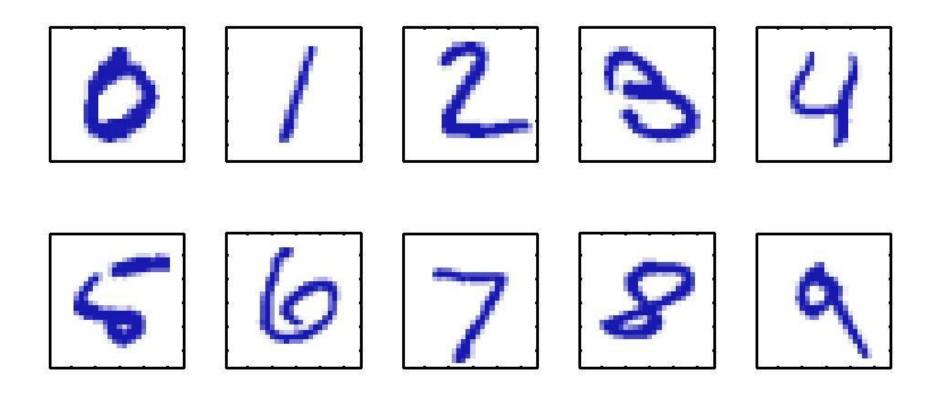


Outlines

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

Example

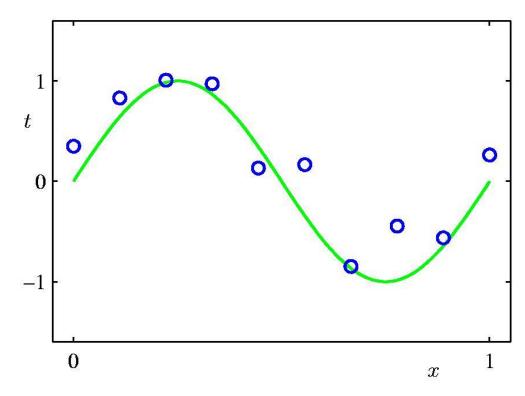
Handwritten Digit Recognition



Outlines

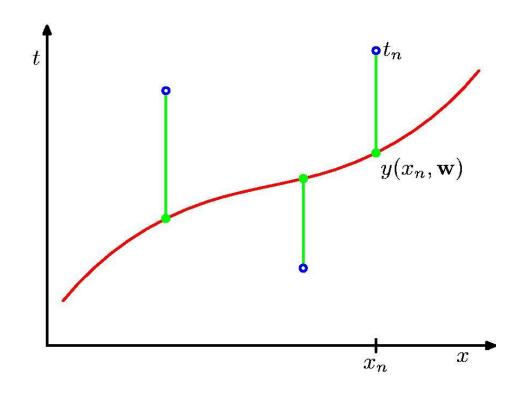
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Polynomial Curve Fitting



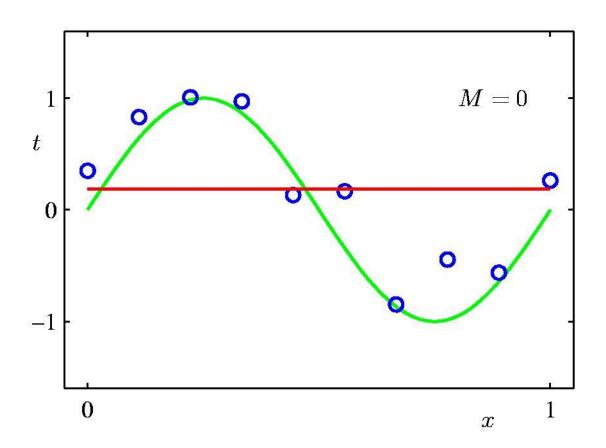
$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Sum-of-Squares Error Function

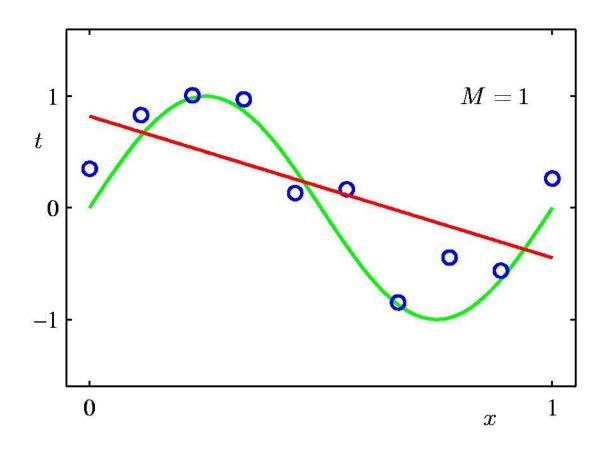


$$E(\mathbf{w}) = \frac{1}{2} \sum_{n=1}^{N} \{y(x_n, \mathbf{w}) - t_n\}^2$$

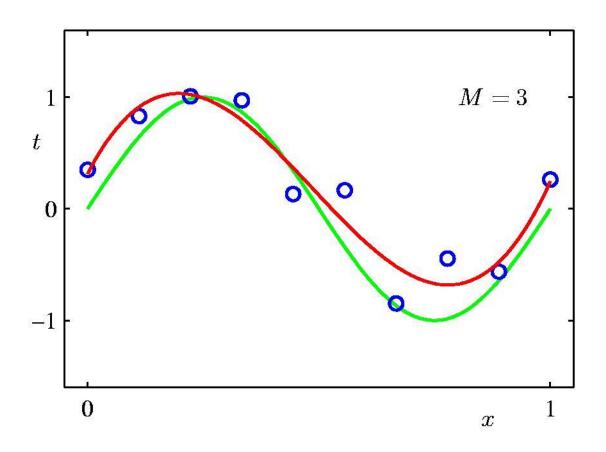
Oth Order Polynomial



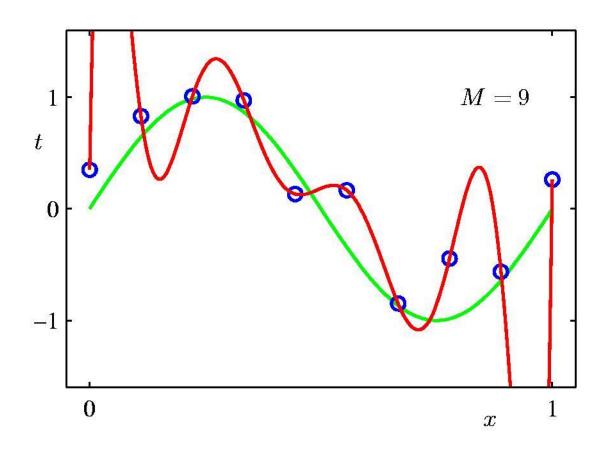
1st Order Polynomial



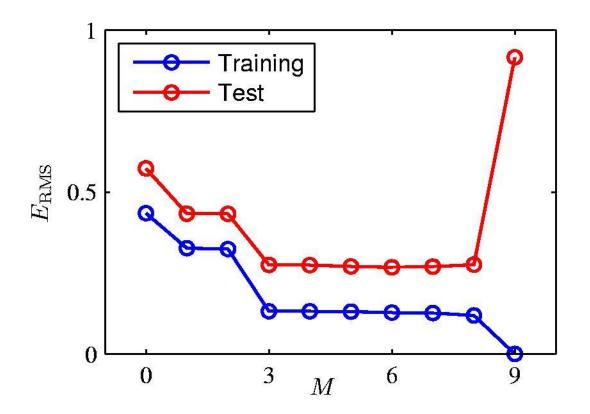
3rd Order Polynomial



9th Order Polynomial



Over-fitting



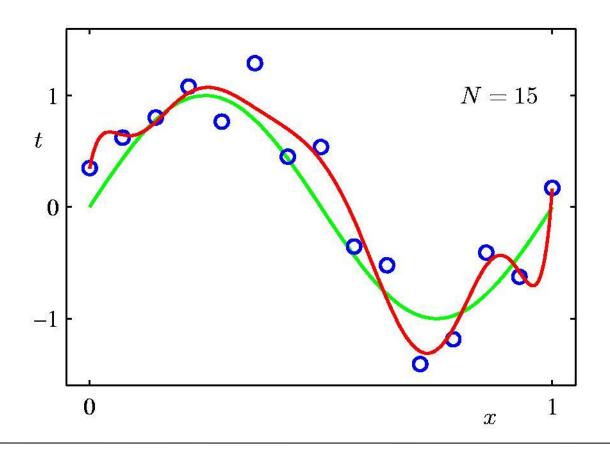
Root-Mean-Square (RMS) Error: $E_{\rm RMS} = \sqrt{2E(\mathbf{w}^\star)/N}$

Polynomial Coefficients

	M=0	M = 1	M = 3	M = 9
$\overline{w_0^{\star}}$	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

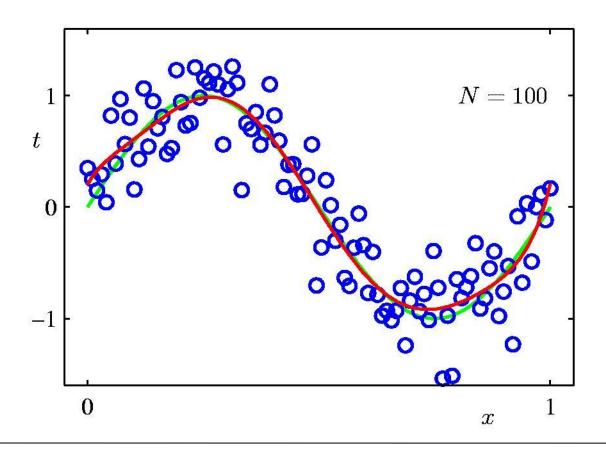
Data Set Size: N=15

9th Order Polynomial



Data Set Size: N = 100

9th Order Polynomial

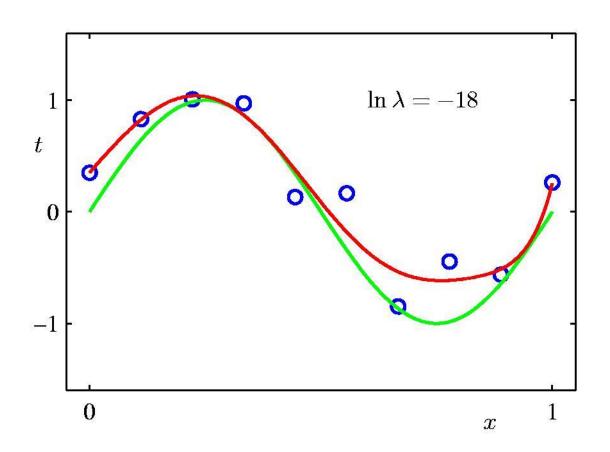


Regularization

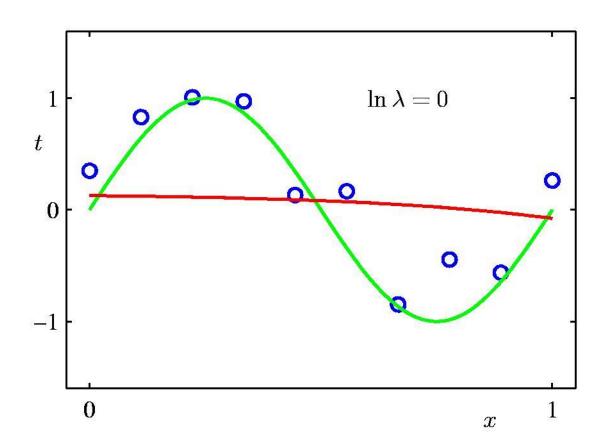
Penalize large coefficient values

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

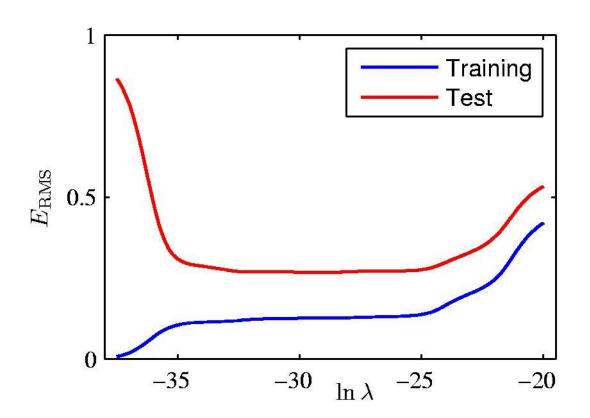
Regularization: $\ln \lambda = -18$



Regularization: $\ln \lambda = 0$



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



Polynomial Coefficients

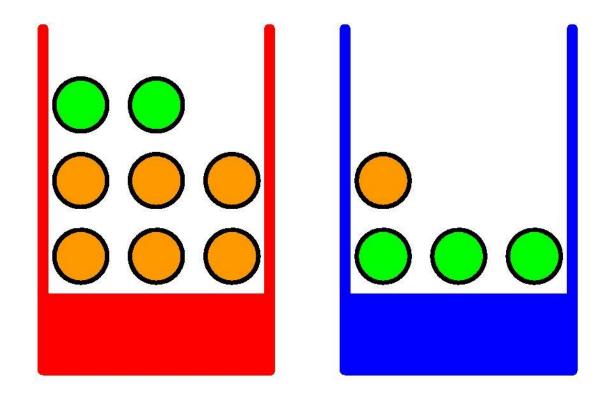
	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$\overline{w_0^{\star}}$	0.35	0.35	0.13
w_1^{\star}	232.37	4.74	-0.05
w_2^\star	-5321.83	-0.77	-0.06
w_3^{\star}	48568.31	-31.97	-0.05
w_4^{\star}	-231639.30	-3.89	-0.03
w_5^{\star}	640042.26	55.28	-0.02
w_6^{\star}	-1061800.52	41.32	-0.01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

Outlines

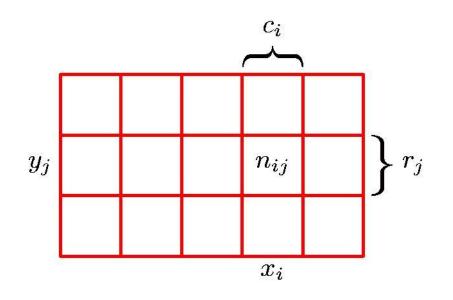
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Probability Theory

Apples and Oranges



Probability Theory



Marginal Probability

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

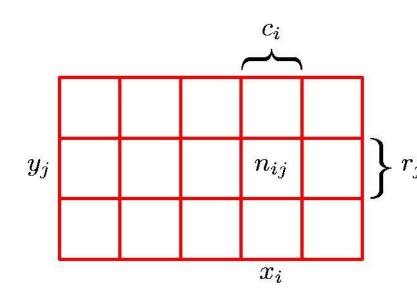
Joint Probability

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

Conditional Probability

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

Probability Theory



Sum Rule

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

Product Rule

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

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

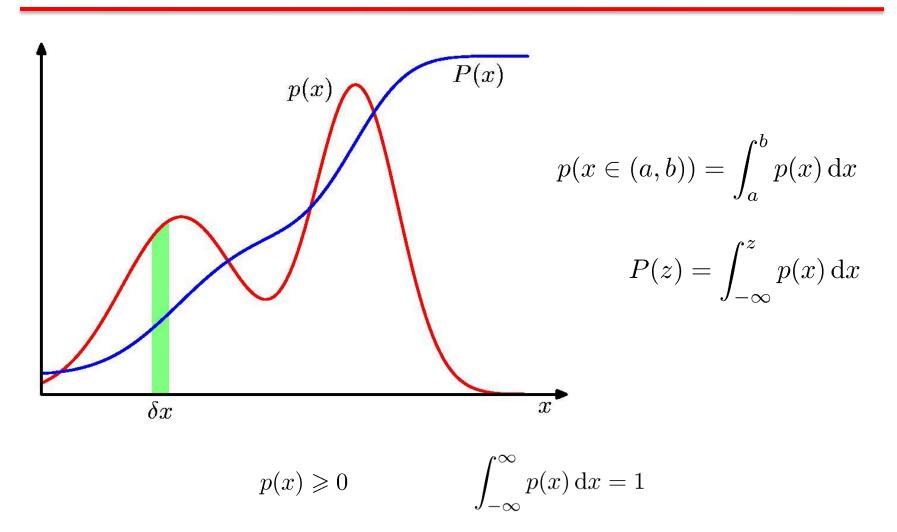
$$p(Y|X) = \frac{p(X|Y)p(Y)}{p(X)}$$

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

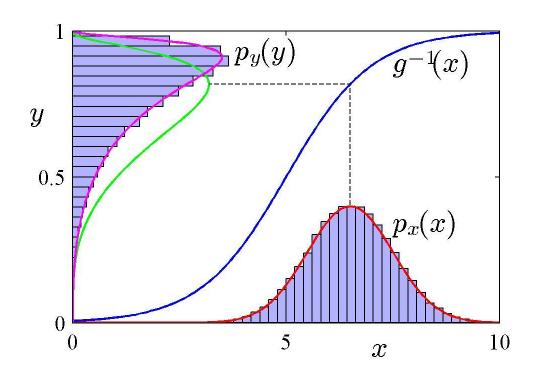
posterior ∝ likelihood × prior

$$p(Y|X)$$
 $p(X|Y)$ $p(Y)$

Probability Densities



Transformed Densities



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

= $p_x(g(y)) |g'(y)|$

$$x = g(y)$$

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

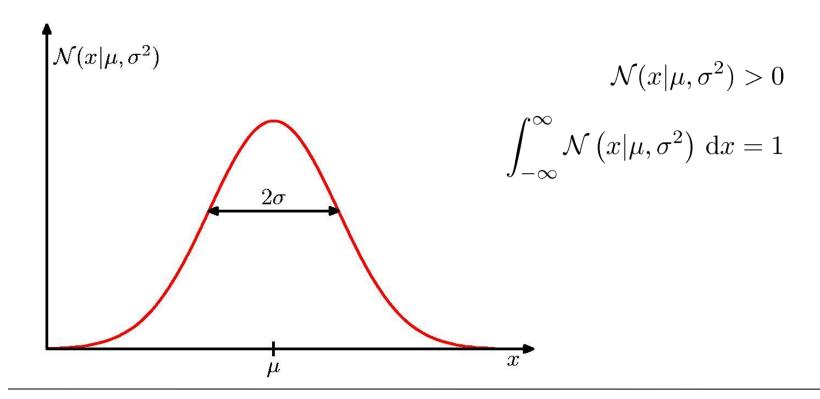
$$\operatorname{var}[f] = \mathbb{E}\left[\left(f(x) - \mathbb{E}[f(x)]\right)^{2}\right] = \mathbb{E}[f(x)^{2}] - \mathbb{E}[f(x)]^{2}$$

$$cov[x, y] = \mathbb{E}_{x,y} [\{x - \mathbb{E}[x]\} \{y - \mathbb{E}[y]\}]$$
$$= \mathbb{E}_{x,y} [xy] - \mathbb{E}[x] \mathbb{E}[y]$$

$$cov[\mathbf{x}, \mathbf{y}] = \mathbb{E}_{\mathbf{x}, \mathbf{y}} [\{\mathbf{x} - \mathbb{E}[\mathbf{x}]\} \{\mathbf{y}^{\mathrm{T}} - \mathbb{E}[\mathbf{y}^{\mathrm{T}}]\}]$$
$$= \mathbb{E}_{\mathbf{x}, \mathbf{y}} [\mathbf{x}\mathbf{y}^{\mathrm{T}}] - \mathbb{E}[\mathbf{x}] \mathbb{E}[\mathbf{y}^{\mathrm{T}}]$$

The Gaussian Distribution

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



Gaussian Mean and Variance

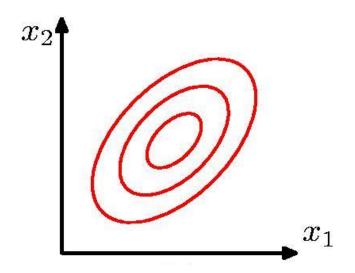
$$\mathbb{E}[x] = \int_{-\infty}^{\infty} \mathcal{N}(x|\mu, \sigma^2) x \, \mathrm{d}x = \mu$$

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

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

The Multivariate Gaussian

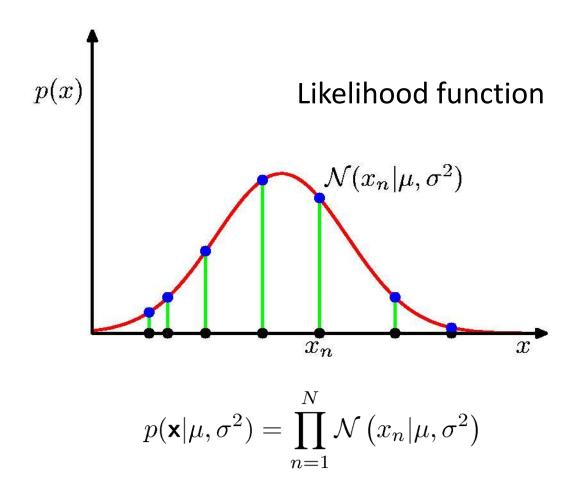
$$\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^{\mathrm{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu})\right\}$$



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Gaussian Parameter Estimation



Maximum (Log) Likelihood

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

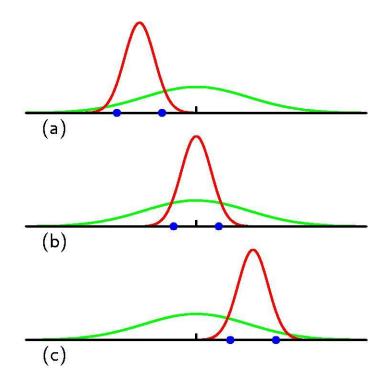
$$\mu_{\text{ML}} = \frac{1}{N} \sum_{n=1}^{N} x_n$$
 $\sigma_{\text{ML}}^2 = \frac{1}{N} \sum_{n=1}^{N} (x_n - \mu_{\text{ML}})^2$

Properties of $\mu_{ m ML}$ and $\sigma_{ m ML}^2$

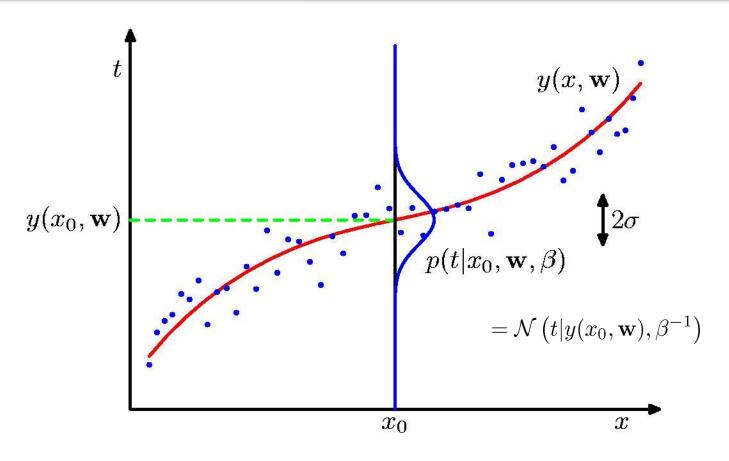
$$\mathbb{E}[\mu_{\mathrm{ML}}] = \mu$$

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

$$\widetilde{\sigma}^2 = \frac{N}{N-1} \sigma_{\text{ML}}^2$$
$$= \frac{1}{N-1} \sum_{n=1}^{N} (x_n - \mu_{\text{ML}})^2$$



Curve Fitting Re-visited



$$(t, x)$$
: training data $\Rightarrow w, \beta$ (w, β, x_0) : $\Rightarrow p(t/x_0, w, \beta)$

Maximum Likelihood

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

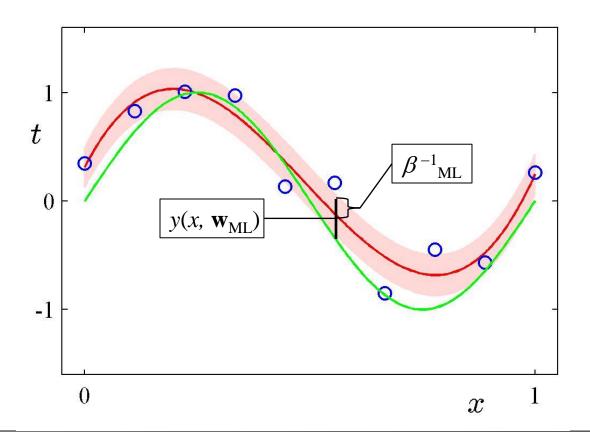
$$\ln p(\mathbf{t}|\mathbf{x}, \mathbf{w}, \beta) = -\underbrace{\frac{\beta}{2} \sum_{n=1}^{N} \left\{ y(x_n, \mathbf{w}) - t_n \right\}^2 + \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi)}_{\beta E(\mathbf{w})}$$

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

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

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

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

$$\begin{array}{c|c} \hline posteriori & \longrightarrow p(\mathbf{w}|\mathbf{x},\mathbf{t},\alpha,\beta) \propto p(\mathbf{t}|\mathbf{x},\mathbf{w},\beta)p(\mathbf{w}|\alpha) & \longleftarrow & priori \\ \hline \\ likelihood & \\ \end{array}$$

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

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

Bayesian Curve Fitting

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

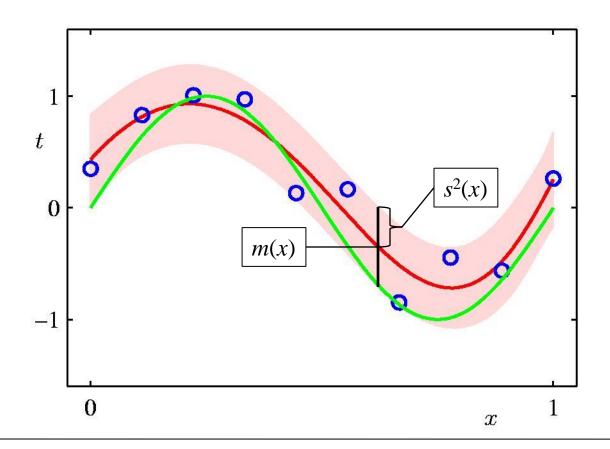
$$m(x) = \beta \phi(x)^{\mathrm{T}} \mathbf{S} \sum_{n=1}^{N} \phi(x_n) t_n$$
 $s^2(x) = \beta^{-1} + \phi(x)^{\mathrm{T}} \mathbf{S} \phi(x)$

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

We will go through more details in a later lecture.

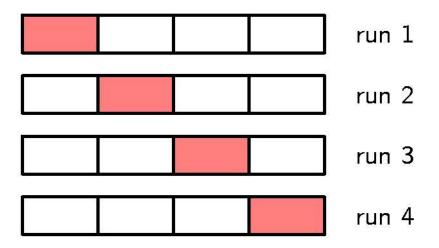
Bayesian Predictive Distribution

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



Model Selection

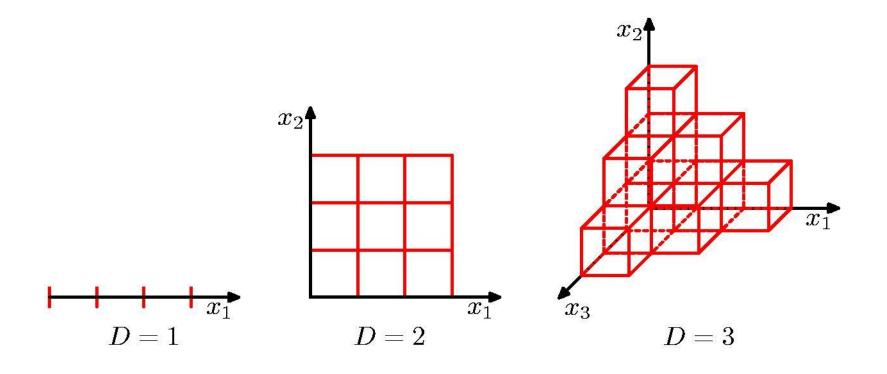
Cross-Validation



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Curse of Dimensionality

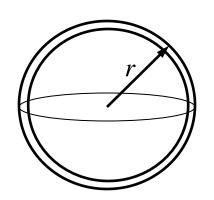


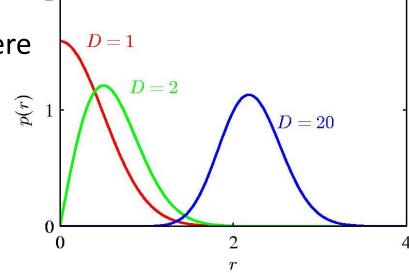
Curse of Dimensionality

Polynomial curve fitting, M=3

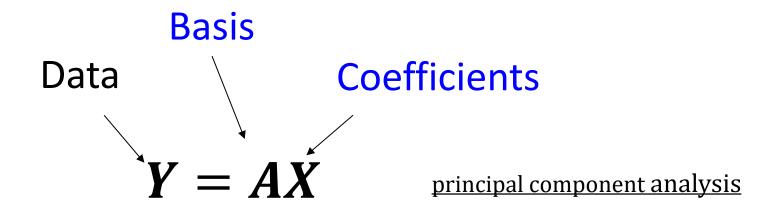
$$y(\mathbf{x}, \mathbf{w}) = w_0 + \sum_{i=1}^{D} w_i x_i + \sum_{i=1}^{D} \sum_{j=1}^{D} w_{ij} x_i x_j + \sum_{i=1}^{D} \sum_{j=1}^{D} \sum_{k=1}^{D} w_{ijk} x_i x_j x_k$$

Gaussian Densities in higher dimensions of a sphere





Reduction of Dimensionality (PCA)



$$\min_{A_i} A_i^T VAR(Y_i) A_i$$

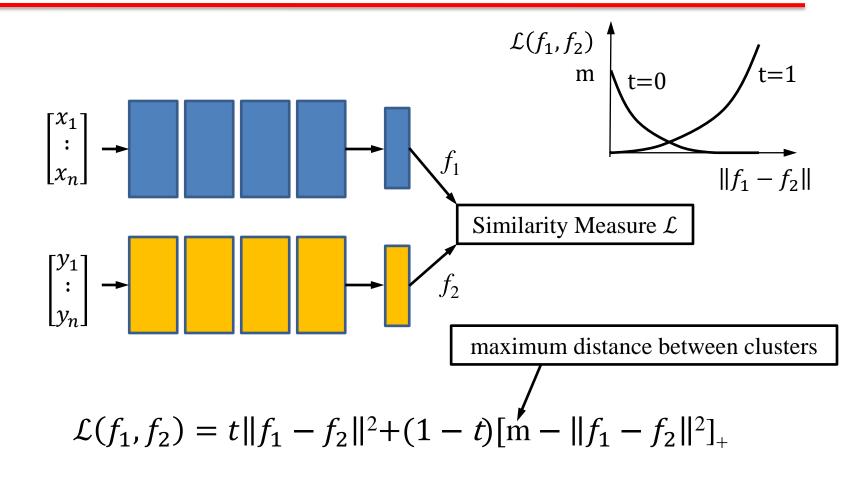
A: rotation

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

 A_i^* : optimal solution

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

Feature Extraction (Contrastive Cost)



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

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Decision Theory

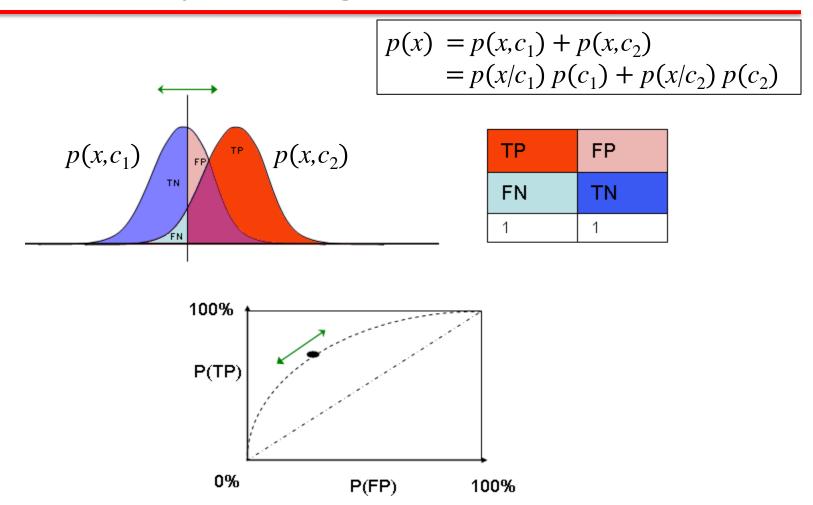
Inference step

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

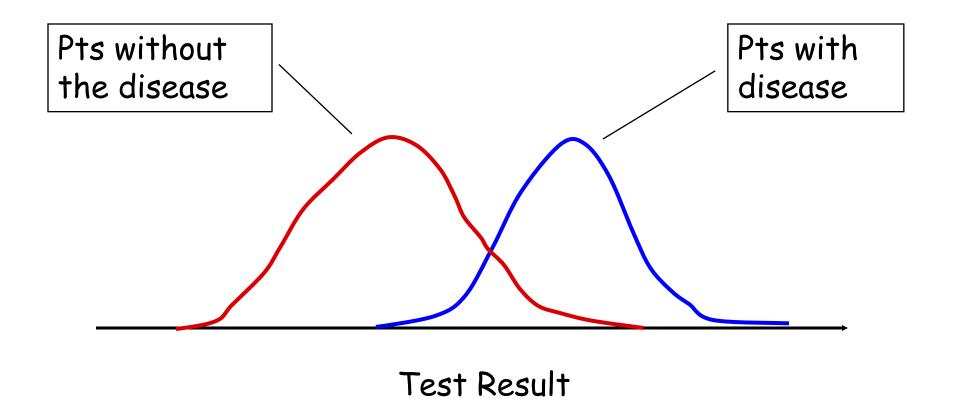
Decision step

For given x, determine optimal t.

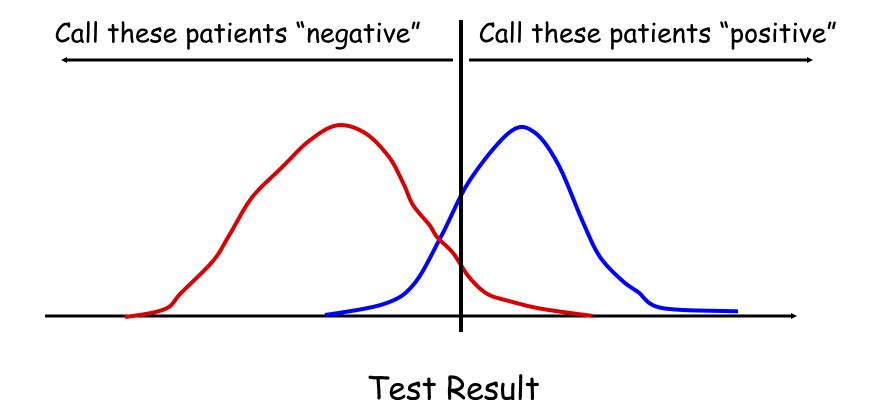
Receiver Operating Characteristic Curve



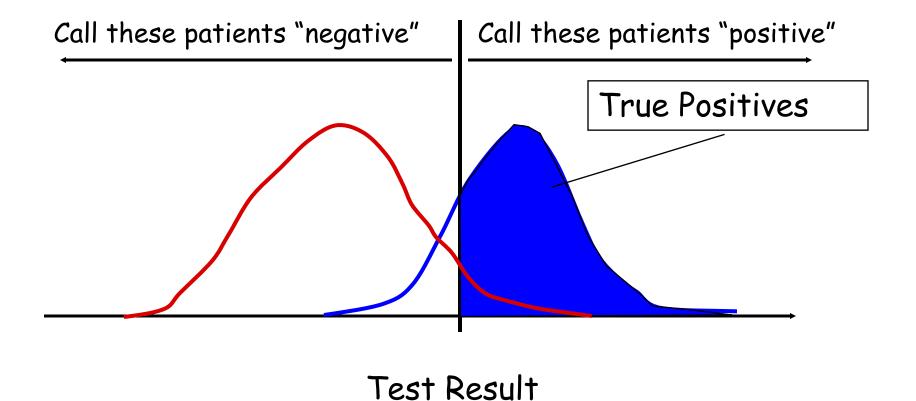
Bimodal Distribution



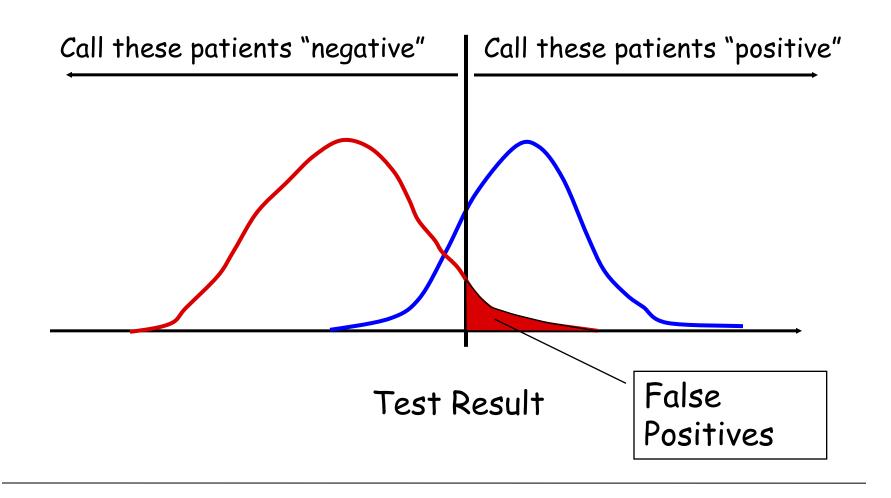
Decision Threshold



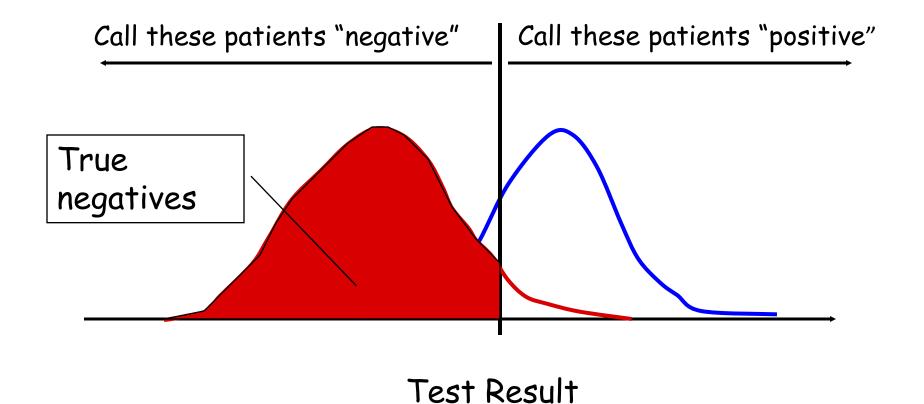
True Positive



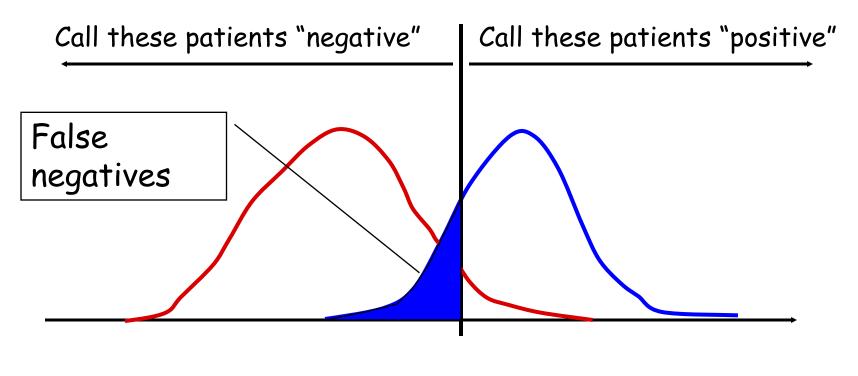
False Positive



True Negative

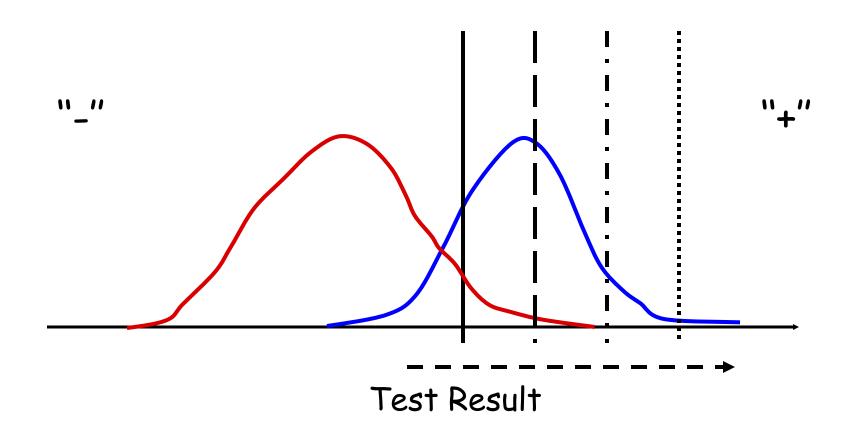


False Negative

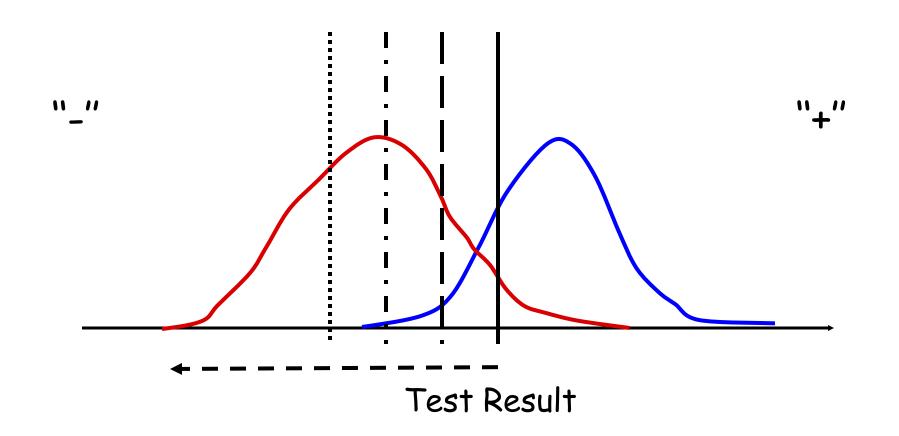


Test Result

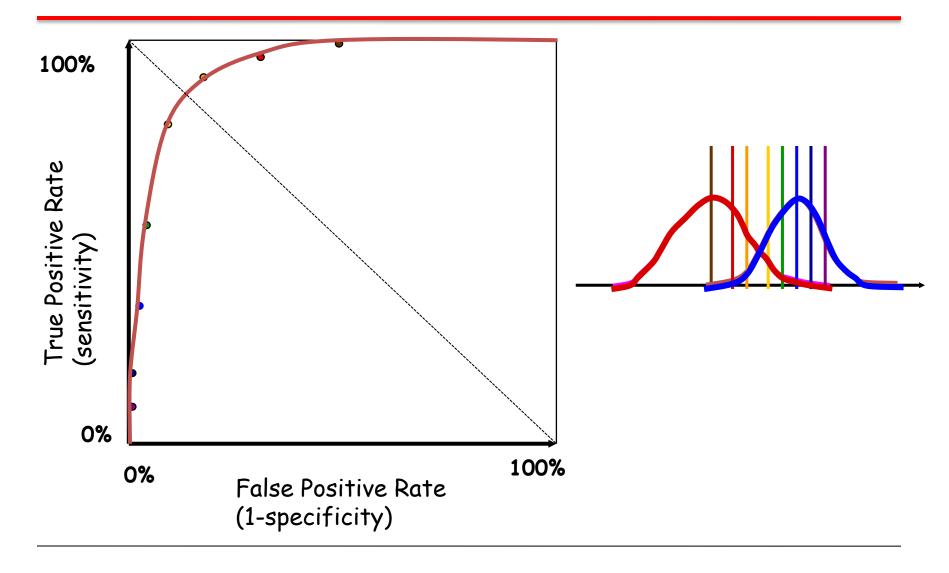
Moving the Threshold: Right



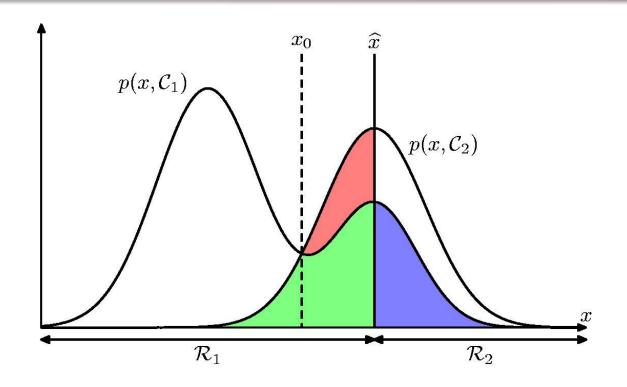
Moving the Threshold: Left



ROC Curve



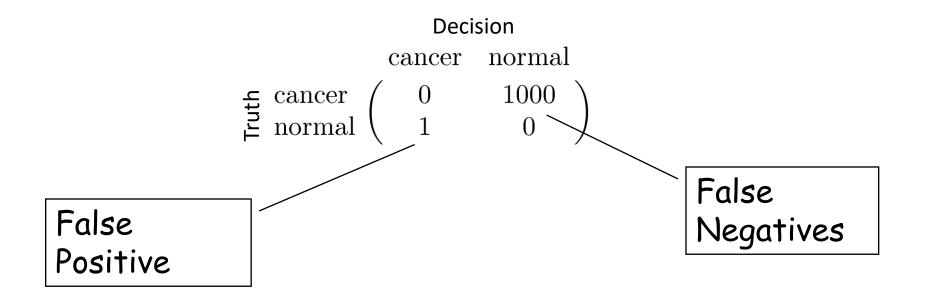
Minimum Misclassification Rate



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

Minimum Expected Loss

Example: classify medical images as 'cancer' or 'normal'



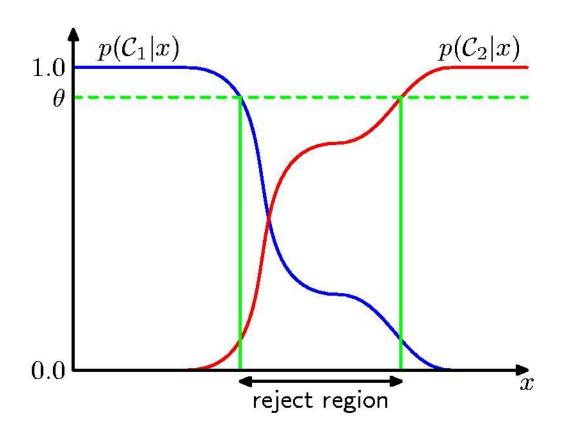
Minimum Expected Loss

$$\mathbb{E}[L] = \sum_{k} \sum_{j} \int_{\mathcal{R}_{j}} L_{kj} p(\mathbf{x}, \mathcal{C}_{k}) d\mathbf{x}$$

Regions \mathcal{R}_i 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 $p(\mathbf{x}, t)$.

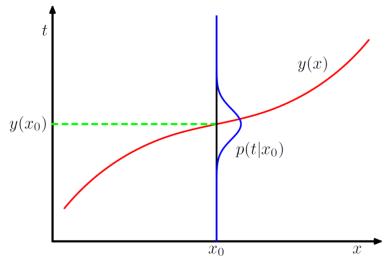
Decision step

For given x, make optimal prediction, y(x), for t.

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

The Expected Squared Loss Function

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



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

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

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

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

y(x): an estimator of the mean of t for given **x**

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

Generative vs Discriminative

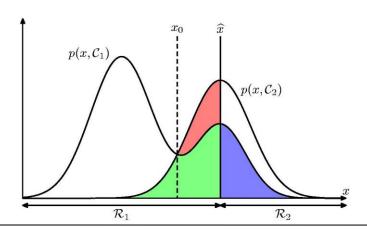
Generative approach:

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

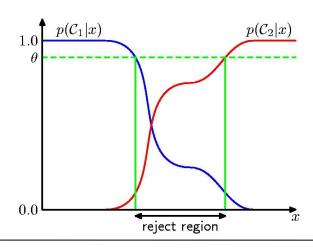
Use Bayes' theorem
$$p(t|\mathbf{x}) = \frac{p(\mathbf{x}|t)p(t)}{p(\mathbf{x})}$$

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

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

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

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

Entropy

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

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 bits

Entropy

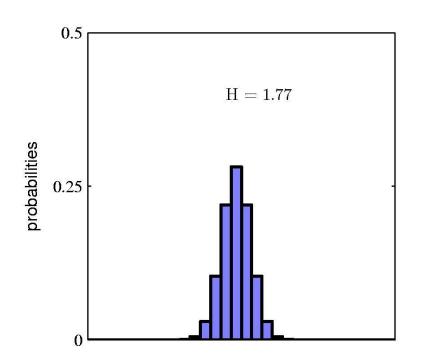
In how many ways can N identical objects be allocated M bins?

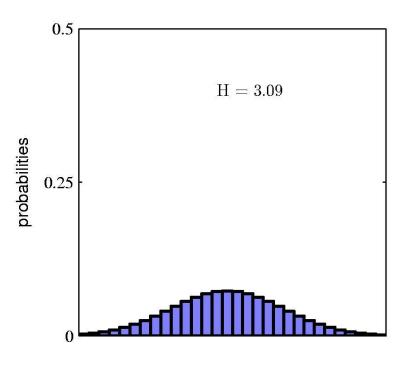
$$W = \frac{N!}{\prod_i n_i!}$$

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

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

Entropy





Differential Entropy

Put bins of width Δ along the real line

$$\lim_{\Delta \to 0} \left\{ -\sum_{i} p(x_i) \Delta \ln p(x_i) \right\} = -\int p(x) \ln p(x) dx$$

Differential entropy maximized (for fixed σ^2) when

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

in which case

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

Conditional Entropy

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

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

The Kullback-Leibler Divergence

$$\begin{aligned} \operatorname{Cross Entropy C}(p||q) & \operatorname{Entropy H}(p) \\ \operatorname{KL}(p||q) & = & -\int p(\mathbf{x}) \ln q(\mathbf{x}) \, \mathrm{d}\mathbf{x} - \left(-\int p(\mathbf{x}) \ln p(\mathbf{x}) \, \mathrm{d}\mathbf{x}\right) \\ & = & -\int p(\mathbf{x}) \ln \left\{\frac{q(\mathbf{x})}{p(\mathbf{x})}\right\} \, \mathrm{d}\mathbf{x} \\ & \operatorname{Cross Entropy} & \operatorname{Negative Entropy} \\ \operatorname{KL}(p||q) & \simeq \frac{1}{N} \sum_{n=1}^{N} \left\{-\ln q(\mathbf{x}_n|\boldsymbol{\theta}) + \ln p(\mathbf{x}_n)\right\} \\ \operatorname{KL}(p||q) & \geqslant 0 & \operatorname{KL}(p||q) \not\equiv \operatorname{KL}(q||p) \end{aligned}$$

KL divergence describes a distance between model p and model q

Cross Entropy for Machine Learning

Goal of Machine Learning: $p(real data) \approx p(model / \theta)$

we assume: $p(training data) \approx p(training data)$

Operation of Machine Learning: $p(training \ data) \approx p(model \ | \ \theta)$

$$\min_{\theta} KL(p(training data) || p(model | \theta))$$

 \Leftrightarrow

 $\min_{\theta} C(p(training data) || p(model | \theta))$

as H(p(training data)) is fixed

Bernoulli model: $p(model / \theta) = \prod_{n} \rho^{t_n} (1 - \rho)^{1 - t_n}$ t_n : training data

Cross entropy: $C = -\sum_{n} t_n \ln \rho + (1 - t_n) \ln (1 - \rho)$ ρ : model parameter

Mutual Information

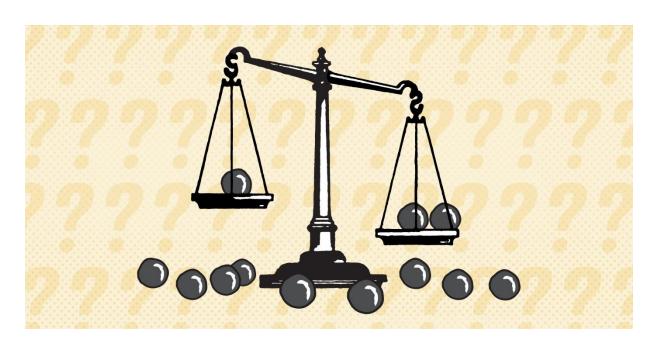
$$I[\mathbf{x}, \mathbf{y}] \equiv KL(p(\mathbf{x}, \mathbf{y}) || p(\mathbf{x}) p(\mathbf{y}))$$

$$= -\iint p(\mathbf{x}, \mathbf{y}) \ln \left(\frac{p(\mathbf{x}) p(\mathbf{y})}{p(\mathbf{x}, \mathbf{y})} \right) d\mathbf{x} d\mathbf{y}$$

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

Mutual information describes the degree of dependence between ${\bf x}$ and ${\bf y}$

Information Gain



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

H[x]: uncertain of balls

H[x|y]:

uncertain of balls after weighing once

X: one ball lighter

y: weighing once

x|**y**: one ball lighter after weighing once

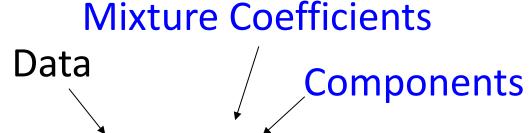
 $H[\mathbf{x}] = \log_2 N$

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

Independent Signal Separation



Independent Component Analysis

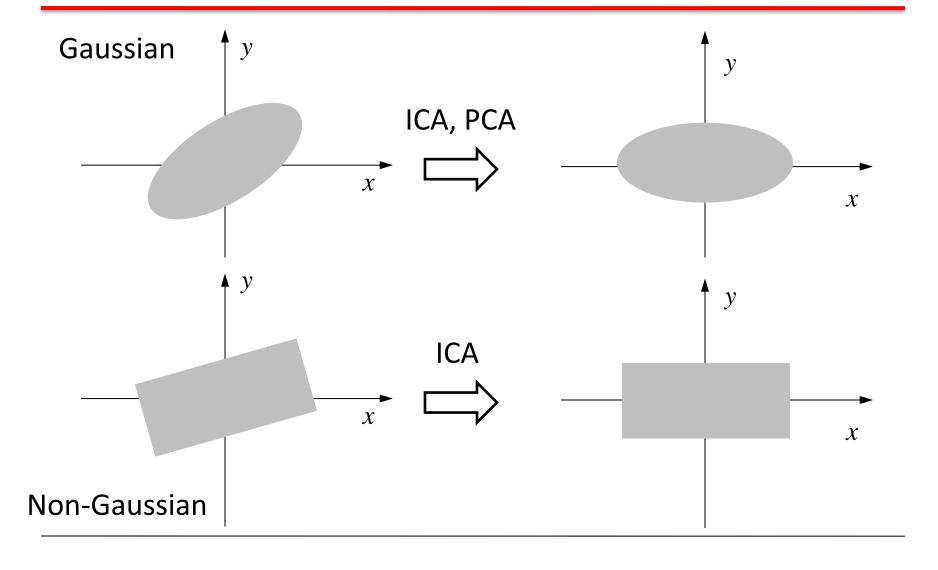


$$Y = AX$$

$$\min_{A} I([X_1, X_2, ..., X_M]|A, Y)$$

After optimization, the components of X become as much independent as possible

Illustration of ICA Operation



Summary

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