having **leverage**  $h_{jj} \doteq 1$  implies that  $\hat{y}_j \approx y_j$  — need one parameter to fit this case.

- ☐ As  $\text{tr}(H) = \sum_{j=1}^n h_{jj} = p$ , the average  $h_{jj}$  is  $p/n$ . If  $h_{jj} > 2p/n$ , then  $j$ th case should be checked (rule of thumb), e.g. by refitting without  $(x_j, y_j)$ .
- ☐ Let  $\hat{y}_{-j}$  be fitted values for (all) data when  $(x_j, y_j)$  is dropped and use **Cook's distance**

$$C_j = \frac{1}{ps^2}(\hat{y} - \hat{y}_{-j})^T(\hat{y} - \hat{y}_{-j}) = \dots = \frac{r_j^2 h_{jj}}{p(1 - h_{jj})}$$

to measure the difference between  $\hat{y}$  and  $\hat{y}_{-j}$ .

- ☐ Large  $C_j$  implies large  $r_j$  and/or large  $h_{jj}$ .
- ☐ Cases with  $C_j > 8/(n - 2p)$  worth a closer look (rule of thumb).
- ☐ High leverage and/or influence need not be bad, just need to be aware of it.
- ☐ These ideas are not very useful in large samples, since the plots become uninformative.

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## Response transformation

- Linear model for  $y$  may be better applied for some transformation  $g(y)$ , especially if some  $y$  are much larger than others, or the variance is non-constant.
- Survival times  $y_{ptj}$  in 10-hour units of animals in a  $3 \times 4$  factorial experiment with four replicates, with (below) average (standard deviation) for the poison  $\times$  treatment combinations:
  - generally see higher SD and mean together,
  - times must be positive, so linear model inappropriate?

Treatment	Poison 1	Poison 2	Poison 3
A	0.31, 0.45, 0.46, 0.43	0.36, 0.29, 0.40, 0.23	0.22, 0.21, 0.18, 0.23
B	0.82, 1.10, 0.88, 0.72	0.92, 0.61, 0.49, 1.24	0.30, 0.37, 0.38, 0.29
C	0.43, 0.45, 0.63, 0.76	0.44, 0.35, 0.31, 0.40	0.23, 0.25, 0.24, 0.22
D	0.45, 0.71, 0.66, 0.62	0.56, 1.02, 0.71, 0.38	0.30, 0.36, 0.31, 0.33

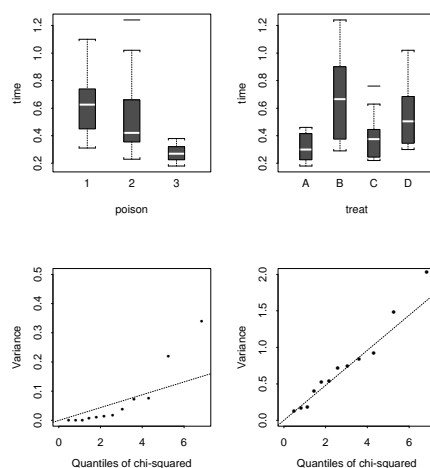
Treatment	Poison 1	Poison 2	Poison 3	Average
A	0.41 (0.07)	0.32 (0.08)	0.21 (0.02)	0.31
B	0.88 (0.16)	0.82 (0.34)	0.34 (0.05)	0.68
C	0.57 (0.16)	0.38 (0.06)	0.24 (0.01)	0.39
D	0.61 (0.11)	0.67 (0.27)	0.33 (0.03)	0.53
Average	0.62	0.55	0.28	0.48

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## Example: Poison data

Upper panels: dependence of responses on the factor levels. Lower left:  $\chi^2_3$  probability plots of the  $3s_{pt}^2$ , where  $s_{pt}^2$  is the sample variance of  $y_{ptj}$ . Lower right: same for  $y_{ptj}^{-1}$ .



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## Box–Cox transformation

- For  $y > 0$ , the **Box–Cox transformation**

$$y^{(\lambda)} = \begin{cases} \frac{y^\lambda - 1}{\lambda}, & \lambda \neq 0, \\ \log y, & \lambda = 0, \end{cases}$$

includes the inverse ( $\lambda = -1$ ), log ( $\lambda = 0$ ), cube and square roots ( $\lambda = \frac{1}{3}, \frac{1}{2}$ ), original scale ( $\lambda = 1$ ) and square ( $\lambda = 2$ ); sometimes map  $y \mapsto y + c > 0$ .

- Suppose normal linear model

$$y^{(\lambda)} \sim \mathcal{N}_n(X\beta, \sigma^2 I_n)$$

applies for some  $\beta$ ,  $\sigma$  and  $\lambda$  to be determined. Here  $X$  contains  $1_n$ , so use of  $y^{(\lambda)}$  just changes intercept and rescales  $\beta$  and  $\sigma$ .

- Use profile log likelihood for  $\lambda$  to choose ‘best’ transformation (usually from list above to aid interpretation).
- Interpretation of  $\beta$  depends on  $\lambda$ , so usually we ignore the fact that  $\lambda$  was estimated, unless we are not interested in  $\beta$  (e.g., when performing ‘automatic’ prediction).

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## Example: Poison data

- Fits of two-way layout model, with interaction:

$$y_{tpj}^{(\lambda)} \sim \mathcal{N}(\mu + \alpha_t + \beta_p + \gamma_{tp}, \sigma^2), \quad t = 1, 2, 3, 4, \quad p = 1, 2, 3, \quad j = 1, 2, 3, 4.$$

- Analyses of variance with responses  $y$  and  $y^{-1}$ . For MS and  $F$  read ‘Mean square’ and ‘ $F$  statistic’.
- The terms explain appreciably more of the variation of  $y^{-1}$ , suggesting that this is a preferable choice of response.

Term	df	Response $y$			Response $y^{-1}$		
		SS	MS	$F$	SS	MS	$F$
Poisons	2	1.033	0.517	23.22	34.88	17.44	72.63
Treatments	3	0.921	0.307	13.81	20.41	6.80	28.34
Treatments $\times$ Poisons	6	0.250	0.042	1.87	1.57	0.26	1.09
Residual	36	0.801	0.022		8.64	0.24	

Regression Methods

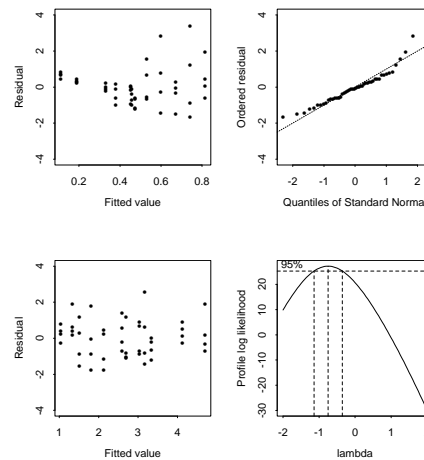
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### Example: Poison data

Top: residuals for model without interactions  $\gamma_{tp}$ ; clearly problematic.

Lower right: profile log likelihood for Box–Cox  $\lambda$ , showing 95% confidence interval.

Lower left: residuals for the two-way layout model (no interactions) for  $1/y$ .



Regression Methods

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### Summary on model-checking

- ☐ Recall the distinction between primary and secondary assumptions. Use of the standard linear model when the secondary assumptions fail leads to inefficient estimation and over-confident uncertainty assessment, but is not usually disastrous per se.
- ☐ When they fail ...
  - **Linearity** (primary): add terms (e.g.,  $x^2$ ) to the model, transform the covariate (e.g., to  $\log x$ ), or question the basic setup;
  - **Constant variance** (secondary): use a response transformation (below), weighted least squares, or question primary aspects. Non-constant variance affects uncertainty assessment, but not estimation;
  - **Lack of correlation (independence)** (secondary): use a correlated error model (e.g., time series or random effects). Dependence affects uncertainty assessment, but not estimation;
  - **normality** (secondary): often does not matter, because the CLT applies to the estimators. It does matter for prediction, which is affected by the distribution of individual responses;
- ☐ Checking leverage and influence may be useful in small and moderate samples, but rarely in large samples. In any case, automatic dropping of outlying and/or influential cases is dangerous!

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**Goals**

- ☐ What to do faced with a set of data?
- ☐ Two main aims:
  - **understand** (science) — maybe have prior idea/hypotheses on how response depends on explanatory variables. Interpretation is key.
  - **predict/control** (technology) — don't really care how  $y$  depends on  $X$ . Interpretation not critical (though this describes only prediction in the narrowest of senses).
- ☐ There is no reason that a single model will do both, or even that there must be a single 'best' model:
  - maybe two models with different interpretations both fit about equally well, and then future work might aim to choose between them;
  - prediction with a mixture of models might be better than using a single model.

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**Meta-algorithm**

- ☐ **Collect** data intended to answer question of interest;
- ☐ **examine** data (graphs, look for outliers, problems with sampling scheme);
- ☐ **choose/construct** response variable (transformations? independence?);
- ☐ **consider** what models are coherent with context of problem (limiting properties, units, similar problems/datasets, covariates that must be included, ...);
- ☐ **iterate**:
  - fit models, compare quality of fits;
  - check interpretations of  $\hat{\beta}$ ,  $\hat{\sigma}^2$  and
  - check fit (diagnostics, outliers, ...)
 until satisfied; finally
- ☐ give **conclusions**—careful interpretation of best model(s) in terms of original problem, consider deficiencies, and explain what extra data might overcome them.

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**Initial examination of data**

- ☐ Plot  $y$  against covariates, look for outliers, non-constant variance, nonlinearity, etc.
- ☐ Plot covariates against each other, look for dependence.
- ☐ Try to understand covariates (e.g., dimensions), are transformations needed?
- ☐ May need to reduce dimension of  $X$  by **regularisation** — many ways to do this (later).

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### Albert Einstein (1879–1955)



'Everything should be made as simple as possible, *but no simpler.*'

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### William of Occam (?1285–1347/9)



Occam's razor: *Pluralitas non est ponenda sine necessitate*: entities should not be multiplied beyond necessity.

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## Automatic variable selection

- ☐ Assume linear model  $E(y) = X\beta$
- ☐  $2^p$  possible subsets of columns of  $X$ , plus transformations, ...
- ☐ Example:  $p = 17$  gives 131072 possible subsets of variables
- ☐ Fast algorithms (e.g., branch and bound, leaps in R) exist visit them all or just subsets (e.g., stepwise), but we need criteria for comparing models.
- ☐ Many proposals for model comparison
  - cross-validation,
  - information criteria (AIC, AIC<sub>c</sub>, BIC, NIC, TIC, ...)
  - Mallows's  $C_p$ ,
  - ...
- ☐ Most involve minimising estimated prediction error for future data *like those observed!*

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## Prediction error

- ☐ True model  $y \sim (\mu, \sigma^2 I_n)$ , we assume (perhaps incorrectly) that  $\mu = X\beta$ , fit  $X_{n \times p}$  and obtain fitted value

$$X\hat{\beta} = Hy \sim (H\mu, \sigma^2 H).$$

- ☐ Terminology
  - the **true model** has  $\mu = X\beta$  and all  $\beta_r \neq 0$ ;
  - a **correct model** has  $\mu = X\beta$  but some  $\beta_r = 0$ ;
  - a **wrong** model has  $\mu \notin \text{span}(X)$ ;so  $(I_n - H)\mu = 0$  if the model is true or correct, and  $(I_n - H)\mu \neq 0$  if it is wrong.
- ☐ The **prediction error** for an independent dataset  $y_+$  with mean vector  $\mu$  is

$$\Delta = n^{-1}E \left\{ (y_+ - X\hat{\beta})^T (y_+ - X\hat{\beta}) \right\} = \begin{cases} n^{-1}\mu^T(I - H)\mu + (1 + p/n)\sigma^2, & \text{wrong,} \\ (1 + q/n)\sigma^2, & \text{true,} \\ (1 + p/n)\sigma^2, & \text{correct,} \end{cases}$$

where  $E(\cdot)$  is over both  $y_+$  and  $y$  and  $p \geq q = \#\{\beta_r : \beta_r \neq 0\}$  when  $\mu \in \text{span}(X)$ .

- ☐ In principle we should write  $\Delta \equiv \Delta(X)$ .

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### Note: Computation of $\Delta$

Let  $y \sim (\mu, \sigma^2 I)$  and fit  $X\beta$ , obtaining fitted value

$$X\hat{\beta} = Hy \sim (H\mu, \sigma^2 H),$$

where  $H\mu = \mu$ , i.e.,  $(I - H)\mu = 0$  if  $\mu \in \text{span}(X)$ , but otherwise  $(I - H)\mu \neq 0$ .

We have a new data set  $y_+ \sim (\mu, \sigma^2 I)$ , and we compute the average error in predicting  $y_+$  using  $X\hat{\beta}$ , i.e.,

$$\Delta = n^{-1} \mathbb{E} \left\{ (y_+ - X\hat{\beta})^T (y_+ - X\hat{\beta}) \right\}.$$

Let  $e_+ = y_+ - X\hat{\beta}$  and note that as the trace of a scalar is the scalar and trace is a linear operator,

$$\mathbb{E}(e_+^T e_+) = \mathbb{E}\{\text{tr}(e_+^T e_+)\} = \mathbb{E}\{\text{tr}(e_+ e_+^T)\} = \text{tr}\{\mathbb{E}(e_+ e_+^T)\} = \text{tr}\{\text{var}(e_+) + \mathbb{E}(e_+) \mathbb{E}(e_+)^T\}.$$

Now as  $y_+$  and  $y$  are independent and  $\text{var}(X\hat{\beta}) = \sigma^2 H$ , we have

$$y_+ - X\hat{\beta} \sim (\mu - H\mu, \sigma^2 I + \sigma^2 H),$$

so the computation above gives

$$\mathbb{E} \left\{ (y_+ - X\hat{\beta})^T (y_+ - X\hat{\beta}) \right\} = \text{tr}\{\sigma^2(I + H) + (I - H)\mu\mu^T(I - H)\} = \sigma^2(n + p) + \mu^T(I - H)\mu,$$

because  $\text{tr}(I + H) = n + p$  and  $I - H$  is symmetric and idempotent, giving

$$\Delta = \begin{cases} n^{-1}\mu^T(I - H)\mu + (1 + p/n)\sigma^2, & \text{wrong model,} \\ (1 + q/n)\sigma^2, & \text{true model,} \\ (1 + p/n)\sigma^2, & \text{correct model.} \end{cases}$$

### Bias/variance trade-off

- ☐ Minimising  $\Delta$  involves balancing the
  - **bias**  $n^{-1}\mu^T(I - H)\mu$ , which is reduced by including useful terms in  $X$ , and
  - **variance**  $(1 + p/n)\sigma^2$ , which is increased by including useless terms in  $X$ .
- ☐ We would like to minimise  $\Delta$ , but it depends on the unknown  $\mu$  and  $\sigma$ .
- ☐ The **cross-validation** estimator of  $\Delta$  splits the data into  $X', y'$  and  $X^*, y^*$ , then
  - for each possible subset  $\mathcal{S}$  of columns of  $X^*$ :
    - ▷ compute  $\hat{\beta}_{\mathcal{S}}^*$  by regressing  $y^*$  on  $X_{\mathcal{S}}^*$ ;
    - ▷ use  $\hat{\beta}_{\mathcal{S}}^*$  to estimate the prediction error for  $\mathcal{S}$  by

$$\hat{\Delta}_{\mathcal{S}} = (n')^{-1} (y' - X_{\mathcal{S}}' \hat{\beta}_{\mathcal{S}}^*)^T (y' - X_{\mathcal{S}}' \hat{\beta}_{\mathcal{S}}^*);$$

- finally choose the set of columns  $\mathcal{S}$  for which  $\hat{\Delta}_{\mathcal{S}}$  is minimised.
- ☐ This estimator depends on the split, and since  $X' \neq X^*$  in general,  $\hat{\Delta}_{\mathcal{S}}$  does not estimate  $\Delta_{\mathcal{S}}$ , so it would be preferable to use the entire dataset ...

## Leave-one-out cross-validation

- Simplest way to use entire dataset is **leave-one-out cross-validation (CV)**, minimising

$$n\hat{\Delta}_{CV} = CV = \sum_{j=1}^n (y_j - x_j^T \hat{\beta}_{-j})^2,$$

where  $\hat{\beta}_{-j}$  is estimate computed without  $(x_j, y_j)$ .

- This seems to require  $n$  fits, but the lemma below implies that with one fit we have

$$CV = \sum_{j=1}^n \frac{(y_j - x_j^T \hat{\beta})^2}{(1 - h_{jj})^2}.$$

**Lemma 14** For a fit  $\hat{y} = Hy$  where  $H$  has  $j$ th diagonal element  $h_{jj}$  and  $\hat{y}_{j,-j}$  is the fitted value for  $y_j$  obtained when  $(x_j, y_j)$  is dropped,

$$y_j - \hat{y}_{j,-j} = \frac{y_j - \hat{y}_j}{1 - h_{jj}},$$

and therefore

$$\sum_{j=1}^n (y_j - \hat{y}_{j,-j})^2 = \sum_{j=1}^n \frac{(y_j - \hat{y}_j)^2}{(1 - h_{jj})^2}.$$

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## Note to Lemma 14

- Consider any linear fit  $\hat{y} = Hy$ , and note that  $\hat{y}_j = \sum_{i=1}^n h_{ji} y_i$ .
- Now suppose we leave out  $(x_j, y_j)$  and compute the corresponding (penalized) estimate

$$\hat{\beta}_{-j} = \operatorname{argmin}_{\beta} \sum_{i \neq j} (y_i - x_i^T \beta)^2 + \lambda p(\beta),$$

and fitted value  $y_j^* = \hat{y}_{j,-j} = x_j^T \hat{\beta}_{-j}$  corresponding to  $x_j$ .

- Inserting  $(x_j, y_j^*)$  back into the dataset used to compute  $\hat{\beta}_{-j}$  changes nothing, because  $(y_j^* - x_j^T \hat{\beta}_{-j})^2 = 0$  and  $p(\beta)$  does not depend on the data. For this new dataset,

$$y_j^* = \sum_{i \neq j} h_{ji} y_i + h_{jj} y_j^* = \sum_{i=1}^n h_{ji} y_i + h_{jj} (y_j^* - y_j) = \hat{y}_j + h_{jj} (y_j^* - y_j)$$

so

$$y_j - y_j^* = y_j - \hat{y}_j + h_{jj} (y_j - y_j^*),$$

leading to

$$y_j - y_j^* = y_j - \hat{y}_{j,-j} = \frac{y_j - \hat{y}_j}{1 - h_{jj}},$$

and thus to the given formula.

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## Generalized cross-validation

- Leave-one-out CV can be unstable if some of the  $h_{jj}$  are large.
- **Generalised cross-validation (GCV)** replaces all the  $h_{jj}$  by their average  $\text{tr}(H)/n = p/n$ , giving

$$\text{GCV} = \sum_{j=1}^n \frac{(y_j - x_j^T \hat{\beta})^2}{(1 - p/n)^2},$$

and hence

$$\text{E}(\text{GCV}) = \mu^T(I - H)\mu/(1 - p/n)^2 + n\sigma^2/(1 - p/n) \approx n\Delta.$$

- Often choose the model that minimises GCV or CV.
- Note that these only require the second-order assumptions.

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## Note: Properties of GCV

We have  $(1 - p/n)^2 \text{GCV} = e^T e$  where  $e = y - X\hat{\beta} = (I - H)y \sim ((I - H)\mu, (I - H)\sigma^2)$ , and

$$\text{E}(e^T e) = \text{E}\{\text{tr}(ee^T)\} = \text{tr}\{\text{E}(e)\text{E}(e)^T + \text{var}(e)\} = \mu^T(I - H)\mu + \sigma^2 \text{tr}(I - H).$$

Now note that  $\text{tr}(I - H) = n - p$  and divide by  $(1 - p/n)^2$  to give (almost) the required result, for which we need also  $(1 - p/n)^{-1} \approx 1 + p/n$ , for  $p \ll n$ .

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## Akaike information criterion

- The above arguments apply only to least squares estimators. More generally, we could aim to minimise the **Kullback–Leibler discrepancy**

$$D(f_\theta, g) = \int \log \left\{ \frac{g(y)}{f(y; \theta)} \right\} g(y) dy \geq 0,$$

between **candidate model**  $f_\theta \equiv f(y; \theta)$  and true model  $g$ , based on  $Y_1, \dots, Y_n \stackrel{\text{iid}}{\sim} g$ .

- Suppose that  $\theta_g$  minimises  $D(f_\theta, g)$  within the family of candidate models, and is estimated by the MLE  $\hat{\theta}$ , with log likelihood  $\hat{\ell}$ .
- We suppose there is an independent sample  $Y_1^+, \dots, Y_n^+ \stackrel{\text{iid}}{\sim} g$  and aim to estimate

$$\text{E}_g \left( \text{E}_g^+ \left[ \sum_{j=1}^n \log \left\{ \frac{g(Y_j^+)}{f(Y_j^+; \hat{\theta})} \right\} \right] \right) = n \text{E}_g \{ D(f_{\hat{\theta}}, g) \}; \quad (2)$$

the outer expectation is over the distribution of  $\hat{\theta}$ , which is independent of  $Y^+$ .

- After tedious expansions we end up trying to minimise the **Akaike information criterion**

$$\text{AIC} = -2\hat{\ell} + 2p \quad (\equiv n \log \text{RSS} + 2p \text{ in linear model}).$$

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## Note: Derivation of AIC

- Taylor series expansion shows that  $\log f(y; \hat{\theta})$  approximately equals

$$\log f(y; \theta_g) + (\hat{\theta} - \theta_g)^T \frac{\partial \log f(y; \theta_g)}{\partial \theta} + \frac{1}{2} (\hat{\theta} - \theta_g)^T \frac{\partial^2 \log f(y; \theta_g)}{\partial \theta \partial \theta^T} (\hat{\theta} - \theta_g),$$

and as  $\theta_g$  minimizes  $D(f_\theta, g)$ ,

$$\int \frac{\partial \log f(y; \theta_g)}{\partial \theta} g(y) dy = 0.$$

Hence taking expectation over  $Y_1^+, \dots, Y_n^+$ , we get

$$nD(f_{\hat{\theta}}, g) = n \int \log \left\{ \frac{g(y)}{f(y; \hat{\theta})} \right\} g(y) dy \doteq nD(f_{\theta_g}, g) + \frac{1}{2} \text{tr} \left\{ (\hat{\theta} - \theta_g)(\hat{\theta} - \theta_g)^T I_g(\theta_g) \right\},$$

where we have used the fact that the trace of a scalar is itself.

- Expectation over the distribution of  $\hat{\theta}$  gives its variance matrix,  $I_g(\theta_g)^{-1} K(\theta_g) I_g(\theta_g)^{-1}$ , and hence

$$nE_g \{D(f_{\hat{\theta}}, g)\} \doteq nD(f_{\theta_g}, g) + \frac{1}{2} \text{tr} \{I_g(\theta_g)^{-1} K(\theta_g)\}, \quad (3)$$

where the second term penalizes the dimension  $p$  of  $\theta$ . The first term here is  $O(n)$  but the second is  $O(p)$ . When  $f_{\theta_g} = g$ ,  $I_g(\theta_g) = K(\theta_g)$  so  $\text{tr} \{I_g(\theta_g)^{-1} K(\theta_g)\} = p$ .

- To build an estimator, note that  $\int \log g(y) g(y) dy$  is constant and can be ignored. Now  $\ell(\hat{\theta}) = \ell(\theta_g) + \{\ell(\hat{\theta}) - \ell(\theta_g)\}$ , so

$$\begin{aligned} E_g \{-\ell(\hat{\theta})\} &= -E_g \{\ell(\theta_g) + \frac{1}{2} W(\theta_g)\} \\ &\doteq nD(f_{\theta_g}, g) - \frac{1}{2} \text{tr} \{I(\theta_g)^{-1} K(\theta_g)\} - n \int \log g(y) g(y) dy, \end{aligned}$$

where we have used the fact that under the wrong model, the likelihood ratio statistic  $W(\theta_g)$  has mean approximately  $\text{tr} \{I(\theta_g)^{-1} K(\theta_g)\}$ . Hence  $-\ell(\hat{\theta})$  tends to underestimate

$nD(f_{\theta_g}, g) - n \int \log g(y) g(y) dy$ . On reflection this is obvious, because  $\ell(\hat{\theta}) \geq \ell(\theta_g)$  by definition of  $\hat{\theta}$ . As  $p$  increases, so will the extent of overestimation.

- An estimator is  $-\ell(\hat{\theta}) + c$ , where  $c$  estimates  $\text{tr} \{I(\theta_g)^{-1} K(\theta_g)\}$ . Two possible choices of  $c$  are  $p$  and  $\text{tr}(\hat{I}^{-1} \hat{K})$ , and these lead to

$$\text{AIC} = 2\{-\ell(\hat{\theta}) + p\}, \quad \text{NIC} = 2\{-\ell(\hat{\theta}) + \text{tr}(\hat{J}^{-1} \hat{K})\}; \quad (4)$$

another possibility is  $\text{BIC} = -2\ell(\hat{\theta}) + p \log n$ .

- The model is chosen to minimize AIC, say, with the factor 2 putting differences of AIC on the same scale as likelihood ratio statistics. Such criteria are used far beyond random samples, and even in cases where the theory above doesn't work.
- In particular, the maximised log-likelihood for a normal-theory linear model with residual sum of squares RSS can be shown to be

$$-\frac{n}{2} \log(2\pi\hat{\sigma}) - \frac{n}{2} \equiv -\frac{n}{2} \log \text{RSS} + \text{constants},$$

which leads to the formula given on the slide.

## Other model selection criteria

- **'Corrected' AIC** for (normal-theory) regression problems:

$$\text{AIC}_c \equiv n \log \hat{\sigma}^2 + n \frac{1 + p/n}{1 - (p+2)/n}.$$

- **Bayes' information criterion**

$$\text{BIC} = -2\hat{\ell} + p \log n.$$

- **Mallows  $C_p$ :**

$$C_p = \frac{SS_p}{s^2} + 2p - n,$$

where  $SS_p$  is RSS for fitted model and  $s^2$  estimates  $\sigma^2$ .

- When the true model is a candidate and  $n \rightarrow \infty$ ,
  - AIC is **inconsistent** — it will not choose the true model with probability one, but tends to pick a more complex model;
  - $\text{AIC}_c$  is also inconsistent but gives better results in finite samples;
  - BIC is **consistent** — it chooses the true model with probability  $\rightarrow 1$ .

These results suppose that the models are fixed, but in practice we also have  $p \rightarrow \infty$  when  $n \rightarrow \infty$ , because we fit ever more complex models when we have more data.

## Simulation experiment

Number of times models were selected using various model selection criteria in 50 repetitions using simulated normal data for each of 20 design matrices. The true model has  $p = 3$ .

$n$		Number of covariates						
		1	2	3	4	5	6	7
10	$C_p$		131	504	91	63	83	128
	BIC		72	373	97	83	109	266
	AIC		52	329	97	91	125	306
	$\text{AIC}_c$	15	398	565	18	4		
20	$C_p$		4	673	121	88	61	53
	BIC		6	781	104	52	30	27
	AIC		2	577	144	104	76	97
	$\text{AIC}_c$		8	859	94	30	8	1
40	$C_p$			712	107	73	66	42
	BIC			904	56	20	15	5
	AIC			673	114	90	69	54
	$\text{AIC}_c$			786	105	52	41	16

### Stepwise methods

- ☐ In principle we might wish to fit all  $2^p$  possible choices of covariates, but in practice this is possible only for 'modest'  $p$ , using **leaps** or similar methods (or approximations).
- ☐ When  $p$  is too large for exhaustive searches, we instead consider subsets of the models, using the methods below (or variants).
- ☐ **Forward selection**: starting from the model with a constant only,
  1. add each remaining term separately to the current model;
  2. if none of these terms improves the fit, stop; otherwise
  3. update the current model to include the most useful new term; go to 1
- ☐ **Backward elimination**: starting from the model with all terms,
  1. if all terms are 'useful', stop; otherwise
  2. update current model by dropping the 'least useful' term; go to 1
- ☐ **Stepwise**: starting from an arbitrary model,
  1. consider three options—add a term, delete a term, swap a term in the model for one not in the model;
  2. if model unchanged, stop; otherwise go to 1
- ☐ 'Useful' means 'reduces the AIC' (but in the past meant 'is significant using an  $F$  test').

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### Stepwise methods: Comments

- ☐ Original formulation of stepwise used  $F$  tests (or even arbitrary numbers!) to assess significance, but this finds spurious models.
- ☐ Systematic search minimising AIC or similar over all possible models is preferable, but is often infeasible.
- ☐ Compare AICs for different models at each step—i.e., use AIC (or  $AIC_c$ ) as objective function.
- ☐ Important not to fixate on a specific model, or assume that there is a single 'best' model, but to consider any models whose AIC is within (say) 2 of the minimum — especially if the interpretations of competing models differ.

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### Example: Nuclear power stations

```
> nuclear
      cost  date t1 t2  cap pr ne ct bw cum.n pt
1  460.05 68.58 14 46  687  0  1  0  0    14  0
2  452.99 67.33 10 73 1065  0  0  1  0     1  0
3  443.22 67.33 10 85 1065  1  0  1  0     1  0
4  652.32 68.00 11 67 1065  0  1  1  0    12  0
5  642.23 68.00 11 78 1065  1  1  1  0    12  0
6  345.39 67.92 13 51  514  0  1  1  0     3  0
7  272.37 68.17 12 50  822  0  0  0  0     5  0
8  317.21 68.42 14 59  457  0  0  0  0     1  0
9  457.12 68.42 15 55  822  1  0  0  0     5  0
10 690.19 68.33 12 71  792  0  1  1  1     2  0
...
32 270.71 67.83  7 80  886  1  0  0  1    11  1
```

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### Example: Nuclear power stations

	Full model			Backward			Forward		
	Est	(SE)	<i>t</i>	Est	(SE)	<i>t</i>	Est	(SE)	<i>t</i>
Constant	−14.24	(4.229)	−3.37	−13.26	(3.140)	−4.22	−7.627	(2.875)	−2.66
date	0.209	(0.065)	3.21	0.212	(0.043)	4.91	0.136	(0.040)	3.38
log(T1)	0.092	(0.244)	0.38						
log(T2)	0.290	(0.273)	1.05						
log(cap)	0.694	(0.136)	5.10	0.723	(0.119)	6.09	0.671	(0.141)	4.75
PR	−0.092	(0.077)	−1.20						
NE	0.258	(0.077)	3.35	0.249	(0.074)	3.36			
CT	0.120	(0.066)	1.82	0.140	(0.060)	2.32			
BW	0.033	(0.101)	0.33						
log(N)	−0.080	(0.046)	−1.74	−0.088	(0.042)	−2.11			
PT	−0.224	(0.123)	−1.83	−0.226	(0.114)	−1.99	−0.490	(0.103)	−4.77
<i>s</i> (df)	0.164 (21)			0.159 (25)			0.195 (28)		

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**M-estimation**

- ☐ The least squares estimates are linear in  $y$  and therefore very sensitive to outliers.
- ☐ When  $y_i \mapsto y_i + c$ ,

$$\hat{\beta} = \sum_{j=1}^n (X^T X)^{-1} x_j y_j \mapsto \sum_{j=1}^n (X^T X)^{-1} x_j y_j + (X^T X)^{-1} x_i c = \hat{\beta} + (X^T X)^{-1} x_i c,$$

which could be arbitrarily far from  $\hat{\beta}$ .

- ☐ Try and fix this by replacing

$$\min_{\beta} \sum_{j=1}^n (y_j - x_j^T \beta)^2 \quad \text{by} \quad \min_{\beta} \sum_{j=1}^n \rho \{ (y_j - x_j^T \beta) / \sigma \},$$

for function  $\rho(\cdot)$  that will give a more robust **M**(aximum likelihood-like)-**e**stimator, or equivalently solving the  $p \times 1$  system of **e**stimating **e**quations

$$\frac{1}{\sigma} \sum_{j=1}^n x_j \rho' \{ (y_j - x_j^T \beta) / \sigma \} = X^T \rho' = 0$$

say, where  $\rho'_{n \times 1}$  has  $j$ th element  $d\rho(u)/du$  for  $u = (y_j - x_j^T \beta) / \sigma$ .

**Choice of  $\rho$** 

- ☐ Choose  $\rho(u)$  to have desirable properties, e.g., to downweight outliers:

$$\rho(u) = u^2/2 \quad (\text{normal errors}),$$

$$\rho(u) = |u| \quad (\text{Laplace errors}),$$

$$\rho(u) = \nu \log(1 + u^2/\nu)/2 \quad (t_\nu \text{ errors}),$$

$$\rho(u) = \begin{cases} u^2/2, & |u| < c, \\ c(2|u| - c)/2, & \text{otherwise,} \end{cases} \quad (\text{Huber function}).$$

- ☐ The function  $\rho'(u)$  is also called the **i**nfluence **f**unction of the estimator, as its value determines what influence an observation at  $u$  has on the estimator:

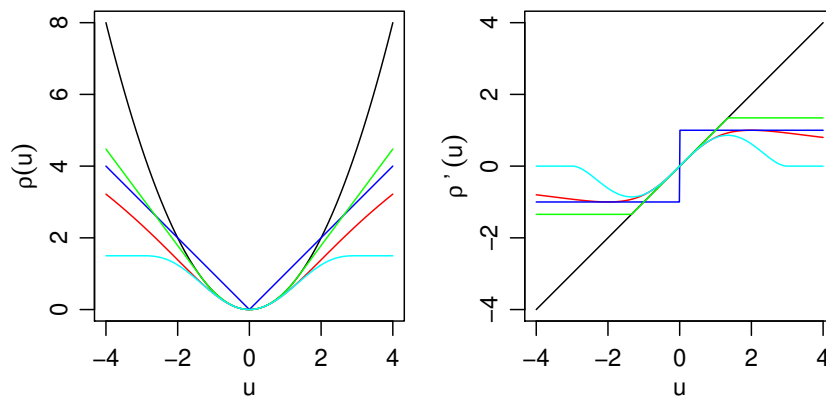
- Huber  $\rho'(u)$  is bounded,
- $t_\nu$  function is bounded and **r**edescending, as  $\lim_{u \rightarrow \pm\infty} \rho'(u) = 0$ ;
- Tukey's **b**iweight

$$\rho'(u) = u \{1 - (u/c)^2\}^2 I(|u| < c),$$

which gives  $\rho'(u) = 0$  when  $|u| > c$ , is also redescending, giving no weight to observations outside  $\pm c$ .

## $\rho$ and $\rho'$

Functions  $\rho$  and  $\rho'$  for least squares (black),  $t_5$  (red), Laplace (blue), Huber (green) and biweight (cyan) estimators.



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## Estimation

- We need to solve

$$X^T \rho' = 0,$$

where  $\rho'$  has  $j$ th element

$$\sigma^{-1} \rho' \{ (y_j - x_j^T \beta) / \sigma \} \propto \frac{\rho' \{ (y_j - x_j^T \beta) / \sigma \}}{y_j - x_j^T \beta} \times (y_j - x_j^T \beta) = w_j(\beta, \sigma) (y_j - x_j^T \beta),$$

say, so we write the estimating equation as

$$X^T W (y - X\beta) = 0,$$

with  $W = \text{diag}\{w_1(\beta, \sigma), \dots, w_n(\beta, \sigma)\}$ .

- We use **iterative weighted least squares**: choose some initial  $\tilde{\beta}$  and  $\sigma$ , then iterate to convergence the steps
  - compute  $W$  using the current  $\tilde{\beta}$ ,
  - compute the weighted least squares estimate,

$$\tilde{\beta} = (X^T W X)^{-1} X^T W y.$$

- Estimate  $\sigma$  using median absolute deviation of residuals  $y_j - x_j^T \tilde{\beta}$  at each iteration, or similar robust scale estimate.

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## M-estimator variance

- Estimator  $\tilde{\beta}$  is solution to  $p \times 1$  system of equations

$$g(y; \beta) = X^T \rho' = 0.$$

- Can show that if the estimating function  $g$  is **unbiased**, i.e.

$$E \{g(Y; \beta); \beta\} = 0, \quad \text{for any } \beta,$$

then under mild regularity conditions

$$\tilde{\beta} \sim \mathcal{N}_p \left( \beta, E \left\{ -\frac{\partial g(Y; \beta)}{\partial \beta^T} \right\}^{-1} \text{var} \{g(Y; \beta)\} E \left\{ -\frac{\partial g(Y; \beta)}{\partial \beta^T} \right\}^{-1} \right).$$

This is another **sandwich** variance matrix, with

$$E \left\{ -\frac{\partial g(Y; \beta)}{\partial \beta^T} \right\} = X^T W_1 X, \quad \text{var} \{g(Y; \beta)\} = X^T W_2 X,$$

so if  $W_1 = A(\sigma)I_n$ ,  $W_2 = \sigma^2 B(\sigma)I_n$ , then

$$\text{var}(\tilde{\beta}) \doteq \sigma^2 (X^T X)^{-1} \times B(\sigma) / A(\sigma)^2.$$

### Note: Sandwich matrix I

- The  $p \times 1$  estimating function is

$$g(y; \beta) = \sum_{j=1}^n x_j \rho' \left( \frac{y_j - x_j^T \beta}{\sigma} \right),$$

and unbiasedness implies that if the individual densities are  $\sigma^{-1} f\{(y_j - x_j^T \beta)/\sigma\}$ , then

$$0 = E\{g(y; \beta)\} = \sum_{j=1}^n x_j \int \rho' \left( \frac{y_j - x_j^T \beta}{\sigma} \right) \sigma^{-1} f \left( \frac{y_j - x_j^T \beta}{\sigma} \right) dy_j = X^T a_{n \times 1},$$

say, where  $a_j$  is the  $j$ th integral above, and setting  $u = (y_j - x_j^T \beta)/\sigma$  shows that all the  $a_j$  equal

$$\int \rho'(u) f(u) du = 0; \quad (5)$$

this is true by symmetry if the error distribution and  $\rho'$  are symmetric around the origin. Now

$$\frac{\partial g(y; \beta)}{\partial \beta^T} = -\frac{1}{\sigma} \sum_{j=1}^n x_j x_j^T \rho'' \left( \frac{y_j - x_j^T \beta}{\sigma} \right),$$

whose expectation is (using the same transformation)

$$\begin{aligned} E \left\{ \frac{\partial g(y; \beta)}{\partial \beta^T} \right\} &= -\frac{1}{\sigma} \sum_{j=1}^n x_j x_j^T E \left\{ \rho'' \left( \frac{Y_j - x_j^T \beta}{\sigma} \right) \right\} \\ &= -\frac{1}{\sigma} \sum_{j=1}^n x_j x_j^T \int \rho''(u) f(u) du = -\frac{1}{\sigma} X^T X A(\sigma), \end{aligned}$$

say.

- The components of these sums are independent, so

$$\text{var} \{g(Y; \beta)\} = \text{var} \left\{ \sum_{j=1}^n x_j \rho' \left( \frac{Y_j - x_j^T \beta}{\sigma} \right) \right\} = \sum_{j=1}^n x_j x_j^T \text{var} \left\{ \rho' \left( \frac{Y_j - x_j^T \beta}{\sigma} \right) \right\},$$

where the substitution  $u = (y_j - x_j^T \beta)/\sigma$  and (5) show that the variance term can be written as

$$\text{var} \left\{ \rho' \left( \frac{Y_j - x_j^T \beta}{\sigma} \right) \right\} = \int \rho'(u)^2 f(u) du = B(\sigma).$$

- The sandwich variance formula is therefore

$$\left\{ -\frac{1}{\sigma} X^T X A(\sigma) \right\}^{-1} X^T X B(\sigma) \left\{ -\frac{1}{\sigma} X^T X A(\sigma) \right\}^{-1} = (X^T X)^{-1} \times \frac{\sigma^2 B(\sigma)}{A(\sigma)^2}.$$

The variance of the LSE is  $\text{var}(Y_j)(X^T X)^{-1}$ , so the asymptotic relative efficiency of the M-estimator based on  $\rho$  and the LSE is

$$\frac{\text{var}(Y_j)}{\sigma^2} \times \frac{A(\sigma)^2}{B(\sigma)}.$$



### Note: Sandwich matrix II

- As a check on this, note that for the normal distribution  $\rho'(u) = u$ ,  $f(u) = (2\pi)^{-1}e^{-u^2/2}$ , so  $A(\sigma) = B(\sigma) = 1$ , which gives ARE of 1. If we take  $\rho'(u) = \text{sign}(u)$  with the normal density, we have  $B(\sigma) = 1$ ,  $A(\sigma) = -2/(2\pi)^{1/2}$ , so the sandwich variance formula gives  $\sigma^2(X^T X)^{-1}\pi/2$ . So using the  $\rho$ -function corresponding to the Laplace distribution when the data are in fact normally distributed leads to an estimator which is  $\pi/2 \approx 1.57$  times more variable than would be the case if the appropriate  $\rho$ -function were used.
- If we take the  $\rho$ -function  $\rho'(u) = u$  corresponding to the normal density, and the errors are in fact Laplace,  $g(u) = (1/2)e^{-|u|}$ , we have

$$A(\sigma) = \int (-1)f(u) du = 1, \quad B(\sigma) = \int u^2 f(u) du = 2$$

and the asymptotic relative efficiency is  $1/2$ .

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### Efficiency

- Efficiency of M-estimators of  $\beta$  relative to LSEs of  $\beta$  is

$$\frac{\text{var}(Y_j)}{\sigma^2} \times \frac{A(\sigma)^2}{B(\sigma)};$$

for example, the Huber estimator is 95% efficient if  $c = 1.345$ .

- In practice need to balance robustness and efficiency, increasing the latter by increasing  $c$ .
- High numbers of outliers can wreck M-estimators.
- Highly robust **least trimmed squares** estimators obtained by minimising

$$\sum_{j=1}^q (y_j - x_j^T \beta)_{(j)}^2,$$

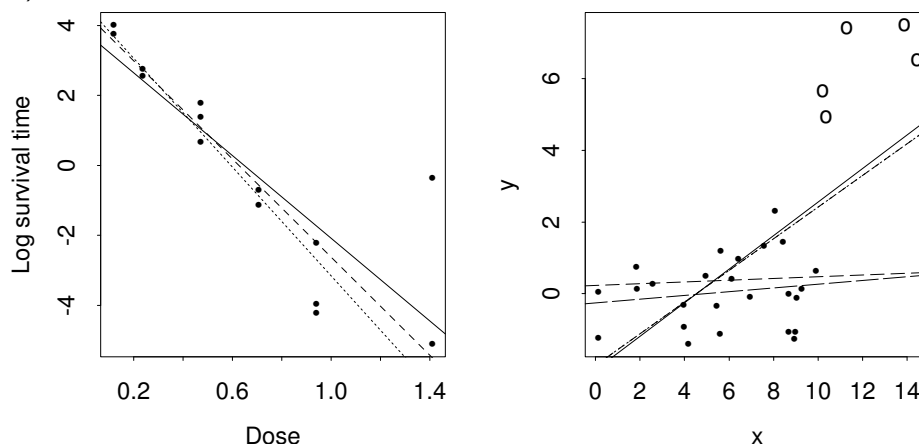
where  $q = \lfloor n/2 \rfloor + \lfloor (p+1)/2 \rfloor$ .

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### Example: Survival data

Left: log survival proportions for rats given doses of radiation, with lines fitted by least squares with (solid) and without (dotted) the outlier, and a Huber fit for the entire data (dashes). Right: simulated data with a batch of outliers (circles), and fits by least squares to all data (solid), least squares to good data only (large dash), Huber (dot-dash), biweight (dashes), and least trimmed squares (medium dash). The Huber and biweight fits are the same to plotting accuracy.



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### Simulation (right-hand panel on slide 86)

Table 1: Bias (standard deviation) of estimators of slope in sample of 25 good data and  $k$  outliers, estimated from 200 replications.

$k$	Least squares		M-estimation		Least trimmed squares
	No outliers	With outliers	Huber	Biweight	
1	0.00 (0.07)	0.17 (0.06)	0.07 (0.07)	0.01 (0.07)	−0.01 (0.13)
2	0.00 (0.07)	0.26 (0.06)	0.13 (0.07)	0.02 (0.09)	0.01 (0.14)
5	0.00 (0.07)	0.41 (0.05)	0.38 (0.06)	0.19 (0.19)	0.01 (0.14)
10	0.00 (0.06)	0.48 (0.04)	0.48 (0.04)	0.46 (0.12)	0.05 (0.20)

Good strategy is initial fit using least trimmed squares, then robust fit using this as starting point.

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## Quantile regression

- The Laplace distribution has

$$\rho(u) = |u| = uI(u \geq 0) - uI(u < 0),$$

and for continuous  $Y$ , the solution to  $E\{\rho'(Y - \theta)\} = 0$  is the median of  $Y$ . Hence

$$\operatorname{argmin} \sum_{j=1}^n \rho(y_j - x_j^T \beta)$$

estimates the median of  $y$  as a linear function of  $X\beta$ .

- **Quantile regression** takes  $\tau \in (0, 1)$  and uses the **check function**

$$\rho_\tau(u) = \tau u I(u \geq 0) - (1 - \tau) u I(u < 0);$$

then

$$\tilde{\beta}_\tau = \operatorname{argmin} \sum_{j=1}^n \rho_\tau(y_j - x_j^T \beta)$$

estimates the  $\tau$  quantile of  $y$  as a linear function of  $X\beta$ .

- For numerical purposes it may be better to smooth the bottom  $\rho$ .
- Note that  $\rho''_\tau(u) = 0$ , so it's better to bootstrap to find  $\operatorname{var}(\tilde{\beta}_\tau)$ .

Regression Methods

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## Expectile regression

- Quantile regression can be used to estimate value-at-risk in finance settings, but it has the drawback of just counting how many residuals are above/below the quantile.
- **Expectile regression** extends the LSE in the same way, taking

$$\rho_\tau(y - \theta) = \eta_\tau(y - \theta) - \eta_\tau(y), \quad \eta_\tau(u) = |I(u \leq 0) - \tau| u^2,$$

so  $\tau = 1/2$  gives the LSE, while taking  $\tau > 1/2$  leads to a more general form of LSE, with good properties for risk estimation in finance applications (coherent elicitable risk measure).

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## Smoking data

Table 2: Lung cancer deaths in British male physicians (Doll and Hill, 1952). The table gives man-years at risk  $T$ /number of cases  $y$  of lung cancer, cross-classified by years of smoking  $t$ , taken to be age minus 20 years, and number of cigarettes smoked per day,  $d$ .

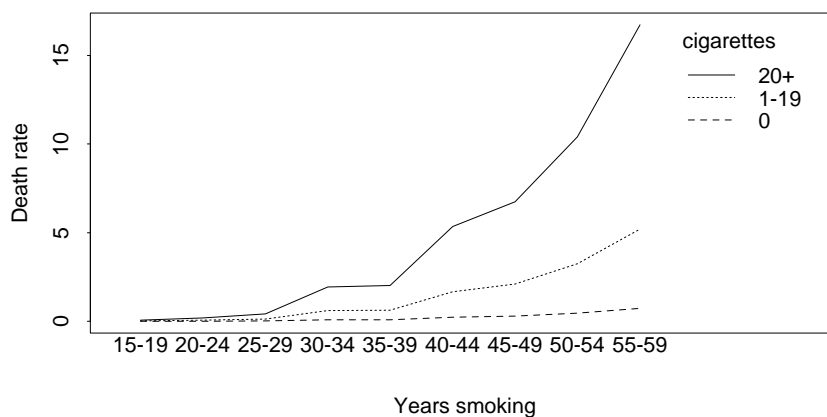
Years of smoking $t$	Daily cigarette consumption $d$						
	Nonsmokers	1-9	10-14	15-19	20-24	25-34	35+
15-19	10366/1	3121	3577	4317	5683	3042	670
20-24	8162	2937	3286/1	4214	6385/1	4050/1	1166
25-29	5969	2288	2546/1	3185	5483/1	4290/4	1482
30-34	4496	2015	2219/2	2560/4	4687/6	4268/9	1580/4
35-39	3512	1648/1	1826	1893	3646/5	3529/9	1336/6
40-44	2201	1310/2	1386/1	1334/2	2411/12	2424/11	924/10
45-49	1421	927	988/2	849/2	1567/9	1409/10	556/7
50-54	1121	710/3	684/4	470/2	857/7	663/5	255/4
55-59	826/2	606	449/3	280/5	416/7	284/3	104/1

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## Smoking data

Lung cancer deaths in British male physicians. The figure shows the rate of deaths per 1000 man-years at risk, for each of three levels of daily cigarette consumption.



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### Smoking data

- Suppose number of deaths  $y$  has Poisson distribution, mean  $T\lambda(d, t)$ , where  $T$  is man-years at risk,  $d$  is number of cigarettes smoked daily and  $t$  is time smoking (years).

- Take

$$\lambda(d, t) = \beta_0 t^{\beta_1} (1 + \beta_2 d^{\beta_3}) :$$

- background rate of lung cancer is  $\beta_0 t^{\beta_1}$  for non-smoker,
- additional risk due to smoking  $d$  cigarettes/day is  $\beta_2 d^{\beta_3}$ .

- With  $x_j = (T_j, d_j, t_j)$ , can write this as

$$y_j \sim \text{Pois}\{\mu(\beta; x_j)\},$$

$$\mu(\beta; x) = T\beta_0 t^{\beta_1} (1 + \beta_2 d^{\beta_3}), \quad j = 1, \dots, n :$$

a nonlinear model with Poisson-distributed response.

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### Comments

- Linear model  $y \sim (X\beta, \sigma^2 I_n)$ 
  - applicable for continuous response  $y \in \mathbb{R}$
  - assumes linear dependence of mean response  $E(y)$  on covariates  $X$
  - sometimes assumes  $y$  normal
- Lots of data not like this
- Need extensions for
  - nonlinear dependence on covariates
  - arbitrary response distribution (binomial, Poisson, exponential, ...)
  - dependent responses
  - variance non-constant (and related to mean?)
  - censoring, truncation, ...
  - ...

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### Simple fixes

- Just fit a linear model anyway
  - Might work as an approximation, but usually extrapolates really badly.
- Fit a linear model to transformed responses
  - E.g., take variance-stabilising transformation for  $y$ , such as  $2\sqrt{y}$  when  $y$  is Poisson
  - Can be helpful, but usually the obvious transformation can't give linearity.
- Instead we attempt to fit the model using likelihood estimation.

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**Revision: Likelihood**

**Definition 15** Let  $y$  be a data set, assumed to be the realisation of a random variable  $Y \sim f(y; \theta)$ , where the unknown parameter  $\theta$  lies in the parameter space  $\Omega_\theta \subset \mathbb{R}^p$ . Then the **likelihood** (for  $\theta$  based on  $y$ ) and the corresponding **log likelihood** are

$$L(\theta) = L(\theta; y) = f_Y(y; \theta), \quad \ell(\theta) = \log L(\theta), \quad \theta \in \Omega_\theta.$$

The **maximum likelihood estimate** (MLE)  $\hat{\theta}$  satisfies  $\ell(\hat{\theta}) \geq \ell(\theta)$ , for all  $\theta \in \Omega_\theta$ . Often  $\hat{\theta}$  is unique and in many cases it satisfies the **score (or likelihood) equation**

$$\frac{\partial \ell(\theta)}{\partial \theta} = 0,$$

which is interpreted as a vector equation of dimension  $p \times 1$  if  $\theta$  is a  $p \times 1$  vector.

The **observed information** and **expected (Fisher) information** are defined as

$$J(\theta) = -\frac{\partial^2 \ell(\theta)}{\partial \theta \partial \theta^\top}, \quad I(\theta) = E\{J(\theta)\};$$

these are  $p \times p$  matrices if  $\theta$  has dimension  $p$ .

**Revision: Maximum likelihood estimator**

- In large samples from a **regular model** in which the true parameter is  $\theta_{p \times 1}^0$ , the maximum likelihood estimator  $\hat{\theta}$  has an approximate normal distribution,

$$\hat{\theta} \sim \mathcal{N}_p\{\theta^0, J(\hat{\theta})^{-1}\},$$

so we can compute an approximate  $(1 - 2\alpha)$  confidence interval for the  $r$ th parameter  $\theta_r^0$  as

$$\hat{\theta}_r \pm z_\alpha v_{rr}^{1/2},$$

where  $v_{rr}$  is the  $r$ th diagonal element of the matrix  $J(\hat{\theta})^{-1}$ .

- This is easily implemented:
- we code the negative log likelihood  $-\ell(\theta)$  (and check the code carefully!);
  - we minimise  $-\ell(\theta)$  numerically, ensuring that the minimisation routine returns  $\hat{\theta}$  and the Hessian matrix  $J(\hat{\theta}) = -\partial^2 \ell(\theta) / \partial \theta \partial \theta^\top|_{\theta=\hat{\theta}}$
  - we compute  $J(\hat{\theta})^{-1}$ , and use the square roots of its diagonal elements,  $v_{11}^{1/2}, \dots, v_{dd}^{1/2}$ , as standard errors for the corresponding elements of  $\hat{\theta}$ .

### Revision: Regular model

We say that a statistical model  $f(y; \theta)$  is **regular (for likelihood inference)** if

1. the true value  $\theta^0$  of  $\theta$  is interior to the parameter space  $\Omega_\theta \subset \mathbb{R}^p$ ;
2. the densities defined by any two different values of  $\theta$  are distinct;
3. there is an open set  $\mathcal{I} \subset \Omega_\theta$  containing  $\theta^0$  within which the first three derivatives of the log likelihood with respect to elements of  $\theta$  exist almost surely, and

$$|\partial^3 \log f(Y_j; \theta) / \partial \theta_r \partial \theta_s \partial \theta_t| \leq g(Y_j)$$

uniformly for  $\theta \in \mathcal{I}$ , where  $0 < E_0\{g(Y_j)\} = K < \infty$ ; and

4. for  $\theta \in \mathcal{I}$  we can interchange differentiation with respect to  $\theta$  and integration, that is,

$$\frac{\partial}{\partial \theta} \int f(y; \theta) dy = \int \frac{\partial f(y; \theta)}{\partial \theta} dy, \quad \frac{\partial^2}{\partial \theta \partial \theta^\top} \int f(y; \theta) dy = \int \frac{\partial^2 f(y; \theta)}{\partial \theta \partial \theta^\top} dy.$$

The results are also true under weaker conditions, for non-identically distributed and dependent data.

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### Revision: Comments on regular models

Condition

1. is needed so that  $\hat{\theta}$  can lie 'on both sides' of  $\theta^0$  and hence can have a limiting normal distribution, once standardized—**fails**, for example, if  $\theta$  has a discrete component (e.g. changepoint  $\gamma \in \{1, \dots, n\}$ );
2. is needed to be able to identify the model on the basis of the data;
3. ensures the validity of Taylor series expansions of  $\ell(\theta)$ —not usually a problem;
4. ensures that the score statistic has a limiting normal distribution—can **fail** in some models — sometimes good news, leading to faster convergence than  $n^{-1/2}$ .

**All the above assumes the postulated model is correct!** — there is a literature on what happens when we fit the wrong model, or if the parameter dimension increases with  $n$ , or ... usually there are no generic results for such cases.

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### Revision: Likelihood ratio statistic

- Model  $f_B(y)$  is **nested** within model  $f_A(y)$  if  $A$  reduces to  $B$  on restricting some parameters:
  - for example, the model  $Y_1, \dots, Y_n \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$  is nested within the model  $Y_1, \dots, Y_n \stackrel{\text{iid}}{\sim} \mathcal{N}(\mu, \sigma^2)$ , because the first is obtained from the second by setting  $\mu = 0$ ;
  - the maximised log likelihoods satisfy  $\hat{\ell}_A \geq \hat{\ell}_B$ , because the more comprehensive model  $A$  contains the simpler model  $B$ .

- The **likelihood ratio statistic** for comparing them is

$$W = 2(\hat{\ell}_A - \hat{\ell}_B).$$

- If the model is regular, the simpler model is true, and  $A$  has  $q$  more parameters than  $B$ , then

$$W \sim \chi_q^2.$$

- This implicitly assumes that ML inference for model  $A$  is OK, so that the approximation  $\hat{\theta}_A \sim \mathcal{N}\{\theta_A, J_A(\hat{\theta}_A)^{-1}\}$  is adequate.

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### Revision: Profile log likelihood

- Consider a regular log likelihood  $\ell(\psi, \lambda)$ , where the **parameter of interest**  $\psi$  is variation independent of the **nuisance parameter**  $\lambda$ , i.e.,  $(\psi, \lambda) \in \Omega_\psi \times \Omega_\lambda$ , and the overall MLE is  $(\hat{\psi}, \hat{\lambda})$ .
- For a confidence set for  $\psi$ , without reference to  $\lambda$ , we use the **profile log likelihood**

$$\ell_p(\psi) = \max_{\lambda \in \Omega_\lambda} \ell(\psi, \lambda) = \ell(\psi, \hat{\lambda}_\psi),$$

say, and, based on the limiting distribution of the likelihood ratio statistic, take as  $(1 - 2\alpha)$  confidence region the set

$$\left\{ \psi \in \Omega_\psi : 2\{\ell(\hat{\psi}, \hat{\lambda}) - \ell(\psi, \hat{\lambda}_\psi)\} \leq \chi_{\dim \psi}^2(1 - 2\alpha) \right\}.$$

- When  $\psi$  is scalar, this yields

$$\left\{ \psi \in \Omega_\psi : \ell(\psi, \hat{\lambda}_\psi) \geq \ell(\hat{\psi}, \hat{\lambda}) - \frac{1}{2}\chi_1^2(1 - 2\alpha) \right\},$$

and  $\frac{1}{2}\chi_1^2(0.95) = 1.92$ .

- Such intervals are generally better than the standard interval  $\hat{\psi} \pm z_\alpha \text{SE}$ , particularly when the distribution of  $\hat{\psi}$  is asymmetric, but require more computation, since they involve many maximisations of  $\ell$ .

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### Model setup

- ☐ Independent random variables  $Y_1, \dots, Y_n$ , with observed values  $y_1, \dots, y_n$ , and covariates  $x_1, \dots, x_n$ .
- ☐ Suppose that probability density of  $Y_j$  is  $f(y_j; \eta_j, \phi)$ , where  $\eta_j = \eta(\beta, x_j)$ , and  $\phi$  is common to all models.
- ☐ Log likelihood is

$$\ell(\beta, \phi) = \sum_{j=1}^n \ell_j(\beta, \phi) = \sum_{j=1}^n \log f\{y_j; \eta(\beta, x_j), \phi\}.$$

- ☐ More generally, just let  $\ell_j(\beta, \phi)$  denote the log likelihood contribution from the  $j$ th observation.
- ☐ Suppose  $\phi$  known (for now), suppress it, and estimate  $\beta$ .

**Example 16 (Normal regression model)** Express the normal regression model in the terms above.

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### Note to Example 16

Here  $Y_j \stackrel{\text{ind}}{\sim} \mathcal{N}(\mu_j, \sigma^2)$  with  $\mu_j = \eta_j = \eta(x_j; \beta)$ , so obviously

$$\eta_j = \eta(x_j; \beta), \quad \phi = \sigma^2, \quad \ell_j \equiv -\frac{1}{2}\{(y_j - \eta_j)^2 / \phi + \log \phi\}.$$

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### Iterative weighted least squares (IWLS)

- ☐ General approach for estimation in regression models, based on Newton–Raphson iteration
- ☐ Assume that  $\phi$  is fixed, and write

$$\ell(\beta) = \sum_{j=1}^n \ell_j\{\eta_j(\beta)\}.$$

- ☐ MLEs  $\hat{\beta}$  usually satisfy

$$\frac{\partial \ell(\hat{\beta})}{\partial \beta_r} = 0, \quad r = 1, \dots, p,$$

or equivalently

$$\frac{\partial \ell(\hat{\beta})}{\partial \beta} = \frac{\partial \eta^T}{\partial \beta} \frac{\partial \ell}{\partial \eta} = \frac{\partial \eta^T}{\partial \beta} u(\hat{\beta}) = \sum_{j=1}^n \frac{\partial \eta_j}{\partial \beta} \frac{\partial \ell_j\{\eta_j(\beta)\}}{\partial \eta_j} = 0, \quad (6)$$

where  $u(\beta)$  is  $n \times 1$  vector with  $j$ th element  $\partial \ell / \partial \eta_j$ .

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## IWLS II

- Newton–Raphson update step:

$$\hat{\beta} = (X^T W X)^{-1} X^T W z,$$

where

$$X_{n \times p} = \partial \eta / \partial \beta^T, \quad (\text{design matrix})$$

$$W_{n \times n} = \text{diag}\{E(-\partial^2 \ell_j / \partial \eta_j^2)\}, \quad (\text{weights})$$

$$z_{n \times 1} = X\beta + W^{-1}u, \quad (\text{adjusted dependent variable})$$

- Thus to obtain MLEs  $\hat{\beta}$  we use the **IWLS algorithm**:
- take an initial  $\hat{\beta}$ . Repeat
  - compute  $X, W, u, z$ ;
  - compute new  $\hat{\beta}$  and replace the preceding value;until changes in  $\ell(\hat{\beta})$  (or, sometimes,  $\hat{\beta}$ , or both) are lower than some tolerance.
- Sometimes a line search is added, if  $\ell(\hat{\beta}_{\text{new}}) < \ell(\hat{\beta}_{\text{old}})$ : i.e., we half the step length and try again.

## Derivation of IWLS algorithm

- To find the maximum likelihood estimate  $\hat{\beta}$  starting from a trial value  $\beta$ , we make a Taylor series expansion in (6), to obtain

$$\frac{\partial \eta^T(\beta)}{\partial \beta} u(\beta) + \left\{ \sum_{j=1}^n \frac{\partial \eta_j(\beta)}{\partial \beta} \frac{\partial^2 \ell_j(\beta)}{\partial \eta_j^2} \frac{\partial \eta_j(\beta)}{\partial \beta^T} + \sum_{j=1}^n \frac{\partial^2 \eta_j(\beta)}{\partial \beta \partial \beta^T} u_j(\beta) \right\} (\hat{\beta} - \beta) \doteq 0. \quad (7)$$

If we denote the  $p \times p$  matrix in braces on the left by  $-J(\beta)$ , assumed invertible, we can rearrange (7) to obtain

$$\hat{\beta} \doteq \beta + J(\beta)^{-1} \frac{\partial \eta^T(\beta)}{\partial \beta} u(\beta). \quad (8)$$

This suggests that maximum likelihood estimates may be obtained by starting from a particular  $\beta$ , using (8) to obtain  $\hat{\beta}$ , then setting  $\beta$  equal to  $\hat{\beta}$ , and iterating (8) until convergence. This is the Newton–Raphson algorithm applied to our particular setting. In practice it can be more convenient to replace  $J(\beta)$  by its expected value

$$I(\beta) = \sum_{j=1}^n \frac{\partial \eta_j(\beta)}{\partial \beta} E \left( -\frac{\partial^2 \ell_j}{\partial \eta_j^2} \right) \frac{\partial \eta_j(\beta)}{\partial \beta^T};$$

the other term vanishes because  $E\{u_j(\beta)\} = 0$ . We write

$$I(\beta) = X(\beta)^T W(\beta) X(\beta), \quad (9)$$

where  $X(\beta)$  is the  $n \times p$  matrix  $\partial \eta(\beta)/\partial \beta^T$  and  $W(\beta)$  is the  $n \times n$  diagonal matrix whose  $j$ th diagonal element is  $E(-\partial^2 \ell_j / \partial \eta_j^2)$ .

- If we replace  $J(\beta)$  by  $X(\beta)^T W(\beta) X(\beta)$  and reorganize (8), we obtain

$$\hat{\beta} = (X^T W X)^{-1} X^T W (X\beta + W^{-1}u) = (X^T W X)^{-1} X^T W z, \quad (10)$$

say, where the dependence of the terms on the right on  $\beta$  has been suppressed. That is, starting from  $\beta$ , the updated estimate  $\hat{\beta}$  is obtained by weighted linear regression of the  $n \times 1$  vector **adjusted dependent variable**

$$z = X(\beta)\beta + W(\beta)^{-1}u(\beta)$$

on the columns of  $X(\beta)$ , using weight matrix  $W(\beta)$ . The maximum likelihood estimates are obtained by repeating this step until the log likelihood, the estimates, or more often both, are essentially unchanged. The variable  $z$  plays the role of the response or dependent variable in the weighted least squares step.

- Often the structure of a model simplifies the estimation of an unknown value of  $\phi$ . It may be estimated by a separate step between iterations of  $\hat{\beta}$ , by including it in the step (8), or from the profile log likelihood  $\ell_p(\phi)$ .

## Examples

**Example 17 (Normal nonlinear model)** Give the components of the IWLS algorithm for the normal nonlinear model.

## Note to Example 17

- Here the mean of the  $j$ th observation is  $\eta_j = \eta(x_j; \beta)$ . The log likelihood contribution  $\ell_j(\eta_j)$  is

$$\ell_j(\eta_j, \sigma^2) \equiv -\frac{1}{2} \left\{ \log \sigma^2 + \frac{1}{\sigma^2} (y_j - \eta_j)^2 \right\},$$

so

$$u_j(\eta_j) = \frac{\partial \ell_j}{\partial \eta_j} = \frac{1}{\sigma^2} (y_j - \eta_j), \quad \frac{\partial^2 \ell_j}{\partial \eta_j^2} = -\frac{1}{\sigma^2};$$

the  $j$ th element on the diagonal of  $W$  is the constant  $\sigma^{-2}$ .

The  $j$ th row of the matrix  $X = \partial \eta / \partial \beta^T$  is  $(\partial \eta_j / \partial \beta_0, \dots, \partial \eta_j / \partial \beta_{p-1})$ , and as  $\eta_j$  is nonlinear as a function of  $\beta$ ,  $X$  depends on  $\beta$ .

After some simplification, we see that the new value for  $\hat{\beta}$  given by (10) is

$$\hat{\beta} \doteq (X^T X)^{-1} X^T (X \beta + y - \eta), \quad (11)$$

where  $X$  and  $\eta$  are evaluated at the current  $\beta$ . Here  $\eta \neq X\beta$  and (11) must be iterated.

- The log likelihood is a function of  $\beta$  only through the sum of squares,  $SS(\beta) = \sum_{j=1}^n \{y_j - \eta_j(\beta)\}^2$ . The profile log likelihood for  $\sigma^2$  is

$$\ell_p(\sigma^2) = \max_{\beta} \ell(\beta, \sigma^2) \equiv -\frac{1}{2} \left\{ n \log \sigma^2 + SS(\hat{\beta}) / \sigma^2 \right\},$$

so the maximum likelihood estimator of  $\sigma^2$  is  $\hat{\sigma}^2 = SS(\hat{\beta})/n$ . Although  $S^2 = SS(\hat{\beta})/(n-p)$  is not unbiased when the model is nonlinear, it turns out to have smaller bias than  $\hat{\sigma}^2$ , and is preferable in applications.

- In some cases the error variance depends on covariates, and we write the variance of the  $j$ th response as  $\sigma_j^2 = \sigma^2(x_j, \gamma)$ . Such models may be fitted by alternating iterative weighted least squares updates for  $\beta$  treating  $\gamma$  as fixed at a current value with those for  $\gamma$  with  $\beta$  fixed, convergence being attained when neither estimates nor log likelihood change materially.

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## Deviance

- Let  $\hat{\eta}_j = \eta_j(\hat{\beta}, x_j)$ , where  $\hat{\beta}$  is MLE of  $\beta$ , giving maximised log likelihood  $\ell(\hat{\beta})$  and  $\hat{\eta}^T = (\hat{\eta}_1, \dots, \hat{\eta}_n)$ .
- Let  $\tilde{\eta}_j$  be the value of  $\eta_j$  that maximises  $\log f(y_j; \eta_j)$ , and let  $\tilde{\eta}^T = (\tilde{\eta}_1, \dots, \tilde{\eta}_n)$ . This corresponds to the **saturated model**, with

$$\# \text{parameters in } \eta = \# \text{observations in } y,$$

which will give the largest likelihood possible.

- Define the **scaled deviance**:

$$D = 2 \sum_{j=1}^n \{ \log f(y_j; \tilde{\eta}_j) - \log f(y_j; \hat{\eta}_j) \} \geq 0.$$

- Small  $D$  implies  $\hat{\eta} \approx \tilde{\eta}$ , so model fits well.
- Large  $D$  implies poor fit — like  $SS(\hat{\beta})$  in linear model.

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## Differences of deviances

- Consider two models:
  - Model  $A$ :  $\beta^T = (\beta_1, \dots, \beta_p) \in \mathbb{R}^p$  vary freely — MLEs  $\hat{\eta}^A = \eta(\hat{\beta}^A)$ ;
  - Model  $B$ :  $(\beta_1, \dots, \beta_q) \in \mathbb{R}^q$  vary freely, but  $\beta_{q+1}, \dots, \beta_p$  are fixed — hence  $q$  free parameters, MLEs  $\hat{\eta}^B = \eta(\hat{\beta}^B)$ .
- Model  $B$  is **nested within** model  $A$ :  $B$  can be obtained by restricting  $A$ .
- Likelihood ratio statistic for comparing the models is

$$2(\hat{\ell}_A - \hat{\ell}_B) = 2 \sum_{j=1}^n \{ \log f(y_j; \hat{\eta}_j^A) - \log f(y_j; \hat{\eta}_j^B) \} = D_B - D_A,$$

and this  $\sim \chi_{p-q}^2$  if the models are regular.

- If  $\phi$  unknown, replace it by an estimate: same distributional approximations will apply.

**Example 18 (Normal linear model)** Find the difference of deviances in the normal linear model.

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## Note to Example 18

- Suppose that the  $y_j$  are normal with means  $\eta_j$  and known variance  $\phi$ . Then

$$\log f(y_j; \eta_j, \phi) = -\frac{1}{2} \{ \log(2\pi\phi) + (y_j - \eta_j)^2 / \phi \}$$

is maximized with respect to  $\eta_j$  when  $\tilde{\eta}_j = y_j$ , giving  $\log f(y_j; \tilde{\eta}_j, \phi) = -\frac{1}{2} \log(2\pi\phi)$ . Therefore the scaled deviance for a model with fitted means  $\hat{\eta}_j$  is

$$D = \phi^{-1} \sum_{j=1}^n (y_j - \hat{\eta}_j)^2,$$

which is just the residual sum of squares for the model, divided by  $\phi$ . If  $\eta_j = x_j^T \beta$  is the correct normal linear model, the distribution of the residual sum of squares is  $\phi \chi_{n-p}^2$ , so values of  $D$  extreme relative to the  $\chi_{n-p}^2$  distribution call the model into question.

- The difference between deviances for nested models  $A$  and  $B$  in which  $\beta$  has dimensions  $p$  and  $q < p$ ,

$$D_B - D_A = \phi^{-1} \sum_{j=1}^n \{ (y_j - \hat{\eta}_j^B)^2 - (y_j - \hat{\eta}_j^A)^2 \} \sim \chi_{p-q}^2$$

when model  $B$  is correct. This distribution is exact for linear models.

- If  $\phi$  is unknown, it is replaced by an estimate. The large-sample properties of deviance differences outlined above still apply, though in small samples it may be better to replace the approximating  $\chi^2$  distribution by an  $F$  distribution with denominator degrees of freedom equal to the degrees of freedom for estimation of  $\phi$ .

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**Model checking**

- Two basic approaches:
  - overall tests either using generic statistic (e.g., chi-squared) or by **model expansion** (e.g., adding a term and testing for significance);
  - **regression diagnostics** for detecting a few possibly dodgy observations.
- Most widely used diagnostics in the linear model  $y = X_{n \times p}\beta + \varepsilon$  are **residuals**  $e_j = y_j - \hat{y}_j$  and (much better) **standardized residuals**

$$r_j = \frac{y_j - \hat{y}_j}{s(1 - h_{jj})^{1/2}}, \quad j = 1, \dots, n,$$

where the **leverage**  $h_{jj}$  is the  $j$ th diagonal element of the hat matrix  $H = X(X^T X)^{-1} X^T$ , and the **Cook statistic**

$$C_j = \frac{1}{ps^2} (\hat{y} - \hat{y}_{-j})^T (\hat{y} - \hat{y}_{-j}) = \frac{r_j^2 h_{jj}}{p(1 - h_{jj})},$$

which measures the effect of deleting the  $j$ th case  $(x_j, y_j)$  on the fitted model.

**Diagnostics in general case**

- Linear model ideas work as approximations (2nd order Taylor series, painful expansions).
- **Leverage**  $h_{jj}$  defined as  $j$ th diagonal element of

$$H = W^{1/2} X (X^T W X)^{-1} X^T W^{1/2},$$

depends in general on  $\hat{\beta}$ , unlike in linear model.

- **Cook statistic** is change in deviance

$$C_j = 2p^{-1} \left\{ \ell(\hat{\beta}) - \ell(\hat{\beta}_{-j}) \right\} \doteq \frac{h_{jj}}{p(1 - h_{jj})} r_{Pj}^2,$$

where  $\hat{\beta}_{-j}$  is MLE when  $j$ th case  $(x_j, y_j)$  is dropped, and  $r_{Pj}$  is **standardized Pearson residual** (see below).

- There are several types of residual (see next page).

## Residuals in general case

- **Deviance residual:**

$$d_j = \text{sign}(\tilde{\eta}_j - \hat{\eta}_j) [2\{\ell_j(\tilde{\eta}_j; \phi) - \ell_j(\hat{\eta}_j; \phi)\}]^{1/2},$$

for which  $\sum d_j^2 = D$  is deviance.

- **Pearson residual:**  $u_j(\hat{\beta}) / \sqrt{w_j(\hat{\beta})}$ .

- Standardized versions

$$r_{Dj} = \frac{d_j}{(1 - h_{jj})^{1/2}}, \quad r_{Pj} = \frac{u_j(\hat{\beta})}{\{w_j(\hat{\beta})(1 - h_{jj})\}^{1/2}},$$

and (even better)

$$r_j^* = r_{Dj} + r_{Dj}^{-1} \log(r_{Pj}/r_{Dj}) \sim N(0, 1)$$

for many models.

- These all reduce to usual standardized residual for normal linear model.

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## Example

**Example 19 (Gumbel linear model)** Give the components of the IWLS algorithm for fitting the linear model

$$y_j = \beta_0 + \beta_1(x_j - \bar{x}) + \tau \varepsilon_j, \quad j = 1, \dots, n,$$

with Gumbel errors having density function

$$f(y_j; \eta_j, \tau) = \tau^{-1} \exp \left\{ -\frac{y_j - \eta_j}{\tau} - \exp \left( -\frac{y_j - \eta_j}{\tau} \right) \right\},$$

where  $\tau > 0$  and  $\eta_j = \beta_0 + \beta_1(x_j - \bar{x})$ ; this distribution is natural for maxima; note that  $\tau^2$  is not the variance.

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### Note to Example 19

- As the data are annual maxima, it is more appropriate to suppose that  $y_j$  has the Gumbel density

$$f(y_j; \eta_j, \tau) = \tau^{-1} \exp \left\{ -\frac{y_j - \eta_j}{\tau} - \exp \left( -\frac{y_j - \eta_j}{\tau} \right) \right\}, \quad (12)$$

where  $\tau$  is a scale parameter and  $\eta_j = \beta_0 + \beta_1(x_j - \bar{x})$ ; here we have replaced the  $\gamma$ s with  $\beta$ s for continuity with the general discussion above.

- In this case

$$\ell_j(\eta_j, \tau) = -\log \tau - \frac{y_j - \eta_j}{\tau} - \exp \left( -\frac{y_j - \eta_j}{\tau} \right), \quad (13)$$

and it is straightforward to establish that

$$\frac{\partial \ell_j(\eta_j, \tau)}{\partial \eta_j} = \tau^{-1} \left\{ 1 - \exp \left( -\frac{y_j - \eta_j}{\tau} \right) \right\}, \quad E \left\{ -\frac{\partial^2 \ell_j(\eta_j, \tau)}{\partial \eta_j^2} \right\} = \tau^{-2},$$

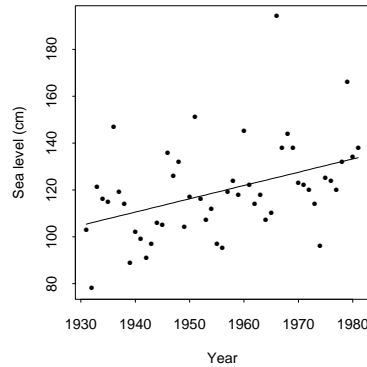
that  $\partial \eta / \partial \beta^T = X$  is the  $n \times 2$  matrix whose  $j$ th row is  $(1, x_j - \bar{x})$ , and  $W = \tau^{-2} I_n$ . Hence (10) becomes  $\hat{\beta} \doteq (X^T X)^{-1} (X\beta + \tau^2 u)$ , where the  $j$ th element of  $u$  is  $\tau^{-1}[1 - \exp\{-(y_j - \eta_j)/\tau\}]$ .

- Here it is simplest to fix  $\tau$ , to obtain  $\hat{\beta}$  by iterating (10) for each fixed value of  $\tau$ , and then to repeat this over a range of values of  $\tau$ , giving the profile log likelihood  $\ell_p(\tau)$  and hence confidence intervals for  $\tau$ . Confidence intervals for  $\beta_0$  and  $\beta_1$  are obtained from the information matrix.
- With starting value chosen to be the least squares estimates of  $\beta$ , and with  $\tau = 5$ , 19 iterations of (10) were required to give estimates and a maximized log likelihood whose relative change was less than  $10^{-6}$  between successive iterations. We then took  $\tau = 5.5, \dots, 40$ , using  $\hat{\beta}$  from the preceding iteration as starting-value for the next; in most cases just three iterations were needed. The left panel of Figure 1 shows a close-up of  $\ell_p(\tau)$ ; its maximum is at  $\hat{\tau} = 14.5$ , and the 95% confidence interval for  $\tau$  is (11.9, 18.1). The maximum likelihood estimates of  $\beta_0$  and  $\beta_1$  are 111.4 and 0.563, with standard errors 2.14 and 0.137; these compare with standard errors 2.61 and 0.177 for the least squares estimates. There is some gain in precision in using the more appropriate model.



## Venice data

**Example 20 (Venice sea level data)** The figure below shows annual maximum sea levels in Venice, from 1931–1981. The very large value in 1966 is not an outlier. The fit of a Gumbel model to the data using IWLS gives MLEs (SEs)  $\hat{\beta}_0 = 111.4$  (2.14) (cm) and  $\hat{\beta}_1 = 0.563$  (0.137) (cm/year). The standard errors for LSEs are 2.61, 0.177, larger than for MLEs with Gumbel model — gain in precision through using appropriate model.

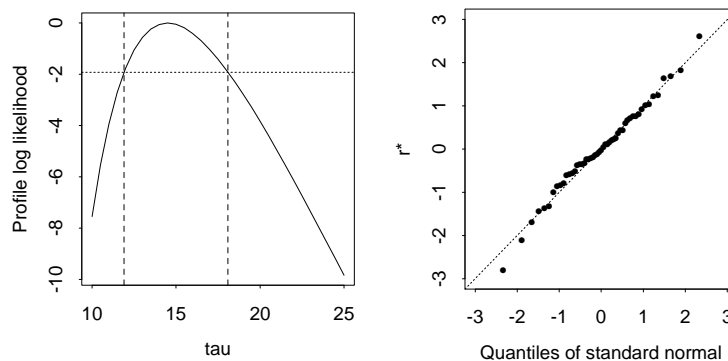


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## Venice data

Figure 1: Gumbel analysis of Venice data. Left panel: profile log likelihood  $\ell_p(\tau) = \max_{\beta} \ell(\beta, \tau)$ , with 95% confidence interval (11.9, 18.1) (cm) for  $\tau$ . Right panel: normal probability plot of residuals  $r_j^*$ .



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## Summary

- For regression problems with independent responses  $y_j$  dependent on parameters  $\beta$  through parameter  $\eta_j = \eta(x_j; \beta)$ , generalise least squares estimation to maximum likelihood estimation, using iterative weighted least squares algorithm: iterate to convergence

$$\hat{\beta} = (X^T W X)^{-1} X^T W z, \quad z = X\beta + W^{-1}u,$$

where

$$X_{n \times p} \equiv X(\beta) = \frac{\partial \eta}{\partial \beta^T}, \quad u_{n \times 1} \equiv u(\eta) = \frac{\partial \ell}{\partial \eta}, \quad W_{n \times n} \equiv W(\eta) = -E \left\{ \frac{\partial^2 \ell}{\partial \eta \partial \eta^T} \right\},$$

with  $\ell$  the log likelihood for the data.

- Standard likelihood theory is used for confidence intervals and model comparison.
- Linear model diagnostics (residuals, leverage, Cook statistics, ...) generalise to this setting.
- Next: generalized linear models (GLMs), wide class of models with exponential family-like response distributions.

**Motivation**

- Need to generalise linear model beyond normal responses, e.g. to data with  $y \in \{0, 1, \dots, m\}$ , or  $y \in \{0, 1, \dots\}$ , or  $y > 0$ .
- Consider **exponential family** response distributions (binomial, Poisson, ...), which have an elegant unifying theory, and encompass many possibilities (in addition to the normal)
- Basic idea is to build models such that

$$E(y) = \mu, \quad g(\mu) = \eta = x^T \beta,$$

where  $g$  is a suitable function, and  $y \sim$  exponential family (almost).

- **Warnings:**
  - **Don't** confuse Generalized Linear Model (GLM) with General Linear Model (GLM, in older books, the latter is  $y = X\beta + \varepsilon$ , with  $\text{cov}(\varepsilon) = \sigma^2 V$  not diagonal);
  - **Don't** write  $y = \mu + \varepsilon$ , since in a GLM the distribution of  $\varepsilon$  usually depends on  $\mu$ .

**Generalized linear model (GLM)**

- Normal linear model has three key aspects:
  - structure for covariates: **linear predictor**,  $\eta = x^T \beta$ ;
  - response distribution:  $y \sim N(\mu, \sigma^2)$ ;
  - linear relation  $\eta = \mu$  between  $\mu = E(y)$  and  $\eta$ .
- GLM extends last two to
  - $Y$  has density/mass function

$$f(y; \theta, \phi) = \exp \left\{ \frac{y\theta - b(\theta)}{\phi} + c(y; \phi) \right\}, \quad y \in \mathcal{Y}, \theta \in \Omega_\theta, \phi > 0, \quad (14)$$

where

- ▷  $\mathcal{Y}$  is the support of  $Y$ ,
- ▷  $\Omega_\theta$  is the parameter space of valid values for  $\theta \equiv \theta(\eta)$ , and
- ▷ the **dispersion parameter**  $\phi$  is often known;
- $\eta = g(\mu)$ , where  $g$  is monotone **link function**
  - ▷ the **canonical link** function giving  $\eta = \theta = b'^{-1}(\mu)$  has nice statistical properties;
  - ▷ but a range of link functions are possible for each distribution of  $Y$ .

## Examples

**Example 21 (GLM density)** Show that the moment-generating function of  $f(y; \theta, \phi)$  is  $M_Y(t) = \exp[\{b(\theta + t\phi) - b(\theta)\}/\phi]$ , and deduce that

$$E(Y) = b'(\theta) = \mu, \quad \text{var}(Y) = \phi b''(\theta) = \phi b''\{b'^{-1}(\mu)\} = \phi V(\mu);$$

the function  $\mu \mapsto V(\mu)$  is known as the **variance function**.

**Example 22 (Poisson distribution)** Write the Poisson mass function as a GLM density, and find its canonical link function.

**Example 23 (Normal distribution)** Write the normal density function as a GLM density, and find its canonical link function.

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## Note to Example 21

- Suppose that  $Y$  has a continuous density; if not the argument below is the same, except that integrals are replaced by summations.
- Let  $\Omega_\theta = \{\theta : b(\theta) < \infty\}$ . Then

$$\begin{aligned} M_Y(t) &= E\{\exp(tY)\} \\ &= \int e^{ty} \exp\left\{\frac{y\theta - b(\theta)}{\phi} + c(y; \phi)\right\} dy \\ &= \int \exp\left\{\frac{y(\theta + t\phi) - b(\theta)}{\phi} + c(y; \phi)\right\} dy. \end{aligned}$$

If  $\theta + t\phi \in \Omega_\theta$ , then

$$\int \exp\left\{\frac{y(\theta + t\phi) - b(\theta + t\phi)}{\phi} + c(y; \phi)\right\} dy = 1,$$

so

$$M_Y(t) = E\{\exp(tY)\} = \exp[\{b(\theta + t\phi) - b(\theta)\}/\phi].$$

- Hence the cumulant-generating function of  $Y$  is

$$K_Y(t) = \log M_Y(t) = \{b(\theta + t\phi) - b(\theta)\}/\phi,$$

and differentiating twice with respect to  $t$  and setting  $t = 0$  yields

$$E(Y) = K'_Y(t)|_{t=0} = b'(\theta), \quad \text{var}(Y) = K''_Y(t)|_{t=0} = \phi b''(\theta).$$

- One can show that  $b(\theta)$  is strictly convex on  $\Omega_\theta$ . Thus  $b'(\theta)$  is a monotonic increasing function of  $\theta$ , so  $b'^{-1}(\cdot)$  exists and is itself monotonic, so  $V(\mu) = b''\{b'^{-1}(\mu)\}$  is well-defined.

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### Note to Example 22

The Poisson density may be written as

$$f(y; \mu) = \exp(y \log \mu - \mu - \log y!), \quad y = 0, 1, \dots, \quad \mu > 0,$$

which has GLM form (14) with  $\theta = \log \mu$ ,  $b(\theta) = e^\theta$ ,  $\phi = 1$ , and  $c(y; \phi) = -\log y!$ . The mean of  $y$  is  $\mu = b'(\theta) = e^\theta = \mu$ , and its variance is  $b''(\theta) = e^\theta = \mu$ , so the variance function is linear:  $V(\mu) = \mu$ .

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### Note to Example 23

The normal density with mean  $\mu$  and variance  $\sigma^2$  may be written

$$f(y; \mu, \sigma^2) = \exp \left\{ -\frac{(y^2 - 2y\mu + \mu^2)}{2\sigma^2} - \frac{1}{2} \log(2\pi\sigma^2) \right\},$$

so

$$\theta = \mu, \quad \phi = \sigma^2, \quad b(\theta) = \frac{1}{2}\theta^2, \quad c(y; \phi) = -\frac{1}{2\phi}y^2 - \frac{1}{2} \log(2\pi\phi).$$

As the first and second derivatives of  $b(\theta)$  are  $\theta$  and 1, we have  $V(\mu) = 1$ ; the variance function is constant.

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### Estimation of $\beta$

**Example 24 (IWLS algorithm)** Find the components of the IWLS algorithm for a GLM.

- If canonical link is used then  $\theta_j = x_j^T \beta$ , so if  $\phi$  is known, then

$$\begin{aligned} \ell(\beta) &= \sum_{j=1}^n \left\{ \frac{y_j x_j^T \beta - b(x_j^T \beta)}{\phi} + c(y_j; \phi) \right\} \\ &= \{y^T X \beta - K(\beta)\} / \phi + C(y; \phi), \end{aligned}$$

say, which in terms of  $\beta$  is a linear exponential family with

- **canonical parameter**  $\beta_{p \times 1}$
- **canonical statistic**  $(X^T y)_{p \times 1}$ ,

and many nice properties then hold.

- If  $X$  is full rank, then  $\ell(\beta)$  is (almost always) strictly concave and has a unique maximum in terms of  $\beta$ .
- Problem: the maximum may be at infinity in certain (rare) cases—this can arise with binomial responses: beware of  $\hat{\theta}_r \approx \pm 36$ .

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### Note to Example 24

- To compute the quantities needed for the IWLS step  $\hat{\beta} = (X^T W X)^{-1} X^T W (X\beta + W^{-1}u)$ , we need

$$X_{n \times p} = \frac{\partial \eta}{\partial \beta^T}, \quad W_{n \times n} = \text{diag}\{E(-\partial^2 \ell_j / \partial \eta_j^2)\}, \quad u_{n \times 1} = \{\partial \ell_j / \partial \eta_j\},$$

where (with  $\phi_j$  instead of  $\phi$  for generality, see the next slide),

$$\ell_j(\beta) = \left\{ \frac{y_j \theta_j - b(\theta_j)}{\phi_j} + c(y_j; \phi_j) \right\}, \quad b'(\theta_j) = \mu_j, \quad \eta_j = g(\mu_j) = x_j^T \beta.$$

- First note that  $\partial \eta_j / \partial \beta_r = x_{jr}$ , so  $X = \partial \eta / \partial \beta^T$  is just a matrix of constants.  
 □ We need the first and second derivatives of  $\ell_j$  with respect to  $\eta_j$ , so we write

$$\frac{\partial \ell_j}{\partial \eta_j} = \frac{\partial \mu_j}{\partial \eta_j} \frac{\partial \theta_j}{\partial \mu_j} \frac{\partial \ell_j}{\partial \theta_j},$$

with

$$\frac{\partial \eta_j}{\partial \mu_j} = g'(\mu_j), \quad \frac{\partial \mu_j}{\partial \theta_j} = b''(\theta_j) = V(\mu_j), \quad \frac{\partial \ell_j}{\partial \theta_j} = \frac{y_j - b'(\theta_j)}{\phi_j},$$

which yields

$$u_j = \frac{\partial \ell_j}{\partial \eta_j} = \frac{y_j - b(\theta_j)}{g'(\mu_j) \phi_j V(\mu_j)} = \frac{y_j - \mu_j}{g'(\mu_j) \phi_j V(\mu_j)} = \frac{A(\theta_j)}{B(\theta_j)},$$

say, where  $E(A) = 0$ . For the second derivative, we note that

$$\frac{\partial^2 \ell_j}{\partial \eta_j^2} = \frac{\partial}{\partial \eta_j} \frac{\partial \ell_j}{\partial \eta_j} = \left( \frac{\partial \mu_j}{\partial \eta_j} \frac{\partial \theta_j}{\partial \mu_j} \frac{\partial}{\partial \theta_j} \right) \frac{\partial \ell_j}{\partial \eta_j} = \frac{\partial \mu_j}{\partial \eta_j} \frac{\partial \theta_j}{\partial \mu_j} \left\{ \frac{A'(\theta_j)}{B(\theta_j)} - \frac{A(\theta_j) B'(\theta_j)}{B(\theta_j)^2} \right\},$$

and on noting that  $B(\theta_j)$  is non-random and  $A'(\theta_j) = -b''(\theta_j) = -V(\mu_j)$ , we obtain

$$w_j = E \left( -\frac{\partial^2 \ell_j}{\partial \eta_j^2} \right) = \frac{1}{g'(\mu_j)} \frac{1}{V(\mu_j)} \frac{V(\mu_j)}{g'(\mu_j) \phi_j V(\mu_j)} = \frac{1}{g'(\mu_j)^2 \phi_j V(\mu_j)}.$$

### Note to Example 24, part II

- From above we see that the components of the score statistic  $u(\beta)$  and the weight matrix  $W(\beta)$  may be expressed in terms of components  $\mu_j$  of the mean vector  $\mu$  as

$$\begin{aligned} u_j &= \frac{\partial \theta_j}{\partial \eta_j} \frac{\partial \ell_j(\theta_j)}{\partial \theta_j} = \frac{y_j - \mu_j}{g'(\mu_j) \phi_j V(\mu_j)}, \\ w_j &= \left( \frac{\partial \theta_j}{\partial \eta_j} \right)^2 \frac{\partial^2 \ell_j(\theta_j)}{\partial \theta_j^2} = \frac{1}{g'(\mu_j)^2 \phi_j V(\mu_j)}, \end{aligned} \quad (15)$$

where  $g'(\mu_j) = dg(\mu_j)/d\mu_j$ . Thus  $\hat{\beta}$  is obtained by iterative weighted least squares regression of response

$$z = X\beta + g'(\mu)(y - \mu) = \eta + g'(\mu)(y - \mu)$$

on the columns of  $X$  using weights (15).

- By using  $y$  as an initial value for  $\mu$  and  $g(y)$  as an initial value for  $\eta = X\beta$ , we avoid needing an initial value for  $\beta$ .
- It may be necessary to modify  $y$  slightly for this initial step. For example if we use the log link for Poisson data, and some  $y_j$  equal zero, then we may need to replace them with some small positive value to avoid taking  $\log 0$  for some components of the initial  $\eta = \log y$ .

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### Estimation of $\phi$

- When  $\phi$  unknown, it is often replaced by  $\phi_j = \phi a_j$ , with known  $a_j$  and  $a_j^{-1}$  treated as a weight. Then we replace the scaled deviance by the **deviance**  $\phi D$ .
- If the model is correct and  $\phi$  is known, then **Pearson's statistic**

$$P = \frac{1}{\phi} \sum_{j=1}^n \frac{(y_j - \hat{\mu}_j)^2}{a_j V(\hat{\mu}_j)} \sim \chi_{n-p}^2,$$

analogously to the sum of squares in a linear model, with  $E(P) \doteq n - p$ .

- The MLE of  $\phi$  can be badly behaved, so usually we prefer the method of moments estimator

$$\hat{\phi} = \frac{1}{n-p} \sum_{j=1}^n (y_j - \hat{\mu}_j)^2 / \{a_j V(\hat{\mu}_j)\},$$

which is obtained by solving the equation  $P = n - p$ , based on noting that  $E(\chi_{n-p}^2) = n - p$ .

- If the data are sparse (e.g., many small binomial or Poisson counts), then standard asymptotic results are suspect.

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## Example: Jacamar data

Table 3: Response (N=not sampled, S = sampled and rejected, E = eaten) of a rufous-tailed jacamar to individuals of seven species of palatable butterflies with artificially coloured wing undersides. Data from Peng Chai, University of Texas.

	<i>Aphrissa boisduvalli</i>	<i>Phoebis argante</i>	<i>Dryas iulia</i>	<i>Pierella luna</i>	<i>Consul fabius</i>	<i>Siproeta stelenes</i> †
	N/S/E	N/S/E	N/S/E	N/S/E	N/S/E	N/S/E
Unpainted	0/0/14	6/1/0	1/0/2	4/1/5	0/0/0	0/0/1
Brown	7/1/2	2/1/0	1/0/1	2/2/4	0/0/3	0/0/1
Yellow	7/2/1	4/0/2	5/0/1	2/0/5	0/0/1	0/0/3
Blue	6/0/0	0/0/0	0/0/1	4/0/3	0/0/1	0/1/1
Green	3/0/1	1/1/0	5/0/0	6/0/2	0/0/1	0/0/3
Red	4/0/0	0/0/0	6/0/0	4/0/2	0/0/1	3/0/1
Orange	4/2/0	6/0/0	4/1/1	7/0/1	0/0/2	1/1/1
Black	4/0/0	0/0/0	1/0/1	4/2/2	7/1/0	0/1/0

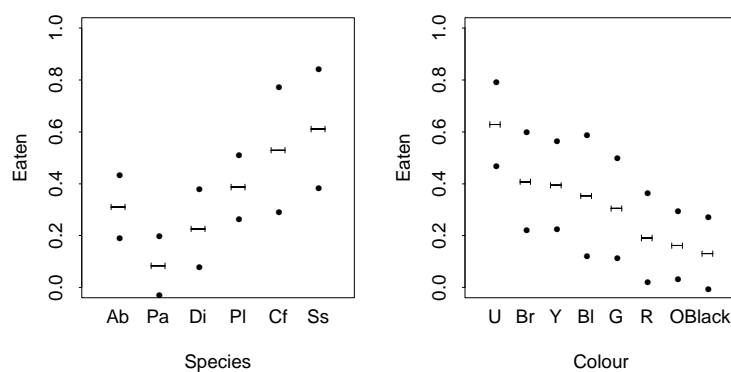
† includes *Philaethria dido* also.

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## Jacamar data

Figure 2: Proportion of butterflies eaten ( $\pm 2SE$ ) for different species and wing colour.



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## Jacamar data

- ☐ How does a bird respond to the species  $s$  and wing colour  $c$  of its prey?
- ☐ Response has 3 (ordered) categories: not attacked (N), attacked but then rejected (S), attacked and eaten (E)
- ☐ The data form an  $8 \times 6$  layout, with a 3-category response in each cell, total  $m_{cs}$
- ☐ Assume that the number in category E (response) is binomial:

$$R_{cs} \sim B(m_{cs}, \pi_{cs}), \quad c = 1, \dots, 8, s = 1, \dots, 6,$$

where  $c$  is colour and  $s$  is species, with probability that bird attacks and eats butterfly is

$$\pi_{cs} = \frac{\exp(\alpha_c + \gamma_s)}{1 + \exp(\alpha_c + \gamma_s)}, \quad c = 1, \dots, 8, s = 1, \dots, 6,$$

so

- large  $\alpha_c$  corresponds to colours that the jacamar likes to eat,
  - large  $\gamma_s$  corresponds to species that it likes.
- ☐ This is a GLM with response  $y_{cs} = r_{cs}/m_{cs}$ ,  $E(y_{cs}) = \pi_{cs}$ , and canonical (logit) link function

$$\eta = \log\{\pi/(1 - \pi)\}, \quad \eta_{cs} = \alpha_c + \gamma_s.$$

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## Jacamar data: Analysis of deviance

Table 4: Deviances and analysis of deviance for models fitted to jacamar data. The lower part shows results for the reduced data, without two outliers.

Terms	Full data		Without outliers	
	df	Deviance	df	Deviance
1	43	134.24	35	73.68
1+Species	38	114.59	31	46.04
1+Colour	36	108.46	28	63.20
1+Species+Colour	31	67.28	24	28.02

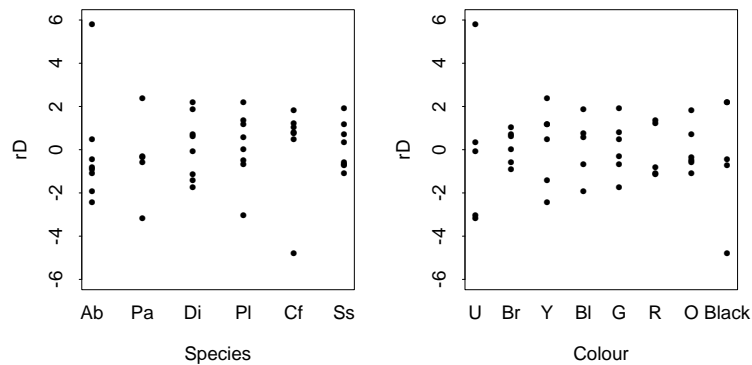
Terms	df	Deviance reduction	Terms	df	Deviance reduction
Species (unadj. for Colour)	5	19.64	Species (adj. for Colour)	5	41.18
Colour (adj. for Species)	7	47.31	Colour (unadj. for Species)	7	25.78
Species (unadj. for Colour)	4	27.63	Species (adj. for Colour)	4	35.18
Colour (adj. for Species)	7	18.03	Colour (unadj. for Species)	7	10.48

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## Jacamar data: Residuals

Figure 3: Standardized deviance residuals  $r_D$  for binomial two-way layout fitted to jacamar data.



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## Jacamar data: Parameter estimates

Table 5: Estimated parameters and standard errors for the jacamar data, without 2 outliers.

<div></div>						
<i>Aphrissa boisduvalli</i>		<i>Phoebis argante</i>	<i>Dryas iulia</i>	<i>Pierella luna</i>	<i>Consul fabius</i>	<i>Siproeta stelenes</i>
-1.99 (0.79)		-2.22 (0.85)	-0.56 (0.67)	0.16 (0.54)	—	1.50 (0.78)
Brown	Yellow	Blue	Green	Red	Orange	Black
0.16 (0.73)	0.33 (0.68)	-0.53 (0.81)	-0.83 (0.75)	-1.93 (0.88)	-1.94 (0.85)	-1.26 (0.86)

- ☐ Interpretation
- ☐ Residual deviance: 28.02, with 24 df
- ☐ Pearson statistic: 25.58, with 24 df
- ☐ Standardized residuals in range  $-2.03$  to  $1.96$ : OK.

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### Example: Chimpanzee data

Table 6: Times in minutes taken by four chimpanzees to learn ten words.

Chimpanzee	Word									
	1	2	3	4	5	6	7	8	9	10
1	178	60	177	36	225	345	40	2	287	14
2	78	14	80	15	10	115	10	12	129	80
3	99	18	20	25	15	54	25	10	476	55
4	297	20	195	18	24	420	40	15	372	190

- ☐ A two-way layout.
- ☐ Times vary from 2 to 476 minutes — need transformation (e.g., logarithm) if use linear model.

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### Chimpanzee data

- ☐ How does learning time depend on word  $w$  and chimp  $c$ ?
- ☐ Response is continuous and positive, so we try fitting the gamma distribution with mean  $\mu$  and shape parameter  $\nu$ , i.e.,

$$f(y; \mu, \nu) = \frac{1}{\Gamma(\nu)} y^{\nu-1} \left(\frac{\nu}{\mu}\right)^{\nu} \exp(-\nu y/\mu), \quad y > 0, \quad \nu, \mu > 0,$$

so dispersion parameter is  $\phi = 1/\nu$  ( $\phi = \nu = 1$  for exponential).

- ☐ Possible link functions:

$$\eta = \log \mu, \text{ (log, most common), } \eta = 1/\mu, \text{ (reciprocal, canonical)}$$

- ☐ Linear model structure:

$$\eta_{cw} = \alpha_c + \gamma_w, \quad c = 1, \dots, 4, w = 1, \dots, 10,$$

but the interpretation of the  $\alpha_c$  and  $\gamma_w$  will depend on the link function.

- ☐ With the log link, the deviances for models 1, 1+Chimp, 1+Word, and 1+Chimp+Word are 60.38, 53.43, 21.19, and 14.97. How many df are there for each model?

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## Chimpanzee data: Analysis of deviance

Table 7: Analysis of deviance for models fitted to chimpanzee data.

Term	df	Deviance reduction	Term	df	Deviance reduction
Chimp (unadj. for Word)	3	6.95	Chimp (adj. for Word)	3	6.22
Word (adj. for Chimp)	9	38.46	Word (unadj. for Chimp)	9	39.19

- ☐ Method of moments estimate is  $\hat{\phi} = 0.432$ , so  $\hat{\nu} = 1/\hat{\phi} = 2.31$ .
- ☐ Use  $F$  tests to assess effects of Word and Chimp, for example obtaining

$$\frac{6.22/3}{0.423} = 4.78 \sim F_{3,27}$$

if there is no difference between the chimps. What is the corresponding statistic for testing differences between words?

- ☐ Residuals suggest that this model, or one with the inverse link, are both adequate, and both are better than fitting a normal linear model to the log times.

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## Summary

- ☐ Generalized linear models extend the classical linear model in two ways:
  - the response distribution is (almost) exponential family, so includes binomial, Poisson, gamma and other distributions in addition to the normal;
  - the relation between the linear predictor  $\eta = x^T\beta$  and the mean  $\mu$  is determined by a wide range of possible link functions.
- ☐ Canonical link functions give particularly simple models and are widely used.
- ☐ Estimates of  $\beta$  are obtained by IWLS, which has a simple form, with no need for initial values.
- ☐ A simple estimate of the dispersion parameter  $\phi$  is available using the method of moments.
- ☐ Models are compared using the analysis of deviance, which generalises the analysis of variance in the classical linear model.
- ☐ Standard likelihood theory results are used for inference (standard errors, confidence intervals, etc.)
- ☐ Standard diagnostics (residuals, ...) extend in a natural way to this setting.

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**Binary response**

- ☐ Response  $Y$  has Bernoulli distribution with

$$P(Y = 1) = \pi, \quad P(Y = 0) = 1 - \pi, \quad 0 < \pi < 1.$$

and  $E(Y) = \mu = \pi$ ,  $\text{var}(Y) = \pi(1 - \pi)$ .

- ☐ Linear link function  $\pi = \eta = x^T \beta$  can give  $\pi \notin [0, 1]$ , so not usually a good idea.
- ☐  $Y$  can be interpreted in terms of a hidden variable/tolerance distribution: let  $Z = x^T \gamma + \sigma \varepsilon$ , where  $\varepsilon \sim F$ . Set  $Y = I(Z > 0)$ , and note that

$$\pi = P(Y = 1) = P(x^T \gamma + \sigma \varepsilon > 0) = P(\varepsilon > -x^T \gamma / \sigma) = 1 - F(-x^T \gamma / \sigma),$$

say. Note that  $\beta = \gamma / \sigma$  is estimable, but  $\gamma$  and  $\sigma$  are not.

- ☐ The corresponding link function is given by

$$\eta = x^T \beta = -F^{-1}(1 - \pi) = g(\pi),$$

so different choices of  $F$  yield different possible link functions.

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**Link functions**

Tolerance distributions and corresponding link functions for binary data.

Distribution $F$		Link function	
Logistic	$e^u / (1 + e^u)$	Logit	$\eta = \log\{\pi / (1 - \pi)\}$
Normal	$\Phi(u)$	Probit	$\eta = \Phi^{-1}(\pi)$
Log Weibull	$1 - \exp(-\exp(u))$	Log-log	$\eta = -\log\{-\log(\pi)\}$
Gumbel	$\exp\{-\exp(-u)\}$	Complementary log-log	$\eta = \log\{-\log(1 - \pi)\}$

- ☐ The logit and probit links are symmetric.
- ☐ Logit (canonical link) is usual choice, good for medical studies (later), with nice interpretation, but the probit is very similar to it and may be preferred in some cases, for its relation to the normal distribution.
- ☐ The log-log and complementary log-log links are asymmetric.

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## Logistic regression

- Commonest choice of link function for proportion data is the **logit**, which gives

$$P(Y = 1) = \pi = \frac{\exp(x^T \beta)}{1 + \exp(x^T \beta)}, \quad P(Y = 0) = 1 - \pi = \frac{1}{1 + \exp(x^T \beta)},$$

leading to a linear model for the **log odds** of success,

$$\log \left\{ \frac{P(Y = 1)}{P(Y = 0)} \right\} = \log \left( \frac{\pi}{1 - \pi} \right) = x^T \beta, \quad \beta \in \mathbb{R}^p.$$

- The likelihood for  $\beta$  based on independent responses  $y_1, \dots, y_n$  with covariate vectors  $x_1, \dots, x_n$  and corresponding probabilities  $\pi_1, \dots, \pi_n$  is

$$L(\beta) = \prod_{j=1}^n \pi_j^{y_j} (1 - \pi_j)^{1-y_j} = \dots = \frac{\exp \left( \sum_{j=1}^n y_j x_j^T \beta \right)}{\prod_{j=1}^n \{1 + \exp(x_j^T \beta)\}},$$

which is a regular exponential family with  $s(y) = X^T y$  and log likelihood

$$\ell(\beta) = (X^T y)^T \beta - \sum_{j=1}^n \log \{1 + \exp(x_j^T \beta)\}, \quad \beta \in \mathbb{R}^p,$$

known as the **logistic regression model**.

## Nodal involvement data

Data on nodal involvement: 53 patients with prostate cancer have nodal involvement ( $r$ ), with five binary covariates age, stage, etc.

$m$	$r$	age	stage	grade	xray	acid
6	5	0	1	1	1	1
6	1	0	0	0	0	1
4	0	1	1	1	0	0
4	2	1	1	0	0	1
4	0	0	0	0	0	0
3	2	0	1	1	0	1
3	1	1	1	0	0	0
3	0	1	0	0	0	1
3	0	1	0	0	0	0
2	0	1	0	0	1	0
2	1	0	1	0	0	1
2	1	0	0	1	0	0
1	1	1	1	1	1	1
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
1	1	0	0	1	0	1
1	0	0	0	0	1	1
1	0	0	0	0	1	0

## Deviances for nodal involvement models

Scaled deviances  $D$  for 32 logistic regression models for nodal involvement data. + denotes a term included in the model.

age	st	gr	xr	ac	df	$D$	age	st	gr	xr	ac	df	$D$
					52	40.71	+	+	+			49	29.76
+					51	39.32	+	+		+		49	23.67
	+				51	33.01	+	+			+	49	25.54
		+			51	35.13	+		+	+		49	27.50
			+		51	31.39	+		+		+	49	26.70
				+	51	33.17	+			+	+	49	24.92
+	+				50	30.90		+	+	+		49	23.98
+		+			50	34.54		+	+		+	49	23.62
+			+		50	30.48		+		+	+	49	19.64
+				+	50	32.67			+	+	+	49	21.28
	+	+			50	31.00	+	+	+	+		48	23.12
	+		+		50	24.92	+	+	+		+	48	23.38
	+			+	50	26.37	+	+		+	+	48	19.22
		+	+		50	27.91	+		+	+	+	48	21.27
		+		+	50	26.72		+	+	+	+	48	18.22
			+	+	50	25.25	+	+	+	+	+	47	18.07

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## Model selection

- ☐ We have 32 competing models, and would like to select the ‘best’, or a few ‘near-best’.
- ☐ In general we have  $2^p$  models, so automatic selection of some sort is helpful.
- ☐ Could use likelihood ratio tests (differences of deviances) to compare competing models, but this involves many correlated tests, so may lead to spurious results.
- ☐ Usually minimise an information criterion, which accounts for the number of parameters in each model, such as

$$\text{AIC} \equiv D + 2p, \quad \text{BIC} \equiv D + p \log n,$$

where  $D$  is the deviance.

- ☐ Recall their properties, with  $p$  fixed and as  $n \rightarrow \infty$ :
  - AIC tends to overfit, i.e., it has a positive probability of choosing a model that is too complex,;
  - BIC applies a stronger penalty, so *if the true model is among those fitted*, it will choose it with probability one;
  - BIC usually yields less complex models than AIC, but they may predict less well.
- ☐ There are many other information criteria, but these are most used in practice.

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### Example: Nodal involvement

- Model with lowest AIC has stage, xray, acid:

$$x^T \hat{\beta} = -3.05 + 1.65I_{\text{stage}} + 1.91I_{\text{xray}} + 1.64I_{\text{acid}},$$

where  $I_{\text{stage}} = 1$  indicates that stage takes its higher level, etc.

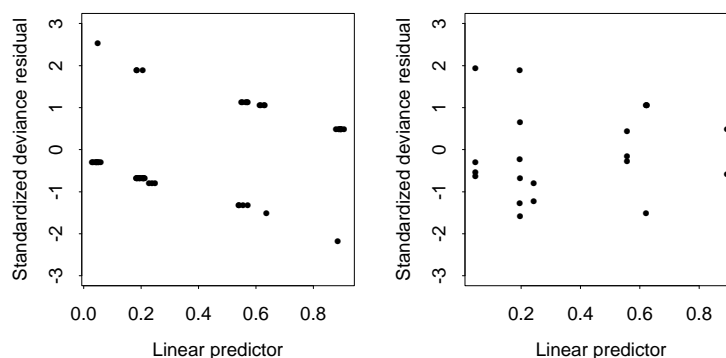
- Interpretation of this model:
  - for an individual with stage, xray and acid at their lowest levels, the fitted probability of nodal involvement is  $e^{-3.05}/(1 + e^{-3.05}) \doteq 0.045$  (though there are no such people in the data, so this involves extrapolation);
  - for someone with only  $I_{\text{stage}} = 1$ , the odds of nodal involvement are  $e^{-3.05+1.65} = e^{-1.4} \doteq 0.25$ , a probability of 0.2;
  - for someone with  $I_{\text{stage}} = I_{\text{xray}} = I_{\text{acid}} = 1$ , the odds of nodal involvement are  $e^{-3.05+1.65+1.91+1.64} \doteq 8.6$ , a probability of 0.9;
- Problems with interpretation of residual deviance of 19.64: how many df? — can amalgamate independent binary responses with same covariates.
- Likewise problems with residuals ...

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### Nodal involvement residuals

Figure 4: Standardized deviance residuals for nodal involvement data, for ungrouped responses (left) and grouped responses (right).



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## Summary

- ☐ Proportion data are often modelled using the Bernoulli/binomial response distributions.
- ☐ Link functions (logit, probit, ...) have interpretations in terms of underlying continuous variables that have been dichotomized.
- ☐ The canonical and most commonly-used link is the logit, and fitting using this yields logistic regression, in which
  - the canonical parameter is the log odds;
  - classical data structures (e.g., the  $2 \times 2$  table) have nice interpretations.
- ☐ The deviance can be used to compare models (so can AIC, BIC, ...), but using its absolute value to assess fit can be dangerous (exercise).
- ☐ Residuals for binary data are not very informative.

**Types of count data**

- $y \in \{0, 1, 2, \dots\}$ , perhaps with upper bound  $m$ , depending on sampling scheme:
  - counts, with no fixed total;
  - $m$  individuals, subdivided into various categories:
    - ▷ **nominal response**—unordered categories (gender, nationality, ...)
    - ▷ **ordinal response**—ordered categories (pain level, spiciness of curry, ...)
- Simplest models:
  - single unbounded response, or Poisson approximation to binomial, takes  $Y \sim \text{Pois}(\mu)$ ;
  - group of responses  $(Y_1, \dots, Y_d)$  with fixed total  $\sum Y_j = m$  has multinomial distribution, probabilities  $(\pi_1, \dots, \pi_d)$  and denominator  $m$ .
- Previous examples:
  - Doll and Hill data on smoking had response  $y$  Poisson with  $\mu = T\lambda(x; \beta)$ ;
  - Jacamar data had ordinal (?) response N/S/E with total N+S+E fixed—multinomial with  $d = 3$

**Poisson and multinomial distributions**

- $Y \sim \text{Pois}(\mu)$  implies that
 
$$f(y; \mu) = \frac{\mu^y}{y!} e^{-\mu}, \quad y = 0, 1, 2, \dots, \quad \mu > 0.$$
- Exponential family with natural parameter  $\theta = \log \mu$ , GLM with canonical logarithmic link,  $x^T \beta = \eta = \log \mu$ .
- If  $Y$  is number of events in Poisson process of rate  $\lambda$  observed for period of length  $T$ , then  $\mu = \lambda T$  and we set  $\eta = x^T \beta + \log T$ 
  - **offset**  $\log T$  is fixed part of linear predictor  $\eta$
- If  $Y_r \stackrel{\text{ind}}{\sim} \text{Pois}(\mu_r)$ ,  $r = 1, \dots, d$ , then the joint distribution of  $Y_1, \dots, Y_d$  given  $Y_1 + \dots + Y_d = m$  is **multinomial**, with denominator  $m$ , and probabilities

$$\pi_1 = \frac{\mu_1}{\sum_{r=1}^d \mu_r}, \quad \dots, \quad \pi_d = \frac{\mu_d}{\sum_{r=1}^d \mu_r}.$$

- If  $(Y_1, \dots, Y_d) \sim \text{Mult}(m; \pi_1, \dots, \pi_d)$ , then marginal and conditional distributions, e.g., of

$$(Y_1 + Y_2, Y_3 + Y_4 + Y_5, Y_6, \dots, Y_d), \quad (Y_1, Y_2, Y_4) \mid (Y_3, Y_5, \dots, Y_d),$$

are also multinomial.

## Log-linear and logistic regressions

- Special case: if  $d = 2$ , then

$$Y_2 \mid Y_1 + Y_2 = m \sim B\left(m, \pi = \frac{\mu_2}{\mu_1 + \mu_2}\right)$$

- If  $\mu_1 = \exp(\gamma + x_1^T \beta)$ ,  $\mu_2 = \exp(\gamma + x_2^T \beta)$ , then

$$\pi = \frac{\exp(\gamma + x_2^T \beta)}{\exp(\gamma + x_1^T \beta) + \exp(\gamma + x_2^T \beta)} = \frac{\exp\{(x_2 - x_1)^T \beta\}}{1 + \exp\{(x_2 - x_1)^T \beta\}},$$

which corresponds to a logistic regression model for  $Y_2$  with denominator  $m$  and probability  $\pi$ .

- Can estimate  $\beta$  using log linear model or logistic model—but can't estimate  $\gamma$  from logistic model.

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## 2.6 Poisson Regression

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### Premier League data

```
> soccer
  month day year   team1   team2 score1 score2
1   Aug  19 2000 Charlton ManchesterC      4      0
2   Aug  19 2000  Chelsea   WestHam      4      2
3   Aug  19 2000 Coventry  Middlesbr      1      3
4   Aug  19 2000   Derby Southampton      2      2
5   Aug  19 2000   Leeds   Everton      2      0
6   Aug  19 2000 Leicester AstonVilla      0      0
7   Aug  19 2000 Liverpool  Bradford      1      0
8   Aug  19 2000 Sunderland   Arsenal      1      0
9   Aug  19 2000 Tottenham   Ipswich      3      1
10  Aug  20 2000 ManchesterU Newcastle      2      0
11  Aug  21 2000   Arsenal  Liverpool      2      0
12  Aug  22 2000  Bradford   Chelsea      2      0
13  Aug  22 2000   Ipswich ManchesterU      1      1
14  Aug  22 2000  Middlesbr Tottenham      1      1
15  Aug  23 2000   Everton   Charlton      3      0
16  Aug  23 2000 ManchesterC Sunderland      4      2
17  Aug  23 2000  Newcastle   Derby      3      2
18  Aug  23 2000 Southampton  Coventry      1      2
19  Aug  23 2000   WestHam  Leicester      0      1
20  Aug  26 2000   Arsenal   Charlton      5      3
...
```

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### Premier League data

- ☐ 380 soccer matches in English Premier League in 2000–2001 season.
- ☐ Data: home score  $y_{ij}^h$  and away score  $y_{ij}^a$  when team  $i$  is at home to team  $j$ , for  $i, j = 1, \dots, 20$ ,  $i \neq j$ .
- ☐ Treat these as Poisson counts with means

$$\mu_{ij}^h = \exp(\Delta + \alpha_i - \beta_j), \quad \mu_{ij}^a = \exp(\alpha_j - \beta_i)$$

where

- $\Delta$  represents the home advantage;
  - $\alpha_i$  and  $\beta_i$  represent the offensive and defensive strengths of team  $i$ .
- ☐ Two possibilities for fitting:
    - Poisson GLM, with 39 parameters;
    - binomial GLM, with 20 parameters.

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### Premier League data: Analysis of deviance

Poisson model			Binomial model		
Terms	df	Deviance reduction	Terms	df	Deviance reduction
Home	1	33.58	Home	1	33.58
Defence	19	39.21	Team	19	79.63
Offence	19	58.85			
Residual	720	801.08	Residual	332	410.65

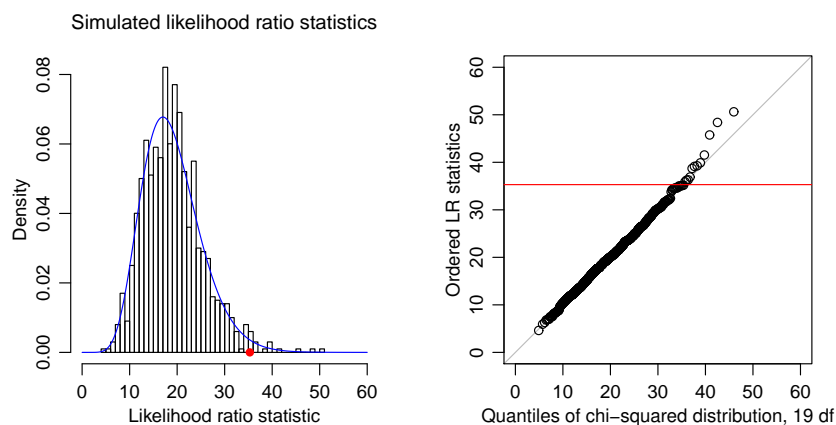
- ☐ There's a strong effect of playing at home, and lots of evidence of differences among the teams—more in offence than defence.
- ☐ Both residual deviances are a little large, but since the counts are small, we don't expect the large-sample  $\chi^2$  distribution to apply well to the residual deviance.
- ☐ Simulations from the fitted model suggest that the residual deviances are not unusually large, so there's no evidence of a lack of fit.

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## Premier League data: Null deviance for defence effect

Defence effect deviance (in red) for the Poisson model is large(ish) relative to  $\chi^2_{19}$  distribution, but the asymptotics seem OK, based on simulations from a model without this effect (i.e., Home + Offence). It seems we can trust asymptotic distributions for differences of deviances, even though the counts are small.

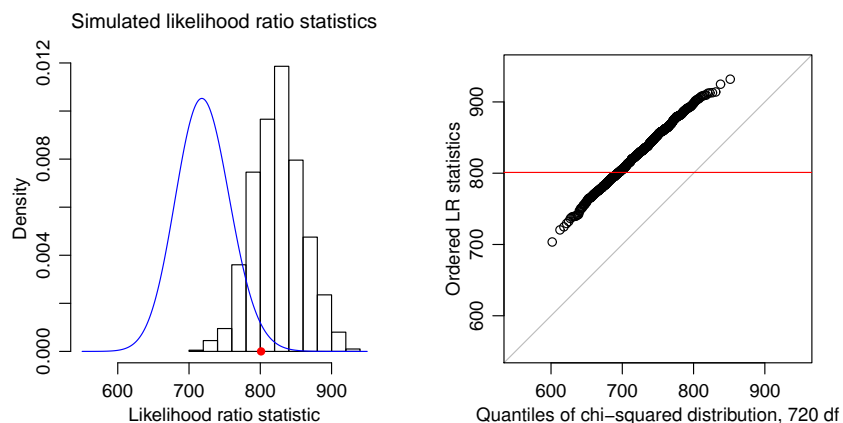


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## Premier League data: Residual deviance

Residual deviance of 801 (in red) for the Poisson model seems large(ish) relative to  $\chi^2_{720}$  distribution, but the asymptotics are suspect because most of the counts are small. Comparison of observed deviance with  $\chi^2_{720}$  distribution shows that 801 is in fact somewhat smaller than average for datasets simulated from the fitted model.



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## Premier League data: Estimates

	Overall ( $\delta$ )	Offensive ( $\alpha$ )	Defensive ( $\beta$ )
Manchester United	0.39	0.22	0.15
Liverpool	0.13	0.12	-0.08
Arsenal	—	0.04	—
Chelsea	-0.09	0.08	-0.22
Leeds	-0.10	0.02	-0.17
Ipswich	-0.16	-0.10	-0.13
Sunderland	-0.33	-0.31	-0.10
Aston Villa	-0.48	-0.31	-0.15
West Ham	-0.53	-0.33	-0.30
Middlesbrough	-0.53	-0.35	-0.17
Charlton	-0.55	-0.21	-0.43
Tottenham	-0.58	-0.28	-0.38
Newcastle	-0.59	-0.35	-0.30
Southampton	-0.60	-0.45	-0.25
Everton	-0.75	-0.32	-0.46
Leicester	-0.77	-0.47	-0.31
Manchester City	-0.90	-0.40	-0.56
Coventry	-0.93	-0.53	-0.52
Derby	-0.93	-0.51	-0.45
Bradford	-1.29	-0.71	-0.62
SEs	0.29	0.20	0.20

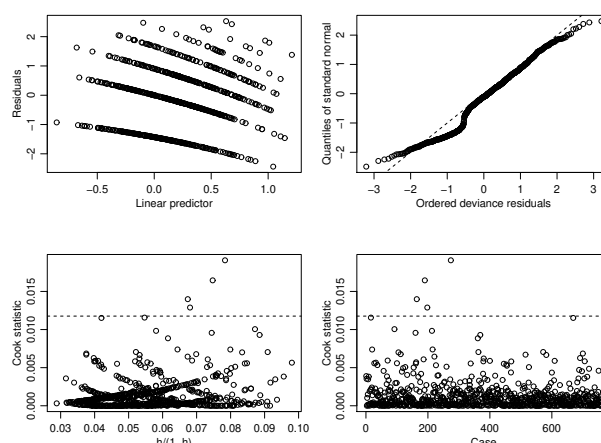
Home advantage:  $\hat{\Delta} = 0.37$  (0.07),  $\exp(\hat{\Delta}) = 1.45$ .

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## Premier League data: Assessment of fit

Diagnostic plots for fitted model: residuals against  $\hat{\eta}$  (top left); normal QQ-plot of residuals (top right); Cook statistic  $C_j$  against leverage ratio  $h_j/(1 - h_j)$  (lower left); Cook statistic  $C_j$  against case number (lower right).



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**Sampling schemes**

- A **contingency table** contains individuals (sampling units) cross-classified by various categorical variables.

- Example: the jacamar data cross-classify butterflies by

$$6 \text{ species} \times 8 \text{ colours} \times 3 \text{ fates}$$

for a total of 144 categories, each with its number of butterflies  $0, 1, \dots, 14$ .

- The sampling scheme underlying a table may fix certain totals. Suppose a pollster wants to find out how people will vote. She might
  - wait in the street for a morning, and get opinions from those people willing to talk to her;
  - wait until she has the views of a fixed number, say  $m$ , of people;
  - wait until she has the views of fixed numbers of men and women.

**Example 25** Find the likelihoods for each of these sampling schemes, under (unrealistic!) assumptions of independence of voters.

**Note to Example 25**

- An  $R \times C$  table arises by randomly sampling a population over a fixed period and then classifying the resulting individuals.
- In the first scheme there are no constraints on the row and column totals, and a simple model is that the count in the  $(r, c)$  cell,  $y_{rc}$ , has a Poisson distribution with mean  $\mu_{rc}$ . The resulting likelihood is

$$\prod_{r,c} \left\{ \frac{\mu_{rc}^{y_{rc}}}{y_{rc}!} e^{-\mu_{rc}} \right\};$$

this is simply the Poisson likelihood for the counts in the  $RC$  groups.

- The pollster may set out with the intention of interviewing a fixed number  $m$  of individuals, stopping only when  $\sum_{rc} y_{rc} = m$ . In this case the data are multinomially distributed, with likelihood

$$\frac{m!}{\prod_{r,c} y_{rc}!} \prod_{r,c} \pi_{rc}^{y_{rc}}, \quad \sum_{r,c} \pi_{rc} = 1,$$

with  $\pi_{rc} = \mu_{rc} / \sum_{s,t} \mu_{st}$  the probability of falling into the  $(r, c)$  cell.

- A third scheme is to interview fixed numbers of men and of women, thus fixing the row totals  $m_r = \sum_c y_{rc}$  in advance. In effect this treats the row categories as subpopulations, and the column categories as the response. This yields independent multinomial distributions for each row, and product multinomial likelihood

$$\prod_r \left\{ \frac{m_r!}{\prod_c y_{rc}!} \prod_c \pi_{rc}^{y_{rc}} \right\}, \quad \sum_c \pi_{1c} = \dots = \sum_c \pi_{Rc} = 1,$$

in which  $\pi_{rc} = \mu_{rc} / \sum_t \mu_{rt}$ .

## Contingency tables and Poisson response models

- Multinomial models can be fitted using Poisson errors, provided the appropriate baseline terms are always included in the linear predictor.
- Write the data as two-way layout, with  $C$  columns and  $R$  rows with fixed totals (e.g.,  $6 \times 8 = 48$  rows each with 3 columns for the jacamar data).
- Consider Poisson model with means  $\mu_{rc} = \exp(\gamma_r + x_{rc}^T \beta)$ :
  - the row parameters  $\gamma_1, \dots, \gamma_R$  are **nuisance parameters**, not of interest;
  - we want inference for the **parameter of interest**,  $\beta$ .
- Corresponding multinomial model has fixed row totals  $m_r$  and probabilities

$$\pi_{rc} = \frac{\mu_{rc}}{\sum_{d=1}^C \mu_{rd}} = \frac{\exp(\gamma_r + x_{rc}^T \beta)}{\sum_{d=1}^C \exp(\gamma_r + x_{rd}^T \beta)} = \frac{\exp(x_{rc}^T \beta)}{\sum_{d=1}^C \exp(x_{rd}^T \beta)},$$

for  $r = 1, \dots, R$ ,  $c = 1, \dots, C$ ; i.e., one multinomial variable for each row.

- The resulting multinomial log likelihood is

$$\begin{aligned} \ell_{\text{Mult}}(\beta; y \mid m) &\equiv \sum_{r=1}^R \sum_{c=1}^C y_{rc} \log \pi_{rc} \\ &= \sum_{r=1}^R \left\{ \sum_{c=1}^C y_{rc} x_{rc}^T \beta - m_r \log \left( \sum_{d=1}^C e^{x_{rd}^T \beta} \right) \right\}. \end{aligned}$$

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## Contingency tables and Poisson response models, II

**Lemma 26** *If parameters  $\tau_r$  for the row margins are included in the above setup, then we can write*

$$\ell_{\text{Pois}}(\beta, \tau) = \ell_{\text{Pois}}(\tau; m) + \ell_{\text{Mult}}(\beta; y \mid m).$$

- Implications:
  - the MLEs of  $\beta$  and  $\tau$  based on the LHS are the same as those from separate maximisations of the terms on the right:
    - ▷  $\hat{\beta}$  equals the MLE for the multinomial model,
    - ▷  $\hat{\tau}_r = m_r$
  - the observed and expected information matrices for  $\beta, \tau$  are block diagonal.
  - SEs based on the multinomial and Poisson models are equal (exercise).
- General conclusion: inferences on  $\beta$  are the same for multinomial and Poisson models,
 

*provided the parameters associated to the margins fixed under the multinomial model, i.e., the  $\gamma_r$ , are included in the Poisson fit.*

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## Note to Lemma 26

- The Poisson model has no conditioning, so with  $\log \mu_{rc} = \gamma_r + x_{rc}^T \beta$  the log likelihood is

$$\ell_{\text{Pois}}(\beta, \gamma) \equiv \sum_{r,c} (y_{rc} \log \mu_{rc} - \mu_{rc}) = \sum_{r=1}^R \left( m_r \gamma_r + \sum_{c=1}^C y_{rc} x_{rc}^T \beta - e^{\gamma_r} \sum_{c=1}^C e^{x_{rc}^T \beta} \right).$$

- Now we reparametrise in terms of the row totals  $\tau_r = \sum_c \mu_{rc}$ , noting that

$$\tau_r = e^{\gamma_r} \sum_{c=1}^C e^{x_{rc}^T \beta}, \quad \gamma_r = \log \tau_r - \log \left\{ \sum_{c=1}^C \exp(x_{rc}^T \beta) \right\},$$

so

$$\begin{aligned} \ell_{\text{Pois}}(\beta, \tau) &\equiv \sum_{r=1}^R (m_r \log \tau_r - \tau_r) + \sum_{r=1}^R \left\{ \sum_{c=1}^C y_{rc} x_{rc}^T \beta - m_r \log \left( \sum_{c=1}^C e^{x_{rc}^T \beta} \right) \right\}, \\ &= \ell_{\text{Pois}}(\tau; m) + \ell_{\text{Mult}}(\beta; y \mid m), \end{aligned}$$

which is the log likelihood corresponding to

- independent Poisson row totals  $m_r$  with means  $\tau_r$ , and, independent of this,
- the multinomial log likelihood for the contingency table.

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## Jacamar data

Response (N=not sampled, S = sampled and rejected, E = eaten) of a rufous-tailed jacamar to individuals of seven species of palatable butterflies with artificially coloured wing undersides. Data from Peng Chai, University of Texas.

	<i>Aphrissa boisduvalli</i>	<i>Phoebis argante</i>	<i>Dryas iulia</i>	<i>Pierella luna</i>	<i>Consul fabius</i>	<i>Siproeta stelenes</i> †
	N/S/E	N/S/E	N/S/E	N/S/E	N/S/E	N/S/E
Unpainted	0/0/14	6/1/0	1/0/2	4/1/5	0/0/0	0/0/1
Brown	7/1/2	2/1/0	1/0/1	2/2/4	0/0/3	0/0/1
Yellow	7/2/1	4/0/2	5/0/1	2/0/5	0/0/1	0/0/3
Blue	6/0/0	0/0/0	0/0/1	4/0/3	0/0/1	0/1/1
Green	3/0/1	1/1/0	5/0/0	6/0/2	0/0/1	0/0/3
Red	4/0/0	0/0/0	6/0/0	4/0/2	0/0/1	3/0/1
Orange	4/2/0	6/0/0	4/1/1	7/0/1	0/0/2	1/1/1
Black	4/0/0	0/0/0	1/0/1	4/2/2	7/1/0	0/1/0

† includes *Philaethria dido* also.

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## Jacamar data: Models

- Let factors  $F$ ,  $S$ ,  $C$  represent the 3 fates, the 6 species, and the 8 colours.
- The models  $C * S$ ,  $C * S + F$ , and  $C * S + C * F$  mean we set

$$\log \mu_{csf} = \alpha_{cs}, \quad \log \mu_{csf} = \alpha_{cs} + \gamma_f, \quad \log \mu_{csf} = \alpha_{cs} + \gamma_{cf}.$$

- The vector of probabilities corresponding to the model with terms  $C * S$  is

$$(\pi_{cs1}, \pi_{cs2}, \pi_{cs3}) = \left( \frac{\mu_{cs1}}{\sum_{f=1}^3 \mu_{csf}}, \frac{\mu_{cs2}}{\sum_{f=1}^3 \mu_{csf}}, \frac{\mu_{cs3}}{\sum_{f=1}^3 \mu_{csf}} \right) = \left( \frac{1}{3}, \frac{1}{3}, \frac{1}{3} \right),$$

and that corresponding to the model with terms  $C * S + F$  is

$$\begin{aligned} (\pi_{cs1}, \pi_{cs2}, \pi_{cs3}) &= \left( \frac{\mu_{cs1}}{\sum_{f=1}^3 \mu_{csf}}, \frac{\mu_{cs2}}{\sum_{f=1}^3 \mu_{csf}}, \frac{\mu_{cs3}}{\sum_{f=1}^3 \mu_{csf}} \right) \\ &= \frac{1}{e^{\gamma_1} + e^{\gamma_2} + e^{\gamma_3}} (e^{\gamma_1}, e^{\gamma_2}, e^{\gamma_3}). \end{aligned}$$

- Exercise: similar computations for  $C * S + C * F$  and  $C * S + C * F + S * F$ .

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## Jacamar data: Analysis of deviance

Deviances for log-linear models fitted to jacamar data.

Terms	df	Deviance
$C * S$	88	259.42
$C * S + F$	86	173.86
$C * S + C * F$	72	139.62
$C * S + S * F$	76	148.23
$C * S + C * F + S * F$	62	90.66
$C * S * F$	0	0

- The null model  $C * S$  is not of interest.
- The first model it is sensible to fit is  $C * S + F$ .
- The best model seems to be  $C * S + C * F + S * F$ , corresponding to independent effects of species and colour, though its deviance is high (but remember the two outlying cells!)

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**Pneumoconiosis data**

Period of exposure  $x$  and prevalence of pneumoconiosis amongst coalminers.

	Period of exposure (years)							
	5.8	15	21.5	27.5	33.5	39.5	46	51.5
Normal	98	51	34	35	32	23	12	4
Present	0	2	6	5	10	7	6	2
Severe	0	1	3	8	9	8	10	5

- ☐ Here

Normal < Present < Severe,

so these are ordinal responses with  $d = 3$  categories and the total in each group (corresponding to each period of exposure) fixed.

- ☐ We imagine that the assigned category stems from an underlying continuous variable, even if this cannot be quantified very well.

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**Models**

- ☐ Assume we have  $n$  independent individuals whose responses  $I_1, \dots, I_n$  fall into the set  $\{1, \dots, L\}$ , corresponding to  $L$  ordered categories, and that

$$\gamma_l = P(I_j \leq l) = \pi_1 + \dots + \pi_l, \quad l = 1, \dots, L, \quad \gamma_L = 1,$$

- ☐ The corresponding likelihood is  $\prod_{j=1}^n \pi_{I_j}$ , where usually the contribution  $\pi_{I_j} \equiv \pi_{I_j}(\eta_j)$  for individual  $j$  will depend on covariates  $x_j$  through a linear predictor  $\eta_j = x_j^T \beta$ .
- ☐ We often want the interpretation of the parameters not to change if we merge adjacent categories, and we can do this using an underlying tolerance distribution, with

$$I_j = l \Leftrightarrow x_j^T \beta + \varepsilon_j \in (\zeta_{l-1}, \zeta_l], \quad \zeta_0 = -\infty < \zeta_1 < \dots < \zeta_{L-1} < \zeta_L = \infty,$$

where the tolerance distribution  $F$  of  $\varepsilon_j$  is often taken to be logistic, giving the **proportional odds model**, in which

$$\pi_l(x_j^T \beta) = P(\zeta_{l-1} < x_j^T \beta + \varepsilon \leq \zeta_l) = F(\zeta_l - x_j^T \beta) - F(\zeta_{l-1} - x_j^T \beta), \quad l = 1, \dots, L;$$

here  $\zeta_1, \dots, \zeta_{L-1}$  are aliased with an intercept  $\beta_0$  and are not usually of interest.

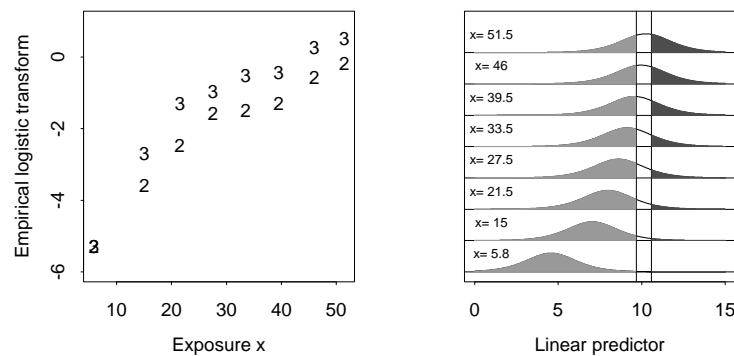
- ☐ Another standard tolerance distribution is  $F(u) = 1 - \exp\{-\exp(u)\}$ .
- ☐ To fit, we just apply IWLS to the multinomial likelihood  $\prod_{j=1}^n \pi_{I_j}$ .

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## Pneumoconiosis data

Pneumoconiosis data analysis, showing how the implied fitted logistic distributions depend on  $x$ . Left: plots of empirical logistic transforms for comparing categories 1 with 2 + 3 and 1 + 2 with 3; the nonlinearity suggests using  $\log x$  as covariate. Right: fitted model, showing probabilities for the three groups with an underlying logistic distribution.



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## Comments on count data

- ☐ Log-linear models are mathematically elegant and useful defaults for count data, with close links to logistic regression, based on the relation between the Poisson and multinomial distributions.
- ☐ Interpretation of log-linear models can be difficult, especially for contingency tables, because marginal and conditional parameters cannot be disentangled.
- ☐ Other models exist that are less elegant mathematically, but are more interpretable statistically.
- ☐ Also possible to fit models for ordinal data, using multinomial models and tolerance distribution interpretation used for binomial data.

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**Overdispersion**

- ☐ Often find that discrete response data are more variable than might be expected from a simple Poisson or binomial model, so we see
  - residual deviances larger than expected
  - residuals more variable than expected under the model
 but otherwise no evidence of systematic lack of fit
- ☐ This is **overdispersion**, perhaps due to effect of unmeasured explanatory variables on the responses.

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**UK monthly AIDS reports 1983–1992**

Diagnosis period		Reporting-delay interval (quarters):									Total reports to end of 1992
Year	Quarter	0 <sup>†</sup>	1	2	3	4	5	6	...	≥14	
	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
1988	1	31	80	16	9	3	2	8	...	6	174
	2	26	99	27	9	8	11	3	...	3	211
	3	31	95	35	13	18	4	6	...	3	224
	4	36	77	20	26	11	3	8	...	2	205
1989	1	32	92	32	10	12	19	12	...	2	224
	2	15	92	14	27	22	21	12	...	1	219
	3	34	104	29	31	18	8	6	...		253
	4	38	101	34	18	9	15	6	...		233
1990	1	31	124	47	24	11	15	8	...		281
	2	32	132	36	10	9	7	6	...		245
	3	49	107	51	17	15	8	9	...		260
	4	44	153	41	16	11	6	5	...		285
1991	1	41	137	29	33	7	11	6	...		271
	2	56	124	39	14	12	7	10	...		263
	3	53	175	35	17	13	11	2			306
	4	63	135	24	23	12	1				258
1992	1	71	161	48	25	5					310
	2	95	178	39	6						318
	3	76	181	16							273
	4	67	66								133

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## AIDS data

- UK monthly reports of AIDS diagnoses 1983–1992, with reporting delay up to several years!
- Example of incomplete contingency table (very common in insurance)
- Chain-ladder model: number of reports in row  $j$  and column  $k$  is Poisson, with mean

$$\mu_{jk} = \exp(\alpha_j + \beta_k).$$

- Analysis of deviance:

Model	df	Deviance reduction	df	Deviance
			464	14184.3
Time (rows)	37	6114.8	427	8069.5
Delay (cols)	14	7353.0	413	716.5

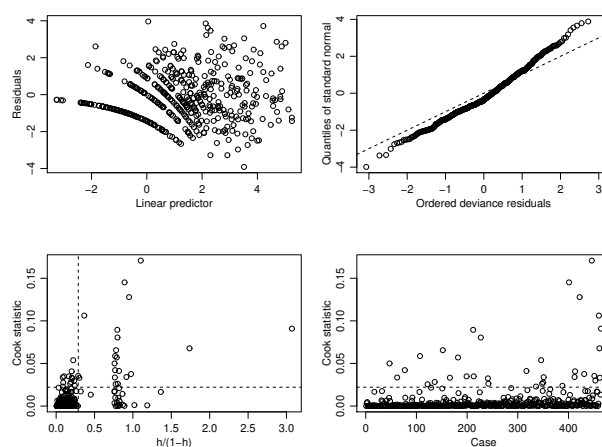
- Residual deviance is obviously far too large for a Poisson model to be OK, but the model is also too complex, since we expect smooth variation in the  $\alpha_j$ .
- Residuals on next page show no obvious problems, just generic overdispersion.

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## AIDS data: Assessment of fit

Diagnostic plots for fitted model: residuals against  $\hat{\eta}$  (top left); normal QQ-plot of residuals (top right); Cook statistic  $C_j$  against leverage ratio  $h_j/(1 - h_j)$  (lower left); Cook statistic  $C_j$  against case number (lower right).

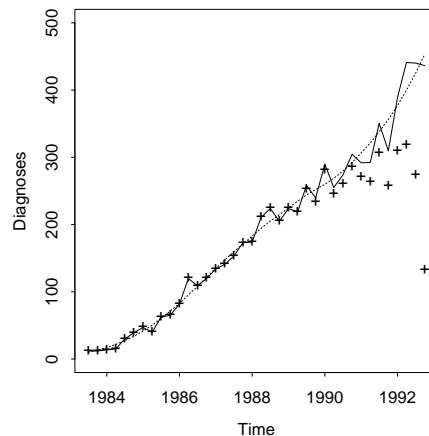


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## AIDS data

- ☐ Data (+) and predicted true numbers based on simple Poisson model (solid) and GAM (dots).
- ☐ The Poisson model and data agree up to where data start to be missing.



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## Dealing with overdispersion

- ☐ Two basic approaches:
  - parametric modelling
  - quasi-likelihood estimation, based only on the variance function

**Example 27 (Linear and quadratic variance functions)** Suppose that, conditional on  $\varepsilon > 0$ ,  $Y \sim \text{Pois}(\mu\varepsilon)$ , where  $E(\varepsilon) = 1$  and  $\text{var}(\varepsilon) = \xi$ . Show that this can lead to either linear or quadratic variance functions, but a lot of data may be needed to distinguish them.

Comparison of variance functions for overdispersed count data. The linear and quadratic variance functions are  $V_L(\mu) = (1 + \xi_L)\mu$  and  $V_Q(\mu) = \mu(1 + \xi_Q\mu)$ , with  $\xi_L = 0.5$  and  $\xi_Q$  chosen so that  $V_L(15) = V_Q(15)$ .

$\mu$	1	2	5	10	15	20	30	40	60
Linear	1.5	3.0	7.5	15.0	22.5	30	45	60	90
Quadratic	1.0	2.1	5.8	13.3	22.5	33	60	93	180

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### Note to Example 27

Let  $\varepsilon$  have unit mean and variance  $\xi > 0$ , and to be concrete suppose that conditional on  $\varepsilon$ ,  $Y$  has the Poisson distribution with mean  $\mu\varepsilon$ . Then

$$E(Y) = E_{\varepsilon} \{E(Y | \varepsilon)\}, \quad \text{var}(Y) = \text{var}_{\varepsilon} \{E(Y | \varepsilon)\} + E_{\varepsilon} \{\text{var}(Y | \varepsilon)\},$$

so the response has mean and variance

$$E(Y) = E_{\varepsilon}(\mu\varepsilon) = \mu, \quad \text{var}(Y) = \text{var}_{\varepsilon}(\mu\varepsilon) + E_{\varepsilon}(\mu\varepsilon) = \mu(1 + \xi\mu).$$

If on the other hand the variance of  $\varepsilon$  is  $\xi/\mu$ , then  $\text{var}(Y) = (1 + \xi)\mu$ . In both cases the variance of  $Y$  is greater than its value under the standard Poisson model, for which  $\xi = 0$ . In the first case the variance function is quadratic, and in the second it is linear.

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### Negative binomial model

**Example 28 (Negative binomial)** In Example 27, if  $\varepsilon$  is gamma with shape parameter  $1/\nu$ , show that

$$f(y; \mu, \nu) = \frac{\Gamma(y + \nu)}{\Gamma(\nu)y!} \frac{\nu^{\nu} \mu^y}{(\nu + \mu)^{\nu+y}}, \quad y = 0, 1, \dots, \quad \mu, \nu > 0,$$

and that quadratic and linear variance functions are obtained on setting  $\nu = 1/\xi$  and  $\nu = \mu/\xi$  respectively.

The log link function  $\log \mu = x^T \beta$  is most natural.

$\xi$  is estimated by maximum likelihood or through Pearson's statistic.

### Example 29 (AIDS data)

- ☐ MLE  $\hat{\xi}_Q = 22.7$  (5.5)
- ☐ Analysis of Deviance (with  $\hat{\xi}_Q$  fixed):

Model	df	Deviance reduction	df	Deviance
			464	7998.3
Time (rows)	37	3582.5	427	4415.8
Delay (cols)	14	3892.2	413	523.6

- ☐ Still somewhat overdispersed?

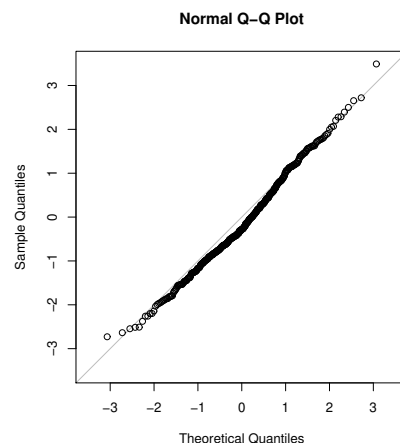
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## AIDS data: Deviance residuals for NB model

Clear improvement over previous plots, even if not perfect.



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## Quasi-likelihood

- ☐ Recall two basic assumptions for the linear model:
  - the responses are uncorrelated with means  $\mu_j = x_j^T \beta$  and equal variances  $\sigma^2$ ;
  - in addition to this, the responses are normally distributed.
- ☐ To avoid parametric modelling, we generalise the second-order assumptions, to

$$E(Y_j) = \mu_j, \quad \text{var}(Y_j) = \phi_j V(\mu_j), \quad g(\mu_j) = \eta_j = x_j^T \beta,$$

where the variance function  $V(\cdot)$  and the link function are taken as known.

- ☐ We obtain estimates  $\tilde{\beta}$  by solving the estimating equation

$$h(\beta; Y) = X^T u(\beta) = \sum_{j=1}^n x_j u_j(\beta) = \sum_{j=1}^n x_j \frac{Y_j - \mu_j}{g'(\mu_j) \phi_j V(\mu_j)} = 0.$$

- ☐ If the mean structure is correct, then  $E(Y_j) = \mu_j$ , so  $E\{h(\beta; Y)\} = 0$ , and under mild conditions  $\tilde{\beta}$  is consistent (but maybe not efficient) as  $n \rightarrow \infty$ .

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## Quasi-likelihood II

Recall that the general variance of an estimator  $\tilde{\beta}$  defined by an estimating equation  $h(\beta; Y)_{p \times 1} = 0_p$  has sandwich form

$$E \left\{ -\frac{\partial h(\beta; Y)}{\partial \beta^T} \right\}^{-1} \text{var} \{h(\beta; Y)\} E \left\{ -\frac{\partial h(\beta; Y)^T}{\partial \beta} \right\}^{-1}.$$

**Lemma 30** *If  $V(\mu)$  is correctly specified, then  $\text{var}(\tilde{\beta}) \doteq (X^T W X)^{-1}$ , where  $W$  is diagonal with  $(j, j)$  element  $\{g'(\mu_j)^2 \phi_j V(\mu_j)\}^{-1}$ .*

- If  $\phi_j = \phi a_j$ , with known  $a_j > 0$  and unknown  $\phi > 0$ , then we obtain
- $\tilde{\beta}$  by fitting the GLM with variance function  $V(\mu)$  and link  $g(\mu)$ ;
  - standard errors by multiplying the standard errors for this fit by  $\hat{\phi}^{1/2}$ , where

$$\hat{\phi} = \frac{1}{n-p} \sum_{j=1}^n \frac{(y_j - \hat{\mu}_j)^2}{a_j g'(\mu_j)^2 V(\hat{\mu}_j)}.$$

### Note to Lemma 30

- Note first that we can write

$$u_j(\beta) \equiv u_j(\mu_j) = \frac{A_j(\mu_j)}{B_j(\mu_j)},$$

where  $A_j(\mu_j) = Y_j - \mu_j$  and  $B_j(\mu_j) = g'(\mu_j)\phi_j V(\mu_j)$ . Only  $A_j$  is random and  $E\{A_j(\mu_j)\} = 0$ . Hence if we let prime denote derivative with respect to  $\mu_j$ ,

$$\frac{\partial u_j(\mu_j)}{\partial \mu_j} = \frac{A'_j(\mu_j)}{B_j(\mu_j)} - \frac{A_j(\mu_j)B'_j(\mu_j)}{B_j^2(\mu_j)}$$

has expectation  $E\{A'_j(\mu_j)\}/B_j(\mu_j) = -1/B_j(\mu_j)$ .

- We require  $E\{-\partial h(\beta; Y)/\partial \beta^T\}$  and  $\text{var}\{h(\beta; Y)\}$ . Now

$$\frac{\partial u_j(\beta)}{\partial \beta^T} = \frac{\partial \eta_j}{\partial \beta^T} \frac{\partial \mu_j}{\partial \eta_j} \frac{\partial u_j(\beta)}{\partial \mu_j} = x_j^T \frac{1}{g'(\mu_j)} u'_j(\mu_j),$$

which gives

$$E\left\{-\frac{\partial h(\beta; Y)}{\partial \beta^T}\right\} = -\sum_{j=1}^n x_j E\left\{\frac{\partial u_j(\beta)}{\partial \beta^T}\right\} = \sum_{j=1}^n x_j x_j^T \frac{1}{g'(\mu_j)^2 \phi_j V(\mu_j)} = X^T W X,$$

where  $W$  is the  $n \times n$  diagonal matrix with  $j$ th element  $\{g'(\mu_j)^2 \phi_j V(\mu_j)\}^{-1}$ . Moreover if in addition the variance function has been correctly specified, then  $\text{var}(Y_j) = \phi_j V(\mu_j)$ , and hence

$$\text{var}\{h(\beta; Y)\} = X^T \text{var}\{u(\beta)\} X = \sum_{j=1}^n x_j x_j^T \frac{\text{var}(Y_j)}{g'(\mu_j)^2 \phi_j^2 V(\mu_j)^2} = X^T W X.$$

Thus the sandwich equals  $(X^T W X)^{-1}$ .

- Had the variance function been wrongly specified, the variance matrix of  $\tilde{\beta}$  would have been  $(X^T W X)^{-1} (X^T W' X) (X^T W X)^{-1}$ , where  $W'$  is a diagonal matrix involving the true and assumed variance functions. Only if the variance function has been chosen very badly will this sandwich matrix differ greatly from  $(X^T W X)^{-1}$ , which therefore provides useful standard errors unless a plot of absolute residuals against fitted means is markedly non-random. In that case the choice of variance function should be reconsidered.

### Quasi-likelihood III

- Under an exponential family model,  $h(\beta; Y)$  is the score statistic, so  $\tilde{\beta}$  is the MLE and is efficient (i.e., it has the smallest possible variance in large samples).
- If not, inference is valid provided  $g$  and  $V$  are correctly chosen, and  $\tilde{\beta}$  is optimal among estimators based on linear combinations of the  $Y_j - \mu_j$ , by extending the Gauss–Markov theorem.
- In fact we can define a **quasi-likelihood**  $Q$  and its score through

$$Q(\beta; Y) = \sum_{j=1}^n \int_{Y_j}^{\mu_j} \frac{Y_j - u}{\phi a_j V(u)} du, \quad h(\beta; Y) = \frac{\partial}{\partial \beta} Q(\beta; Y),$$

and a (quasi-)deviance as  $D = -2\phi Q(\beta; Y)$ .

- To compare models  $A, B$  with numbers of parameters  $p_B < p_A$  and deviances  $D_B > D_A$ , we use the fact that

$$\frac{(D_B - D_A)/(p_A - p_B)}{\hat{\phi}_A} \underset{\sim}{\sim} F_{p_A - p_B, n - p_A},$$

if the simpler model  $B$  is adequate. This is easy in R.

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### AIDS example

```
> aids.ql <- glm(y~factor(time)+factor(delay),family=quasipoisson,data=aids.in)
> anova(aids.ql,test="F")
```

Analysis of Deviance Table

Model: quasipoisson, link: log

Response: y

Terms added sequentially (first to last)

	Df	Deviance	Resid. Df	Resid. Dev	F	Pr(>F)
NULL			464	14184.3		
factor(time)	37	6114.8	427	8069.5	92.638	< 2.2e-16 ***
factor(delay)	14	7353.0	413	716.5	294.402	< 2.2e-16 ***

---

Signif. codes: 0 '\*\*\*' 0.001 '\*\*' 0.01 '\*' 0.05 '.' 0.1 ' ' 1

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## Summary

- ☐ Overdispersion is widespread in count and proportion data.
- ☐ We deal with it either by
  - parametric modelling, or
  - quasi-likelihood (QL) estimation, which involves assumptions only on the mean-variance relationship.
- ☐ QL estimators equal the ML ones, but SEs are inflated by  $\hat{\phi}^{1/2}$ .
- ☐ (Quasi-)deviance can also be defined, and used for model comparison, with  $F$  tests replacing  $\chi^2$  tests.

**Tall and wide regressions**

- ☐ So far we have supposed that we have a **tall regression**:
  - the number of units  $n$  exceeds the number of variables  $p$ ,
  - the design matrix  $X$  has rank  $p$ .
- ☐ In many 'modern' settings we instead have a **wide regression**:
  - $n$  and  $p$  are comparable,  $p > n$ , maybe even  $p \gg n$ ;
  - in genomics, for example (typically)  $n = O(10^2, 10^3)$ ,  $p = O(10^5, 10^6)$ ;
  - hence  $\text{rank}(X) = \min(n, p) = n$ .
- ☐ Even tall  $X$  may be 'almost singular', making  $\beta$  'almost inestimable'.
- ☐ Solutions:
  - subset selection (drop certain columns of  $X$ );
  - seek different good explanations of response variation, not single model;
  - regularisation (often with prediction in mind).
- ☐ Certain regularisation methods (e.g., lasso) also perform subset selection.

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**Different good explanations**

- ☐ With  $p > n$ , perhaps  $p \gg n$ ,  $X$  is rank-deficient and many  $\beta$  may give  $X\beta = y$ .
- ☐ To find important variables we include intrinsic variables (gender, ...) in all models, and then
  - choose some  $k$  (preferably  $\leq 15$ ) such that  $k < n$  and suppose that  $p < k^a$  (let  $a = 3$  for easy visualisation);
  - assign each variable to a cell of a hyper-cube with coordinates  $\{1, \dots, k\}^a$ ;
  - fit a linear model containing each set of  $k$  variables corresponding to the  $ak^{a-1}$  rows, columns, ... of the cube, so each variable appears in  $a$  distinct models;
  - for each such model, retain the two variables that are most significant.
- ☐ Iterate the above procedure, retaining only the most significant variables at each stage, aiming for a final set of 10–20 variables, for which a careful analysis is performed, perhaps leading to several different good explanations of the response variation.
- ☐ Some cells of the hyper-cube may be empty, and important variables might be assigned to several cells.
- ☐ The above design is a form of **balanced incomplete block design (BIBD)** (with  $k^a$  treatments and  $ak^{a-1}$  blocks).
- ☐ See Cox and Battey (2017, PNAS)

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## Why regularise?

- ☐ Columns of  $X$  **collinear** if there exists a non-zero vector  $v_{p \times 1}$  such that  $Xv = 0$ , i.e.,  $\text{rank}(X) < p$ .
- ☐ Then  $X^T X$  has no unique inverse, and  $\hat{\beta}$  is not unique.
- ☐ Similar problems if  $Xv \doteq 0$ : consider distribution of the (squared) distance of  $\hat{\beta}$  from its target  $\beta$ , i.e.,

$$Q = \|\hat{\beta} - \beta\|^2 = (\hat{\beta} - \beta)^T (\hat{\beta} - \beta),$$

and find (in normal model) that

$$E(Q) = \sigma^2 \sum_{r=1}^p d_r^{-2}, \quad \text{var}(Q) = 2\sigma^4 \sum_{r=1}^p d_r^{-4},$$

where the  $d_r$  are the singular values of  $X = UDV^T$ .

- ☐ Collinearity often measured using **condition number**  $(d_p/d_1)^{1/2}$ , but its statistical meaning is unclear.
- ☐ Simplest way to remove collinearity: drop columns from  $X$ . But which?

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## Note on collinearity

- ☐ When  $p < n$  and  $m = p$  we have  $y \sim (X\beta, \sigma^2 I_n) \sim (UD\gamma, \sigma^2 I_n)$ , where  $\gamma = V^T \beta$ , and as  $\gamma$  is just an orthogonal transformation of  $\beta$  and (in this case)  $\hat{\gamma} = V^T \hat{\beta}$ , we have

$$(\hat{\beta} - \beta)^T (\hat{\beta} - \beta) = (\hat{\gamma} - \gamma)^T (\hat{\gamma} - \gamma).$$

- ☐ Having  $y \sim (UD\gamma, \sigma^2 I_n)$  implies that

$$\hat{\gamma} = \{(UD)^T UD\}^{-1} (UD)^T y = (D^T D)^{-1} D^T U^T y = \text{diag}(d_1^{-1}, \dots, d_p^{-1}, 0, \dots, 0) U^T y,$$

so

$$\text{var}(\hat{\gamma}) = \sigma^2 \text{diag}(d_1^{-2}, \dots, d_p^{-2}).$$

Thus if  $d_p \approx 0$ , there is at least one direction in which  $\gamma$ , i.e.,  $v^T \beta$  for some  $v_{p \times 1}$ , is extremely poorly determined.

- ☐ Under the normal model the  $\hat{\gamma}_r$  are independent  $\mathcal{N}(\gamma_r, \sigma^2/d_r^2)$ , so  $\hat{\gamma}_r - \gamma_r \stackrel{D}{=} \sigma Z_r/d_r$ , where  $Z_1, \dots, Z_p \stackrel{\text{iid}}{\sim} \mathcal{N}(0, 1)$ , giving

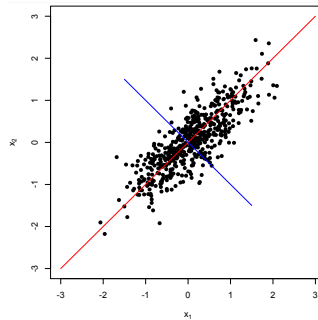
$$Q = (\hat{\gamma} - \gamma)^T (\hat{\gamma} - \gamma) \stackrel{D}{=} \sum_{r=1}^p \sigma^2 Z_r^2 / d_r^2,$$

and as  $E(Z_r^2) = 1$  and  $\text{var}(Z_r^2) = 2$  we get the desired results.

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## Principal component regression



- ☐ Assume columns of  $X$  have been centered, then
  - regress  $y$  on  $u_1, \dots, u_{m'}$ , then
  - choose  $m' \leq m$  to trade off model dimension  $m'$  and good fit.
- ☐ Used to reduce variance, to deal with collinearity, for dimension reduction, and regularisation, but generally hard to interpret results in terms of original columns of  $X$ .
- ☐ Assumes that high variation in  $X$  corresponds to high variation in  $y$ : is this true?
- ☐ Alternative:  $\max_{a_1} \text{corr}(y, Xa_1)$ , then  $\max_{a_2} \text{corr}(y, Xa_2)$  subject to  $\|a_r\| = 1$ ,  $a_1^T a_2 = 0$ , etc.

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## Regularisation

- ☐ Subset selection/PC regression take only a subset of (transformed) columns of  $X$ , but discreteness (retain/delete) of process increases variance of predictions.
- ☐ Regularisation via shrinkage aims to make this smoother, as more continuity should decrease the overall variance.
- ☐ Typically we first center both  $y$  and  $X$  so that the intercept is zero, i.e., map

$$y \mapsto (I_n - H)y, \quad X \mapsto (I_n - H)X, \quad \text{with} \quad H = 1_n(1_n^T 1_n)^{-1} 1_n^T,$$

sometimes we also rescale to give the columns of  $X$  unit variance.

- ☐ Then we minimise the sum of squares subject to a penalty on  $\beta$ , taking

$$\hat{\beta}_\lambda = \underset{\beta}{\text{argmin}} \quad \|y - X\beta\|_2^2 + \lambda p(\beta), \quad \lambda > 0,$$

where among many possibilities,

- $p(\beta) = \|\beta\|_2^2 = \sum_{r=1}^p \beta_r^2$  gives **ridge regression** (aka Tikhonov regularisation);
- $p(\beta) = \|\beta\|_1 = \sum_{r=1}^p |\beta_r|$  gives the **lasso** (aka  $L_1$  regularisation);
- $p(\beta) = (1 - \alpha)\|\beta\|_2^2 + \alpha\|\beta\|_1$  for  $0 \leq \alpha \leq 1$  gives the **elastic net**;
- $p(\beta) = \sum_{g=1}^G p_g^{1/2} \|\beta_g\|_2$ , with  $\beta_g$  being  $p_g \times 1$  sub-vectors of  $\beta$ , gives the **grouped lasso**, which penalises factors with parameters  $\beta_g$ .

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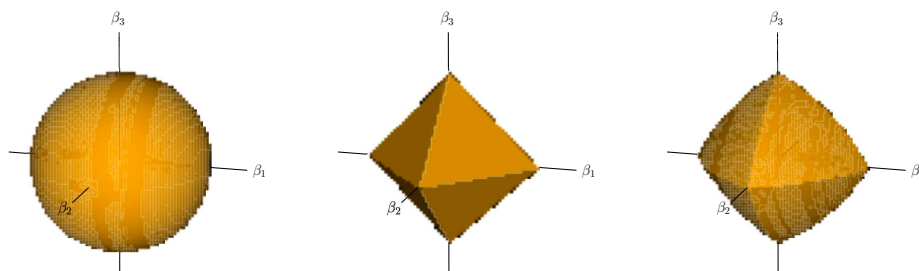
## Bound form

- Equivalently we can take the **bound form** of the minimisation problem, i.e.,

$$\text{minimise}_{\beta} \quad \|y - X\beta\|_2^2 \quad \text{subject to} \quad p(\beta) \leq t,$$

for some  $t \geq 0$ , where setting  $t = \infty$  just gives the least squares estimates.

- Below: constraint balls for ridge (left), lasso (centre) and elastic-net (right) regularisation. The sharp corners of the last two allow for variable selection as well as shrinkage.



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## Ridge regression

- Writing the criterion in matrix form gives

$$\hat{\beta}_{\lambda} = \operatorname{argmin}_{\beta} \quad (y - X\beta)^T(y - X\beta) + \lambda\beta^T\beta,$$

and using the singular value decomposition  $X = UDV^T$  gives

$$\begin{aligned} \hat{\beta}_{\lambda} &= (X^T X + \lambda I_p)^{-1} X^T y \\ &= V(D^T D + \lambda I_p)^{-1} D^T U^T y \\ &= \sum_{d_j > 0} v_j \times \frac{d_j}{d_j^2 + \lambda} u_j^T y, \end{aligned}$$

i.e., a linear combination of the  $v_j$  with coefficients  $u_j^T y d_j / (d_j^2 + \lambda)$  that are more shrunk towards zero when  $d_j$  is small.

- The fitted value is a linear combination of the principal components of  $X$ ,

$$\hat{y}_{\lambda} = X\hat{\beta}_{\lambda} = H_{\lambda}y = \sum_{d_j > 0} u_j \times \frac{1}{1 + \lambda/d_j^2} u_j^T y,$$

with increasing shrinkage as  $j$  increases and  $\lambda/d_j^2$  increases (sketch).

- Hence the SVD of  $X$  gives the ridge solution for all  $\lambda \geq 0$ .

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## Bias-variance tradeoff

**Lemma 31** Under the second-order assumptions  $y \sim (X\beta, \sigma^2 I_n)$ , with  $n > p$  and  $\text{rank}(X) = p$ ,  $\hat{\beta}_\lambda$  has bias vector and variance matrix

$$-\sum_{r=1}^p v_r \times \frac{1}{1 + d_r^2/\lambda} v_r^T \beta, \quad \sigma^2 \sum_{r=1}^p \frac{d_r^2}{(d_r^2 + \lambda)^2} v_r v_r^T.$$

- As  $\lambda \rightarrow \infty$ , the bias increases to  $-\beta$  and the variance decreases to zero.
- The interpretation of  $\lambda$  is unclear, but by analogy with the usual linear model we define the degrees of freedom to be

$$\text{tr}(H_\lambda) = \text{tr}\{X(X^T X + \lambda I_p)^{-1} X^T\} = \sum_{r=1}^p \frac{d_r^2}{d_r^2 + \lambda},$$

which

- starts at  $p$  provided  $d_p > 0$ , corresponding to a standard least squares fit with  $\lambda = 0$ , and
- is monotone decreasing in  $\lambda$ , and hence gives a more interpretable measure of regularity.

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## Note to Lemma 31

- The objective function for ridge regression is

$$y^T y - 2y^T X\beta + \beta^T (X^T X + \lambda I_p) \beta,$$

and differentiation with respect to  $\beta$  gives first and second derivatives

$$-2yX^T + 2(X^T X + \lambda I_p)\beta, \quad X^T X + \lambda I_p.$$

The second derivative matrix is positive definite for any  $\lambda > 0$ , and setting the first to 0 gives

$$\hat{\beta}_\lambda = (X^T X + \lambda I_p)^{-1} X^T y.$$

- Setting  $X = UDV^T$  gives  $X^T y = VD^T U^T y = \sum_{d_j > 0} v_j d_j u_j^T y$  and

$$(X^T X + \lambda I_p)^{-1} = (VD^T DV^T + \lambda I_p)^{-1} = \{V(D^T D + \lambda I_p)V^T\}^{-1} = VS_\lambda V^T,$$

where  $S_\lambda = \text{diag}(d_1^2 + \lambda, \dots, d_r^2 + \lambda)^{-1}$  exists because all its elements are positive. Hence

$$\hat{\beta}_\lambda = (X^T X + \lambda I_p)^{-1} X^T y = VS_\lambda V^T (VD^T U^T) y = \sum_{d_j > 0} \frac{d_j}{d_j^2 + \lambda} u_j^T y \times v_j.$$

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## Note II to Lemma 31

- Under the second-order assumptions

$$E(\hat{\beta}_\lambda) = VS_\lambda V^T V D^T U^T U D V^T \beta = \sum_{r=1}^p \frac{d_r^2}{d_r^2 + \lambda} v_r^T \beta \times v_r,$$

$$\text{var}(\hat{\beta}_\lambda) = VS_\lambda D^T U^T \text{cov}(y) \{VS_\lambda D^T U^T\}^T = \sigma^2 V \text{diag} \left\{ \frac{d_1^2}{(d_1^2 + \lambda)^2}, \dots, \frac{d_p^2}{(d_p^2 + \lambda)^2} \right\} V^T.$$

The latter is just the given formula for the variance, and the bias is

$$E(\hat{\beta}_\lambda) - \beta = \sum_{r=1}^p \frac{d_r^2}{d_r^2 + \lambda} v_r^T \beta \times v_r - \sum_{r=1}^p v_r v_r^T \beta = - \sum_{r=1}^p \frac{\lambda}{d_r^2 + \lambda} v_r^T \beta \times v_r$$

- Finally,

$$\text{tr}(H_\lambda) = \text{tr}\{(UDV^T)VS_\lambda V^T(UDV^T)^T\} = \text{tr}\{U^T U DS_\lambda D^T\} = \sum_{r=1}^p \frac{d_r^2}{d_r^2 + \lambda},$$

as required.

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## Choice of $\lambda$

- Can aim to choose  $\lambda$  for best prediction at an individual  $x_+$ , minimising

$$\text{MSE}(x_+, \lambda) = E\{(x_+^T \hat{\beta}_\lambda - x_+^T \beta)^2\} = \{x_+^T \text{Bias}(\hat{\beta}_\lambda)\}^2 + x_+^T \text{var}(\hat{\beta}_\lambda) x_+,$$

or the generalisation to a matrix  $X_+$ .

- Usually choose  $\lambda$  to minimise the cross-validation sum of squares

$$\text{CV}(\lambda) = \sum_{j=1}^n (y_j - \hat{y}_{\lambda, -j})^2 = \sum_{j=1}^n \frac{(y_j - \hat{y}_{\lambda, j})^2}{(1 - h_{jj, \lambda})^2}$$

(recall Lemma 14), or the generalized cross-validation sum of squares

$$\text{GCV}(\lambda) = \sum_{j=1}^n \frac{(y_j - \hat{y}_{\lambda, j})^2}{\{1 - \text{tr}(H_\lambda)/n\}^2},$$

where  $\hat{y}_{\lambda, j}$  and  $\hat{y}_{\lambda, -j}$  are the fitted values for  $y_j$  predicted from ridge fits with and without case  $j$ , and  $h_{jj, \lambda}$  is the  $j$ th diagonal element of  $H_\lambda$ .

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### Example: Cement data

```
> cement
  x1 x2 x3 x4    y
1   7 26  6 60  78.5
2   1 29 15 52  74.3
3  11 56  8 20 104.3
4  11 31  8 47  87.6
5   7 52  6 33  95.9
6  11 55  9 22 109.2
7   3 71 17  6 102.7
8   1 31 22 44  72.5
9   2 54 18 22  93.1
10 21 47  4 26 115.9
11  1 40 23 34  83.8
12 11 66  9 12 113.3
13 10 68  8 12 109.4
```

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### Example: Cement data

Parameter	Full model		Reduced model	
	Estimate	Standard error	Estimate	Standard error
$\beta_0$	62.41	70.07	71.64	14.14
$\beta_1$	1.55	0.74	1.45	0.12
$\beta_2$	0.51	0.72	0.42	0.19
$\beta_3$	0.10	0.75		
$\beta_4$	-0.14	0.71	-0.24	0.17

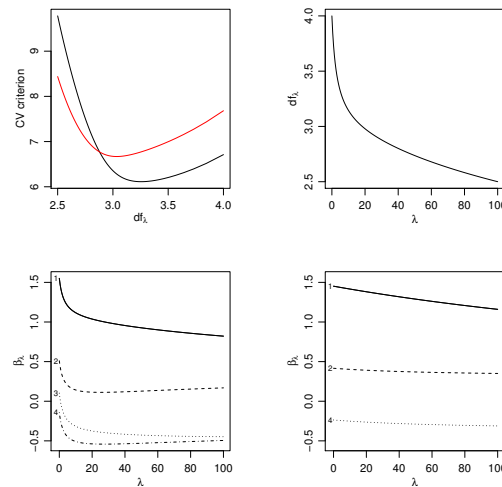
- ☐ The next slide shows results for ridge fits for these models.
- ☐ Looks like 3 df is optimal for prediction.
- ☐ The singular values for the centred  $X$  matrix are 78.8, 28.5, 12.2, 1.7, and those for the centred and scaled  $X$  matrix are 5.18, 4.35, 1.50, 0.14, so it matters which is used.
- ☐ The singular values for the (centred) reduced matrix are 78.8, 19.8 and 9.15.
- ☐ The shrinkage due to increasing  $\lambda$  occurs more slowly for the reduced model

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### Example: Cement data/Ridge analysis

Top left: CV (black) and GCV (red) as functions of degrees of freedom  $df_\lambda$ . Top right: dependence of  $df_\lambda$  on  $\lambda$ . Bottom left:  $\hat{\beta}_\lambda$  as a function of  $\lambda$ , with all four covariates. Bottom right:  $\hat{\beta}_\lambda$  as a function of  $\lambda$ , with  $x_1, x_2$ , and  $x_4$  only.



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### Comments

- ☐ Be careful with software: any pre-processing of  $X$  is not always described.
- ☐ The literature on ridge regression is very large and very dispersed, with many variants and many connections to ML techniques.
- ☐ Bayesian interpretation:  $\hat{\beta}_\lambda$  is the posterior mean/mode for  $\beta$  in the model

$$y | \beta \sim \mathcal{N}_n(\beta_0 1_n + X\beta, \sigma^2 I_n), \quad \beta \sim \mathcal{N}_p(0, \sigma^2 I_p / \lambda), \quad \sigma^2, \lambda > 0,$$

with  $X$  centred, an improper uniform prior on  $\beta_0$  and  $\sigma^2$  and  $\lambda$  fixed. The latter can be estimated/chosen using **empirical Bayes** or **REML** (later).

- ☐ Similar Bayesian interpretation as posterior mode (not mean) for other penalties.
- ☐ In 'ordinary ridge' the penalisation is the same for all elements of  $\beta$  and shrinkage is towards the origin. More generally, we could minimise

$$\|y - \beta_0 1_n - X\beta\|^2 + \lambda(\beta - \beta')^T W(\beta - \beta'),$$

corresponding to shrinkage towards  $\beta'$  according to dispersion matrix  $W$ , equivalent to taking prior

$$\beta \sim \mathcal{N}_p(\beta', \sigma^2 W^{-1} / \lambda), \quad \sigma^2, \lambda > 0,$$

above.

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## Lasso

- **Lasso (least absolute shrinkage and selection operator)** (aka **basis pursuit**) solves

$$\text{minimise}_{\beta} \quad \|y - X\beta\|_2^2 \quad \text{such that} \quad \|\beta\|_1 \leq t,$$

or equivalently finds

$$\tilde{\beta}_{\lambda} = \operatorname{argmin}_{\beta} \quad (y - X\beta)^T(y - X\beta) + \lambda\|\beta\|_1, \quad \lambda > 0.$$

- If  $t > t_0 = \|\hat{\beta}\|_1$  then  $\lambda = 0$  and  $\tilde{\beta}_{\lambda} = \hat{\beta}$ , whereas if  $t \approx t_0/2$  then the estimates are shrunk by a factor around 0.5 on average, with

$$\lim_{\lambda \rightarrow \infty} \tilde{\beta}_{\lambda} = 0, \quad \lim_{\lambda \rightarrow 0} \tilde{\beta}_{\lambda} = (X^T X)^{-1} X^T y = \hat{\beta}$$

- Orthogonal design matrix  $X^T X = I_p$  gives **soft thresholding** function

$$\tilde{\beta}_{\lambda,r} = g_{\lambda}(\hat{\beta}_r) = \begin{cases} 0, & |\hat{\beta}_r| < \lambda, \\ \operatorname{sign}(\hat{\beta}_r)(|\hat{\beta}_r| - \lambda), & \text{otherwise,} \end{cases} \quad r = 1, \dots, p,$$

and this happens in general: if the constraints bite, then some of the  $\tilde{\beta}_{\lambda,r}$  are zero.

### Note on soft thresholding

- We have  $X^T X = I_p$  and hence  $\hat{\beta} = X^T y$ . The Lagrangian

$$L = \frac{1}{2}(y^T y - 2y^T X\beta + \beta^T \beta) + \lambda \left( \sum_{r=1}^p |\beta_r| - t \right)$$

is a sum of two convex functions and therefore is convex in  $\beta$ . Apart from constants, we can write

$$2L \equiv \sum_{r=1}^p (\beta_r^2 - 2\hat{\beta}_r \beta_r + 2\lambda |\beta_r|) - 2p\lambda t,$$

which is differentiable except at  $\beta_r = 0$ . This is a sum of  $p$  separate functions which can be minimised individually, and in which we replace  $\beta_r$  by the scalar  $\beta$ .

- In each case, either the minimum is at  $\beta = 0$  or elsewhere. Differentiation gives

$$\partial L / \partial \beta = \beta - \hat{\beta} + \lambda \text{sign}(\beta),$$

and

$$\lim_{\beta \rightarrow 0_+} \partial L / \partial \beta = \lambda - \hat{\beta}, \quad \lim_{\beta \rightarrow 0_-} \partial L / \partial \beta = -\lambda - \hat{\beta}.$$

For a minimum at  $\beta = 0$  we must have  $\lambda - \hat{\beta} > 0$  and  $-\lambda - \hat{\beta} < 0$ , or equivalently  $|\hat{\beta}| < \lambda$ . Elsewhere  $\partial L / \partial \beta = 0$  gives

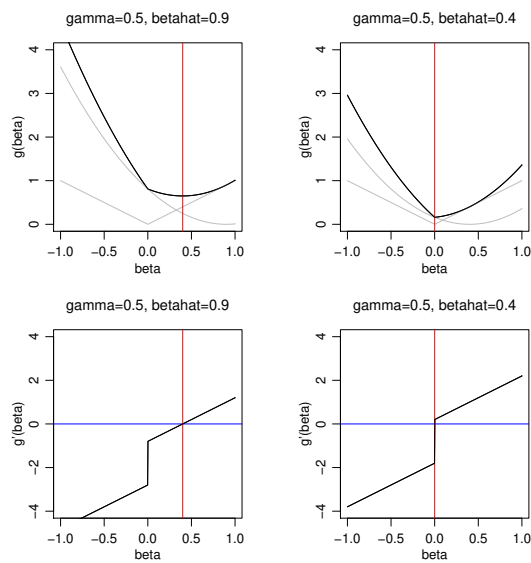
$$\tilde{\beta} = \hat{\beta} - \lambda \text{sign}(\tilde{\beta}),$$

so if  $\tilde{\beta} > 0$ , then  $\tilde{\beta} = \hat{\beta} - \lambda$ , whereas if  $\tilde{\beta} < 0$ , then  $\tilde{\beta} = \hat{\beta} + \lambda$ . This leads to the function  $g_\lambda(\cdot)$  given on the slide.

- The top graphs on slide 196 show grey lines corresponding to  $|\beta|$  and  $(\beta - \hat{\beta})^2$ ; the black line is their sum. In both cases  $\lambda = 0.5$ . In the left panel with  $\hat{\beta} = 0.9$  the minimum is at  $\beta = 0.4$ , and on the right panel with  $\hat{\beta} = 0.4$  the minimum is at  $\beta = 0$ .

The lower panels show the corresponding derivatives (black) and the value of  $\beta$  (red) at which they equal zero (shown by the blue horizontal line). If  $\hat{\beta}$  is sufficiently far from zero, then the intersection will not be at zero, but otherwise it is.

## Soft thresholding

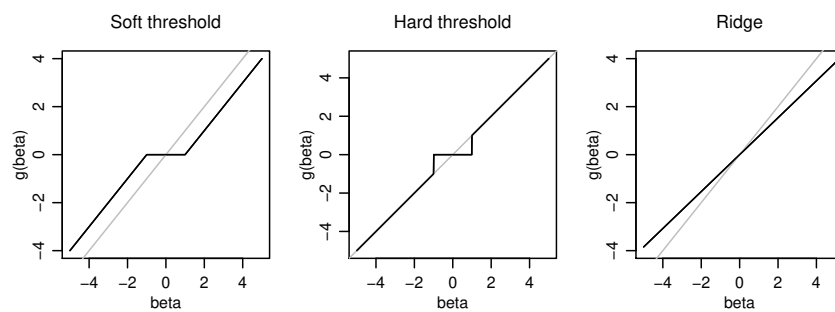


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## Threshold functions

- Soft threshold of lasso (left), hard threshold of subset selection (middle), no threshold of ridge (right).



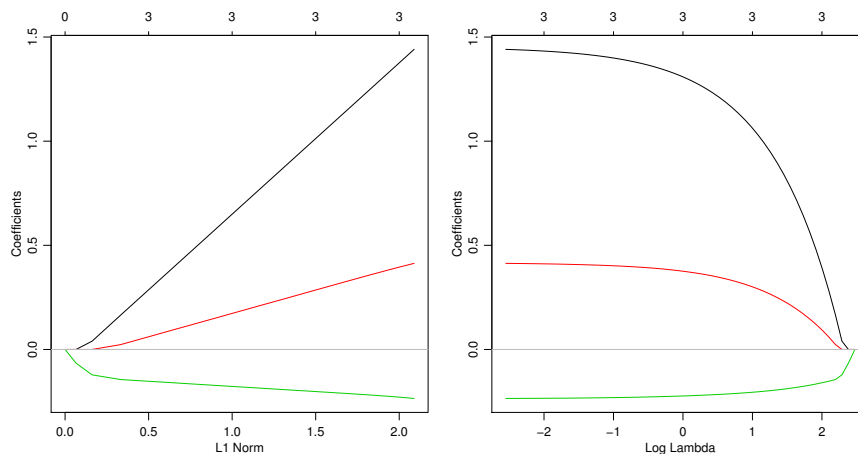
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## Example: cement data

- Estimated coefficients for lasso fit against  $L_1$  norm and  $\lambda$ :



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## Comments

- **Least angle regression (LAR)** is similar to the lasso, and the LAR algorithm can compute the lasso solution path for all  $\lambda$  in  $O(n)$  operations (as with ridge).
- For any regression model we can define the **degrees of freedom** as

$$\sigma^{-2} \sum_{j=1}^n \text{cov}(y_j, \hat{y}_j) = \text{tr}\{\text{cov}(y, \hat{y})\} / \sigma^2;$$

this reduces to previous definitions but can be computed in more situations.

- **Theory**: one can ask about the properties of  $\tilde{\beta}_\lambda$  in suitable settings (e.g.,  $n, p \rightarrow \infty$  with  $p/n \rightarrow c > 0$ ). Then under certain conditions one can show that the selection of variables is consistent (i.e., the probability that the variables with  $\beta_r \neq 0$  are selected tends to 1), but that the  $\tilde{\beta}_\lambda$  are inconsistent (because soft thresholding implies that  $|\tilde{\beta}_{\lambda,r}|$  is systematically smaller than  $|\beta_r|$ ).
- Many (many!) variants and related procedures exist to overcome such problems.
- **Computation**: lasso and elastic net penalisations available in R package `glmnet` and extend to generalized linear models and more general regressions (later).

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**Background and motivation**

- All the models so far have involved just one level of randomness, corresponding to ‘measurement error’ on individual responses.
- Complex layering of randomness can arise in applications, and then conclusions may depend on how it is dealt with.
- Two conceptually different set-ups (which may give the same models):
  - observational/experimental setup generates several layers of randomness;
  - we find it useful to treat the parameters of some model as drawn from a distribution.
 The first concerns logical properties of the data, whereas the second is a modelling assumption.

**Example: Blood pressure**

- Blood pressure data:  $P = 25$  patients each made  $V = 16$  visits to a clinic, and on each occasion their systolic and diastolic blood pressures were measured twice.
- Consider just the diastolic pressure. We expect there to be variation
  - between patients,
  - between visits within patients, and
  - between measurements within visits,
 which we could model as

$$y_{pvm} = \mu + b_p + e_{pv} + \varepsilon_{pvm}, \quad p = 1, \dots, P, v = 1, \dots, V, m = 1, \dots, M,$$

where

- $\mu$  is the population mean diastolic blood pressure (DBP),
- $b_p$  is the difference between the patient and population mean DBP,
- $e_{pv}$  is the difference between this and the mean DBP on the  $v$ th visit, and
- $\varepsilon_{pvm}$  is the difference between the mean DBP for the  $p$ th patient at the  $v$ th visit and the  $m$ th measurement on that visit,

and

$$b_p \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma_b^2) \perp\!\!\!\perp e_{pv} \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma_e^2) \perp\!\!\!\perp \varepsilon_{pvm} \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2).$$

### Example: Blood pressure

```

patno patient visno dbp1 dbp2 sbp1 sbp2
1307      1      7   95   85  150  130
1307      1      8   85   85  140  140
1307      1      9   90   90  150  150
1307      1     10   80   80  135  135
1307      1     11   80   80  130  125
1307      1     12   85   85  150  155
.
.
1307      1     19   80   80  130  130
1307      1     20   80   80  140  140
1307      1     21   90   85  145  140
1307      1     22   75   75  130  130
1418      2      7  104  106  160  148
1418      2      8   98  104  158  162
.
.
9202     25     21   91   90  142  139
9202     25     22   80   78  162  160

```

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### Fixed and random effects

	Chimpanzee	Word									
		1	2	3	4	5	6	7	8	9	10
	1	178	60	177	36	225	345	40	2	287	14
	2	78	14	80	15	10	115	10	12	129	80
	3	99	18	20	25	15	54	25	10	476	55
	4	297	20	195	18	24	420	40	15	372	190

- ☐ Times (min) for four chimpanzees to learn each of ten words.
- ☐ A possible model for log time is

$$y_{cw} \mid \alpha_c, \beta_w \stackrel{\text{ind}}{\sim} \mathcal{N}(\mu + \alpha_c + \beta_w, \sigma^2), \quad c = 1, \dots, C = 4, w = 1, \dots, W = 10.$$

- ☐ The  $\alpha_c$  and/or the  $\beta_w$  would be considered as constant **fixed effects** if we were interested in the relative linguistic abilities of these particular chimps and/or if we planned further tests with these particular words.
- ☐ Either (or both) of the  $\alpha_c$  and  $\beta_w$  might be considered to be **random effects** if they were thought to be sampled from a larger population whose variation is of interest.

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## Two distinctions

- We distinguish **fixed** and **random** effects (above).
- We distinguish **nested** and **crossed** effects:
  - in the blood pressure data, replicate measurements at each visit are **nested** within visit, because there is no logical connection between  $y_{p,v_1,1}$  and  $y_{p,v_2,1}$  (we could permute the final index  $m$  within each patient/visit combination without changing the data structure). Likewise if we ignore any possible time effects between visits, we could consider that visits are nested within patients;
  - in the chimp data, the effects are **crossed**, because permuting chimps or words would entail permuting entire rows or columns of the data table: there is a logical connection between  $y_{c_1w}$  and  $y_{c_2w}$ , and between  $y_{cw_1}$  and  $y_{cw_2}$ ;
- In R syntax, with patient and visit number declared as factors, for nested effects we write

`y ~ patient/visno`

read as ‘separate effects for visit number within the levels of patient’ and for crossed effects with chimp and word declared as factors we write

`y ~ chimp + word`

## Nested model ANOVA

- For the nested model

$$y_{pvm} = \mu + b_p + e_{pv} + \varepsilon_{pvm}, \quad p = 1, \dots, P, v = 1, \dots, V, m = 1, \dots, M,$$

and using the notation we met in the exercises, we write

$$y_{pvm} - \bar{y}_{...} = y_{pvm} - \bar{y}_{pv.} + \bar{y}_{pv.} - \bar{y}_{p..} + \bar{y}_{p..} - \bar{y}_{...},$$

and note that

$$\begin{aligned} y_{pvm} - \bar{y}_{pv.} &= \varepsilon_{pvm} - \bar{\varepsilon}_{pv.}, \\ \bar{y}_{pv.} - \bar{y}_{p..} &= e_{pv} + \bar{\varepsilon}_{pv.} - (\bar{e}_{p.} + \bar{\varepsilon}_{p..}), \\ \bar{y}_{p..} - \bar{y}_{...} &= b_p + \bar{e}_{p.} + \bar{\varepsilon}_{p..} - (\bar{b}_{.} + \bar{e}_{..} + \bar{\varepsilon}_{...}), \end{aligned}$$

so the overall sum of squares is

$$\begin{aligned} \sum_{p,v,m} (y_{pvm} - \bar{y}_{...})^2 &= \sum_{p,v,m} (y_{pvm} - \bar{y}_{pv.})^2 + \sum_{p,v,m} (\bar{y}_{pv.} - \bar{y}_{p..})^2 + \sum_{p,v,m} (\bar{y}_{p..} - \bar{y}_{...})^2 \\ &= \sum_{p,v,m} (y_{pvm} - \bar{y}_{pv.})^2 + M \sum_{p,v} (\bar{y}_{pv.} - \bar{y}_{p..})^2 + VM \sum_p (\bar{y}_{p..} - \bar{y}_{...})^2, \end{aligned}$$

where these terms are independent sums of squares for variables that are

$$\mathcal{N}(0, \sigma^2), \quad \mathcal{N}(0, \sigma_e^2 + \sigma^2/M), \quad \mathcal{N}\{0, \sigma_b^2 + \sigma_e^2/V + \sigma^2/(VM)\}.$$

## Nested model ANOVA II

□ Hence

$$\sum_{p,v,m} (y_{pvm} - \bar{y}_{pv.})^2 \sim \sigma^2 \chi_{PV(M-1)}^2,$$

$$\sum_{p,v,m} (\bar{y}_{pv.} - \bar{y}_{p..})^2 \sim M(\sigma_e^2 + \sigma^2/M) \chi_{P(V-1)}^2 \stackrel{D}{=} (M\sigma_e^2 + \sigma^2) \chi_{P(V-1)}^2,$$

$$\sum_{p,v,m} (\bar{y}_{p..} - \bar{y}_{...})^2 \sim VM \left( \sigma_b^2 + \frac{\sigma_e^2}{V} + \frac{\sigma^2}{VM} \right) \chi_{P-1}^2 \stackrel{D}{=} (VM\sigma_b^2 + M\sigma_e^2 + \sigma^2) \chi_{P-1}^2,$$

so we can estimate the components of variance  $\sigma^2$ ,  $\sigma_e^2$  and  $\sigma_b^2$  from the ANOVA table.

□ The interpretation of the ANOVA depends on whether we regard  $\delta_b^2 = \sum_p (b_p - \bar{b}.)^2$  and  $\delta_e^2 = \sum_{p,v} (e_{pv} - \bar{e}_{p.})^2$  as random or fixed:

Term	df	Sum of squares	E(Mean square) when terms below random		
			$\varepsilon$	$\varepsilon, e$	$\varepsilon, e, b$
Between patients	$P - 1$	$\sum (\bar{y}_{p..} - \bar{y}_{...})^2$	$VM\delta_b^2 + M\delta_e^2 + \sigma^2$	$VM\delta_b^2 + M\sigma_e^2 + \sigma^2$	$VM\sigma_b^2 + M\sigma_e^2 + \sigma^2$
Between visits within patients	$P(V - 1)$	$\sum (\bar{y}_{pv.} - \bar{y}_{p..})^2$	$M\delta_e^2 + \sigma^2$	$M\sigma_e^2 + \sigma^2$	$M\sigma_e^2 + \sigma^2$
Between measures within visits	$PV(M - 1)$	$\sum (y_{pvm} - \bar{y}_{pv.})^2$	$\sigma^2$	$\sigma^2$	$\sigma^2$

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## Nested and crossed ANOVA

□ Nested analysis of the blood pressure data:

```
summary( aov(dbp ~ patient/visno, data=blood.dia) )
              Df Sum Sq Mean Sq F value Pr(>F)
patient      24  23059    960.8   124.29 <2e-16 ***
patient:visno 375  39082    104.2    13.48 <2e-16 ***
Residuals    400   3092     7.7
```

□ Likewise, crossed analysis of the chimpanzee data:

```
summary( aov(log(y)~chimp+word,data=chimps) )
              Df Sum Sq Mean Sq F value Pr(>F)
chimp         3    5.33    1.778    2.719  0.0642 .
word         9   45.69    5.077    7.765 1.5e-05 ***
Residuals    27   17.65    0.654
```

There are  $C - 1$  degrees of freedom for chimps,  $W - 1$  for words, and  $(C - 1)(W - 1)$  for the residual.

□ In both cases, we can use the ANOVA table to estimate the variance components and then perform **synthesis of variance**: e.g., how large would  $W$  need to be to distinguish the learning abilities of two chimps with probability 0.95?

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### Example: Blood pressure

- Solving the equations

$$\sigma^2 = 7.7, \quad M\sigma_e^2 + \sigma^2 = 104.2, \quad VM\sigma_b^2 + M\sigma_e^2 + \sigma^2 = 960.8,$$

gives (in units of millimeters of mercury, mmHg)

$$\hat{\sigma} = 2.8, \quad \hat{\sigma}_e = 6.9, \quad \hat{\sigma}_b = 5.2,$$

so the largest variation is between different visits within patients, while that between measurements on a single visit is smallest.

- Different comparisons require appropriate baseline variances:

- if we are interested in how patient  $p$ 's response varies from visit to visit, we use

$$\bar{y}_{pv_1\cdot} - \bar{y}_{pv_2\cdot} = \mu + b_p + e_{pv_1} + \bar{\varepsilon}_{pv_1\cdot} - (\mu + b_p + e_{pv_2} + \bar{\varepsilon}_{pv_2\cdot}) \sim \mathcal{N}(0, 2\sigma_e^2 + 2\sigma^2/M),$$

as a basis for a test of a significant difference, whereas to compare average blood pressures for two different patients we use

$$\bar{y}_{p_1\cdot\cdot} - \bar{y}_{p_2\cdot\cdot} = b_{p_1} + \bar{e}_{p_1\cdot} + \bar{\varepsilon}_{p_1\cdot\cdot} - (b_{p_2} + \bar{e}_{p_2\cdot} + \bar{\varepsilon}_{p_2\cdot\cdot}) \sim \mathcal{N}\{0, 2\sigma_b^2 + 2\sigma_e^2/V + 2\sigma^2/(VM)\}.$$

- **Split-unit designs** are set up to make the most important comparisons within units (here patients) and less important ones between units, and the ANOVA reflects this.

### General form

- We could have written the nested model above as

$$y = 1_n\mu + X_b b + X_e e + \varepsilon,$$

with design matrices  $X_b$  and  $X_e$  for the patient and visit-within-patient effects.

- Then if

- $b$  and  $e$  are treated as fixed (ordinary parameters),

$$y \sim \mathcal{N}_n(1_n\mu + X_b b + X_e e, \sigma^2 I_n),$$

- $b$  is treated as fixed but  $e \sim \mathcal{N}_{PV}(0, \sigma_e^2 I_{PV})$ , then

$$y \sim \mathcal{N}_n(1_n\mu + X_b b, \sigma_e^2 X_e X_e^T + \sigma^2 I_n),$$

- and if  $b \sim \mathcal{N}_P(0, \sigma_b^2 I_P)$  independent of  $e \sim \mathcal{N}_{PV}(0, \sigma_e^2 I_{PV})$ , then

$$y \sim \mathcal{N}_n(1_n\mu, \sigma_b^2 X_b X_b^T + \sigma_e^2 X_e X_e^T + \sigma^2 I_n).$$

- Hence random  $e$  or  $b$  give patterned covariance matrices depending on their variances.

## Summary

- Components of variance ANOVA is easily performed directly for balanced data.
- Standard ANOVA tables have different interpretations, depending on which components of variance are taken to be random or fixed.
- Extensions are needed to deal with more complex settings, with unbalanced data, or with non-linear or non-normal errors — hence **mixed models**, i.e., models with both random and fixed parts, arising in many different settings (and with different names):
  - components of variance (as above),
  - classical experimental design (split-plot designs, ...),
  - repeated measures,
  - longitudinal models,
  - multi-level models,
  - hierarchical models.
- Can subsume linear versions into the **linear mixed model**, which can be extended to nonlinear models, GLMs, ...

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## Linear mixed model

- The **linear mixed model** may be written as

$$y_{n \times 1} = X_{n \times p} \beta_{p \times 1} + Z_{n \times q} b_{q \times 1} + \varepsilon_{n \times 1}, \quad b \sim N_q(0, \Omega_b), \quad \varepsilon \sim N_n(0, \Omega),$$

where

- $\beta$  represents the **fixed effects**,
  - $b$  represents the **random effects**, and
  - usually  $\Omega = \sigma^2 I_n$ .
- Equivalently,

$$y \mid b \sim N_n(X\beta + Zb, \Omega), \quad b \sim N_q(0, \Omega_b),$$

which gives marginal response distribution

$$y \sim N_n(X\beta, Z\Omega_b Z^T + \Omega), \quad Z\Omega_b Z^T + \Omega = \sigma^2 \Delta^{-1}(\psi),$$

say, with  $\psi$  the vector of distinct variance ratios appearing in  $\Delta^{-1}$  (e.g.,  $\sigma_b^2/\sigma^2, \dots$ ).

- Although  $\Omega$  is often diagonal,  $Z\Omega_b Z^T$  is not, so inverting  $Z\Omega_b Z^T + \Omega$  involves  $O(n^3)$  flops in general, and we should try and avoid working with  $\Delta$ .

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### Maximum likelihood estimation

- Let  $\tilde{b}$  denote the MLE of  $b$  for fixed  $\beta$  (and  $\psi$ ). Then

$$\begin{aligned} f(y; \beta, \sigma^2, \psi) &= \int f(y | b; \beta, \sigma^2, \psi) f(b; \sigma^2, \psi) db \\ &= f(y, \tilde{b}; \beta, \sigma^2, \psi) \times \frac{(2\pi)^{q/2}}{|Z^T \Omega^{-1} Z + \Omega_b^{-1}|^{1/2}} \\ &\propto \frac{f(y | \tilde{b}; \beta, \sigma^2, \psi) f(\tilde{b} | \sigma^2, \psi)}{|Z^T \Omega^{-1} Z + \Omega_b^{-1}|^{1/2}}, \end{aligned}$$

so (apart from additive constants)  $-2 \log f(y; \beta, \sigma^2, \psi)$  equals

$$(y - X\beta - Z\tilde{b})^T \Omega^{-1} (y - X\beta - Z\tilde{b}) + \tilde{b}^T \Omega_b^{-1} \tilde{b} + \log\{|\Omega| |\Omega_b| |Z^T \Omega^{-1} Z + \Omega_b^{-1}|\}.$$

- The first two (quadratic) terms here depend on  $\beta$  and  $b$ , so given  $\psi$  and  $\sigma^2$  we can find  $\hat{\beta}_\psi$  and  $\tilde{b}(\hat{\beta}_\psi)$  explicitly, and thus obtain  $\ell_p(\psi)$ .
- By noting that

$$f(b | y; \beta, \sigma^2, \psi) = f(y | b; \beta, \sigma^2, \psi) f(b; \sigma^2, \psi) / f(y; \beta, \sigma^2, \psi)$$

and taking logs, we obtain

$$b | y \sim \mathcal{N}_q \left\{ \tilde{b}, (Z^T \Omega^{-1} Z + \Omega_b^{-1})^{-1} \right\}, \quad \tilde{b} = (Z^T \Omega^{-1} Z + \Omega_b^{-1})^{-1} Z^T \Omega^{-1} (y - X\beta).$$

### Note on maximum likelihood estimation

- Suppressing the parameters  $\beta$ ,  $\sigma^2$  and  $\psi$  for now, we write the log integrand in

$$f(y) = \int f(y, b) db = \int f(y | b) f(b) db$$

in the form

$$\log f(y, b) = \log f(y, \tilde{b}) - \frac{1}{2} (b - \tilde{b})^T H(\tilde{b}) (b - \tilde{b}),$$

where the linear term of the Taylor series equals zero, because it is evaluated at the maximising value  $\tilde{b}$ , and the given Taylor series is exact because the log likelihood is quadratic.

- On ignoring terms not involving  $b$  we have

$$-2 \log f(y, b) = -2 \log f(y | b) - 2 \log f(b) \equiv (y - X\beta - Zb)^T \Omega^{-1} (y - X\beta - Zb) + b^T \Omega_b^{-1} b,$$

so

$$H(b) \equiv H = Z^T \Omega^{-1} Z + \Omega_b^{-1}$$

does not depend on  $b$ , and thus

$$\begin{aligned} f(y) &= f(y, \tilde{b}) \int \exp \left\{ -\frac{1}{2} (b - \tilde{b})^T H (b - \tilde{b}) \right\} db \\ &= f(y, \tilde{b}) \times (2\pi)^{q/2} |H|^{-1/2} = f(y, \tilde{b}) \times \frac{(2\pi)^{q/2}}{|Z^T \Omega^{-1} Z + \Omega_b^{-1}|^{1/2}}, \end{aligned}$$

as announced; the integral equals the normalising constant for a  $\mathcal{N}_q(\tilde{b}, H^{-1})$  density.



### Reminder: Matrix inversion formulae

- Assume that any inverses needed below exist.
- The (Sherman–Morrison)–Woodbury formula

$$(A + BCD)^{-1} = A^{-1} - A^{-1}B(C^{-1} + DA^{-1}B)^{-1}DA^{-1}$$

is easily checked by multiplying the formula above by  $A + BCD$ .

- For the partitioned matrix  $A$  and its correspondingly partitioned inverse,

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}, \quad A^{-1} = \begin{pmatrix} A^{11} & A^{12} \\ A^{21} & A^{22} \end{pmatrix},$$

we have

$$\begin{aligned} A^{11} &= (A_{11} - A_{12}A_{22}^{-1}A_{21})^{-1}, & A^{12} &= -A_{11}^{-1}A_{12}A^{22}, \\ A^{21} &= -A_{22}^{-1}A_{21}A^{11}, & A^{22} &= (A_{22} - A_{21}A_{11}^{-1}A_{12})^{-1}, \end{aligned}$$

as is also easily checked.

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### Inference on $\beta$

- Since

$$y \sim \mathcal{N}_n(X\beta, Z\Omega_b Z^T + \Omega),$$

weighted least squares gives

$$\hat{\beta} = \{X^T(Z\Omega_b Z^T + \Omega)^{-1}X\}^{-1}X^T(Z\Omega_b Z^T + \Omega)^{-1}y,$$

with

$$\hat{\beta} \sim \mathcal{N}_p[\beta, \{X^T(Z\Omega_b Z^T + \Omega)^{-1}X\}^{-1}],$$

where in general we need  $O(n^3)$  flops to invert the  $n \times n$  matrix  $Z\Omega_b Z^T + \Omega$ .

- For cheaper calculation of  $\text{var}(\hat{\beta})$ , we use the inversion formulae and obtain

$$\begin{pmatrix} \text{var}(\hat{\beta})_{p \times p} & \cdot \\ \cdot & \cdot \end{pmatrix} = \begin{pmatrix} X^T\Omega^{-1}X & X^T\Omega^{-1}Z \\ Z^T\Omega^{-1}X & Z^T\Omega^{-1}Z + \Omega_b^{-1} \end{pmatrix}_{(p+q) \times (p+q)}^{-1},$$

which involves only  $O\{n(p+q)^2\}$  flops, as  $\Omega$  is usually diagonal.

- Note that  $\text{var}(b | y) = (Z^T\Omega^{-1}Z + \Omega_b^{-1})^{-1}$  can be obtained as a by-product.
- In practice these formulae would be evaluated at the MLEs  $\hat{\sigma}^2$  and  $\hat{\psi}$  and used to compute confidence intervals etc. for elements of  $\beta$ .

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## Inference on random effects

- **Conventional terminology**: we **estimate** parameters  $\beta$  and **predict** random variables  $b$ .
- To find the best predictor  $\tilde{b}(y)$  of  $b$  we minimise

$$E_{b,y} \left[ \left\{ \tilde{b}(y) - b \right\}^T \left\{ \tilde{b}(y) - b \right\} \right],$$

which gives  $\tilde{b}(y) = E(b | y)$ , with (Woodbury formula):

$$\begin{aligned} E(b | y) &= (Z^T \Omega^{-1} Z + \Omega_b^{-1})^{-1} Z^T \Omega^{-1} (y - X\beta), \\ \text{var}(b | y) &= (Z^T \Omega^{-1} Z + \Omega_b^{-1})^{-1}. \end{aligned}$$

- Replace parameters  $\beta$ ,  $\sigma^2$ ,  $\psi$  by estimates to get **best linear unbiased predictor (BLUP)**  $\tilde{b}$  and its estimated variance.
- Residuals

$$\begin{aligned} y - X\hat{\beta} &= Z\tilde{b} + y - X\hat{\beta} - Z\tilde{b} \\ &= Z\tilde{b} + \left\{ I_n - Z \left( Z^T \hat{\Omega}^{-1} Z + \hat{\Omega}_b^{-1} \right)^{-1} Z^T \hat{\Omega}^{-1} \right\} (y - X\hat{\beta}), \end{aligned}$$

split into two parts, with  $Z\tilde{b}$  attributable to random effects, and the second the usual residual  $y - X\hat{\beta}$  shrunk towards zero; this estimates  $\varepsilon$ .

## Note on conditional mean and variance

- First we write

$$\tilde{b}(y) - b = \tilde{b}(y) - E(b | y) + E(b | y) - b,$$

expand  $\{\tilde{b}(y) - b\}^T \{\tilde{b}(y) - b\}$  and take expectation over  $b$  conditional on  $y$  to get

$$E \left[ \{\tilde{b}(y) - b\}^T \{\tilde{b}(y) - b\} | y \right] = \left\{ \tilde{b}(y) - E(b | y) \right\}^T \left\{ \tilde{b}(y) - E(b | y) \right\} + \text{var}(b | y),$$

which is minimised when  $\tilde{b}(y) = E(b | y)$ . Any other choice will give a larger expectation when we take  $E_y$ , so this is optimal.

- To obtain  $E(b | y)$ , we note that

$$\begin{pmatrix} y \\ b \end{pmatrix} \sim \mathcal{N}_{n+q} \left\{ \begin{pmatrix} X\beta \\ 0 \end{pmatrix}, \begin{pmatrix} \Omega + Z\Omega_b Z^T & Z\Omega_b \\ \Omega_b Z^T & \Omega_b \end{pmatrix} \right\},$$

so using standard formulae for conditional normal distributions, we have

$$\begin{aligned} E(b | y) &= \Omega_b Z^T (\Omega + Z\Omega_b Z^T)^{-1} (y - X\beta), \\ \text{var}(b | y) &= \Omega_b - \Omega_b Z^T (\Omega + Z\Omega_b Z^T)^{-1} Z\Omega_b. \end{aligned}$$

- The Woodbury formula applied to the conditional variance gives

$$\text{var}(b | y) = (Z^T \Omega^{-1} Z + \Omega_b^{-1})^{-1}$$

as required.

- For the conditional mean we apply the Woodbury formula to  $(\Omega + Z\Omega_b Z^T)^{-1}$  and get

$$\begin{aligned} E(b | y) &= \Omega_b Z^T \left\{ \Omega^{-1} - \Omega^{-1} Z (\Omega_b^{-1} + Z^T \Omega^{-1} Z)^{-1} Z^T \Omega^{-1} \right\} (y - X\beta) \\ &= \Omega_b \left\{ I_q - Z^T \Omega^{-1} Z (\Omega_b^{-1} + Z^T \Omega^{-1} Z)^{-1} \right\} Z^T \Omega^{-1} (y - X\beta) \\ &= \Omega_b \left\{ \Omega_b^{-1} (\Omega_b^{-1} + Z^T \Omega^{-1} Z)^{-1} \right\} Z^T \Omega^{-1} (y - X\beta), \end{aligned}$$

as required, where we wrote the term in braces in the second line as

$$I - B(A + B)^{-1} = A(A + B)^{-1}, \text{ with } A = \Omega_b^{-1} \text{ and } B = Z^T \Omega^{-1} Z.$$

## REML

- Problems with the usual MLEs:
  - the MLEs  $\hat{\sigma}^2$  and  $\hat{\psi}$  are downwardly biased (no adjustment for estimation of  $\beta$ );
  - variance ratios  $\psi_r \geq 0$ , so maybe  $\hat{\psi}_r = 0$ , making usual asymptotic properties fail;
  - $n$  can be very large in applications, raising computational issues.
- **Restricted maximum likelihood (REML) estimation** is often used to reduce the bias:
  - a form of **marginal likelihood**, i.e., based on the marginal density of a statistic  $s = s(y)$ ;
  - but can also be derived as a **conditional likelihood**, based on the conditional density of  $y$  given a statistic  $s(y)$ .
- REML maximised using Newton–Raphson or EM algorithms.

**Lemma 32** A restricted log likelihood for  $\sigma^2$  and  $\psi$  is

$$\ell(\hat{\beta}_\psi, \sigma^2, \psi) + \frac{p}{2} \log \sigma^2 - \frac{1}{2} \log |X^T \Delta X|$$

i.e.,

$$\frac{1}{2} \log |\Delta| - \frac{1}{2} \log |X^T \Delta X| - \frac{1}{2\sigma^2} (y - X\hat{\beta}_\psi)^T \Delta (y - X\hat{\beta}_\psi) - \frac{n-p}{2} \log \sigma^2.$$

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## Note to Lemma 32

- Suppose  $f(y; \alpha, \beta)$  depends on two parameters, that interest is focused on  $\alpha$ , and that for fixed  $\alpha$  there is a sufficient statistic  $s_\alpha$  for  $\beta$ . Then

$$f(y; \alpha, \beta) = f(y | s_\alpha; \alpha) f(s_\alpha; \alpha, \beta),$$

and since the first density on the right is a proper conditional density not depending on  $\beta$ , we can base inference for  $\alpha$  on

$$\log f(y | s_\alpha; \alpha) = \log f(y; \alpha, \beta) - \log f(s_\alpha; \alpha, \beta).$$

- In the normal mixed model we take  $\alpha = (\sigma^2, \psi)$ . If all the variance parameters are fixed, then  $s_\alpha = \hat{\beta}_\alpha = (X^T \Delta X)^{-1} X^T \Delta y$  is sufficient for  $\beta$ ; its distribution is  $\mathcal{N}_p\{\beta, \sigma^2 (X^T \Delta X)^{-1}\}$ .

- Apart from constants, the logarithm of the required conditional density is therefore

$$\begin{aligned} \log f(y; \sigma^2, \psi, \beta) - \log f(\hat{\beta}_\psi; \sigma^2, \psi, \beta) &\equiv -\frac{n}{2} \log \sigma^2 + \frac{1}{2} \log |\Delta| - \frac{1}{2\sigma^2} (y - X\beta)^T \Delta (y - X\beta) \\ &\quad + \frac{p}{2} \log \sigma^2 - \frac{1}{2} \log |X^T \Delta X| \\ &\quad + \frac{1}{2\sigma^2} (\hat{\beta}_\psi - \beta)^T X^T \Delta X (\hat{\beta}_\psi - \beta), \end{aligned}$$

which reduces to the given form on writing

$$y - X\beta = (y - X\hat{\beta}_\psi) + X(\hat{\beta}_\psi - \beta)$$

in the first quadratic term and expanding out, noting that the cross-product vanishes because

$$\begin{aligned} (\hat{\beta}_\psi - \beta)^T X^T \Delta (y - X\hat{\beta}_\psi) &= (\hat{\beta}_\psi - \beta)^T X^T \Delta \{y - X(X^T \Delta X)^{-1} X^T \Delta y\} \\ &= (\hat{\beta}_\psi - \beta)^T \{X^T \Delta y - X^T \Delta X (X^T \Delta X)^{-1} X^T \Delta y\} = 0. \end{aligned}$$

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## Example: Rat growth

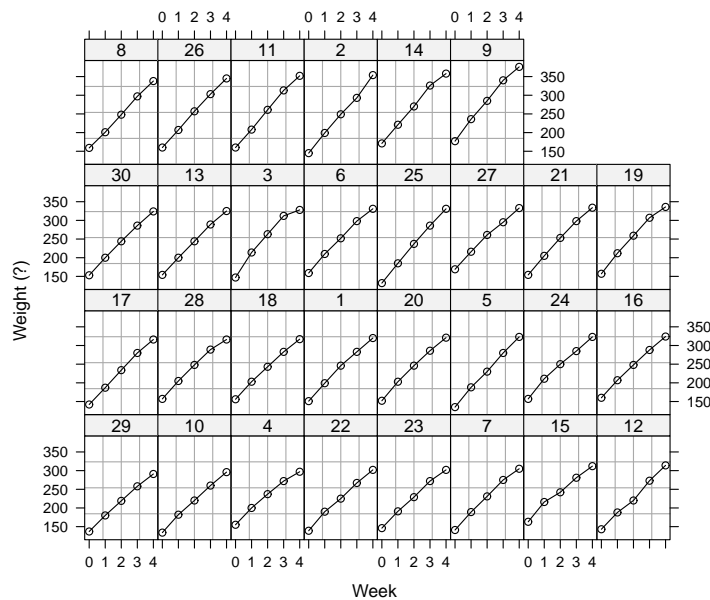
Weights (units unknown) of 30 young rats over a five-week period

	Week					Week				
	1	2	3	4	5	1	2	3	4	5
1	151	199	246	283	320	16	160	207	248	288
2	145	199	249	293	354	17	142	187	234	280
3	147	214	263	312	328	18	156	203	243	283
4	155	200	237	272	297	19	157	212	259	307
5	135	188	230	280	323	20	152	203	246	286
6	159	210	252	298	331	21	154	205	253	298
7	141	189	231	275	305	22	139	190	225	267
8	159	201	248	297	338	23	146	191	229	272
9	177	236	285	340	376	24	157	211	250	285
10	134	182	220	260	296	25	132	185	237	286
11	160	208	261	313	352	26	160	207	257	303
12	143	188	220	273	314	27	169	216	261	295
13	154	200	244	289	325	28	157	205	248	289
14	171	221	270	326	358	29	137	180	219	258
15	163	216	242	281	312	30	153	200	244	286

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## Example: Rat growth



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### Example: Rat growth

#### Example 33 (Rat growth data)

□ Write

$$y_{jt} = \beta_0 + b_{j0} + (\beta_1 + b_{j1})x_{jt} + \varepsilon_{jt}, \quad t = 1, \dots, 5, j = 1, \dots, 30,$$

where the random variables  $(b_{j0}, b_{j1})$  have a joint normal distribution with mean vector zero and unknown variance matrix and the  $\varepsilon_{jt} \stackrel{\text{iid}}{\sim} \mathcal{N}(0, \sigma^2)$ . In matrix terms,

$$\begin{pmatrix} y_{j1} \\ \vdots \\ y_{j5} \end{pmatrix} = \begin{pmatrix} 1 & x_{j1} \\ \vdots & \vdots \\ 1 & x_{j5} \end{pmatrix} \begin{pmatrix} \beta_0 \\ \beta_1 \end{pmatrix} + \begin{pmatrix} 1 & x_{j1} \\ \vdots & \vdots \\ 1 & x_{j5} \end{pmatrix} \begin{pmatrix} b_{j0} \\ b_{j1} \end{pmatrix} + \begin{pmatrix} \varepsilon_{j1} \\ \vdots \\ \varepsilon_{j5} \end{pmatrix}, \quad j = 1, \dots, 30;$$

the overall model with  $n = 150$  is obtained by stacking these expressions.

□ We set  $(x_{j1}, \dots, x_{j5}) = (0, \dots, 4)$ , so that  $\beta_0$  is the mean weight in week 1.

□  $p = 2$  parameters;  $q = 60$  since two random variables per rat.

### Example: Rat growth

```
> rat.growth
  rat week   y
1    1    0 151
2    1    1 199
3    1    2 246
4    1    3 283
5    1    4 320
6    2    0 145
...
> fit.reml <- lme(fixed= y~week, random=~week|rat, data=rat.growth)
> summary(fit.reml)
Linear mixed-effects model fit by REML
Data: rat.growth
      AIC      BIC    logLik
1096.58 1114.563 -542.2899

Random effects:
Formula: ~week | rat
Structure: General positive-definite, Log-Cholesky parametrization
          StdDev   Corr
(Intercept) 10.932986 (Intr)
week          3.534747 0.184
Residual      5.817426

Fixed effects: y ~ week
              Value Std.Error DF  t-value p-value
(Intercept) 156.05333 2.1589786 119 72.28109      0
week         43.26667 0.7275228 119 59.47122      0
Correlation:
      (Intr)
week 0.007
```

## Example: Rat growth

Results from fit of mixed model to rat growth data, using REML. Values in parentheses are for ML fit. In each case  $\hat{\sigma}^2 = 5.82^2$ .

Parameter	Fixed		Random	
	Estimate	Standard error	Variance	Correlation
Intercept	156.05	2.16 (2.13)	10.93 <sup>2</sup> (10.71 <sup>2</sup> )	
Slope	43.27	0.73 (0.72)	3.53 <sup>2</sup> (3.46 <sup>2</sup> )	0.18 (0.19)

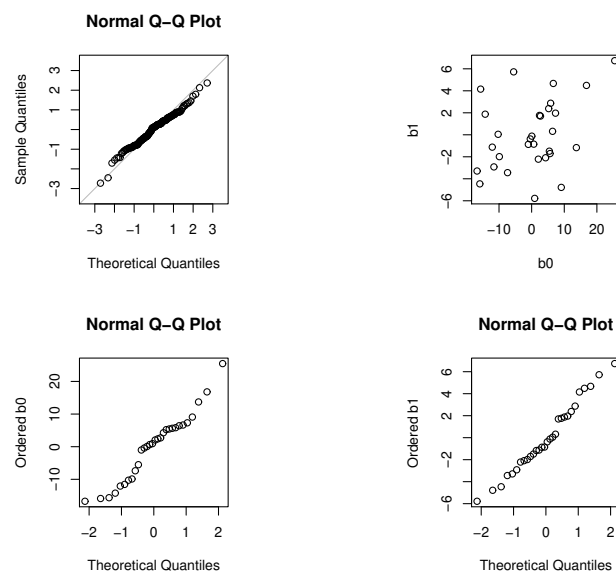
- ☐ REML estimates of  $\Omega_b$  slightly larger than ML estimates, but effect is small since  $p = 2$ .
- ☐ Estimated mean weight in week 1 is 156, but SD of individual rats around this is 11.
- ☐ Correlation between slope and intercept is small but positive: initially heavier rats tend to gain weight faster.
- ☐ Variation around individual slopes is given by  $\hat{\sigma}$ , smaller than for the intercept variance.
- ☐ Shrinkage of intercept estimates, shown on next page, is small in this case.
- ☐ Residuals look acceptably normal.

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## Example: Rat growth

Residuals and random effects



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## Comments

- Testing for non-zero variance components involves tests on the boundary of the parameter space, which have nasty asymptotic properties: if  $\psi = 0$ , then a likelihood ratio statistic for testing  $\psi = 0$  satisfies  $W \sim \frac{1}{2}\chi_0^2 + \frac{1}{2}\chi_1^2$  as  $n \rightarrow \infty$ , meaning that

$$P_0(W = 0) = \frac{1}{2}, \quad P_0(W > w) = \frac{1}{2}P(\chi_1^2 > w), \quad w > 0.$$

Unfortunately,

- $P_0(W = 0)$  can be very different from  $\frac{1}{2}$  even in large samples, and
  - in more complex problems, the limiting distribution can be much more complex.
- Sometimes clearer to write a mixed model in **multi-level model** form

$$y = X\beta + Z_L b_L + \cdots + Z_0 b_0,$$

where the  $q_l \times 1$  vectors  $b_l$  are all mutually independent with means zero and variance matrices  $\Omega_l$ , so  $Y \sim \mathcal{N}_n(X\beta, \sum_{l=0}^L Z_l \Omega_l Z_l^T)$ , where  $Z_0 = I_n$ ,  $b_0 = \varepsilon$  and  $\Omega_0 = \sigma^2 I_n$ .

- The same basic approaches apply in **nonlinear mixed models** and **generalized linear mixed models (GLMMs)**, but integrals appear everywhere and have to be approximated numerically, leading to nastier computations.

**Motivation**

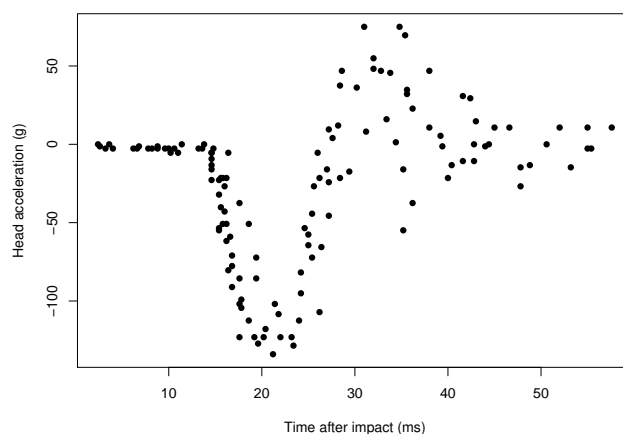
- Normal linear model has two main aspects:
  - **systematic variation**,  $E(y) = \mu$ , and  $\mu = X\beta$  with parameters  $\beta$ ;
  - **stochastic variation**,  $y \sim \mathcal{N}_n(\mu, \sigma^2 I_n)$ .
- Can relax the stochastic assumption using other distributions or second-order assumptions, but still have parametric model for the systematic part.
- Often want to relax systematic part for more flexible models, for
  - exploratory data analysis — ‘will a linear model be adequate?’
  - confirmatory data analysis — ‘I’ve fitted a linear model, is it adequate?’
  - general modelling — ‘the data are too complex/too large to expect a simple parametric model to work, so what can I do?’
  - semiparametric modelling — ‘I will use a parametric model for the effects of interest, but can I model nuisance effects more flexibly?’
- Introduce **‘semi-parametric’** regression models—widely used in applications.

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**Example: Motorcycle data**

Measurements of head acceleration (g) at time after impact (ms) in a simulated motorcycle accident, used to test crash helmets:



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### Example: Spring barley data

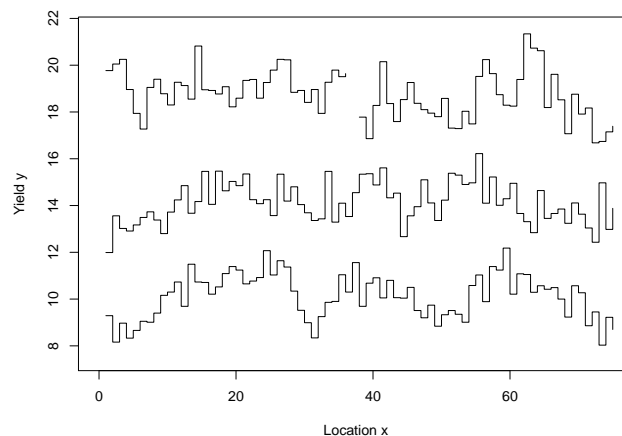
Plot yield at harvest for 75 varieties of spring barley sown in 3 blocks each of 75 plots:

Location $x$	Block 1		Block 2		Block 3	
	Variety	Yield $y$	Variety	Yield $y$	Variety	Yield $y$
1	57	9.29	49	7.99	63	11.77
2	39	8.16	18	9.56	38	12.05
3	3	8.97	8	9.02	14	12.25
4	48	8.33	69	8.91	71	10.96
5	75	8.66	29	9.17	22	9.94
6	21	9.05	59	9.49	46	9.27
7	66	9.01	19	9.73	6	11.05
8	12	9.40	39	9.38	30	11.40
9	30	10.16	67	8.80	16	10.78
10	32	10.30	57	9.72	24	10.30
11	59	10.73	37	10.24	40	11.27
12	50	9.69	26	10.85	64	11.13
13	5	11.49	16	9.67	8	10.55
14	23	10.73	6	10.17	56	12.82
15	14	10.71	47	11.46	32	10.95
16	68	10.21	36	10.05	48	10.92
17	41	10.52	64	11.47	54	10.77
18	1	11.09	63	10.63	37	11.08
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$

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### Example: Spring barley data



Yield as a function of location for the three blocks, with yields for blocks 2 and 3 offset by the addition of 4 and of 7 respectively. Value 37 in block 3 is missing.

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## Comments

- The motorcycle data are pairs  $(x_1, y_1), \dots, (x_n, y_n)$ , with

$$y_j \stackrel{\text{ind}}{\sim} (\mu(x_j), \sigma^2), \quad j = 1, \dots, n,$$

with  $\mu$  unspecified and  $x_1, \dots, x_n \in \mathcal{X}$ , say (ignoring the heteroscedasticity). We might aim to estimate the function  $\mu(\cdot)$  using a **scatterplot smoother**.

- For the spring barley data we could envisage an **additive model**

$$y_{bx} \stackrel{\text{ind}}{\sim} (\beta_{v(b,x)} + \mu_b(x), \sigma^2), \quad b = 1, 2, 3, x = 1, \dots, 75,$$

where

- $\beta_{v(b,x)}$  denotes mean yield for the variety  $v(b, x)$  planted at location  $x$  of block  $b$ , and
- $\mu_b(x)$  represents smooth variation in the mean yield in block  $b$ , as fertility changes with location  $x$ .

In this case we are mostly interested in the variety effects  $\beta_1, \dots, \beta_{75}$ , but need to account for changes in the (nuisance functions)  $\mu_b$ .

- More generally we might have random effects (the  $\beta_v$ ?) and/or non-linear models and/or non-Gaussian responses ...

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## Polynomial regression

- Fit polynomial of degree  $p - 1$ , i.e.,

$$\mu(x_j) = \beta_0 + \beta_1 x_j + \dots + \beta_{p-1} x_j^{p-1},$$

and choose  $\beta_0, \dots, \beta_{p-1}$  to minimise the sum of squares

$$\sum_{j=1}^n \{y_j - \mu(x_j)\}^2 = \sum_{j=1}^n \left\{ y_j - (\beta_0 + \beta_1 x_j + \dots + \beta_{p-1} x_j^{p-1}) \right\}^2,$$

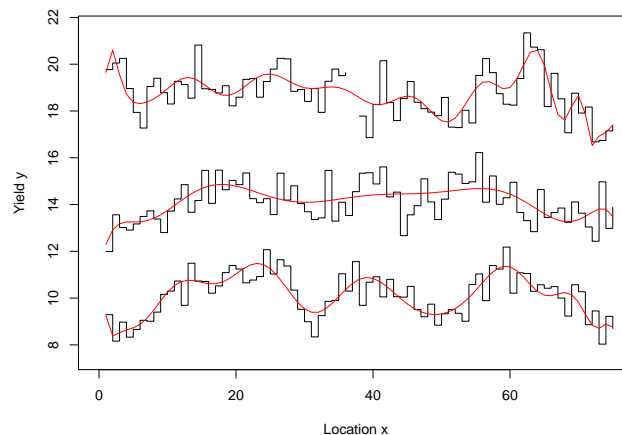
giving  $\hat{\beta}_{p \times 1} = (X^T X)^{-1} X^T y$ , where  $(j, i)$  element of  $n \times p$  matrix  $X$  is  $x_j^{i-1}$ .

- Comments:
  - easily copes with missing values/unequally spaced observations;
  - use orthogonal polynomials to avoid numerical problems if  $n, k$  large;
  - sensitivity to observations at extremities of series often leads to poor fit;
  - usually doesn't work well because polynomials are too restrictive — infinite differentiability everywhere is generally too restrictive.

Regression Methods

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## Spring barley data and polynomial fits



Yield as a function of location for the three blocks, with yields for blocks 2 and 3 offset by the addition of 4 and of 7 respectively, with fitted polynomials of degrees 20, 10 and 50.

Regression Methods

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## Basis functions

- ☐ We seek to estimate a function  $\mu(x)$  based on data  $(x_1, y_1), \dots, (x_n, y_n)$ .
- ☐ There are  $n$  parameters  $\mu_1 = \mu(x_1), \dots, \mu_n = \mu(x_n)$  (plus noise, ...), so we assume that  $\mu(x)$  belongs to a suitable class of functions, defined for  $x \in \mathcal{X}$ .
- ☐ Simple linear model is

$$\mu_{n \times 1} = B_{n \times p} \beta_{p \times 1}, \quad \text{rank}(B) = p \leq n,$$

with the columns of  $B$  evaluations at  $x_1, \dots, x_n$  of **basis functions**.

- ☐ The basis functions may be
  - **global** (e.g., polynomials, trigonometric/Fourier functions),
  - **local** (e.g., splines),
  - **multiscale** (e.g., wavelets).
- ☐ We choose the basis for
  - suitability for the problem at hand (e.g., suitably smooth), and
  - computational reasons—want fast, preferably  $\mathcal{O}(n)$ , handling of  $n \times n$  matrices.
- ☐ Focus on **spline functions**, on which there is a huge literature, starting with a very simple example.

Regression Methods

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## Piecewise linear basis

- Place **knots** of a univariate  $x$  at  $x_1^* < \dots < x_K^*$ , and define **tent functions**

$$b_1(x) = \begin{cases} (x_2^* - x)/(x_2^* - x_1^*), & x_1^* \leq x \leq x_2^*, \\ 0, & \text{otherwise,} \end{cases}$$

$$b_k(x) = \begin{cases} (x - x_{k-1}^*)/(x_k^* - x_{k-1}^*), & x_{k-1}^* < x \leq x_k^*, \\ (x_{k+1}^* - x)/(x_{k+1}^* - x_k^*), & x_k^* < x \leq x_{k+1}^*, \end{cases} \quad k = 2, \dots, K-1,$$

$$b_K(x) = \begin{cases} (x - x_{K-1}^*)/(x_K^* - x_{K-1}^*), & x_{K-1}^* \leq x \leq x_K^*, \\ 0, & \text{otherwise :} \end{cases}$$

these are non-zero only in  $(x_{k-1}^*, x_{k+1}^*)$  (**compact support**) and take value 1 at  $x_k^*$ .

- An exact linear interpolant of data  $y_1, \dots, y_K$  at the knots is the function

$$\mu(x) = \sum_{k=1}^K b_k(x)y_k = B(x)^T y,$$

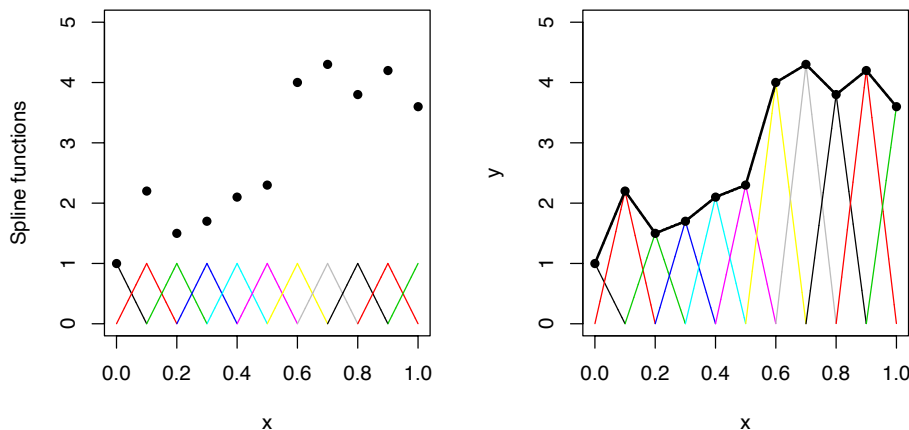
which by construction

- passes through the points  $(x_k^*, y_k)$  and
- is linear between the knots.

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## Piecewise linear basis II



- Left: piecewise linear basis functions  $b_k(x)$  and data  $(x_k^*, y_k)$ .
- Right: functions  $b_k(x)y_k$  and linear interpolant (bold).

Regression Methods

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## Statistical use

- Aim for summary of  $n$  observations, so interpolation not useful.
- Could use  $K < n$  knots, but fit tends to depend heavily on their locations, so better to use high(ish)  $K$  and impose structure by penalising roughness of  $\mu(x)$ :

$$\hat{\beta}_\lambda = \operatorname{argmin}_\beta \left\{ \|y - B\beta\|^2 + \lambda \sum_{k=2}^{K-1} \{\mu(x_{k-1}^*) - 2\mu(x_k^*) + \mu(x_{k+1}^*)\}^2 \right\}.$$

- The second term sums squared numerical second derivatives at the internal knots, and  $\lambda$  imposes the degree of penalisation:
  - $\lambda = 0$  (no penalty) gives the interpolant,
  - $\lambda \rightarrow \infty$  forces the second derivatives to be zero, so gives a straight-line fit.
- On setting  $\beta_k = \mu(x_k^*)$  and writing

$$\begin{pmatrix} \beta_1 - 2\beta_2 + \beta_3 \\ \beta_2 - 2\beta_3 + \beta_4 \\ \beta_3 - 2\beta_4 + \beta_5 \\ \vdots \end{pmatrix} = \begin{pmatrix} 1 & -2 & 1 & 0 & 0 & 0 & \cdots \\ 0 & 1 & -2 & 1 & 0 & 0 & \cdots \\ 0 & 0 & 1 & -2 & 1 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \vdots \end{pmatrix} = D_{(K-2) \times K} \beta_{K \times 1},$$

the penalty is  $\sum_{k=2}^{K-1} (\beta_{k-1} - 2\beta_k + \beta_{k+1})^2 = (D\beta)^T D\beta = \beta^T D^T D\beta = \beta^T S\beta$ , say.

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## Penalized fit

- The penalty matrix  $S$  is of side  $K \times K$  but of rank  $K - 2$ , because

$$S1_K = Sx_{K \times 1}^* = 0_K :$$

the null space of  $S$  consists of all straight lines  $\beta_0 1_K + \beta_1 x^*$ , which are unpenalised.

- Hence (recalling ridge regression),

$$\hat{\beta}_\lambda = \operatorname{argmin}_\beta \{ \|y - B\beta\|^2 + \lambda \beta^T S\beta \} = (B^T B + \lambda S)^{-1} B^T y$$

giving

$$\text{fitted values} \quad \hat{y} = B\hat{\beta}_\lambda = B(B^T B + \lambda S)^{-1} B^T y = H_\lambda y,$$

$$\text{equivalent degrees of freedom} \quad \operatorname{df}_\lambda = \operatorname{tr}(H_\lambda) = \sum_{k=1}^K \frac{1}{1 + \eta_k \lambda},$$

where

- $\eta_1 \leq \cdots \leq \eta_K \in [0, 1]$  are the eigenvalues of  $(B^T B)^{-1/2} S (B^T B)^{-1/2}$ ,
- $\eta_1 = \eta_2 = 0$ , corresponding to the null space of  $S$ , so
- $\operatorname{df}_\lambda$  is monotone decreasing in  $\lambda$ , with

$$(\lambda = 0) \quad K \geq \operatorname{df}_\lambda \geq 2 \quad (\lambda \rightarrow \infty).$$

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## A useful lemma

**Lemma 34** Let  $A$  and  $B$  be  $q \times q$  positive semi-definite matrices such that  $(A + \lambda B)^{-1}$  exists for some  $\lambda > 0$ . Let  $\eta$  be an eigenvalue of  $(A + \lambda B)^{-1}A$ . Then

- ☐ if  $B$  is invertible then

$$\eta = \frac{\eta_B}{\lambda + \eta_B},$$

where  $\eta_B$  is an eigenvalue of  $B^{-1/2}AB^{-1/2}$ , whereas

- ☐ if  $A$  is invertible then

$$\eta = \frac{1}{1 + \lambda\eta_A},$$

where  $\eta_A$  is an eigenvalue of  $A^{-1/2}BA^{-1/2}$ ;

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## Note to Lemma 34

Exercise!

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## Choosing $K$ and $\lambda$

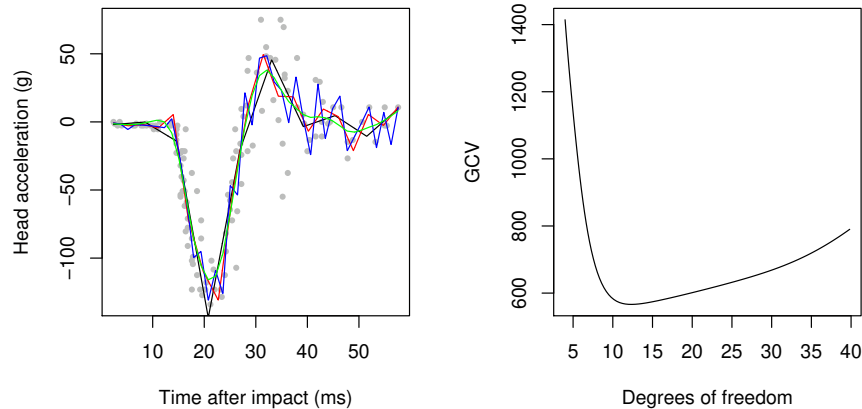
- ☐ So far we have taken  $K = n$ , but this is unnecessary:
  - theory suggests that as  $n \rightarrow \infty$  we need  $K = O(n^{1/5})$  or even  $O(n^{1/9})$  to get near-optimal estimation of  $\mu(x)$ , when  $\mu$  lies in reasonable function classes;
  - in practice we take  $K$  (more than) large enough to give enough flexibility (increasing it if results are suspect,  $K = 9$  by default in `mgcv`), and allow  $\lambda$  to determine the smoothness of the curve;
  - typically the knots  $x_k^*$  are placed at equally-spaced quantiles of  $x$ ; so
  - from now on we suppose that  $K \leq n$ .
- ☐ Under second-order assumptions we choose  $\lambda$  by minimising one of the
  - cross-validation sum of squares,  $CV(\lambda)$ ,
  - generalized cross-validation sum of squares,  $GCV(\lambda)$ .
- ☐ If there is no penalisation ( $\lambda = 0$ ) then we have a standard linear model, and the basis functions are called **regression splines**.
- ☐ Under normal-theory assumptions we link to the mixed model and use REML to estimate  $\sigma^2$  and  $\lambda$ .

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### Example: Motorcycle data



- ☐ Left: linear spline fits with  $\lambda = 0$  and  $K = 10$  (black), 20 (red), 40 (blue), and optimal GCV choice of  $\lambda$  with  $K = 40$  (green)
- ☐ Right: GCV( $\lambda$ ) as a function of  $\text{df}_\lambda$  for  $K = 40$ .
- ☐ In practice we should deal with the obvious heteroscedasticity.

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### Bayesian formulation

- ☐ Spectral theorem:  $S = U L U^T$ , where  $L = \text{diag}(0, 0, \eta_3, \dots, \eta_K)$  contains the eigenvalues of  $S$  and  $U$  is orthogonal;  $S$  has rank  $K - 2$ .
- ☐ With  $L^- = \text{diag}(0, 0, \eta_3^{-1}, \dots, \eta_K^{-1})$ , the **generalized inverse**  $S^- = U L^- U^T$  has rank  $K - 2$ .
- ☐ To express our prior belief that  $\mu(x)$  should be smooth, we write

$$y \mid \beta \sim \mathcal{N}_n(B\beta, \sigma^2 I_n), \quad \beta \sim \mathcal{N}_K(0, \sigma^2 S^- / \lambda),$$

which gives

$$-2 \log f(y, \beta \mid \sigma^2, \lambda) \equiv \|y - B\beta\|^2 / \sigma^2 + n \log \sigma^2 + \lambda (\beta - 0)^T S (\beta - 0) / \sigma^2 + K \log(\sigma^2 / \lambda),$$

so minimising this with respect to  $\beta$  to obtain its **maximum a posteriori (MAP)** estimate gives

$$\hat{\beta}_\lambda = \underset{\beta}{\text{argmin}} \{ \|y - B\beta\|^2 + \lambda \beta^T S \beta \} = (B^T B + \lambda S)^{-1} B^T y,$$

this is also the posterior mean of  $\beta$  given  $y$ , so the posterior mean for  $\mu(x)$  is  $B \hat{\beta}_\lambda = H_\lambda y$ , say.

- ☐ This also can be seen as a mixed model ...

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### Mixed model formulation

- Recalling that  $S = ULU^T$ , we have the 1–1 reparametrisation

$$\beta = U \text{diag}(1, 1, \eta_3^{-1/2}, \dots, \eta_K^{-1/2}) \theta = UL_* \theta,$$

say, where  $L_*$  has rank  $K$  and  $L_*^T L L_* = \text{diag}(0, 0, 1, \dots, 1)$ , so

$$B\beta = BUL_*\theta, \quad \beta^T S \beta = \theta^T L_*^T U^T (ULU^T) UL_* \theta = \theta^T L_*^T L L_* \theta = \sum_{k=3}^K \theta_k^2.$$

- On writing  $\theta^T = (\beta^{*T}, b^T) = (\beta_1^*, \beta_2^*, b_1, \dots, b_{K-2})$ , the smoothing prior is the (proper)

$$b \sim \mathcal{N}_{K-2}(0, \sigma^2 I_{K-2}/\lambda),$$

and  $\beta^*$  is unpenalized, so if  $X$  and  $Z$  represent the first two and last  $K - 2$  columns of  $BUL_*$ , we can formulate the penalised smooth as a mixed model

$$y \mid b \sim \mathcal{N}_n(X\beta^* + Zb, \sigma^2 I_n), \quad b \sim \mathcal{N}_{K-2}(0, \sigma^2 I_{K-2}/\lambda),$$

and estimate  $\lambda$  and  $\sigma^2$  using REML.

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### Summary

- Using penalised basis functions is equivalent to fitting a linear mixed model
  - with linear splines and a roughness penalty, where
  - the null space of the penalty matrix corresponds to a straight-line fit (unpenalized), and
  - the degree of smoothing (equivalent degrees of freedom) is chosen by GCV or REML.
- Spline fits depend on number of knots  $\equiv$  number of basis functions — need not be  $O(n)$ .
- Equivalent to a Bayesian formulation.
- Can also fit unpenalised regression splines.
- Next: splines, inference, additive models, generalized additive models

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## Splines

- The  $p$ th degree spline basis with knots  $x_1^* < \dots < x_K^*$  is

$$1, x, \dots, x^p, (x - x_1^*)_+^p, \dots, (x - x_K^*)_+^p,$$

where  $u_+ = \max(u, 0)$  is the **positive part function**.

- The resulting basis matrix  $B$  is highly collinear and gives an implausible statistical model.
- **B-spline** bases span the same linear space, but have better numerical properties. They are defined by adding **boundary knots**  $x_0^*$  and  $x_{K+1}^*$  and setting up an **augmented knot sequence**

$$\tau_1 \leq \dots \leq \tau_M \leq x_0^* \leq \tau_{M+1} = x_1^* \leq \dots \leq \tau_{M+K} = x_K^* \leq x_{K+1}^* \leq \tau_{K+1+M} \leq \dots \leq \tau_{K+2M};$$

typically the  $\tau_k$  outside  $[x_0^*, x_{K+1}^*]$  are set to the boundary knot values. Then

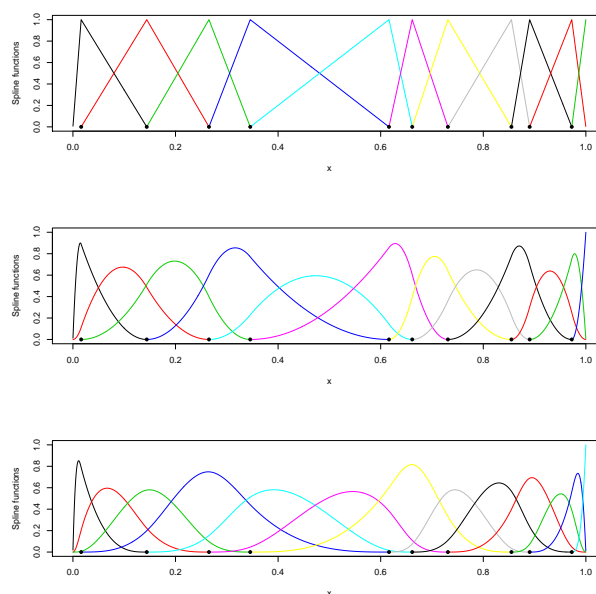
$$B_{k,1}(x) = I(\tau_k \leq x < \tau_{k+1}), \quad k = 1, \dots, K + 2M - 1,$$

$$B_{k,m}(x) = \frac{x - \tau_k}{\tau_{k+m-1} - \tau_k} B_{k,m-1}(x) + \frac{\tau_{k+m} - x}{\tau_{k+m} - \tau_{k+1}} B_{k+1,m-1}(x), \quad k = 1, \dots, K + 2M - m,$$

where we set  $B_{k,1} \equiv 0$  if  $\tau_k = \tau_{k+1}$  (avoiding division by zero).

- Cubic splines ( $p = 3, M = 4$ ) give visually smooth functions.
- $K = 10$  on the next slide, with  $M = 2$  (linear),  $M = 3$  (quadratic) and  $M = 4$  (cubic), and the  $\tau_k$  set to equal the boundary knots.

## Linear, quadratic and cubic B-splines



## Natural cubic spline

- Suppose the  $x_j$  are distinct (no loss of generality, see later) and

$$a < x_1 < \dots < x_n < b, \quad \mathcal{X} = [a, b] \subset \mathbb{R}.$$

- A **natural cubic spline** adds the constraint that the function is linear outside  $[x_1, x_n]$ , and thus avoids high variance due to quadratic and higher terms outside this interval.
- A natural cubic spline
  - has  $K = n$  knots, at  $x_1 < \dots < x_n$ ,
  - is a cubic polynomial on each interval between knots,
  - is continuous, with continuous first and second derivatives at each knot, and
  - is linear on  $[a, x_1]$  and  $[x_n, b]$ , with zero second and third derivatives at  $x_1$  and  $x_n$ ,
  - has

$$2 + 4(n - 1) + 2 \text{ parameters} - 3n \text{ linear constraints} = n$$

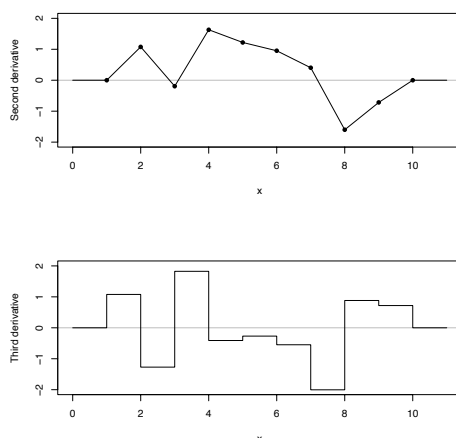
degrees of freedom (df), which can be split into

- ▷ 2 df for a linear fit, plus
- ▷  $n - 2$  df for the second derivatives  $\mu''(x_2), \dots, \mu''(x_{n-1})$ .

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## Natural cubic spline



- A natural cubic spline may be constructed by integrating a linear second derivative function  $\mu''(x)$  which is determined by  $\mu''(x_2), \dots, \mu''(x_{K-1})$  and because  $\mu''(x) \equiv 0$  for  $x \notin (x_1, x_K)$ .
- On integrating twice we gain two constants:  $\mu(x) = \beta_0 + \beta_1 x + \int_0^x \int_0^{x'} \mu''(u) du dx'$ .
- Above  $x_1 = 1, \dots, x_{10} = 10$ , so the spline is determined by  $\mu''(2), \dots, \mu''(9)$  and the line.

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## Optimality of natural cubic splines

- Let  $\mathcal{S}_2(\mathcal{X})$  denote the set of functions  $\mu$  differentiable on  $\mathcal{X} = [a, b]$  with absolutely continuous first derivative  $\mu'$ : i.e., there exists an integrable function  $\mu''$  such that  $\int_a^x \mu''(u) du = \mu'(x) - \mu'(a)$  for  $x \in \mathcal{X}$ .
- Clearly any  $\mu$  with two continuous derivatives on  $\mathcal{X}$  lies in  $\mathcal{S}_2(\mathcal{X})$ .

**Theorem 35** Suppose  $n \geq 2$ , that  $a < x_1 < \dots < x_n < b$ , and that  $\mu$  is the natural cubic spline interpolating  $y_1, \dots, y_n$  at  $x_1, \dots, x_n$ . If  $\tilde{\mu} \in \mathcal{S}_2(\mathcal{X})$  also interpolates the  $y_j$ , then

$$\int_{\mathcal{X}} \tilde{\mu}''^2 \geq \int_{\mathcal{X}} \mu''^2,$$

with equality iff  $\tilde{\mu} \equiv \mu$ .

- Thus  $\mu$  minimises the **roughness penalty**  $\lambda \int_{\mathcal{X}} \mu''^2$  in a larger class of functions than that to which it belongs, making it a natural choice as an interpolant, because minimising

$$\sum_{j=1}^n \{y_j - \tilde{\mu}(x_j)\}^2 + \lambda \int_{\mathcal{X}} \tilde{\mu}''(x)^2 dx$$

for  $\tilde{\mu} \in \mathcal{S}_2(\mathcal{X})$  will automatically result in a natural cubic spline  $\mu$ : if  $\tilde{\mu}(x_j) = \mu(x_j)$ , then the penalty is reduced by using  $\mu$ .

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## Note to Theorem 35

Let  $\nu = \tilde{\mu} - \mu \in \mathcal{S}_2(\mathcal{X})$ , and note that  $\nu(x_j) = 0$  for each  $j$ , since  $\mu(x_j) = \tilde{\mu}(x_j) = y_j$ . The natural boundary conditions imply that  $\mu''(a) = \mu''(b) = 0$ , so integration by parts yields

$$0 = [\mu''(x)\nu'(x)]_a^b = \int_{\mathcal{X}} (\mu''\nu')' = \int_{\mathcal{X}} \mu''\nu'' + \int_{\mathcal{X}} \mu''' \nu',$$

and hence the facts that  $\mu'''$  is piecewise constant and that  $\nu(x_j) = 0$  yields

$$\int_{\mathcal{X}} \mu''\nu'' = - \int_{\mathcal{X}} \mu''' \nu' = - \sum_{j=1}^{n-1} \mu'''(x_j^+) \int_{x_j}^{x_{j+1}} \nu' = - \sum_{j=1}^{n-1} \mu'''(x_j^+) \{\nu(x_{j+1}) - \nu(x_j)\} = 0.$$

Hence

$$\int_{\mathcal{X}} \tilde{\mu}''^2 = \int_{\mathcal{X}} (\mu'' + \nu'')^2 = \int_{\mathcal{X}} \mu''^2 + 2 \int_{\mathcal{X}} \mu''\nu'' + \int_{\mathcal{X}} \nu''^2 = \int_{\mathcal{X}} \mu''^2 + \int_{\mathcal{X}} \nu''^2 \geq \int_{\mathcal{X}} \mu''^2,$$

with equality iff  $\nu''(x) \equiv 0$ . This occurs iff  $\nu(x)$  is linear, but since  $\nu(x_j) = 0$  at at least two points,  $\nu(x) = 0$  for all  $x \in \mathcal{X}$ .

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## Roughness penalty and equivalent formulations

**Theorem 36** *In the setting above, the roughness measure can be expressed as*

$$\int_{\mathcal{X}} \mu''(x)^2 dx = \mu^T S \mu = \gamma^T R \gamma,$$

where

$$\begin{aligned} \mu^T &= (\mu(x_1), \dots, \mu(x_n)), \quad \gamma^T = (\mu''(x_2), \dots, \mu''(x_{n-1})), \\ Q^T \mu &= R \gamma, \\ \text{and} \quad S_{n \times n}, \quad R_{(n-2) \times (n-2)}, \quad Q_{n \times (n-2)} &\text{ all have rank } n-2. \end{aligned}$$

Moreover

- the fit is linear outside  $(x_1, x_n)$ , so  $\mu''(x_1) = \mu''(x_n) = 0$ ,
- $Q$  and  $R$  are band matrices, leading to  $O(n)$  matrix manipulations, and
- imposing the roughness penalty corresponds to using the prior  $\gamma \sim \mathcal{N}_{n-2}(0, \sigma^2 \psi R^{-1})$  for Bayesian inference, or a mixed effects model

$$\mu = \beta_0 1_n + \beta_1 x_{n \times 1} + Z_{n \times (n-2)} b, \quad b \sim \mathcal{N}_{n-2}(0, \sigma^2 \psi I_{n-2}),$$

for a suitable basis matrix  $Z$  and  $\psi = \lambda^{-1}$ .

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### Note 1 to Theorem 36

- Let  $\mathcal{X} = [a, b]$  and suppose that  $a < x_1 < \dots < x_n < b$ ; sometimes below we set  $x_0 = a$  and  $x_{n+1} = b$ . If  $\mu(x)$  is a cubic spline on  $\mathcal{X}$ , then  $\mu''(x)$  is continuous and piecewise linear.
- Taking  $\mu''(a) = \mu''(x_1) = \mu''(b) = \mu''(x_n) = 0$  implies that  $\mu''(x) = 0$  outside  $[x_1, x_n]$ , so there is no contribution to  $\int (\mu'')^2$  from outside  $[x_1, x_n]$ ; this makes sense because the penalty should not depend on  $a$  and  $b$ . The optimal  $\mu(x)$  will be linear outside  $[x_1, x_n]$ , because the corresponding  $\mu''$  is zero outside this set.
- Write  $\gamma_j = \mu''(x_j)$ , parametrise  $\mu''(x)$  in terms of  $\gamma_2, \dots, \gamma_{n-1}$ , set  $h_j = x_j - x_{j-1}$ , and obtain

$$\mu''(x) = \frac{\gamma_j(x - x_{j-1}) + \gamma_{j-1}(x_j - x)}{h_j}, \quad x_{j-1} \leq x \leq x_j, \quad j = 1, \dots, n+1, \quad (16)$$

where  $\gamma_0 = \gamma_1 = \gamma_n = \gamma_{n+1} = 0$ ; note that  $\mu'''(x) = (\gamma_j - \gamma_{j-1})/h_j$  on  $[x_{j-1}, x_j]$ . Now

$$\begin{aligned} \int_{x_{j-1}}^{x_j} \mu''(x)^2 dx &= \frac{1}{3h_j^2(\gamma_j - \gamma_{j-1})} [\gamma_j(x - x_{j-1}) + \gamma_{j-1}(x_j - x)]^3 \Big|_{x_{j-1}}^{x_j} \\ &= \frac{1}{3h_j^2(\gamma_j - \gamma_{j-1})} (h_j^3 \gamma_j^3 - h_j^3 \gamma_{j-1}^3) \\ &= \frac{h_j}{3} (\gamma_j^2 + \gamma_j \gamma_{j-1} + \gamma_{j-1}^2), \end{aligned}$$

so

$$\int_{\mathcal{X}} \mu''(x)^2 dx = \int_{x_1}^{x_n} \mu''(x)^2 dx = \sum_{j=2}^n \int_{x_{j-1}}^{x_j} \mu''(x)^2 dx = \frac{1}{3} \sum_{j=2}^n h_j (\gamma_j^2 + \gamma_j \gamma_{j-1} + \gamma_{j-1}^2).$$

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## Note II to Theorem 36

- Recalling that  $\gamma_1 = \gamma_n = 0$ , we see that  $\int_{\mathcal{X}} \mu''(x)^2 dx$  equals

$$\frac{1}{3} \{h_2\gamma_2^2 + h_3(\gamma_3^2 + \gamma_3\gamma_2 + \gamma_2^2) + \cdots + h_{n-1}(\gamma_{n-1}^2 + \gamma_{n-1}\gamma_{n-2} + \gamma_{n-2}^2) + h_n\gamma_{n-1}^2\} = \gamma^T R \gamma,$$

say, where

$$R_{(n-2) \times (n-2)} = \frac{1}{6} \begin{pmatrix} 2(h_2 + h_3) & h_3 & 0 & \cdots & 0 \\ h_3 & 2(h_3 + h_4) & h_4 & \ddots & \vdots \\ 0 & h_4 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & h_{n-1} \\ 0 & \cdots & 0 & h_{n-1} & 2(h_{n-1} + h_n) \end{pmatrix}, \quad \gamma = \begin{pmatrix} \gamma_2 \\ \vdots \\ \gamma_{n-1} \end{pmatrix}.$$

As  $\gamma^T R \gamma$  equals a non-negative integral that is zero iff  $\gamma = 0$ ,  $R$  is positive definite, and it is symmetric by construction. It is also strictly diagonal dominant, i.e.,  $|r_{jj}| > \sum_{i \neq j} |r_{ji}|$  (which also implies that it is invertible).

The unusual labelling of the elements of  $\gamma$ , starting from  $\gamma_2$ , simplifies things below.

- **Aside for time series experts:** if we regard  $R$  as the precision (inverse variance) matrix of a Gaussian distribution for  $\gamma$ , then we see that

$$\text{corr}(\gamma_r, \gamma_s \mid \text{rest}) = \begin{cases} -h_{r+1}/\{4(h_r + h_{r+1})(h_{r+1} + h_{r+2})\}^{1/2}, & s = r + 1, \\ 0, & \text{otherwise,} \end{cases}$$

corresponding to a Markov process. If the  $x_j$  are equally-spaced, then all the  $h_j$  are equal and  $\text{corr}(\gamma_r, \gamma_s \mid \text{rest}) = I(r = s) - I(|r - s| = 1)/4$  is PACF of an AR(1) model.

- Integration by parts yields

$$\int_{\mathcal{X}} \mu''(x)^2 dx = [\mu'(x)\mu''(x)]_a^b - \int_{\mathcal{X}} \mu'''(x)\mu'(x) dx,$$

where the first term on the right-hand side equals zero because  $\mu''(a) = \mu''(b) = 0$ , and as the third derivative is constant on each interval  $(x_1, x_2], \dots, (x_{n-1}, x_n]$  and zero elsewhere, the second term on the right-hand side equals

$$\begin{aligned} - \sum_{j=1}^{n-1} \mu'''(x_j^+) \int_{x_j}^{x_{j+1}} \mu'(x) dx &= \sum_{j=1}^{n-1} \frac{\gamma_{j+1} - \gamma_j}{h_{j+1}} (\mu_j - \mu_{j+1}) \\ &= \sum_{j=2}^{n-1} \gamma_j \left( \frac{\mu_{j+1} - \mu_j}{h_{j+1}} - \frac{\mu_j - \mu_{j-1}}{h_j} \right) \\ &= \gamma^T Q_{(n-2) \times n}^T \mu, \end{aligned} \tag{17}$$

say, because  $\gamma_1 = \gamma_n = 0$ ; here and below,  $\mu^T = (\mu_1, \dots, \mu_n)$ , where  $\mu_j = \mu(x_j)$ . If we label the  $n - 2$  rows of  $Q^T \mu$  like those of  $\gamma$  (i.e., starting at row  $j = 2$ ), then the  $j$ th row of  $Q^T \mu$  is

$$\frac{\mu_{j+1} - \mu_j}{h_{j+1}} - \frac{\mu_j - \mu_{j-1}}{h_j}, \quad j = 2, \dots, n - 1,$$

so  $Q^T$  is tridiagonal and fast (i.e., linear in  $n$ ) matrix operations with it are possible.

- Note that  $Q^T \mathbf{1}_n = 0$  and  $Q^T x = 0$ , which verifies that linear functions are not penalised.

### Note III to Theorem 36

- If we integrate  $\mu''(x)$  twice, we see that for  $x_{j-1} \leq x \leq x_j$  we can write

$$\mu(x) = \frac{(x - x_{j-1})\mu_j + (x_j - x)\mu_{j-1}}{h_j} - \frac{1}{6}(x - x_{j-1})(x_j - x) \left\{ \left(1 + \frac{x - x_{j-1}}{h_j}\right) \gamma_{j-1} + \left(1 + \frac{x_j - x}{h_j}\right) \gamma_j \right\}.$$

Hence the first derivatives at  $x_1, \dots, x_n$  from the right and from the left may be written as

$$\begin{aligned} \mu'(x_j^+) &= (\mu_{j+1} - \mu_j)/h_{j+1} - \frac{1}{6}h_{j+1}(2\gamma_j + \gamma_{j+1}), \\ \mu'(x_j^-) &= (\mu_j - \mu_{j-1})/h_j + \frac{1}{6}h_j(\gamma_{j-1} + 2\gamma_j). \end{aligned}$$

As  $\gamma_1 = \gamma_n = 0$  the limits at  $x_1$  and  $x_n$  reduce to

$$\mu'(x_1^+) = \frac{\mu_2 - \mu_1}{h_2} - \frac{1}{6}h_2\gamma_2, \quad \mu'(x_n^-) = \frac{\mu_n - \mu_{n-1}}{h_n} + \frac{1}{6}h_n\gamma_{n-1}. \quad (18)$$

Outside  $[x_1, x_n]$  the function  $\mu(x)$  is linear and may be written as

$$\mu(x) = \begin{cases} \mu_1 - (x_1 - x)\mu'(x_1^+), & x \leq x_1, \\ \mu_n + (x - x_n)\mu'(x_n^-), & x \geq x_n, \end{cases}$$

which guarantees that  $\mu'(x)$  is continuously differentiable at  $x_1$  and  $x_n$ .

- Now  $\mu(x)$  is everywhere continuous, has  $\mu''(x_j^+) = \mu''(x_j^-) = \gamma_j$  for each  $j$ , and  $\mu'$  is continuous at  $x_1$  and  $x_n$ , so to make  $\mu$  a natural cubic spline we must ensure that  $\mu'$  is continuous at  $x_2, \dots, x_{n-1}$ , i.e.,  $\mu'(x_j^-) = \mu'(x_j^+)$  for  $j = 2, \dots, n-1$ . Thus (18) yields

$$\frac{\mu_{j+1} - \mu_j}{h_{j+1}} - \frac{\mu_j - \mu_{j-1}}{h_j} = \frac{1}{6}h_j\gamma_{j-1} + \frac{1}{3}(h_j + h_{j+1})\gamma_j + \frac{1}{6}h_{j+1}\gamma_{j+1}, \quad j = 2, \dots, n-1,$$

which on comparison with (17) can be written in matrix form as  $Q^T \mu = R\gamma$ .

- Hence using invertibility of  $R$  we can write the penalty as

$$\int_{\mathcal{X}} \mu''(x)^2 dx = \gamma^T Q^T \mu = \gamma^T R\gamma = \mu^T Q R^{-1} Q^T \mu = \mu^T S \mu.$$

- The  $n \times 1$  vector  $\mu$  lies in the vector space  $\mathbb{R}^n$ , and we can form a basis of this space starting with the vectors  $1_n$  and  $x = (x_1, \dots, x_n)^T$  and then adding any  $n-2$  linearly independent vectors. In particular, on integrating (16) up to  $x$ , twice, we see that we can write

$$\mu(x) = \beta_0 + \beta_1 x + \sum_{j=2}^{n-1} p_j(x)\gamma_j, \quad x \in \mathcal{X}, \quad (19)$$

where the term  $\beta_0 + \beta_1 x$  comes from the constants of integration and the cubic polynomials  $p_j(x)$  stem from integrating the linear functions  $\mu''(x)$  in each of the intervals  $[x_{j-1}, x_j]$ . On evaluating (19) at  $x_1, \dots, x_n$  we obtain

$$\mu = \beta_0 1_n + \beta_1 x + P\gamma, \quad \beta_0, \beta_1, \gamma_2, \dots, \gamma_{n-1} \in \mathbb{R},$$

where the  $n \times (n-2)$  matrix  $P$  has rank  $n-2$ , because its first row consists of zeros and rows  $2, \dots, n-1$  are lower triangular (as  $\mu(x)$  involved integration from  $a$  to  $x$ ).



### Note IV to Theorem 36

- Recall that  $Q^T 1_n = Q^T x = 0$ , giving  $Q^T \mu = Q^T P \gamma$ , and thus

$$\gamma^T R \gamma = \mu^T Q R^{-1} Q^T \mu = \gamma^T P^T Q R^{-1} Q^T P \gamma = \gamma^T (P^T Q R^{-1}) R (R^{-1} Q^T P) \gamma,$$

which implies that  $P^T Q R^{-1} = I_{n-2}$ . Hence  $Q_{n \times (n-2)}$  and  $S_{n \times n} = Q R^{-1} Q^T$  have rank  $n - 2$ .

- Now consider a model in which  $\mu = \beta_0 + \beta_1 x + P \gamma$  and  $\gamma$  is random, with

$$y \mid \gamma \sim \mathcal{N}_n(\mu, \sigma^2 I_n), \quad \gamma \sim \mathcal{N}_{n-2}(0, \sigma^2 \lambda^{-1} R^{-1}), \quad \lambda > 0. \quad (20)$$

Apart from constants, the logarithm of the posterior density  $f(\beta_0, \beta_1, \gamma \mid y; \sigma^2, \lambda)$  equals

$$\log f(y \mid \gamma) + \log f(\gamma) = -\{(y - \mu)^T (y - \mu) + \lambda \gamma^T R \gamma\} / (2\sigma^2) - \frac{2n-2}{2} \log \sigma^2 + \frac{n-2}{2} \log \lambda,$$

and for fixed  $\sigma^2$  and  $\lambda$  the values of  $\beta_0$ ,  $\beta_1$  and  $\gamma$  that maximise  $f(\beta_0, \beta_1, \gamma \mid y; \sigma^2, \lambda)$  are found by minimising the penalised sum of squares

$$(y - \mu)^T (y - \mu) + \lambda \gamma^T R \gamma = \sum_{j=1}^n \{y_j - \mu(x_j)\}^2 + \lambda \int_{\mathcal{X}} \mu''(x)^2 dx.$$

- As  $R$  is not diagonal, the elements of  $\gamma$  in (20) are not independent, but we can use the spectral decomposition to diagonalise  $R$ , writing  $\gamma^T R \gamma = (A\gamma)^T (A\gamma) = b^T b$ , say, where  $A$  is invertible and  $R = A^T A$ , so  $R^{-1} = A^{-1} (A^T)^{-1}$  and  $AR^{-1}A^T = I_{n-2}$ . Thus

$$b = A\gamma \sim \mathcal{N}_{n-2}(0, \sigma^2 \lambda^{-1} AR^{-1}A^T) = \mathcal{N}_{n-2}(0, \sigma^2 \psi I_{n-2}), \quad \psi = \lambda^{-1}.$$

In this parametrization we have

$$\mu = \beta_0 1_n + \beta_1 x + P \gamma = \beta_0 1_n + \beta_1 x + Zb, \quad Z = PA^{-1},$$

and with the stated normal distribution for  $b$  we see that this is a mixed model with fixed effect  $\beta_0 1_n + \beta_1 x$  and random effect  $Zb$ .

- Hence imposing the 'natural' smoothness penalty based on  $\int (\mu'')^2$  is equivalent to Bayesian inference using an improper (constant) prior for  $\beta_0$  and  $\beta_1$  and a proper Gaussian prior for  $\gamma$ ,

$$\gamma \sim \mathcal{N}_{n-2}(0, \sigma^2 \psi R^{-1})$$

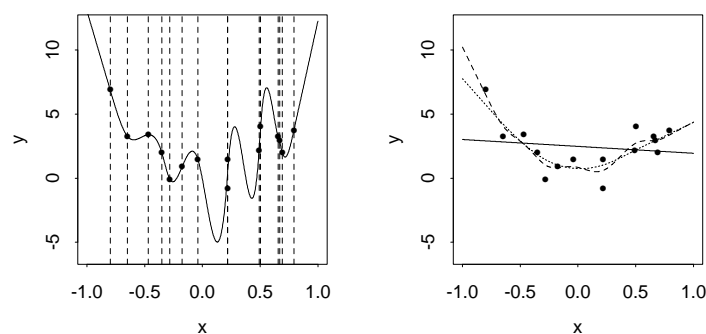
or using the mixed effects model with

$$\mu = X\beta + Zb = \beta_0 1_n + \beta_1 x + Zb, \quad b \sim \mathcal{N}_{n-2}(0, \sigma^2 \psi I_{n-2}),$$

or any other equivalent formulation in terms of an invertible transformation of the columns of  $Z$ .

- In this setup we could set  $\psi = 0$  (equivalent to  $\lambda = \infty$ ), corresponding to fitting the fixed effects alone. Testing  $\psi = 0$  against  $\psi > 0$  corresponds to testing a linear model against the spline fit in which  $b \neq 0$ .

## Natural cubic spline



- ☐ The unpenalized natural cubic spline on the left passes perfectly through the 15 points, but is very sensitive to their values: think of beads on wires.
- ☐ On the right we see the effect of a roughness penalty with 2 (solid), 7 (dashes) and 3.7 (dots) df.

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## Variants

- ☐ Obvious generalisation allows weight matrix  $W = \text{diag}(w_1, \dots, w_n)$ .
- ☐ If the  $x_1, \dots, x_n$  are not unique, write  $E(y) = N_{n \times n'} \mu_{n' \times 1}$  in terms of the means  $\mu$  at the  $n'$  unique elements of  $x$ , and minimise

$$(y - N\mu)^T W (y - N\mu) + \lambda \mu^T S \mu.$$

where  $S_{n' \times n'}$  arises as before as the roughness penalty on  $\mu(x)$ .

- ☐ Could use a truncated power basis of degree  $p - 1$  with knots at  $x_1^*, \dots, x_q^*$ , i.e.,

$$\mu(x) = \beta_0 + \beta_1 x + \dots + \beta_{p-1} x^{p-1} + \sum_{i=1}^q b_i (x - x_i^*)_+^{p-1},$$

set  $\theta^T = (\beta^T, b^T)$  where  $\beta^T = (\beta_0, \dots, \beta_{p-1})$ ,  $b^T = (b_1, \dots, b_q)$  and minimise

$$(y - B\theta)^T W (y - B\theta) + \lambda \theta^T S \theta$$

where the penalty matrix  $S$  does not affect  $\beta$ . This gives

$$\hat{\theta}_\lambda = (B^T W B + \lambda S)^{-1} B^T W y, \quad \hat{y} = B(B^T W B + \lambda S)^{-1} B^T W y = H_\lambda y.$$

Since  $\beta$  is unpenalised,  $H_\lambda y$  tends to the polynomial fit when  $\lambda \rightarrow \infty$ .

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### Equivalent degrees of freedom

- ☐ Fitted values are  $\hat{y} = H_\lambda y$ .
- ☐ With  $B = (X_{n \times p}, Z_{n \times q})$  and  $X$  unpenalised by  $S_{(p+q) \times (p+q)}$ , we define the **equivalent degrees of freedom** of the fit as

$$\text{df}_\lambda = \text{tr}(H_\lambda) = \text{tr}\{B(B^T W B + \lambda S)^{-1} B^T W\} = \text{tr}\{(B^T W B + \lambda S)^{-1} B^T W B\} = \sum_{j=1}^{p+q} \frac{1}{1 + \eta_j \lambda}$$

where  $\eta_1, \dots, \eta_{p+q} \in [0, 1]$  are eigenvalues of  $(B^T W B)^{-1/2} S (B^T W B)^{-1/2}$ .

- ☐ Since the column space of  $X$  is unpenalised,  $p$  of the eigenvalues of  $H_\lambda$  must equal 1: since  $S$  has rank  $q$ ,  $p$  of the  $\eta_j$  equal 0, so

$$\text{df}_\lambda \rightarrow \begin{cases} p, & \lambda \rightarrow \infty, \\ p + q, & \lambda \rightarrow 0. \end{cases}$$

- ☐ We specify smoothness using either  $\lambda$  or  $\text{df}_\lambda$  (preferable, as easier to interpret).
- ☐ Nothing above required  $X$  to consist only of polynomials; it could contain ordinary unpenalized covariates ...

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### Note on equivalent degrees of freedom

Using the lemma we obtain

$$\text{tr}(H_\lambda) = \text{tr}\{B(B^T W B + \lambda S)^{-1} B^T W\} = \text{tr}\{(B^T W B + \lambda S)^{-1} B^T W B\} = \sum_{j=1}^{p+q} \frac{1}{1 + \lambda \eta_j},$$

where  $B^T W B$  is invertible and  $\eta_1 < \dots < \eta_{p+q}$  are the eigenvalues of  $(B^T W B)^{-1/2} S (B^T W B)^{-1/2}$ . Since  $S$  has rank  $q$ ,  $\eta_1 = \dots = \eta_p = 0$ , and therefore

$$p \leq \sum_{j=1}^{p+q} \frac{1}{1 + \lambda \eta_j} \leq p + q,$$

with the limits attained when  $\lambda \rightarrow \infty$  and  $\lambda \rightarrow 0$  respectively.

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## Choice of $\lambda$

- Cross-validation and generalized cross-validation criteria are

$$\text{CV}(\lambda) = \sum_{j=1}^n \left\{ \frac{y_j - \hat{y}_j}{1 - h_{jj}(\lambda)} \right\}^2, \quad \text{GCV}(\lambda) = \sum_{j=1}^n \left\{ \frac{y_j - \hat{y}_j}{1 - \text{tr}(H_\lambda)/n} \right\}^2.$$

where  $h_{jj}(\lambda)$  is  $j$ th diagonal element of  $H_\lambda$ .

- CV and GCV only use second-order assumptions, but tend to give curves that are too variable (df too high), and so do approaches based on minimising Mallows'  $C_p$ .
- If linear mixed model

$$y | b \sim \mathcal{N}_n(X\beta + Zb, \Omega), \quad b \sim \mathcal{N}_q(0, \Omega_b)$$

is credible, then can estimate  $\sigma^2$  and the vector of variance ratios  $\psi$  by ordinary ML or get the REML estimates by maximising

$$\ell_R(\psi, \sigma^2) \equiv \frac{1}{2} \log |\Delta| - \frac{1}{2} \log |X^T \Delta X| - \frac{1}{2\sigma^2} (y - X\hat{\beta}_\psi)^T \Delta (y - X\hat{\beta}_\psi) - \frac{n-p}{2} \log \sigma^2,$$

where

$$\hat{\beta}_\psi = (X^T \Delta X)^{-1} X^T \Delta y, \quad Z \Omega_b Z^T + \Omega = \sigma^2 \Delta^{-1}(\psi);$$

this involves taking a grid of values of  $\psi$ , or iterating on  $\psi$ , or ...

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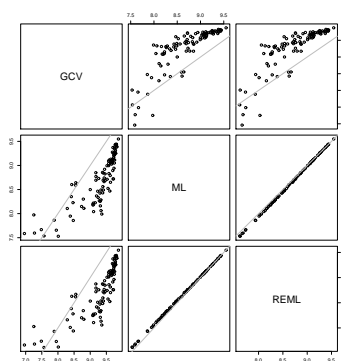
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## Simulation

Equivalent degrees of freedom (EDF) estimated by GCV, ML and REML for 100 replicate datasets simulated by

$$y_j | x_j \stackrel{\text{iid}}{\sim} \mathcal{N} \left\{ 1.5 \phi \left( \frac{x_j - 0.35}{0.15} \right) - \phi \left( \frac{x_j - 0.8}{0.04} \right), 0.1^2 \right\}, \quad x_j \stackrel{\text{iid}}{\sim} U(0, 1), \quad j = 1, \dots, 100.$$

The EDF for GCV is almost always larger than for the other two, which are essentially identical in this case.

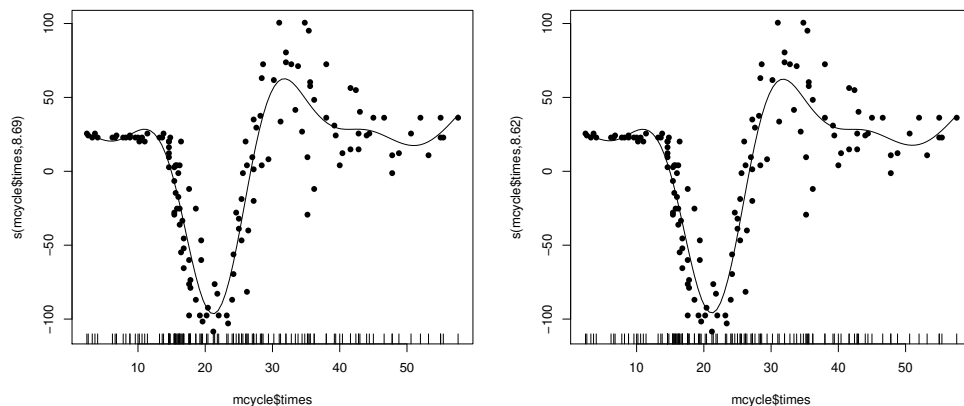


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## Motorcycle data

Spline fits estimated using GCV (left) and REML (right), giving EDF=8.69 and 8.62. Both fits are questionable for small  $x$  because of the heteroscedasticity.



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## More splines

- Sometimes cyclic effects (e.g., seasonality, diurnal variation) must be modelled smoothly, so (e.g.) December joins smoothly onto January. Then the penalty and spline basis must be modified accordingly, to give a **cyclic (cubic) spline**.
- **P-splines** are a version of B-splines (usually with equally-spaced knots) in which a difference penalty is applied to the parameters to control the wiggleness of  $\mu$ , e.g.,

$$\sum_{k=1}^{K-1} w_k (\beta_{k+1} - \beta_k)^2 = \beta^T D^T W D \beta, \quad \text{with} \quad D = \begin{pmatrix} -1 & 1 & 0 & 0 & \dots \\ 0 & -1 & 1 & 0 & \dots \\ \cdot & \cdot & \cdot & \cdot & \dots \end{pmatrix},$$

and  $W = \text{diag}(w_1, \dots, w_{K-1})$ . These are easy to set up and flexible, but messy if the knots are not equi-distant and the penalty is less readily interpreted.

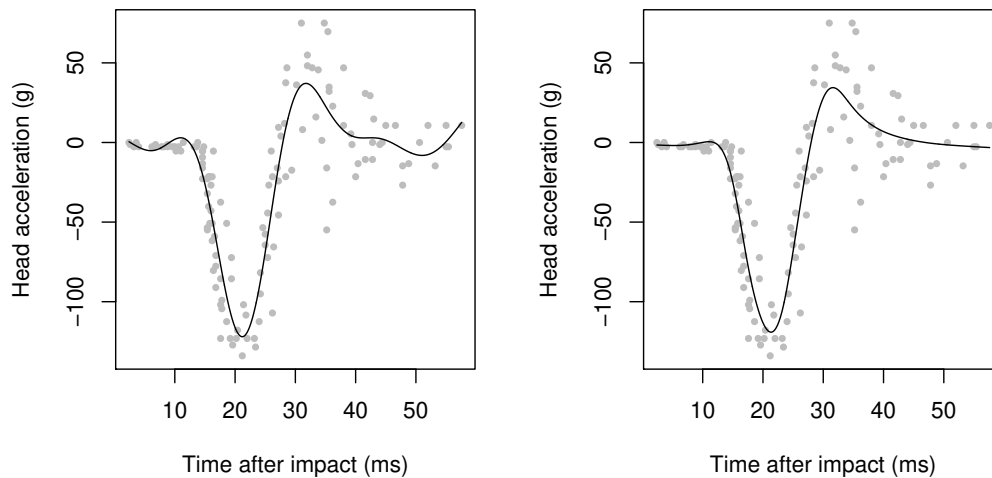
- For an **adaptive spline** we can let  $w_k \equiv w_k(x)$  vary with  $x$ , for example setting  $w(x) = B(x)\lambda_{L \times 1}$  and thus having  $D^T W D = \sum_l \lambda_l D^T \text{diag}\{B_l(x)\} D$ , where  $B_l(x)$  is the  $l$ th column of  $B(x)$ , then estimating the vector  $\lambda$ .
- Other possibilities include (Wood, 2017, Chapter 5)
  - **shape-constrained splines** to impose, e.g., monotonicity on the fit;
  - **thin-plate**, **Duchon** and **tensor product** splines used in spatial problems; and
  - **soap film splines** used when smoothing over complex domains.

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### Motorcycle data: adaptive fit

Standard (left) and adaptive (right) spline fits, the latter with  $K = 40$  and  $L = 5$ :



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## 4.4 Additive Models

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### Generalisations

- We've discussed estimation of a single function  $\mu(x)$ , but in applications we may have
  - covariates to be treated parametrically,
  - several smooth functions,
  - non-normal response variable,
  - random effects.
- To include ordinary covariates, we write

$$y \mid b \sim (B\theta, \sigma^2 I_n), \quad B\theta = X\beta + Zb,$$

where

- $X$  represents the ordinary covariates, plus any polynomial columns for smooth components,
- the 'fixed effects' parameter vector  $\beta$  is not penalized,
- $Z$  is the basis representation for the smooth function,
- the 'random effects' vector  $b$  is penalized,
- and everything 'goes through as before'.

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## Additive model

- We suppose

$$y_j \stackrel{\text{ind}}{\sim} (\mu_1(x_j) + \mu_2(z_j), \sigma^2), \quad j = 1, \dots, n,$$

where  $\mu_1, \mu_2$  belong to suitable classes of 'smooth' functions; for example if

$$x \equiv \text{time}, \quad z \equiv \text{space},$$

then  $\mu_1$  is defined on  $\mathcal{X}_1 \subset \mathbb{R}$  and  $\mu_2$  is defined on  $\mathcal{X}_2 \subset \mathbb{R}^2$ .

- This **additive model** might also include ordinary covariates.
- There is an identifiability problem, since we could map

$$\mu_1(x) \mapsto \mu_1(x) + a, \quad \mu_2(z) \mapsto \mu_2(z) - a, \quad a \in \mathbb{R},$$

and the fitted values would not change, so we must constrain  $\mu_1$  and  $\mu_2$ .

- As before, we use bases for  $\mu_1$  and  $\mu_2$ , writing

$$y = B\theta + \varepsilon = \begin{pmatrix} X_1 & X_2 \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \end{pmatrix} + \begin{pmatrix} Z_1(x) & Z_2(z) \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} + \varepsilon,$$

where we shall penalise the  $q_1$  elements of  $b_1$  and the  $q_2$  elements of  $b_2$ .

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## Estimation

- We minimise the penalised sum of squares

$$(y - B\theta)^T(y - B\theta) + \theta^T S_\lambda \theta,$$

where

$$S_\lambda = \lambda_1 S_1 + \lambda_2 S_2, \quad S_r = \text{diag}(0, \dots, 0, 1, \dots, 1, 0, \dots, 0), \quad r = 1, 2,$$

and the 1s on the diagonals of  $S_r$  correspond to the coefficients to be penalised.

- The solution for fixed  $\lambda_1, \lambda_2$  is the same as before, i.e.,

$$\hat{\theta} = (B^T B + S_\lambda)^{-1} B^T y,$$

where  $\hat{\theta} \equiv \hat{\theta}_\lambda$ , and we've now absorbed the smoothing parameters into  $S_\lambda$ , giving fitted values in terms of the smoothing matrix,

$$\hat{y} = B\hat{\theta} = B(B^T B + S_\lambda)^{-1} B^T y = H_\lambda y.$$

- Now we must decide
  - how many degrees of freedom for each smooth?
  - how to select the smoothing parameters?

Regression Methods

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## Effective degrees of freedom

- Denote the usual (unpenalized) least squares estimate of  $\theta_{(p+q) \times 1}$  by

$$\hat{\theta} = (B^T B)^{-1} B^T y,$$

and note that we can write

$$\hat{\theta}_\lambda = H_\lambda y = (B^T B + S_\lambda)^{-1} B^T y = (B^T B + S_\lambda)^{-1} B^T B \hat{\theta} = P_\lambda \hat{\theta},$$

say, where  $P_\lambda$  shows how penalisation shrinks  $\hat{\theta}$  towards  $\hat{\theta}_\infty = (\hat{\beta}^T, 0^T)^T$ .

- If  $\lambda \approx 0$ , then  $P_\lambda \approx I_{p+q}$  and the degrees of freedom of the two fits are both  $\approx p + q$ , but as  $\lambda \rightarrow \infty$ ,  $P_\lambda$  tends to the projection matrix onto the column space of  $X_{n \times p}$ .
- On slide 254 with just one smooth term we defined

$$\text{df}_\lambda = \text{tr}(S_\lambda) = \text{tr}(P_\lambda) = \sum_{r=1}^{p+q} P_{\lambda,rr} \in (p, p+q),$$

which gives the usual definition for a linear model.

- With several smooth terms,  $\theta^T = (\beta^T, b_1^T, \dots, b_M^T)$ , say, we define the **effective degrees of freedom**  $\text{df}_{\lambda_m}$  associated to the  $m$ th smooth as being the sum of those  $P_{\lambda,rr}$  that correspond to the elements of  $b_m$  in  $\theta$ .

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## Selection of $\lambda$

- Usual suspects:
  - cross-validation sum of squares,  $\text{CV}(\lambda)$ ,
  - generalized cross-validation sum of squares,  $\text{GCV}(\lambda)$ , and
  - REML.
- The first two involve a grid search over values of  $(\log-) \lambda$ , and can be expensive.
- We discuss implementation of the third, which in principle could be cheaper, later.

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## Identifiability

- The identifiability problem is solved by **centering** the fitted smooth, i.e., enforcing

$$1_n^T Z_{n \times q} b_{q \times 1} = 0$$

for each smooth term.

- In general we can use a QR decomposition. If  $C_{m \times q} b_{q \times 1} = 0_{m \times 1}$ , with  $m < q$ , write

$$C_{q \times m}^T = Q_{q \times q} R_{q \times m} = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix},$$

where  $Q$  is orthogonal,

- $Q_1$  has dimension  $q \times m$ ,
- $Q_2$  has dimension  $q \times (q - m)$ , and
- $R_1$  has dimension  $m \times m$  and is upper triangular.

Then if we set  $b_{q \times 1} = Q_2 b'_{(q-m) \times 1}$ , we have

$$Cb = R^T Q^T b = \begin{pmatrix} R_1^T & 0 \end{pmatrix} \begin{pmatrix} Q_1^T \\ Q_2^T \end{pmatrix} Q_2 b' = \begin{pmatrix} R_1^T & 0 \end{pmatrix} \begin{pmatrix} 0 \\ I_{q-m} \end{pmatrix} b' = 0.$$

- Thus the constraint is satisfied if we replace  $Z_{n \times q}$  by  $(ZQ_2)_{n \times (q-1)}$ ; this reduces  $b$  to dimension  $(q - 1) \times 1$ . This is efficiently implemented using Householder operations.

Regression Methods

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## Numerical aspects

- We need to minimise

$$(y - B\theta)^T (y - B\theta) + \theta^T S_\lambda \theta,$$

where  $n$  and  $q$  may be large. Let  $A_\lambda$  be a square root matrix of  $S_\lambda$ , i.e.,  $A_\lambda^T A_\lambda = S_\lambda$ , and note that

$$\left\| \begin{pmatrix} y \\ 0 \end{pmatrix}_{(n+q) \times 1} - \begin{pmatrix} B \\ A_\lambda \end{pmatrix}_{(n+q) \times q} \theta_{q \times 1} \right\|^2 = \|y - B\theta\|^2 + \theta^T S_\lambda \theta$$

has the form of an augmented least squares problem.

- $A_\lambda$  can be found using Choleski decomposition with  $\mathcal{O}(q^3)$  operations.
- The least squares problem can be solved stably and efficiently using standard orthogonal matrix methods, even for very large  $n + q$ .
- To estimate  $\lambda$  by generalized cross-validation: set  $k = 1$ ,  $\lambda_1 = 10^{-8}$ ,  $k_{\max} = 60$ , then while  $k < k_{\max}$ ,
  - compute  $\text{GCV}(\lambda_k)$  using the methods above,
  - set  $\lambda_k \leftarrow 1.5\lambda_k$ ,
  - set  $k \leftarrow k + 1$ ,
- stop and output fit for best value of  $\lambda$

Regression Methods

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## Numerical aspects: REML

- With the linear model

$$y | b \sim \mathcal{N}_n(X\beta + Zb, \sigma^2 I_n), \quad b \sim \mathcal{N}_k(0, \sigma^2 S_\lambda),$$

we get restricted log likelihood

$$\ell(\sigma^2, \lambda) \equiv -\frac{1}{2} \log |U_\lambda| - \frac{1}{2} \log |X^\top U_\lambda^{-1} X| - \frac{1}{2\sigma^2} y^\top P_\lambda y - \frac{n-q}{2} \log \sigma^2,$$

where  $U_\lambda = ZS_\lambda Z^\top + I_n$  and  $P_\lambda = U_\lambda^{-1} - U_\lambda^{-1} X (X^\top U_\lambda^{-1} X)^{-1} X^\top U_\lambda^{-1}$ .

- Given  $\lambda$ , there is an explicit formula for  $\hat{\sigma}^2$ , so we finally seek

$$\hat{\lambda} = \operatorname{argmax} \left\{ -\frac{1}{2} \log |U_\lambda| - \frac{1}{2} \log |X^\top U_\lambda^{-1} X| - \frac{n-q}{2} \log y^\top P_\lambda y \right\},$$

which involves some unpleasant matrix differentials, e.g.,

$$\frac{\partial Q^{-1}}{\partial \lambda} = -Q^{-1} \frac{\partial Q}{\partial \lambda} Q^{-1}, \quad \frac{\partial \log |Q|}{\partial \lambda} = \operatorname{tr} \left( Q^{-1} \frac{\partial Q}{\partial \lambda} \right)$$

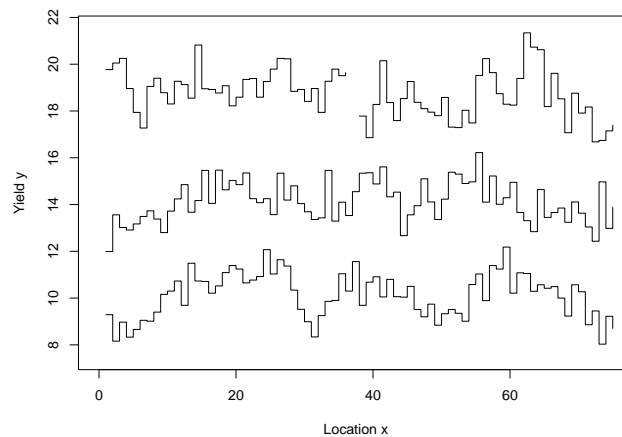
but is just a function of  $\lambda$ . Reasonably efficient computational methods are available . . .

## Example: Spring barley data

Plot yield at harvest for 75 varieties of spring barley sown in 3 blocks each of 75 plots:

Location $t$	Block 1		Block 2		Block 3	
	Variety	Yield $y$	Variety	Yield $y$	Variety	Yield $y$
1	57	9.29	49	7.99	63	11.77
2	39	8.16	18	9.56	38	12.05
3	3	8.97	8	9.02	14	12.25
4	48	8.33	69	8.91	71	10.96
5	75	8.66	29	9.17	22	9.94
6	21	9.05	59	9.49	46	9.27
7	66	9.01	19	9.73	6	11.05
8	12	9.40	39	9.38	30	11.40
9	30	10.16	67	8.80	16	10.78
10	32	10.30	57	9.72	24	10.30
11	59	10.73	37	10.24	40	11.27
12	50	9.69	26	10.85	64	11.13
13	5	11.49	16	9.67	8	10.55
14	23	10.73	6	10.17	56	12.82
15	14	10.71	47	11.46	32	10.95
16	68	10.21	36	10.05	48	10.92
17	41	10.52	64	11.47	54	10.77
18	1	11.09	63	10.63	37	11.08
⋮	⋮	⋮	⋮	⋮	⋮	⋮

### Example: Spring barley data



Yield as a function of location for the three blocks, with yields for blocks 2 and 3 offset by the addition of 4 and of 8 respectively. Value 37 in block 3 (corresponding to variety 27) is missing.

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### Example: Spring barley data

- We fit a model with parametric variety effects and smooth effects for the fertility patterns in the blocks,

$$y_{n \times 1} \sim (X_{n \times 75} \beta_{75 \times 1} + Z_1 \gamma_1 + Z_2 \gamma_2 + Z_3 \gamma_3, \sigma^2 I_n),$$

where

- $n = 224$ , as one of the responses is missing,
  - $X$  is a matrix of indicators (0/1) of which variety is in which plot in each block,
  - $\beta$  are the variety effects, with the model parametrized without an overall mean,
  - $Z_m$  of dimension  $n \times (p_m + q_m)$  corresponds to the basis functions for the smooth in block  $m$ , and
  - $\gamma_m$  are of dimensions  $(p_m + q_m) \times 1$ , for  $m = 1, 2, 3$ , corresponding to the smooth effects, and
  - $p_m + q_m = 9$  by default (after centering) when using `gam` in R package `mgcv`.
- Taking  $p_m = 2$  would correspond to null smooth  $\beta_0 + \beta_1 x$  for each block (i.e., linear fertility pattern), but the identifiability constraints impose  $\beta_0 = 0$ . Hence in fact  $p_m = 1$  for a linear baseline smooth and the degrees of freedom for the smooth terms lie in  $[1, 9]$  (see slide 273).

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### Example: Spring barley data

```
library(SMPracticals)
data(barley)

library(mgcv)

# ML fit of variety as fixed effect, with GCV estimation of lambdas,
# with splines for fertility gradients within each block

fit.gcv <- gam(y~Variety-1+s(Location,by=Block),data=barley)

# fit of variety as fixed effect, with REML estimation of lambdas,
# with splines for fertility gradients within each block

fit <- gam(y~Variety-1+s(Location,by=Block),method="REML",data=barley)

# REML fit with variety as a random effect and splines for fertilities

fit.re <- gam(y~s(Variety,bs="re")+s(Location,by=Block),method="REML",
              data=barley)
```

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### Example: Spring barley data

- ☐ Using GCV the smooths have  $df_\lambda = 8.3, 6.8, 6.3$ , with  $\hat{\sigma} = 0.65$  and  $AIC = 513.1$ , the residual degrees of freedom is  $224 - 75 - 8.3 - 6.8 - 6.3 \approx 130.6$ , with SEs around 0.4 for the estimated variety effects (0.54 for variety 27).
- ☐ Using REML the smooths have  $df_\lambda = 7.2, 3, 6.1$ , with  $\hat{\sigma} = 0.66$  and  $AIC = 518.3$ , the residual degrees of freedom is 132.7, with SEs around 0.4 for the estimated variety effects (0.53 for variety 27).
- ☐ The estimated smoothing parameters are  $\hat{\lambda}_1 = 0.0029$ ,  $\hat{\lambda}_2 = 0.18$  and  $\hat{\lambda}_3 = 0.0078$ .
- ☐ The effective degrees of freedom for the smooth terms, with the totals:

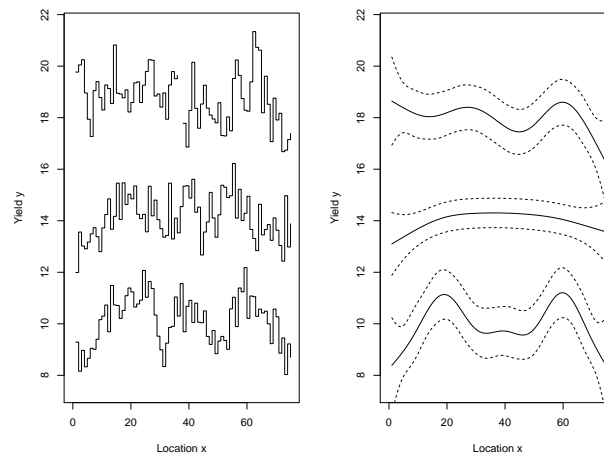
Block	$P_{\lambda,rr}$									Total
1	1.00	1.07	0.90	0.7	0.65	0.17	0.38	1.31	1	7.18
2	0.61	0.21	0.12	-0.2	0.03	-0.26	0.01	1.49	1	3.00
3	0.99	1.04	0.76	0.4	0.41	-0.18	0.18	1.47	1	6.07

- ☐ The  $P_{\lambda,rr}$  need not be positive, though their total for each smooth is positive.
- ☐ In applications it would be wise to check whether increasing  $q_m$  would lead to very different fits.

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### Example: Spring barley data



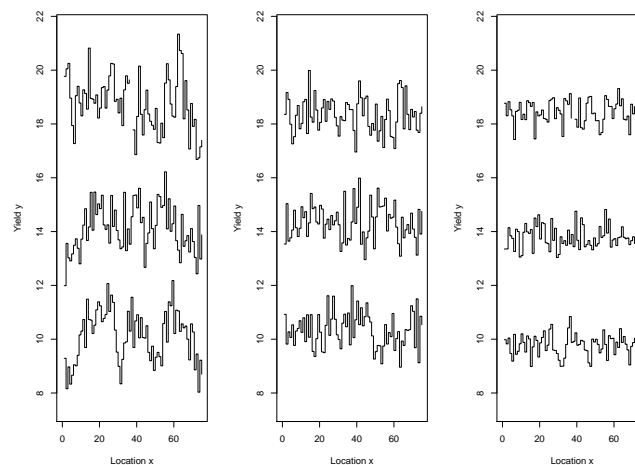
Left: data (offset by adding 4 and 8 to blocks 2 and 3).

Right: estimated fertility patterns (with estimated df 7.2, 3, 6.1) and 95% unconditional pointwise confidence intervals, fitted using REML. The intervals are wider for blocks 1 and 3.

Regression Methods

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### Example: Spring barley data



Left: data (offset by adding 4 and 8 to blocks 2 and 3).

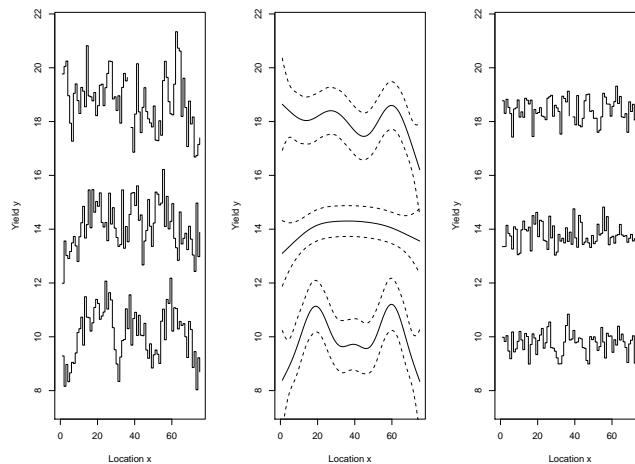
Center: Estimated variety effects (also offset)

Right: residuals (also offset, and showing serial autocorrelation?)

Regression Methods

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### Example: Spring barley data



Left: data (offset by adding 4 and 8 to blocks 2 and 3).  
 Center: estimated fertility patterns (REML), also offset.  
 Right: residuals.

Regression Methods

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### Example: Spring barley data

- ☐ Should the varieties be treated as randomly selected from a population of varieties?
- ☐ If so, we use the same basis matrix  $X$  as in the previous model, but add a penalty matrix  $\lambda_\beta S_\beta$  and minimise the penalised sum of squares

$$(y - B\theta)^T(y - B\theta) + \theta^T S_\lambda \theta,$$

where

$$S_\lambda = \lambda_\beta S_\beta + \lambda_1 S_1 + \lambda_2 S_2 + \lambda_3 S_3,$$

where  $S_\beta = \text{diag}(I_{75}, 0)$ .

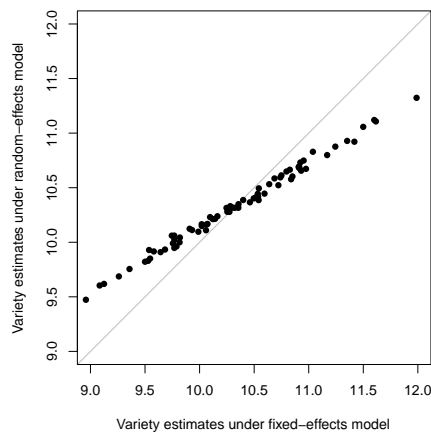
- ☐ The effective degrees of freedom for this model are 44.8 for  $\beta$  and 7.5, 3.9 and 6.4 for the splines.
- ☐ The optimal smoothing parameters are  $\hat{\lambda}_\beta = 1.76$ ,  $\hat{\lambda}_1 = 0.0027$ ,  $\hat{\lambda}_2 = 0.073$  and  $\hat{\lambda}_3 = 0.0070$ .
- ☐ The fixed-effects model has 75 degrees of freedom for  $\beta$ , so this is substantial shrinkage; the estimated standard deviation drops from 0.65 to 0.39.
- ☐ The estimates under the random-effects model have standard errors around 0.31 (0.36 for variety 27), compared to 0.41 (0.54 for variety 27) for the fixed-effects model.
- ☐ The next slide compares the estimates.

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### Example: Spring barley data

Comparison of estimated variety effects under fixed-effects and random-effects models:



Regression Methods

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## 4.5 Inference for Spline Fits

slide 279

### Error of a linear smoother

**Lemma 37** A linear smoother giving  $\hat{y} = H_\lambda y$  applied to data  $y \sim (\mu, \sigma^2 I_n)$  satisfies

$$E \left\{ \sum_{j=1}^n (\hat{y}_j - \mu_j)^2 \right\} = \|(I - H_\lambda)\mu\|^2 + \sigma^2 \text{tr}(H_\lambda^T H_\lambda),$$

where terms on the right represent the squared bias and variance contributions to the overall mean squared error.

This suggests that (as in the usual linear model):

- there is a bias  $(I - H_\lambda)\mu$  unless  $\mu$  lies in the kernel of the matrix  $I - H_\lambda$ , which will happen only if
  - the columns of the fitted  $X$  contain all the true covariates, and
  - there is no need for smoothing, i.e., the spline columns are unnecessary;
- another EDF definition could be  $\text{tr}(H_\lambda^T H_\lambda)$ , since in the linear model case, the second term would be  $\text{tr}(H^T H) = \text{tr}(H) = p$ .

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### Note to Lemma 37

Since

$$(\hat{y}_j - \mu_j)^2 = \{\hat{y}_j - E(\hat{y}_j)\}^2 + 2\{\hat{y}_j - E(\hat{y}_j)\}\{E(\hat{y}_j) - \mu_j\} + \{E(\hat{y}_j) - \mu_j\}^2,$$

the expectation is clearly

$$\begin{aligned} \sum_{j=1}^n \text{var}(\hat{y}_j) + \sum_{j=1}^n \{E(\hat{y}_j) - \mu_j\}^2 &= \text{tr}\{\text{var}(\hat{y})\} + (H_\lambda \mu - \mu)^T (H_\lambda \mu - \mu) \\ &= \text{tr}\{\text{var}(H_\lambda y)\} + \|(I - H_\lambda)\mu\|^2 \\ &= \text{tr}\{H_\lambda \text{var}(y) H_\lambda^T\} + \|(I - H_\lambda)\mu\|^2 \\ &= \sigma^2 \text{tr}(H_\lambda H_\lambda^T) + \|(I - H_\lambda)\mu\|^2, \end{aligned}$$

as required.

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### Inference

- So far we have discussed only ‘point estimation’ of the smooth function  $\mu(x)$ , but in applications we also want
  - pointwise confidence intervals for  $\mu(x)$ ,
  - overall confidence bands for  $\{\mu(x) : x \in \mathcal{S}\}$ , where  $\mathcal{S}$  is some subset of  $\mathcal{X}$ , and
  - tests of hypotheses such as ‘is the spline part needed?’ and ‘is the curve monotonic?’
- Simplest approach to pointwise inference for  $\mu(x)$  is to note that since the spline estimator is linear, we can write  $\hat{\mu}(x) = a_x^T y$ , giving

$$\text{var}\{\hat{\mu}(x)\} = a_x^T \text{var}(y) a_x = \sigma^2 a_x^T a_x$$

when  $\text{var}(y) = \sigma^2 I_n$ .

- This leads to the **(1 - 2α) variability band**,

$$\hat{\mu}(x) \pm \hat{\sigma} \sqrt{a_x^T a_x} \times t_{\text{df}_{\text{res}}}(1 - \alpha),$$

where  $\text{df}_{\text{res}}$  is the residual degrees of freedom; this does not account for the bias of  $\hat{\mu}(x)$  or the estimation of  $\lambda$ .

- The use of  $t_{\text{df}_{\text{res}}}(1 - \alpha)$  is intended to allow for estimation of  $\sigma$ ; for a pointwise 95% variability band we often take  $t_{\text{df}_{\text{res}}}(1 - \alpha) \approx 2$ .

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## Bayesian connection

- Simplest approach to uncertainty estimation is via the Bayesian posterior  $\beta | y \sim \mathcal{N}_p(\hat{\beta}, V_\beta)$ , simulation from which gives posterior inference on an arbitrary function  $a(\beta)$ .
- For a linear function  $a(\beta) = A\beta$  based on an  $a \times p$  matrix of coefficients  $A$ ,

$$A\beta | y \sim \mathcal{N}_a(A\hat{\beta}, AV_\beta A^T), \quad V_\beta = \sigma^2(X^T X + S_\lambda)^{-1},$$

so if  $a(\beta) = X\beta$  then  $A = X$  and the posterior variance is  $XV_\beta X^T$ .

- Bayesian credible intervals have good frequentist properties, averaged over the domain of  $x$ . To see this, note first that  $A\hat{\beta}$  has (frequentist) MSE

$$\begin{aligned} \mathbb{E}(\|A\hat{\beta} - A\beta\|^2) &= \mathbb{E}\left\{\|A\{\hat{\beta} - \mathbb{E}(\hat{\beta})\}\|^2\right\} + \|A\{\mathbb{E}(\hat{\beta}) - \beta\}\|^2 \\ &= \text{tr}\{A\text{var}(\hat{\beta})A^T\} + \|A(F\beta - \beta)\|^2 \\ &= \text{tr}\left\{\sigma^2 A(X^T X + S_\lambda)^{-1} X^T X (X^T X + S_\lambda)^{-1} A^T\right\} \\ &\quad + \text{tr}\left\{A(X^T X + S_\lambda)^{-1} S_\lambda \beta \beta^T S_\lambda^T (X^T X + S_\lambda)^{-1} A^T\right\} \end{aligned}$$

where  $F = (X^T X + S_\lambda)^{-1} X^T X$ , giving  $F - I = -(X^T X + S_\lambda)^{-1} S_\lambda$ .

- This is a bias-variance decomposition, with the first term a variance (which we can approximate) and the second a squared bias (which depends on the unknown  $\beta$ ).

## Bayesian connection II

- To estimate the bias term we note that the Bayesian prior  $\beta \sim \mathcal{N}_p(0, \sigma^2 S_\lambda^{-1})$  gives

$$\mathbb{E}(\beta\beta^T) = \text{var}(\beta) = \sigma^2 S_\lambda^{-1}$$

and replacing this in the bias gives that the MSE is  $\sigma^2 \text{tr}\{A(X^T X + S_\lambda)^{-1} A^T\}$ .

- Now we introduce a random index variable  $J$  that chooses the rows  $a_j^T$  of  $A$  with equal probabilities, and hope to choose constants  $d$  and  $c_j$  such that

$$\text{ACP} = \mathbb{P}\left\{|a_J^T \hat{\beta} - a_J^T \beta| \leq dc_J\right\} = 1 - \alpha;$$

i.e., the **average coverage probability (ACP)** has a desired value averaged over  $y$ ,  $\beta$  and  $J$ .

- We define random variables

$$V = a_J^T \{\hat{\beta} - \mathbb{E}(\hat{\beta})\} / c_J, \quad B = a_J^T \{\mathbb{E}(\hat{\beta}) - \beta\},$$

so  $\mathbb{E}(V) = 0$ ,  $B$  is random because of  $J$ , and  $\mathbb{E}(B) \approx 0$  but  $\text{var}(B) \ll \text{var}(V)$ . To compute  $\text{var}(V + B)$  we therefore need to choose  $d$  and  $C = \text{diag}(c_1, \dots, c_a)$  such that

$$\text{var}\{C^{-1}A(\hat{\beta} - \beta)\} = \mathbb{E}\left\{\|C^{-1}A(\hat{\beta} - \beta)\|^2\right\} = \sigma^2 \text{tr}\{C^{-1}A(X^T X + S_\lambda)^{-1} A^T C^{-1}\},$$

i.e.,  $C = \text{diag}\{A(X^T X + S_\lambda)^{-1} A^T\}^{1/2}$  and  $d = \sigma^2 z_{1-\alpha/2}$ .

## Bayesian connection: Example

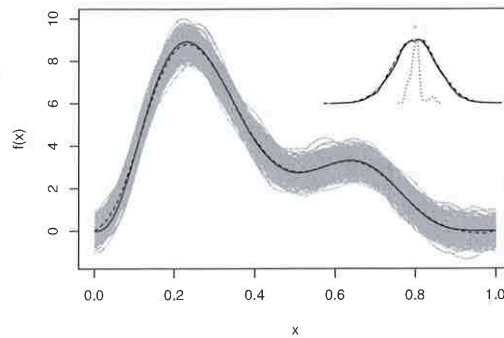


Figure 6.7 The Nychka (1988) idea. The main black curve shows a true function  $f(x)$ , while the grey curves show 500 replicate spline estimates  $\hat{f}(x)$ . The dashed curve is  $\mathbb{E}\hat{f}(x)$ . Inset at top right are scaled kernel smooth estimates of the distributions of the sampling error,  $\hat{f} - \mathbb{E}\hat{f}$  (continuous black); the bias,  $\mathbb{E}\hat{f} - f$ , evaluated at a random  $x$  (dotted) and  $\hat{f} - f$  evaluated at a random  $x$  (dashed). In grey is the normal approximation to the dashed curve. Evaluation at a random  $x$  turns the bias into a random variable, which has substantially lower variance than the approximately normal  $\hat{f} - \mathbb{E}\hat{f}$ . Hence the sum of the randomized bias and sampling error is approximately normally distributed. The variance of this sum turns out to be well approximated by the Bayesian posterior covariance for  $f$ .

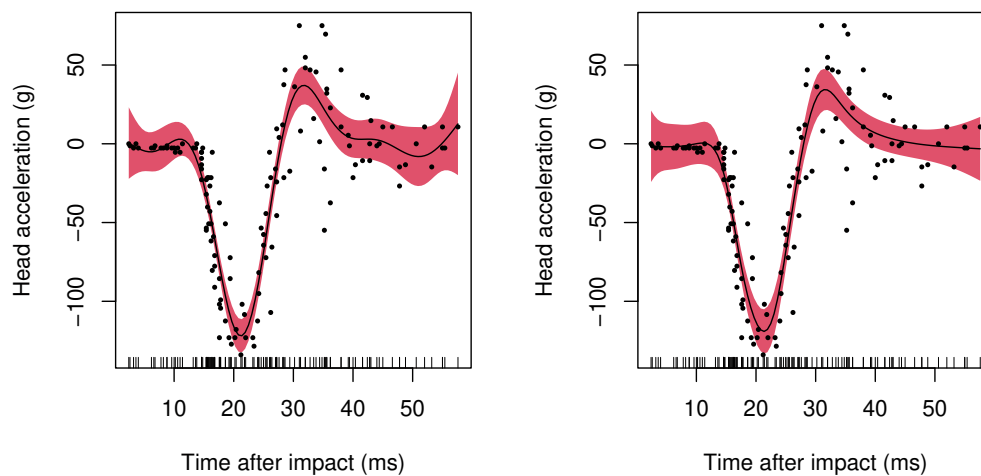
(Wood, 2017)

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## Motorcycle data: adaptive fit

Standard (left) and adaptive (right) spline fits, the latter with  $K = 40$  and  $L = 5$ , and 95% pointwise confidence intervals:



Regression Methods

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## Discussion

- ☐ The basic ideas of spline smoothing extend to the additive model:
  - use of basis functions to represent smooth curves;
  - penalization of parameters/random effects to impose smoothness;
  - REML/GCV estimation of smoothing parameters  $\lambda$ ;
  - linear estimation using shrinkage matrix  $S_\lambda$ ;
  - effective degrees of freedom defined using eigenvalues of  $S_\lambda$ ,  
with
  - inclusion of (unpenalized) parameters for covariate effects;
  - different smoothers for different variables, penalised individually.
- ☐ Penalization corresponds to Bayesian model, with smoothing parameters estimated from the data (empirical Bayes estimation).

**Generalized additive model**

- Now we write

$$E(y) = \mu, \quad g(\mu) = \eta = B\theta = X\beta + Zb,$$

where

- $y$  follows a GLM (or more general) distribution,
- $g(\cdot)$  is a link function,
- the rest is as before ...

giving a **generalized additive model (GAM)**.

- For a general treatment, suppose we have a penalized log likelihood,

$$\ell_\lambda(\theta) = \ell(\theta) - \frac{1}{2}\theta^T S_\lambda \theta = \sum_{j=1}^n \ell_j\{\eta_j(\theta)\} - \frac{1}{2}\theta^T S_\lambda \theta,$$

where  $\theta_{m \times 1}$  (with  $m = p + q$ ) contains both 'fixed-effects'  $\beta_{p \times 1}$  and 'random-effects'  $b_{q \times 1}$ , the latter penalized using a symmetric positive semidefinite  $m \times m$  matrix  $S_\lambda$ , and the underlying observations  $y_1, \dots, y_n$  giving likelihood contributions  $\ell_1, \dots, \ell_n$  are assumed to be independent.

- Now we apply the argument leading to the IWLS algorithm to  $\ell_\lambda$ , leading to the **penalized iterative weighted least squares (PIWLS)** algorithm.

**PIWLS**

- For fixed  $\lambda$ , we apply (ridge regression) iterative weighted least squares with update step

$$\hat{\theta}_\lambda = (B^T W B + S_\lambda)^{-1} B^T W z,$$

where  $S_\lambda$  is the penalty matrix, and

$$B_{n \times m} = \partial \eta / \partial \theta^T, \quad (\text{design matrix})$$

$$W_{n \times n} = \text{diag}(w_1, \dots, w_n), \quad w_j = \{E(-\partial^2 \ell_j / \partial \eta_j^2)\}, \quad (\text{weights})$$

$$u_{n \times 1} = \partial \ell / \partial \eta, \quad (\text{score vector}),$$

$$z_{n \times 1} = B\theta + W^{-1}u, \quad (\text{adjusted dependent variable}).$$

It is easier (but less stable) to use the (random)  $-\partial^2 \ell_j / \partial \eta_j^2$  in place of  $E(-\partial^2 \ell_j / \partial \eta_j^2)$ .

- Thus to obtain (penalized) MLEs  $\hat{\theta}_\lambda$  we use the **PIWLS algorithm**:
- fix  $\lambda$  and take an initial  $\hat{\theta}_\lambda$ . Repeat
- compute  $\eta, B, W, u, z$ ;
  - compute new  $\hat{\theta}_\lambda = (B^T W B + S_\lambda)^{-1} B^T W z$ ;
- until changes in  $\ell_\lambda(\hat{\theta}_\lambda)$  (or  $\hat{\theta}_\lambda$ , or both) are lower than some tolerance.
- We may add a line search: if  $\ell_\lambda(\hat{\theta}_{\lambda, \text{new}}) < \ell_\lambda(\hat{\theta}_{\lambda, \text{old}})$ , halve the step length and try again.

### Note: Derivation of PIWLS algorithm

- To find the estimate  $\hat{\theta}_\lambda$  starting from a trial value  $\theta$ , we make a Taylor series expansion in the score equation

$$0 = \frac{\partial \ell_\lambda(\hat{\theta}_\lambda)}{\partial \theta} \doteq \frac{\partial \ell_\lambda(\theta)}{\partial \theta} + \frac{\partial^2 \ell_\lambda(\theta)}{\partial \theta \partial \theta^T} (\hat{\theta}_\lambda - \theta),$$

where

$$\frac{\partial \ell_\lambda(\theta)}{\partial \theta} = B^T u(\theta) - S_\lambda \theta, \quad \frac{\partial^2 \ell_\lambda(\theta)}{\partial \theta_r \partial \theta_s} = \sum_{j=1}^n \frac{\partial \eta_j(\theta)}{\partial \theta_r} \frac{\partial^2 \ell_j(\theta)}{\partial \eta_j^2} \frac{\partial \eta_j(\theta)}{\partial \theta_s} + \sum_{j=1}^n \frac{\partial^2 \eta_j(\theta)}{\partial \theta_r \partial \theta_s} u_j(\theta) + S_{\lambda, r, s},$$

where  $B \equiv B(\theta) = \partial \eta / \partial \theta^T$ . If we use the approximation

$$-\frac{\partial^2 \ell_\lambda(\theta)}{\partial \theta \partial \theta^T} \doteq B^T W B + S_\lambda, \quad W = \text{diag} \{ -E(\partial^2 \ell_j / \partial \eta_j^2) \},$$

where the diagonal matrix of second derivatives is replaced by its expectation, then

$$\begin{aligned} 0 &\doteq B^T u(\theta) - S_\lambda \theta - (B^T W B + S_\lambda)(\hat{\theta}_\lambda - \theta) \\ &= B^T u(\theta) + B^T W B \theta - (B^T W B + S_\lambda) \hat{\theta}_\lambda. \end{aligned}$$

If  $B^T W B + S_\lambda$  is invertible, this gives

$$\hat{\theta}_\lambda \doteq (B^T W B + S_\lambda)^{-1} B^T (u + W B \theta) = (B^T W B + S_\lambda)^{-1} B^T W z,$$

where  $z = B \theta + W^{-1} u$ , as required.

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### Relation with least squares

- With fixed  $\lambda$ , the penalized MLE

$$\hat{\theta}_\lambda = (B^T W B + S_\lambda)^{-1} B^T W z$$

results from fixing  $\theta$ , and then iteratively solving the minimization problem

$$\min_{\theta} \left\| \begin{pmatrix} W^{1/2} z \\ 0 \end{pmatrix}_{(n+m) \times 1} - \begin{pmatrix} W^{1/2} B \\ Q_\lambda \end{pmatrix}_{(n+m) \times m} \theta_{m \times 1} \right\|^2,$$

where  $Q_\lambda$  is a matrix square root of  $S_\lambda$ , i.e.,  $Q_\lambda^T Q_\lambda = S_\lambda$ .

- The corresponding smoothing matrix is taken to be

$$H_\lambda = B(B^T W B + S_\lambda)^{-1} B^T W,$$

and the effective degrees of freedom for a smooth component are defined as the sum of the corresponding diagonal elements of

$$P_\lambda = (B^T W B + S_\lambda)^{-1} B^T W B,$$

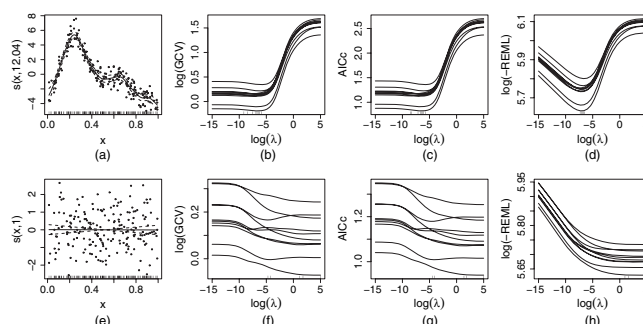
with both  $H_\lambda$  and  $P_\lambda$  evaluated at the final step of the iteration.

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## Numerical example from Wood (2011, JRSSB)

The usual methods (AIC, GCV, ...) for choosing  $\lambda$  are available, but we focus on likelihood methods; see below.



**Fig. 1.** Example comparison of GCV, AICc and REML criteria: (a) some  $(x, y)$ -data modelled as  $y_i = f(x_i) + \varepsilon_i$ ,  $\varepsilon_i$  independent and identically distributed  $N(0, \sigma^2)$  where smooth function  $f$  was represented by using a rank 20 thin plate regression spline (Wood, 2003); (b)–(d) various smoothness selection criteria plotted against logarithmic smoothing parameters, for 10 replicates of the data (each generated from the same ‘truth’) (note how shallow the GCV and AICc minima are relative to the sampling variability, resulting in rather variable optimal  $\lambda$ -values (which are shown as a rug plot), and a propensity to undersmooth; in contrast the REML optima are much better defined, relative to the sampling variability, resulting in a smaller range of  $\lambda$ -estimates); (e)–(h) are equivalent to (a)–(d), but for data with no signal, so that the appropriate smoothing parameter should tend to  $\infty$  (note GCV’s and AICc’s occasional multiple minima and undersmoothing in this case, compared with the excellent behaviour of REML; ML (which is not shown) has a similar shape to REML)

## Approaches to iteration

- ☐ Having chosen how to choose  $\lambda$  for fixed  $\theta$ , there are two main algorithms:
  - **performance iteration** — repeat { fix  $\lambda$ , update  $\theta$  with one step of PIWLS, update  $\lambda$  } to convergence;
  - **outer iteration** — repeat { fix  $\lambda$ , iterate PIWLS to convergence, update  $\lambda$  } to convergence.
- ☐ Performance iteration
  - can be faster,
  - but since the objective function for  $\theta$  changes at each step, it may not converge—especially in the context of **concurvity** (collinearity for curves ...), when two or more smooth functions are (almost) confounded.
- ☐ Outer iteration
  - is computationally more burdensome,
  - but will converge to a (local) optimum.

### Choice of $\lambda$

- The choice of  $\lambda$  can be based on the marginal density of  $y$ ,

$$f(y; \beta, \lambda) = \int f(y | b; \beta) f(b; \lambda) db,$$

which has no closed form in general (but is Gaussian if both  $f$ s are Gaussian).

- Various ways to approximate the integral:
  - quadrature (doesn't work well when  $\dim(b)$  is high);
  - simulation (e.g., importance sampling, same problems as quadrature);
  - Laplace approximation;
  - use the EM algorithm to avoid approximating the integral.
- We focus on Laplace approximation.

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### Laplace approximation

**Lemma 38** Let  $h(u)$  be a smooth convex function defined for  $u \in \mathbb{R}^m$ , with a minimum at  $u = \tilde{u}$ , where  $\partial h(\tilde{u})/\partial u = 0$  and the matrix of partial derivatives  $h_2 \equiv \partial^2 h(\tilde{u})/\partial u \partial u^T$  is positive definite, and let

$$I_n = \int_{\mathbb{R}^m} e^{-nh(u)} du.$$

Then  $I_n = \tilde{I}_n \{1 + O(n^{-1})\}$ , and its **Laplace approximation** is

$$\tilde{I}_n = \frac{(2\pi)^{m/2}}{|nh_2|^{1/2}} e^{-nh(\tilde{u})}.$$

- For marginal density approximation we let  $\theta = (\beta_{p \times 1}^T, b_{q \times 1}^T)^T \sim \mathcal{N}_m(0, S_\lambda^{-1})$ , and write

$$f(y; \beta, \lambda) = \int f(y; \theta) f(\theta; \lambda) d\theta = \frac{|S_\lambda|_+^{1/2}}{(2\pi)^{m/2}} \int \exp\{\ell_\lambda(\theta)\} d\theta,$$

where  $\beta$  is unpenalised,  $|S_\lambda|_+$  is the product of the non-negative eigenvalues of  $S_\lambda$ , and

$$\ell_\lambda(\theta) = \ell(\theta) - \frac{1}{2}\theta^T S_\lambda \theta = O(n);$$

the assumptions of Lemma 38 should be satisfied by  $h(u) \equiv -n^{-1}\ell_\lambda(\theta)$ .

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## Note on Lemma 38

- Close to  $\tilde{u}$  a Taylor series expansion gives

$$h(u) \doteq h(\tilde{u}) + h'(\tilde{u})^T(u - \tilde{u}) + \frac{1}{2}(u - \tilde{u})^T h''(\tilde{u})(u - \tilde{u}) = h(\tilde{u}) + \frac{1}{2}(u - \tilde{u})^T h_2(u - \tilde{u})$$

so if we set  $z = (nh_2)^{1/2}(u - \tilde{u})$  then  $u = \tilde{u} + (nh_2)^{-1/2}z$ ,  $du/dz = (nh_2)^{-1/2}$ , and arguing heuristically (ignoring the third and higher terms),

$$\begin{aligned} I_n &\doteq e^{-nh(\tilde{u})} \int e^{-n(u-\tilde{u})^T h_2(u-\tilde{u})/2} du \\ &= e^{-nh(\tilde{u})} \int_{-\infty}^{\infty} e^{-z^2/2} \frac{du}{dz} dz \\ &= \left( \frac{(2\pi^m)}{|nh_2|} \right)^{1/2} e^{-nh(\tilde{u})}, \end{aligned}$$

because the  $m$ -dimensional normal density has unit integral.

- A more detailed accounting is needed to get the error term. Take the scalar case ( $m = 1$ ) for simplicity. We start by writing

$$\begin{aligned} nh(u) &\doteq nh(\tilde{u}) + \frac{1}{2}nh_2(u - \tilde{u})^2 + \frac{1}{6}nh_3(u - \tilde{u})^3 + \frac{1}{24}nh_4(u - \tilde{u})^4 + \dots \\ &= nh(\tilde{u}) + \frac{1}{2}z^2 + \frac{1}{6}\frac{h_3/h_2^{3/2}}{n^{1/2}}z^3 + \frac{1}{24}\frac{h_4/h_2^2}{n}z^4 + O(n^{-3/2}) \\ &= nh(\tilde{u}) + \frac{1}{2}z^2 + \frac{A}{n^{1/2}}z^3 + \frac{B}{n}z^4 + O(n^{-3/2}) \end{aligned}$$

say. Hence

$$\begin{aligned} e^{-nh(u)} &= e^{-nh(\tilde{u}) - \frac{1}{2}z^2} \left\{ 1 - \frac{A}{n^{1/2}}z^3 - \frac{B}{n}z^4 + \frac{1}{2} \left( -\frac{A}{n^{1/2}}z^3 - \frac{B}{n}z^4 \right)^2 + O(n^{-3/2}) \right\} \\ &= e^{-nh(\tilde{u}) - \frac{1}{2}z^2} \left\{ 1 - \frac{A}{n^{1/2}}z^3 - \frac{B}{n}z^4 + \frac{1}{2}\frac{A^2}{n}z^6 + O(n^{-3/2}) \right\}. \end{aligned}$$

- As the odd moments of the normal density are zero, integration with respect to  $z$  leaves only the  $n^{-1}$  term and the next remaining term is  $O(n^{-2})$ . The fourth and sixth moments of the standard normal distribution are respectively 3 and 15, and

$$15A^2/2 - 3B = 15(h_3/h_2^{3/2}/6)^2/2 - 3\{h_4/(24h_2)\} = \frac{15h_3^2}{72h_2^3} - \frac{h_4}{8h_2^2} = \frac{5h_3^2}{24h_2^3} - \frac{h_4}{8h_2^2},$$

as required. The same argument works for  $m > 1$ , but it is more of a bloodbath.



### Comments on Laplace approximations

- ☐ The  $O(1/n)$  error is relative, so the approximation is often surprisingly accurate;
- ☐ since the odd moments of the normal density are all zero, the expansion has only terms whose orders are even powers of  $n^{-1/2}$ , i.e.,  $n^{-1}, n^{-2}, \dots$ ;
- ☐  $\tilde{I}_n$  involves only  $h$  and the hessian matrix  $h_2$  at  $\tilde{u}$ , so is easily found, numerically if necessary;
- ☐ the series is asymptotic, so the partial sums may not converge, and including additional terms may not be useful;
- ☐ as most of the normal probability lies within  $\pm 3$  standard deviations of the mean, the limits of the integral are almost irrelevant provided they are far enough away from  $\tilde{u}$ ;
- ☐ if

$$I_n = \int_{-\infty}^{\infty} e^{-nh(u)} du, \quad J_n = \int_{-\infty}^{\infty} e^{-nh^*(u)} du,$$

where  $h^*(u) = h(u) + O(n^{-1})$ , then

$$(I_n/J_n) \div (\tilde{I}_n/\tilde{J}_n) = 1 + O(n^{-2}),$$

so two Laplace approximations can be better than one.

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### Approximate REML

- ☐ Laplace approximation gives the approximate restricted log likelihood

$$\ell_p(\lambda) \equiv \frac{1}{2} \log |S_\lambda| + -\frac{1}{2} \log |B^T W B^T + S_\lambda| + \ell(\hat{\theta}_\lambda) - \frac{1}{2} \hat{\theta}_\lambda^T S_\lambda \hat{\theta}_\lambda + O_p(n^{-1}),$$

where  $O_p(n^{-1})$  is a (random) term of order  $n^{-1}$  and

$$\hat{\theta}_\lambda = (B^T W B + S_\lambda)^{-1} B^T W z$$

results from iterating PIWLS to convergence for fixed  $\lambda$  and satisfies  $\partial \ell_\lambda(\hat{\theta}_\lambda) / \partial \theta = 0$ .

- ☐ The expression for  $\hat{\theta}_\lambda$  contains

$$B \equiv B(\hat{\theta}_\lambda), \quad W \equiv W(\hat{\theta}_\lambda), \quad z = B(\hat{\theta}_\lambda) \hat{\theta}_\lambda + W^{-1}(\hat{\theta}_\lambda) u(\hat{\theta}_\lambda),$$

which involve the first two derivatives of the log likelihood contributions  $\ell_j$ .

- ☐ Newton–Raphson maximization of  $\ell_p(\lambda)$  requires its first two derivatives, so we need

$$\frac{\partial \hat{\theta}_\lambda}{\partial \lambda}, \quad \frac{\partial^2 \hat{\theta}_\lambda}{\partial \lambda \partial \lambda^T},$$

which will involve the third and fourth derivatives of the  $\ell_j$  ... could be painful.

- ☐ A version of this is implemented in `mgcv`.

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## UK monthly AIDS reports 1983–1992

Diagnosis period		Reporting-delay interval (quarters):									Total reports to end of 1992
Year	Quarter	0 <sup>†</sup>	1	2	3	4	5	6	...	≥14	
	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮
1988	1	31	80	16	9	3	2	8	...	6	174
	2	26	99	27	9	8	11	3	...	3	211
	3	31	95	35	13	18	4	6	...	3	224
	4	36	77	20	26	11	3	8	...	2	205
1989	1	32	92	32	10	12	19	12	...	2	224
	2	15	92	14	27	22	21	12	...	1	219
	3	34	104	29	31	18	8	6	...		253
	4	38	101	34	18	9	15	6	...		233
1990	1	31	124	47	24	11	15	8	...		281
	2	32	132	36	10	9	7	6	...		245
	3	49	107	51	17	15	8	9	...		260
	4	44	153	41	16	11	6	5	...		285
1991	1	41	137	29	33	7	11	6	...		271
	2	56	124	39	14	12	7	10	...		263
	3	53	175	35	17	13	11	2			306
	4	63	135	24	23	12	1				258
1992	1	71	161	48	25	5					310
	2	95	178	39	6						318
	3	76	181	16							273
	4	67	66								133

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## AIDS data

- ☐ Chain-ladder model: number of reports in row  $j$  and column  $k$  is Poisson, with mean

$$\mu_{jk} = \exp(\alpha_j + \beta_k),$$

but

- why should there be different parameters  $\alpha_j$  and  $\beta_k$  for every row and column?
- Wouldn't smooth variation be more plausible?

- ☐ Better models (maybe?):

$$\mu_{jk} = \exp\{s(j) + \beta_k\}, \quad \mu_{jk} = \exp\{s(j) + s(k)\},$$

where the time effect  $s(j)$  and the delay effect  $s(k)$  vary smoothly.

- ☐ Should also account for the overdispersion ...

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## Example: AIDS data

```
library(mgcv); library(boot)
data(aids)
aids.in <- aids[c(1:570)[as.logical(1-aids$dud)],] # these are elements in the two-way table
aids.glm <- glm(y~factor(time)+factor(delay),family=quasipoisson,data=aids.in)
aids.gam1 <- mgcv::gam(y~s(time,k=20)+factor(delay)-1,family=quasipoisson,data=aids.in)
plot(aids.gam1,page=1)
> anova(aids.gam1)
```

Formula:

```
y ~ s(time, k = 20) + factor(delay)
```

Parametric Terms:

	df	F	p-value
factor(delay)	14	261.6	<2e-16

Approximate significance of smooth terms: # Ref.df can be ignored

	edf	Ref.df	F	p-value
s(time)	4.891	6.129	189.1	<2e-16

```
aids.gam2 <- mgcv::gam(y~s(time,k=20)+s(delay,k=15),family=quasipoisson,data=aids.in)
> anova(aids.gam2)
```

Formula:

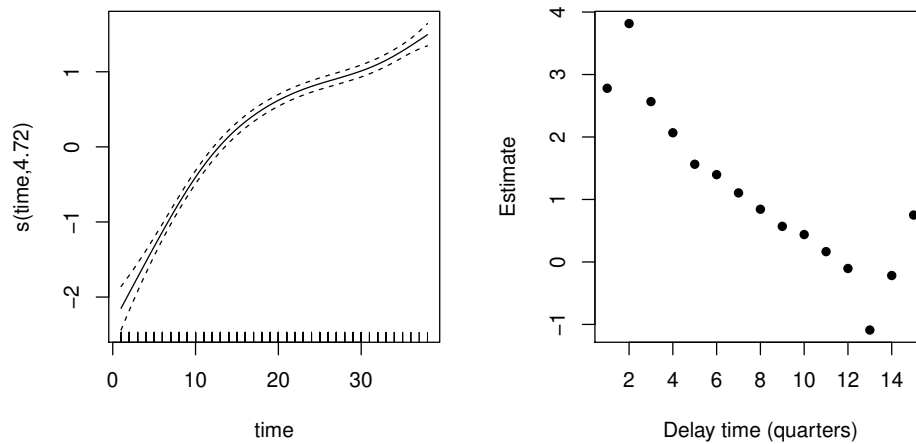
```
y ~ s(time, k = 20) + s(delay, k = 15)
```

Approximate significance of smooth terms:

	edf	Ref.df	F	p-value
s(time)	4.896	6.134	189.0	<2e-16
s(delay)	11.453	12.754	285.5	<2e-16

The fits are very similar, but aids.gam2 has slightly lower AIC of 792.0 compared to 792.1 — these are so similar that the choice should be based on interpretability rather than on AIC.

### Example: AIDS data

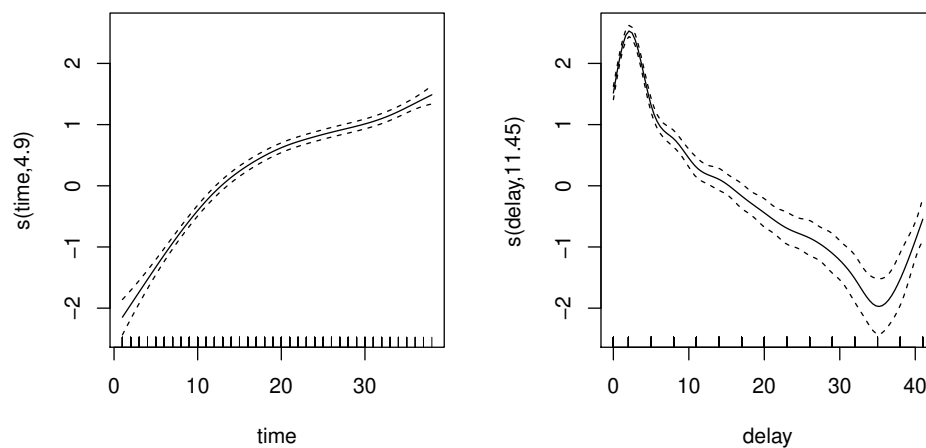


Estimates of (centered) smooth functions  $s(j)$  and parameters based on `plot(aids.gam1)` and `coef(aids.gam1)`.

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### Example: AIDS data

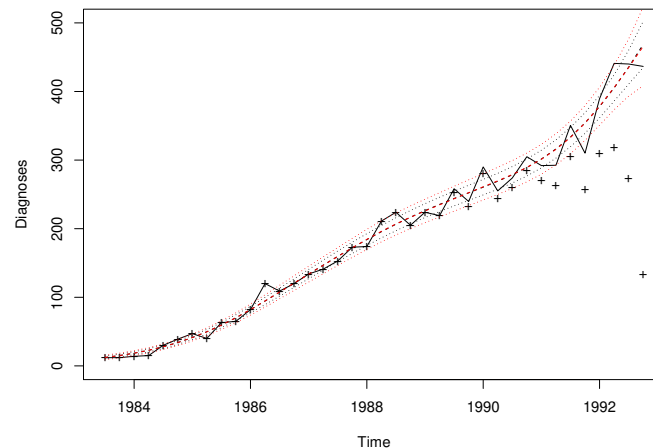


Estimates of (centered) smooth functions  $s(j)$  and  $s(k)$  based on `plot(aids.gam2)`.

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### Example: AIDS data



Numbers of recorded deaths (+), with estimated mean deaths per quarter based on chain-ladder model (solid) and on Poisson (black dashes) and quasi-likelihood GAMs with Poisson variance function  $V(\mu) = \mu$  (red dashes). The last two estimates have 95% pointwise confidence intervals (dots) based on the fit (treating the smoothing parameters as fixed). To make these I had to compute the fitted means for the missing lower right triangle of the data table.

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### Closing

- ☐ The basic ideas of regression, dependence of a response on explanatory variables, extend far beyond the linear model, to
  - non-linear dependence on explanatory variables;
  - general response distributions (Poisson, binomial, ...);
  - random effects models—some parameters treated as random, and others as fixed;
  - smooth curve fitting by basis function methods in (generalized) additive models.
- ☐ Unifying themes are:
  - (semi-)parametric modelling using basis functions;
  - maximum likelihood inference;
  - estimation using iterative weighted least squares algorithms;
  - penalized fitting to allow for random effects/basis functions;
  - analysis of deviance;
  - residuals and other diagnostics.

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