



ChE-609

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Basics of machine learning for chemistry and materials science

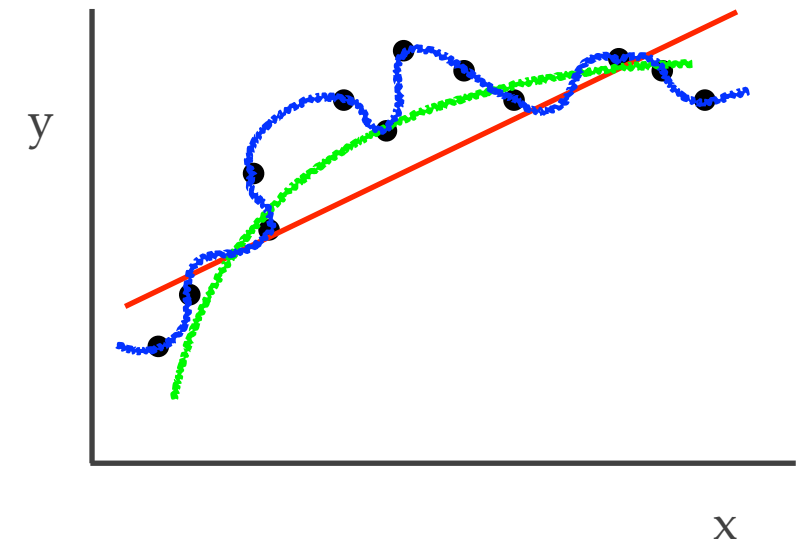
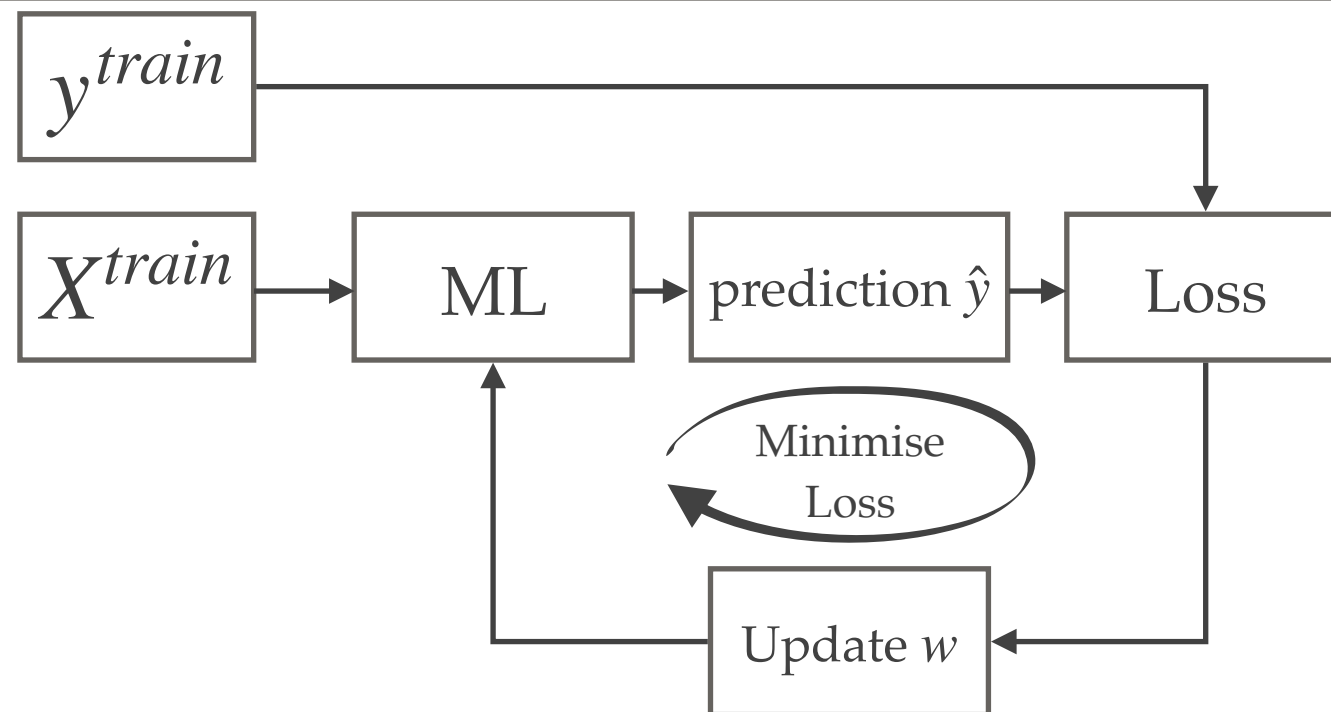


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Model complexity and error



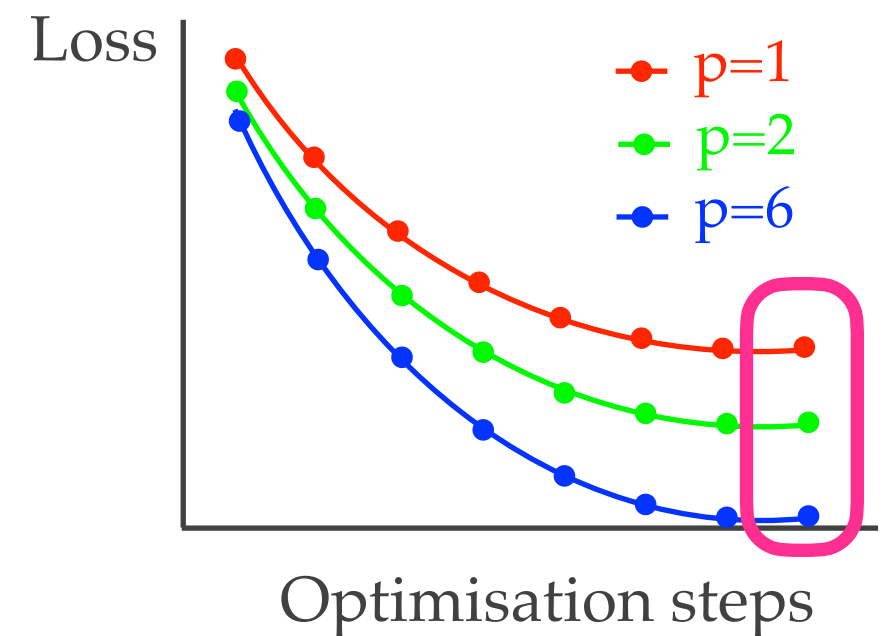
Adding nonlinear terms: polynomial order p

$$\hat{y}_{ML}(x^*) = x^* w = \begin{bmatrix} 1 & x^* & (x^*)^2 & \dots & (x^*)^p \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ \vdots \\ w_p \end{bmatrix}$$

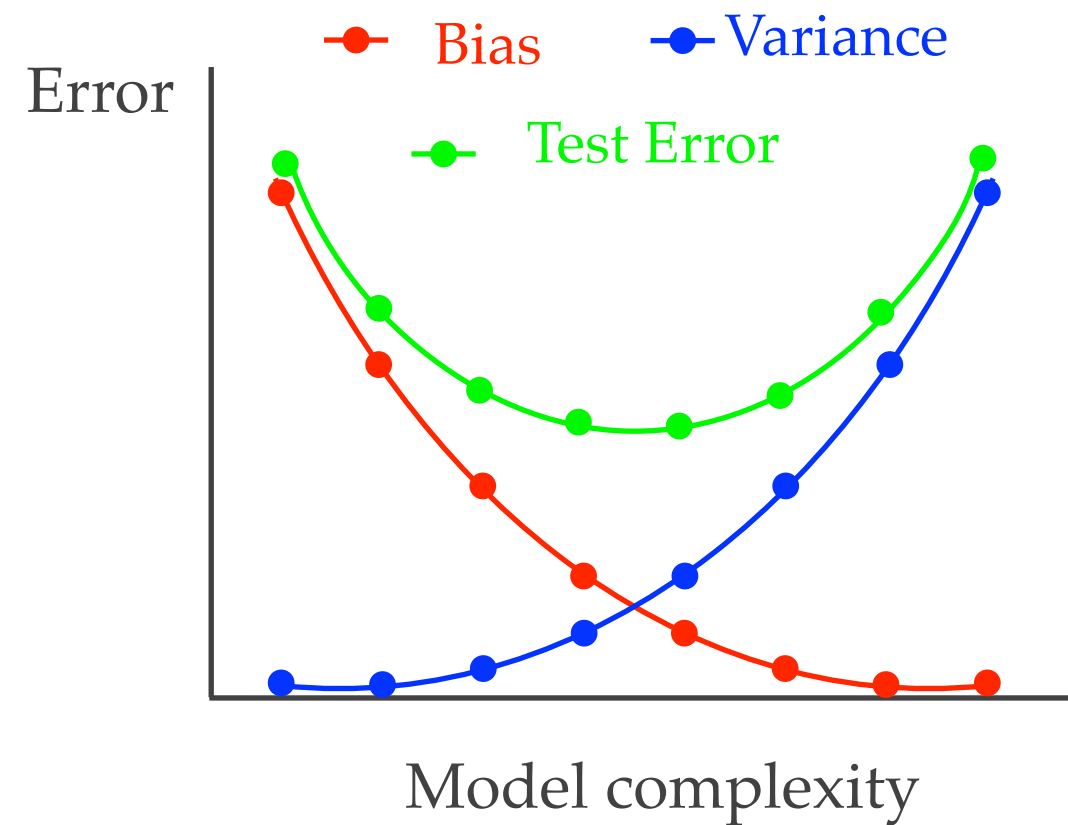
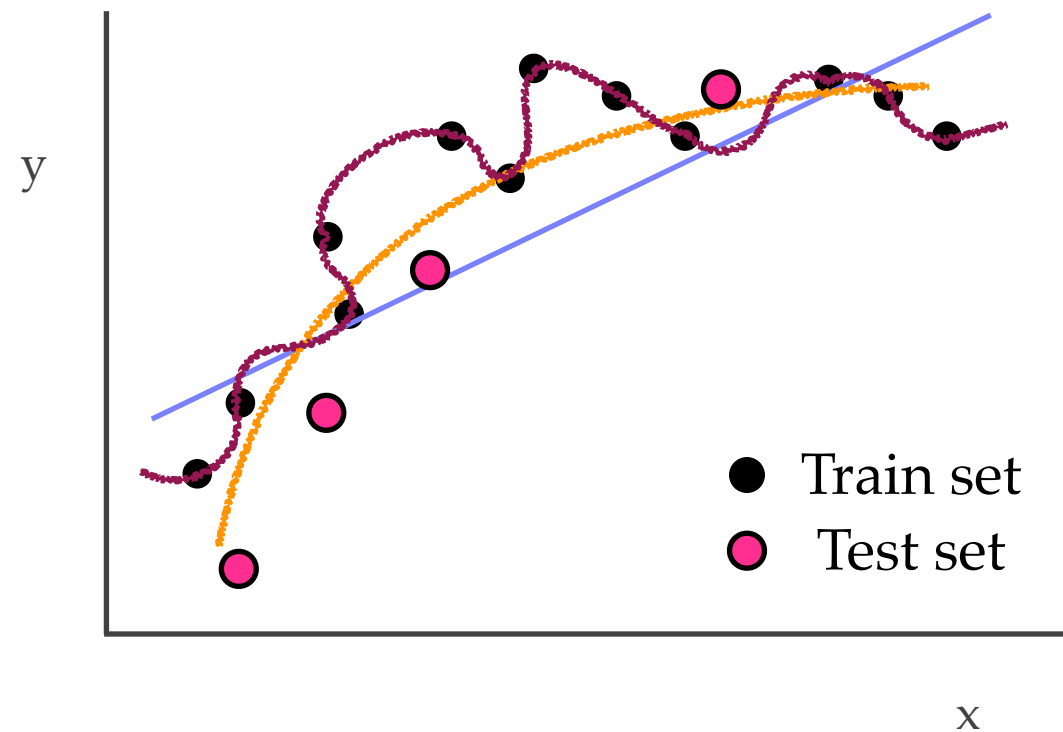
Matrix form:

$$\hat{y}_{ML}(X) = Xw = \begin{bmatrix} 1 & x^1 & (x^1)^2 & \dots & (x^1)^p \\ \vdots & \vdots & \ddots & & \vdots \\ 1 & x^m & (x^m)^2 & \dots & (x^m)^p \end{bmatrix} \begin{bmatrix} w_0 \\ \vdots \\ w_p \end{bmatrix}$$

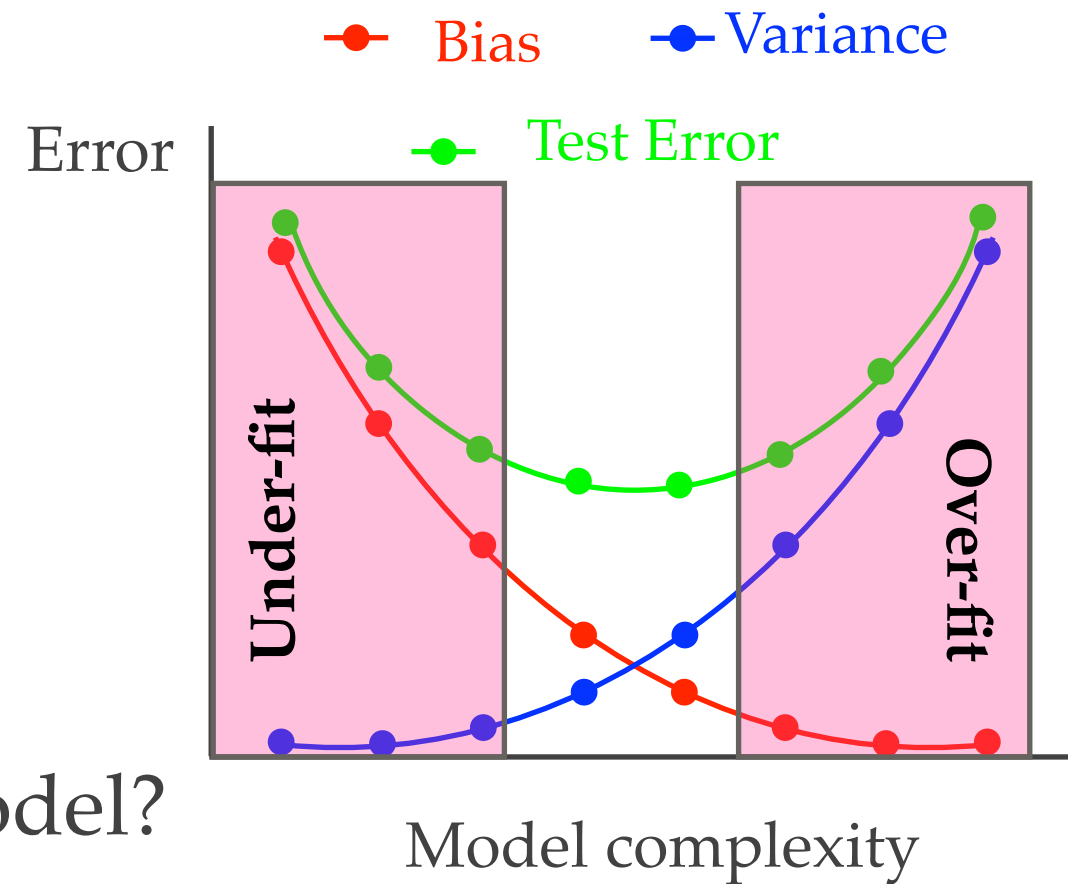
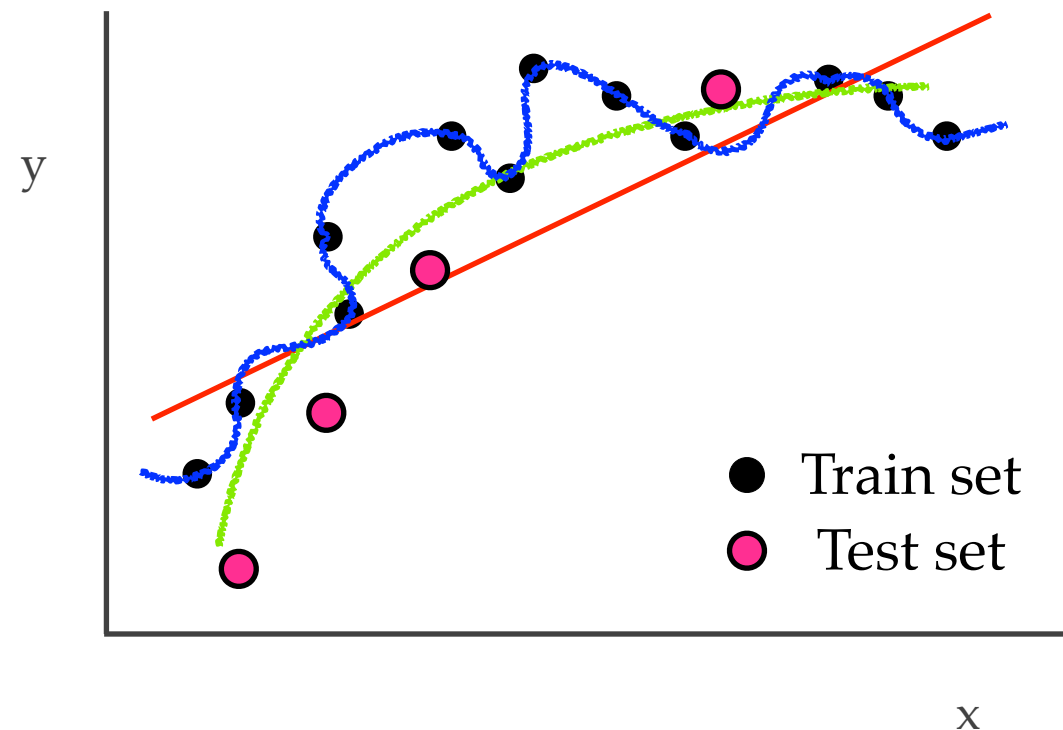
Loss function: $\mathcal{L} = \|\hat{y}_{ML} - y\|_2^2 = \|Xw - y\|_2^2$



Bias –variance tradeoff

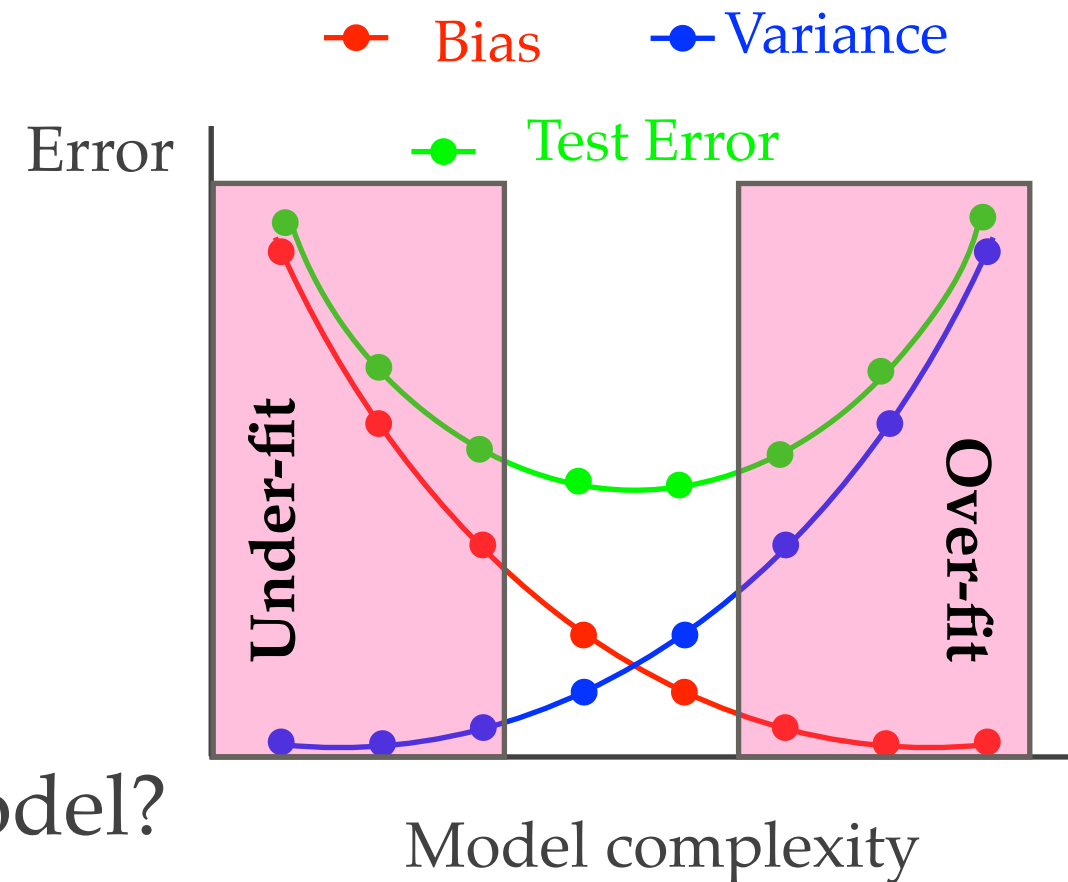
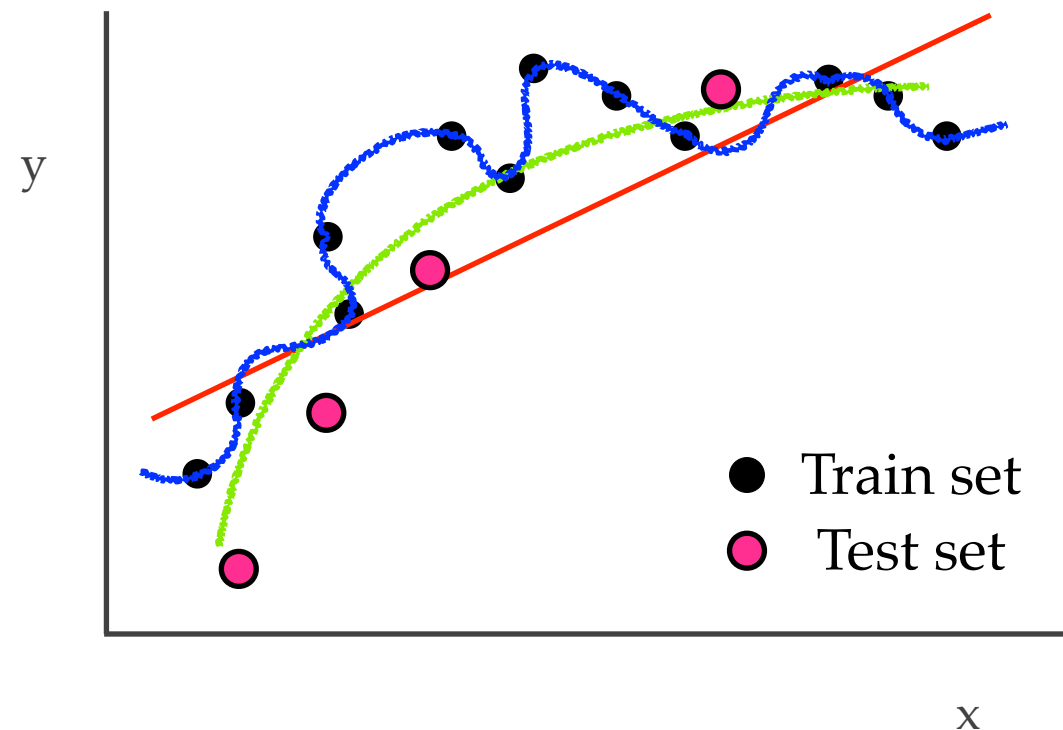


Bias –variance tradeoff



How to include this in the model?

Bias –variance tradeoff: regularisation



How to include this in the model?

Regularise the loss function: $\mathcal{L} = \|\hat{y}_{ML} - y\|_2^2 + \lambda \|w\|_2^2$

Penalising the terms with large weight