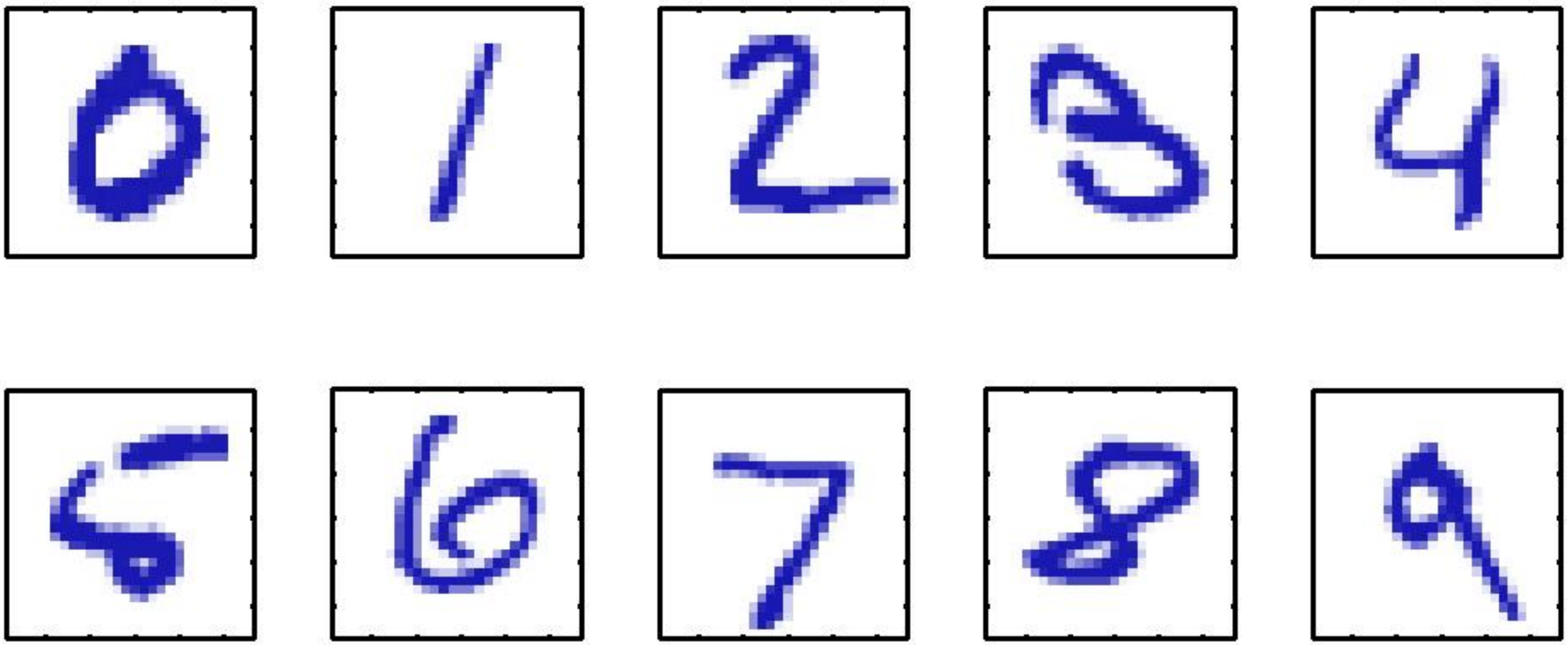
PATTERN RECOGNITION AND MACHINE LEARNING

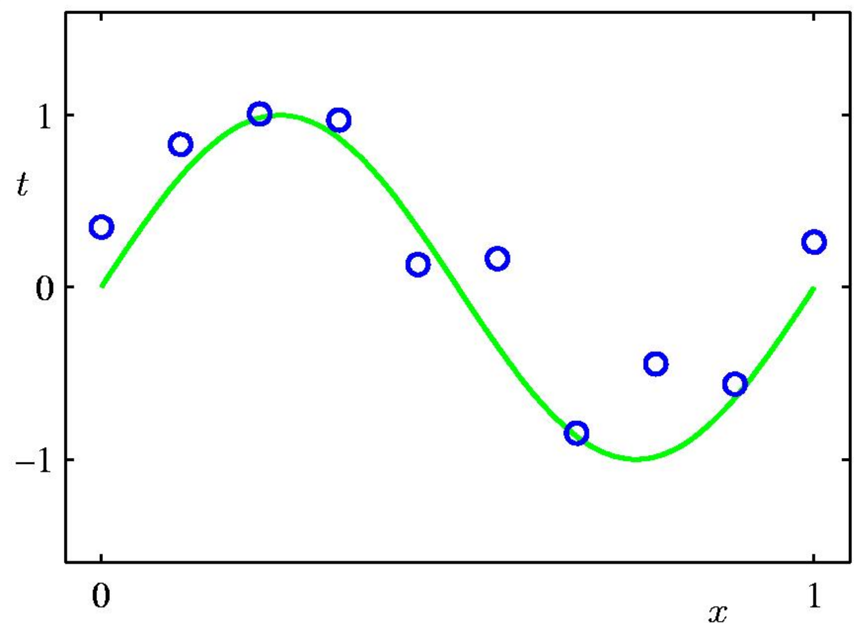
CHAPTER 1: INTRODUCTION

Example

Handwritten Digit Recognition



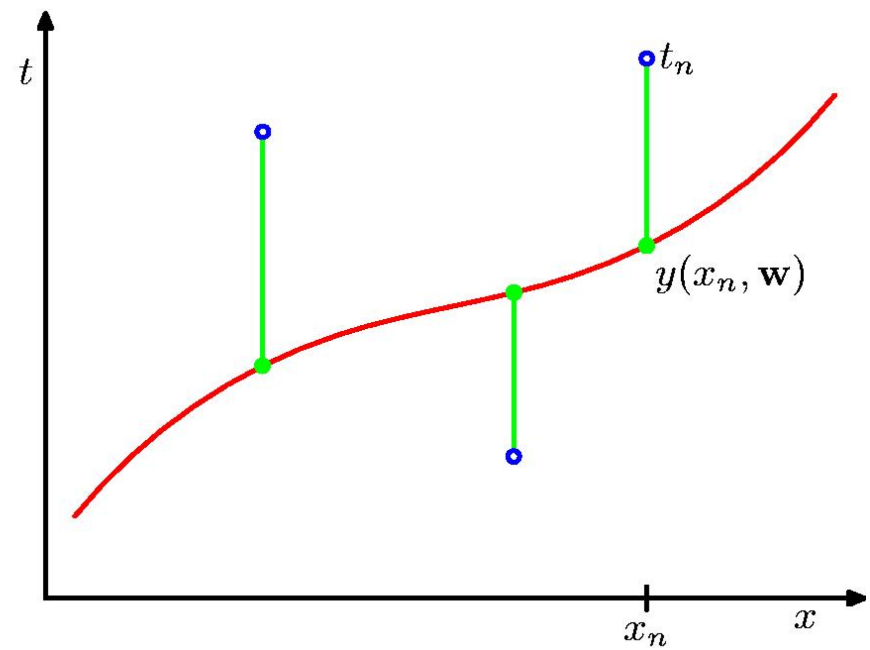
Polynomial Curve Fitting



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

- The input data set x of 10 points was generated by choosing values of x_n, for n = 1, . . . , 10, spaced uniformly in range [0, 1].
- The target data set t was obtained by first computing the corresponding values of the function sin(2πx) and then adding a small level of random noise having a Gaussian distribution to each corresponding value t_n.

Sum-of-Squares Error Function

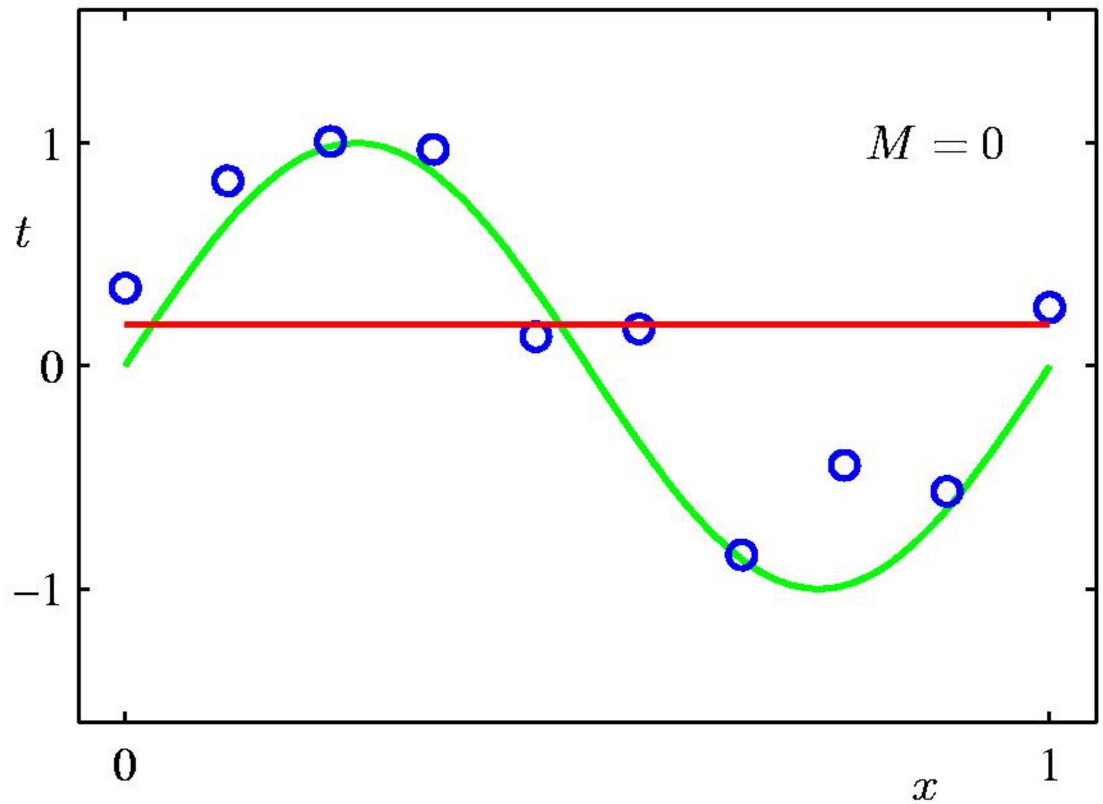


$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2$$

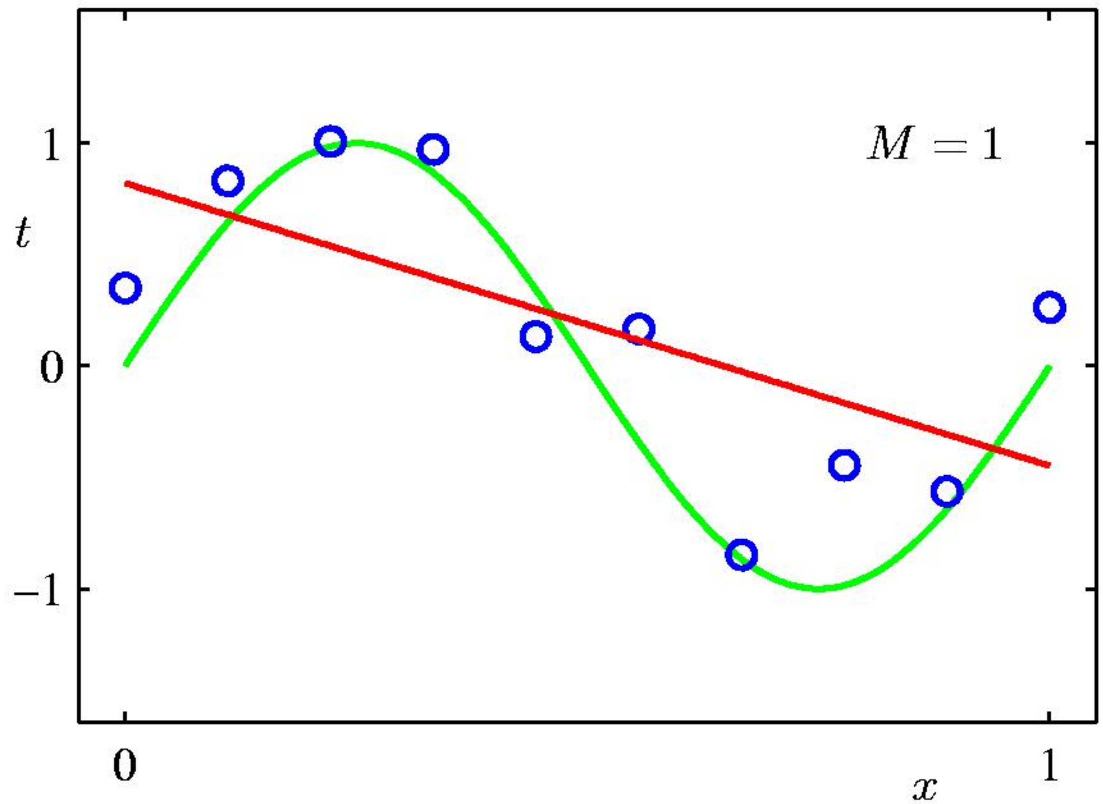
Note: E(w) is a quadratic function w.r.t. each w_i. Thus the partial derivative of E(w) w.r.t. each w_i is a linear function of w's.

This method is also called **Linear Least Squares**

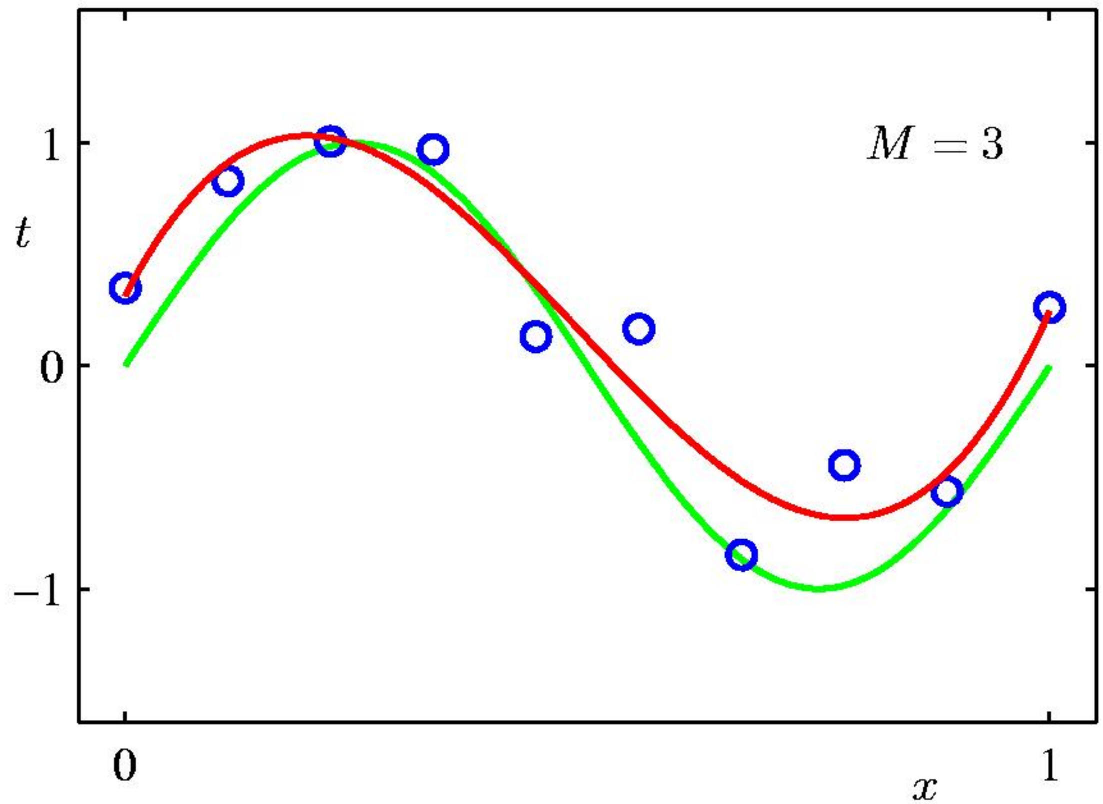
0^{th} Order Polynomial



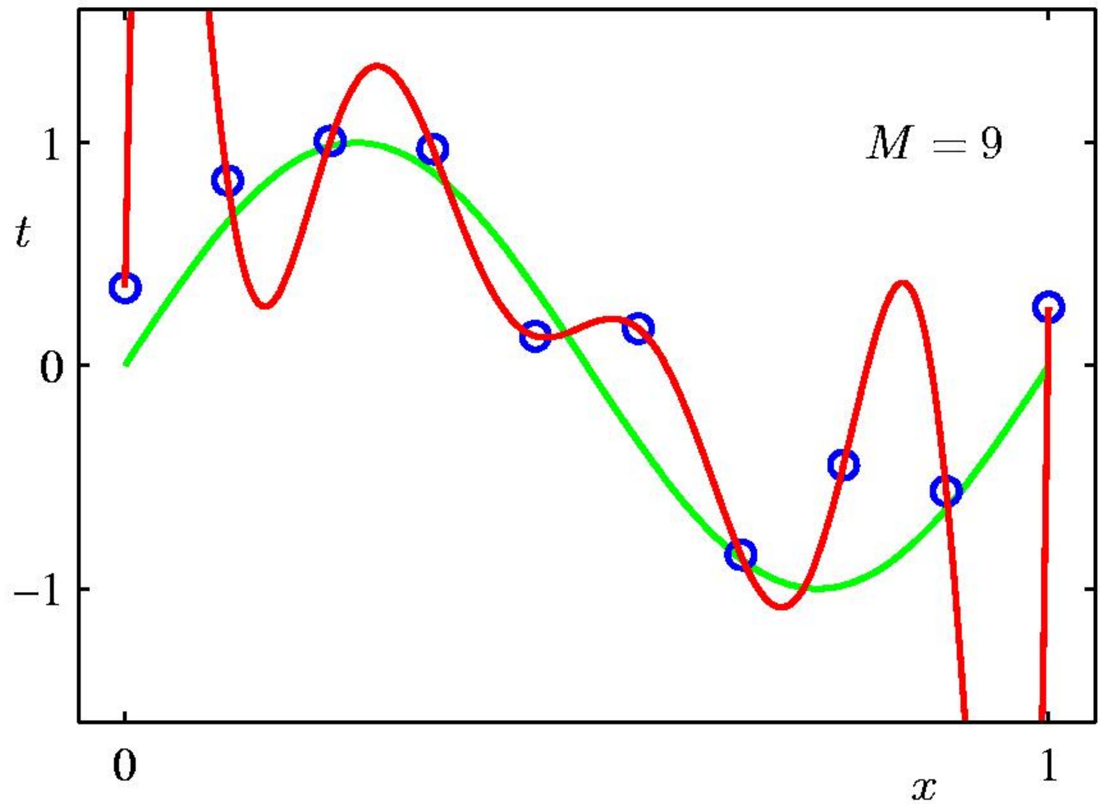
1st Order Polynomial



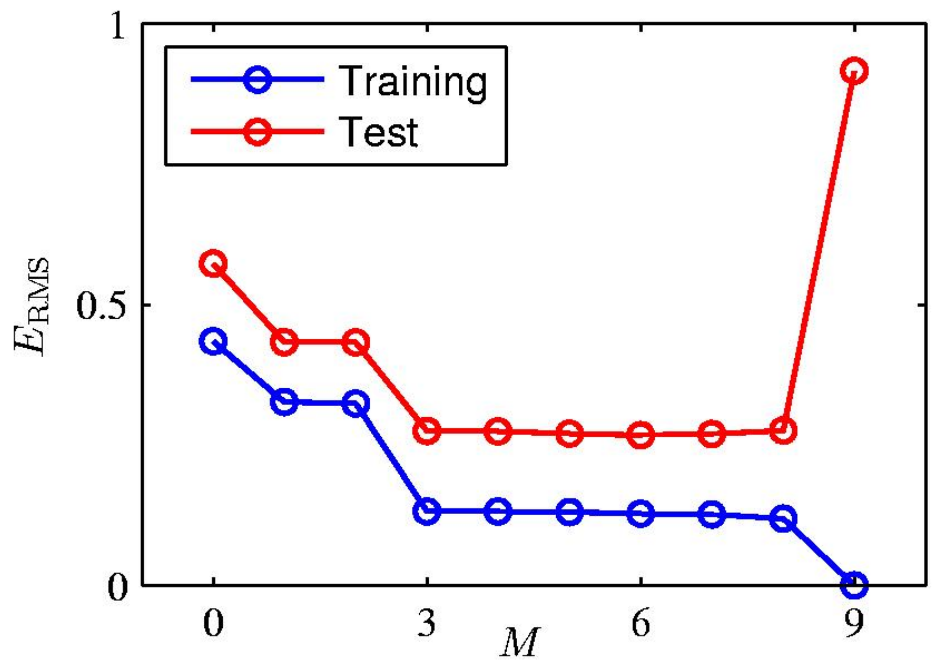
3rd Order Polynomial



9th Order Polynomial



Over-fitting



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

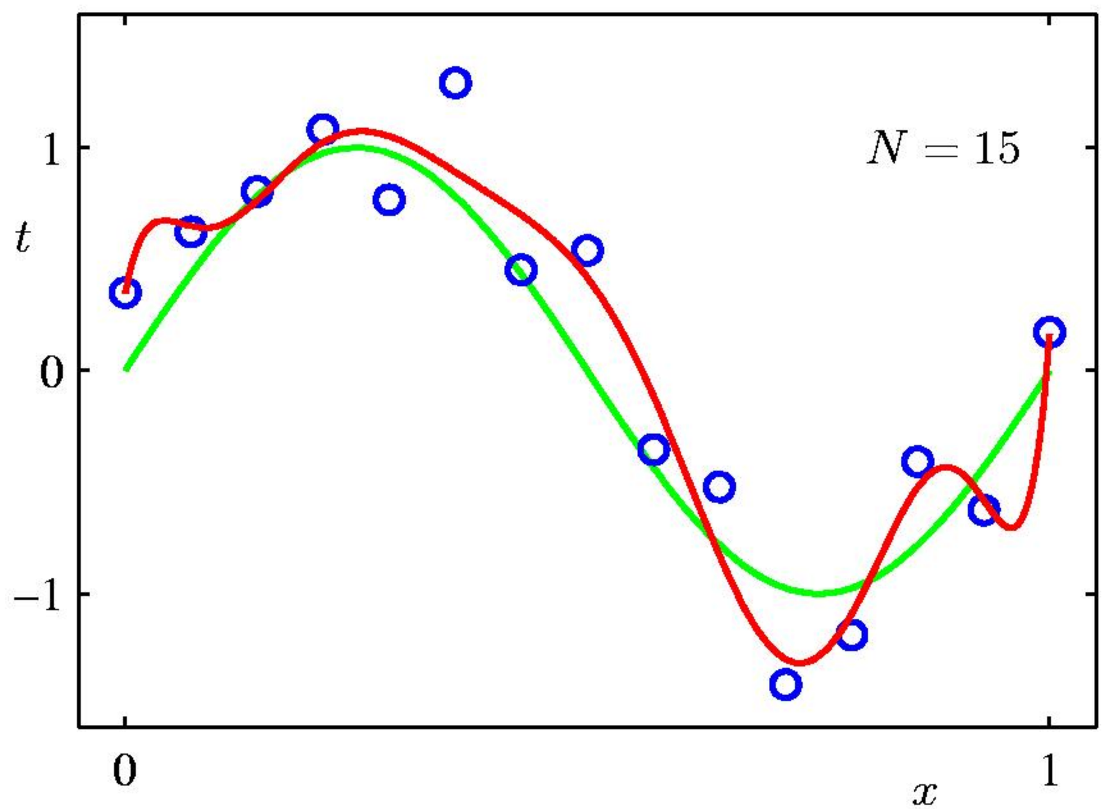
Test set: 100 data points generated using exactly the same procedure used to generate the training set points but with new choices for the random noise values included in the target values t_n.

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

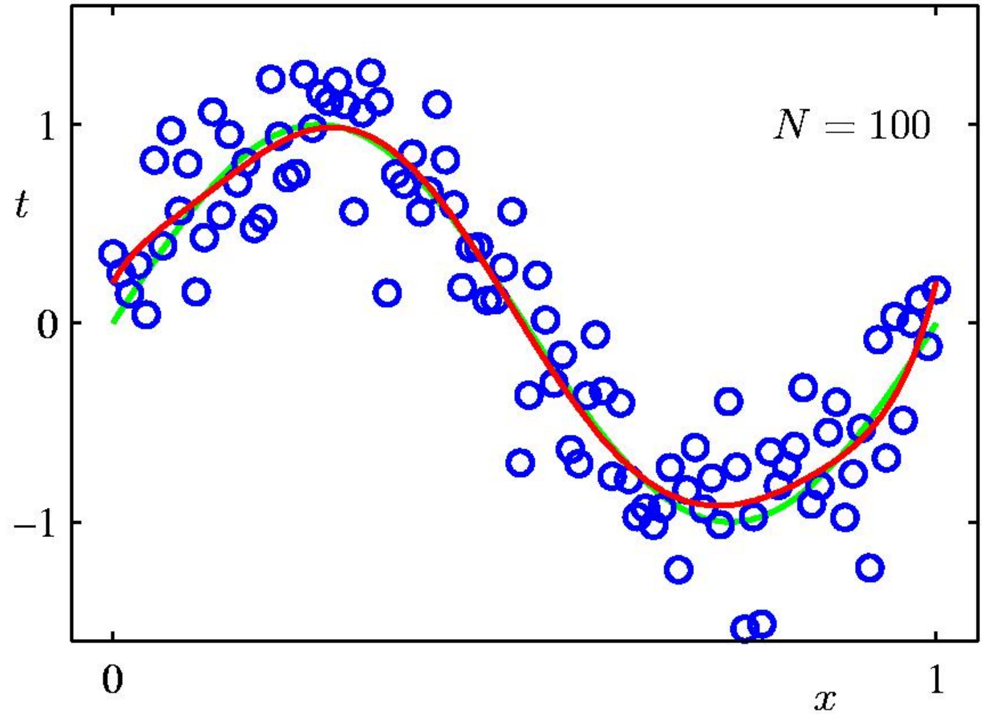
Data Set Size: $N = 15$

9th Order Polynomial



Data Set Size: $N = 100$

9th Order Polynomial



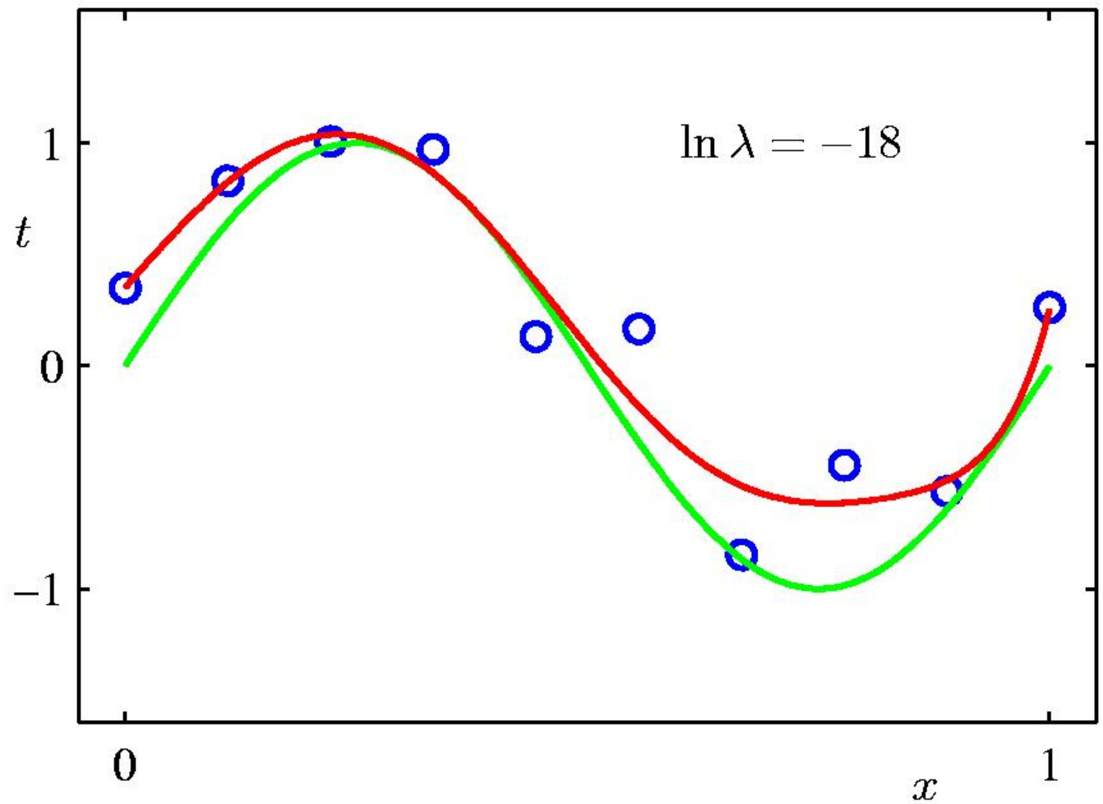
One rough heuristic that is sometimes advocated is that the number of data points should be no less than some multiple (say 5 or 10) of the number of adaptive parameters in the model. (However, the number of parameters is not necessarily the most appropriate measure of model complexity - a measure of how hard it is to learn from limited data.)

Regularization

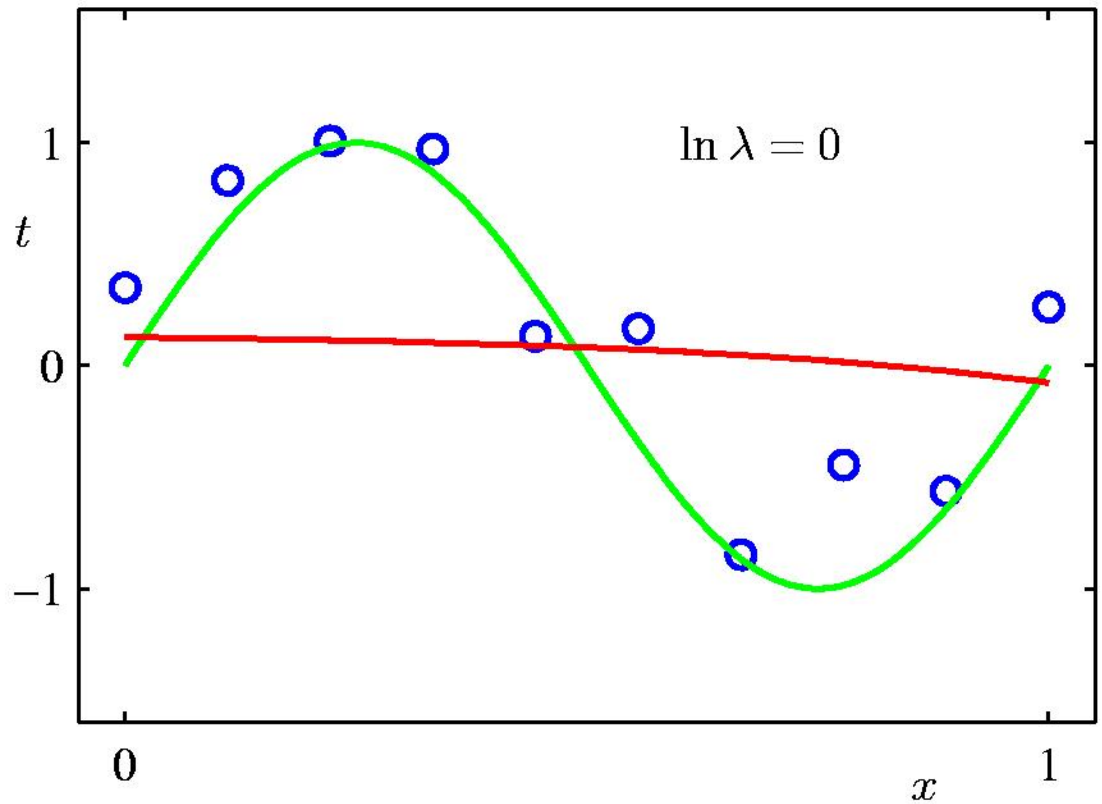
Penalize large coefficient values

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

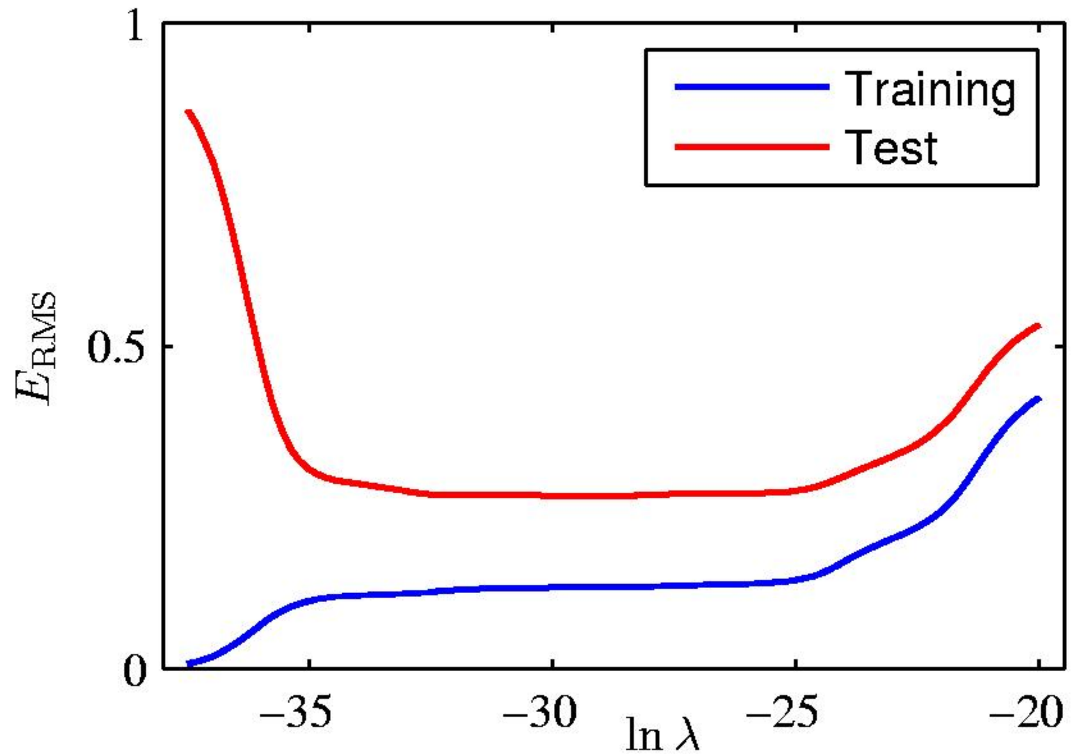
Regularization: $\ln \lambda = -18$



Regularization: $\ln \lambda = 0$



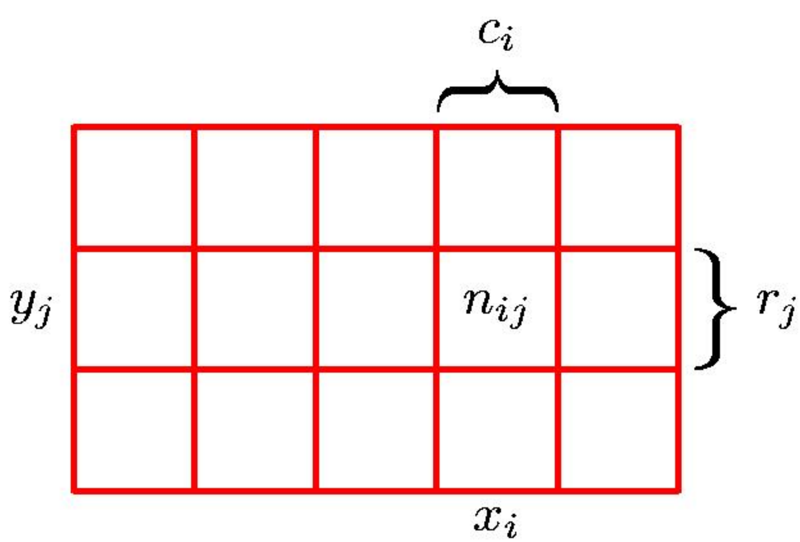
Regularization: E_{RMS} vs. $\ln \lambda$



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

Probability Theory



Marginal Probability

$$p(X = x_i) = \frac{c_i}{N}.$$

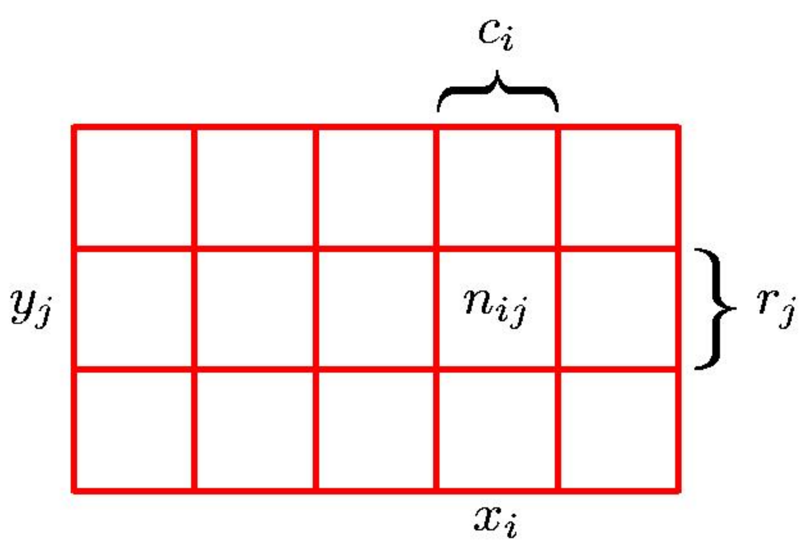
Joint Probability

$$p(X = x_i, Y = y_j) = \frac{n_{ij}}{N}$$

Conditional Probability

$$p(Y = y_j | X = x_i) = \frac{n_{ij}}{c_i}$$

Probability Theory



Sum Rule

$$p(X = x_i) = \frac{c_i}{N} = \frac{1}{N}\sum_{j=1}^{L} n_{ij}$$
$$= \sum_{j=1}^{L} p(X = x_i, Y = y_j)$$

Product Rule

$$\begin{aligned} p(X = x_i, Y = y_j) &= \frac{n_{ij}}{N} = \frac{n_{ij}}{c_i} \cdot \frac{c_i}{N} \\ &= p(Y = y_j | X = x_i) p(X = x_i) \end{aligned}$$

The Rules of Probability

Sum Rule $$p(X) = \sum_Y p(X,Y)$$

Product Rule $$p(X,Y) = p(Y|X)p(X)$$

Also: $p(X, Y) = p(X | Y)\, p(Y)$

Thus:

1. $p(X) = \sum_Y p(X|Y)p(Y)$
2. $p(Y | X)\, p(X) = p(X | Y)\, p(Y)$

Bayes' Theorem

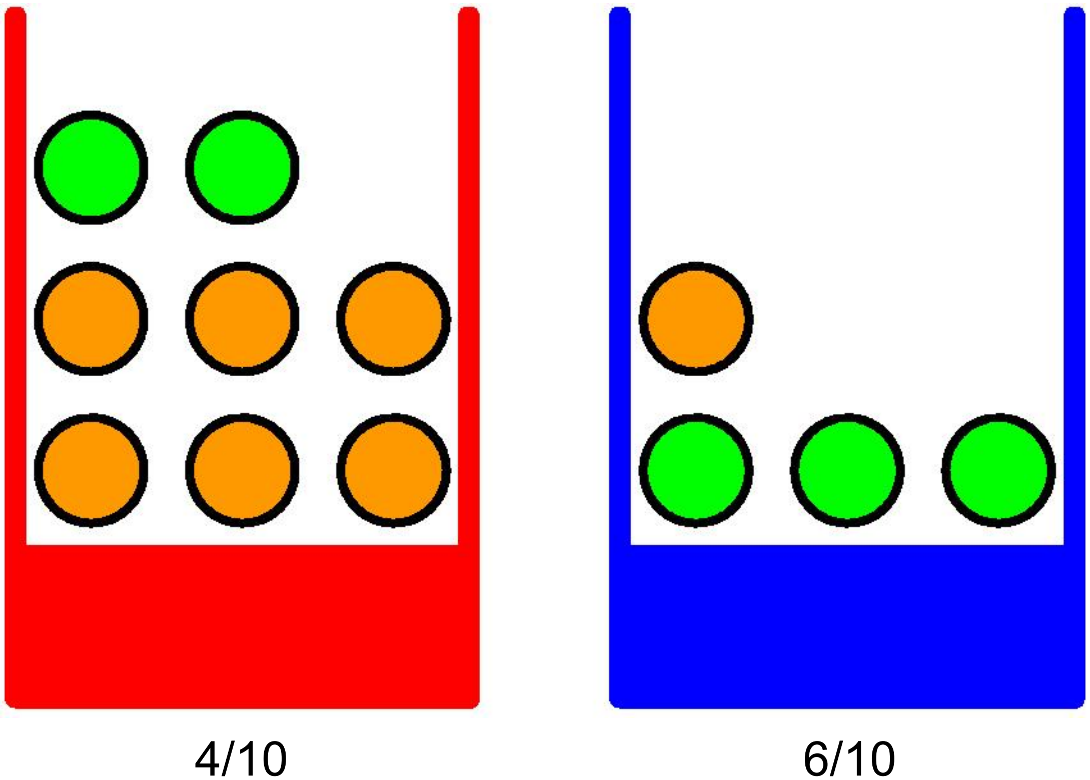
$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

$$p(X) = \sum_{Y} p(X|Y)p(Y)$$

posterior ∝ likelihood × prior

Probability Theory

Apples and Oranges



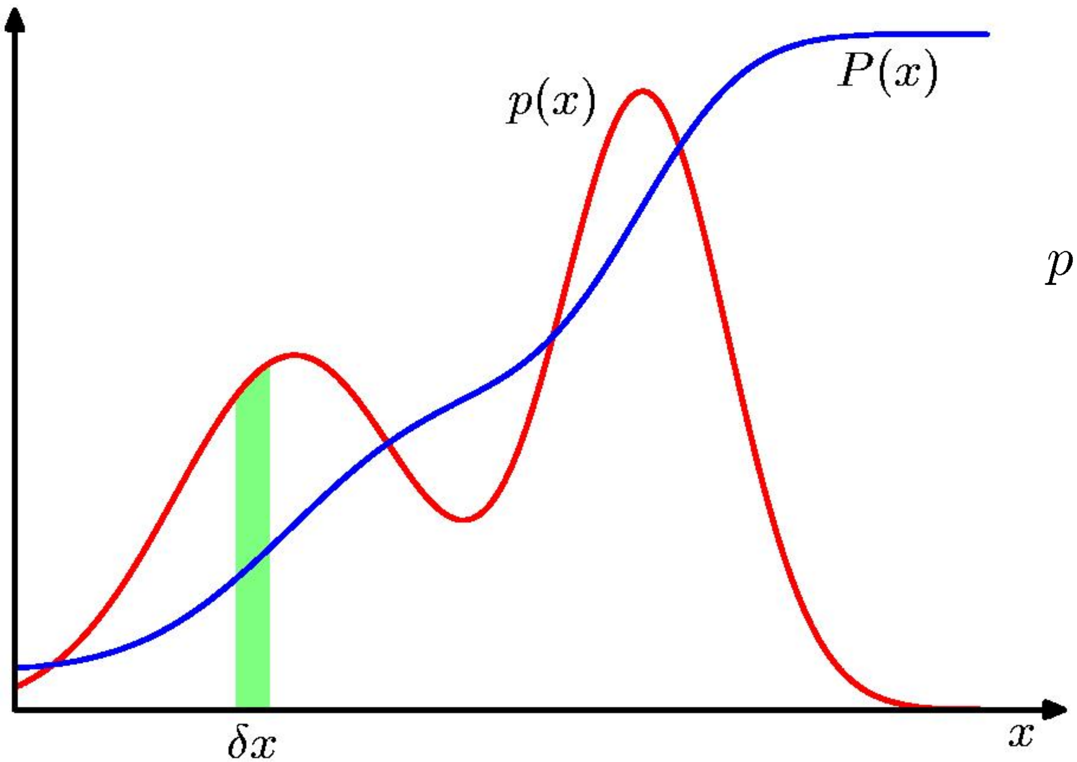
Bayes' Theorem Generalized

$$P(W|T) = p(T|W)\ p(W)\ /\ p(T)$$

$$P(W|T, X) = p(T|X, W)\ p(W|X)\ /\ p(T|X)$$

$$P(T|X) = \text{sum over W of }\ p(T|X, W)\ p(W|X)$$

Probability Densities



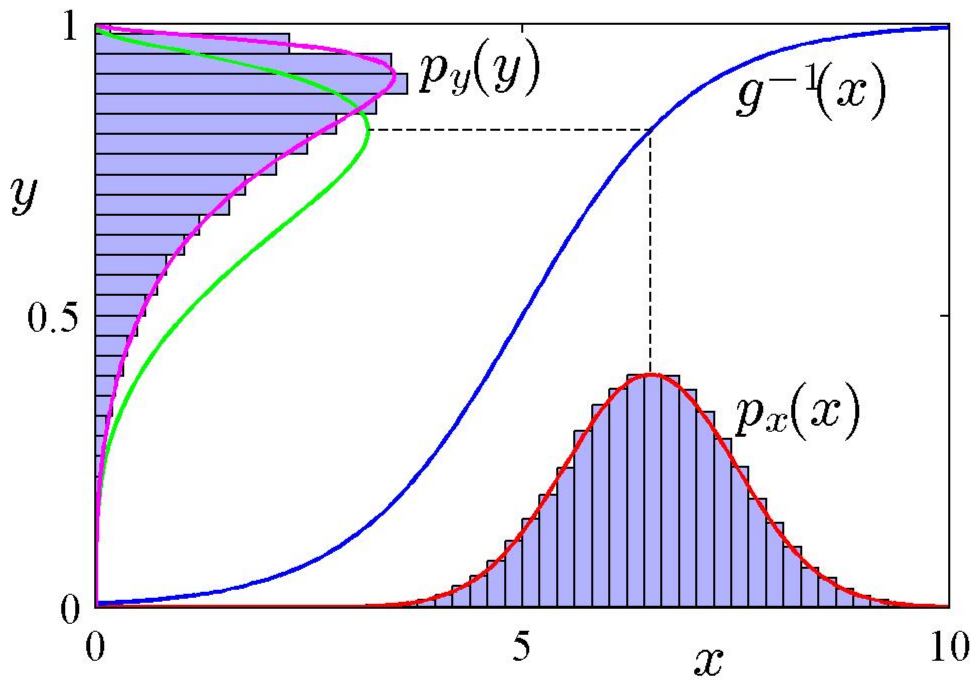
$$p(x \in (a, b)) = \int_a^b p(x)\,\mathrm{d}x$$

$$P(z) = \int_{-\infty}^{z} p(x)\,\mathrm{d}x$$

$$P'(x) = p(x)$$

$$p(x) \geqslant 0 \qquad \int_{-\infty}^{\infty} p(x)\,\mathrm{d}x = 1$$

Transformed Densities



Suppose $x = g(y)$

$$p_y(y) = p_x(x)\left|\frac{\mathrm{d}x}{\mathrm{d}y}\right| = p_x(g(y))\,|g'(y)|$$

Expectations

$$\mathbb{E}[f] = \sum_x p(x) f(x)$$

$$\mathbb{E}[f] = \int p(x) f(x) \, \mathrm{d}x$$

$$\mathbb{E}_x[f|y] = \sum_x p(x|y) f(x)$$

Conditional Expectation
(discrete)

$$\mathbb{E}[f] \simeq \frac{1}{N} \sum_{n=1}^{N} f(x_n)$$

Approximate Expectation
(discrete and continuous)

Variances and Covariances

$$\mathrm{var}[f] = \mathbb{E}\left[(f(x) - \mathbb{E}[f(x)])^2\right] = \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2$$

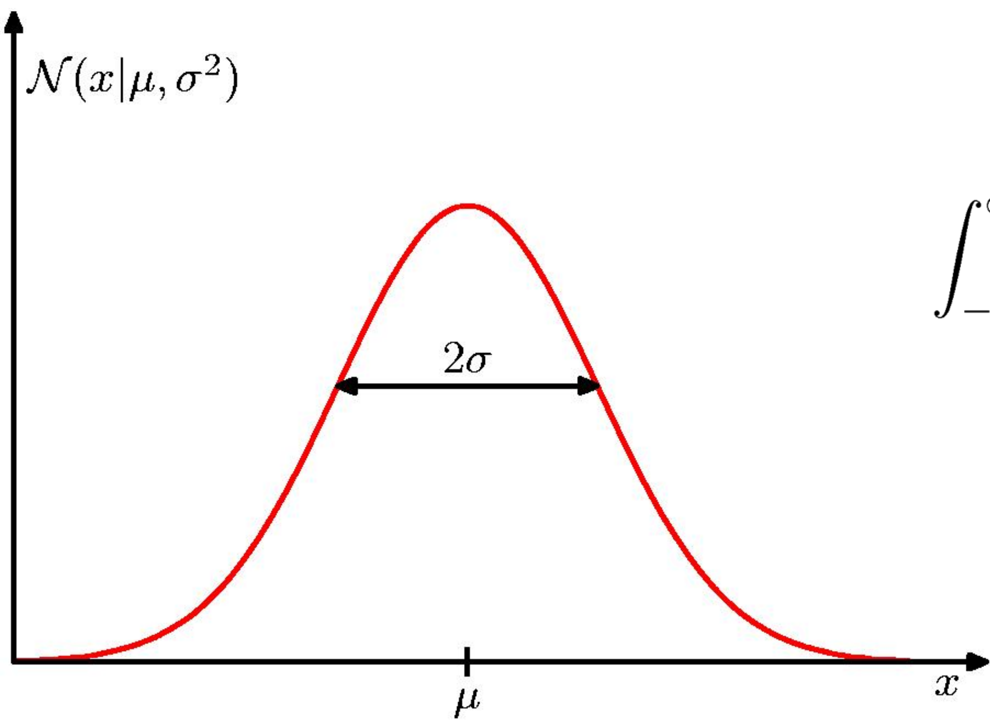
$$\mathrm{var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2$$ (standard deviation's square)

$$\begin{aligned} \mathrm{cov}[x, y] &= \mathbb{E}_{x,y}\left[\{x - \mathbb{E}[x]\}\{y - \mathbb{E}[y]\}\right] \\ &= \mathbb{E}_{x,y}[xy] - \mathbb{E}[x]\mathbb{E}[y] \end{aligned}$$

$$\begin{aligned} \mathrm{cov}[\mathbf{x}, \mathbf{y}] &= \mathbb{E}_{\mathbf{x},\mathbf{y}}\left[\{\mathbf{x} - \mathbb{E}[\mathbf{x}]\}\{\mathbf{y}^{\mathrm{T}} - \mathbb{E}[\mathbf{y}^{\mathrm{T}}]\}\right] \\ &= \mathbb{E}_{\mathbf{x},\mathbf{y}}[\mathbf{x}\mathbf{y}^{\mathrm{T}}] - \mathbb{E}[\mathbf{x}]\mathbb{E}[\mathbf{y}^{\mathrm{T}}] \end{aligned}$$ (a symmetric matrix)

The Gaussian Distribution

$$\mathcal{N}\left(x|\mu,\sigma^2\right) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{-\frac{1}{2\sigma^2}(x-\mu)^2\right\}$$



$$\mathcal{N}(x|\mu,\sigma^2) > 0$$

$$\int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu,\sigma^2\right) \, \mathrm{d}x = 1$$

Gaussian Mean and Variance

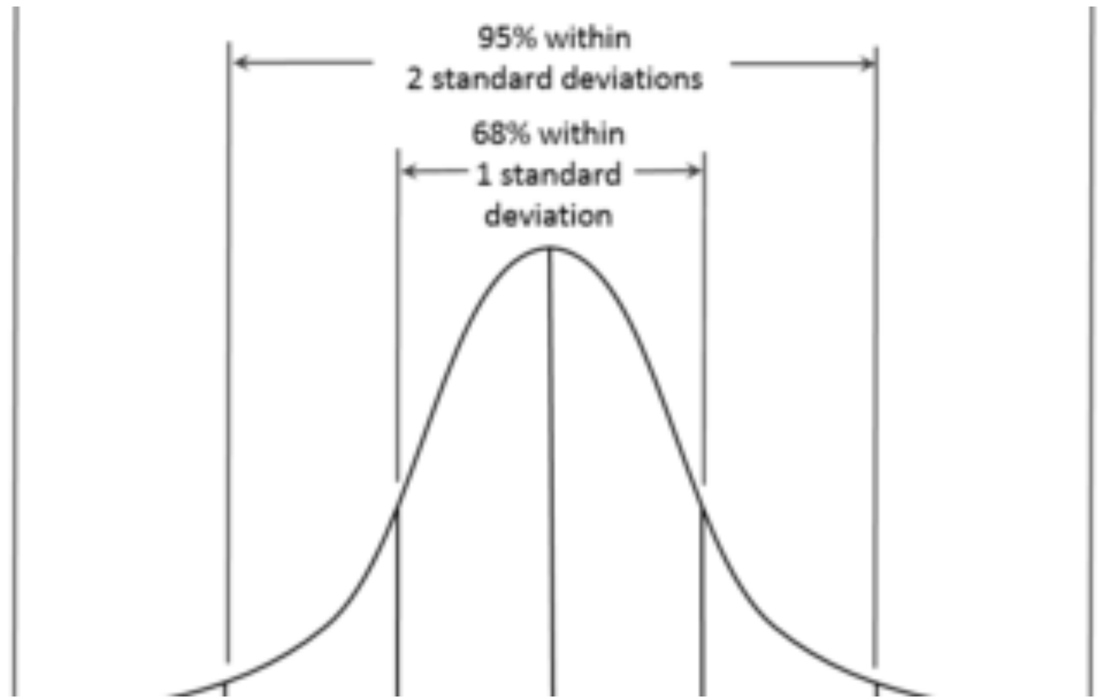
$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) x \, \mathrm{d}x = \mu$$ (mean)

$$\mathbb{E}[x^2] = \int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) x^2 \, \mathrm{d}x = \mu^2 + \sigma^2$$

$$\mathrm{var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2$$ (variance)

$\beta = 1/\sigma^2$ (precision – the bigger β is, the smaller σ is, thus the more "precise" the distribution is.)

The Gaussian Distribution



For the normal distribution, the values less than one standard deviation away from the mean account for 68.27% of the set; while two standard deviations from the mean account for 95.45%; and three standard deviations account for 99.73%.

The Multivariate Gaussian

Gaussian distribution defined over a D-dimensional vector x of continuous variables:

$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu},\boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}}\frac{1}{|\boldsymbol{\Sigma}|^{1/2}}\exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

where the **D**-dimensional vector μ is called the mean, the **D x D** symmetric matrix Σ is called the covariance, and **|Σ|** denotes the determinant of Σ.