Machine Learning

Lecture 2: Polynomial Curve Fitting

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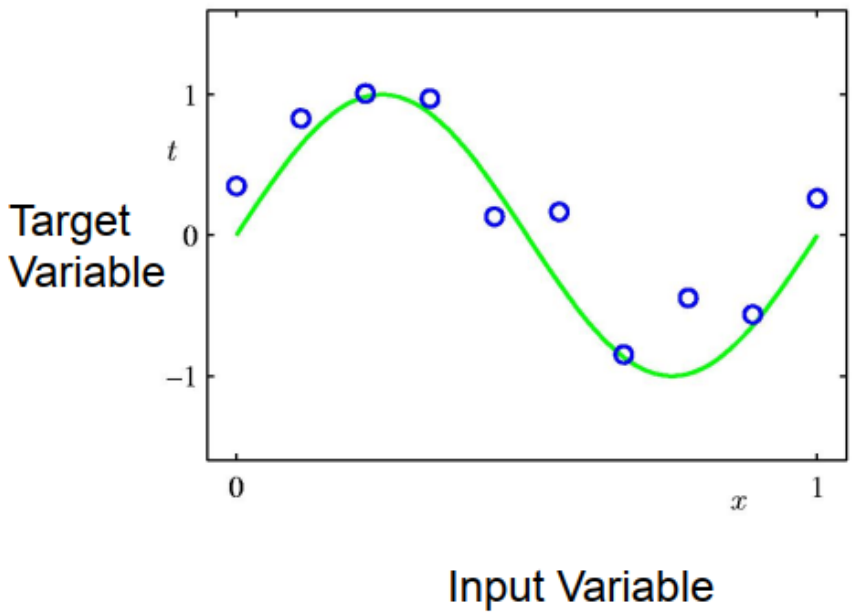
Simple Regression Problem

- Problem:
  - Observe Real-valued input variable x
  - Use x to predict value of target variable t
- We consider an artificial example using synthetically generated data
  - Because we know the process that generated the data, it can be used for comparison against a learned model

Synthetic Data for Regression

- Data generated from the function $\sin(2\pi\ x)$
  - Where x is the input
- Random noise in target values



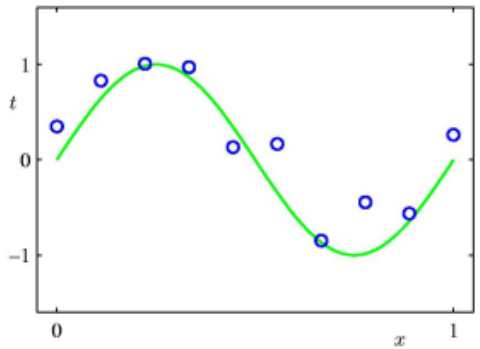
Input values $\{x_n\}$ generated uniformly in range $(0,1)$. Corresponding target values $\{t_n\}$ Obtained by first computing corresponding values of $\sin\{2\pi x\}$ then adding random noise with a Gaussian distribution with std dev 0.3

Training Set

- N observations of x

  $\mathrm{x} = (x_1,..,x_\mathrm{N})^\mathrm{T}$

  $\mathrm{t} = (t_1,..,t_\mathrm{N})^\mathrm{T}$
- Goal is to exploit training set to predict value $\hat{t}$ for some new value $\hat{x}$
- Inherently a difficult problem
- Probability theory provides framework for expressing uncertainty in a precise, quantitative manner
- Decision theory allows us to make a prediction that is optimal according to appropriate criteria



Data Generation:
$\mathrm{N} = 10$
Spaced uniformly in range $[0,1]$
Generated from $\sin(2\pi x)$ by adding small Gaussian noise
Noise typical due to unobserved variables

A Simple Approach to Curve Fitting

- Fit the data using a *polynomial function*

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

  - where M is the order of the polynomial
- Is higher value of M better? We'll see shortly!
- Coefficients $w_0, \ldots w_M$ are collectively denoted by vector $\mathbf{w}$
- It is a nonlinear function of x, but a linear function of the unknown parameters
- Have important properties and are called Linear Models

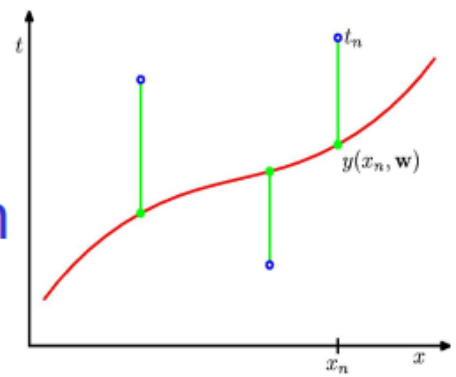
Error Function

- We can obtain a fit by minimizing an error function
  - Sum of squares of the errors between the predictions $y(x_n, \mathbf{w})$ for each data point x_n and target value t_n

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

  - Factor ½ included for later convenience

Red line is best polynomial fit



- Solve by choosing value of w for which small as possible

Minimization of Error Function

- Error function is a quadratic in coefficients w
- Thus derivative with respect to coefficients will be linear in elements of w
- Thus error function has a unique solution which can be found in closed form
  - Unique minimum denoted w^*
- Resulting polynomial is $y(x, \mathrm{w}^*)$

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

Since $y(x, \mathrm{w}) = \sum_{j=0}^{M} w_j x^j$

$$\frac{\partial E(\mathrm{w})}{\partial w_i} = \sum_{n=1}^{N}\{y(x_n, \mathrm{w}) - t_n\}x_n^i$$

$$= \sum_{n=1}^{N}\{\sum_{j=0}^{M} w_j x_n^j - t_n\}x_n^i$$

Setting equal to zero

$$\sum_{n=1}^{N}\sum_{j=0}^{M} w_j x_n^{i+j} = \sum_{n=1}^{N} t_n x_n^i$$

Set of M+1 equations (i=0,..,M) over M+1 variables are solved to get elements of w*

Solving Simultaneous equations

- $\mathrm{A}\mathbf{w}=\mathbf{b}$

  where A is $N \times (M+1)$

  $\mathbf{w}$ is $(M+1) \times 1$: set of weights to be determined

  $\mathbf{b}$ is $N \times 1$

- Can be solved using matrix inversion

  $\mathbf{w}=\mathrm{A}^{-1}\mathbf{b}$

- Or by using Gaussian elimination

Solving Linear Equations

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\ \vdots \qquad & \quad \vdots \qquad \quad \vdots \quad \vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n &= b_m \end{aligned}$$

$$x_1 \begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{bmatrix} + x_2 \begin{bmatrix} a_{12} \\ a_{22} \\ \vdots \\ a_{m2} \end{bmatrix} + \cdots + x_n \begin{bmatrix} a_{1n} \\ a_{2n} \\ \vdots \\ a_{mn} \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

1. Matrix Formulation: $\mathbf{Ax}=\mathbf{b}$
Solution: $\mathbf{x}=\mathbf{A}^{-1}\mathbf{b}$

Here $m=n=M+1$

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}, \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

2. Gaussian Elimination followed by back-substitution

$$\begin{aligned} x + 3y - 2z &= 5 \\ 3x + 5y + 6z &= 7 \\ 2x + 4y + 3z &= 8 \end{aligned}$$

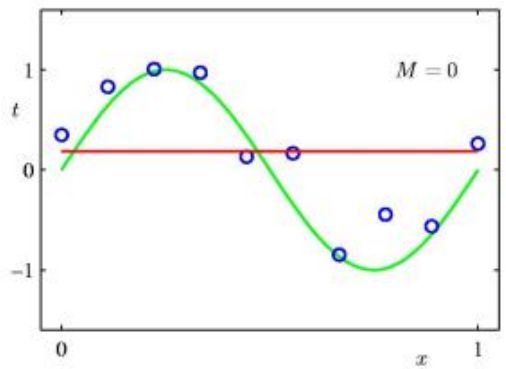
$L_2\text{-}3L_1 \rightarrow L_2$ $\quad$ $L_3\text{-}2L_1 \rightarrow L_3$ $\quad$ $-L_2/4 \rightarrow L_2$

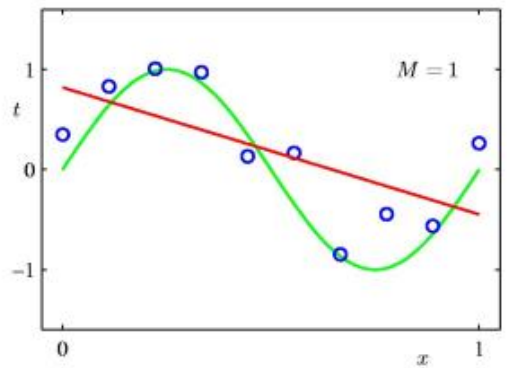
$$\left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 3 & 5 & 6 & 7 \\ 2 & 4 & 3 & 8 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 0 & -4 & 12 & -8 \\ 2 & 4 & 3 & 8 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 0 & -4 & 12 & -8 \\ 0 & -2 & 7 & -2 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 0 & 1 & -3 & 2 \\ 0 & -2 & 7 & -2 \end{array}\right]$$

$$\sim \left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 0 & 1 & -3 & 2 \\ 0 & 0 & 1 & 2 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 3 & -2 & 5 \\ 0 & 1 & 0 & 8 \\ 0 & 0 & 1 & 2 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 3 & 0 & 9 \\ 0 & 1 & 0 & 8 \\ 0 & 0 & 1 & 2 \end{array}\right] \sim \left[\begin{array}{ccc|c} 1 & 0 & 0 & -15 \\ 0 & 1 & 0 & 8 \\ 0 & 0 & 1 & 2 \end{array}\right]$$

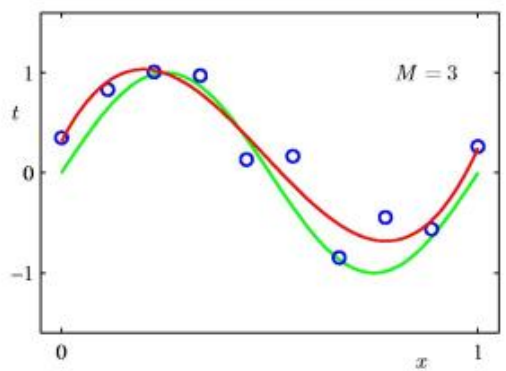
Choosing the order of M

- Model Comparison or Model Selection
- Red lines are best fits with
  - $M = 0,1,3,9$ and $N=10$

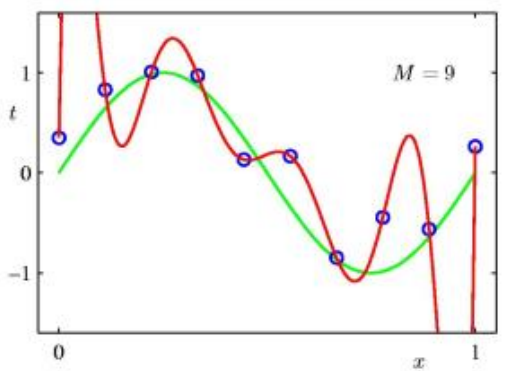




← Poor representations of $\sin(2\pi x)$



← Best Fit to $\sin(2\pi x)$



Over Fit Poor representation of $\sin(2\pi x)$

Generalization Performance

- Consider separate *test* set of 100 points
- For each value of M evaluate

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

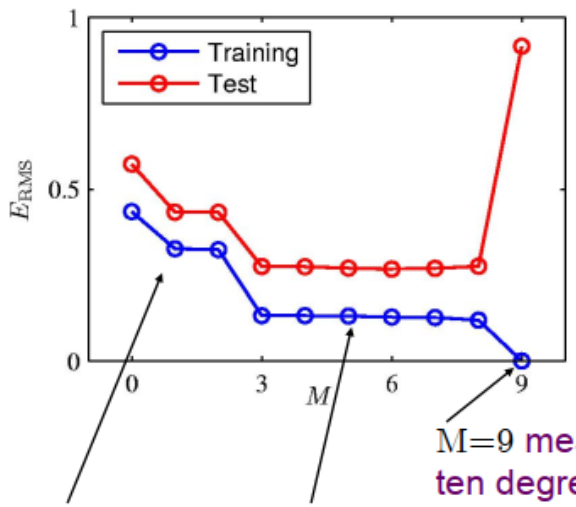
$$y(x, \mathrm{w}^*) = \sum_{j=0}^{M} w_j^* x^j$$

for training data and test data

- Use RMS error

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

  - Division by N allows different sizes of N to be compared on equal footing
  - Square root ensures E_{RMS} is measured in same units as t



Poor due to Inflexible polynomials

Small Error

M=9 means ten degrees of freedom. Tuned exactly to 10 training points (wild oscillations in polynomial)

Values of Coefficients w^* for different polynomials of order M

	$M=0$	$M=1$	$M=6$	$M=9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

As M increases magnitude of coefficients increases

At M=9 finely tuned to random noise in target values

Increasing Size of Data Set

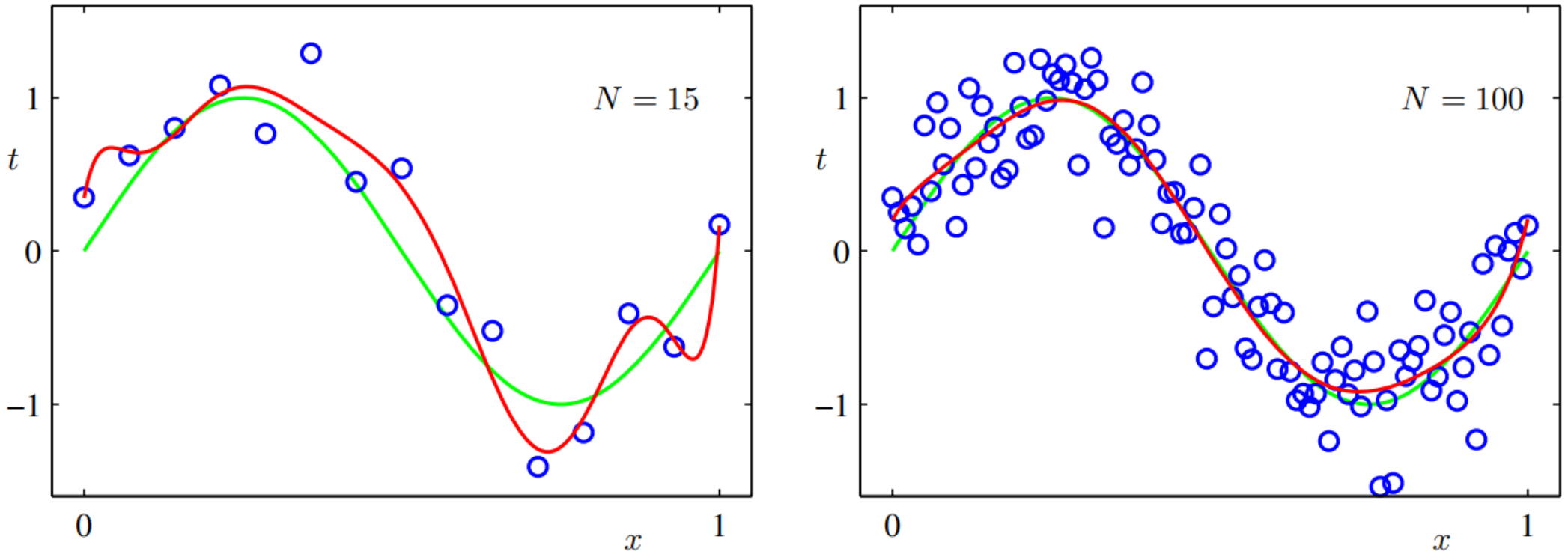


Figure 1.6 Plots of the solutions obtained by minimizing the sum-of-squares error function using the $M = 9$ polynomial for $N = 15$ data points (left plot) and $N = 100$ data points (right plot). We see that increasing the size of the data set reduces the over-fitting problem.

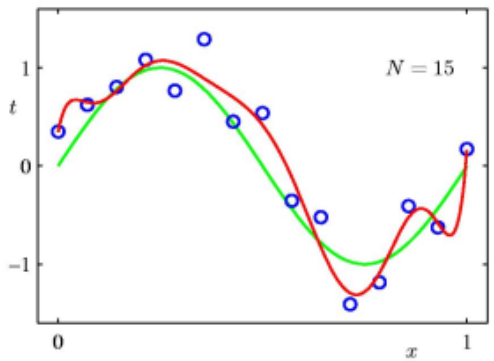
Increasing Size of Data Set

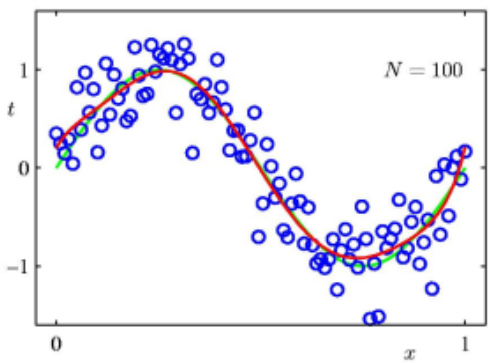
N=15, 100

For a given model complexity overfitting problem is less severe as size of data set increases

Larger the data set, the more complex we can afford to fit the data

Data should be no less than 5 to 10 times adaptive parameters in model





Least Squares is case of Maximum Likelihood

- Unsatisfying to limit the number of parameters to size of training set
- More reasonable to choose model complexity according to problem complexity
- Least squares approach is a specific case of maximum likelihood
  - Over-fitting is a general property of maximum likelihood
- Bayesian approach avoids over-fitting problem
  - No. of parameters can greatly exceed no. of data points
  - Effective no. of parameters adapts automatically to size of data set

Regularization of Least Squares

- Using relatively complex models with data sets of limited size
- Add a penalty term to error function to discourage coefficients from reaching large values

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

where

$$\|\mathrm{w}^2\| \equiv w^T w = w_0^2 + w_1^2 + .. + w_M^2$$

- λ determines relative importance of regularization term to error term
- Can be minimized exactly in closed form
- Known as *shrinkage* in statistics
  Weight decay in neural networks

Effect of Regularizer

M=9 polynomials using regularized error function

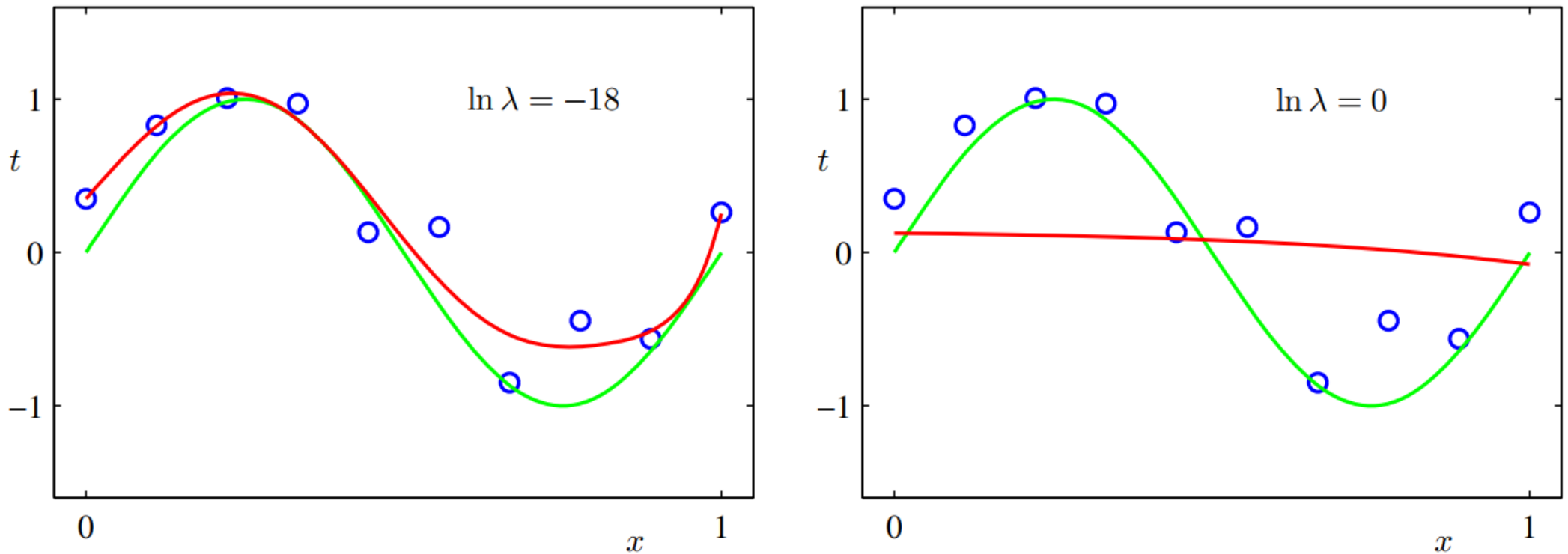


Figure 1.7 Plots of $M = 9$ polynomials fitted to the data set shown in Figure 1.2 using the regularized error function (1.4) for two values of the regularization parameter λ corresponding to $\ln \lambda = -18$ and $\ln \lambda = 0$. The case of no regularizer, i.e., $\lambda = 0$, corresponding to $\ln \lambda = -\infty$, is shown at the bottom right of Figure 1.4.

Effect of Regularizer

M=9 polynomials using regularized error function

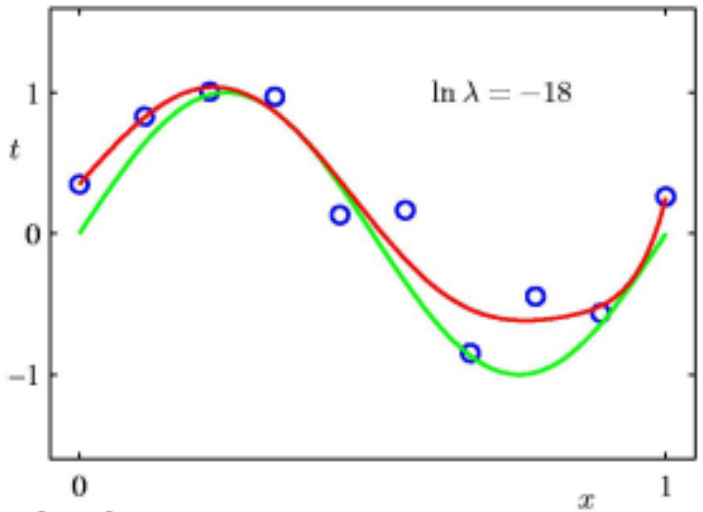
Table of the coefficients $\mathbf{w}^\star$ for $M = 9$ polynomials with various values for the regularization parameter λ. Note that $\ln \lambda = -\infty$ corresponds to a model with no regularization, i.e., to the graph at the bottom right in Figure 1.4. We see that, as the value of λ increases, the typical magnitude of the coefficients gets smaller.

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

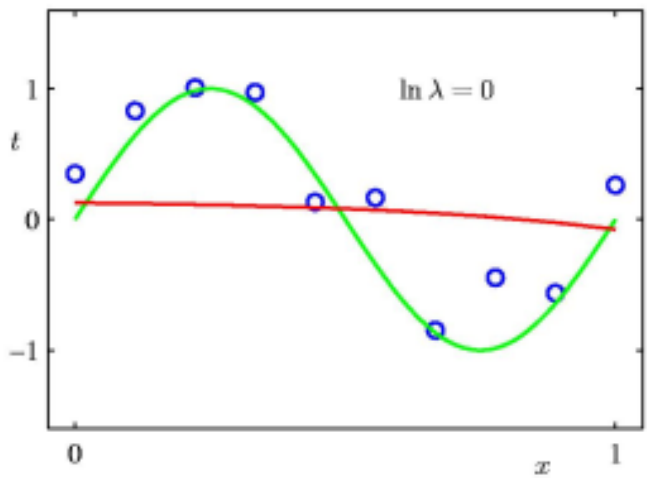
Effect of Regularizer

$M=9$ polynomials using regularized error function

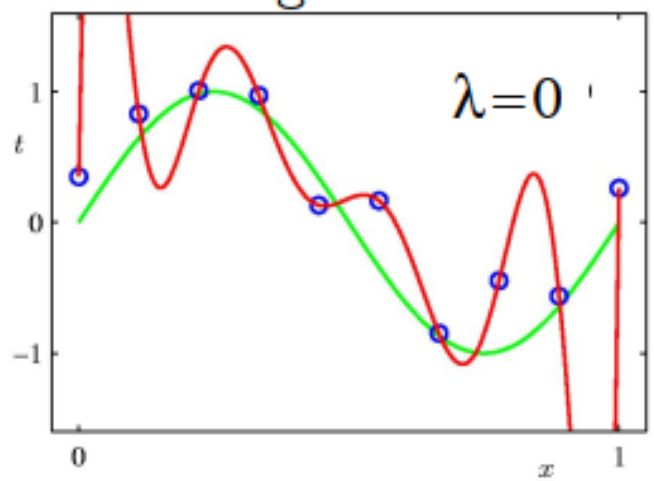
Optimal



Large Regularizer

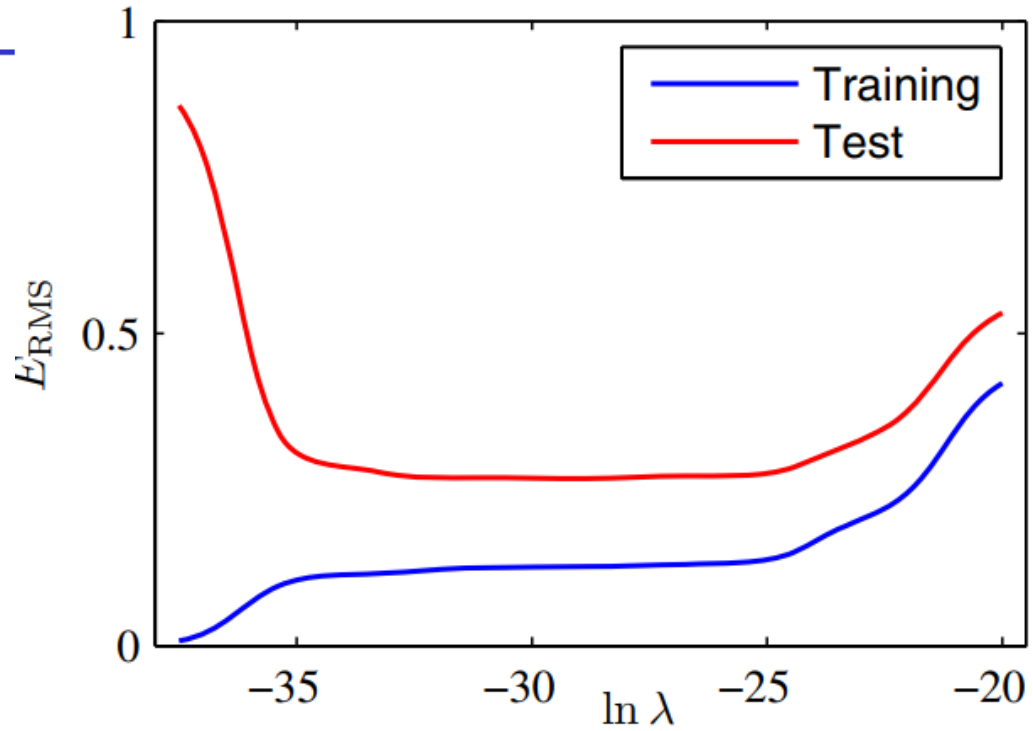


No Regularizer



Impact of Regularization on Error

- λ controls the complexity of the model and hence degree of over-fitting
  - Analogous to choice of M
- Suggested Approach:
- Training set
  - to determine coefficients $\mathbf{w}$
  - For different values of (M or λ)
- Validation set (holdout)
  - to optimize model complexity (M or λ)



Summary of Curve Fitting

- Partitioning data into *training set* (to determine coefficients w) and a separate *validation set* (or *hold-out* set) to optimize model complexity M or λ
- More sophisticated approaches are not as wasteful of training data
- More principled approach is based on probability theory
- Classification is a special case of regression where target value is discrete values

References

- Chapter 1, Pattern Recognition and Machine Learning, C. Bishop.