Regularization

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Introduction to Machine Learning

EPFL

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When Linear Models Are Too Flexible

In the old days

Typically $n > p$ (much more data than predictors)

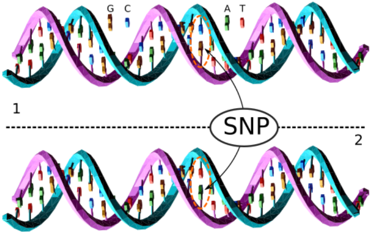
For example: predict blood pressure based on age, gender and body mass index (BMI) (e.g. $n = 200$ patients, $p = 3$).

Nowadays: Big Data

Often $n \approx p$ or $n < p$

For example: predict blood pressure based on 500 000 single nucleotide polymorphisms (SNP) ($n = 200$, $p = 500\,000$).

$\Rightarrow$ **Linear Model perfectly fits the training data.**



Making Linear Models Less Flexible

Idea 1: Fix some parameters at zero

$$\hat{y} = f(x) = f(x_1, x_2, \ldots, x_p) = \beta_0 + \underbrace{\beta_1}_{\cancel{\neq 0}} \cancel{x_1} + \underbrace{\beta_2}_{\cancel{\neq 0}} \cancel{x_2} + \beta_3 x_3 + \cdots + \underbrace{\beta_{p-1}}_{\cancel{\neq 0}} \cancel{x_{p-1}} + \beta_p x_p$$

Problem: Many different models to fit; $\binom{p+1}{m}$ combinations of m non-fixed parameters.

Idea 2: constrain the parameters

Minimize the original loss $L(\beta)$ under the constraint $\|\beta\|_2^2 = \sum_{i=1}^{p} \beta_i^2 \leq S$.

This is equivalent to replacing the original loss $L(\beta)$ by

$$L_{\mathrm{L2}}(\beta) = L(\beta) + \lambda \|\beta\|_2^2$$

Note: idea 2 does not put the parameters to zero. Instead it decreases the flexibility by restricting the space of possible parameter values.

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Ridge Regression (L2 Regularization)

$$L_{\mathrm{L2}}(\theta) = L(\theta) + \lambda \|\theta\|_2^2$$

with **regularization constant** λ and (squared) **L2 norm** $\|\theta\|_2^2 = \sum_{i=1}^{p} \theta_i^2$.

1. The regularization constant λ is a hyper-parameter.
2. Often the intercept θ_0 is not regularized.
3. If $\lambda = 0$: original loss (no penalty)
4. The larger λ, the stronger the impact of the penalty on the result.
5. With increasing λ the model becomes less flexible.
6. With increasing λ all parameters tend to zero; it happens rarely that one is exactly zero.

Lasso (L1 Regularization)

$$L_{\mathrm{L1}}(\theta) = L(\theta) + \lambda\|\theta\|_1$$

with **regularization constant** λ and **L1 norm** $\|\theta\|_1 = \sum_{i=1}^{p} |\theta_i|$.

Points 1-5 from ridge regression are also valid for the Lasso. However:

6. With large λ some parameters are exactly zero (in contrast to ridge regression).

Quiz

- The Lasso tends to have larger variance (when fitted on different training sets from the same data generator) but smaller bias (relative to the true data generator) than linear regression.
- Indicate which is correct: as we increase S from 0 to a large value in L2 regularized linear regression the training error will be

  A) inverted U shape. B) U shape.
  C) steadily increasing. D) steadily decreasing. E) constant.
- Indicate which is correct: as we increase S from 0 to a large value in L2 regularized linear regression the test error will be

  A) inverted U shape. B) U shape.
  C) steadily increasing. D) steadily decreasing. E) constant.

Analytical Solutions for Simple Linear Regression

Notation: $\langle x \rangle = \frac{1}{n}\sum_{i=1}^{n} x_i$

Ridge Regression

$$L(\theta, \lambda) = \langle (y - \theta_0 - \theta_1 x)^2 \rangle + \lambda \theta_1^2$$

$$\theta_1 = \frac{\langle xy \rangle - \langle x \rangle \langle y \rangle}{\langle x^2 \rangle - \langle x \rangle^2 + \lambda}, \qquad \theta_0 = \langle y \rangle - \theta_1 \langle x \rangle$$

Lasso

$$L(\theta, \lambda) = \frac{1}{2}\langle (y - \theta_0 - \theta_1 x)^2 \rangle + \lambda |\theta_1|$$

$$\theta_1 = \frac{\langle xy \rangle - \langle x \rangle \langle y \rangle - \mathrm{sign}(\theta_1)\lambda}{\langle x^2 \rangle - \langle x \rangle^2} \text{ or } 0 \text{ if } |\langle xy \rangle - \langle x \rangle \langle y \rangle| < \lambda$$

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An Alternative Formulation of Regularization

Thanks to a result from constraint optimization (see Karush-Kuhn-Tucker conditions, a generalization of Lagrange multipliers) the above formulations of Ridge Regression and the Lasso are equivalent to a constraint optimization problem:

Ridge Regression

minimize $L(\theta)$ under the constraint that $\|\theta\|_2^2 \leq S$.

The parameters are confined to a p-ball of radius S with center at the origin.

Lasso

minimize $L(\theta)$ under the constraint that $\|\theta\|_1 \leq S$.

The parameters are confined to a hypercube with edge length S, center at the origin and corners on the axes.

S is a (complicated) function of λ and the original loss $L(\theta)$.
With increasing S the model becomes more flexible.

Standardized Inputs for Regularization

Problem

Assume we find in multiple linear regression on the weather data the following parameters

X_1	LUZ_pressure	[hPa]	$\theta_1 = -1$	[km/h/hPa]
X_2	LUZ_temperature	[°C]	$\theta_2 = 0.5$	[km/h/°C]

We could have measured the pressure in Pa and get the equivalent result

X_1	LUZ_pressure	[Pa]	$\theta_1 = -1/100$	[km/h/Pa]
X_2	LUZ_temperature	[°C]	$\theta_2 = 0.5$	[km/h/°C]

With regularization $\lambda(\theta_1^2 + \theta_2^2)$ we would get different results for measurements in hPa and in Pa, because θ_1 contributes less to the penalty in the latter case.

Solution

Standardize all predictors, such that they have mean 0 and variance 1:

$$\tilde{X}_i = (X_i - \bar{X}_i)/\sqrt{\mathrm{Var}(X_i)}$$

Scaling of the Regularization Constant with n

With total loss $L(\theta) = \sum_{i=1}^n \ell(y_i, f(x_i)) + \lambda\|\theta\|_2^2$
the effective regularization depends on the size of the data set.

This is not the case, with average loss

$$L(\theta) = \frac{1}{n}\sum_{i=1}^n \ell(y_i, f(x_i)) + \lambda\|\theta\|_2^2 \tag{1}$$

or (equivalently) scaled regularization term

$$L(\theta) = \sum_{i=1}^n \ell(y_i, f(x_i)) + n \cdot \lambda\|\theta\|_2^2 \tag{2}$$

Version Eq. 1 or Eq. 2 is usually implemented in software packages like scikit-learn or MLJLinearModels.jl. Check the documentation if unsure!

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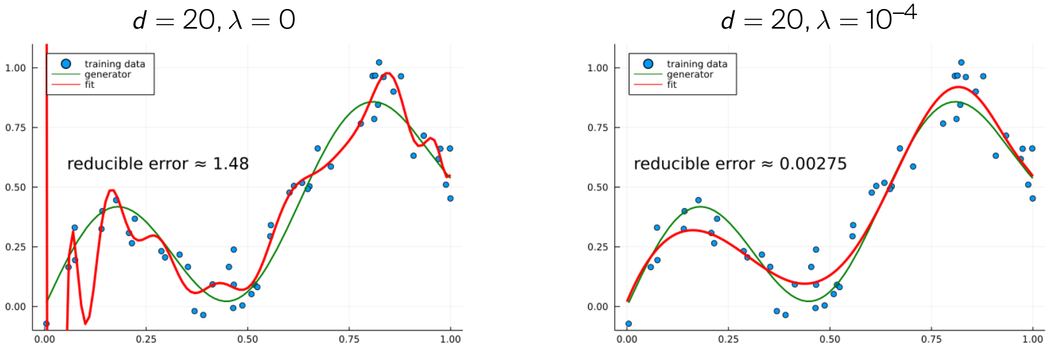
Polynomial Ridge Regression



With a little bit of L2 regularization ($\lambda = 10^{-4}$)
one can prevent overfitting of polynomials with high degrees.

Multiple Logistic Ridge Regression on the Spam Data

$n = 2000$ emails, $p = 801$ features (size of the lexicon)

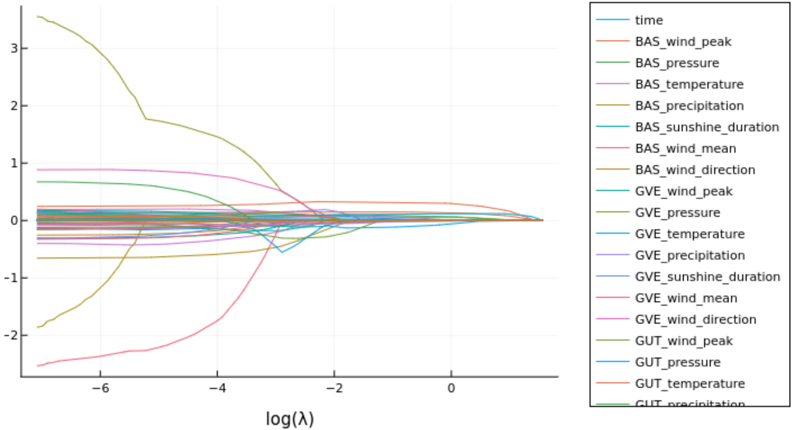
Without regularization

training misclassification rate: 0.0015
test misclassification rate: 0.048

With L2 regularization

training misclassification rate: 0.013
test misclassification rate: 0.041

The Lasso Path for the Weather Data



The Lasso path is useful to identify the most important predictors.

There are specialized efficient methods to compute the Lasso path.

As we lower λ (from right to left), `BER_wind_peak` is the first non-zero factor, `BAS_wind_peak` the second and `LUZ_wind_mean` the third.

Summary

- Regularization allows to lower the flexibility of a model by restricting the parameters to certain areas of the parameter space.
- L1 regularization leads to sparse models with some parameters exactly zero $\Rightarrow$ great for interpretability.

Suggested Reading

- 6.2 Shrinkage Methods
- 6.4 Considerations in High Dimensions