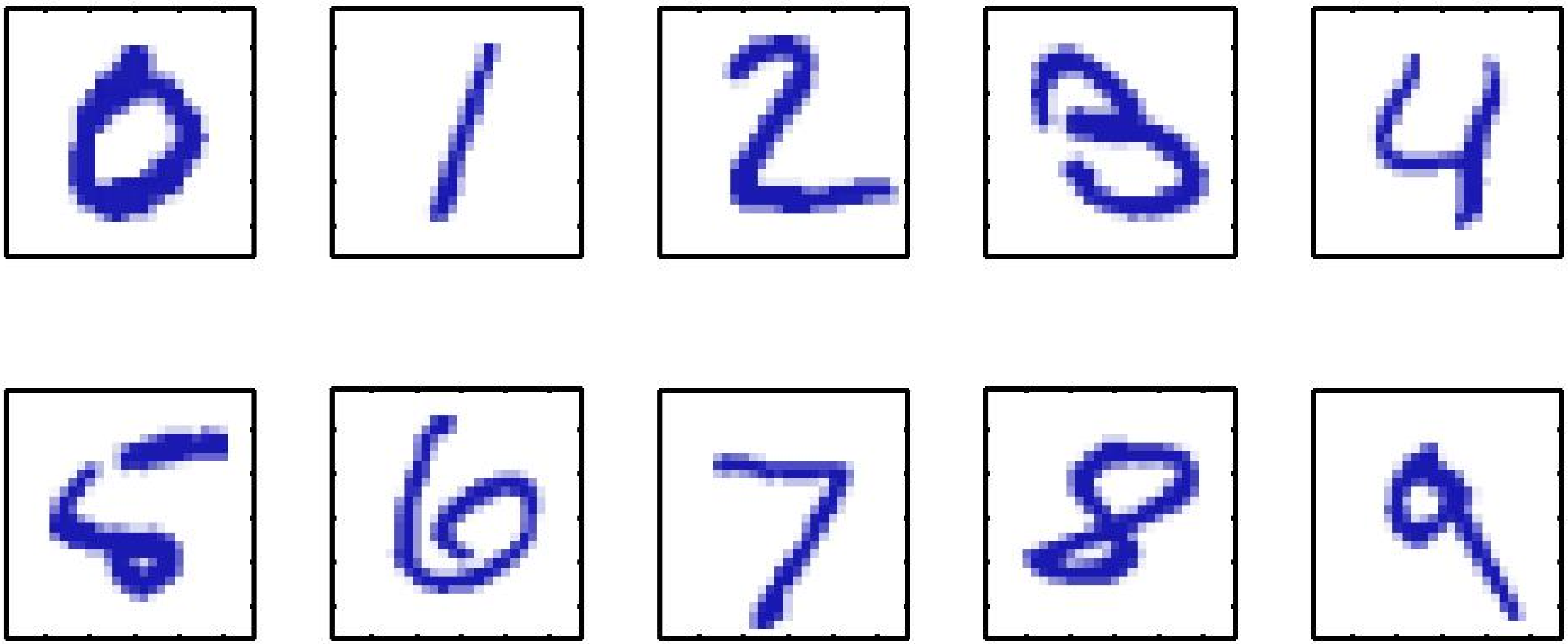
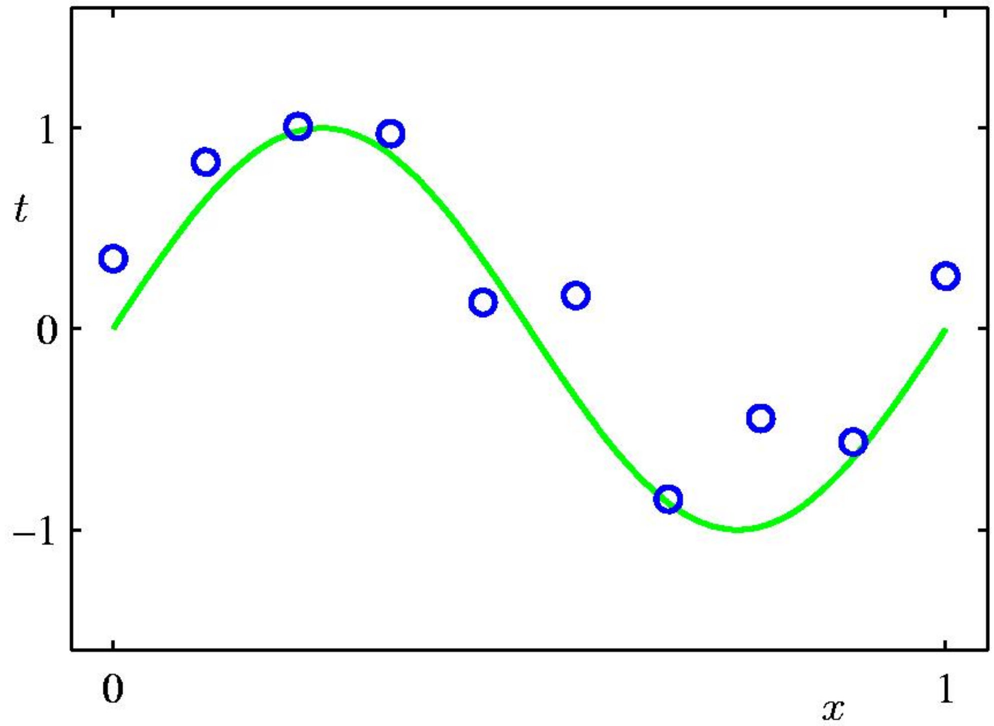
Curve Fitting, Linear Regression， Regularization

Example

Handwritten Digit Recognition

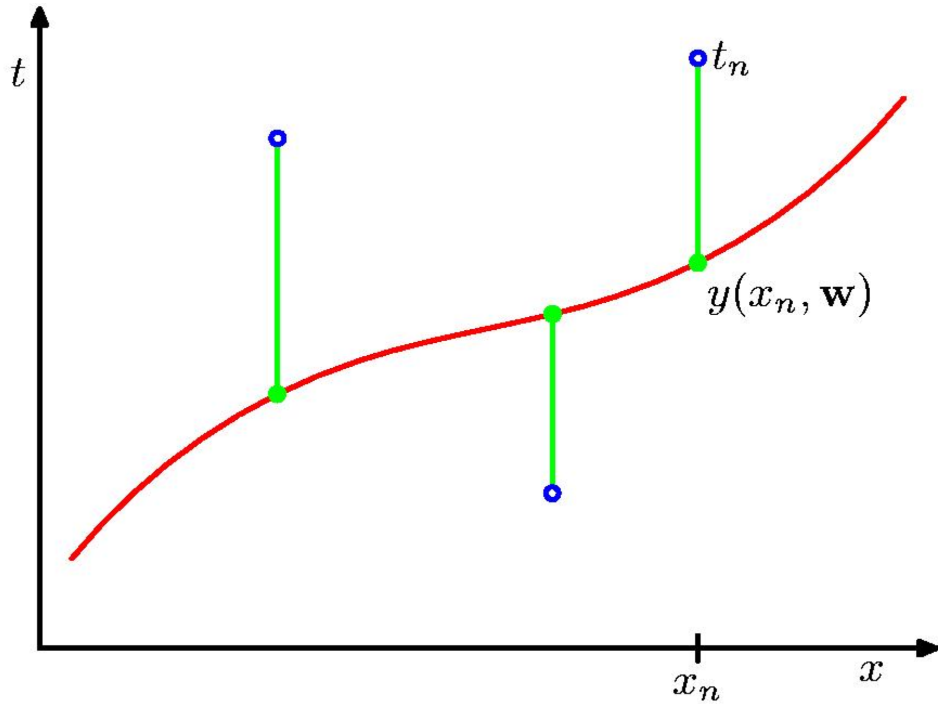


Polynomial Curve Fitting



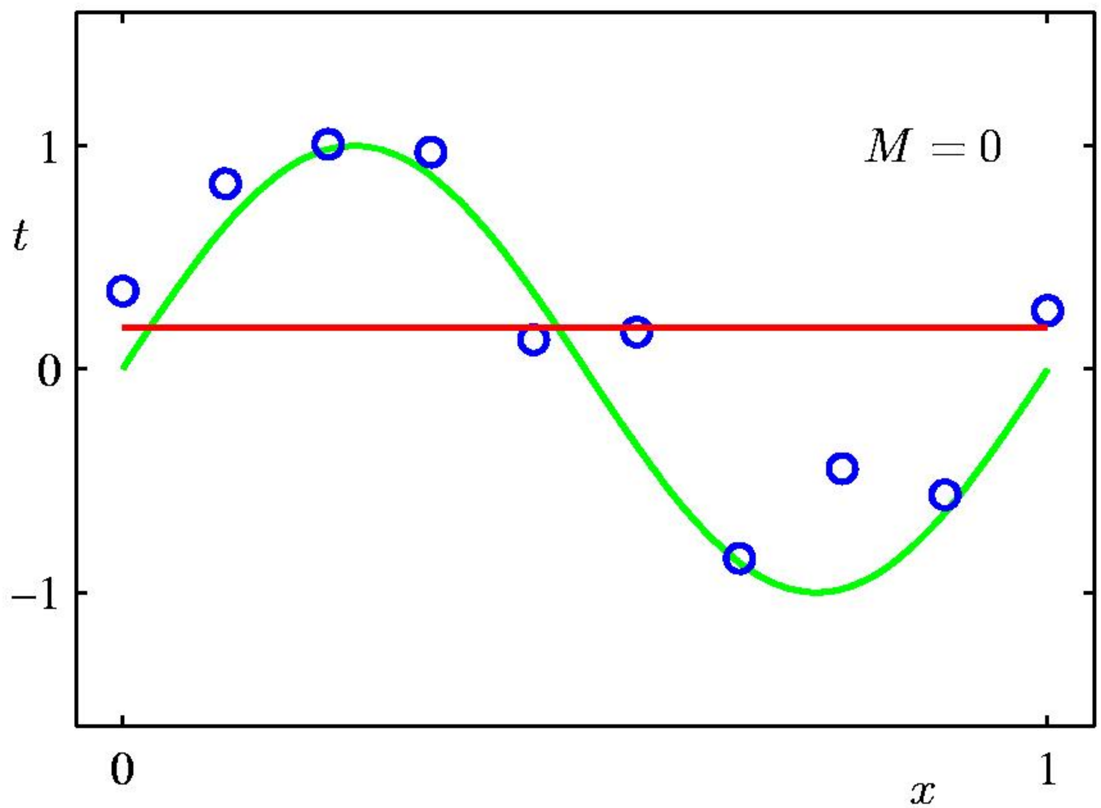
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Sum-of-Squares Error Function

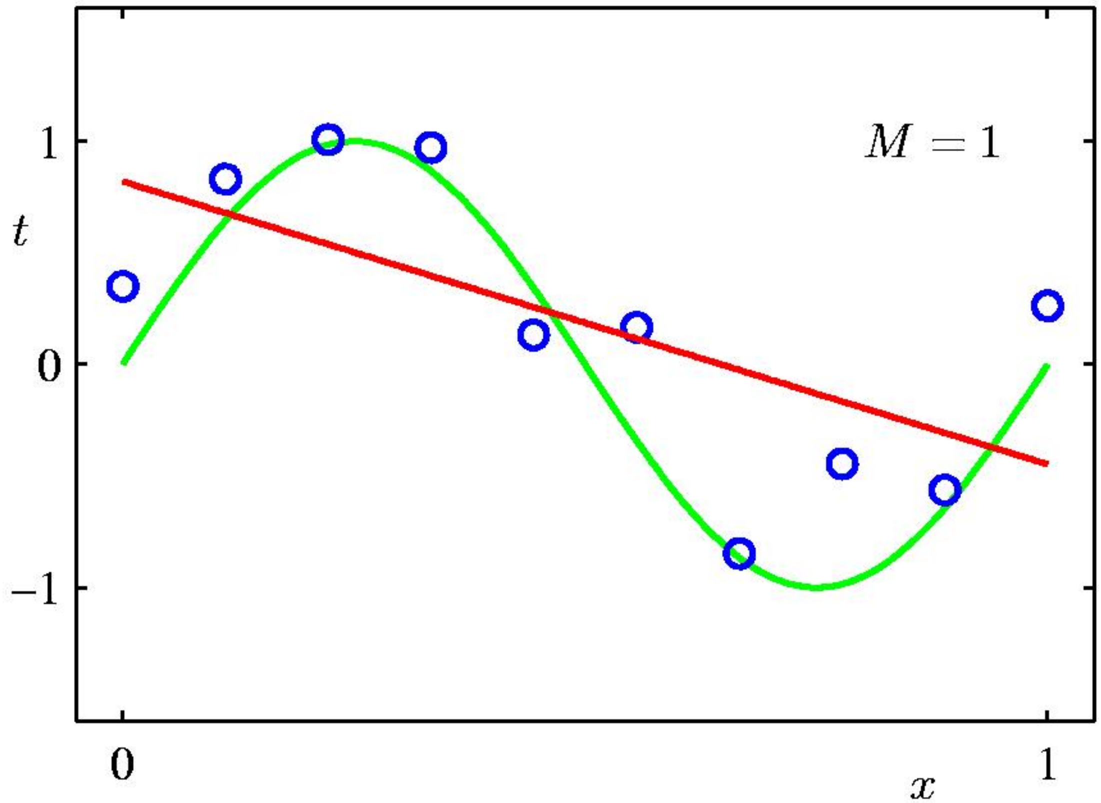


$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2$$

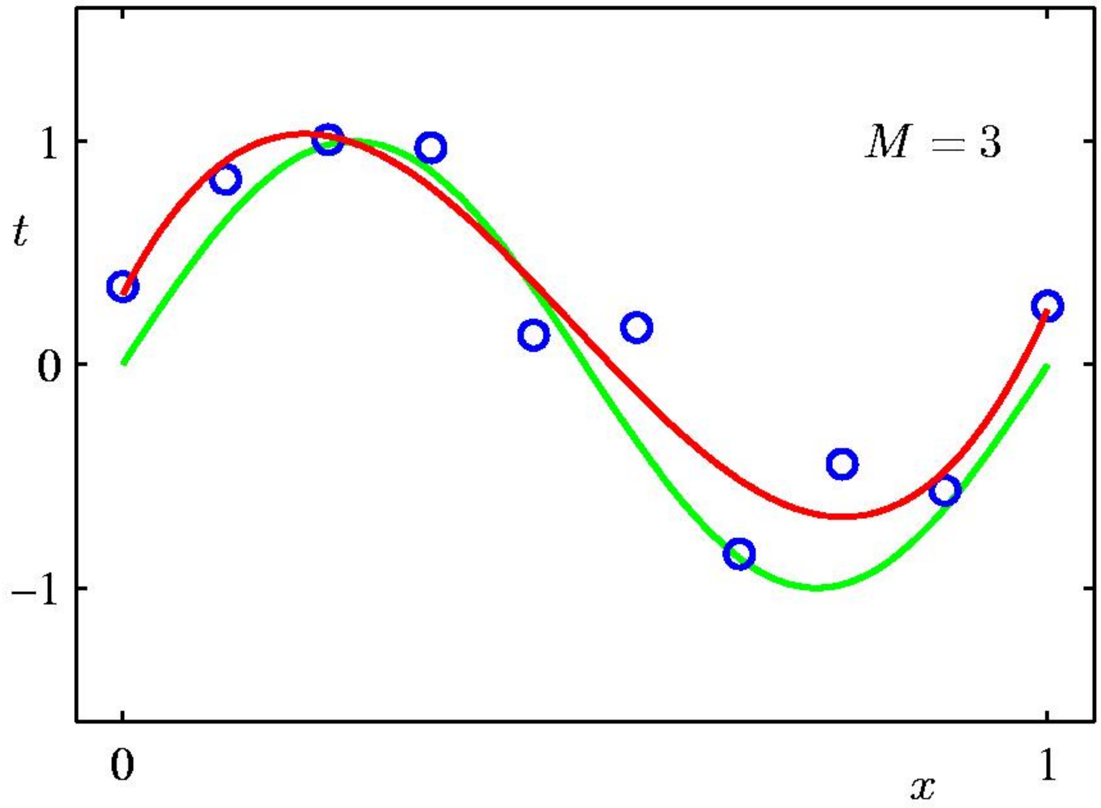
0^{th} Order Polynomial



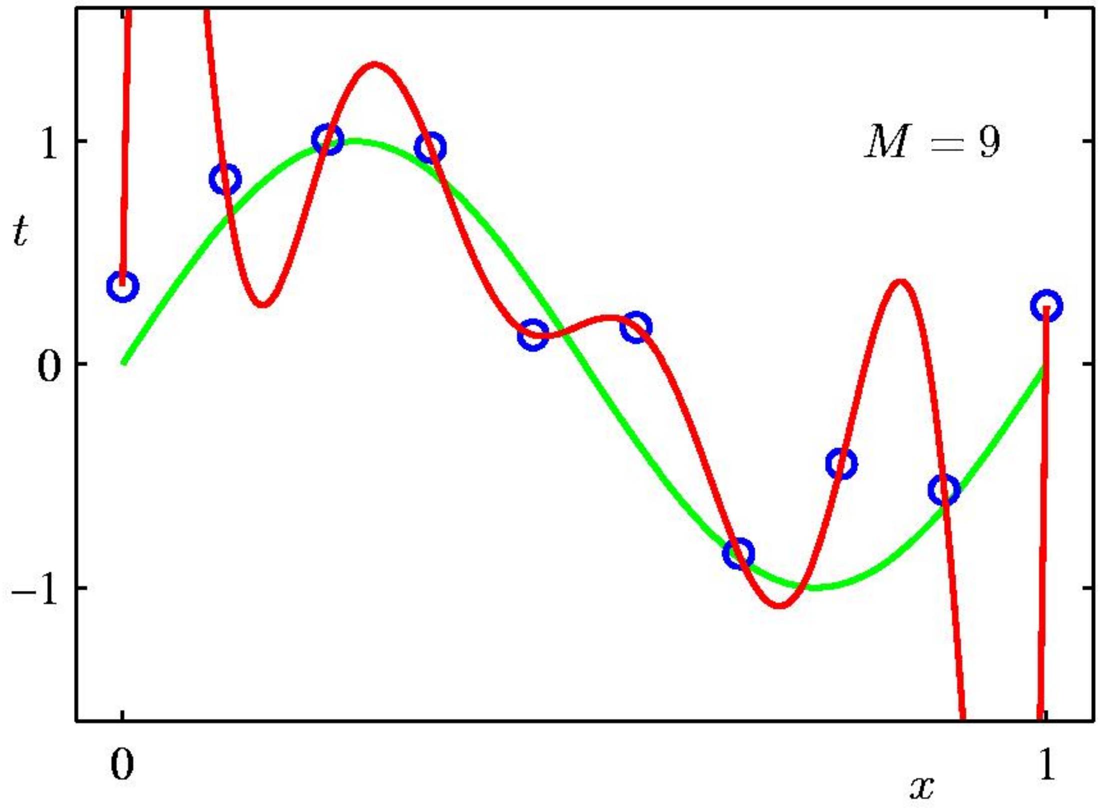
1st Order Polynomial



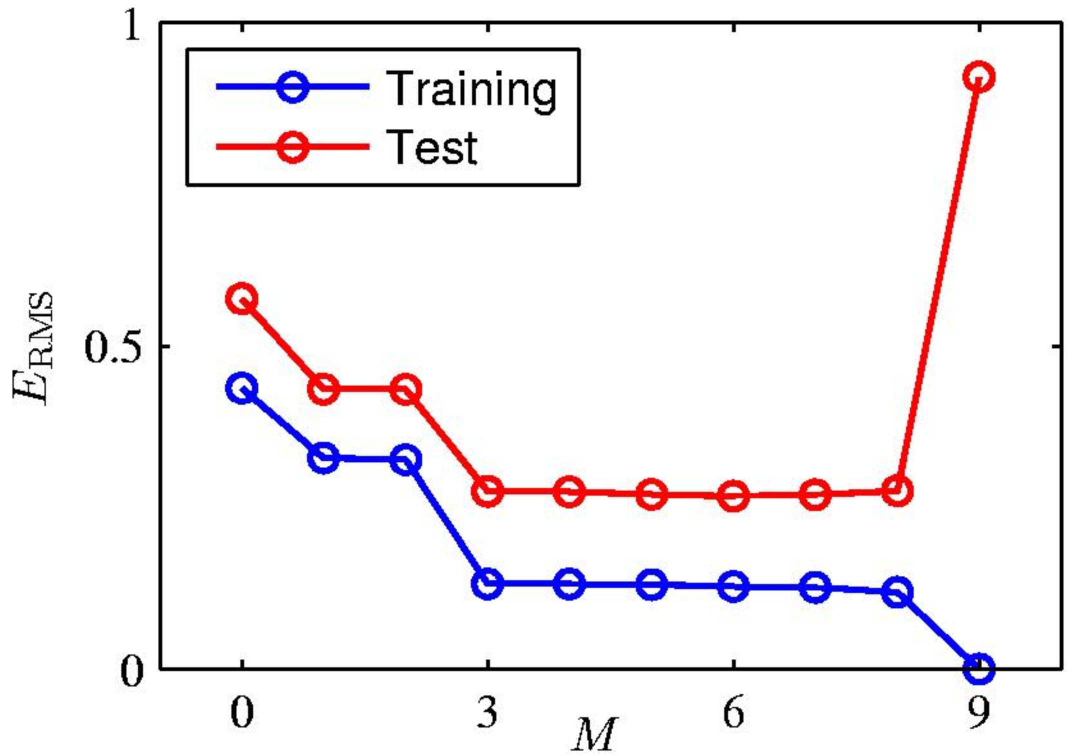
3rd Order Polynomial



9^{th} Order Polynomial



Over-fitting



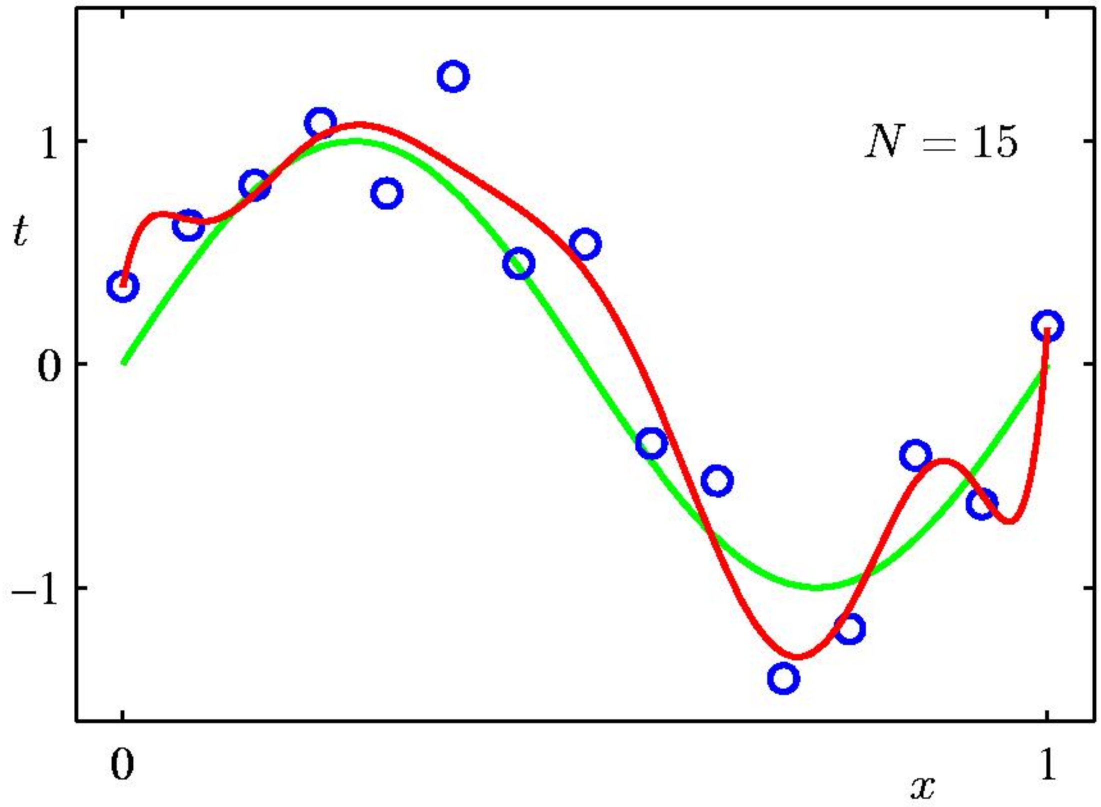
Root-Mean-Square (RMS) Error: $E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$

Polynomial Coefficients

	$M=0$	$M=1$	$M=3$	$M=9$
$w_0^\star$	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

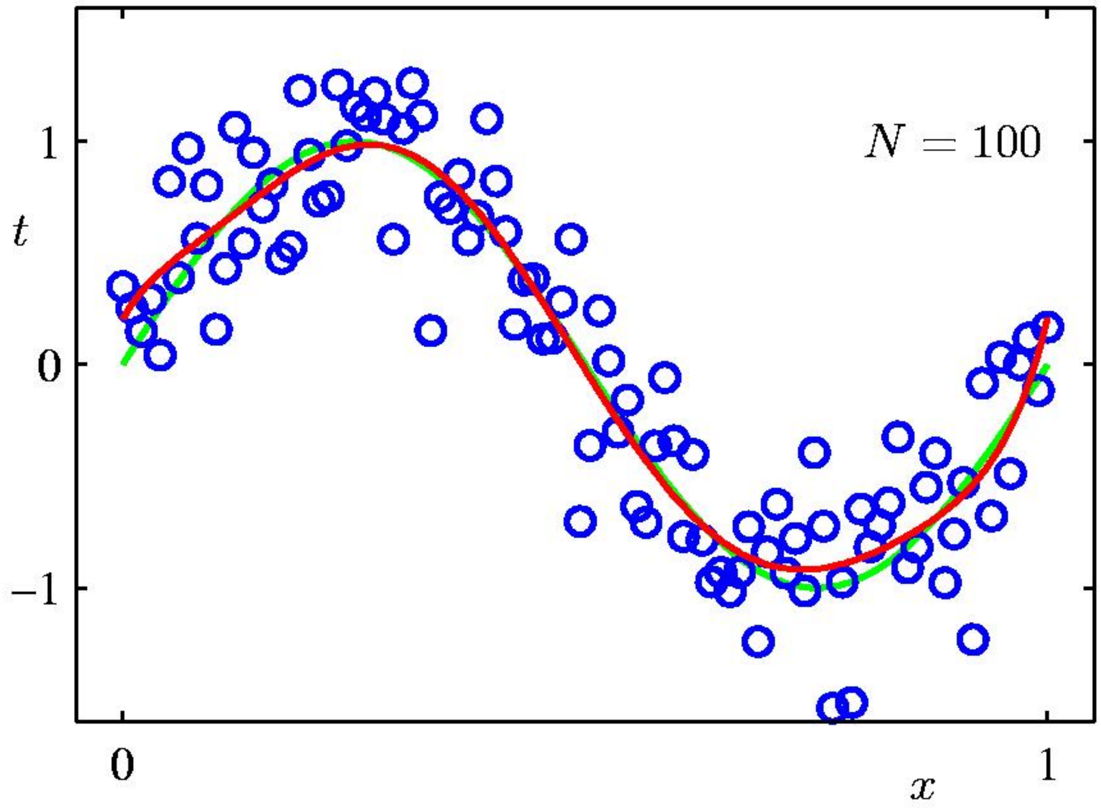
Data Set Size: $N = 15$

9th Order Polynomial



Data Set Size: $N = 100$

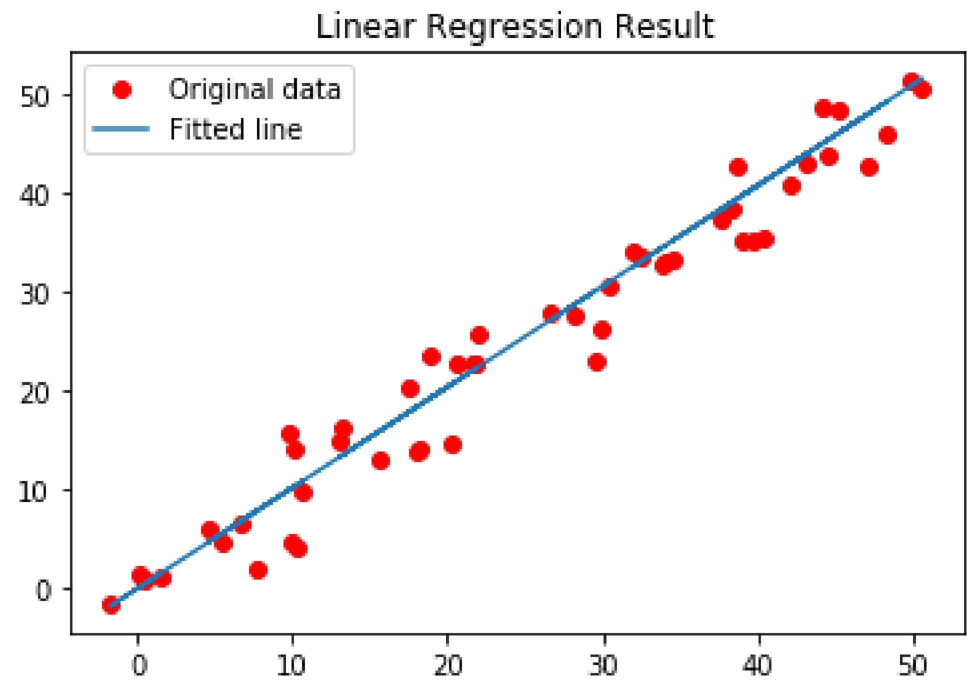
9th Order Polynomial



Regularization

Penalize large coefficient values

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


Linear Regression Result
Original data
Fitted line
50
40
30
20
10
0
0
10
20
30
40
50

Heat Flux	Skin Temperature
10.858	31.002
10.617	31.021
10.183	31.058
9.7003	31.095
9.652	31.133
10,086	31,188
9.459	31,226
8.3972	31,263
7.6251	31,319
7.1907	31,356
7.046	31.412
6.9494	31.468
6.7081	31.524

Heat Flux	Skin Temperature
6.3221	31.581
6.0325	31.618
5.7429	31.674
5.5016	31.712
5.2603	31.768
5,1638	31,825
5,0673	31.862
4.9708	31.919
4,8743	31.975
4.7777	32.013
4.7295	32.07
4.633	32.126
4.4882	32.164

Heat Flux	Skin Temperature
4.3917	32.221
4.2951	32.259
4.2469	32.296
4.0056	32.334
3.716	32.391
3,523	32.448
3,4265	32.505
3,3782	32,543
3,4265	32.6
3.3782	32.657
3.3299	32,696
3,3299	32.753
3.4265	32.791

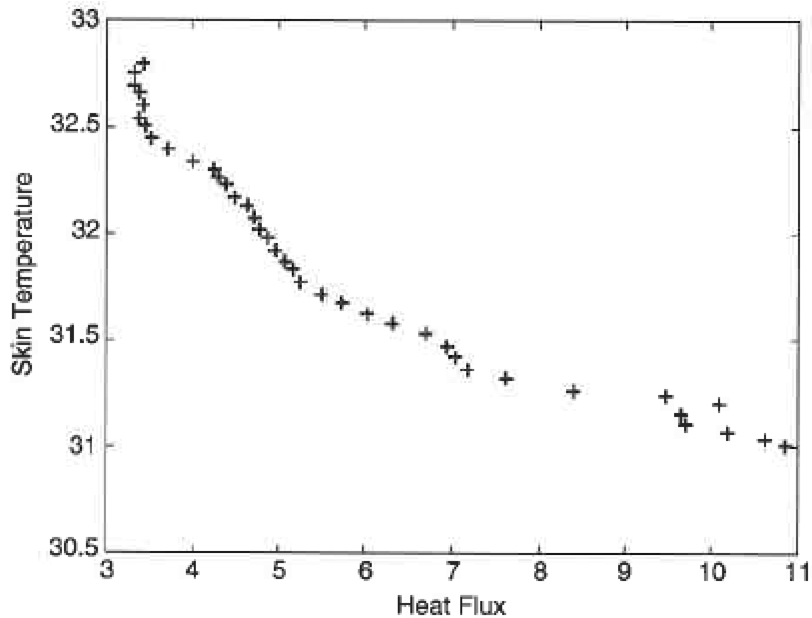


Figure D.1. Measurements of heat flux and skin temperature of a person.

D.2.1 Least Square Method

Suppose we wish to fit the following linear model to the observed data:

$$f(x) = \omega_1 x + \omega_0, \tag{D.3}$$

where ω_0 and ω_1 are parameters of the model and are called the **regression coefficients**. A standard approach for doing this is to apply the **method of least squares**, which attempts to find the parameters (ω_0, ω_1) that minimize the sum of the squared error

$$SSE = \sum_{i=1}^{N} [y_i - f(x_i)]^2 = \sum_{i=1}^{N} [y_i - \omega_1 x - \omega_0]^2, \tag{D.4}$$

which is also known as the **residual sum of squares**.

This optimization problem can be solved by taking the partial derivative of E with respect to ω_0 and ω_1, setting them to zero, and solving the corresponding system of linear equations.

$$\begin{aligned}
\frac{\partial E}{\partial \omega_0} &= -2\sum_{i=1}^{N}[y_i - \omega_1 x_i - \omega_0] = 0 \\
\frac{\partial E}{\partial \omega_1} &= -2\sum_{i=1}^{N}[y_i - \omega_1 x_i - \omega_0]x_i = 0
\end{aligned} \tag{D.5}$$

These equations can be summarized by the following matrix equation, which is also known as the **normal equation**:

$$\begin{pmatrix} N & \sum_i x_i \\ \sum_i x_i & \sum_i x_i^2 \end{pmatrix} \begin{pmatrix} \omega_0 \\ \omega_1 \end{pmatrix} = \begin{pmatrix} \sum_i y_i \\ \sum_i x_i y_i \end{pmatrix}. \tag{D.6}$$

Since $\sum_i x_i = 229.9$, $\sum_i x_i^2 = 1569.2$, $\sum_i y_i = 1242.9$, and $\sum_i x_i y_i = 7279.7$, the normal equations can be solved to obtain the following estimates for the parameters.

$$\begin{aligned}
\begin{pmatrix} \hat{\omega}_0 \\ \hat{\omega}_1 \end{pmatrix} &= \begin{pmatrix} 39 & 229.9 \\ 229.9 & 1569.2 \end{pmatrix}^{-1} \begin{pmatrix} 1242.9 \\ 7279.7 \end{pmatrix} \\
&= \begin{pmatrix} 0.1881 & -0.0276 \\ -0.0276 & 0.0047 \end{pmatrix} \begin{pmatrix} 1242.9 \\ 7279.7 \end{pmatrix} \\
&= \begin{pmatrix} 33.1699 \\ -0.2208 \end{pmatrix}
\end{aligned}$$

$$f(x) = 33.17 - 0.22x.$$

Figure D.2 shows the line corresponding to this model.

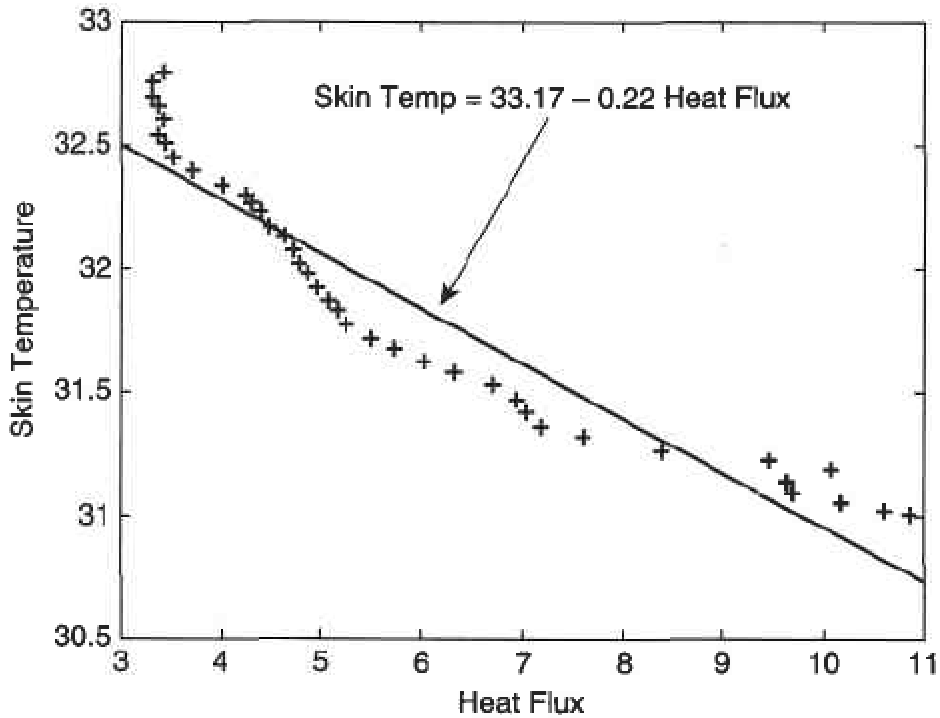
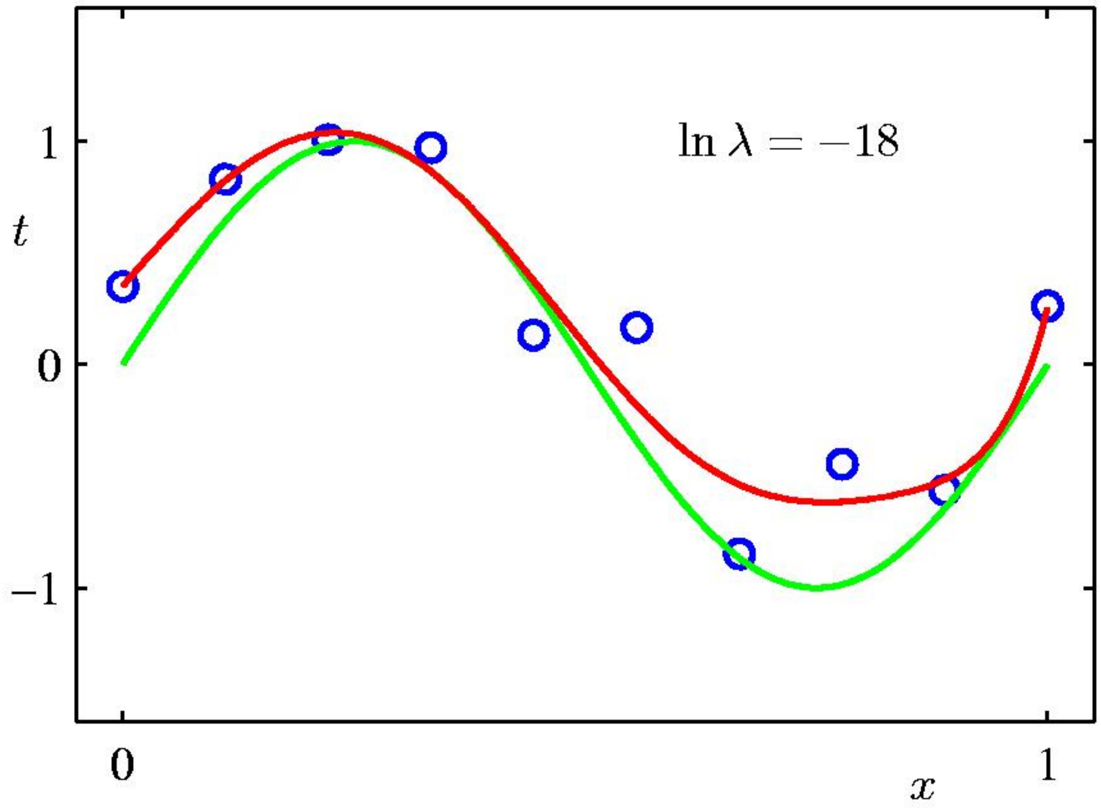
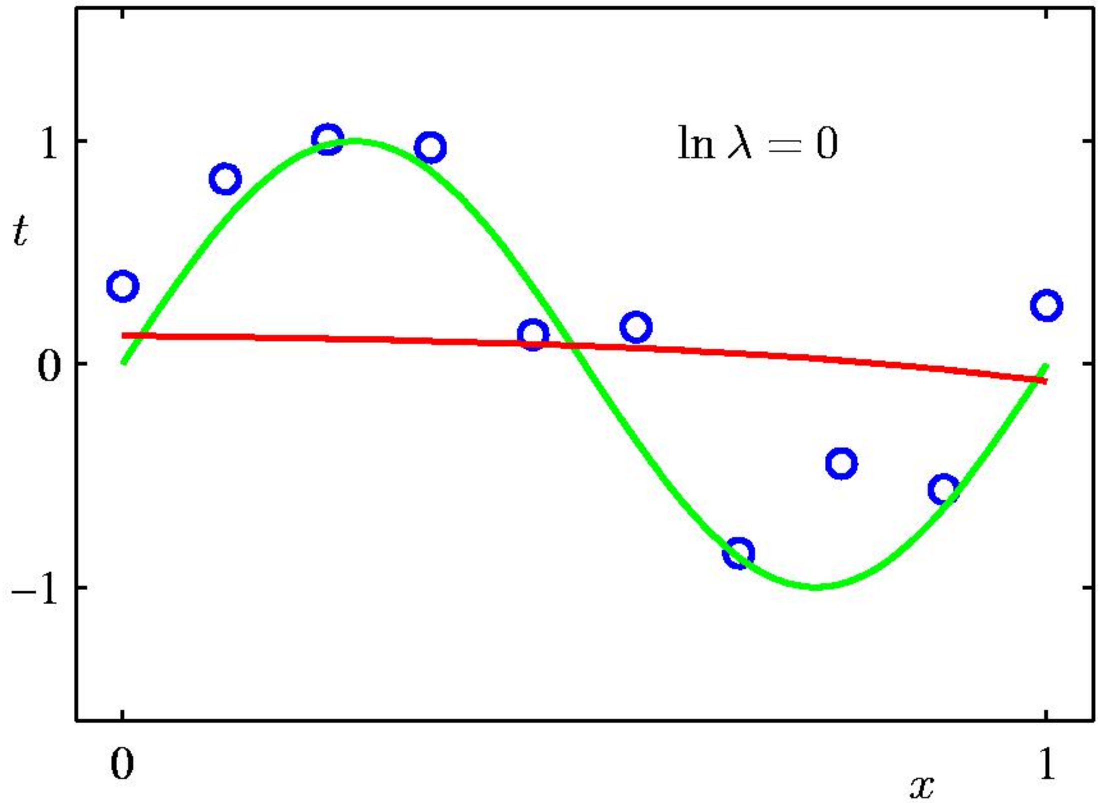


Figure D.2. A linear model that fits the data given in Figure D.1.

Regularization: $\ln \lambda = -18$



Regularization: $\ln \lambda = 0$



Polynomial Coefficients

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	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