NATIONAL UNIVERSITY OF
SCIENCES AND TECHNOLGOY

Machine Learning

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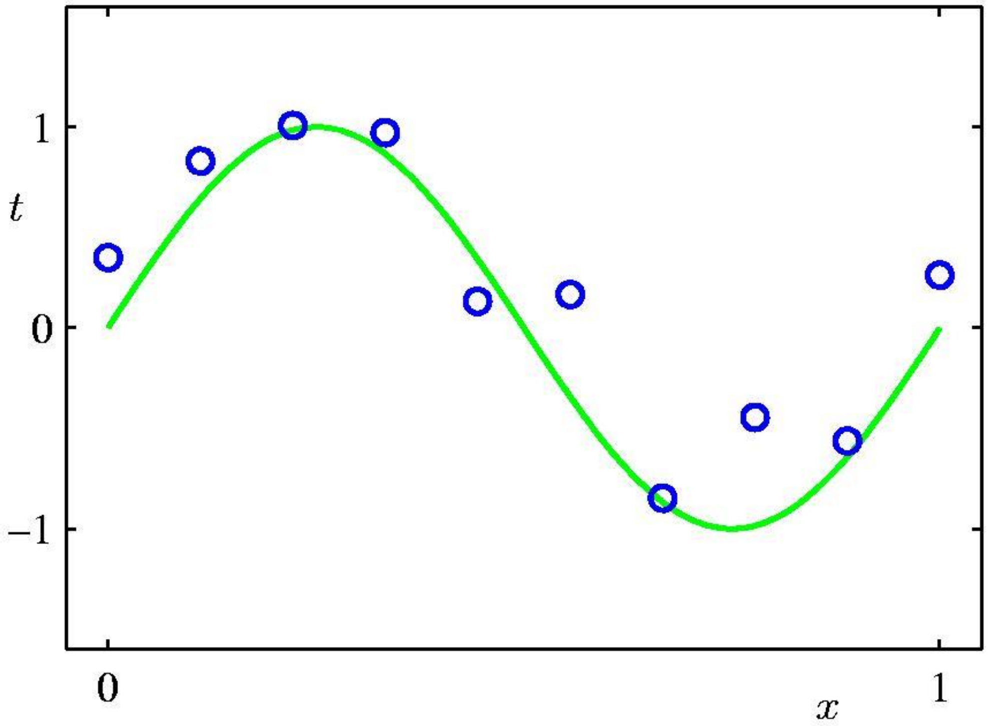
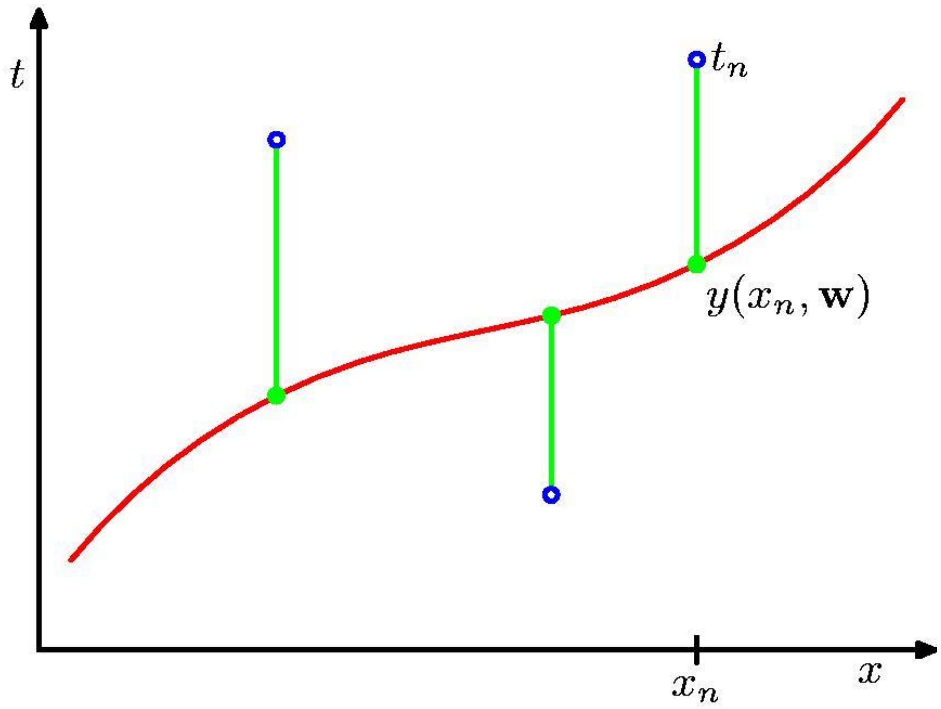
Polynomial Curve Fitting



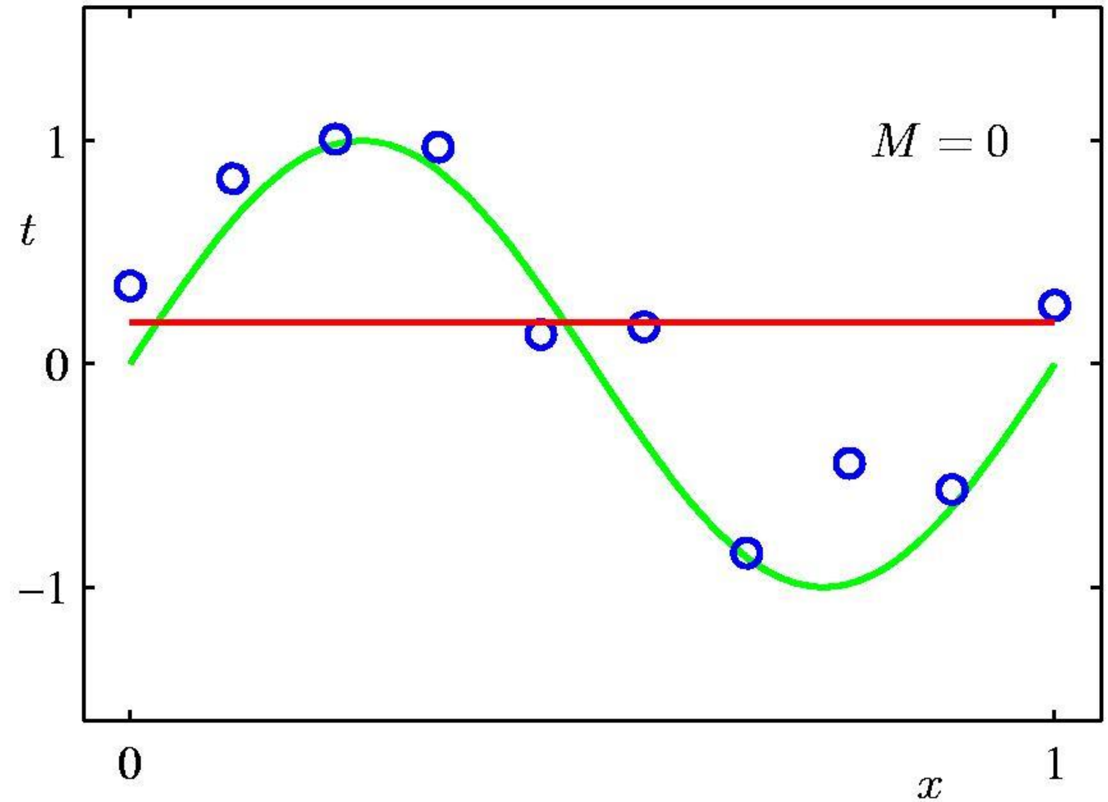
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Sum-of-Squares Error Function



$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2$$

0^{th} Order Polynomial



Fitting a Polynomial

$$\begin{bmatrix} N & \sum_{i=1}^{N} x_i & \cdots & \sum_{i=1}^{N} x_i^k \\ \sum_{i=1}^{N} x_i & \sum_{i=1}^{N} x_i^2 & \cdots & \sum_{i=1}^{N} x_i^{k+1} \\ \vdots & \vdots & \vdots & \vdots \\ \sum_{i=1}^{N} x_i^k & \sum_{i=1}^{N} x_i^{k+1} & \cdots & \sum_{i=1}^{N} x_i^{2k} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_k \end{bmatrix} = \begin{bmatrix} \sum_{i=1}^{N} y_i \\ \sum_{i=1}^{N} x_i y_i \\ \vdots \\ \sum_{i=1}^{N} x_i^k y_i \end{bmatrix}$$

a : Polynomial coefficient

k : The degree of the polynomial

N : The number of points to be regressed

ϵ : Error

Fitting a Polynomial

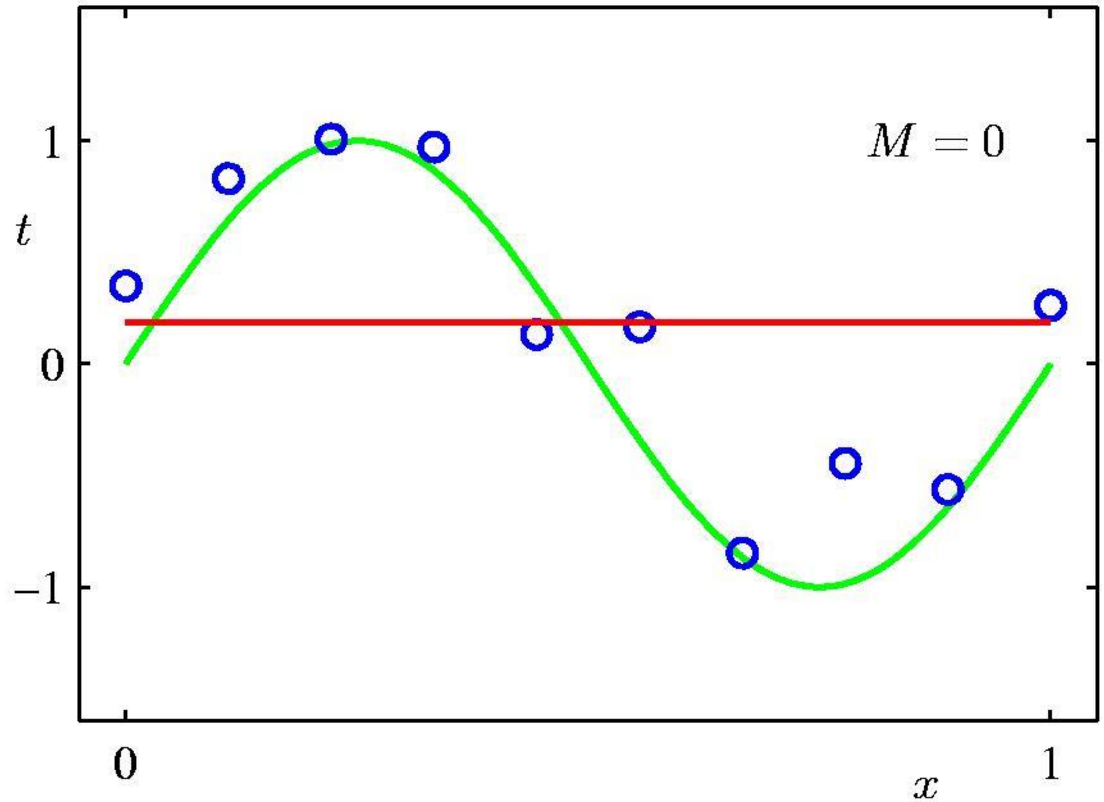
Cramer's rule allows you to solve the linear system of equations to find the regression coefficients using the determinants of the square matrix M. Each of the coefficients a_k may be determined using the following equation:

$$a_k = \frac{det(M_i)}{det(M)}$$

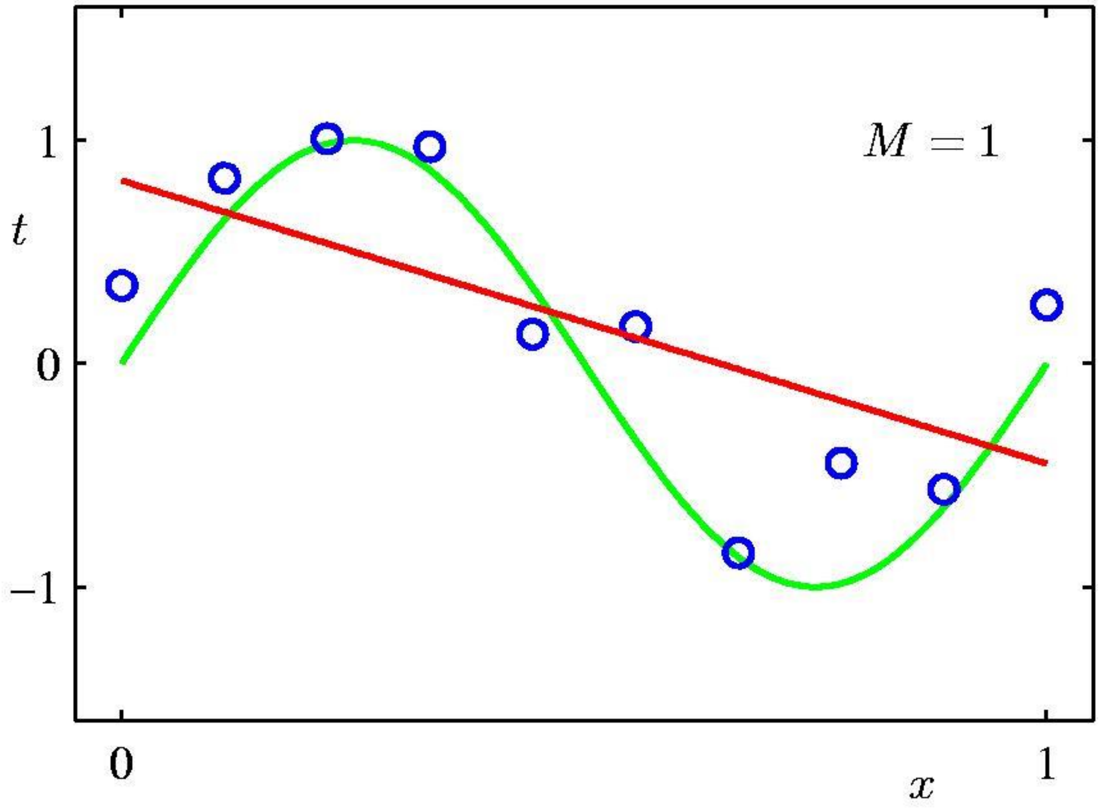
Fitting a Polynomial

$$M_0 = \begin{bmatrix} \sum_{i=1}^{N} y_i & \sum_{i=1}^{N} x_i & \cdots & \sum_{i=1}^{N} x_i^k \\ \sum_{i=1}^{N} x_i y_i & \sum_{i=1}^{N} x_i^2 & \cdots & \sum_{i=1}^{N} x_i^{k+1} \\ \vdots & \vdots & \vdots & \vdots \\ \sum_{i=1}^{N} x_i^k y_i & \sum_{i=1}^{N} x_i^{k+1} & \cdots & \sum_{i=1}^{N} x_i^{2k} \end{bmatrix}$$

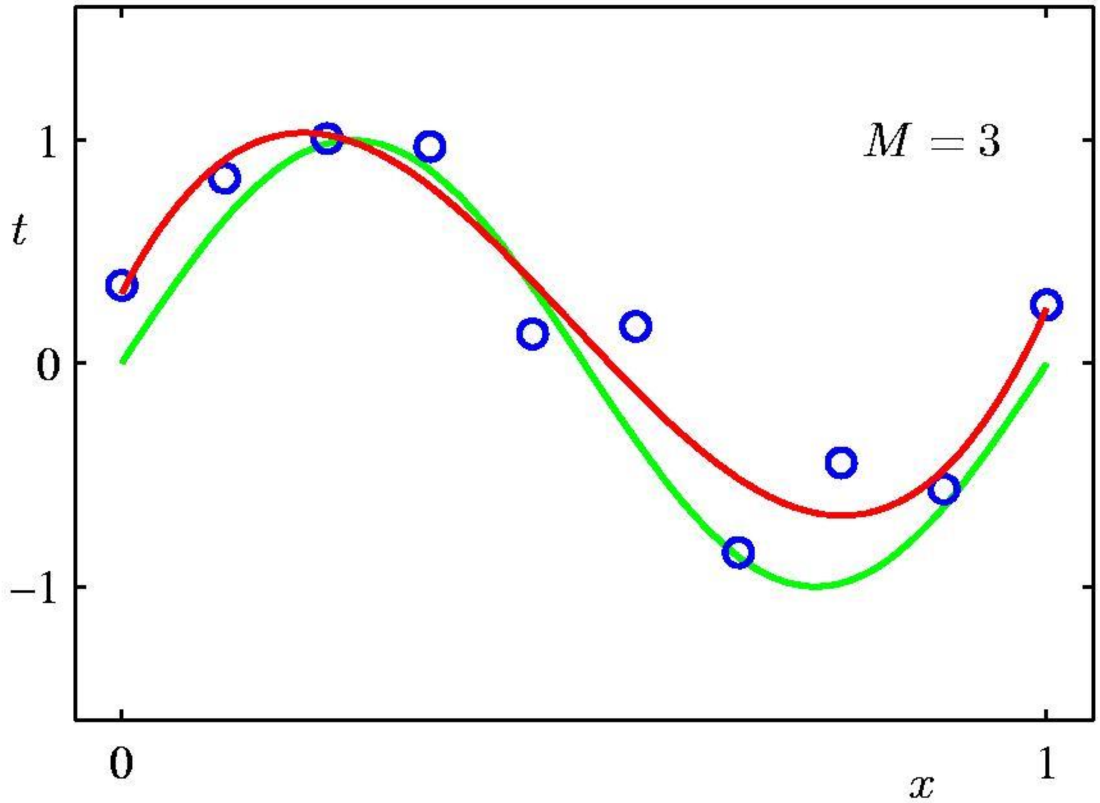
0th Order Polynomial



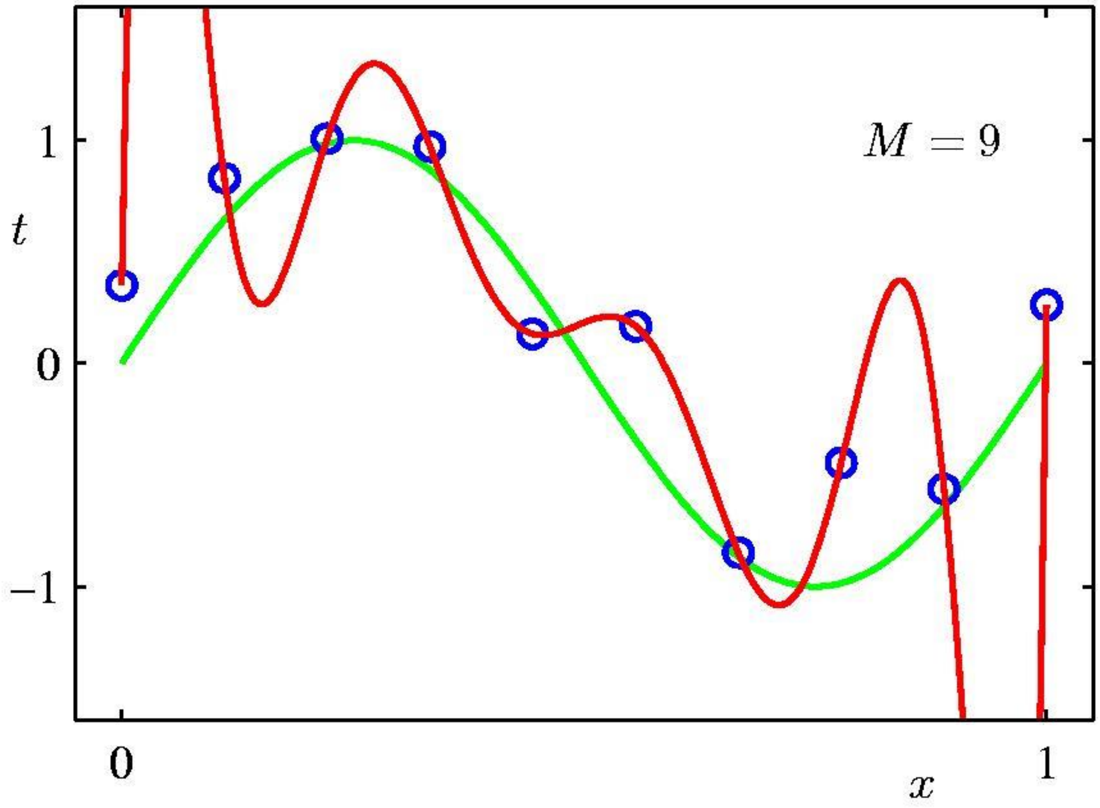
1st Order Polynomial



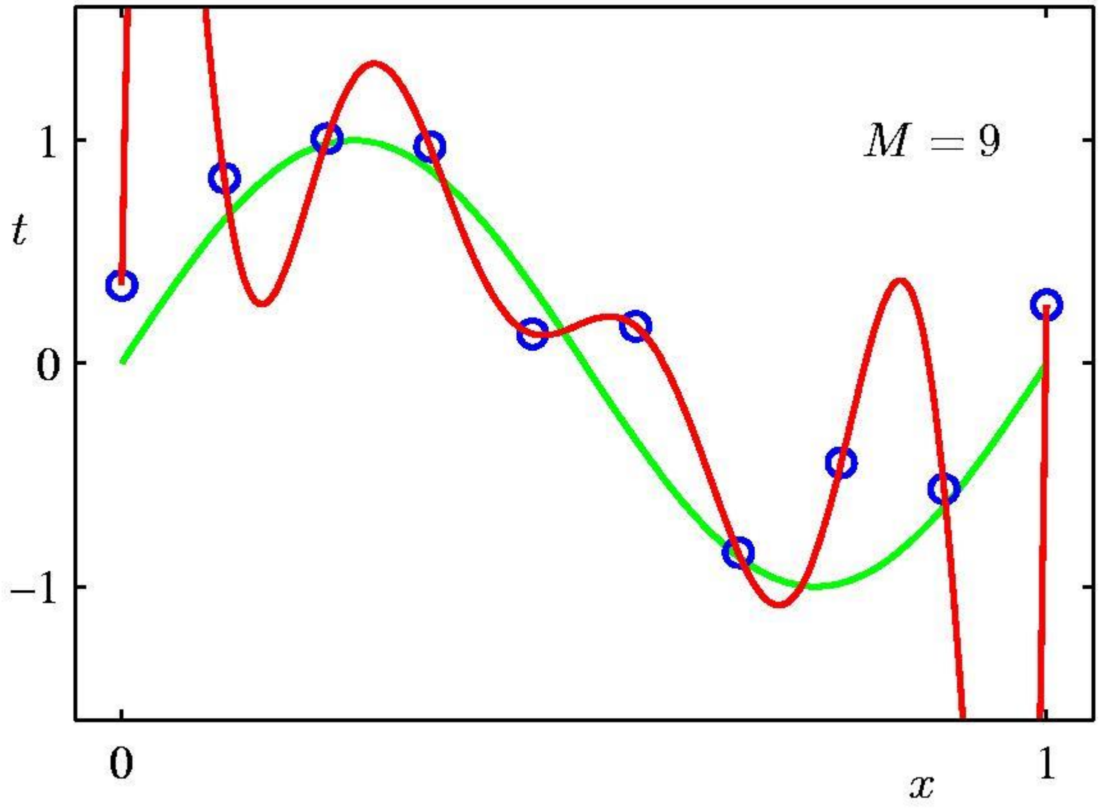
3rd Order Polynomial



9th Order Polynomial



9^{th} Order Polynomial

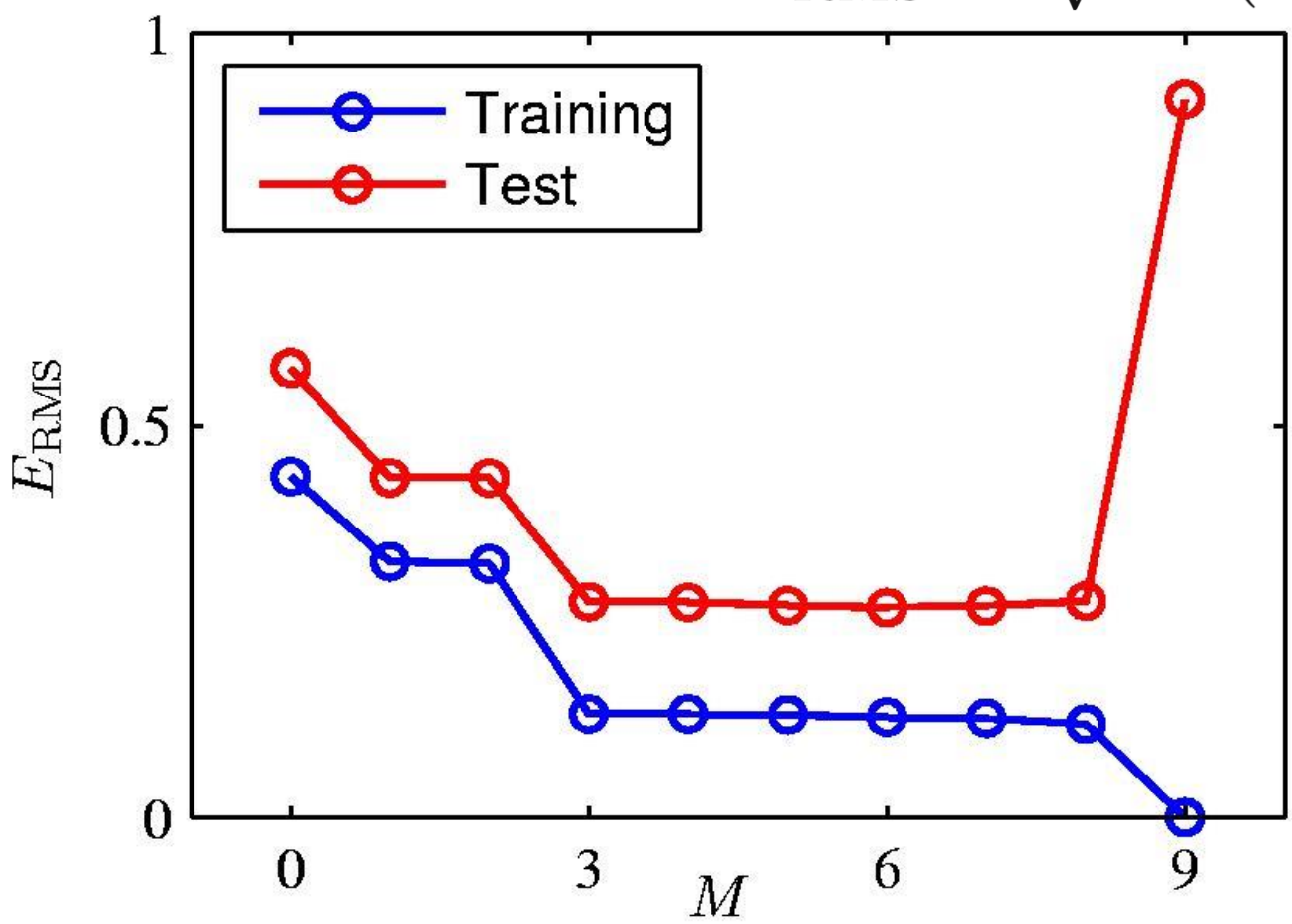


What about Generalization?

Typical Challenges in Machine Learning

Over-fit

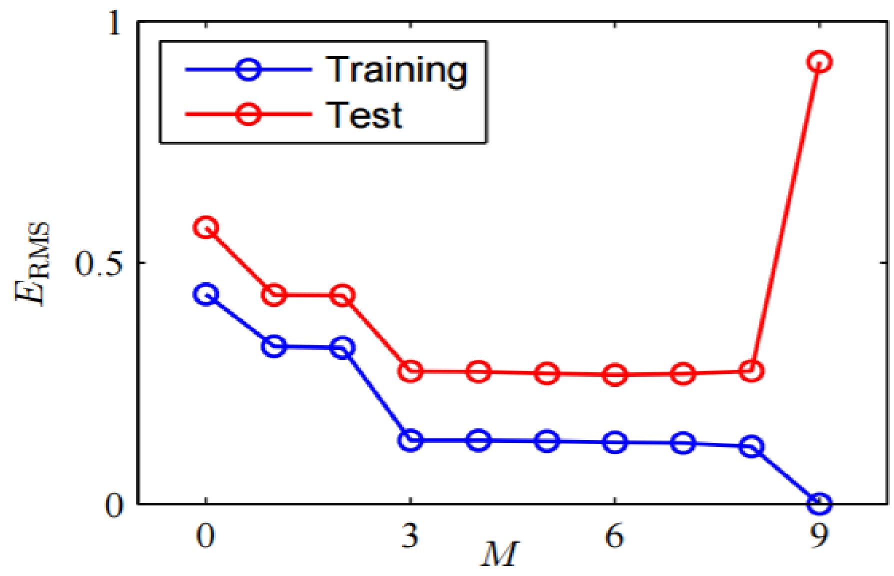
$$E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^{\star})/N}$$



Overfitting

Fix the training set size, vary H complexity (e.g., degree of polynomials)

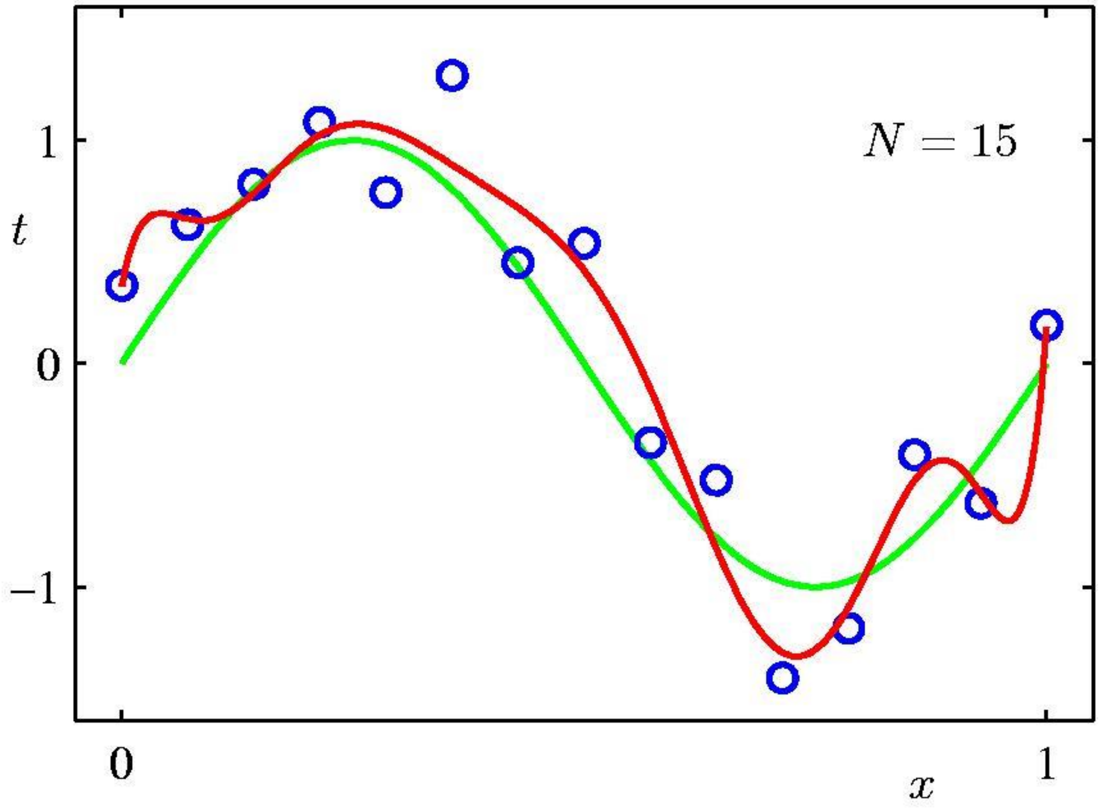
Example from Bishop, Figure 1.5



For any given N, some h of sufficient complexity fits the data but may have very bad generalization error!!

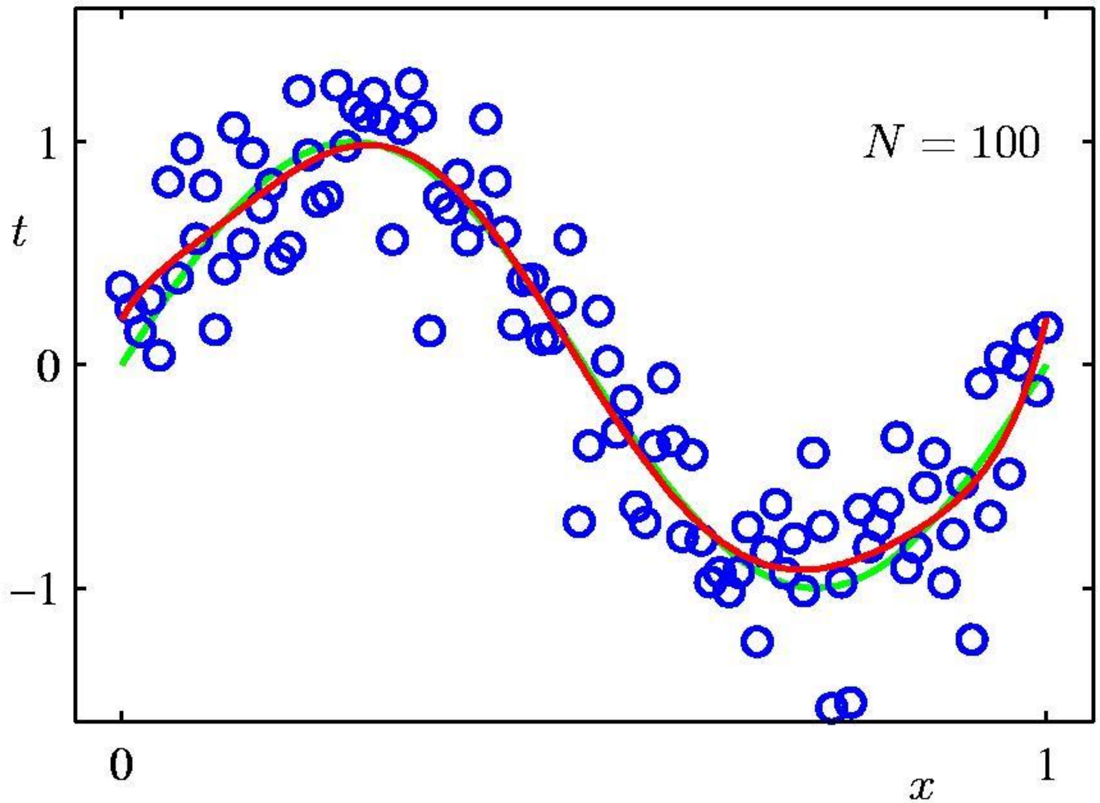
Data Set Size:

9th Order Polynomial fitted on 15 samples



Data Set Size:

9^{th} Order Polynomial fitted on 100 samples

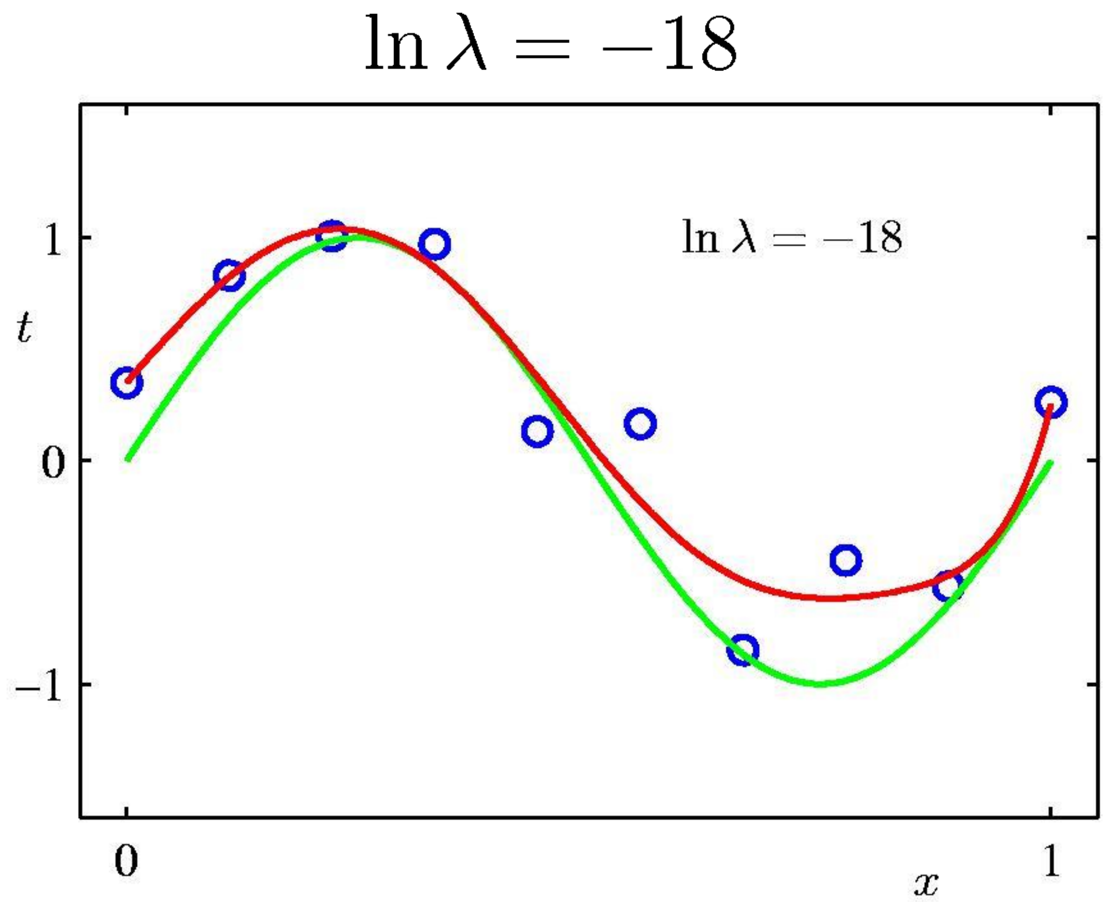


Regularization

- Penalize large coefficient values

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2 + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

Regularization:



Cross-validation

- Regularization helps but still need to pick λ
- Want to minimize test-set error, but we have no test set!
- Idea: make one (a validation set) by pretending we can't see the labels
- Try different values of λ, learn $\hat{h}^{\lambda}$ on rest of data,

test $\hat{h}^{\lambda}$ on validation set, pick best λ, train on all

- Problem: small validation set $\Rightarrow$ large error in estimated loss
- large validation set $\Rightarrow$ small training set $\Rightarrow$ bad $\hat{h}^{\lambda}$

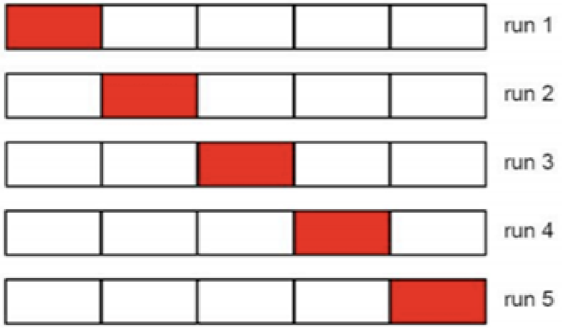
Cross-validation contd.

- K-fold cross-validation: divide data into *K* blocks
- For k=1 to k

 train on blocks except *kth* block, test on *kth* block

average the results, choose best λ

Common cases: *K=5,10* or *K=N (LOOCV)*



High computational cost*: K folds* × many choices of model *or* λ