MACHINE LEARNING

CHAPTER 1: PRELIMINARY

Learning Objectives

1、What is pattern recognition?

2、What are curve fitting and regularization?

3、What are ML and MAP Bayesian inferences?

4、How to deal with the curse of dimensionality?

5、What is the relationship between decision theory and machine learning?

6、What are generative and discriminative models?

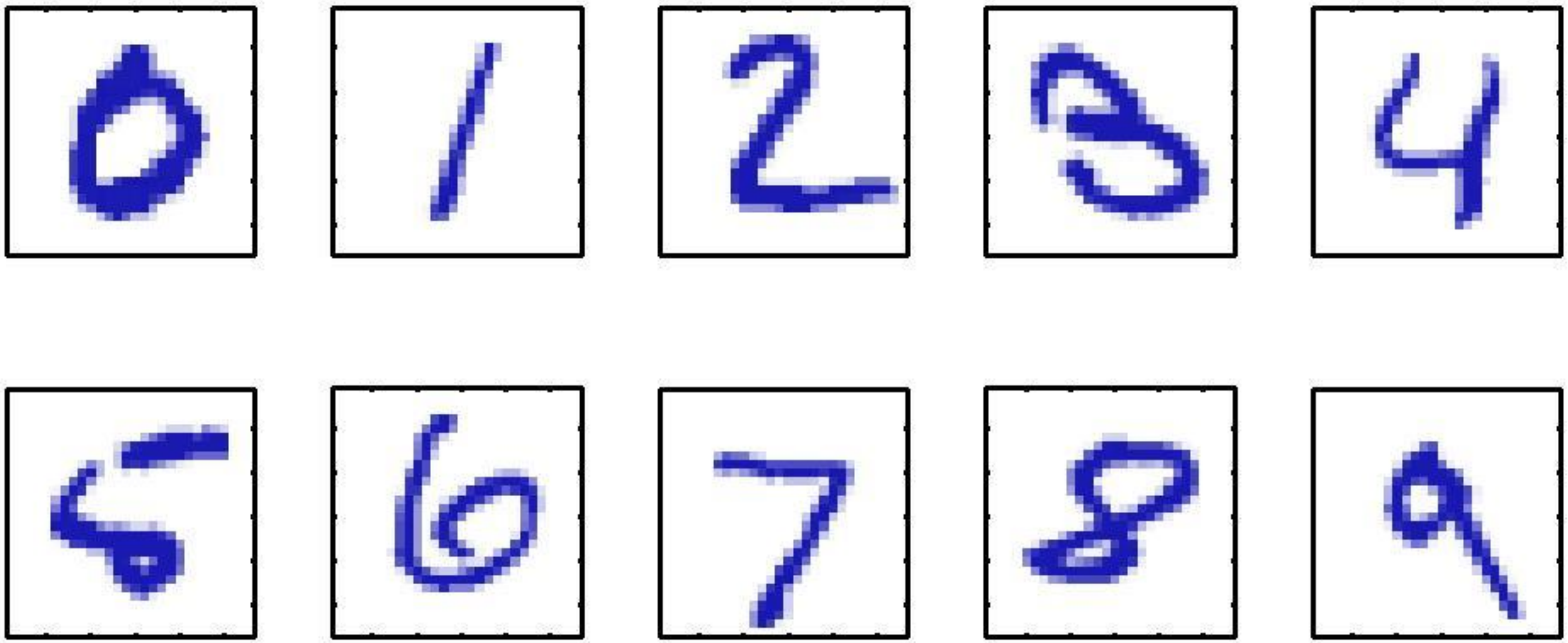
7、How to use entropy、KL divergence and mutual information for machine learning?

Outlines

- Pattern Recognition
- Curve Fitting and Regularization
- Probabilities and Gaussian Distributions
- Bayesian Inferences (ML and MAP)
- Curse of Dimensionality
- Decision Theory
- Entropy and Information

Example

Handwritten Digit Recognition



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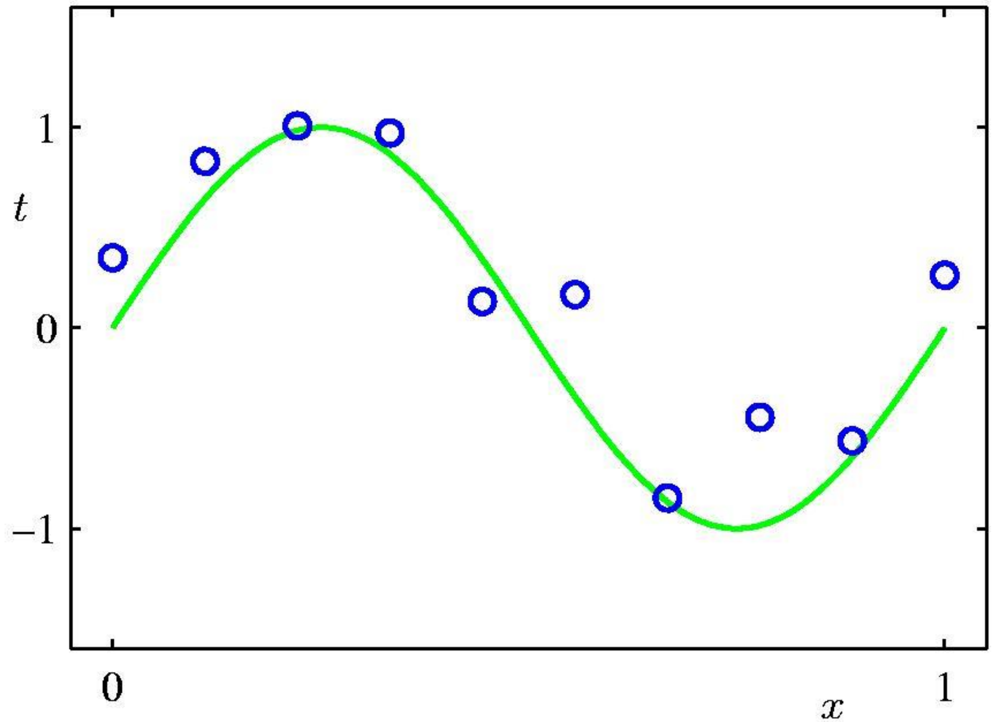
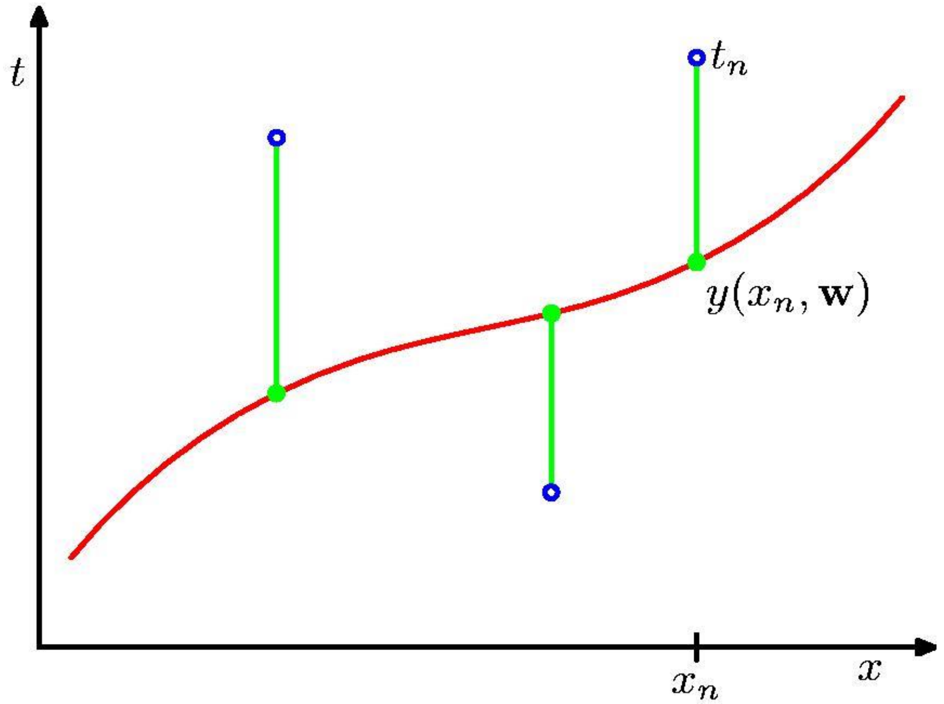
Polynomial Curve Fitting



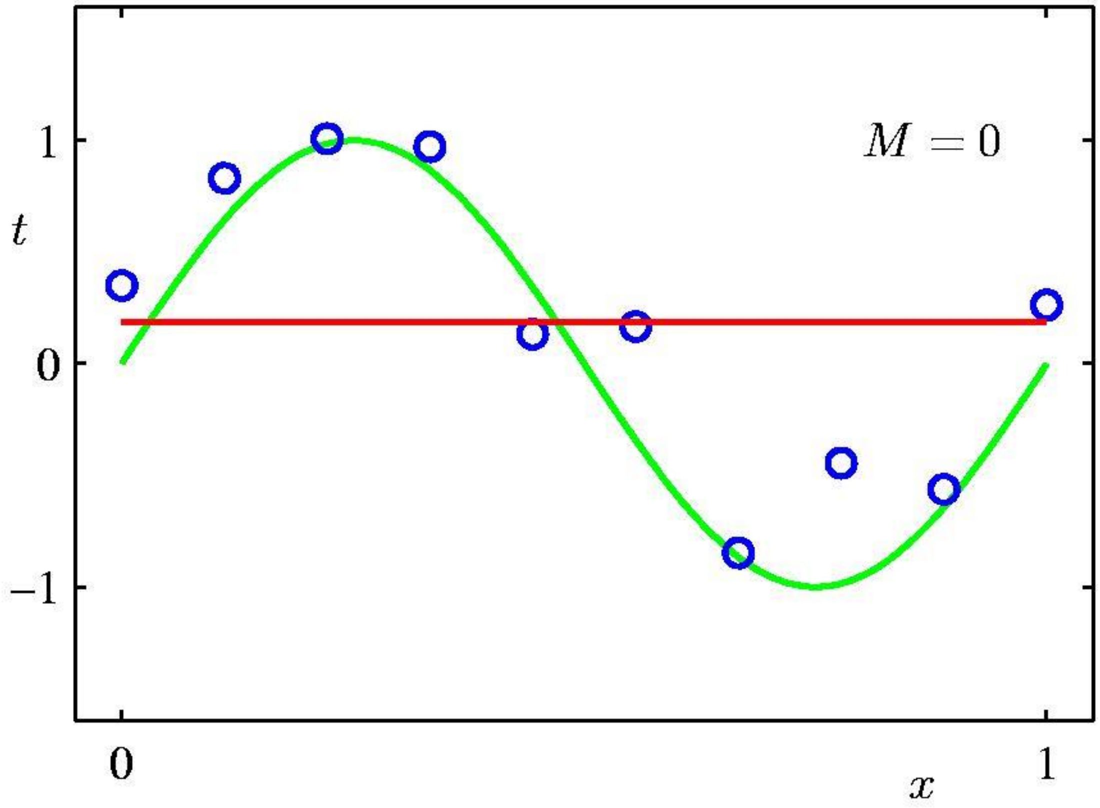
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Sum-of-Squares Error Function

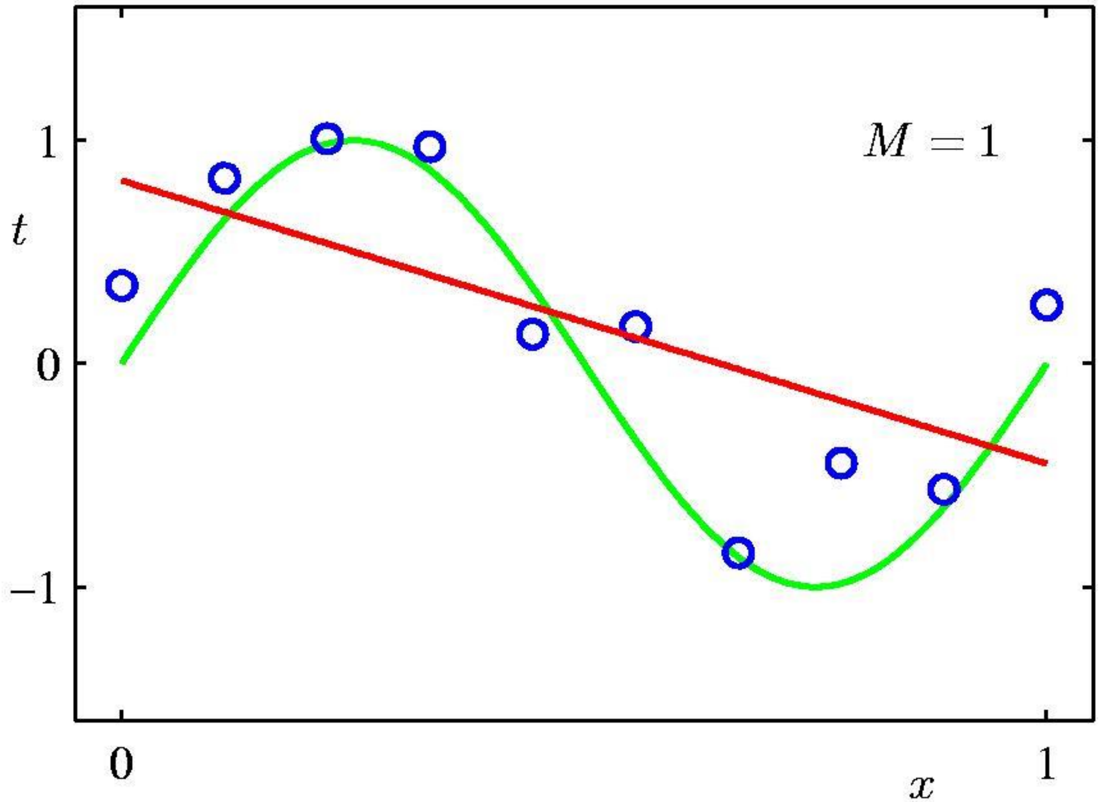


$$E(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{y(x_n, \mathbf{w}) - t_n\}^2$$

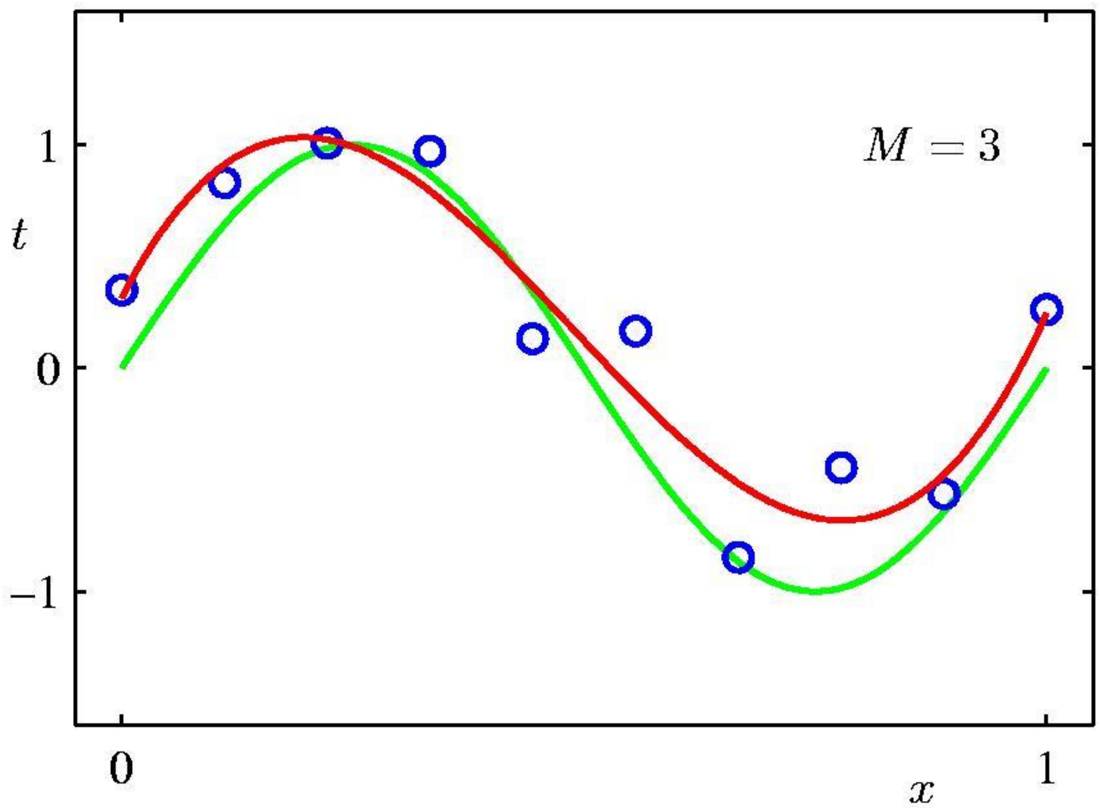
0^{th} Order Polynomial



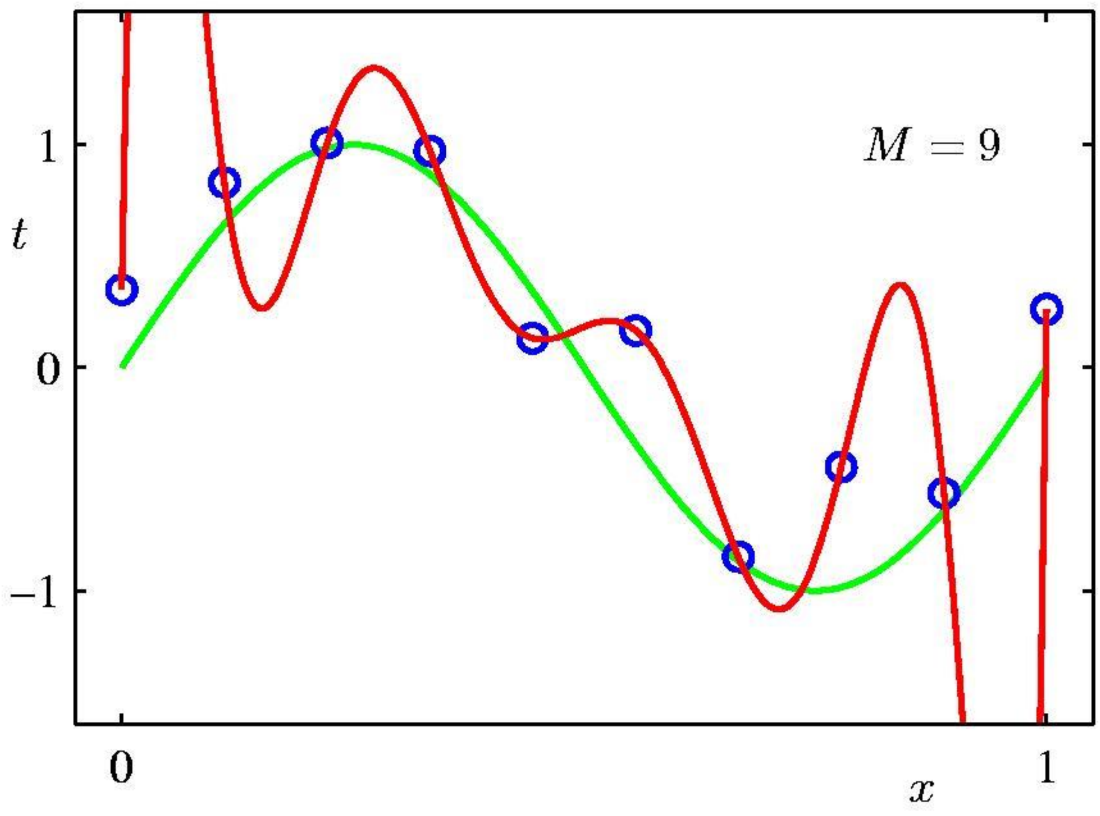
1st Order Polynomial



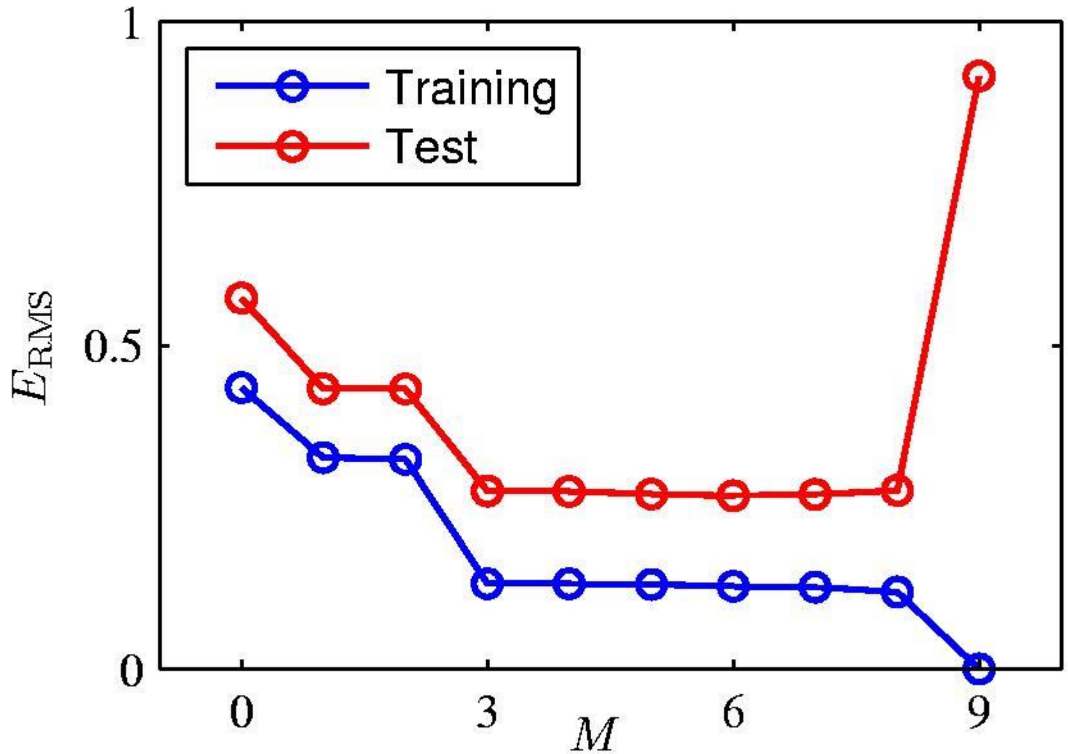
3rd Order Polynomial



9th Order Polynomial



Over-fitting



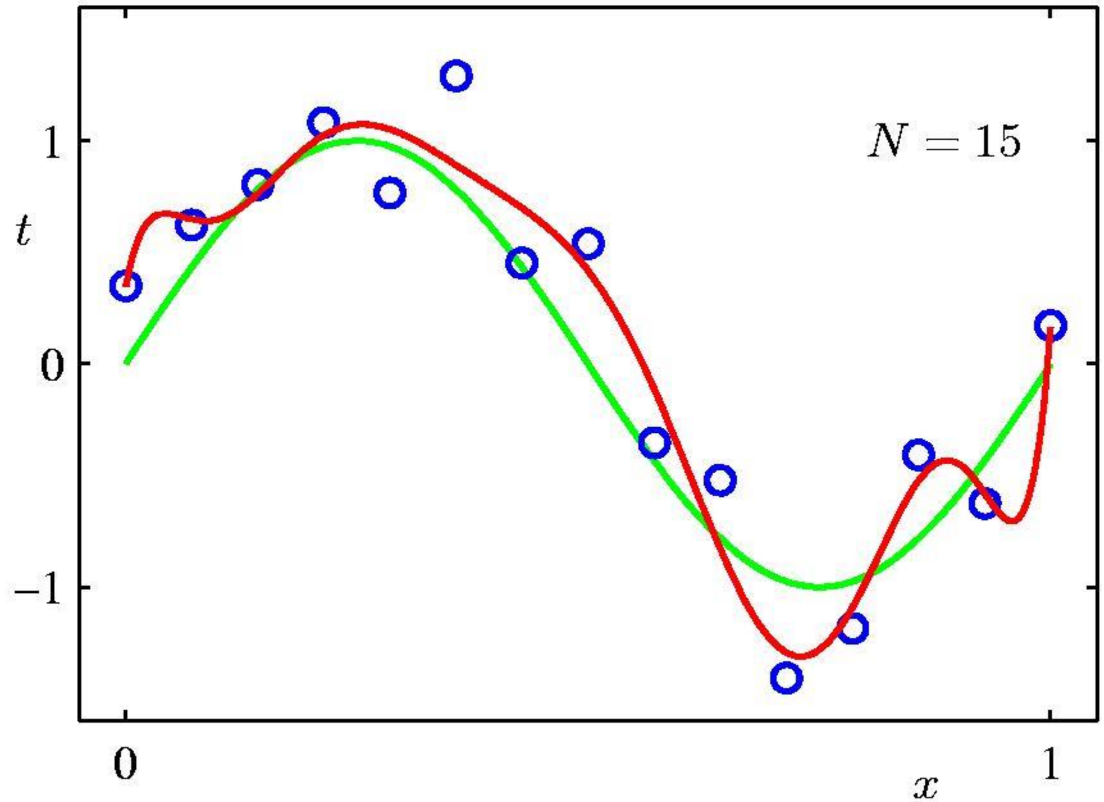
Root-Mean-Square (RMS) Error: $E_{\mathrm{RMS}} = \sqrt{2E(\mathbf{w}^\star)/N}$

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

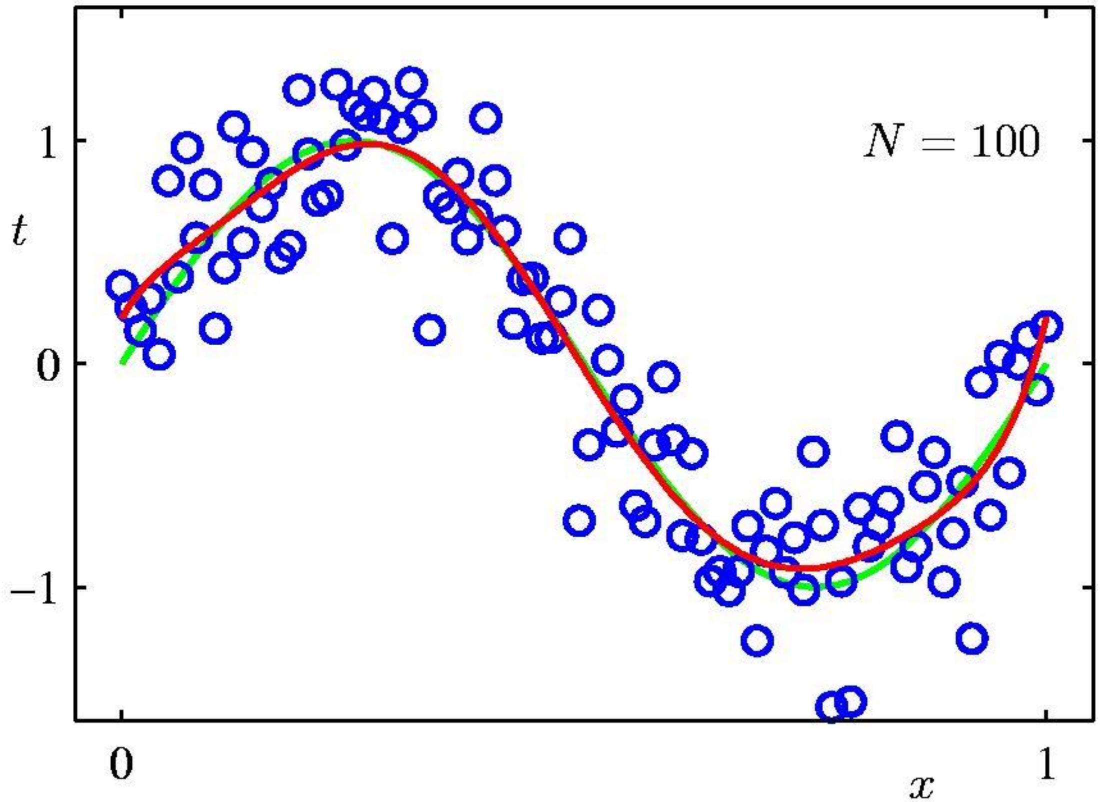
Data Set Size: $N = 15$

9th Order Polynomial



Data Set Size: $N = 100$

9th Order Polynomial

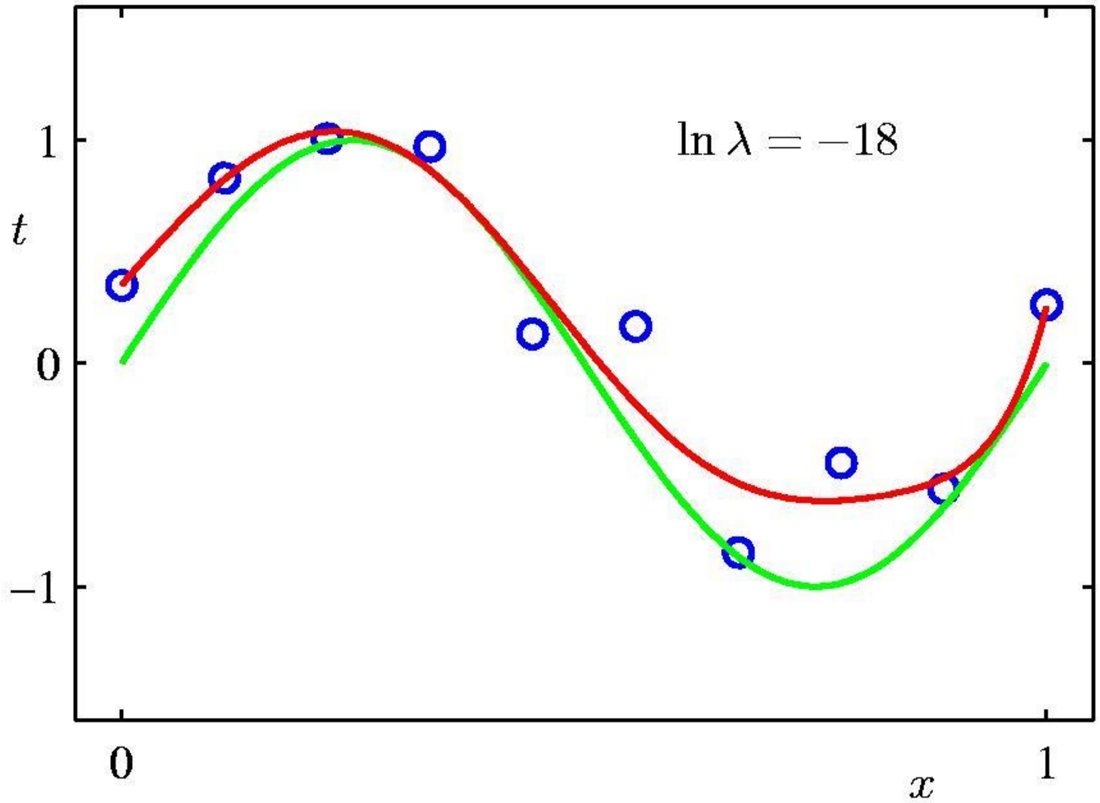


Regularization

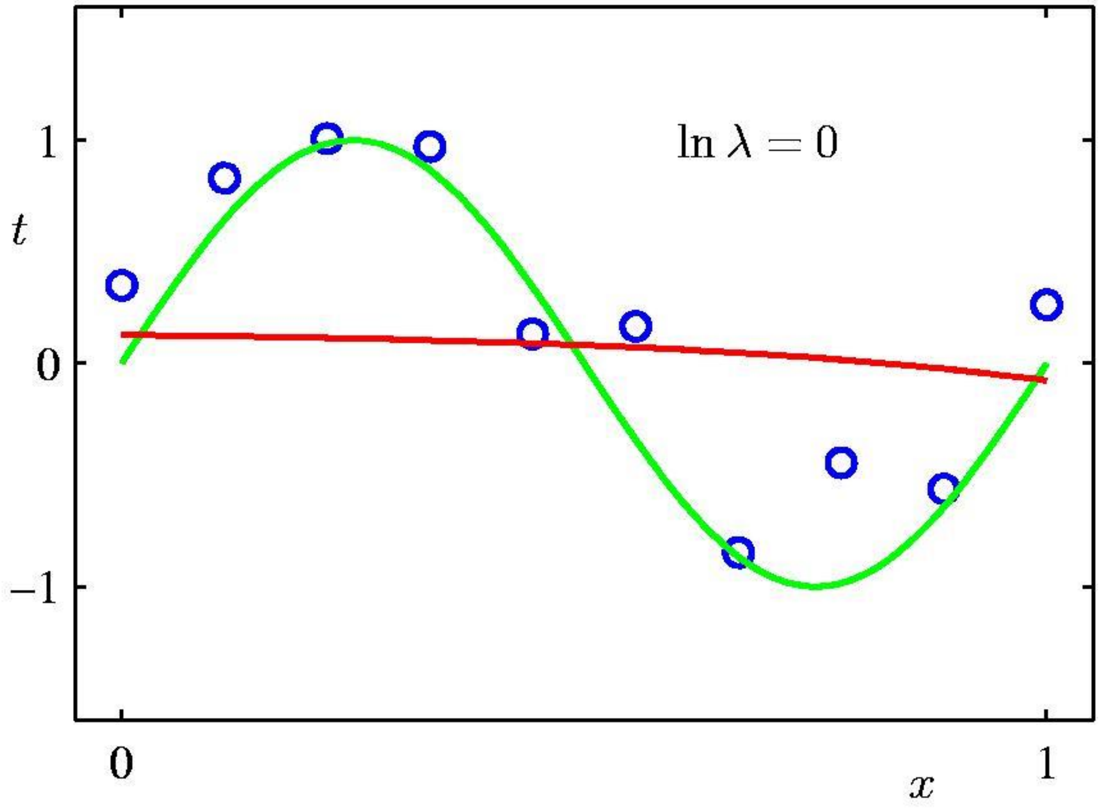
Penalize large coefficient values

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

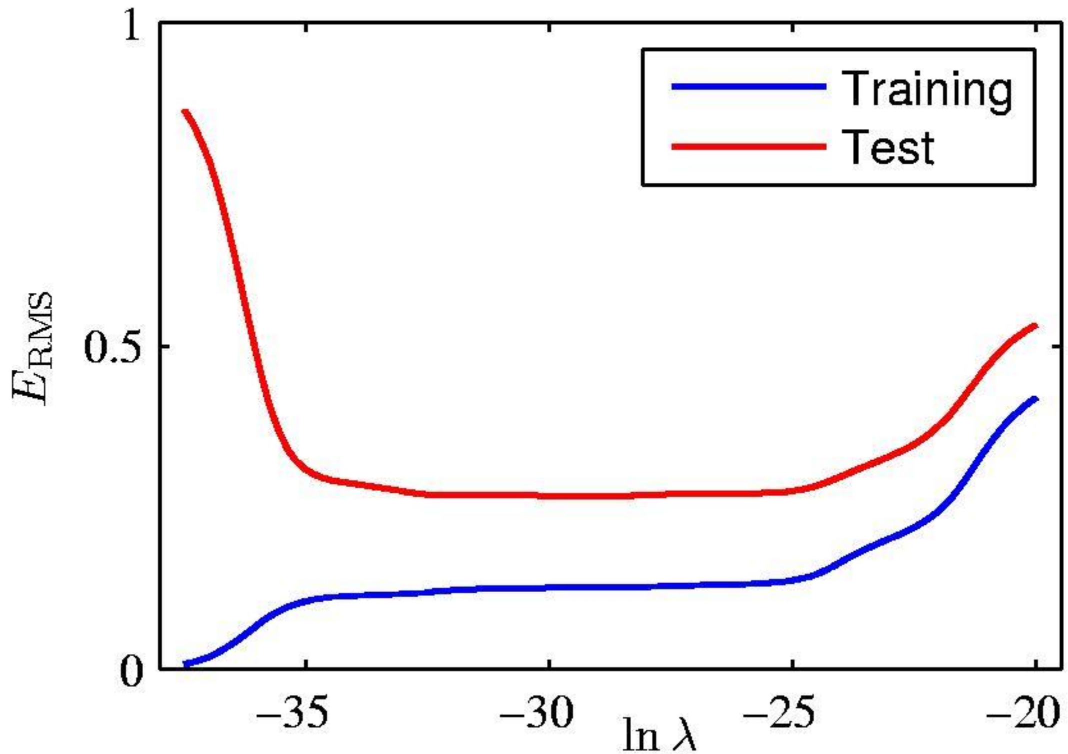
Regularization: $\ln \lambda = -18$



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

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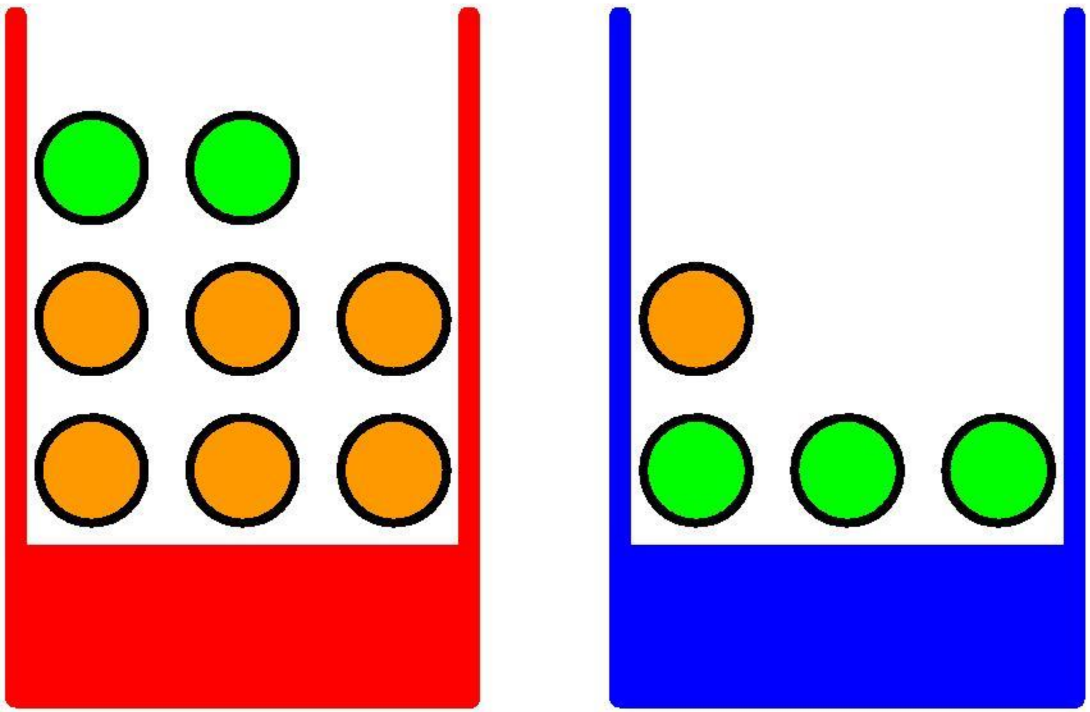
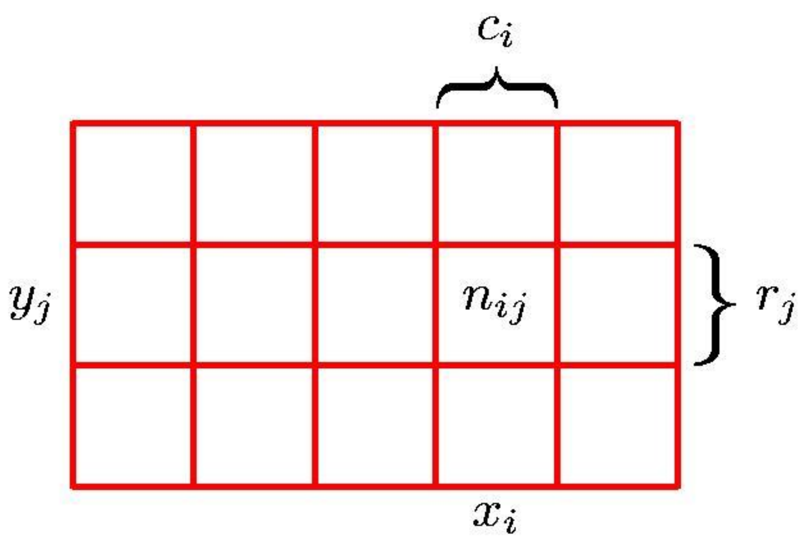
Probability Theory

Apples and Oranges



Probability Theory



Marginal Probability

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

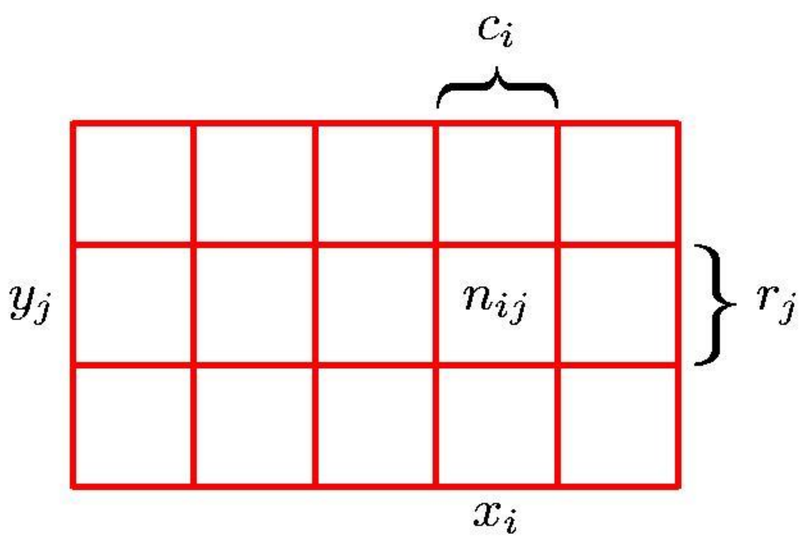
Joint Probability

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

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

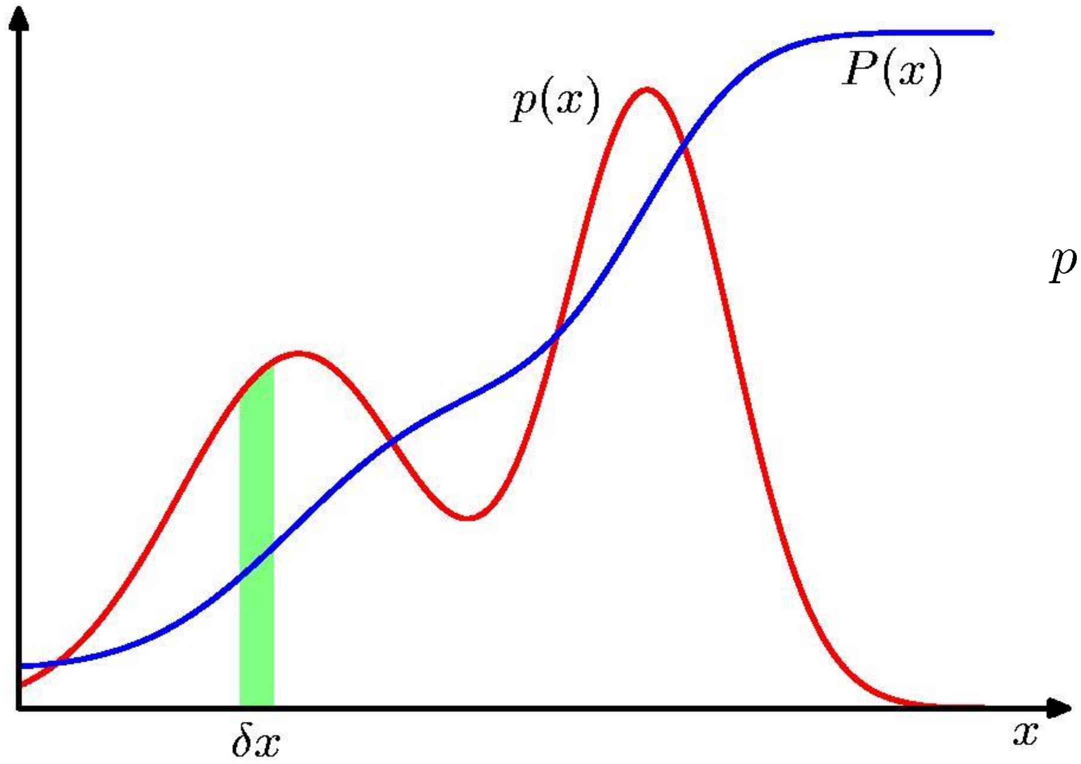
$$\boxed{p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}}$$

$$p(X) = \sum_Y p(X|Y)p(Y) \quad \text{: normalization}$$

posterior $\propto$ likelihood $\times$ prior

$p(Y|X)$ $\qquad$ $p(X|Y)$ $\qquad$ $p(Y)$

Probability Densities

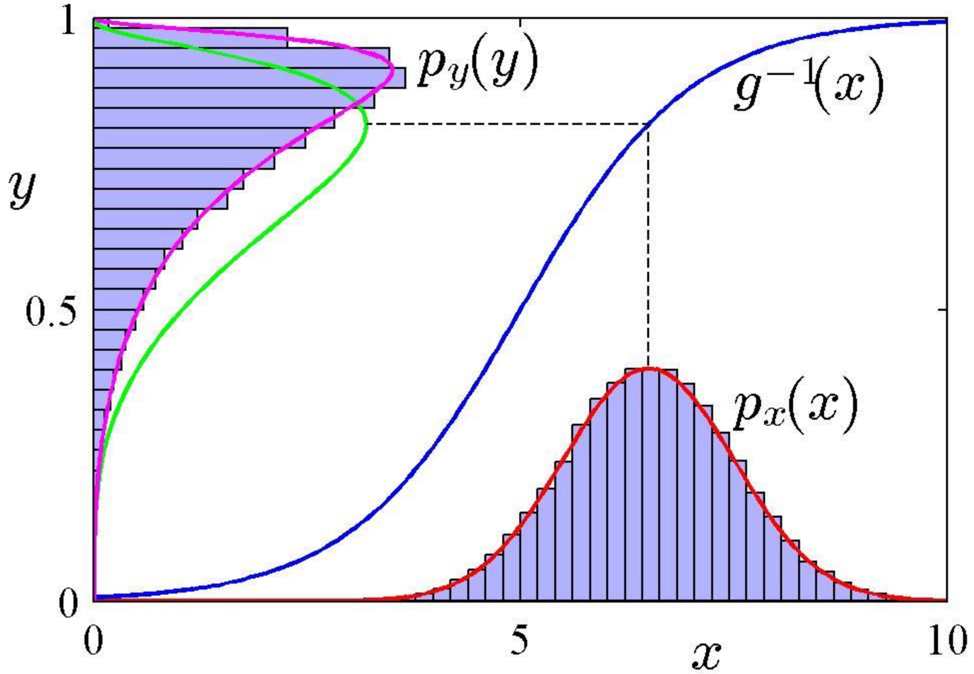


$$p(x \in (a, b)) = \int_a^b p(x)\,\mathrm{d}x$$

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

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

Transformed Densities



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

$x = g(y)$

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

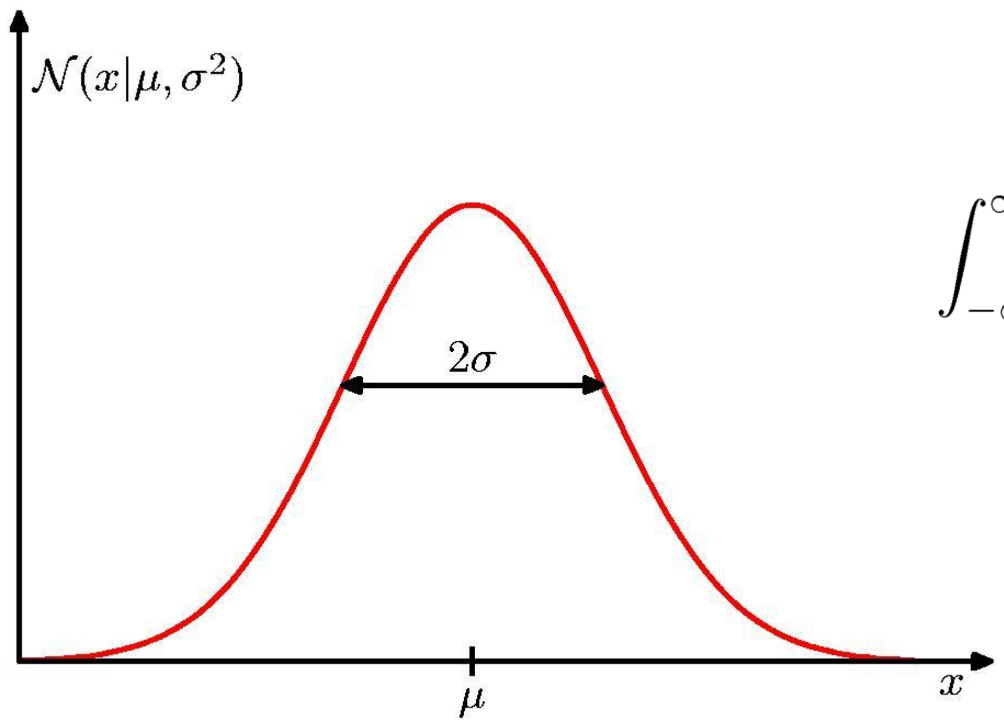
$$\mathrm{var}[f] = \mathbb{E}\left[(f(x) - \mathbb{E}[f(x)])^2\right] = \mathbb{E}[f(x)^2] - \mathbb{E}[f(x)]^2$$

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

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

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

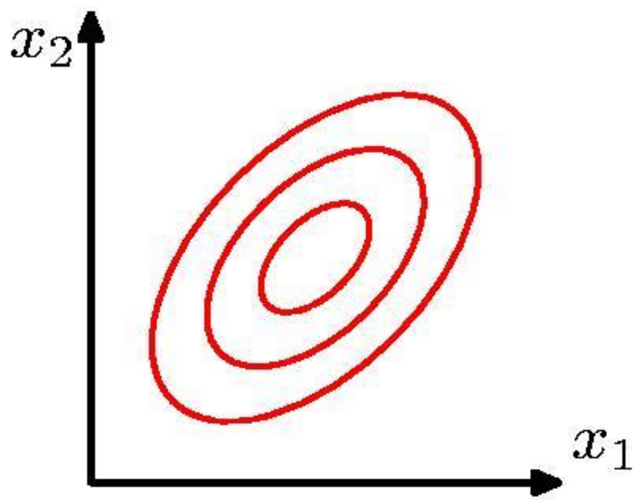
$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}\left(x|\mu, \sigma^2\right) x \,\mathrm{d}x = \mu$$

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

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

The Multivariate Gaussian

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



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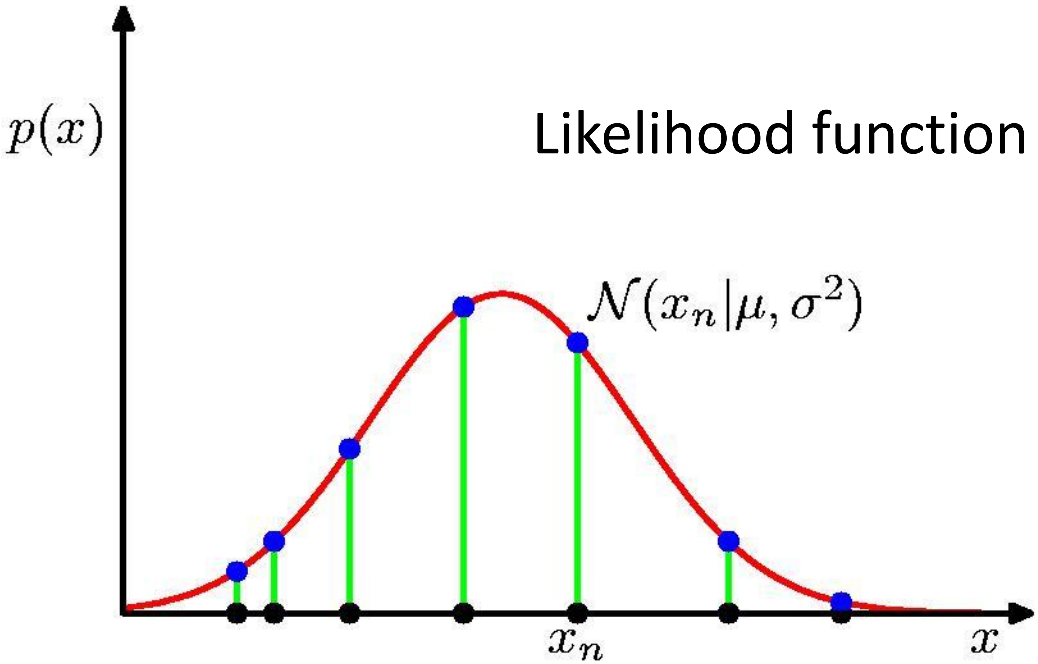
Gaussian Parameter Estimation



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

Maximum (Log) Likelihood

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

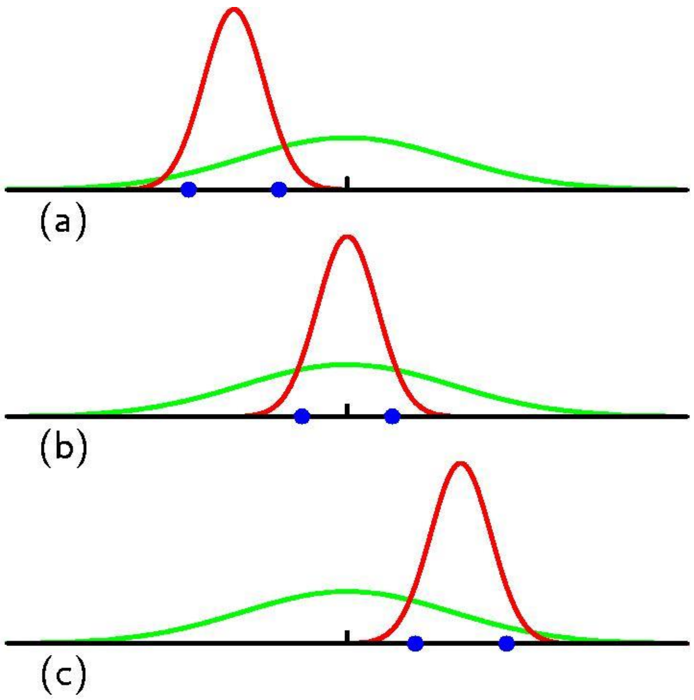
$$\mu_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N}x_n \qquad \sigma^2_{\mathrm{ML}} = \frac{1}{N}\sum_{n=1}^{N}(x_n-\mu_{\mathrm{ML}})^2$$

Properties of μ_{ML} and σ^2_{ML}

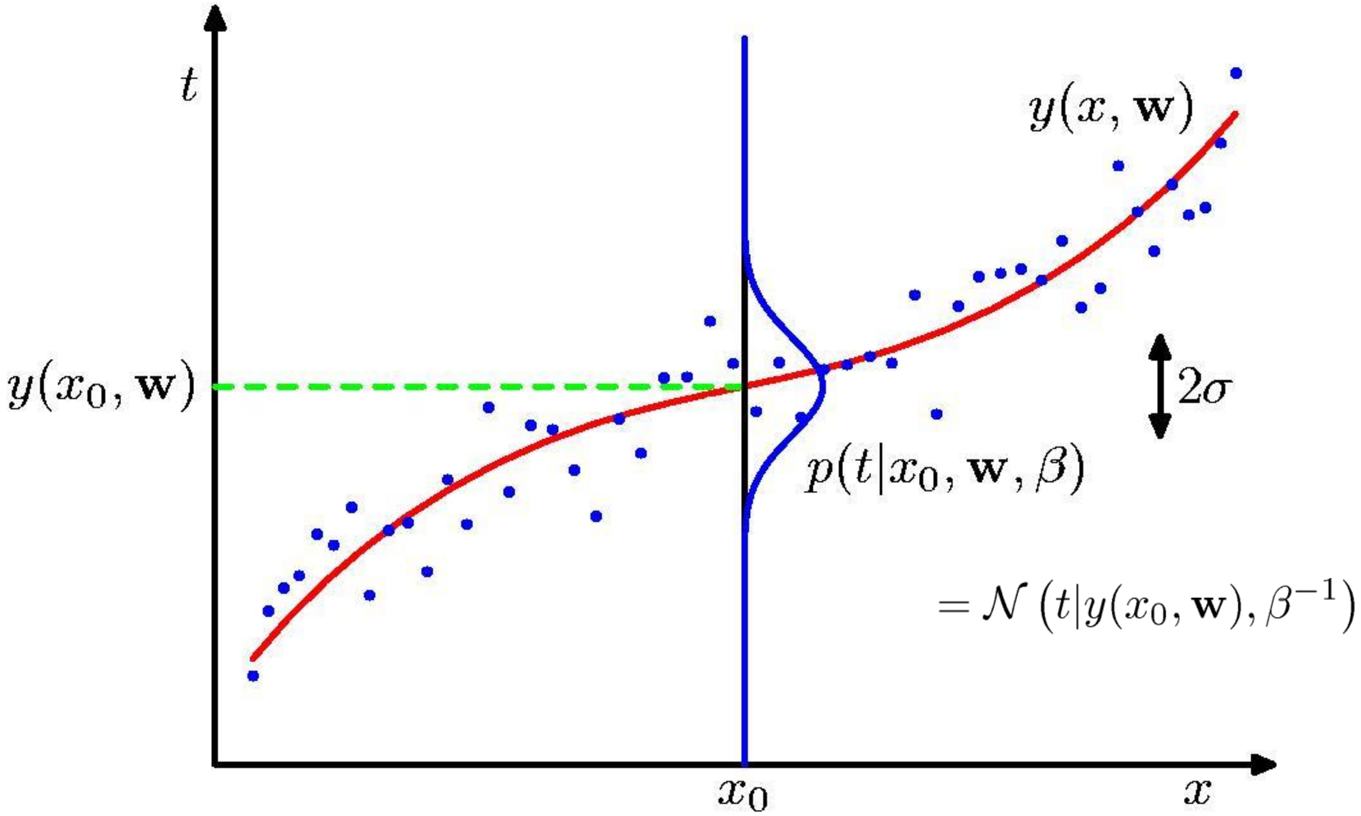
$$\mathbb{E}[\mu_{\mathrm{ML}}] = \mu$$

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

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



Curve Fitting Re-visited



$(\boldsymbol{t}, \boldsymbol{x})$: training data $\Rightarrow \boldsymbol{w}, \boldsymbol{\beta}$ $\qquad (\boldsymbol{w}, \beta, x_0)$: $\Rightarrow p(t|\, x_0, \boldsymbol{w}, \beta)$

Maximum Likelihood

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

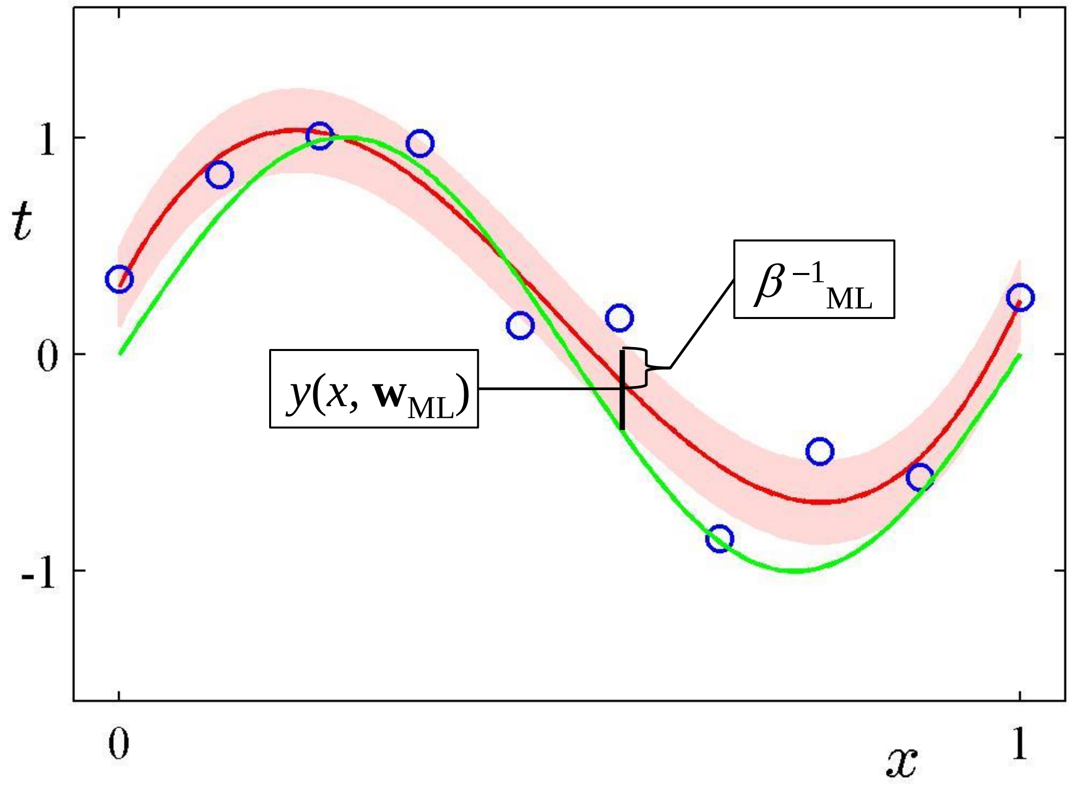
$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = \underbrace{-\frac{\beta}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2}_{\beta E(\mathbf{w})} + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)$$

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

MAP: Maximum *A Posteriori*

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

posteriori

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

priori

likelihood

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

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

Bayesian Curve Fitting

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

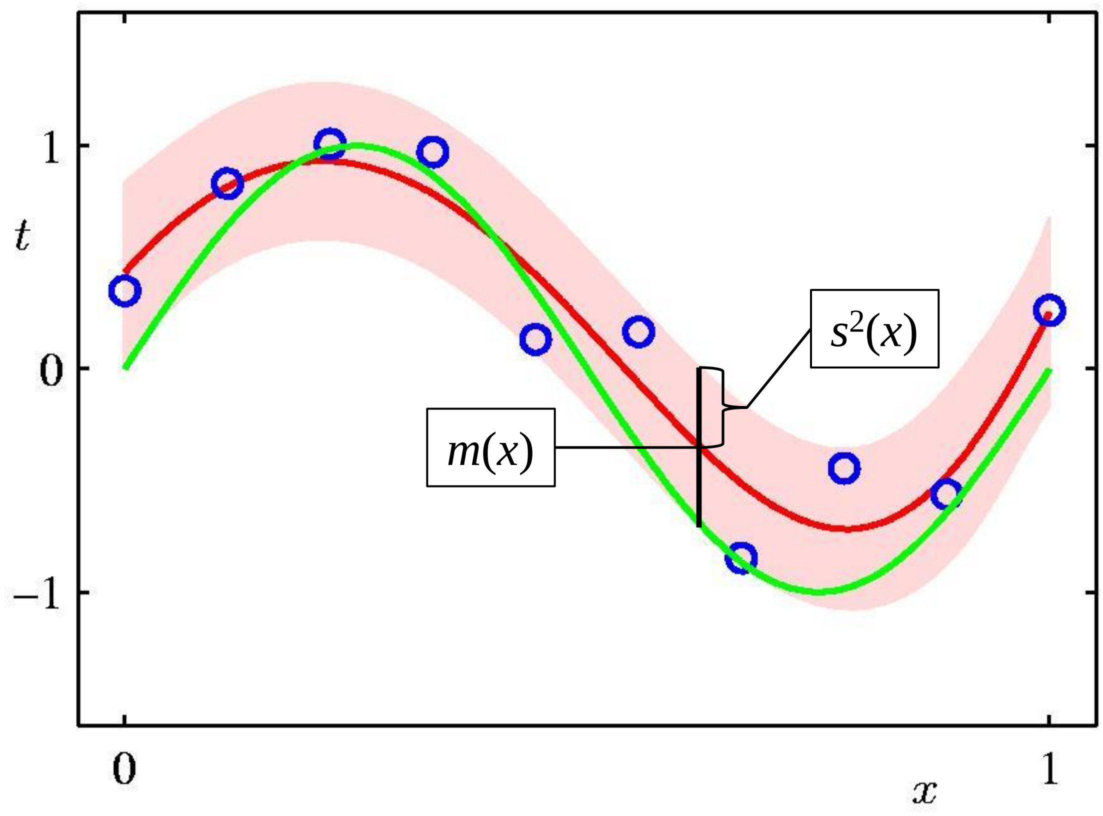
$$m(x) = \beta \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S} \sum_{n=1}^{N} \boldsymbol{\phi}(x_n) t_n \qquad s^2(x) = \beta^{-1} + \boldsymbol{\phi}(x)^{\mathrm{T}} \mathbf{S} \boldsymbol{\phi}(x)$$

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

We will go through more details in a later lecture.

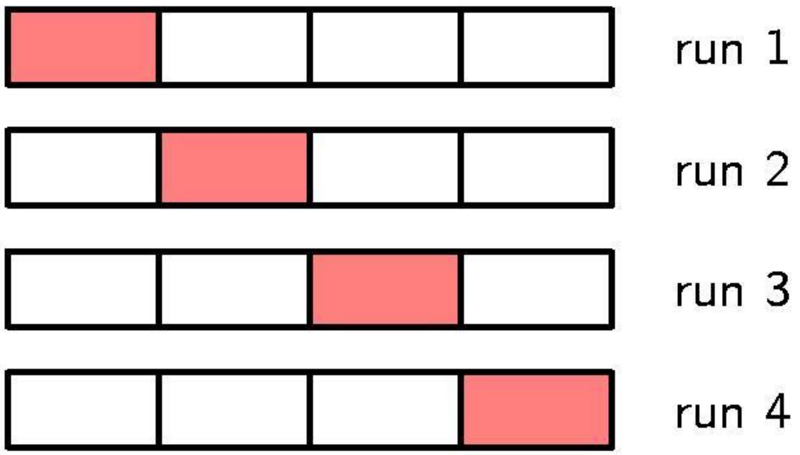
Bayesian Predictive Distribution

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



Model Selection

Cross-Validation



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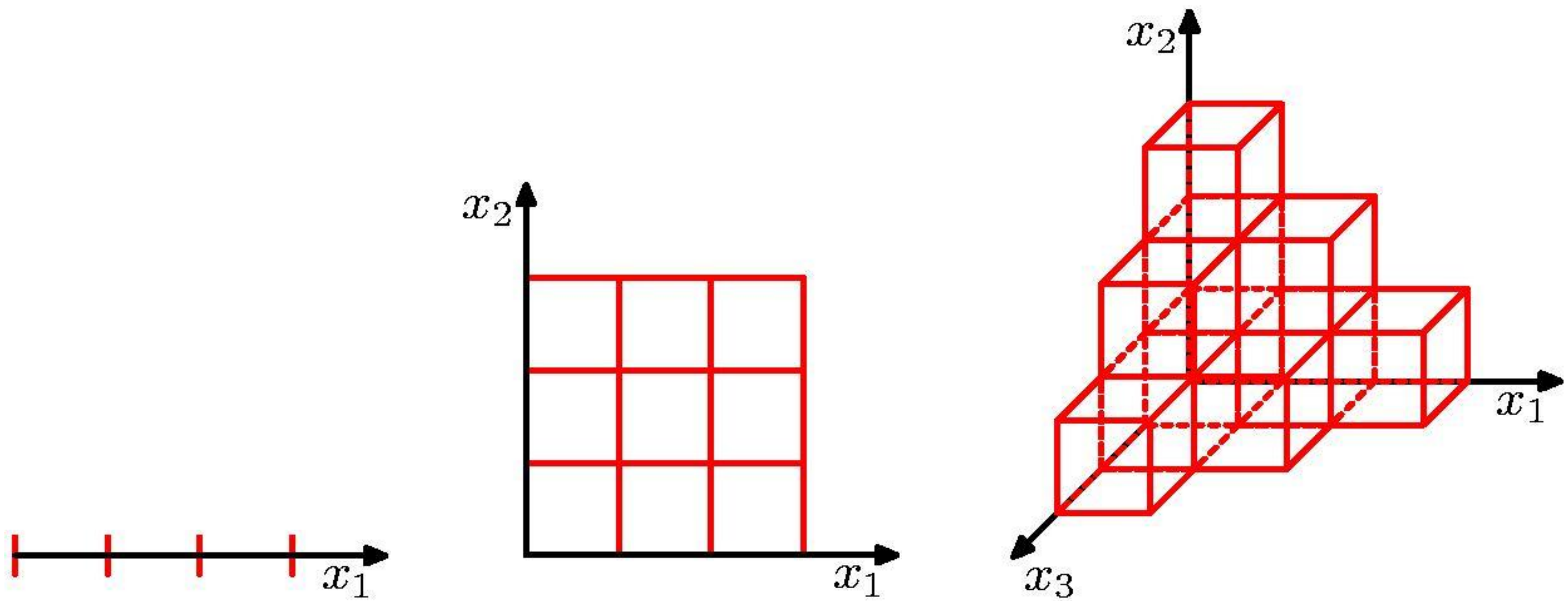
Curse of Dimensionality



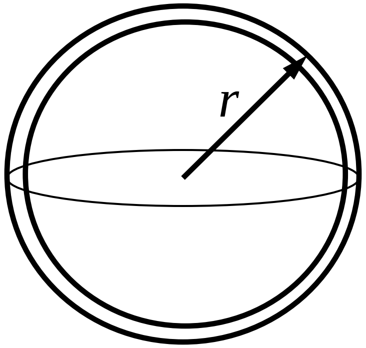
$D = 1$ $D = 2$ $D = 3$

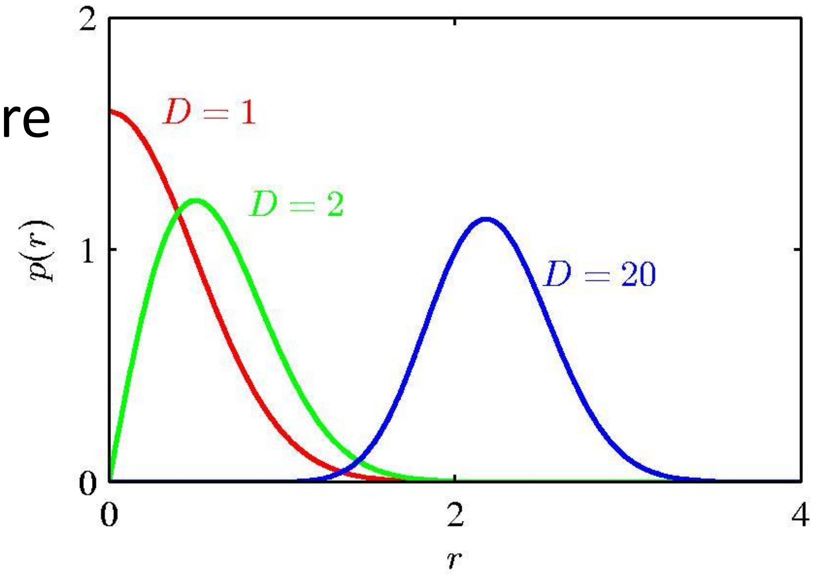
Curse of Dimensionality

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 of a sphere





Reduction of Dimensionality (PCA)

Basis

Data

Coefficients

$$\boldsymbol{Y} = \boldsymbol{A}\boldsymbol{X}$$

principal component analysis

$$\boxed{\min_{A_i} {A_i}^T COV(Y_i) A_i}$$

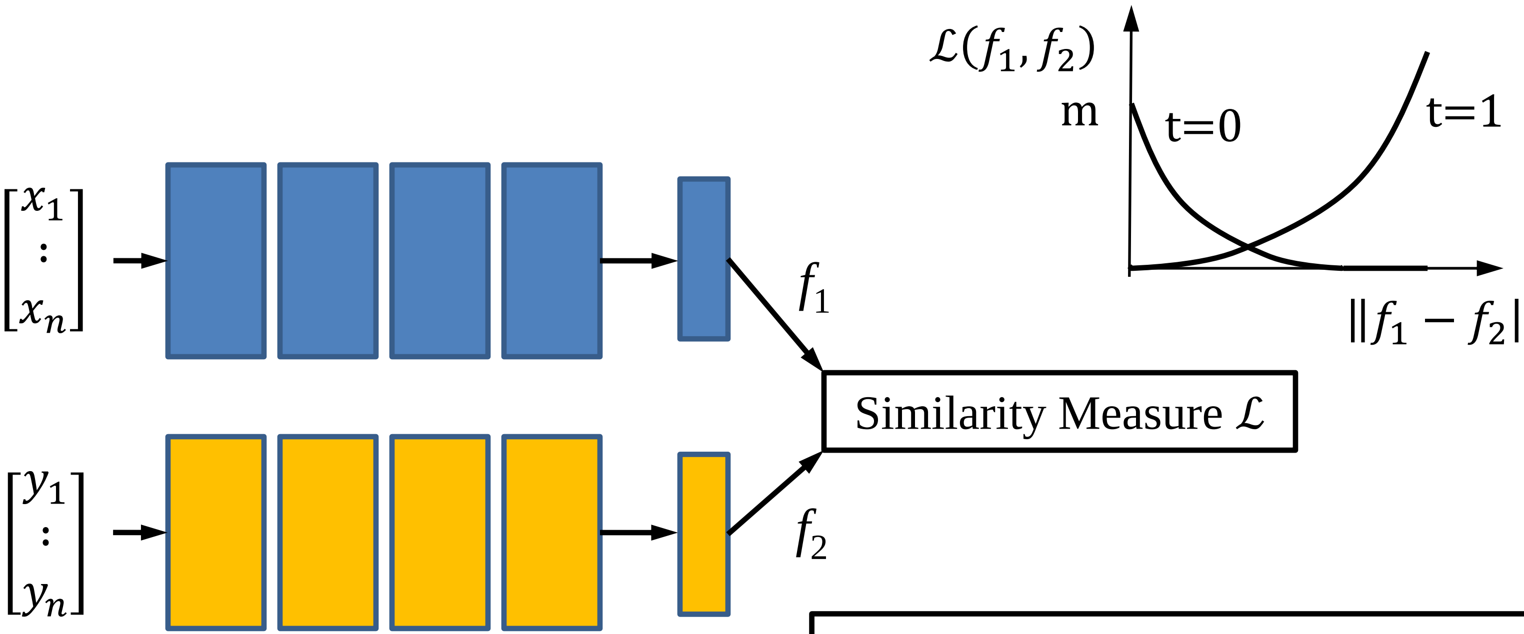
A: rotation

$$A_i^{*T} COV(Y_i) A_i^* = \lambda_i$$

A_i^*: optimal solution

$$s.t. \qquad {A_i}^T A_i = 1 \qquad E[Y_i] = \mathbf{0}$$

Feature Extraction (Contrastive Loss)



maximum distance between clusters

$$\mathcal{L}(f_1, f_2) = t\|f_1 - f_2\|^2 + (1 - t)[\mathrm{m} - \|f_1 - f_2\|^2]_+$$

t =1: two vectors belong to the same category; $[\ ]_+$: non-negative

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Decision Theory

Inference step

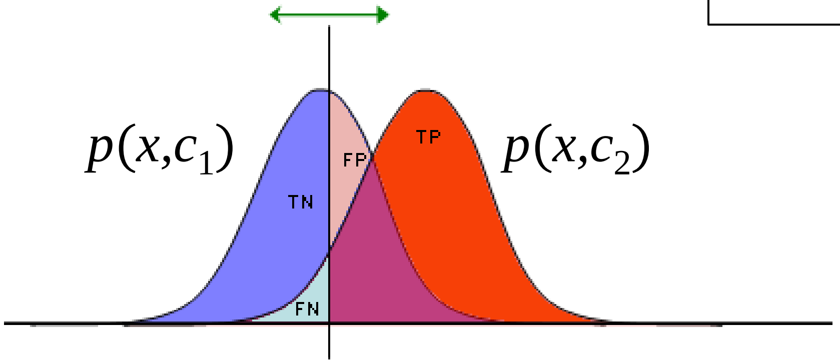
Determine either $p(t|\mathbf{x})$ or $p(\mathbf{x}, t)$.

Decision step

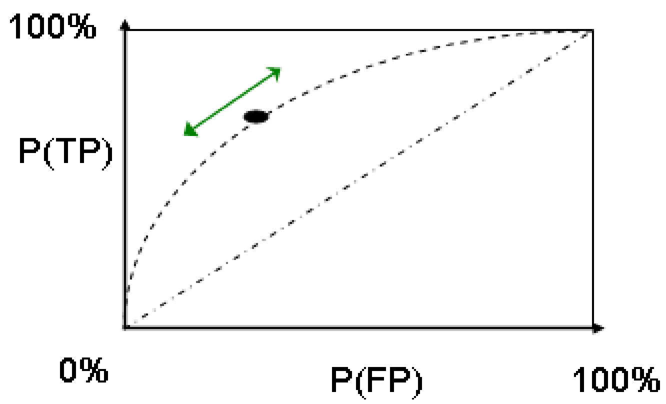
For given $\mathbf{x}$, determine optimal t.

Receiver Operating Characteristic Curve

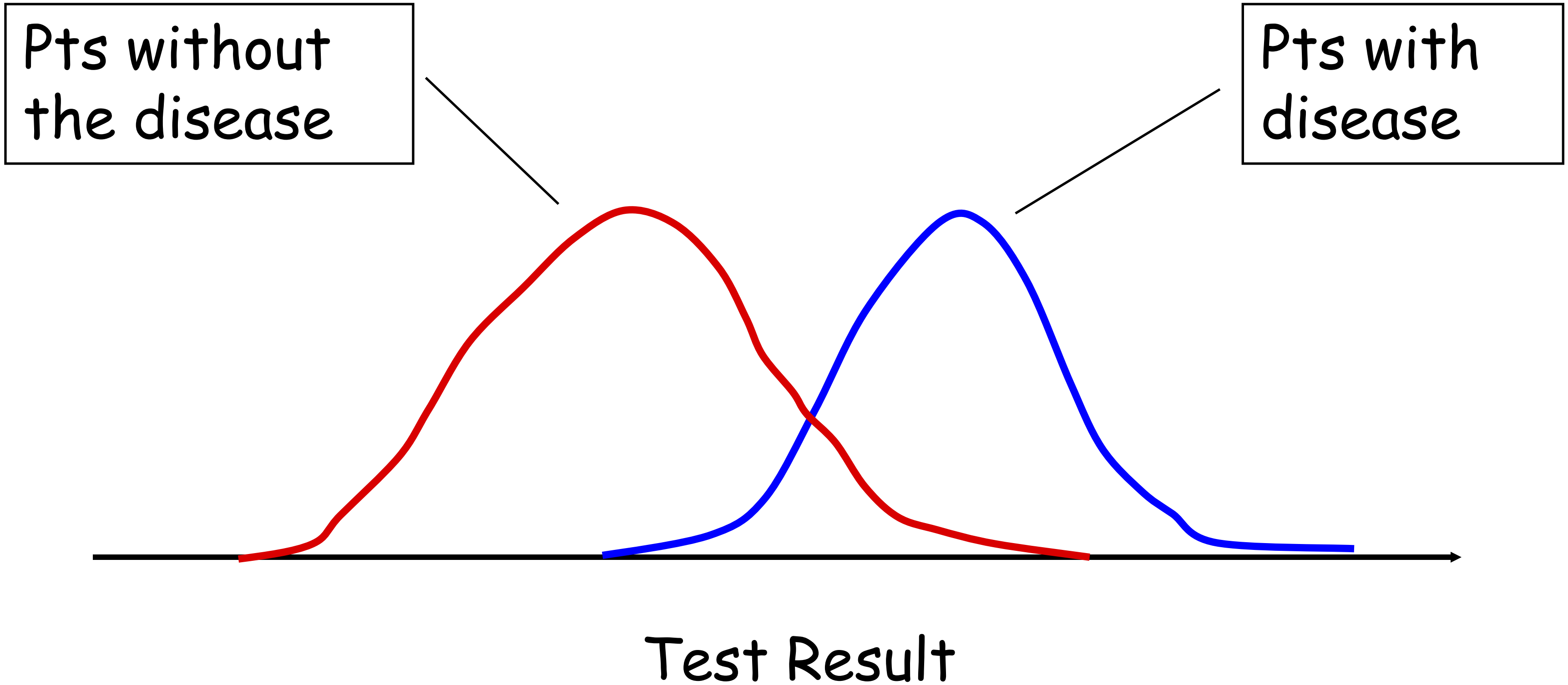
$$\begin{aligned} p(x) &= p(x,c_1) + p(x,c_2) \\ &= p(x|c_1)\, p(c_1) + p(x|c_2)\, p(c_2) \end{aligned}$$



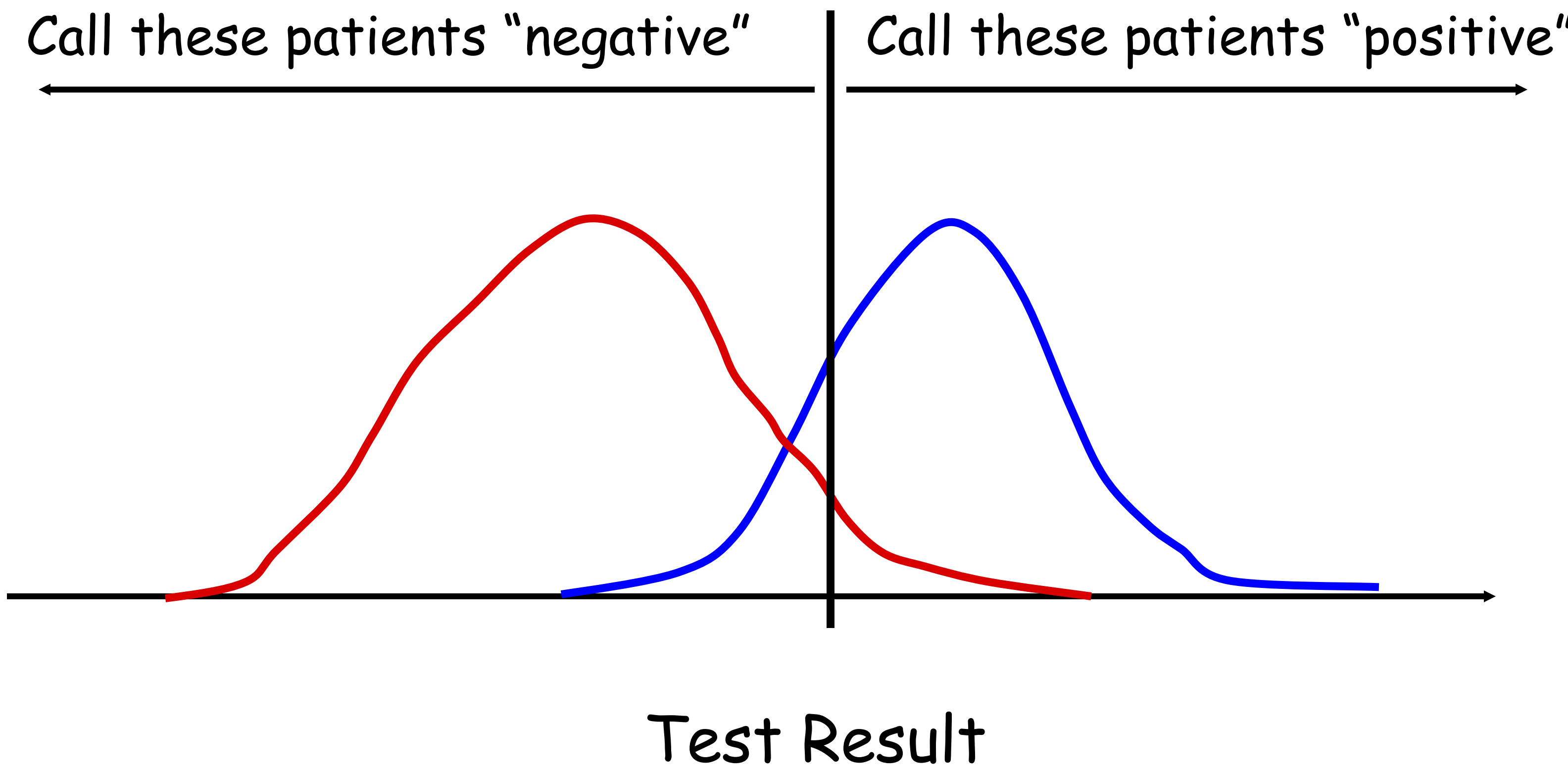
TP	FP
FN	TN
1	1



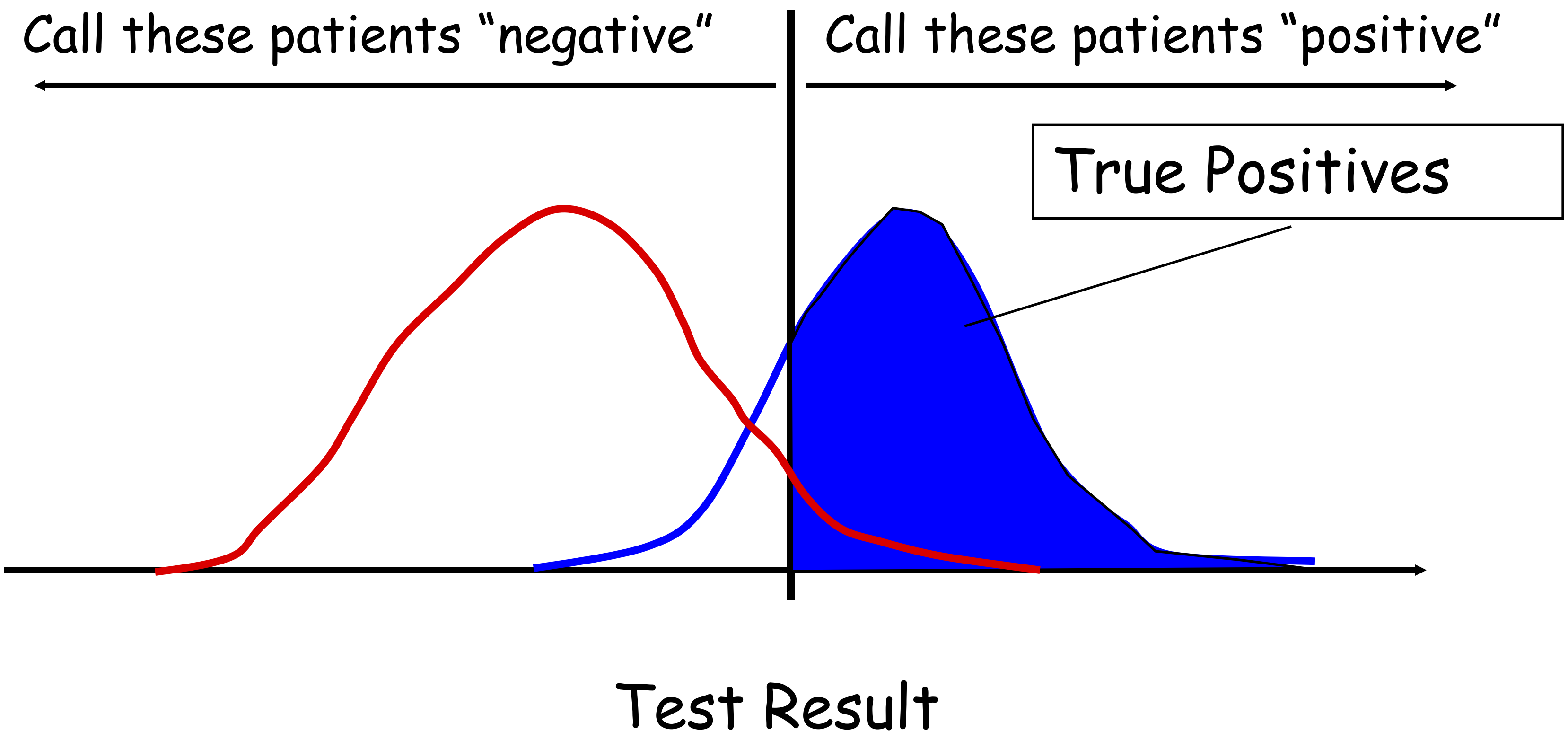
Bimodal Distribution



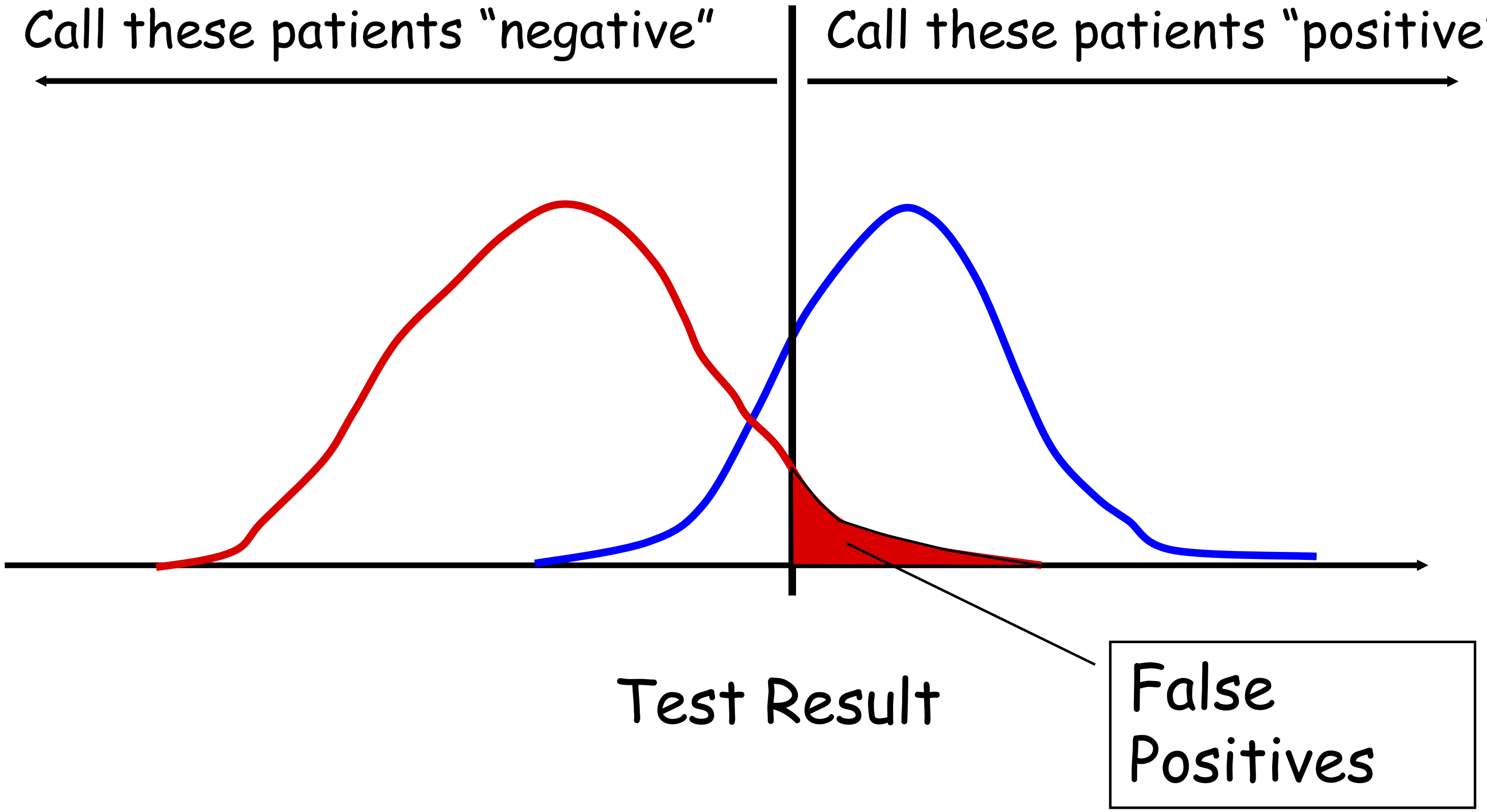
Decision Threshold



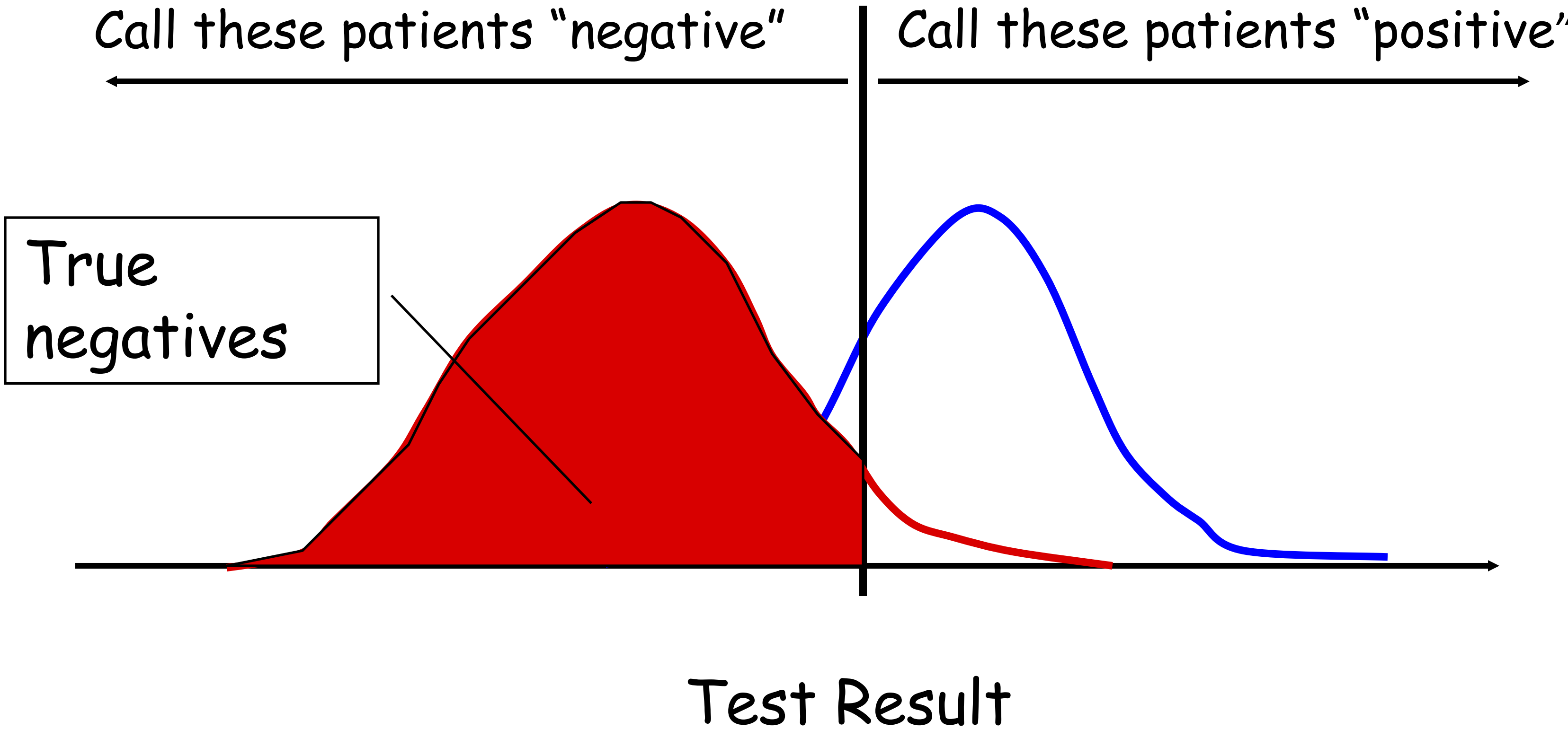
True Positive



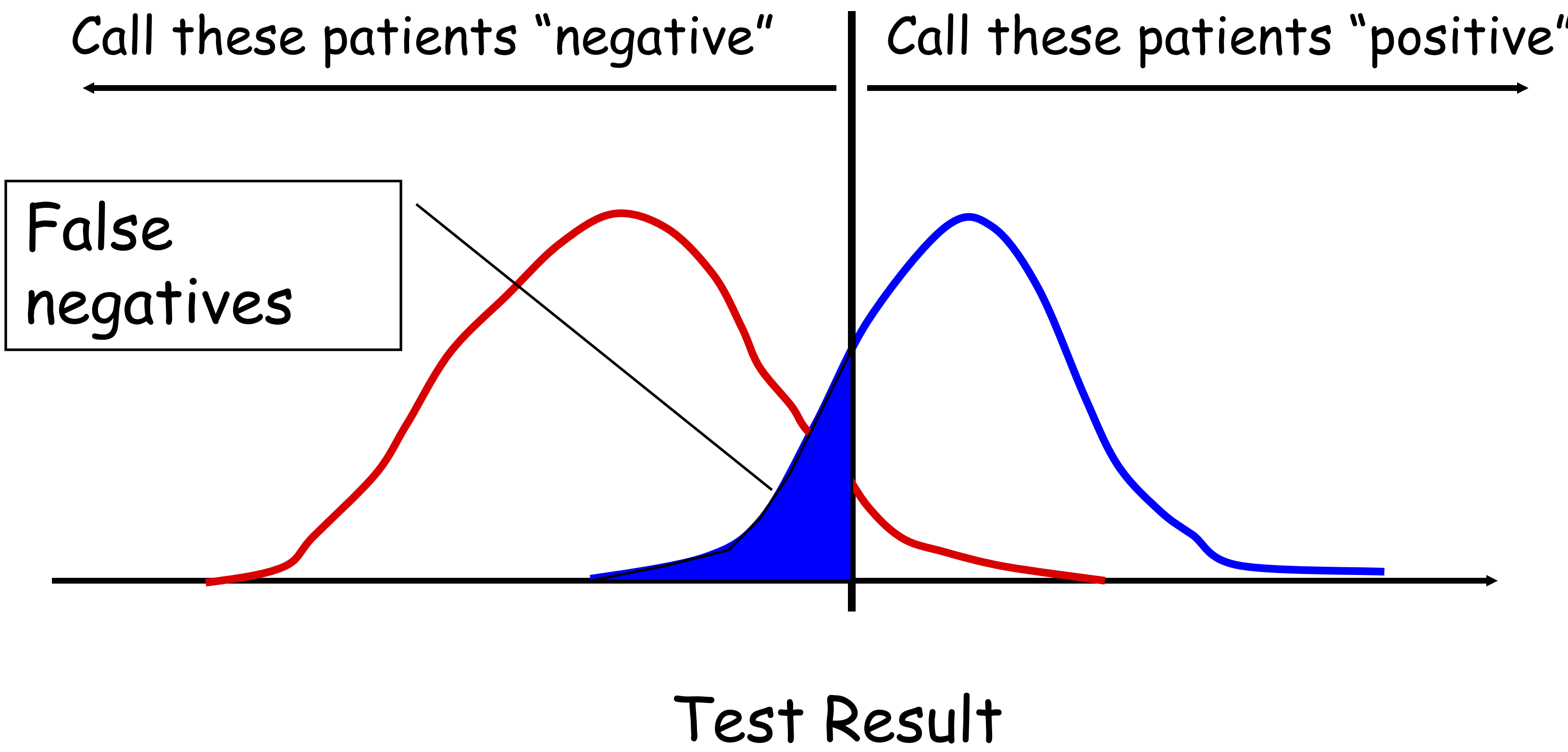
False Positive



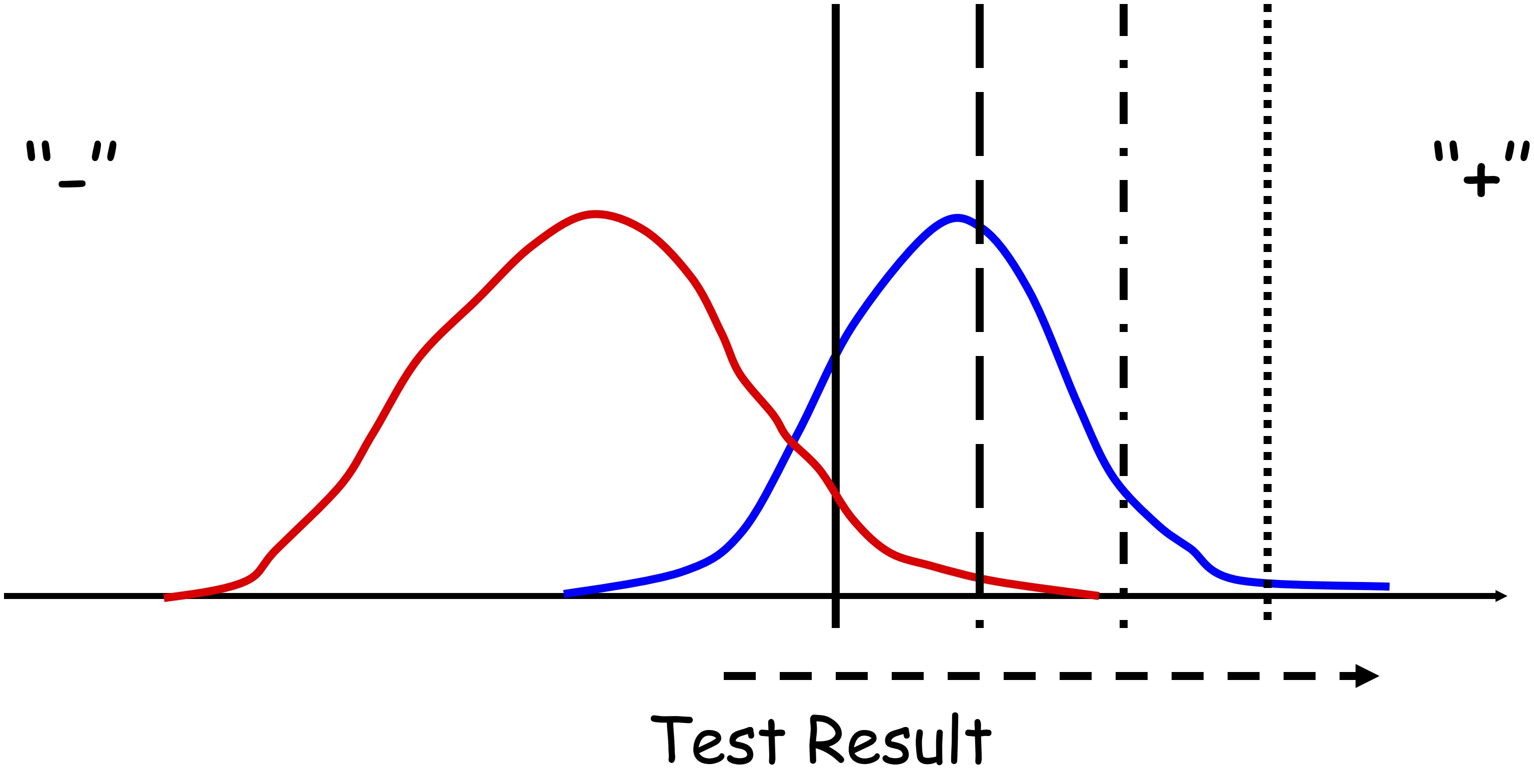
True Negative



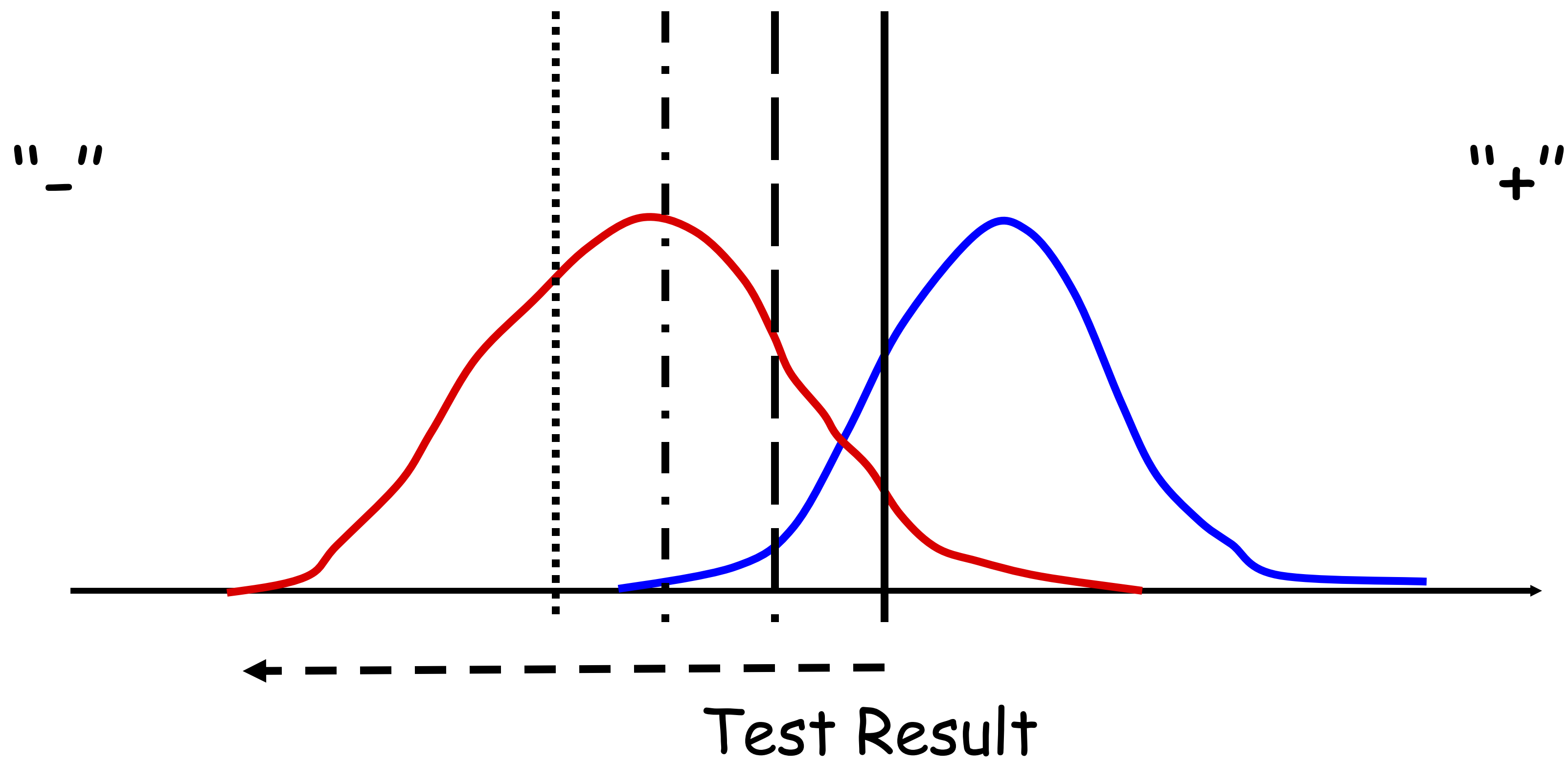
False Negative



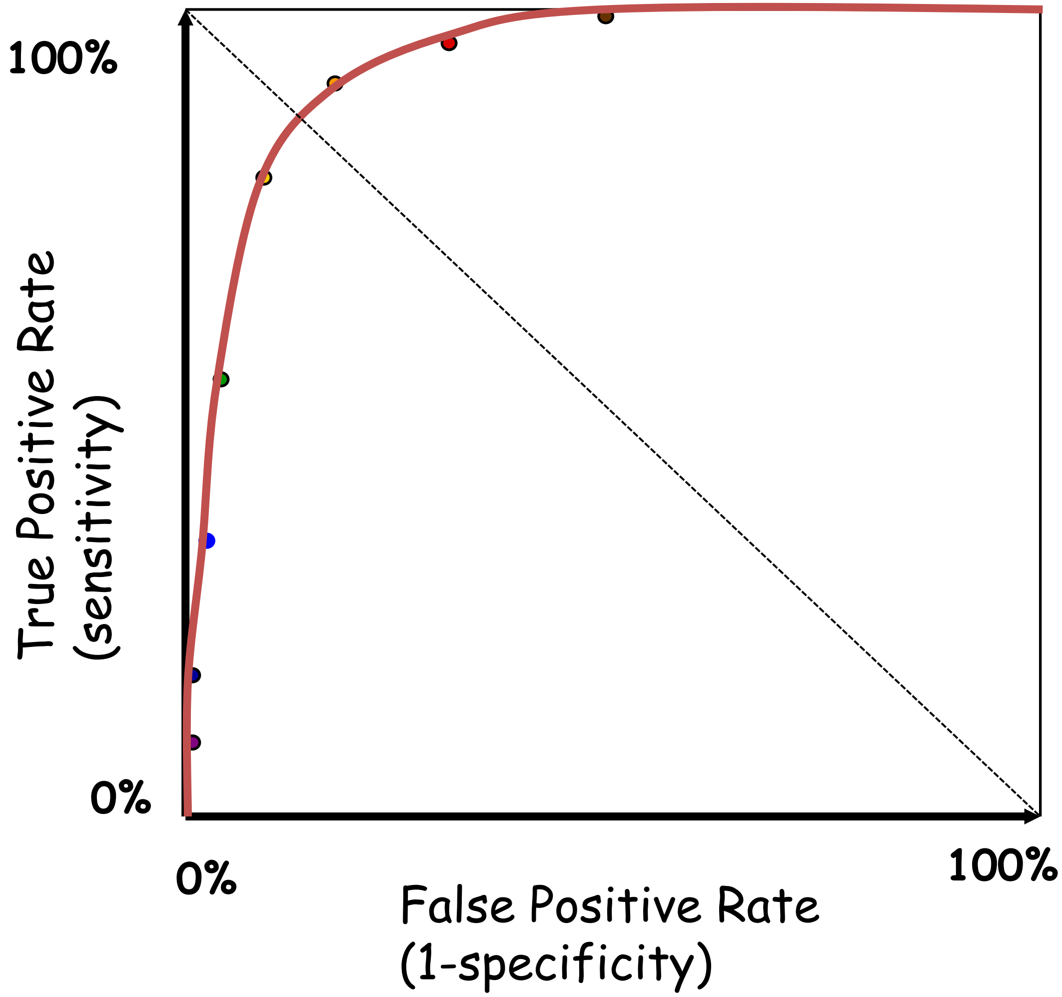
Moving the Threshold: Right

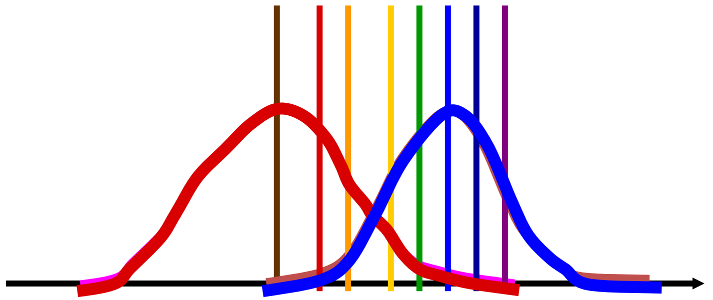


Moving the Threshold: Left

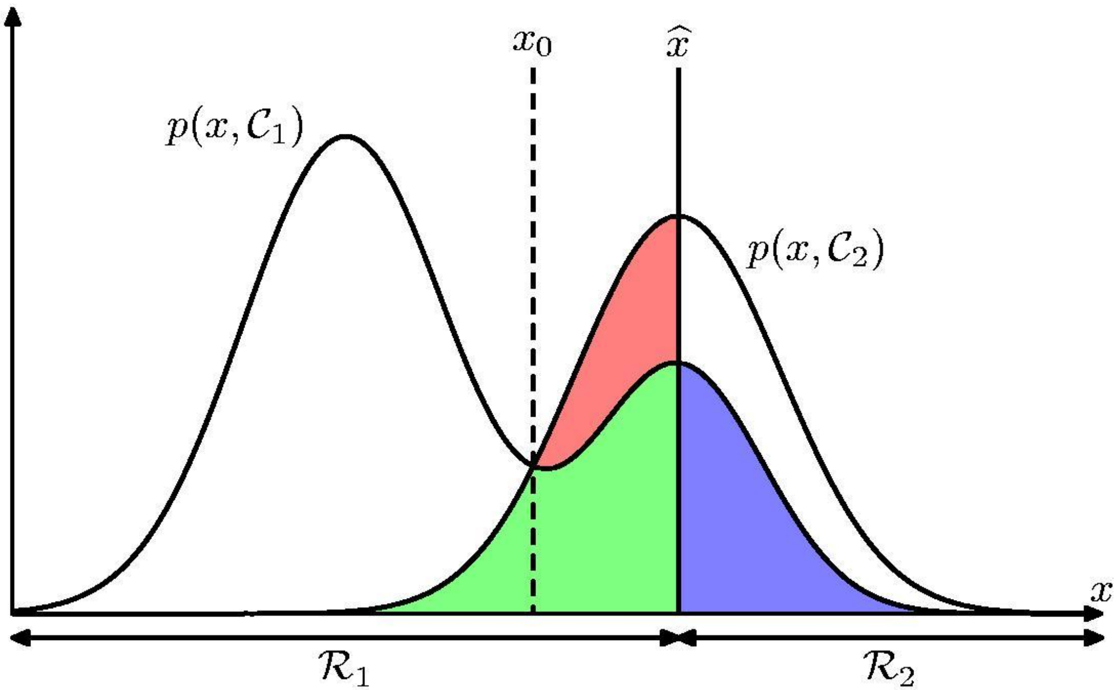


ROC Curve


100%
0%
True Positive Rate
(sensitivity)
0%
100%
False Positive Rate
(1-specificity)



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’

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

False Positive

False Negatives

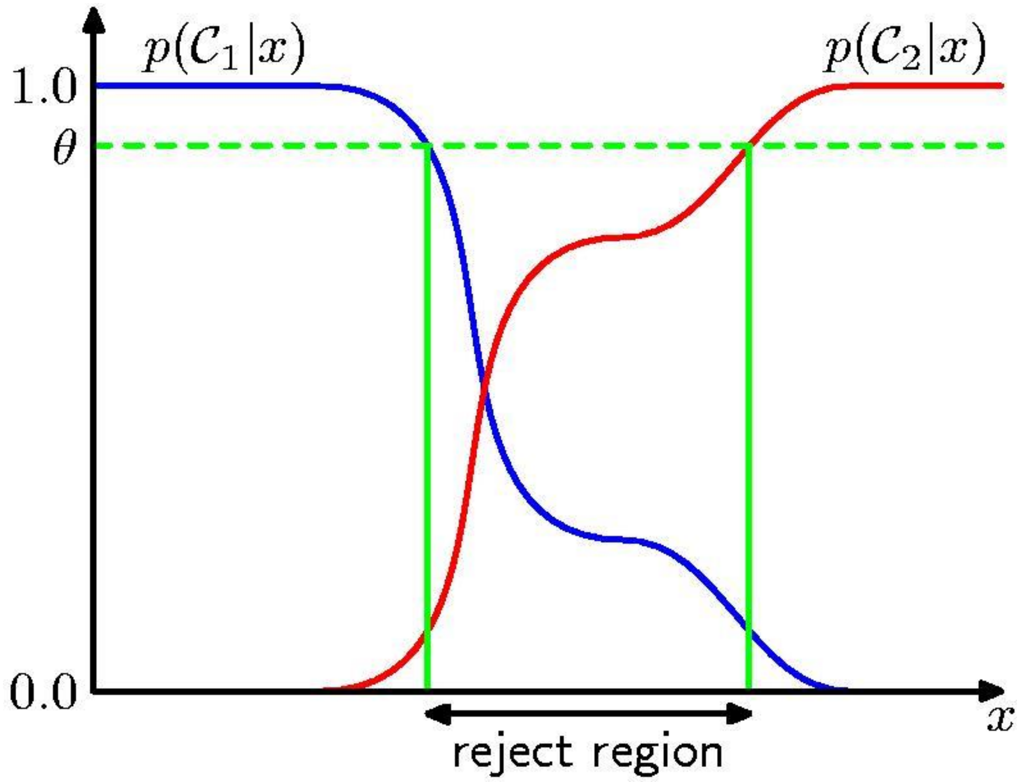
Minimum Expected Loss

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

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

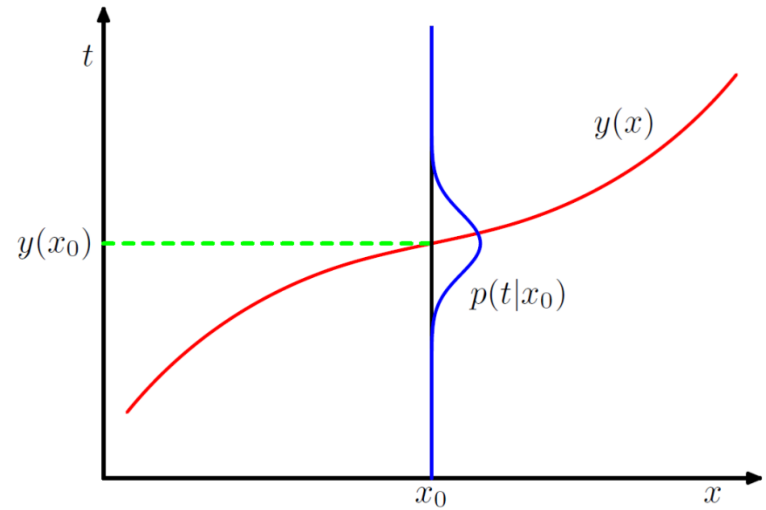
Decision step

For given x, make optimal prediction, $y(\mathrm{x})$, 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 Expected Squared Loss Function

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



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

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

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

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

predictor

noise

$y(x)$: an estimator of the mean of t for given $\mathbf{x}$

https://stats.stackexchange.com/questions/228561/loss-functions-for-regression-proof

Generative vs Discriminative

Generative approach:

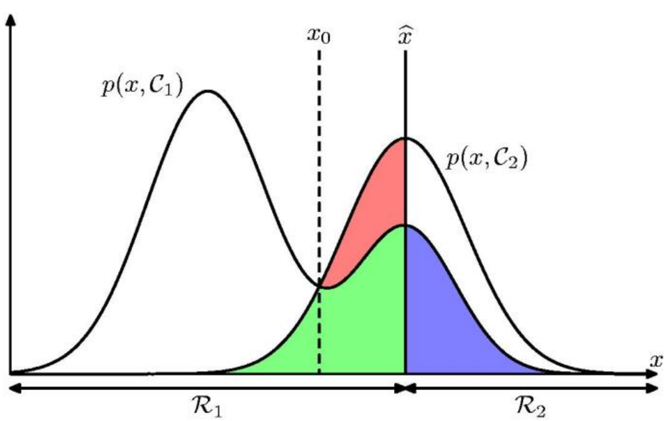
Model $p(t, \mathbf{x}) = p(\mathbf{x}|t)p(t)$

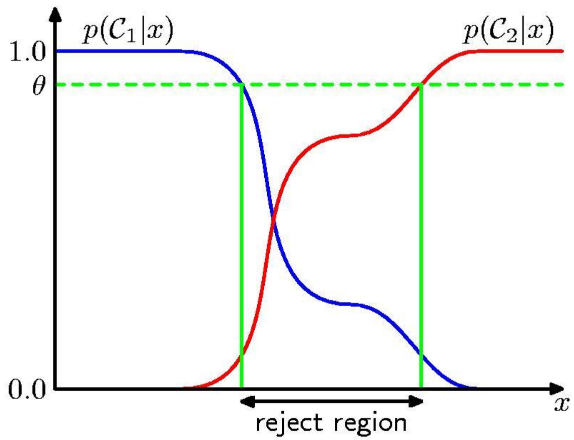
Use Bayes' theorem $p(t|\mathbf{x}) = \dfrac{p(\mathbf{x}|t)p(t)}{p(\mathbf{x})}$

Discriminative approach:

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

t : category





Outlines

- Pattern Recognition
- Curve Fitting and Regularization
- Probabilities and Gaussian Distributions
- Bayesian Inferences (ML and MAP)
- Curse of Dimensionality
- Decision Theories
- Entropy and Information

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

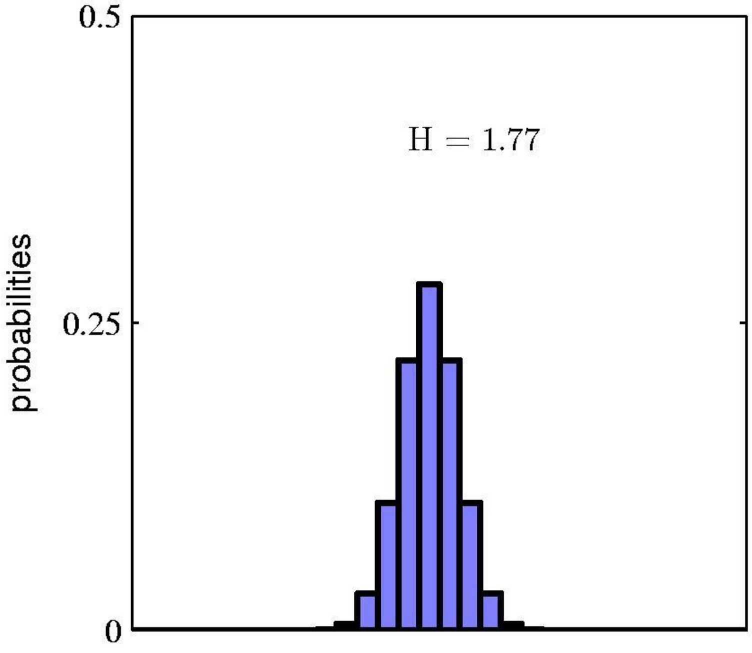
In how many ways can N identical objects be allocated M bins?

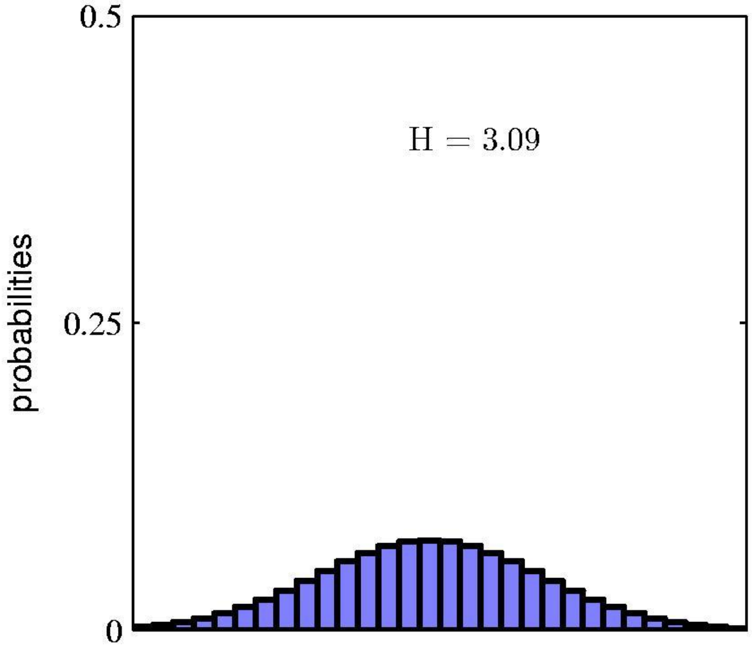
$$W = \frac{N!}{\prod_i n_i!}$$

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

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

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

$$
\begin{aligned}
\mathrm{KL}(p\|q) &= \overbrace{-\int p(\mathbf{x}) \ln q(\mathbf{x})\, \mathrm{d}\mathbf{x}}^{\text{Cross Entropy } \mathrm{C}(p\|q)} - \left(\overbrace{-\int p(\mathbf{x}) \ln p(\mathbf{x})\, \mathrm{d}\mathbf{x}}^{\text{Entropy } \mathrm{H}(p)} \right) \\
&= -\int p(\mathbf{x}) \ln \left\{ \frac{q(\mathbf{x})}{p(\mathbf{x})} \right\} \mathrm{d}\mathbf{x}
\end{aligned}
$$

$$
\mathrm{KL}(p\|q) \simeq \frac{1}{N} \sum_{n=1}^{N} \{ \overbrace{-\ln q(\mathbf{x}_n|\boldsymbol{\theta})}^{\text{Cross Entropy}} + \overbrace{\ln p(\mathbf{x}_n)}^{\text{Negative Entropy}} \}
$$

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

KL divergence describes a distance between model p and model q

Cross Entropy for Machine Learning

Goal of Machine Learning： $p(\,\textit{real data}\,) \approx p(\,\textit{model} \mid \theta\,)$

we assume： $p(\,\textit{training data}\,) \approx p(\,\textit{real data}\,)$

Operation of Machine Learning： $p(\textit{training data}\,) \approx p(\textit{model} \mid \theta\,)$

$$\boxed{\min_{\theta} \mathrm{KL}(p(\,\textit{training data}\,) \,||\, p(\textit{model} \mid \theta)\,)}$$

$$\Leftrightarrow \boxed{\min_{\theta} \mathrm{C}(p(\,\textit{training data}\,) \,||\, p(\textit{model} \mid \theta)\,)}$$

as $\mathrm{H}(p(\,\textit{training data}\,)\,)$ is fixed

Cross Entropy for Machine Learning

$$\boxed{C(p(\textit{training data}) \,||\, p(\textit{model} \,|\, \theta))}$$

Bernoulli model: $p(\textit{model} \mid \theta) = \rho^{t}(1-\rho)^{1-t}$

Cross entropy : $C = -\frac{1}{N}\sum_n t_n \ln\rho + (1-t_n)\ln(1-\rho)$

t_n: *training data*

ρ: *model parameter*

Gaussian model: $p(\textit{model} \mid \theta) \propto e^{-0.5(t-\mu)^2}$

Cross entropy : $C \propto \frac{1}{N}\sum_n (t_n - \mu)^2$

t_n: *training data*

μ: *model parameter*

Mutual Information

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

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

Mutual information describes the degree of dependence between **x** and **y**

Information Gain

$\mathrm{H}[\mathbf{x}]$: uncertain of balls

$\mathrm{H}[\mathbf{x}|\mathbf{y}]$:
uncertain of balls after weighing once

$\mathbf{x}$: one ball lighter

$\mathbf{y}$: weighing once

$\mathbf{x}|\mathbf{y}$: one ball lighter after weighing once

$$\mathrm{I}[\mathbf{x},\mathbf{y}] = \mathrm{H}[\mathbf{x}] - \mathrm{H}[\mathbf{x}|\mathbf{y}] = \log_2 3$$

$$\mathrm{H}[\mathbf{x}] = \log_2 N$$

After weighing $\frac{\mathrm{N}}{3}$ times, all the uncertainties can be removed

Independent Signal Separation

Independent Component Analysis

Mixture Coefficients

Data

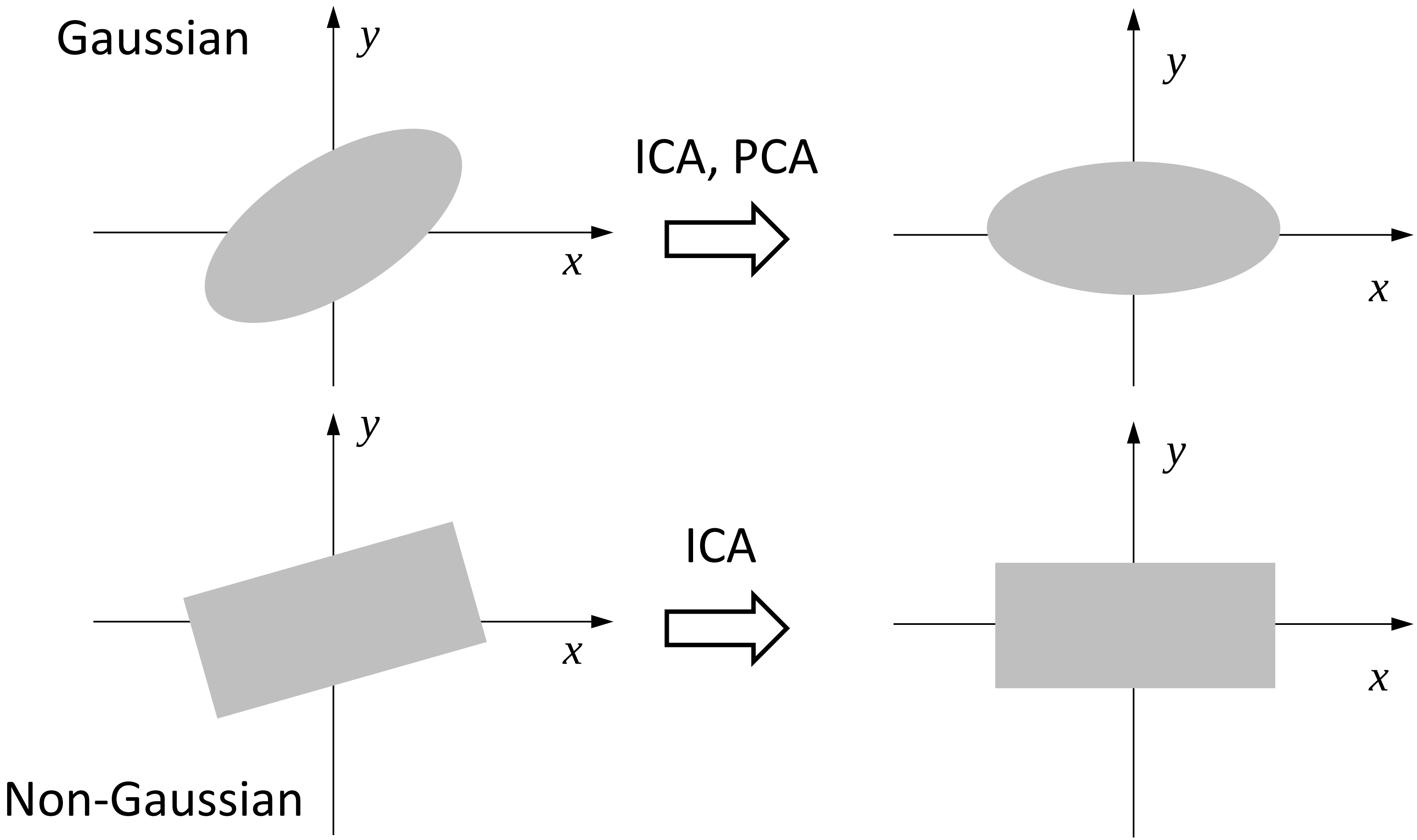
Components

$$Y = AX$$

$$\boxed{\min_{\mathrm{A}} I([X_1, X_2, \dots, X_M] \mid A, Y)}$$

After optimization, the components of $\boldsymbol{X}$ become as much independent as possible

Illustration of ICA Operation



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