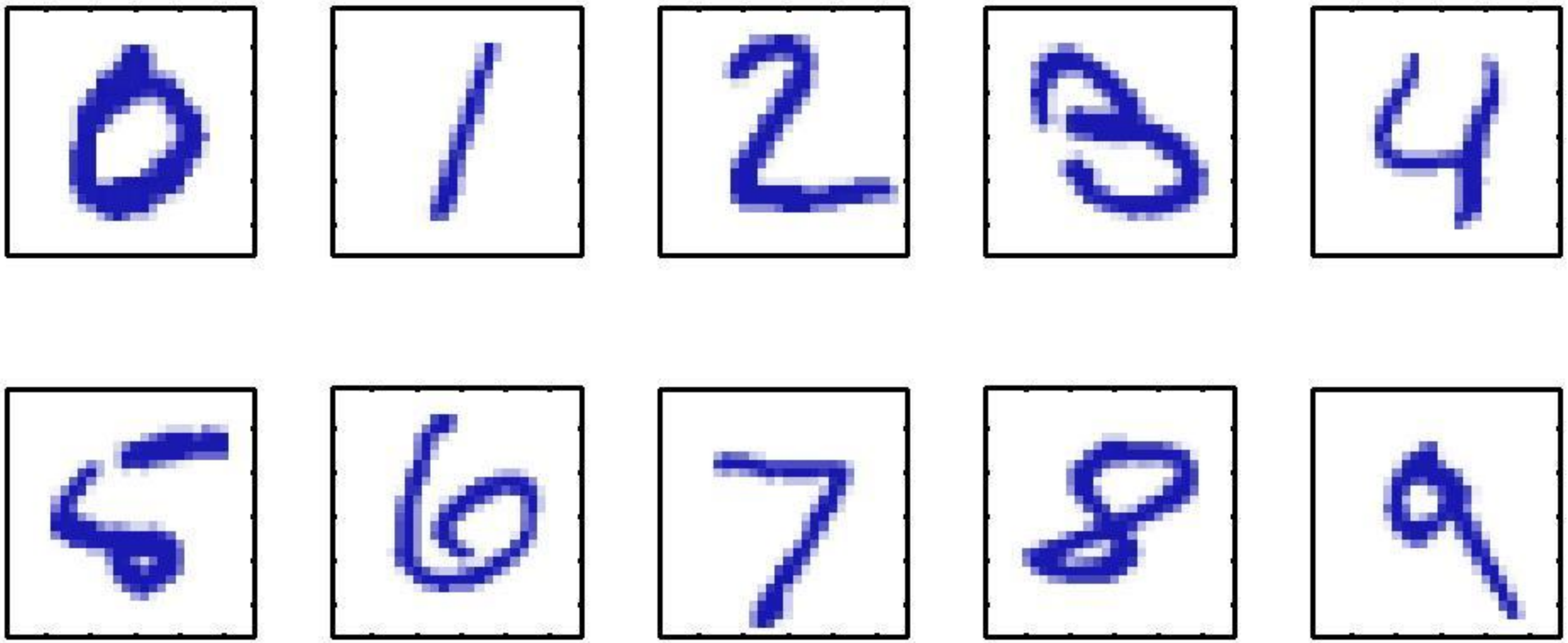
PATTERN RECOGNITION AND MACHINE LEARNING

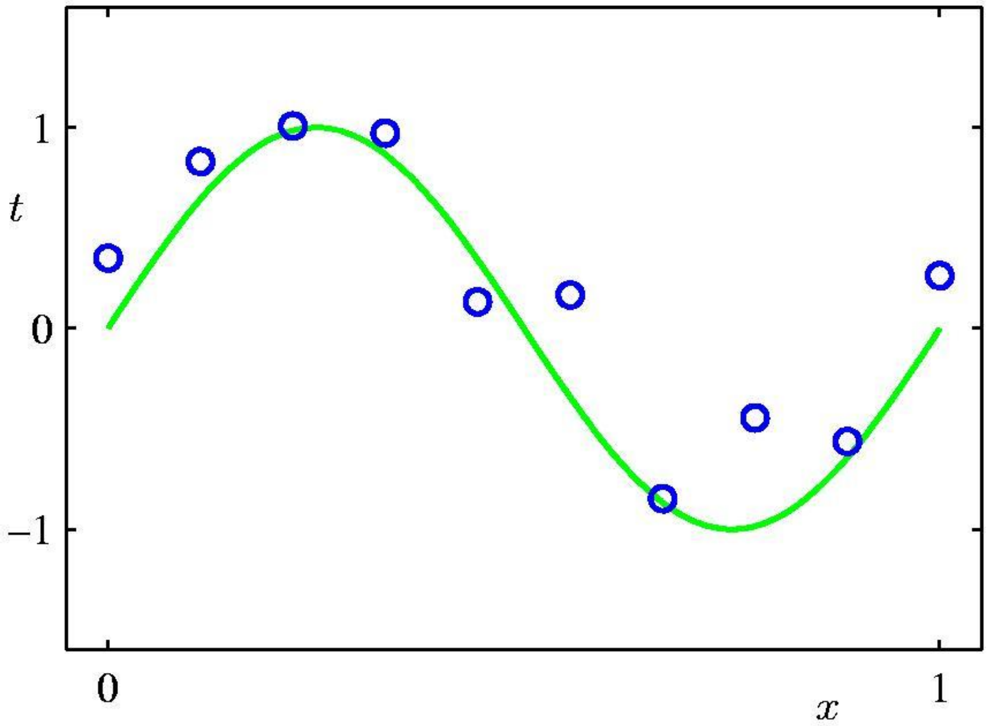
CHAPTER 1: INTRODUCTION

Example

Handwritten Digit Recognition

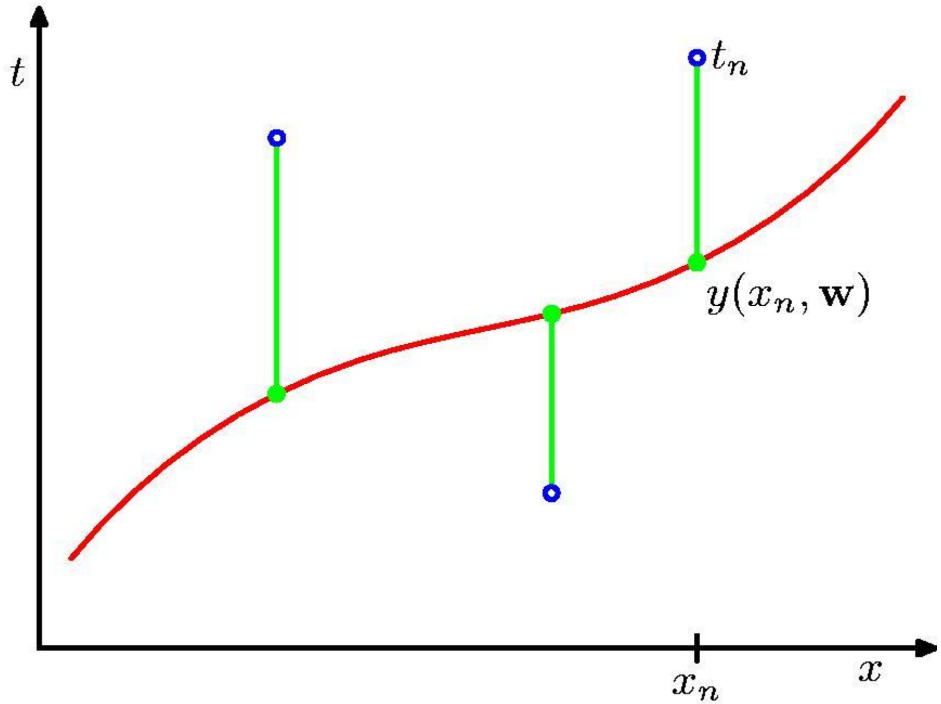


Polynomial Curve Fitting



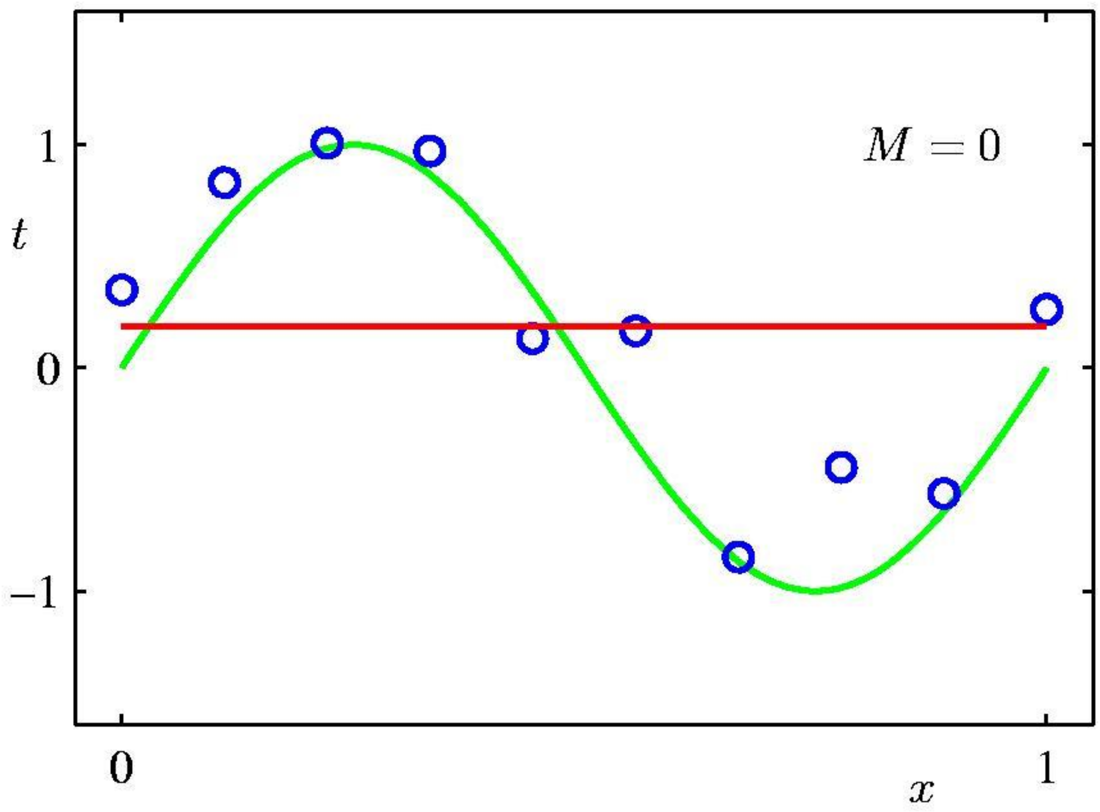
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Sum-of-Squares Error Function

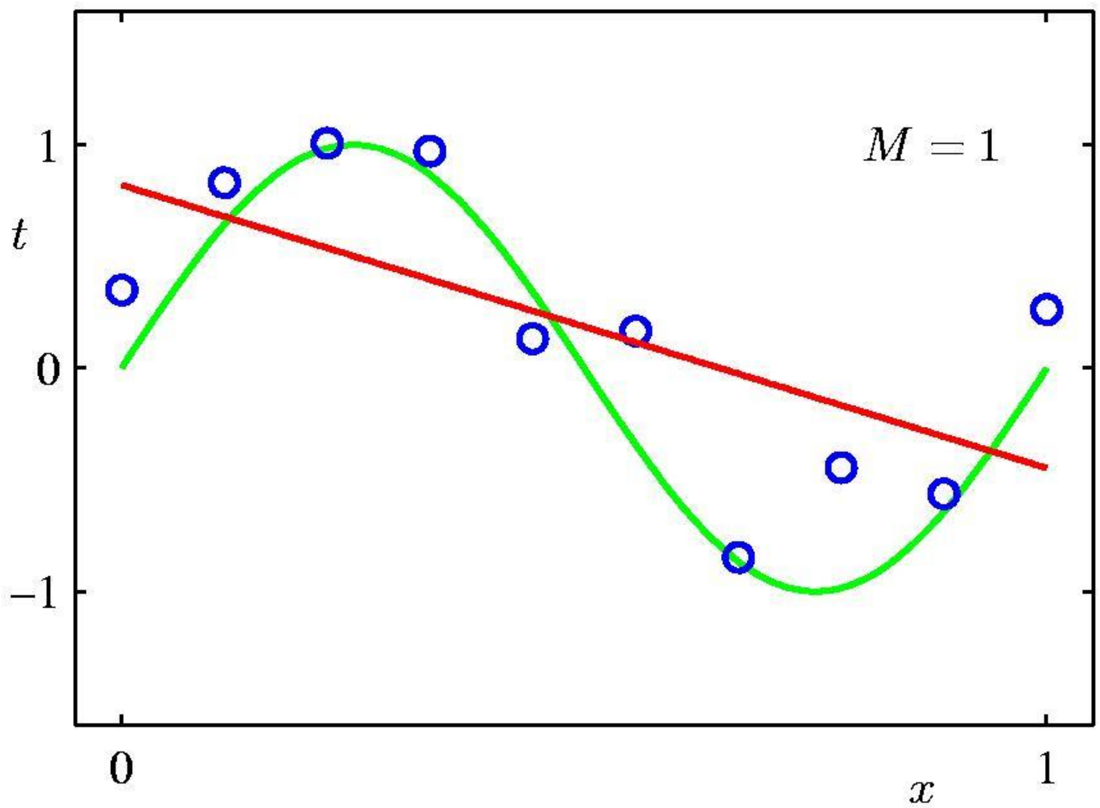


$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2$$

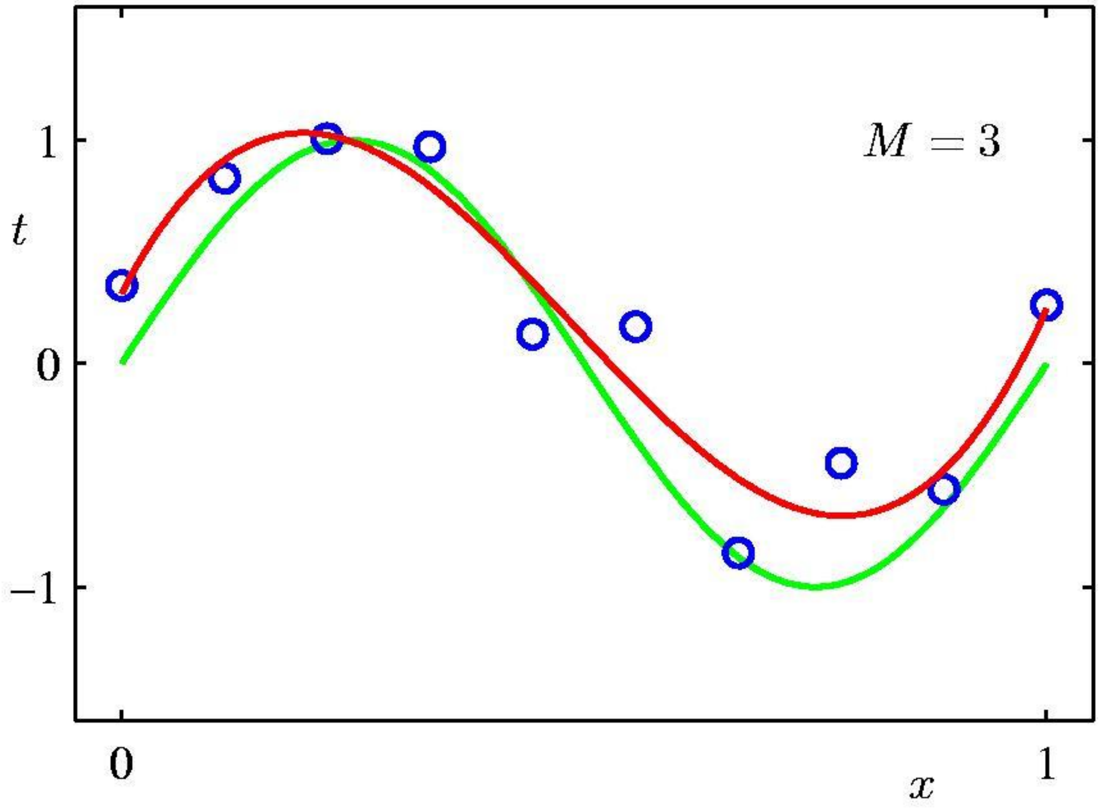
0^{th} Order Polynomial



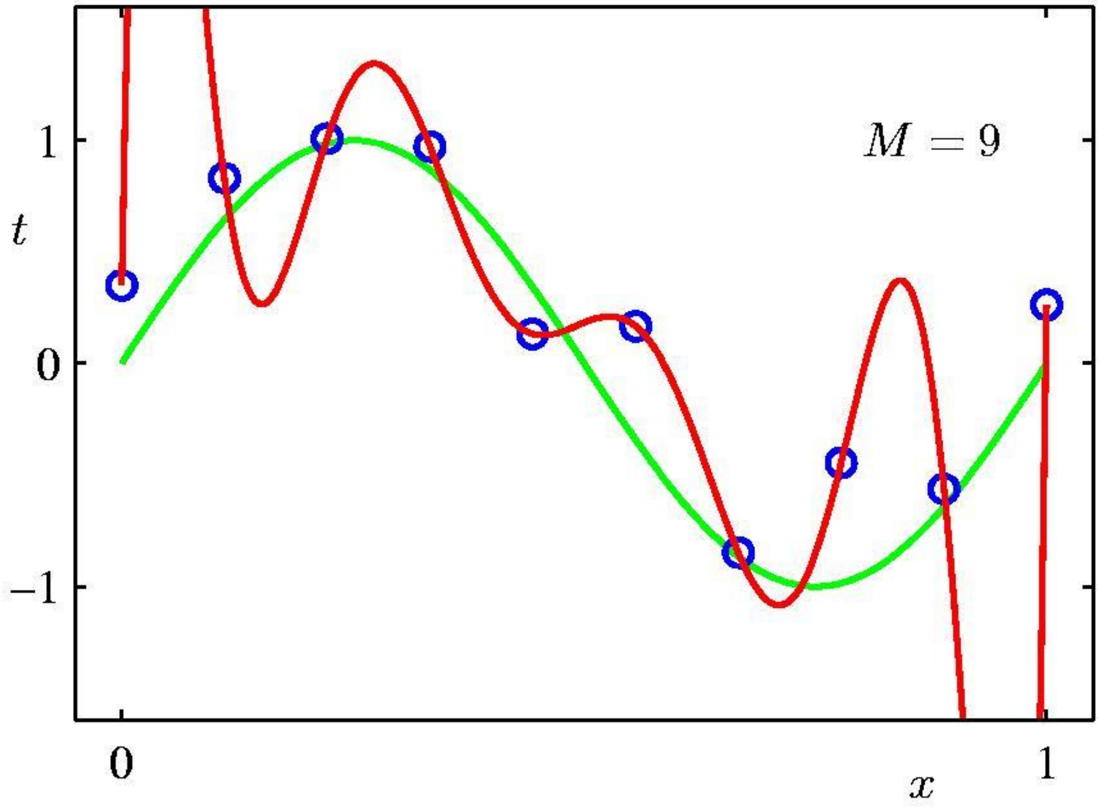
1st Order Polynomial



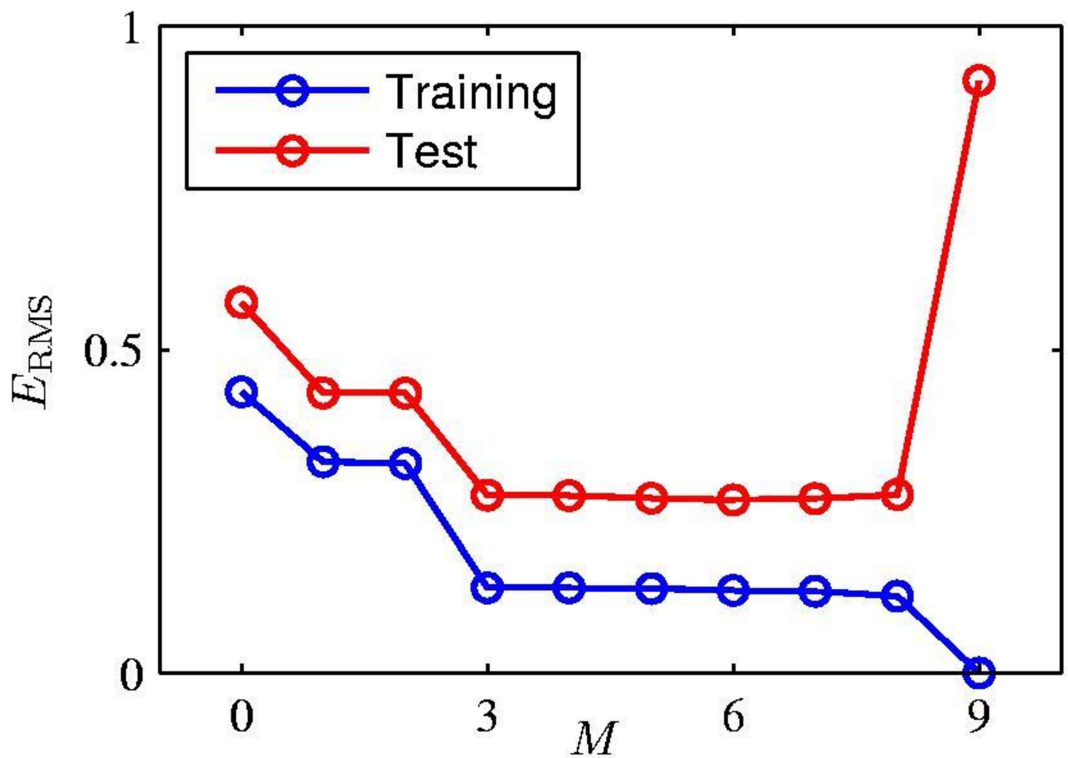
3rd Order Polynomial



9^{th} Order Polynomial



Over-fitting



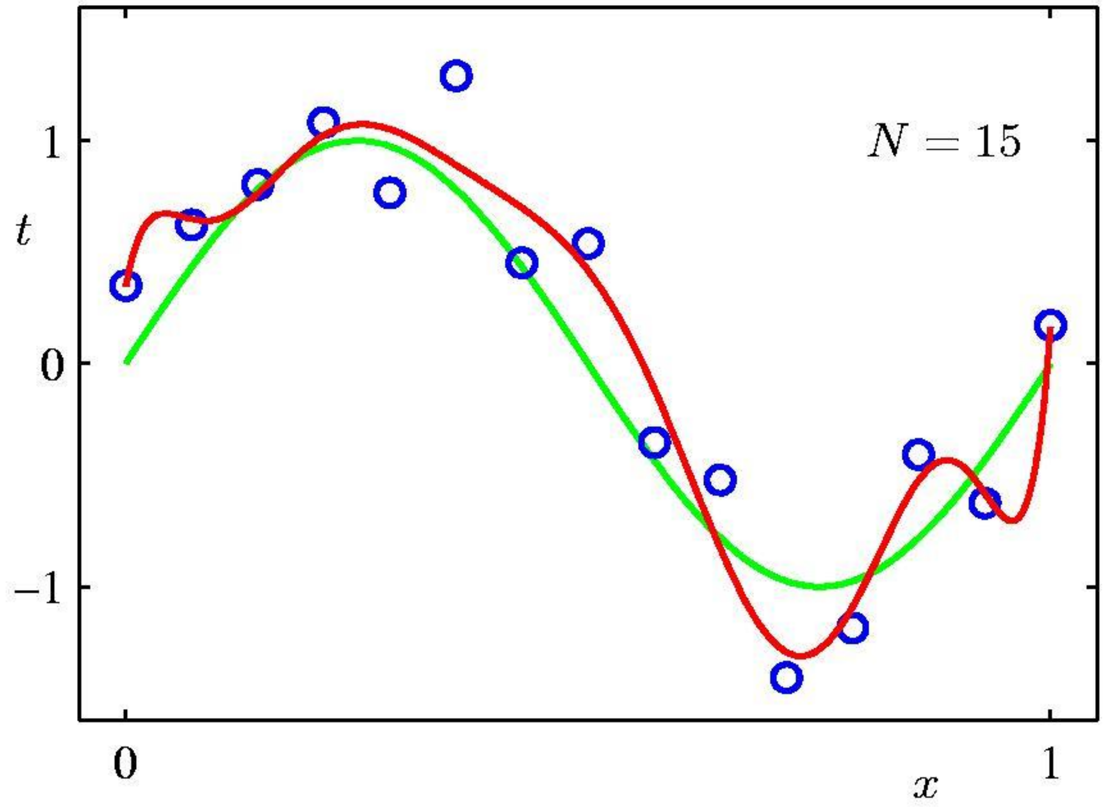
Root-Mean-Square (RMS) Error: $E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$

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

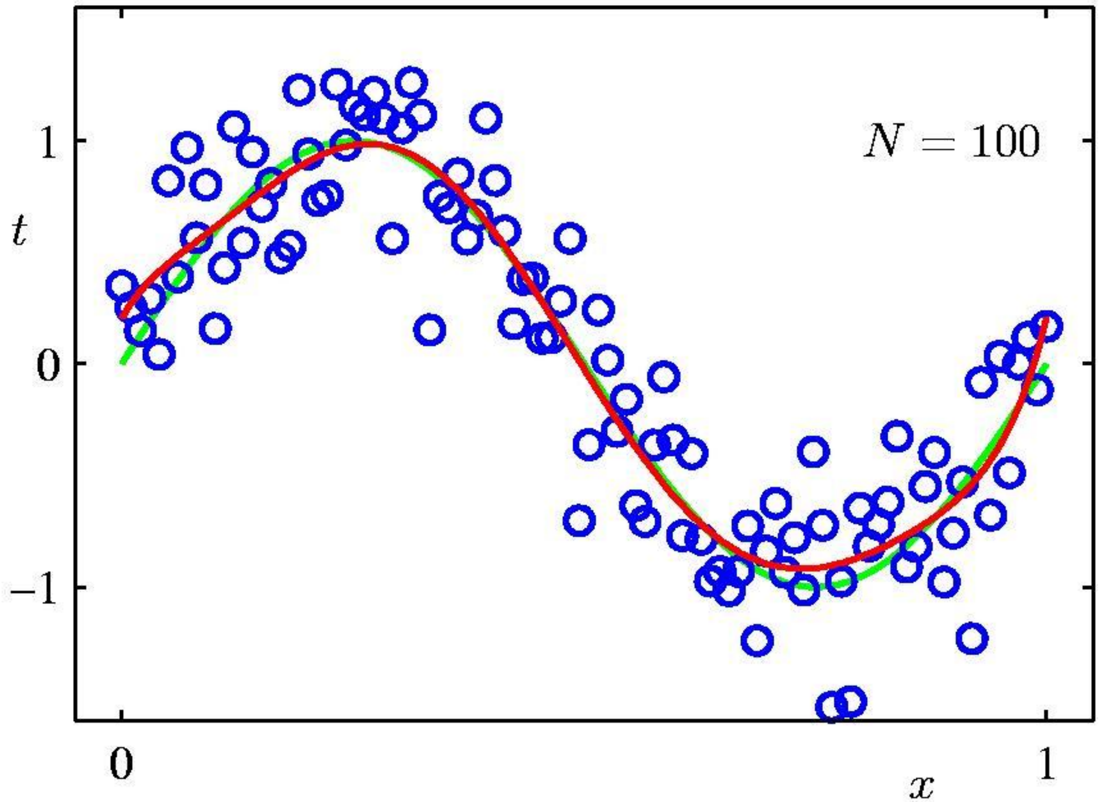
Data Set Size: $N = 15$

9^{th} Order Polynomial



Data Set Size: $N = 100$

9th Order Polynomial

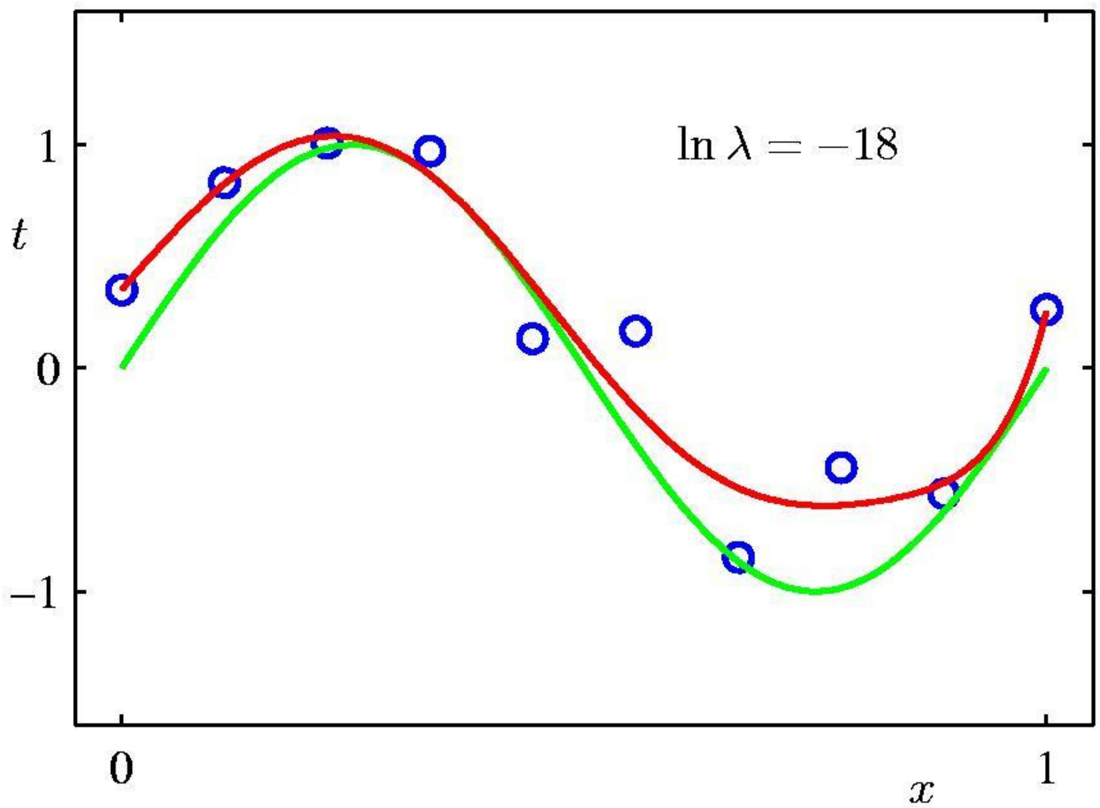


Regularization

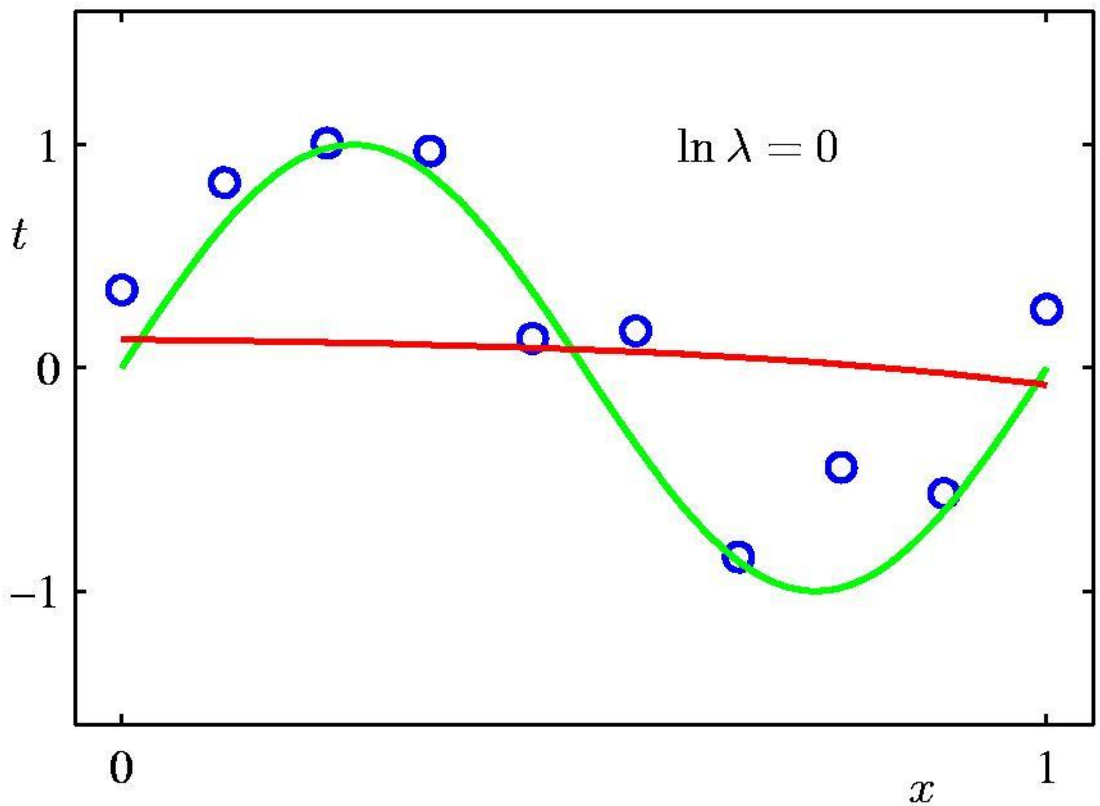
Penalize large coefficient values

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

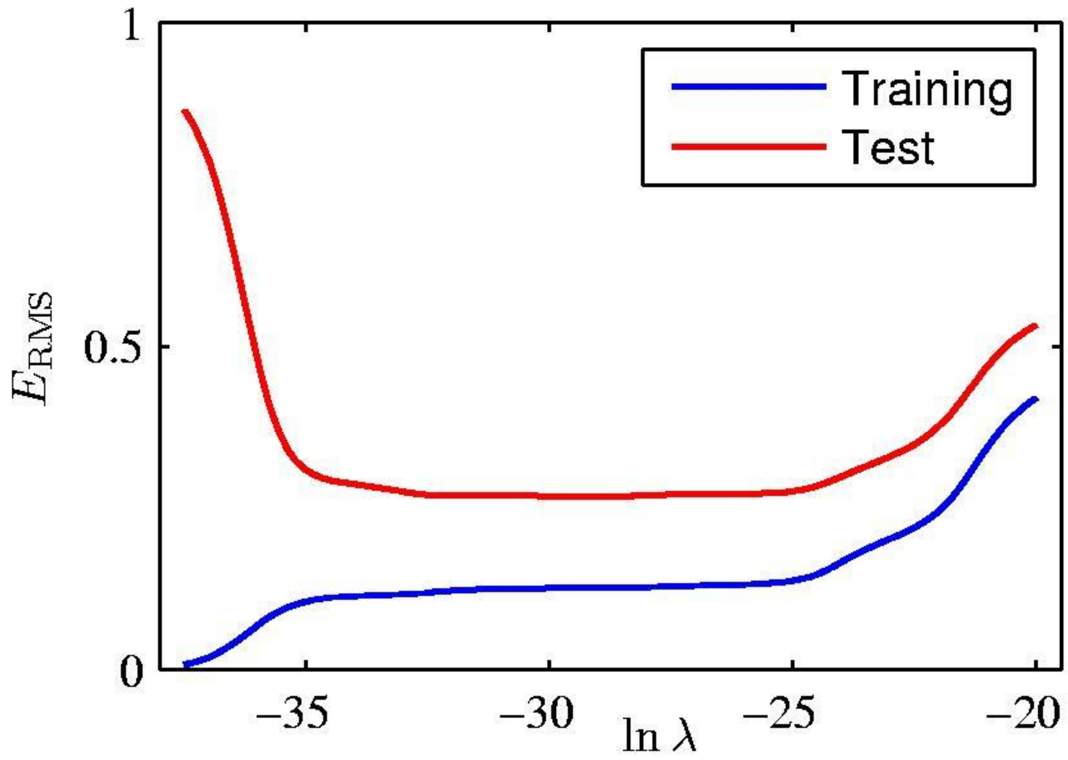
Regularization: $\ln \lambda = -18$



Regularization: $\ln \lambda = 0$



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

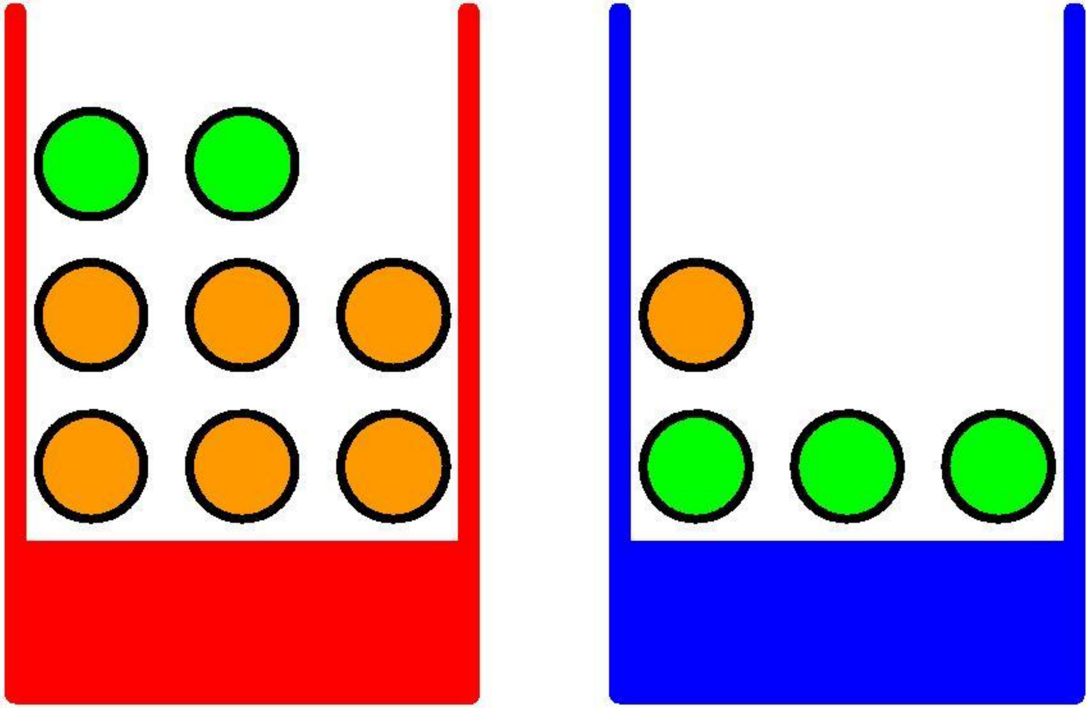


Polynomial Coefficients

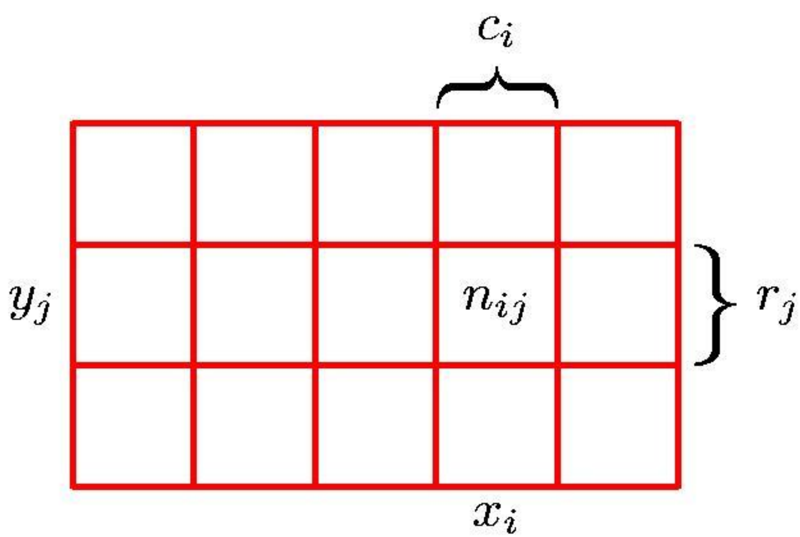
	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$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

Apples and Oranges



Probability Theory



Marginal Probability

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

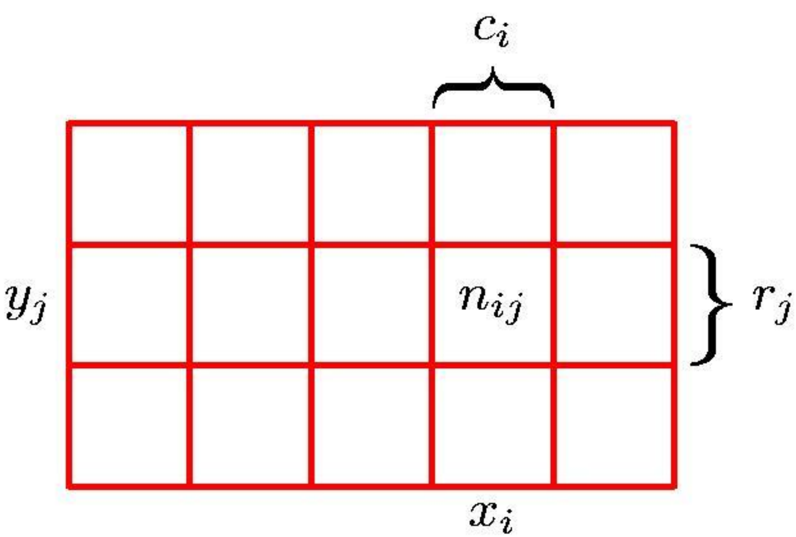
Joint Probability

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

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

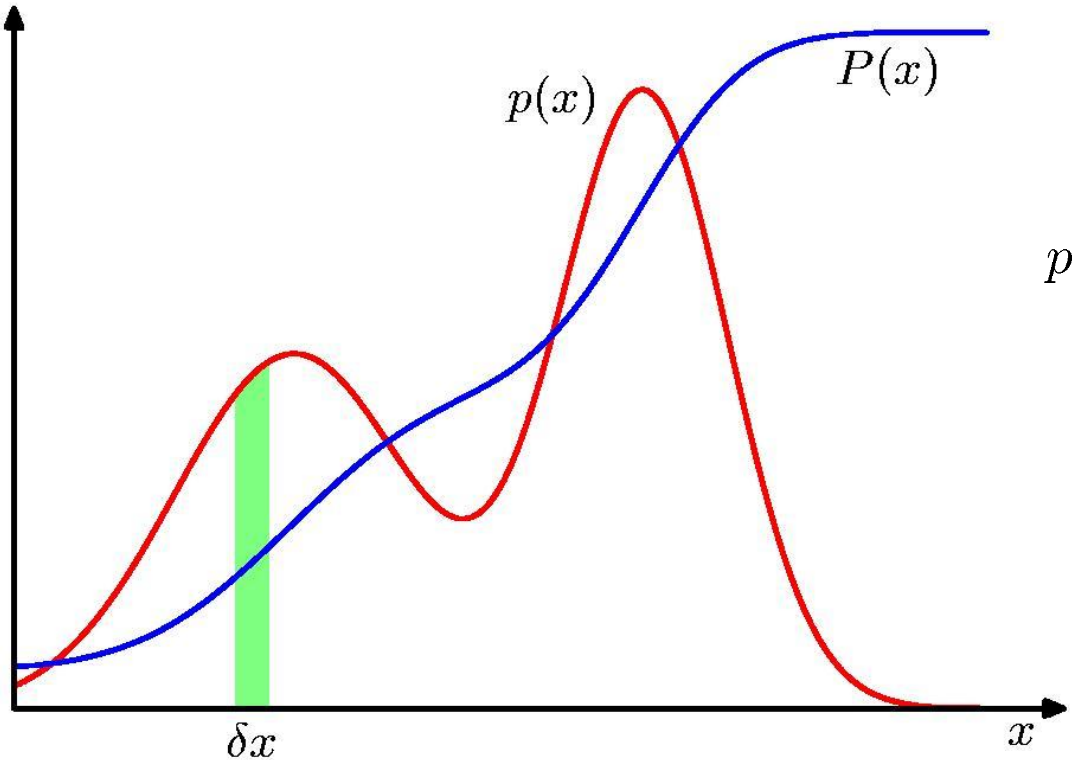
Bayes' Theorem

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

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

posterior $\propto$ likelihood × prior

Probability Densities

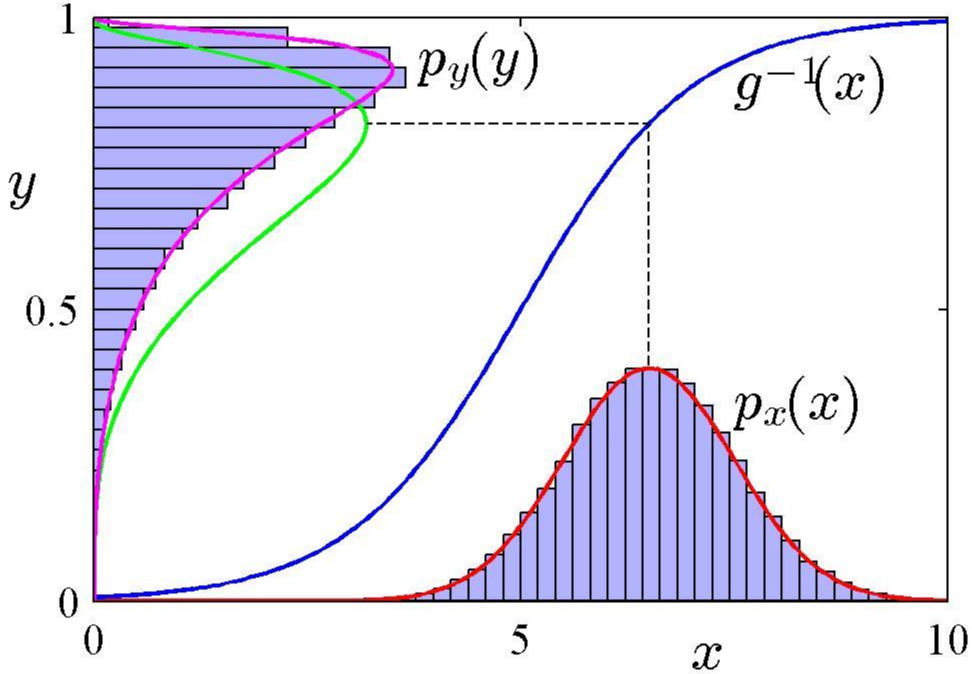


$$p(x \in (a, b)) = \int_a^b p(x)\,\mathrm{d}x$$

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

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

Transformed Densities



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

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

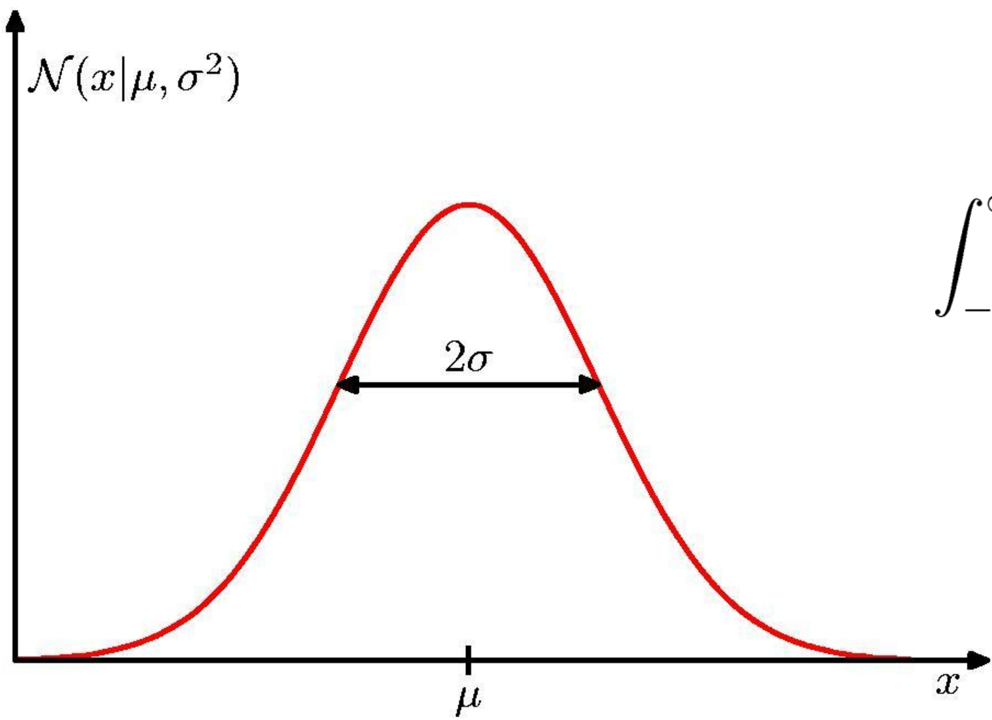
$$\mathrm{var}[f] = \mathbb{E}\left[\left(f(x) - \mathbb{E}[f(x)]\right)^2\right] = \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2$$

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

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

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

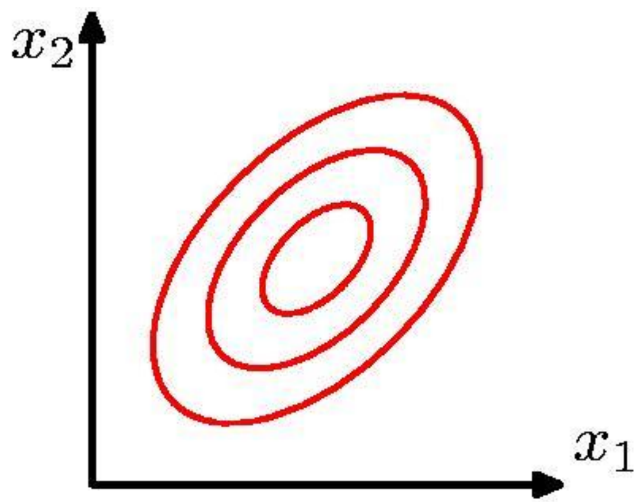
$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) x \, \mathrm{d}x = \mu$$

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

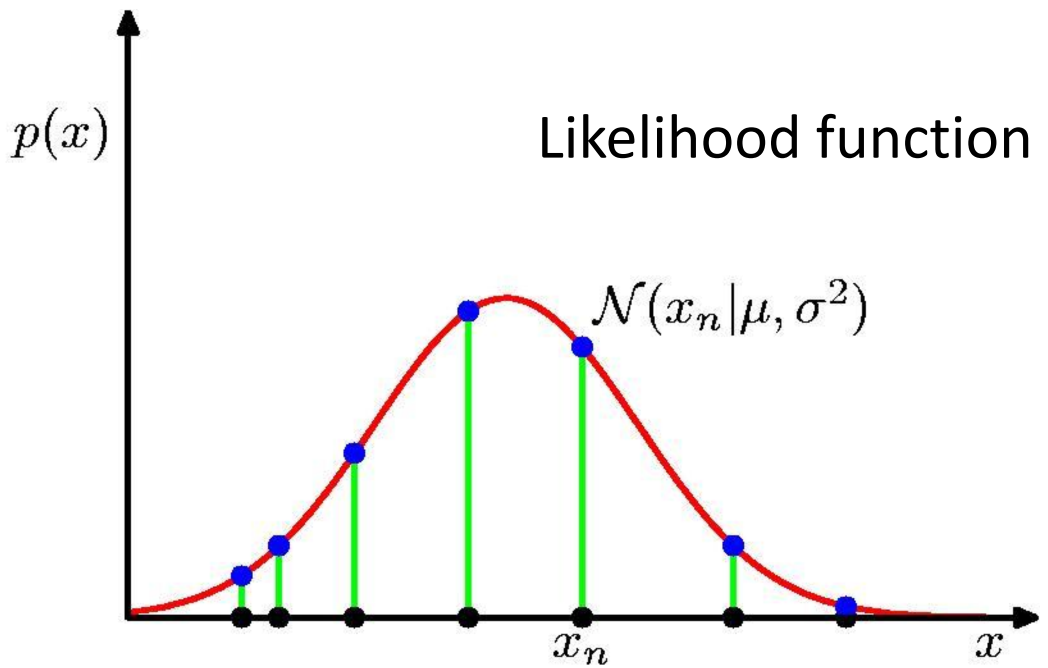
$$\mathrm{var}[x] = \mathbb{E}[x^2] - \mathbb{E}[x]^2 = \sigma^2$$

The Multivariate Gaussian

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



Gaussian Parameter Estimation



$$p(\mathbf{x}|\mu,\sigma^2) = \prod_{n=1}^{N} \mathcal{N}\left(x_n|\mu,\sigma^2\right)$$

Maximum (Log) Likelihood

$$\ln p\left(\mathbf{x}|\mu,\sigma^2\right) = -\frac{1}{2\sigma^2}\sum_{n=1}^{N}(x_n-\mu)^2 - \frac{N}{2}\ln\sigma^2 - \frac{N}{2}\ln(2\pi)$$

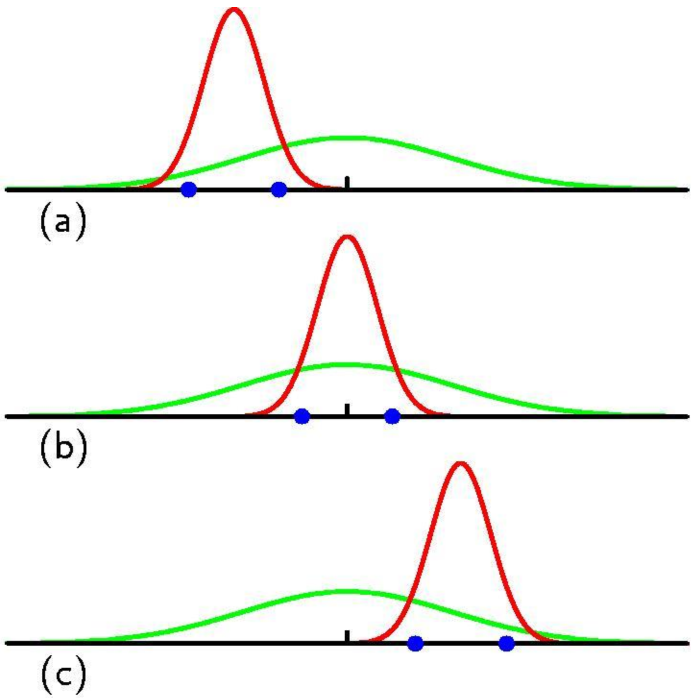
$$\mu_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N}x_n \qquad \sigma^2_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N}(x_n-\mu_{\mathrm{ML}})^2$$

Properties of μ_{ML} and σ^2_{ML}

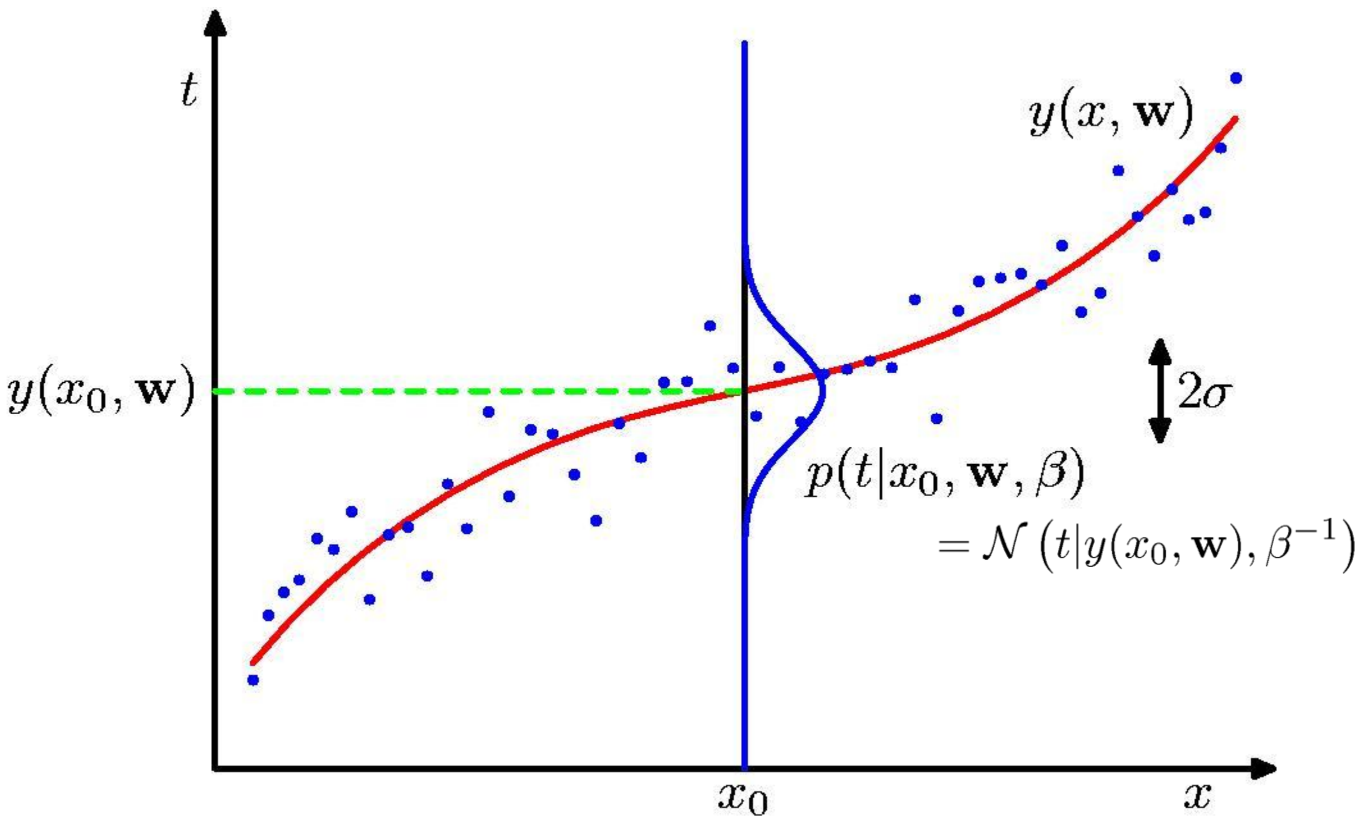
$$\mathbb{E}[\mu_{\mathrm{ML}}] = \mu$$

$$\mathbb{E}[\sigma^2_{\mathrm{ML}}] = \left(\frac{N-1}{N}\right)\sigma^2$$

$$\begin{aligned}\widetilde{\sigma}^2 &= \frac{N}{N-1}\sigma^2_{\mathrm{ML}} \\ &= \frac{1}{N-1}\sum_{n=1}^{N}(x_n - \mu_{\mathrm{ML}})^2\end{aligned}$$



Curve Fitting Re-visited



Maximum Likelihood

$$p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \prod_{n=1}^{N} \mathcal{N}\left(t_n | y(x_n, \mathbf{w}), \beta^{-1}\right)$$

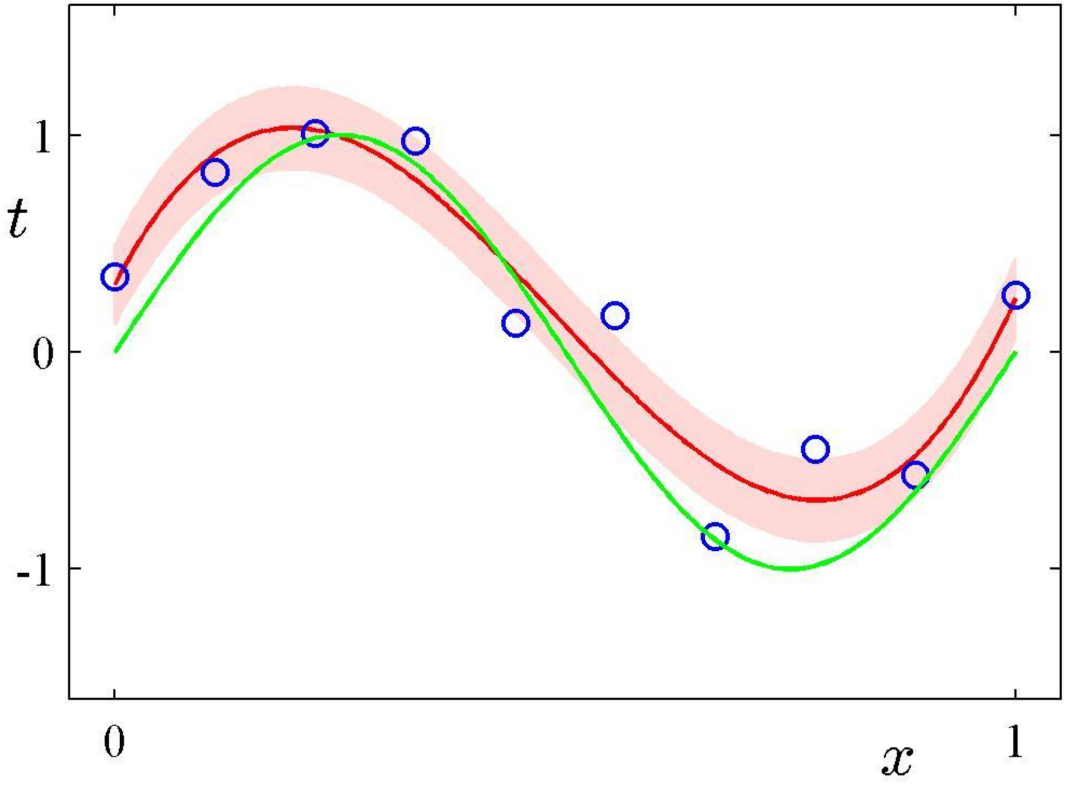
$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \underbrace{-\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2}_{\beta E(\mathbf{w})} + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$$

Determine $\mathbf{w}_{\mathrm{ML}}$ by minimizing sum-of-squares error, $E(\mathbf{w})$.

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

Predictive Distribution

$$p(t|x, \mathbf{w}_{\mathrm{ML}}, \beta_{\mathrm{ML}}) = \mathcal{N}\left(t|y(x, \mathbf{w}_{\mathrm{ML}}), \beta_{\mathrm{ML}}^{-1}\right)$$



MAP: A Step towards Bayes

$$p(\mathbf{w}|\alpha) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \alpha^{-1}\mathbf{I}) = \left(\frac{\alpha}{2\pi}\right)^{(M+1)/2} \exp\left\{-\frac{\alpha}{2}\mathbf{w}^{\mathrm{T}}\mathbf{w}\right\}$$

$$p(\mathbf{w}|\mathbf{x}, \mathbf{t}, \alpha, \beta) \propto p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta)p(\mathbf{w}|\alpha)$$

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

Determine $\mathbf{w}_{\mathrm{MAP}}$ by minimizing regularized sum-of-squares error, $\widetilde{E}(\mathbf{w})$.

Bayesian Curve Fitting

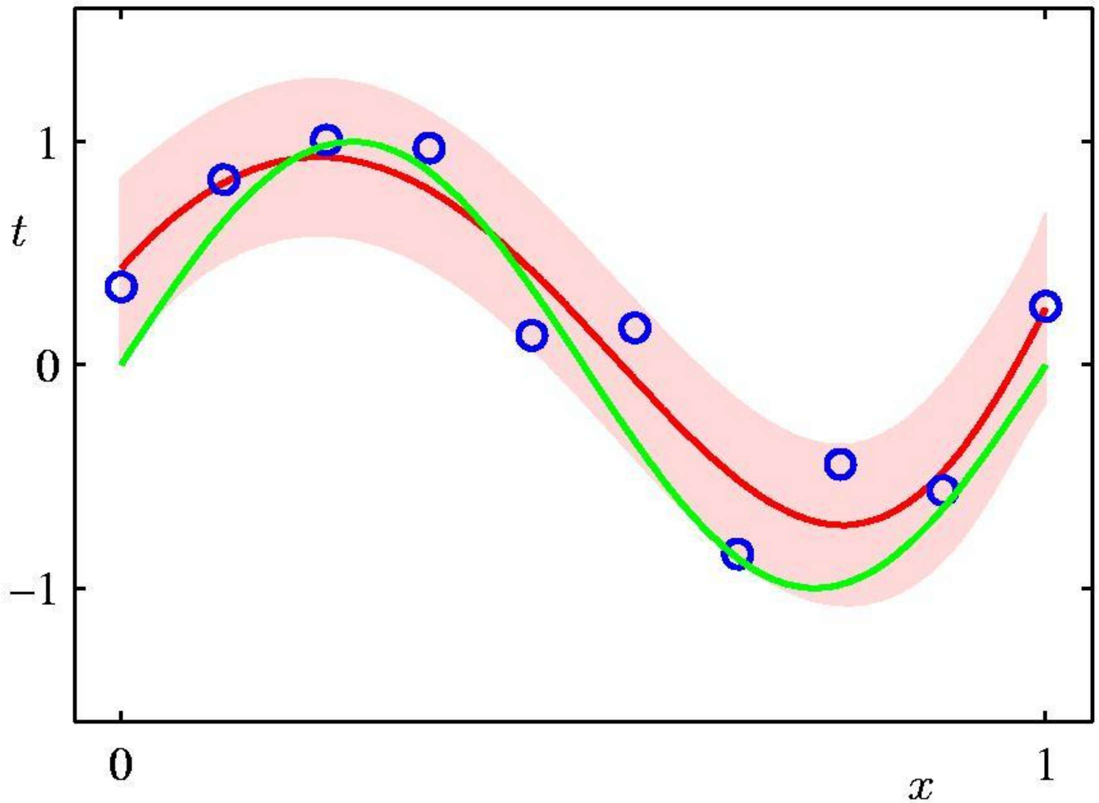
$$p(t|x,\mathbf{x},\mathbf{t}) = \int p(t|x,\mathbf{w})p(\mathbf{w}|\mathbf{x},\mathbf{t})\,\mathrm{d}\mathbf{w} = \mathcal{N}\left(t|m(x), s^2(x)\right)$$

$$m(x) = \beta\boldsymbol{\phi}(x)^{\mathrm{T}}\mathbf{S}\sum_{n=1}^{N}\boldsymbol{\phi}(x_n)t_n \qquad s^2(x) = \beta^{-1} + \boldsymbol{\phi}(x)^{\mathrm{T}}\mathbf{S}\boldsymbol{\phi}(x)$$

$$\mathbf{S}^{-1} = \alpha\mathbf{I} + \beta\sum_{n=1}^{N}\boldsymbol{\phi}(x_n)\boldsymbol{\phi}(x_n)^{\mathrm{T}} \qquad \boldsymbol{\phi}(x_n) = \left(x_n^0, \ldots, x_n^M\right)^{\mathrm{T}}$$

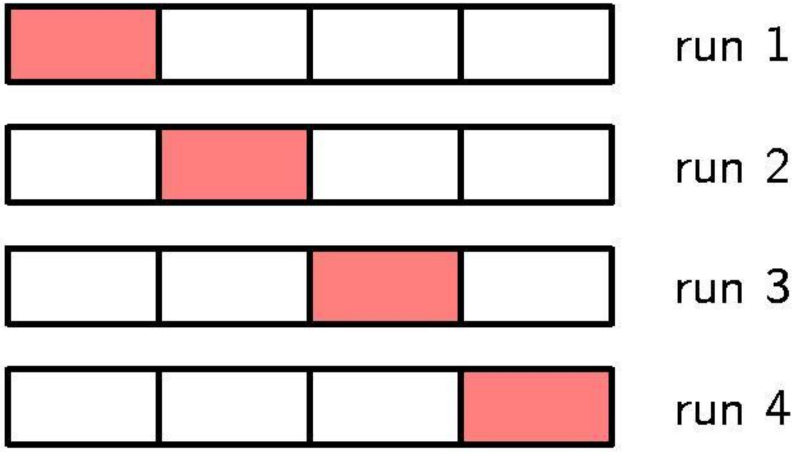
Bayesian Predictive Distribution

$$p(t|x, \mathbf{x}, \mathbf{t}) = \mathcal{N}\left(t|m(x), s^2(x)\right)$$

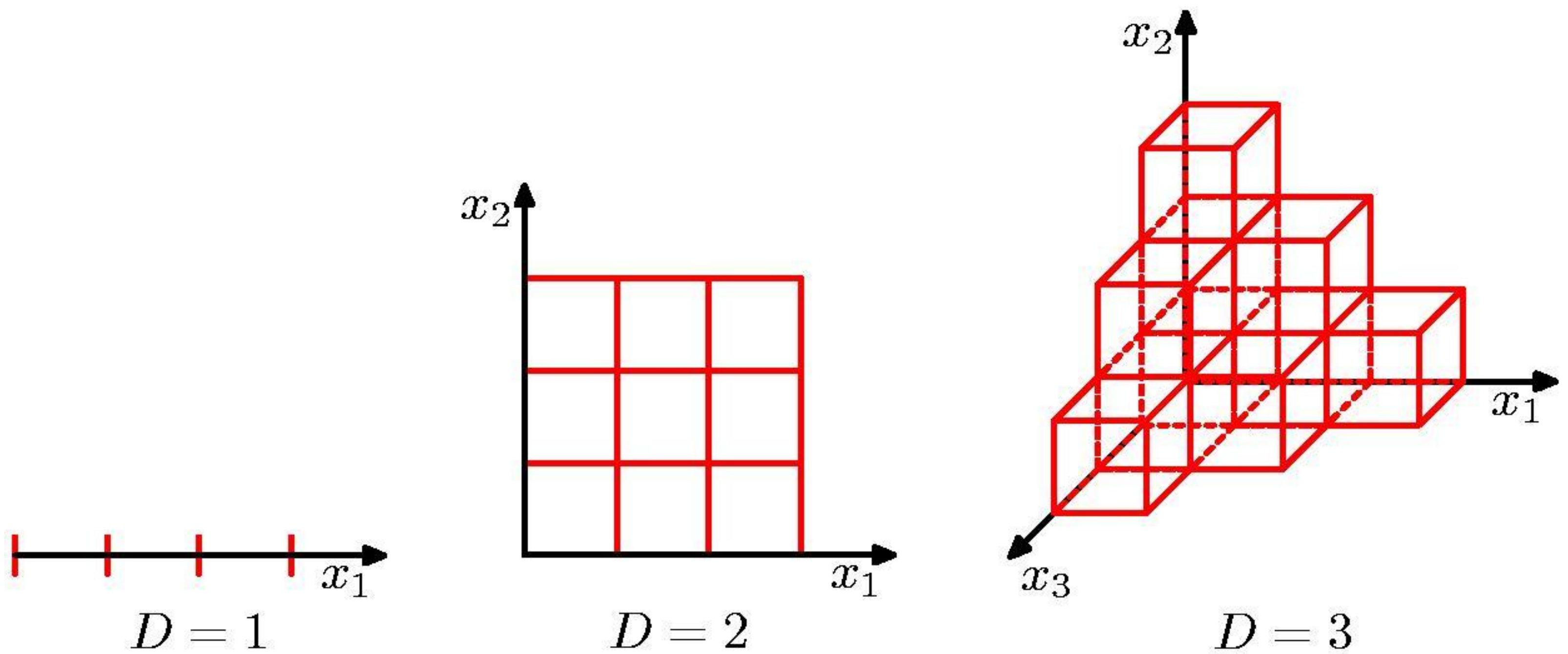


Model Selection

Cross-Validation



Curse of Dimensionality

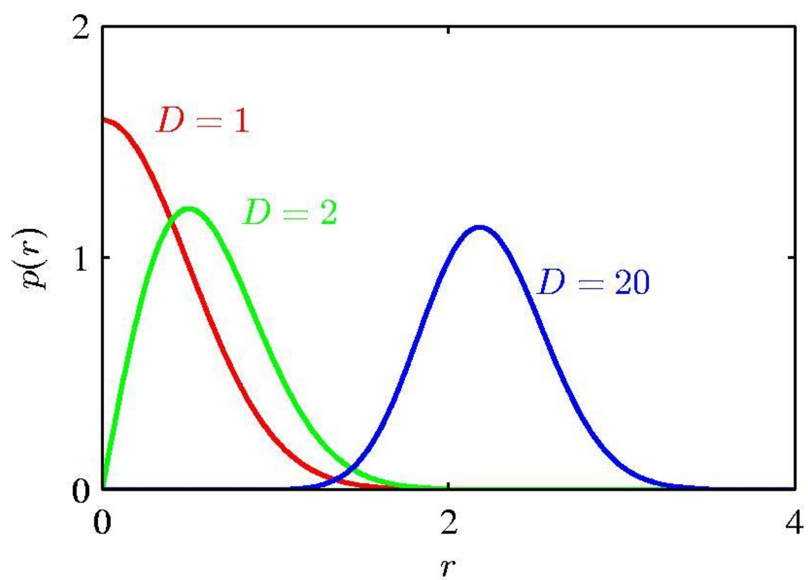


Curse of Dimensionality

Polynomial curve fitting, $M = 3$

$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{i=1}^{D} w_i x_i + \sum_{i=1}^{D} \sum_{j=1}^{D} w_{ij} x_i x_j + \sum_{i=1}^{D} \sum_{j=1}^{D} \sum_{k=1}^{D} w_{ijk} x_i x_j x_k$$

Gaussian Densities in higher dimensions



Decision Theory

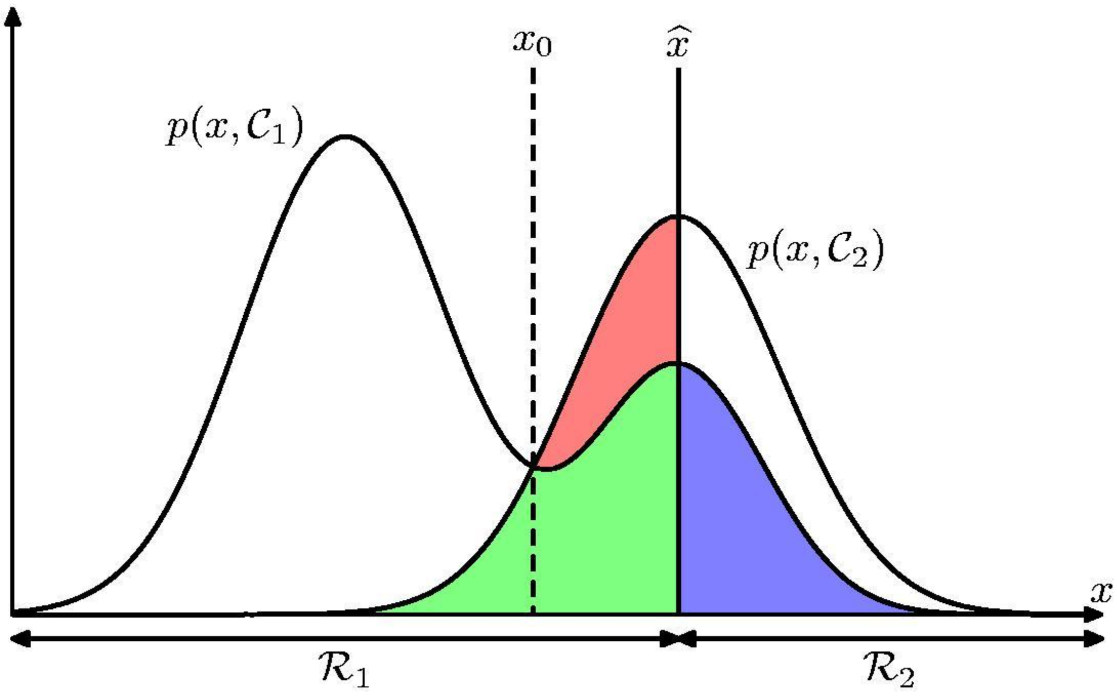
Inference step

Determine either $p(t|\mathbf{x})$ or $p(\mathbf{x}, t)$.

Decision step

For given $\mathbf{x}$, determine optimal t.

Minimum Misclassification Rate



$$\begin{aligned} p(\text{mistake}) &= p(\mathbf{x} \in \mathcal{R}_1, \mathcal{C}_2) + p(\mathbf{x} \in \mathcal{R}_2, \mathcal{C}_1) \\ &= \int_{\mathcal{R}_1} p(\mathbf{x}, \mathcal{C}_2)\,\mathrm{d}\mathbf{x} + \int_{\mathcal{R}_2} p(\mathbf{x}, \mathcal{C}_1)\,\mathrm{d}\mathbf{x}. \end{aligned}$$

Minimum Expected Loss

Example: classify medical images as ‘cancer’ or ‘normal’

$$\begin{array}{ccc} & \multicolumn{2}{c}{\text{Decision}} \\ & \text{cancer} & \text{normal} \end{array}$$

$$\text{Truth}\quad \begin{array}{c} \text{cancer} \\ \text{normal} \end{array} \begin{pmatrix} 0 & 1000 \\ 1 & 0 \end{pmatrix}$$

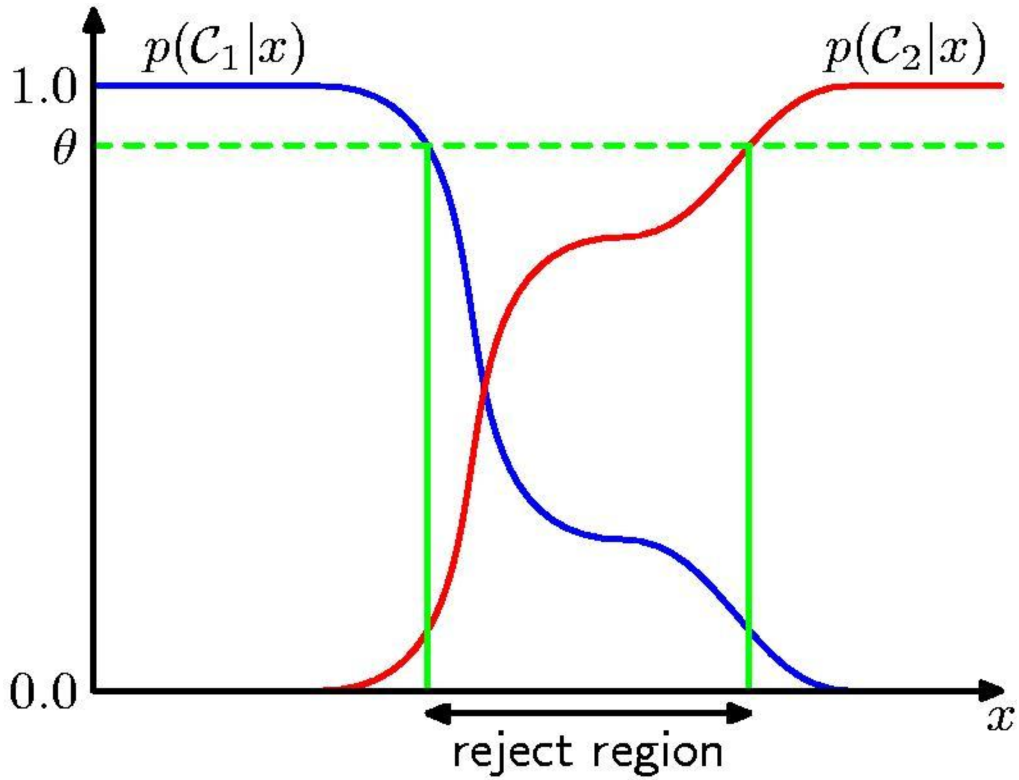
Minimum Expected Loss

$$\mathbb{E}[L] = \sum_k \sum_j \int_{\mathcal{R}_j} L_{kj} p(\mathbf{x}, \mathcal{C}_k) \, \mathrm{d}\mathbf{x}$$

Regions $\mathcal{R}_j$ are chosen to minimize

$$\mathbb{E}[L] = \sum_k L_{kj} p(\mathcal{C}_k | \mathbf{x})$$

Reject Option



Why Separate Inference and Decision?

- Minimizing risk (loss matrix may change over time)
- Reject option
- Unbalanced class priors
- Combining models

Decision Theory for Regression

Inference step

Determine $p(\mathbf{x}, t)$.

Decision step

For given $\mathbf{x}$, make optimal prediction, $y(\mathbf{x})$, for t.

Loss function: $$\mathbb{E}[L] = \iint L(t, y(\mathbf{x}))p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

The Squared Loss Function

$$\mathbb{E}[L] = \iint \{y(\mathbf{x}) - t\}^2 p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

$$\begin{aligned}\{y(\mathbf{x}) - t\}^2 &= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}] + \mathbb{E}[t|\mathbf{x}] - t\}^2 \\ &= \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2 + 2\{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}\{\mathbb{E}[t|\mathbf{x}] - t\} + \{\mathbb{E}[t|\mathbf{x}] - t\}^2\end{aligned}$$

$$\mathbb{E}[L] = \int \{y(\mathbf{x}) - \mathbb{E}[t|\mathbf{x}]\}^2 p(\mathbf{x})\,\mathrm{d}\mathbf{x} + \int \mathrm{var}\,[t|\mathbf{x}]\,p(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

$$y(\mathbf{x}) = \mathbb{E}[t|\mathbf{x}]$$

Generative vs Discriminative

Generative approach:

Model $p(t, \mathbf{x}) = p(\mathbf{x}|t)p(t)$

Use Bayes' theorem $p(t|\mathbf{x}) = \dfrac{p(\mathbf{x}|t)p(t)}{p(\mathbf{x})}$

Discriminative approach:

Model $p(t|\mathbf{x})$ directly

Entropy

$$\mathrm{H}[x] = -\sum_{x} p(x) \log_2 p(x)$$

Important quantity in

- coding theory
- statistical physics
- machine learning

Entropy

Coding theory: x discrete with 8 possible states; how many bits to transmit the state of x?

All states equally likely

$$\mathrm{H}[x] = -8 \times \frac{1}{8} \log_2 \frac{1}{8} = 3 \text{ bits.}$$

Entropy

x	a	b	c	d	e	f	g	h
$p(x)$	$\frac{1}{2}$	$\frac{1}{4}$	$\frac{1}{8}$	$\frac{1}{16}$	$\frac{1}{64}$	$\frac{1}{64}$	$\frac{1}{64}$	$\frac{1}{64}$
code	0	10	110	1110	111100	111101	111110	111111

$$\begin{aligned}\mathrm{H}[x] &= -\frac{1}{2}\log_2\frac{1}{2} - \frac{1}{4}\log_2\frac{1}{4} - \frac{1}{8}\log_2\frac{1}{8} - \frac{1}{16}\log_2\frac{1}{16} - \frac{4}{64}\log_2\frac{1}{64} \\ &= 2 \text{ bits}\end{aligned}$$

$$\begin{aligned}\text{average code length} &= \frac{1}{2}\times 1 + \frac{1}{4}\times 2 + \frac{1}{8}\times 3 + \frac{1}{16}\times 4 + 4\times\frac{1}{64}\times 6 \\ &= 2 \text{ bits}\end{aligned}$$

Entropy

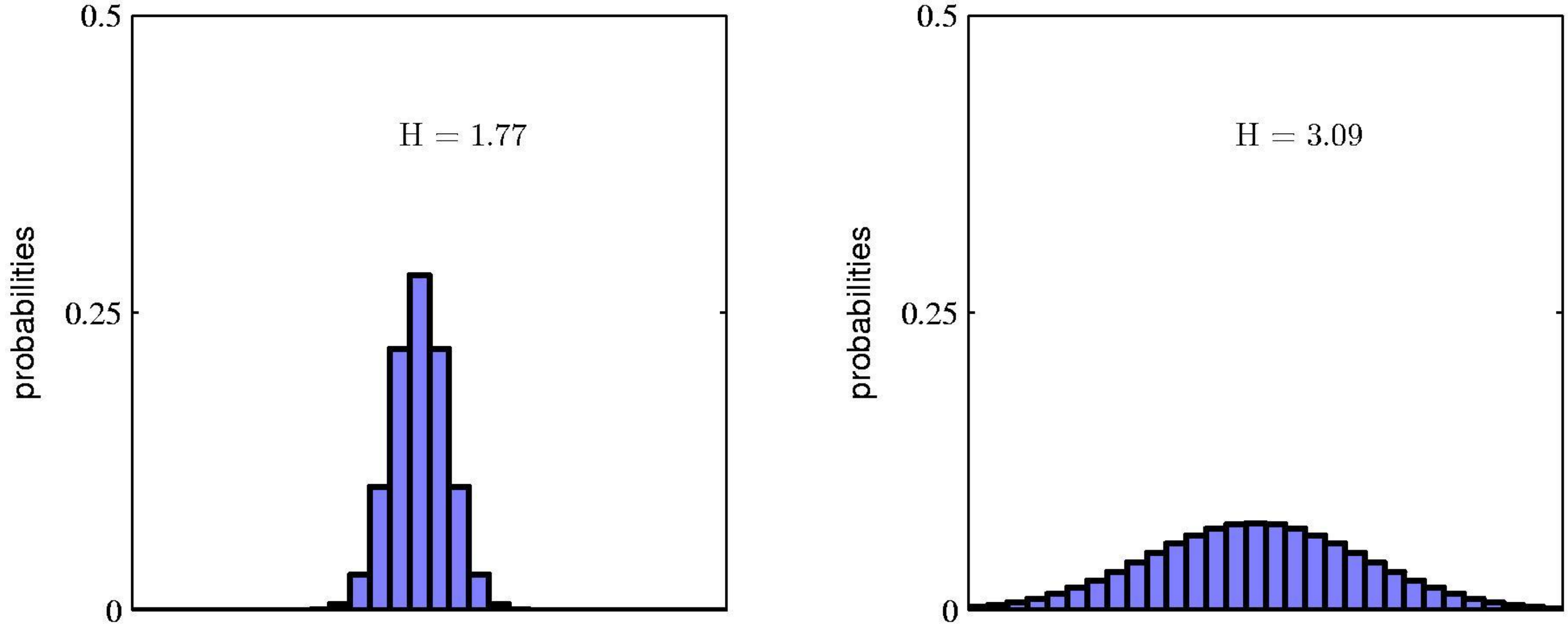
In how many ways can N identical objects be allocated M bins?

$$W = \frac{N!}{\prod_i n_i!}$$

$$\mathrm{H} = \frac{1}{N} \ln W \simeq - \lim_{N \to \infty} \sum_i \left(\frac{n_i}{N}\right) \ln \left(\frac{n_i}{N}\right) = - \sum_i p_i \ln p_i$$

Entropy maximized when $\forall i : p_i = \frac{1}{M}$

Entropy



Differential Entropy

Put bins of width Δ along the real line

$$\lim_{\Delta \to 0} \left\{ - \sum_i p(x_i) \Delta \ln p(x_i) \right\} = - \int p(x) \ln p(x) \, \mathrm{d}x$$

Differential entropy maximized (for fixed σ^2) when

$$p(x) = \mathcal{N}(x|\mu, \sigma^2)$$

in which case

$$\mathrm{H}[x] = \frac{1}{2} \left\{ 1 + \ln(2\pi\sigma^2) \right\}.$$

Conditional Entropy

$$\mathrm{H}[\mathbf{y}|\mathbf{x}] = -\iint p(\mathbf{y}, \mathbf{x}) \ln p(\mathbf{y}|\mathbf{x}) \, \mathrm{d}\mathbf{y} \, \mathrm{d}\mathbf{x}$$

$$\mathrm{H}[\mathbf{x}, \mathbf{y}] = \mathrm{H}[\mathbf{y}|\mathbf{x}] + \mathrm{H}[\mathbf{x}]$$

The Kullback-Leibler Divergence

$$\begin{aligned}\mathrm{KL}(p\|q) &= -\int p(\mathbf{x})\ln q(\mathbf{x})\,\mathrm{d}\mathbf{x} - \left(-\int p(\mathbf{x})\ln p(\mathbf{x})\,\mathrm{d}\mathbf{x}\right)\\ &= -\int p(\mathbf{x})\ln\left\{\frac{q(\mathbf{x})}{p(\mathbf{x})}\right\}\,\mathrm{d}\mathbf{x}\end{aligned}$$

$$\mathrm{KL}(p\|q) \simeq \frac{1}{N}\sum_{n=1}^{N}\left\{-\ln q(\mathbf{x}_n|\boldsymbol{\theta}) + \ln p(\mathbf{x}_n)\right\}$$

$$\mathrm{KL}(p\|q) \geqslant 0 \qquad\qquad \mathrm{KL}(p\|q) \not\equiv \mathrm{KL}(q\|p)$$

Mutual Information

$$\begin{aligned} \mathrm{I}[\mathbf{x}, \mathbf{y}] &\equiv \mathrm{KL}(p(\mathbf{x}, \mathbf{y}) \| p(\mathbf{x})p(\mathbf{y})) \\ &= -\iint p(\mathbf{x}, \mathbf{y}) \ln \left(\frac{p(\mathbf{x})p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} \right) \mathrm{d}\mathbf{x} \, \mathrm{d}\mathbf{y} \end{aligned}$$

$$\mathrm{I}[\mathbf{x}, \mathbf{y}] = \mathrm{H}[\mathbf{x}] - \mathrm{H}[\mathbf{x}|\mathbf{y}] = \mathrm{H}[\mathbf{y}] - \mathrm{H}[\mathbf{y}|\mathbf{x}]$$