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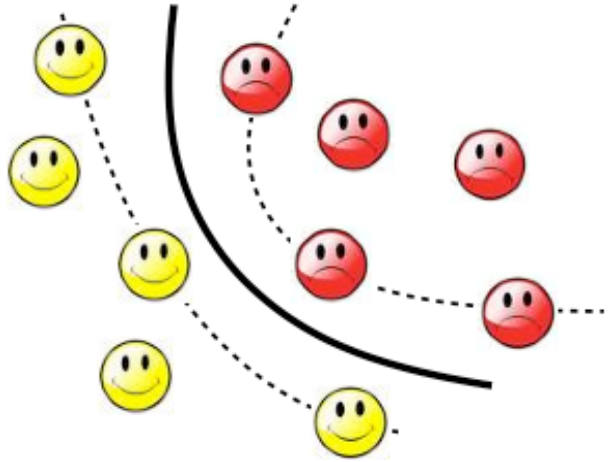

Machine Learning and Data Mining (COMP 5318)

Review

Fabio Ramos

Conditional Probabilities

- One of the most important concepts in all of Data Mining and Machine Learning
- P(A|B) = P(A,B)/P(B) …assuming P(B) not equal 0.
  – Conditional probability of A given B has occurred.
- Probability it will rain tomorrow given it has rained today.
  – P(A|B) = P(AB)/P(B) = 0.1/0.4 = 1/4 = 0.25
  – In general P(A|B) is not equal to P(B|A)

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Bayes' Rule

Posterior

Prior

$$P(A \mid B) = \frac{P(B \mid A)P(A)}{P(B)}$$

$$P(hypothesis \mid Data) = \frac{P(data \mid hypothesis)P(hypothesis)}{P(data)}$$

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Bayes' Rule

- P(A|B) = P(AB)/P(B); P(B|A) = P(BA)|P(A)
- Now P(AB) = P(BA)
- Thus P(A|B)P(B) = P(B|A)P(A)
- Thus P(A|B) = [P(B|A)P(A)]/[P(B)]
  - This is called Bayes Rule
  - Basis of almost all prediction
  - Latest theories hypothesise that human memory and action is Bayes' rule in action.

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Example

The ASX market goes up 60% of the days of a year. 40% of the time it stays the same or goes down. The day the ASX is up, there is a 50% chance that the Shanghai Index is up. On other days there is 30% chance that Shanghai goes up. Suppose The Shanghai market is up. What is the probability that ASX was up.

- Define A1 as "ASX is up"; A2 is "ASX is not up"
  Define S1 as "Shanghai is up"; S2 is "Shanghai is not up"
- We want to calculate P(A1|S1) ?
- P(A1) = 0.6; P(A2) = 0.4;
  P(S1|A1) = 0.5; P(S1|A2) = 0.3
- P(S2|A1) = 1 – P(S1|A1) = 0.5;
  P(S2|A2) = 1 – P(S1|A2) = 0.7;

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Example cont.

- We want to calculate P(A1|S1) ?
- P(A1) = 0.6; P(A2) = 0.4;
  P(S1|A1) = 0.5; P(S1|A2) = 0.3
  P(S2|A1) = 1 – P(S1|A1) = 0.5;
  P(S2|A2) = 1 – P(S1|A2) = 0.7;
- P(A1|S1) = P(S1|A1)P(A1)/(P(S1))
- How do we calculate P(S1) ?

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Example cont.

- P(S1) = P(S1,A1) + P(S1,A2) [Key Step]
  = P(S1|A1)P(A1) + P(S1|A2)P(A2)
  = 0.5 x 0.6 + 0.3 x 0.4
  = 0.42
- Finally,
  P(A1|S1) = P(S1|A1)P(A1)/P(S1)
  = (0.5 x 0.6)/0.42
  = 0.71

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PCA

The central idea of principal component analysis (PCA) is to reduce the dimensionality of a data set consisting of a large number of interrelated variables, while retaining as much as possible of the variation present in the data set. This is achieved by transforming to a new set of variables, the principal components (PCs), which are uncorrelated, and which are ordered so that the first few *retain most of the variation present in* all *of the original variables.*
[Jolliffe, Pricipal Component Analysis, 2nd edition]

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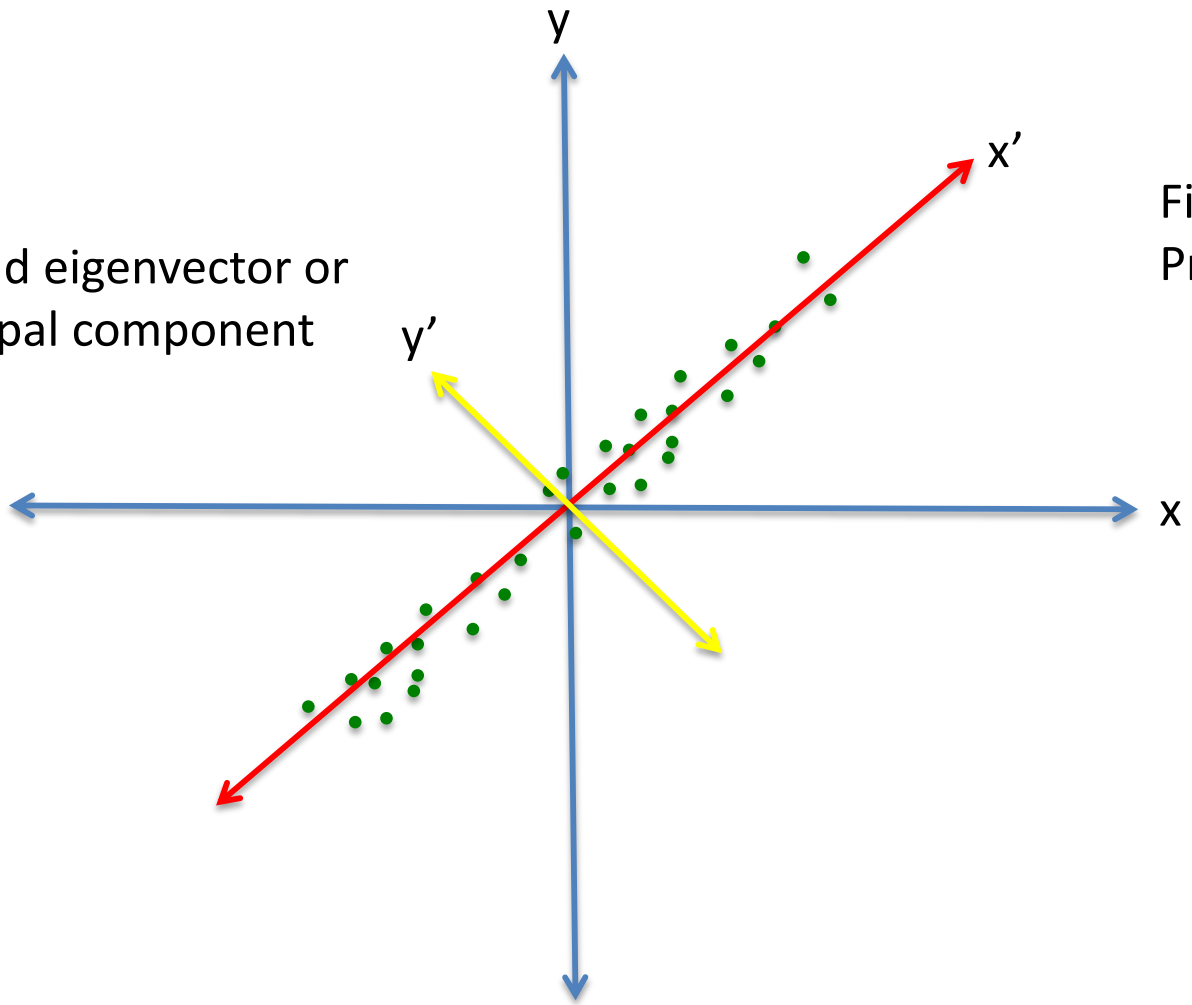
Geometric intuition



Second eigenvector or
Principal component

First eigenvector or
Principal component

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PCA Theorem

Theorem:

Each x_j can be written as: $$\mathbf{x}_j = \bar{\mathbf{x}} + \sum_{i=1}^{i=n} g_{ji}\mathbf{e}_i$$

where e_i are the n eigenvectors of Q with non-zero eigenvalues.

Notes:

1. The eigenvectors e_1 e_2 … e_n span an ***eigenspace***
2. e_1 e_2 … e_n are N x 1 orthonormal vectors (directions in N-Dimensional space)
3. The scalars g_{ji} are the coordinates of x_j in the space.

$$g_{ji} = (\mathbf{x}_j - \bar{\mathbf{x}}).\mathbf{e}_i$$

PCA to compress data

- Expressing x in terms of e_1 … e_n has not changed the size of the data
- However, if the points are highly correlated many of the coordinates of x will be zero or closed to zero.

note: this means they lie in a lower-dimensional linear subspace

PCA to compress data

- Sort the eigenvectors e_i according to their eigenvalue:

$$\lambda_1 \geq \lambda_2 \geq \ldots \lambda_n$$

- Assuming that $\lambda_i \approx 0$ if $i > k$

- Then

$$\mathbf{x}_j \approx \bar{\mathbf{x}} + \sum_{i=1}^{i=k} g_{ji}\mathbf{e}_i$$

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Loss functions

- Squared error, 0-1 loss

$$
\begin{aligned}
L(y, \hat{y}) &= (y - \hat{y})^2 \\
L(y, \hat{y}) &= I(y \neq \hat{y})
\end{aligned}
$$

- Minimize risk (expected loss, empirical loss)

$$
\begin{aligned}
R(\hat{f}) &= E_{\mathbf{x},y} L(f(\mathbf{x}), \hat{f}(\mathbf{x})) \\
\hat{R}(\hat{f}) &= \frac{1}{n} \sum_{i=1}^{n} L(y_i, \hat{f}(\mathbf{x}_i))
\end{aligned}
$$

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

Naïve Bayes Classifier

Generative model:

$$p(\mathbf{x}, \mathcal{C}_k) = p(\mathcal{C}_k)p(\mathbf{x}_n|\mathcal{C}_k) = \pi\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \Sigma_k)$$

class posterior

class conditional density

class prior

$$p(\mathcal{C}_k|\mathbf{x}) = \frac{p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)}{\sum_{\mathcal{C}_j} p(\mathbf{x}|\mathcal{C}_j)p(\mathcal{C}_j)}$$

normalising constant

Example of Naïve Bayes Classifier

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Name	Give Birth	Can Fly	Live in Water	Have Legs	Class
human	yes	no	no	yes	mammals
python	no	no	no	no	non-mammals
salmon	no	no	yes	no	non-mammals
whale	yes	no	yes	no	mammals
frog	no	no	sometimes	yes	non-mammals
komodo	no	no	no	yes	non-mammals
bat	yes	yes	no	yes	mammals
pigeon	no	yes	no	yes	non-mammals
cat	yes	no	no	yes	mammals
leopard shark	yes	no	yes	no	non-mammals
turtle	no	no	sometimes	yes	non-mammals
penguin	no	no	sometimes	yes	non-mammals
porcupine	yes	no	no	yes	mammals
eel	no	no	yes	no	non-mammals
salamander	no	no	sometimes	yes	non-mammals
gila monster	no	no	no	yes	non-mammals
platypus	no	no	no	yes	mammals
owl	no	yes	no	yes	non-mammals
dolphin	yes	no	yes	no	mammals
eagle	no	yes	no	yes	non-mammals

A: attributes

M: mammals

N: non-mammals

$$P(A \mid M) = \frac{6}{7} \times \frac{6}{7} \times \frac{2}{7} \times \frac{2}{7} = 0.06$$

$$P(A \mid N) = \frac{1}{13} \times \frac{10}{13} \times \frac{3}{13} \times \frac{4}{13} = 0.0042$$

$$P(A \mid M)P(M) = 0.06 \times \frac{7}{20} = 0.021$$

$$P(A \mid N)P(N) = 0.004 \times \frac{13}{20} = 0.0027$$

Give Birth	Can Fly	Live in Water	Have Legs	Class
yes	no	yes	no	?

P(A|M)P(M) > P(A|N)P(N)

=> Mammals

Logistic Regression

- Assumes a parametric form for directly estimating P($Y \mid X$). For binary concepts, this is:

$$P(Y=1 \mid X) = \frac{1}{1+\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

$$P(Y=0 \mid X) = 1 - P(Y=1 \mid X)$$

$$= \frac{\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}{1+\exp(w_0 + \sum_{i=1}^{n} w_i X_i)}$$

- Equivalent to a one-layer backpropagation neural net.
- Logistic regression is the source of the sigmoid function used in backpropagation.
- Objective function for training is somewhat different.

Logistic Regression Training

- Weights are set during training to maximise the **conditional data likelihood** :

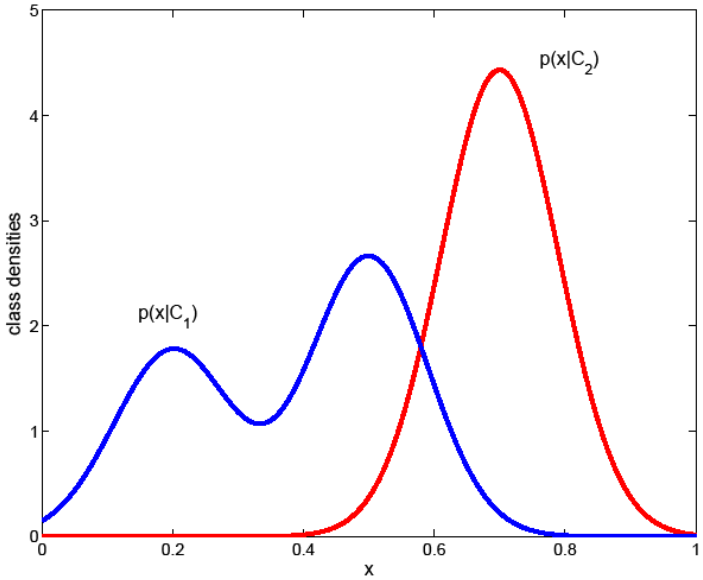
$$W \leftarrow \underset{W}{\operatorname{argmax}} \prod_{d \in D} P(Y^d \mid X^d, W)$$

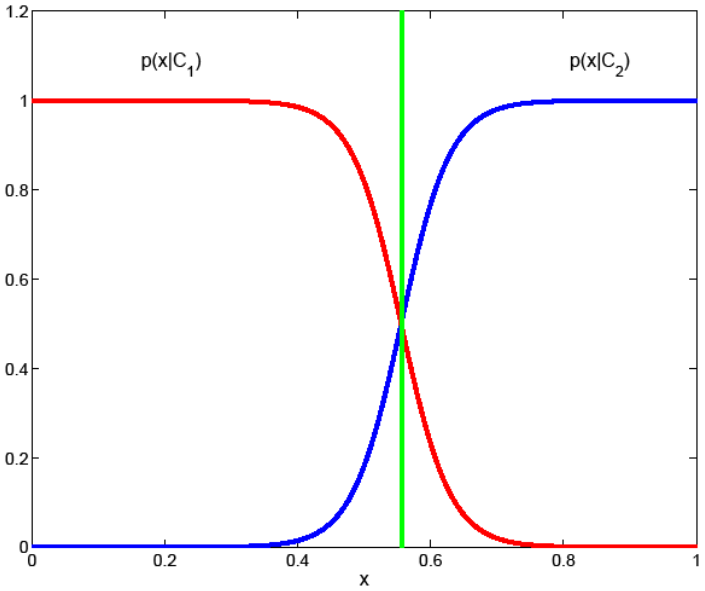
where D is the set of training examples and Y^d and X^d denote, respectively, the values of Y and X for example d.

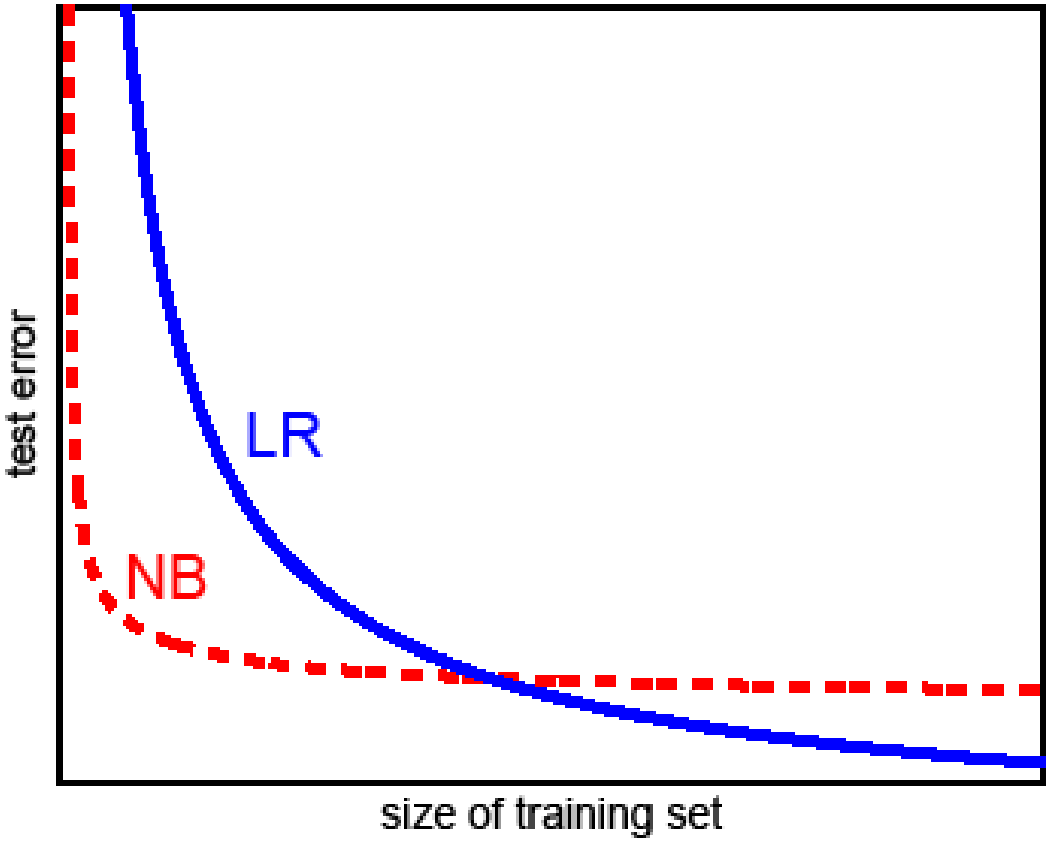
- Equivalently viewed as maximising the **conditional log likelihood** (CLL)

$$W \leftarrow \underset{W}{\operatorname{argmax}} \sum_{d \in D} \ln P(Y^d \mid X^d, W)$$

Logistic Regression vs NB







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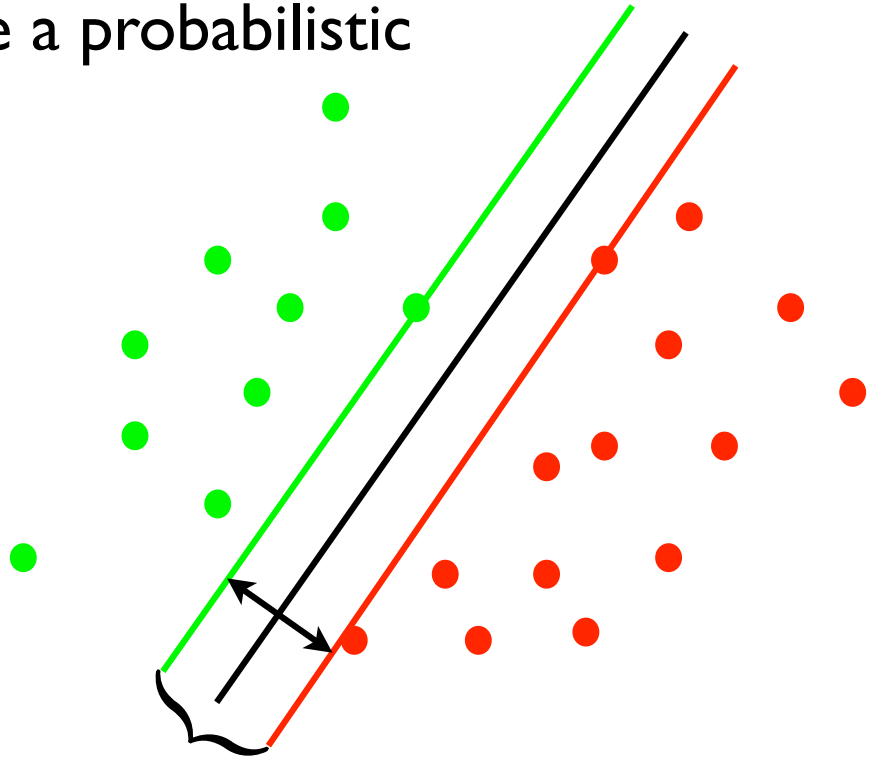
Maximum margin

Things to note

- The boundary is defined by only a few points (support vectors)
- Difficult to define a probabilistic explanation



Maximum margin classifiers (1)

Given a training set

Inputs $\mathbf{x}_1, \ldots, \mathbf{x}_N$

Targets

$t_1, \ldots, t_N$ where $t_n \in \{-1, 1\}$

Linear classifier

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}} \boldsymbol{\phi}(\mathbf{x}) + b$$

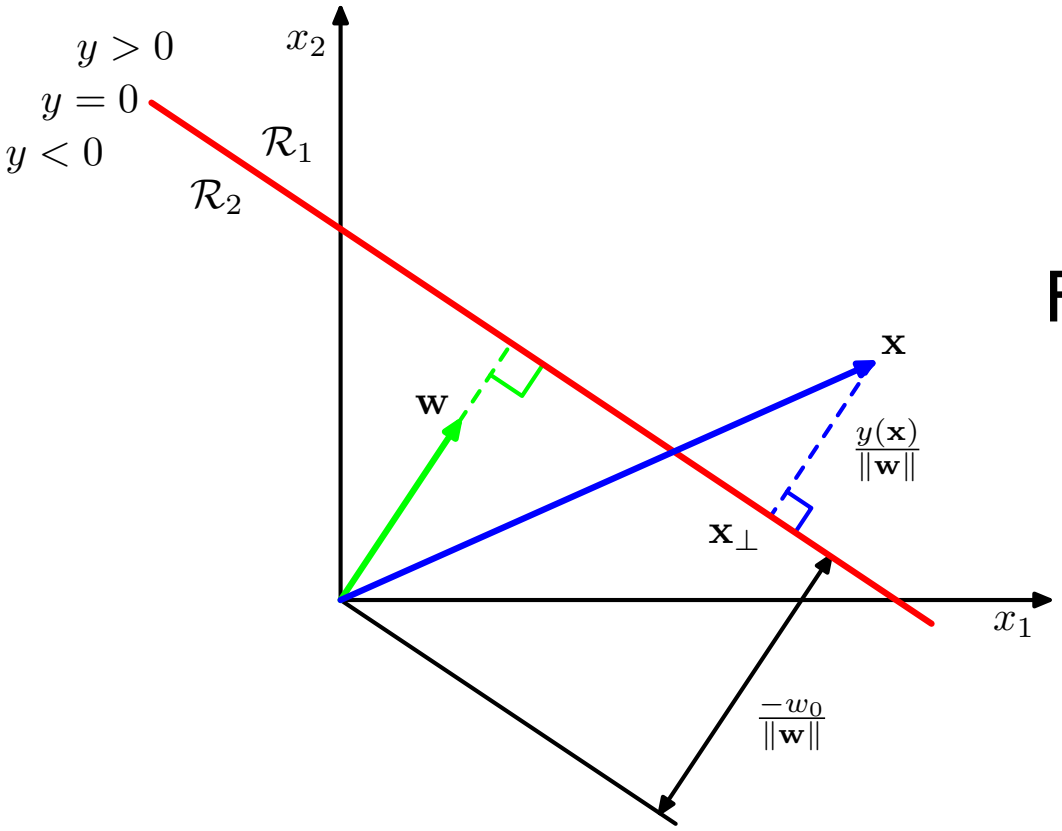
Basis function

Output sign of $y(\mathbf{x})$

so that $t_n y(\mathbf{x}_n) > 0$

for all points in the training set

Maximum margin classifiers(2)



Assuming $\phi(\mathbf{x}) = \mathbf{x}$

$$y(\mathbf{x}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + w_0$$

For points in the boundary

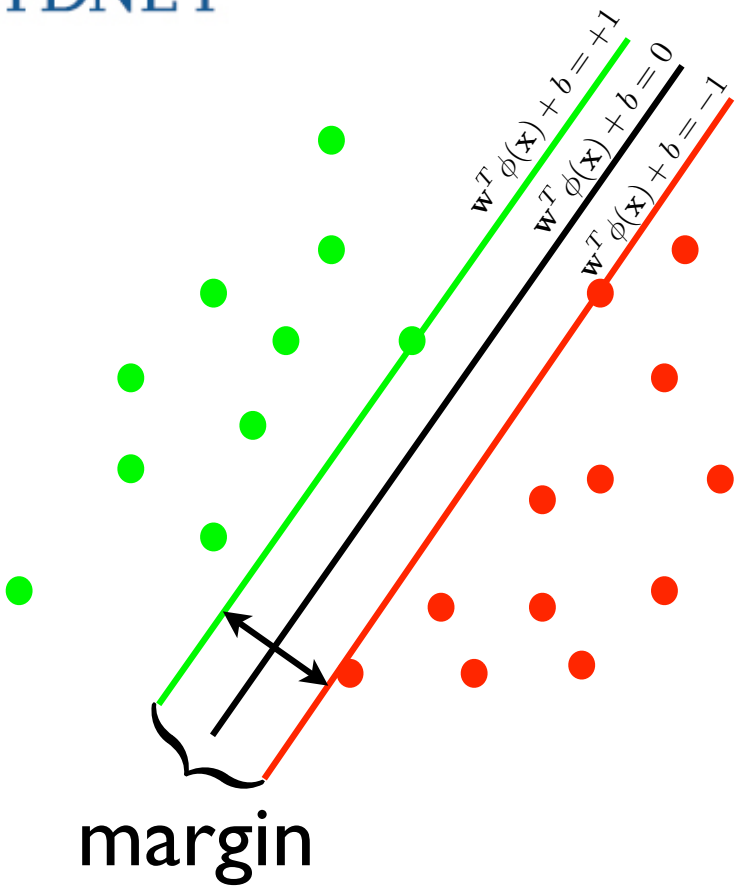
$$y(\mathbf{x}) = 0 \quad \text{and}$$

$$\frac{\mathbf{w}^{\mathrm{T}}\mathbf{x}}{\|\mathbf{w}\|} = -\frac{w_0}{\|\mathbf{w}\|}$$

For arbitrary $\mathbf{x}$

$$\mathbf{x} = \mathbf{x}_\perp + r\frac{\mathbf{w}}{\|\mathbf{w}\|} \quad \text{and} \quad r = \frac{y(\mathbf{x})}{\|\mathbf{w}\|}$$

Support Vector Machines



Quadratic programming

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

s.t.

$$t_n\left(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)+b\right)\geqslant 1, \quad n=1,\ldots,N$$

- Solve efficiently by quadratic programming (QP)
- Hyperplane defined by support vectors

The Dual SVM formulation

Quadratic programming

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2$$

s.t.

$$t_n\left(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)+b\right) \geqslant 1, \quad n = 1, \ldots, N$$

Lagrangian function

$$L(\mathbf{w}, b, \mathbf{a}) = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{n=1}^{N} a_n \left\{t_n(\mathbf{w}^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}_n)+b) - 1\right\}$$

setting the derivatives w.r.t. $\mathbf{w}$ and b equal to zero:

$$\begin{aligned} \mathbf{w} &= \sum_{n=1}^{N} a_n t_n \boldsymbol{\phi}(\mathbf{x}_n) \\ 0 &= \sum_{n=1}^{N} a_n t_n. \end{aligned}$$

$$\widetilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

Kernel trick

$$k(\mathbf{x}, \mathbf{x}') = \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{x}')$$

s.t.

$$\begin{aligned} a_n &\geqslant 0, \qquad n = 1, \ldots, N, \\ \sum_{n=1}^{N} a_n t_n &= 0. \end{aligned}$$

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Kernel SVMs

- Solve the QP problem

$$\widetilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2}\sum_{n=1}^{N}\sum_{m=1}^{N} a_n a_m t_n t_m k(\mathbf{x}_n, \mathbf{x}_m)$$

with respect to $\mathbf{a}$ subject to the constraints

$$\begin{aligned} a_n &\geqslant 0, \qquad n = 1, \ldots, N, \\ \sum_{n=1}^{N} a_n t_n &= 0. \end{aligned}$$

- Support vectors satisfy

$$t_n \left(\sum_{m \in \mathcal{S}} a_m t_m k(\mathbf{x}_n, \mathbf{x}_m) + b \right) = 1$$

- For query points compute

$$y(\mathbf{x}) = \sum_{n=1}^{N} a_n t_n k(\mathbf{x}, \mathbf{x}_n) + b.$$

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Think about kernels not features

Polynomial kernel

$$
\begin{aligned}
k(\mathbf{x}, \mathbf{z}) &= \left(1 + \mathbf{x}^{\mathrm{T}}\mathbf{z}\right)^2 = (1 + x_1 z_1 + x_2 z_2)^2 \\
&= 1 + 2x_1 z_1 + 2x_2 z_2 + x_1^2 z_1^2 + 2x_1 z_1 x_2 z_2 + x_2^2 z_2^2 \\
&= (1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, \sqrt{2}x_1 x_2, x_2^2)(1, \sqrt{2}z_1, \sqrt{2}z_2, z_1^2, \sqrt{2}z_1 z_2, z_2^2)^{\mathrm{T}} \\
&= \boldsymbol{\phi}(\mathbf{x})^{\mathrm{T}}\boldsymbol{\phi}(\mathbf{z}).
\end{aligned}
$$

Gaussian kernel

$$k(\mathbf{x}, \mathbf{z}) = \exp(-\gamma\|\mathbf{x} - \mathbf{z}\|^2)$$

Infinite dimensional feature space!

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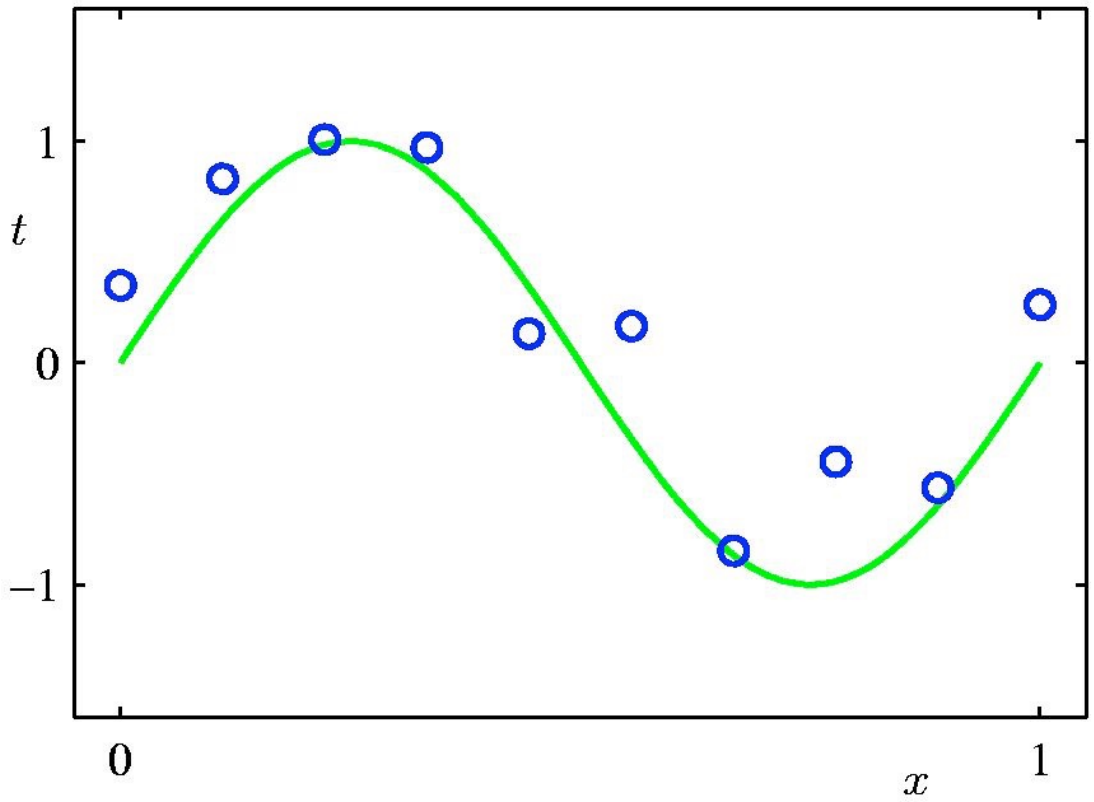
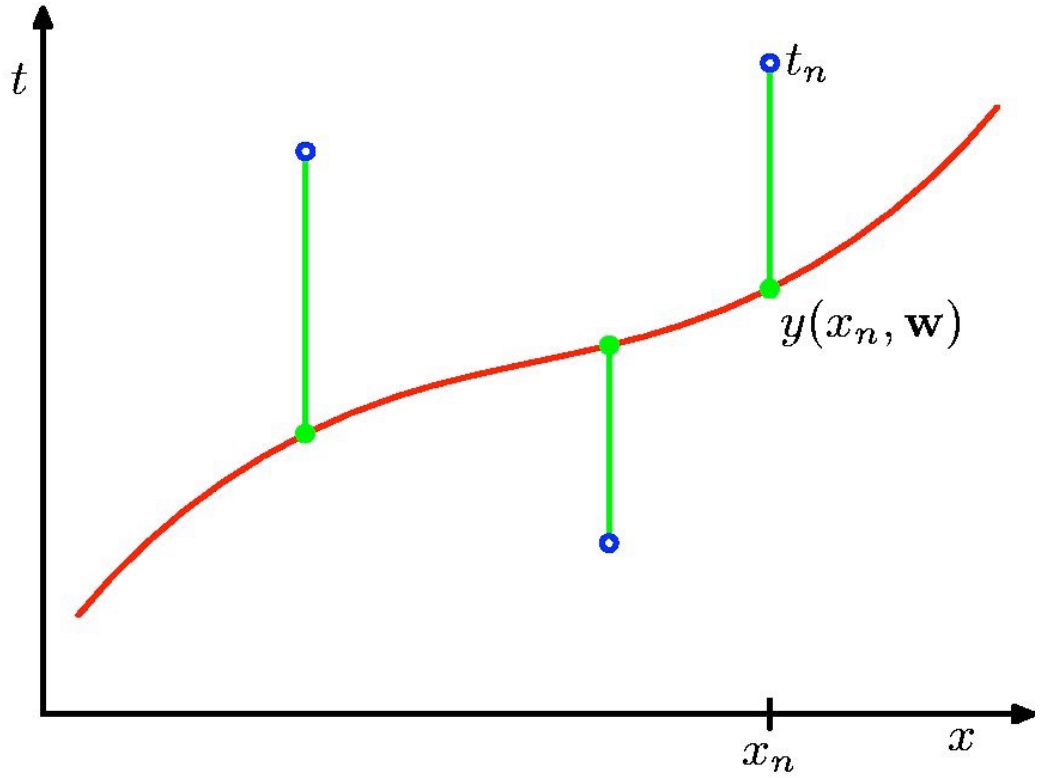
Polynomial Curve Fitting



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

Sum-of-Squares Error Function



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

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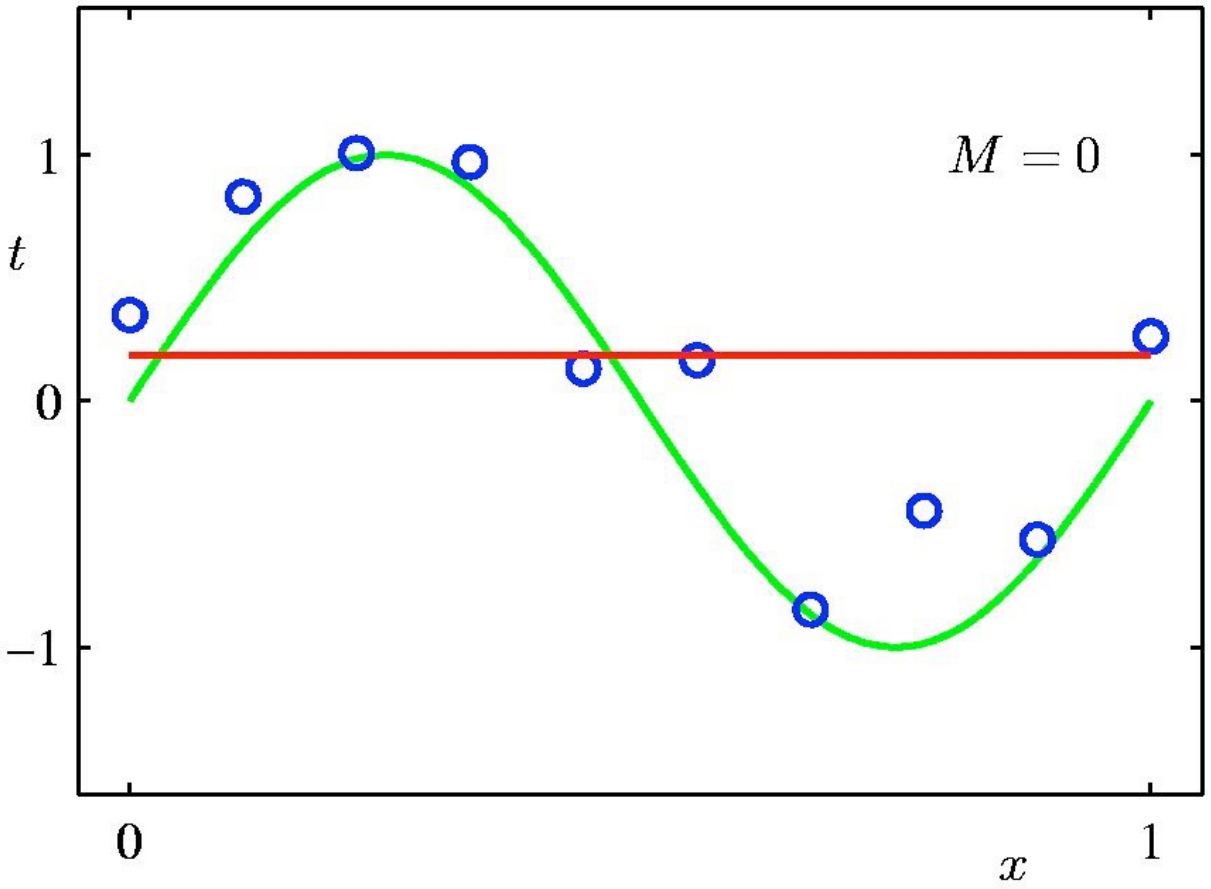
0th Order Polynomial



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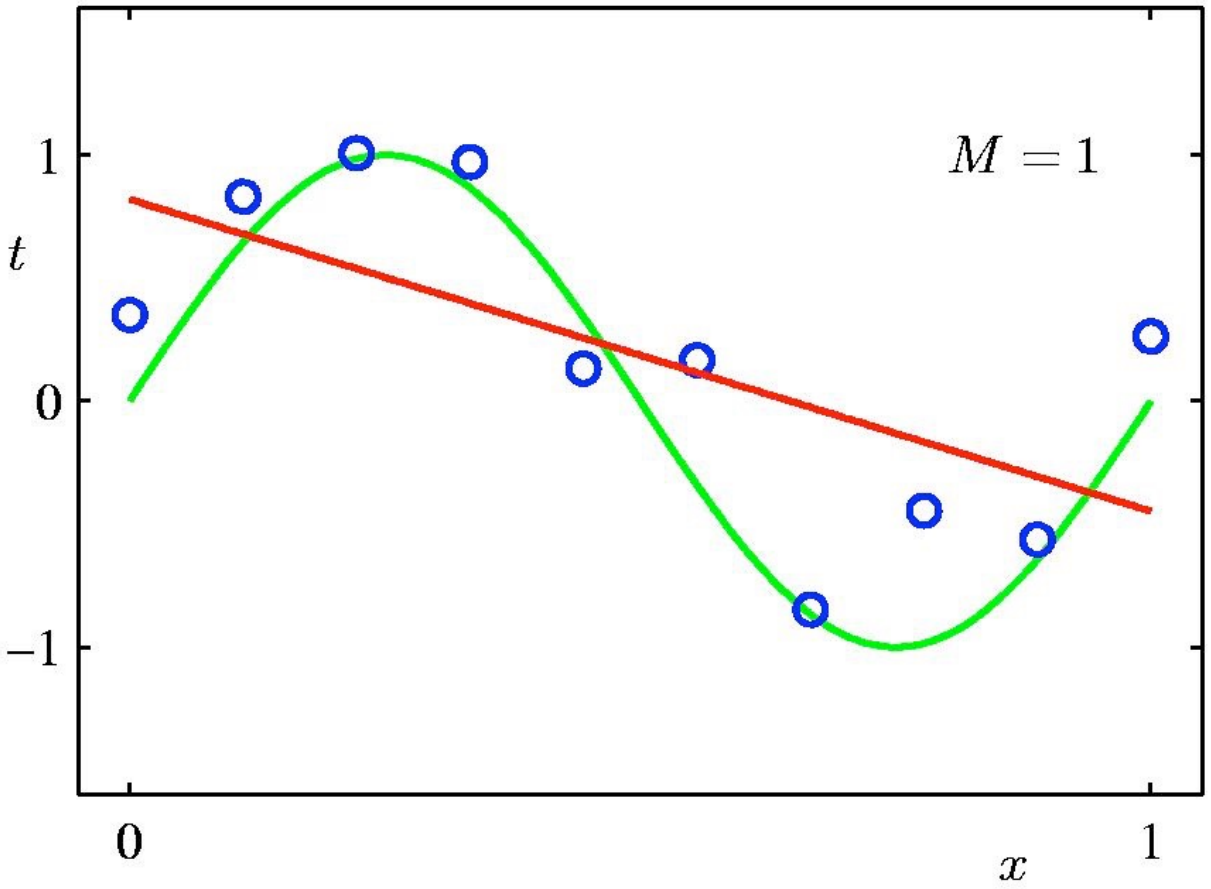
1st Order Polynomial



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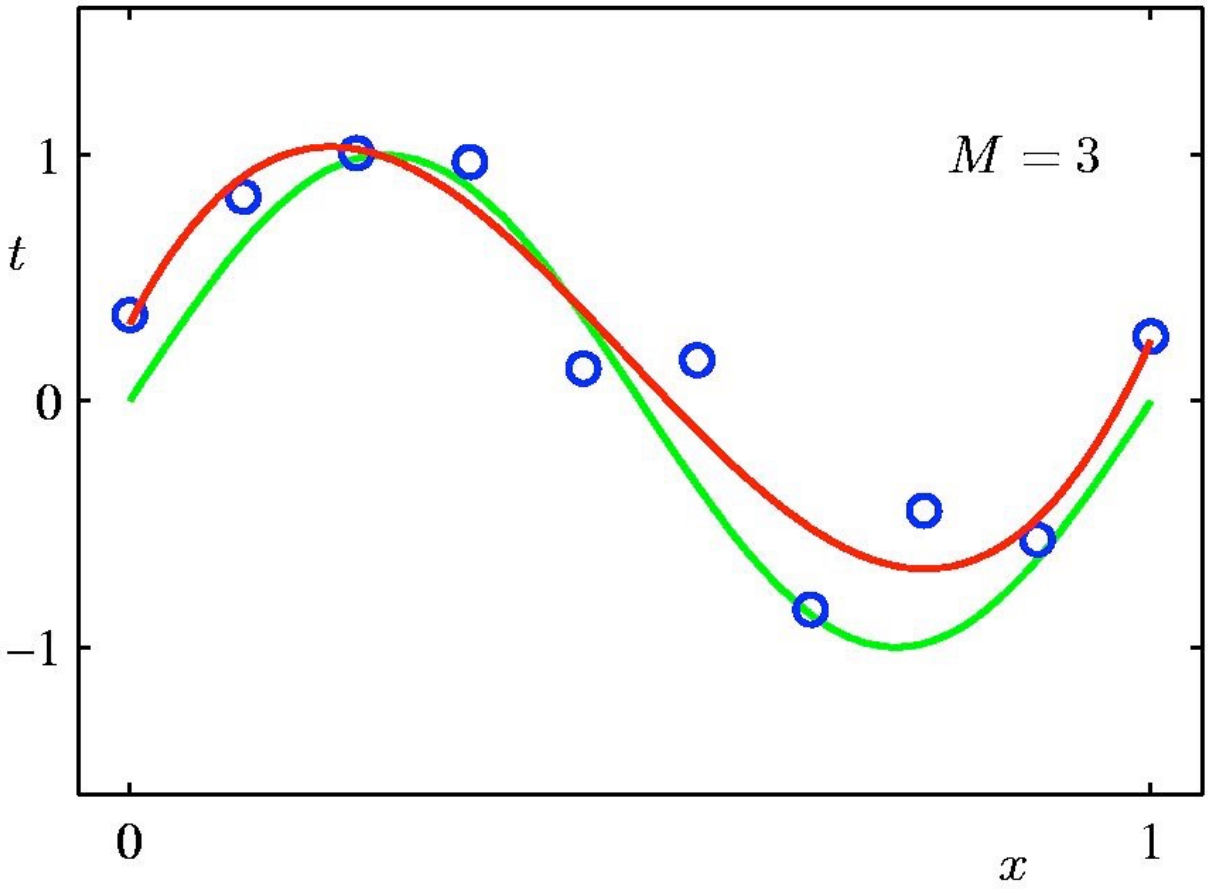
3rd Order Polynomial



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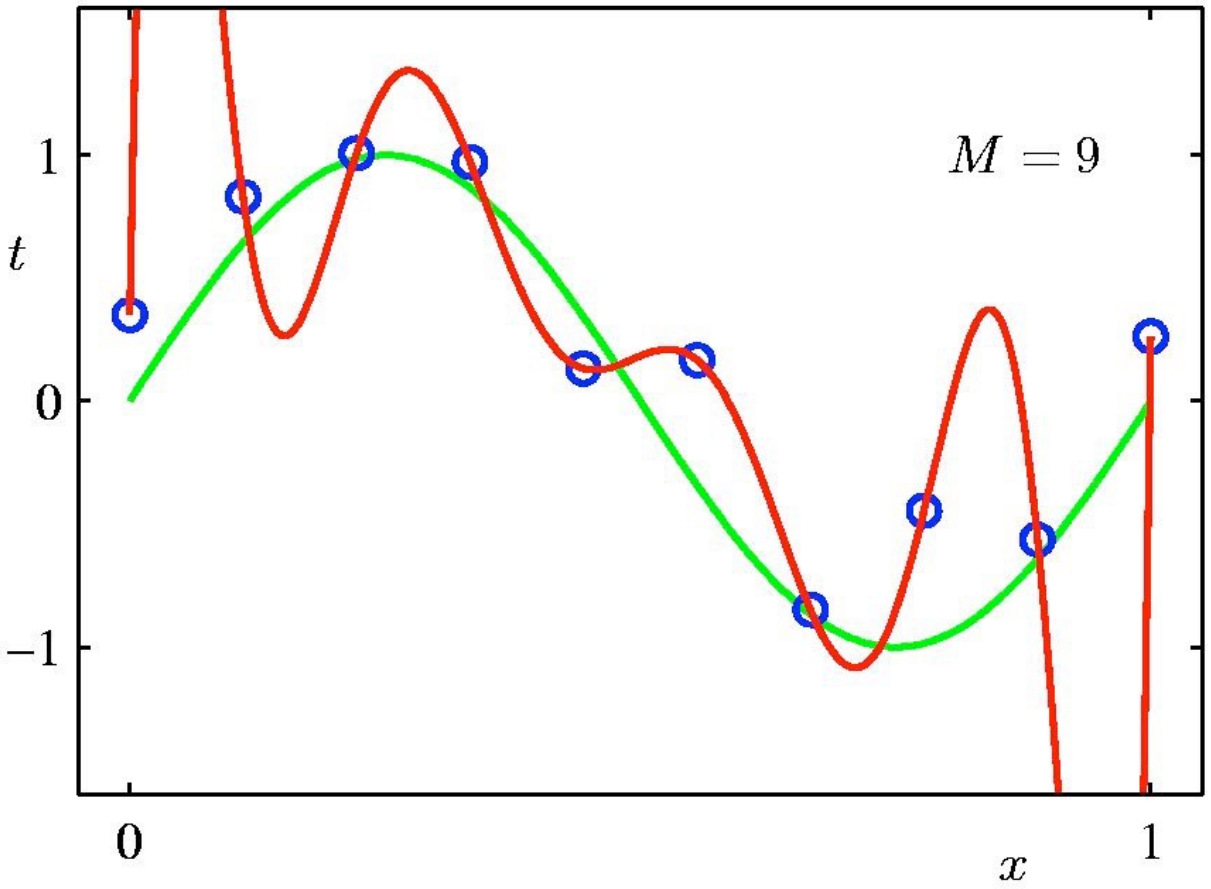
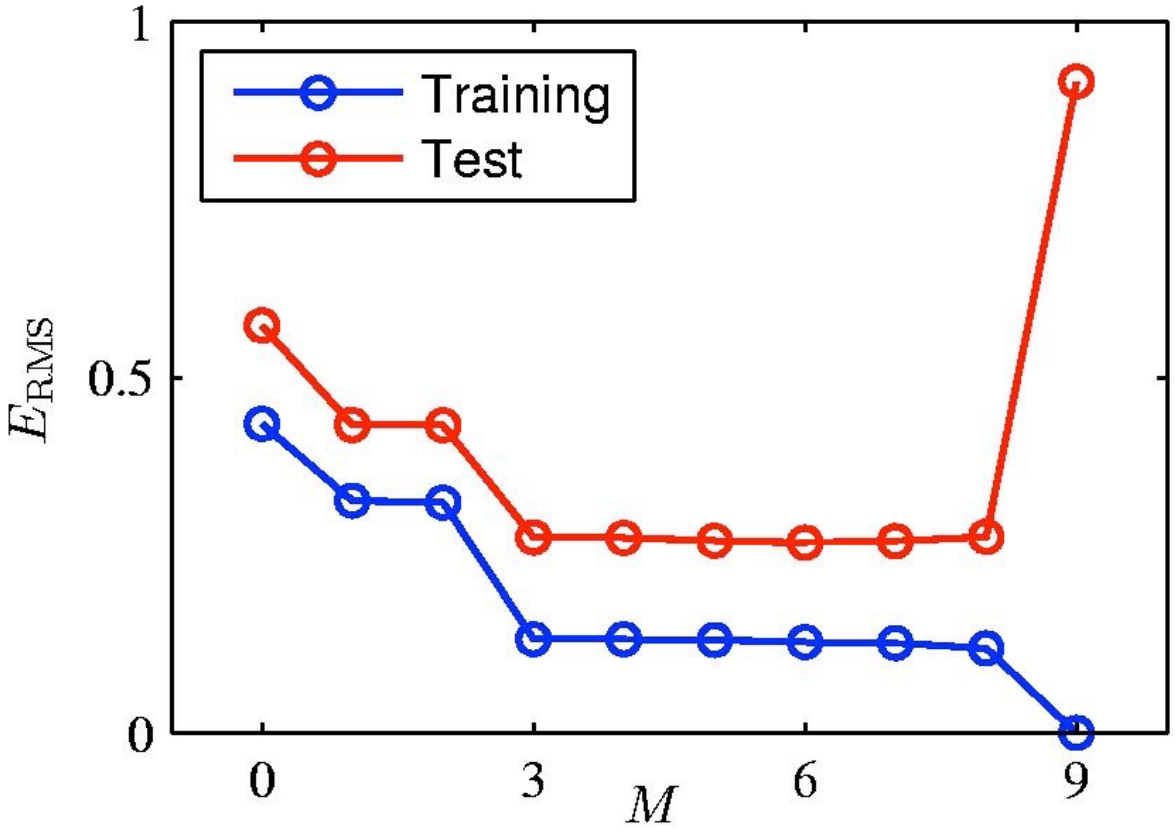
9th Order Polynomial



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

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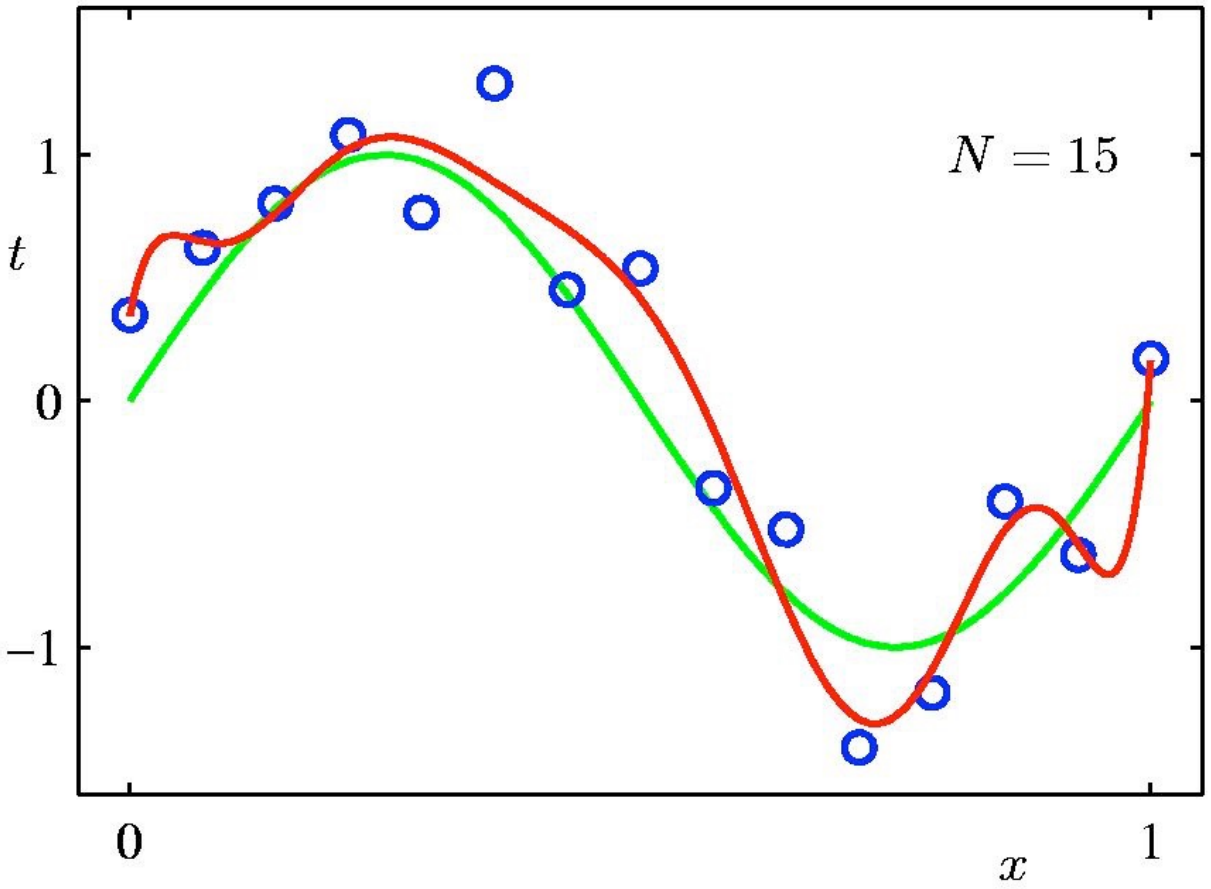
Data Set Size: $N = 15$

9th Order Polynomial



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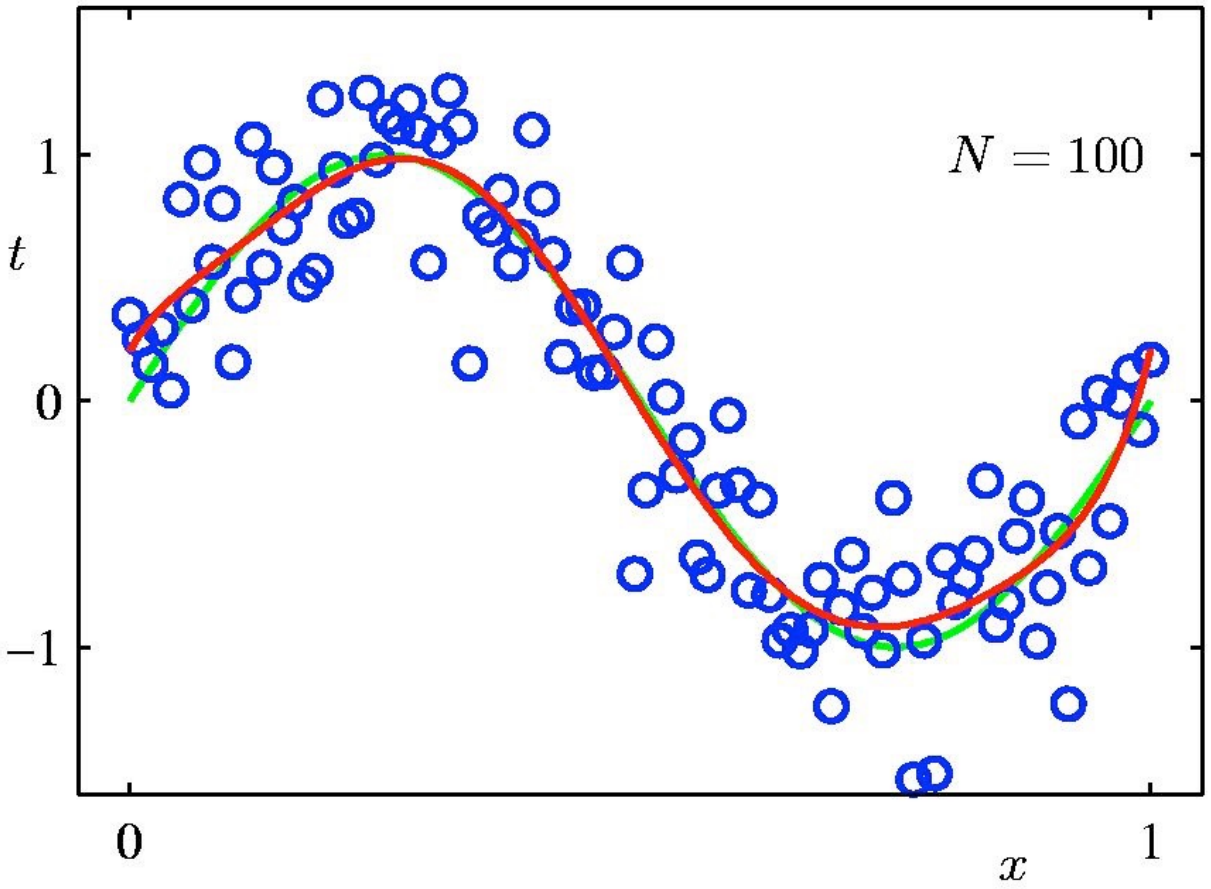
Data Set Size: $N = 100$

9th Order Polynomial



Regularisation

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

Penalise large coefficient values

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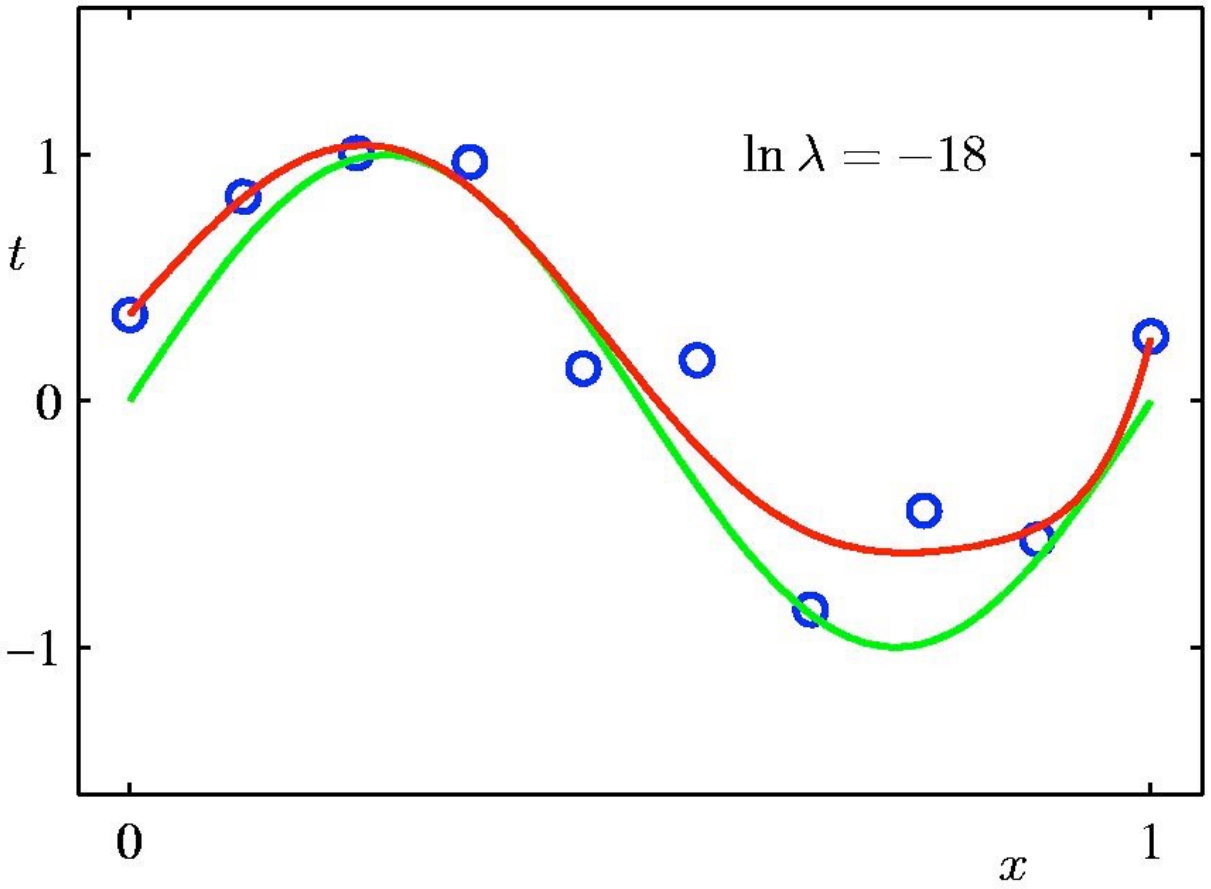
Regularisation: $\ln \lambda = -18$



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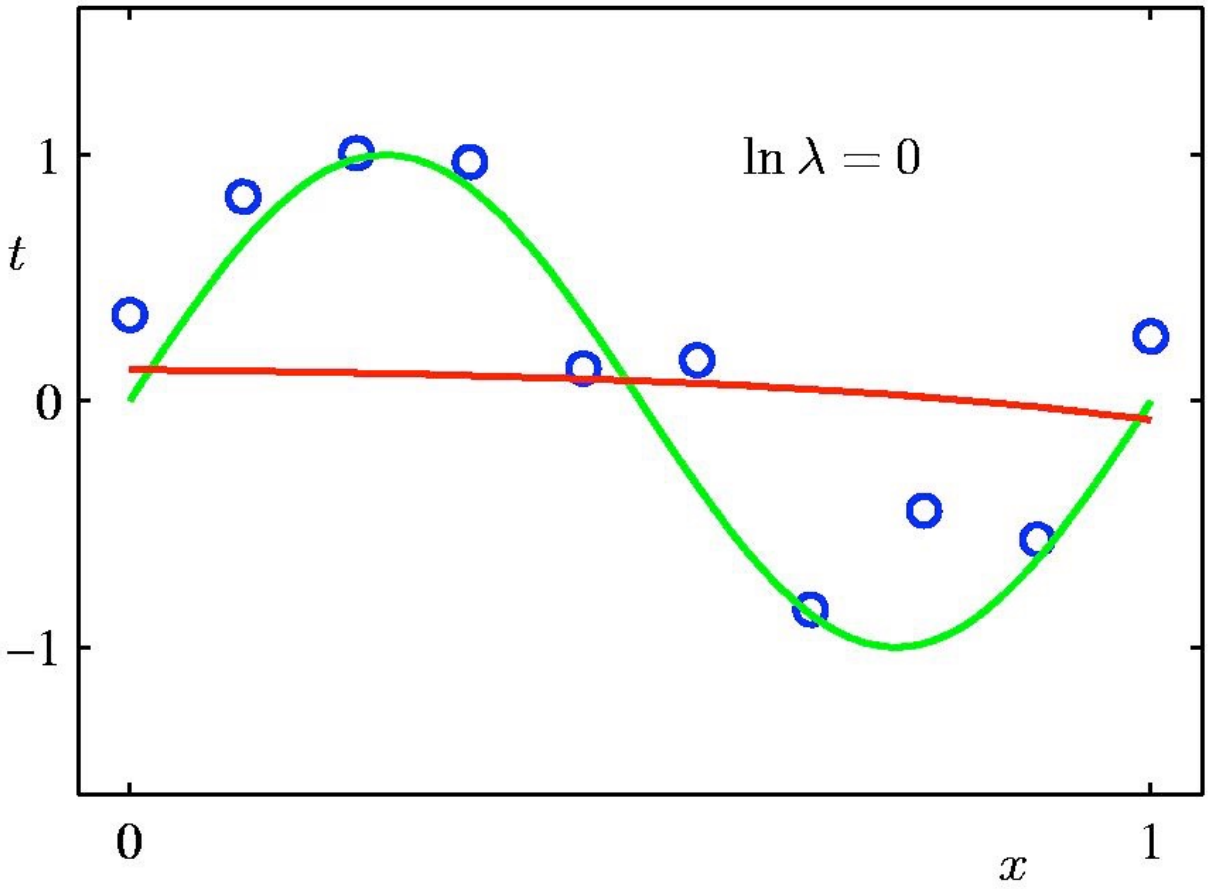
Regularisation: $\ln \lambda = 0$



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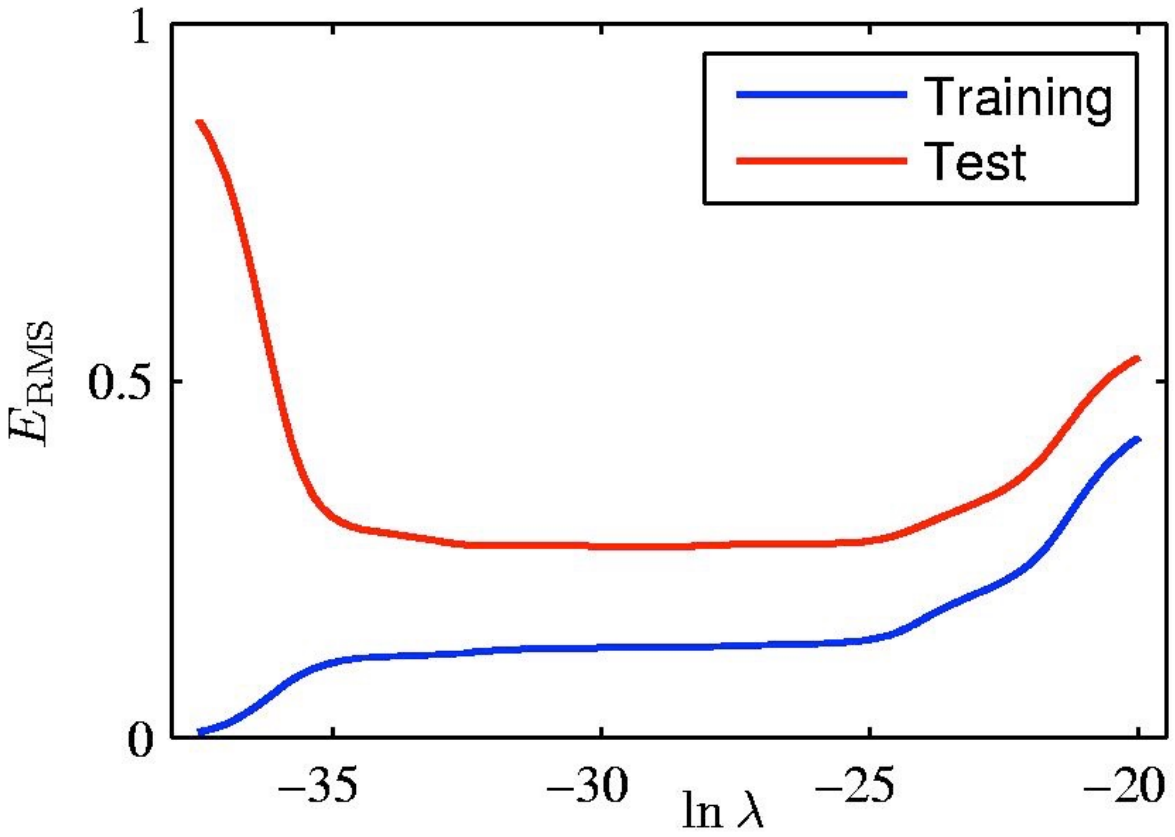
Regularisation: E_{RMS} vs. $\ln \lambda$



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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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 minimising sum-of-squares error, $E(\mathbf{w})$.

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

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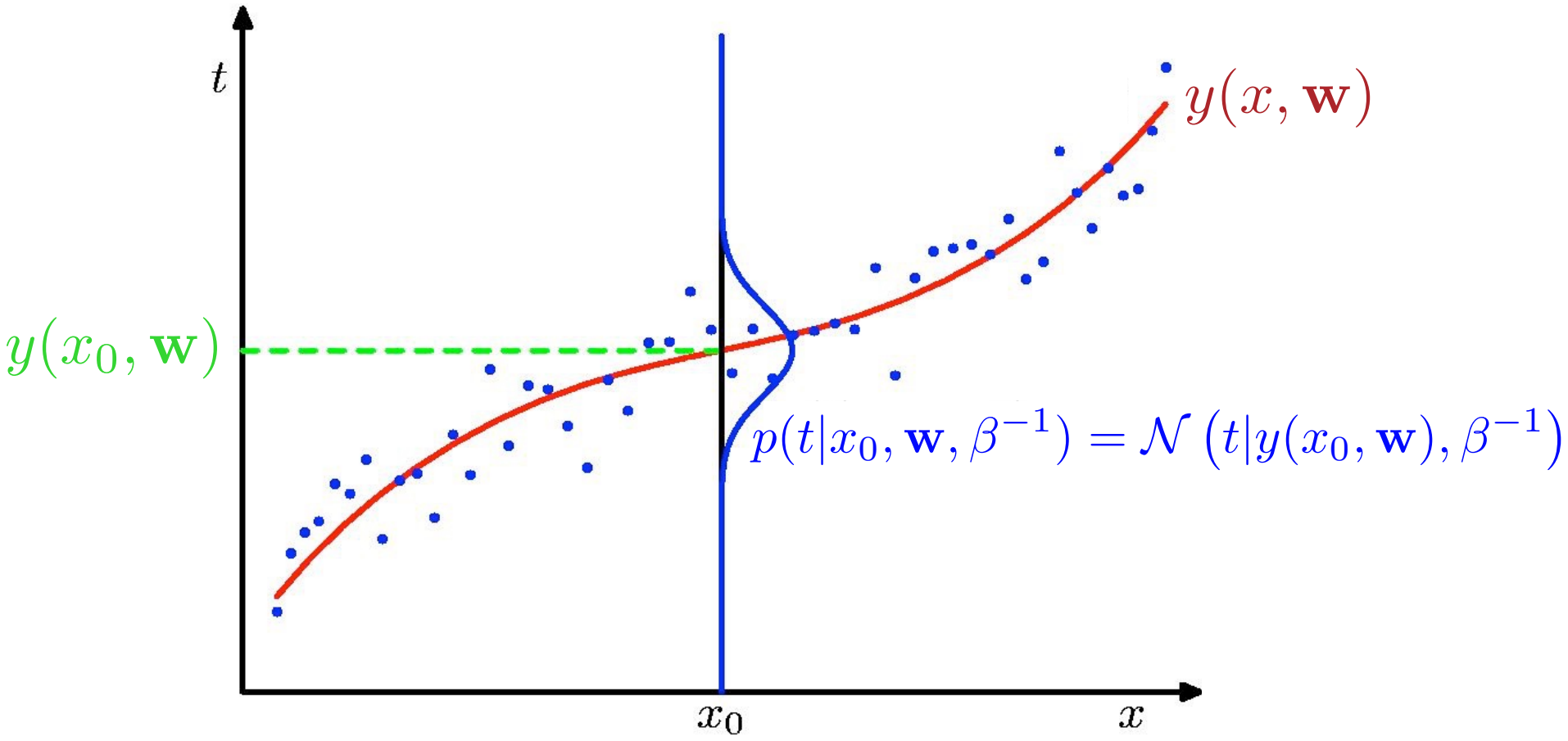
Curve Fitting Re-visited



Bayesian Linear Regression

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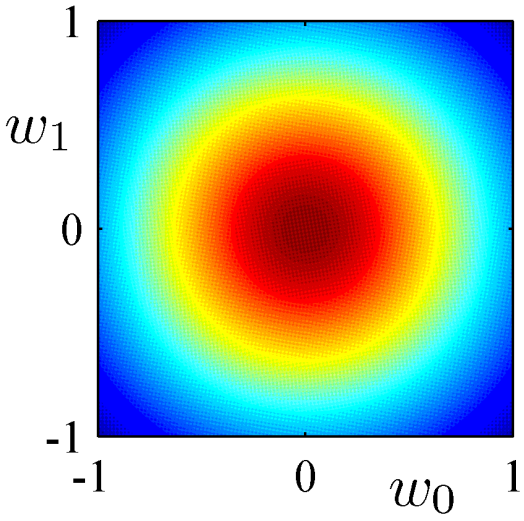
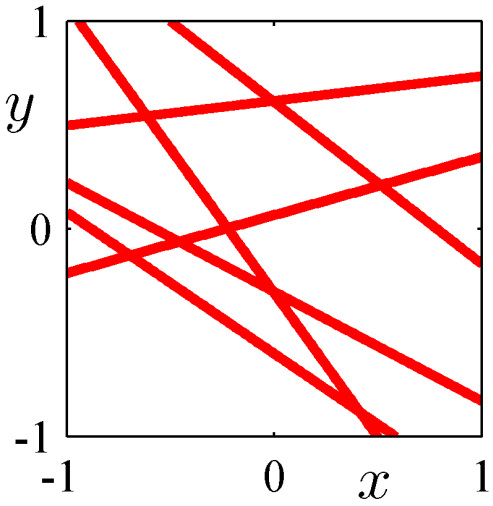
Example:

0 Points Observed

Prior



Data Space



Bayesian Linear Regression

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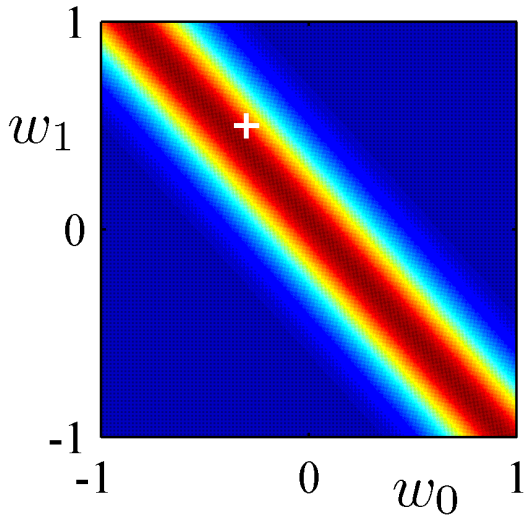
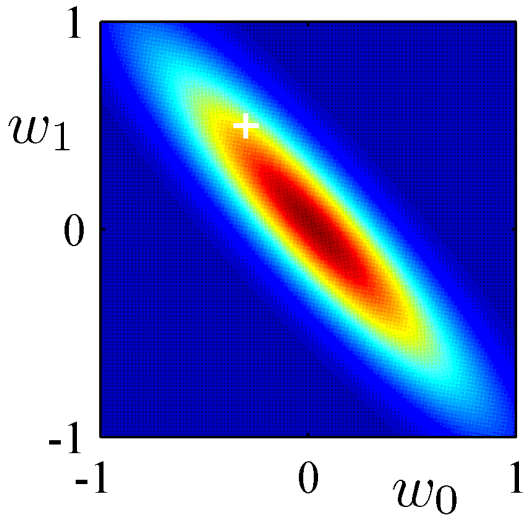
Example:

1 Point Observed

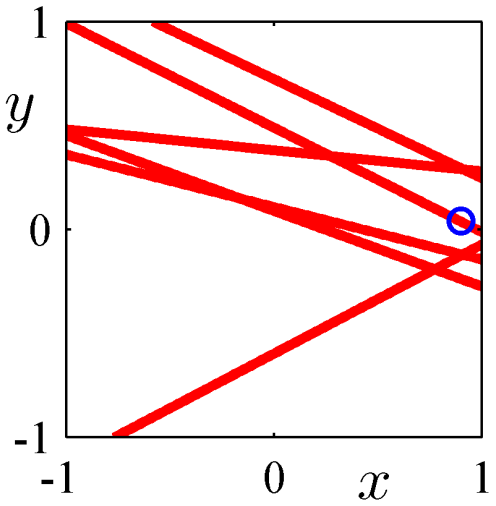
Likelihood



Posterior



Data Space



Bayesian Linear Regression

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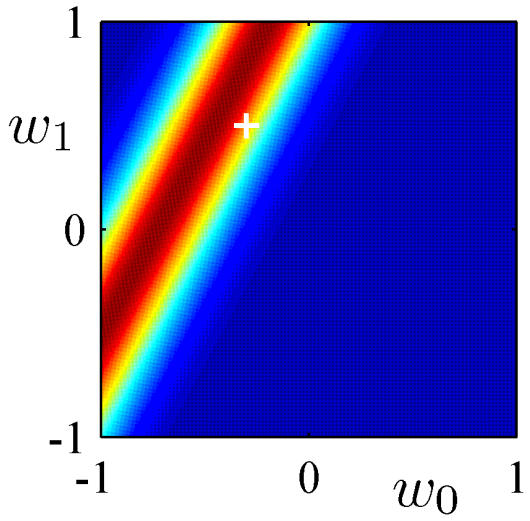
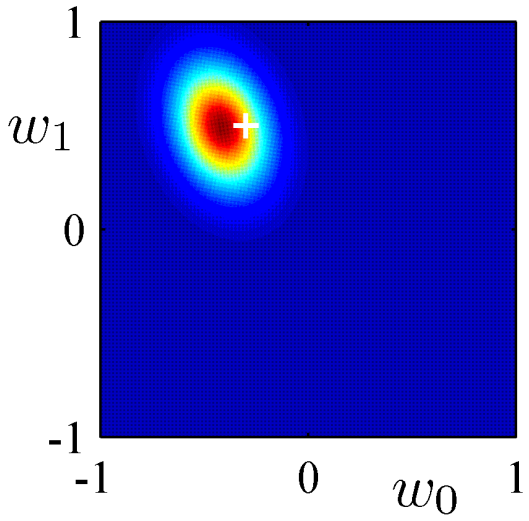
Example:

2 Points Observed

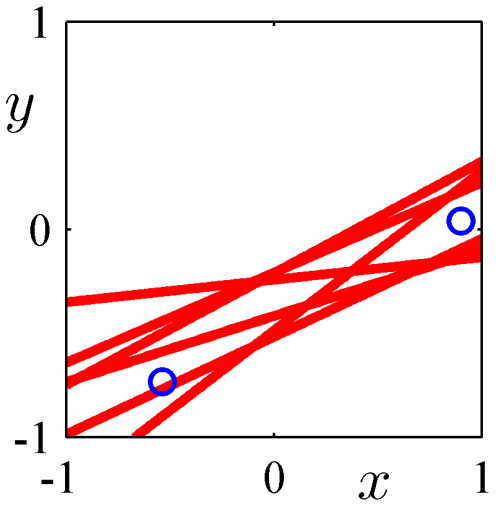
Likelihood



Posterior



Data Space



Bayesian Linear Regression

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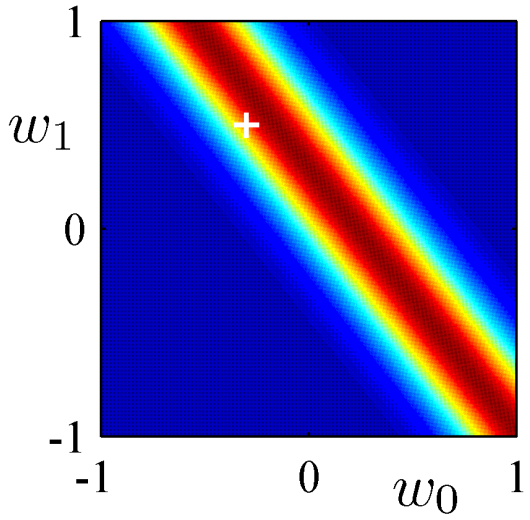
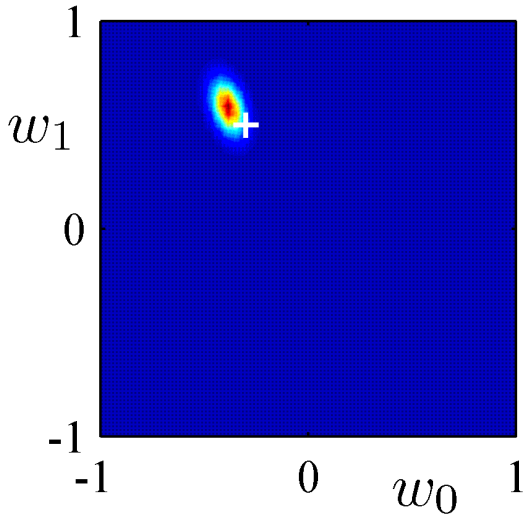
Example:

20 Points Observed

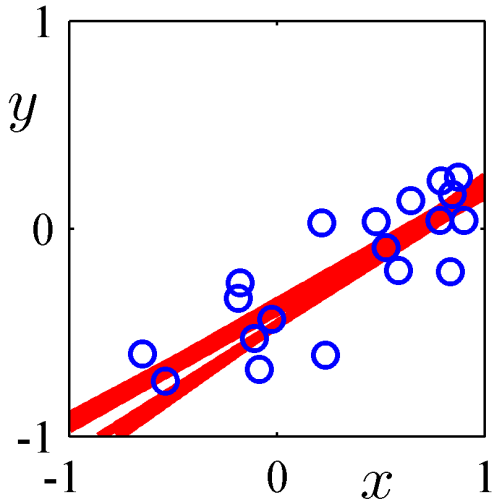
Likelihood



Posterior



Data Space



Clustering

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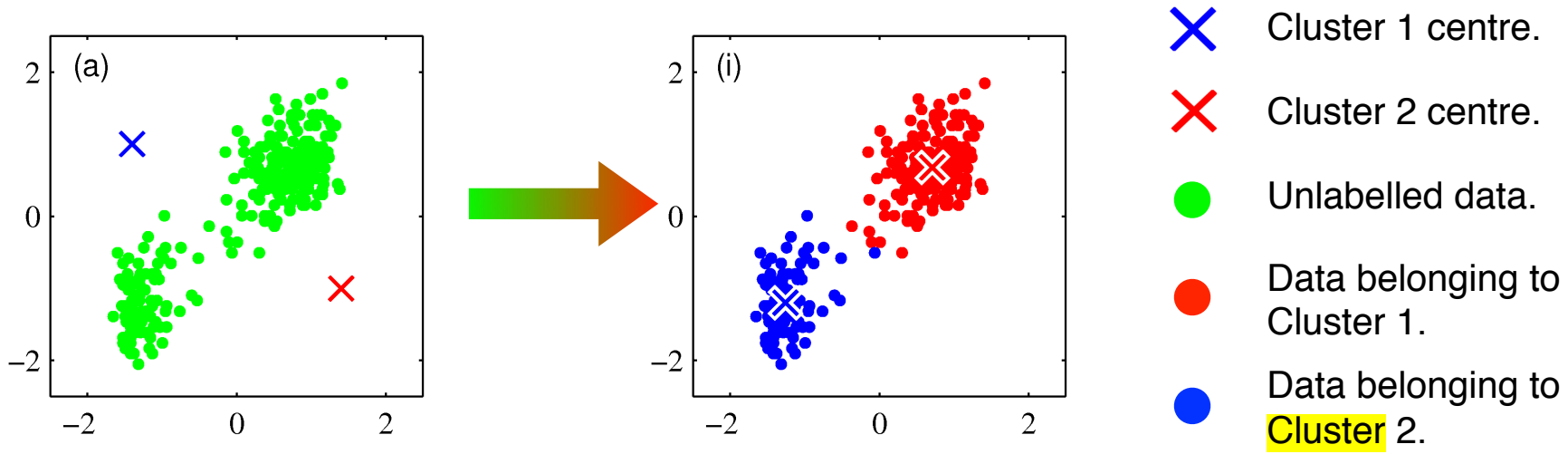
Process of grouping similar objects together.



Learn a set of clusters and assign data to a specific cluster.

Deterministic: Hard assignment to each cluster (K-means).

Probabilistic: Model assignment as a discrete latent variable. (Mixtures of Gaussians, Dirichlet Process)

K-Means

Objective function:

$$J = \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

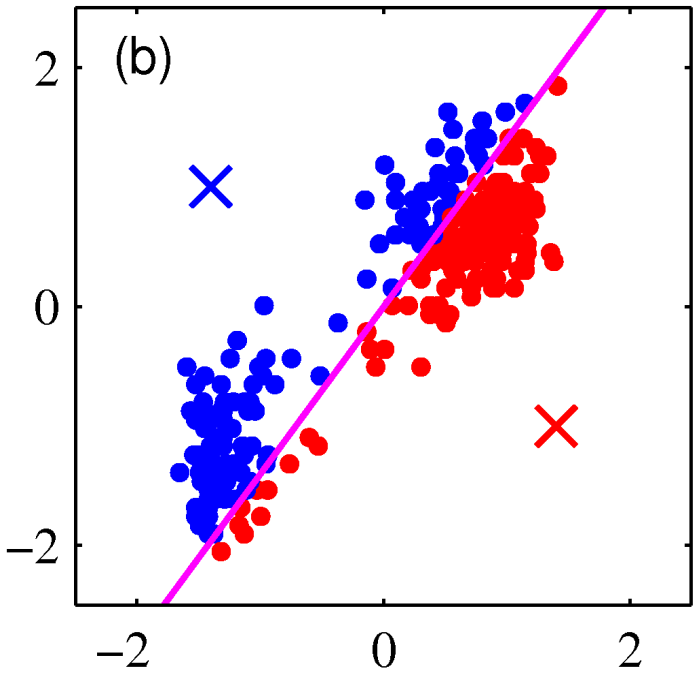
Represents the sum of the squares of the distances of each datapoint to its assigned prototype vector.

Goal: Find $\{r_{nk}\}$ and $\{\boldsymbol{\mu}_k\}$ that minimise J.

$$\{r_{nk}, \boldsymbol{\mu}_k\}^\star = \underset{\{r_{nk}, \boldsymbol{\mu}_k\}}{\operatorname{argmin}} \sum_{n=1}^{N} \sum_{k=1}^{K} r_{nk} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$$

K-Means Example

Number of clusters: $K = 2$

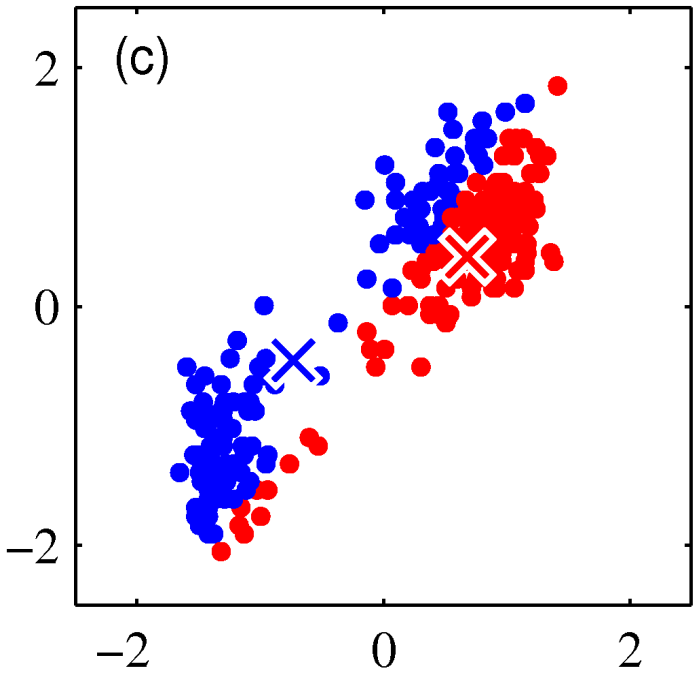


1 Data Preprocessing
2 Initialise $\{\boldsymbol{\mu}_k\}$
3 Repeat until convergence or Max Iterations
4 Minimise J w.r.t. $\{r_{nk}\}$ keeping $\{\boldsymbol{\mu}_k\}$ fixed.
5 Minimise J w.r.t. $\{\boldsymbol{\mu}_k\}$ keeping $\{r_{nk}\}$ fixed.

Each data point is assigned to the closest cluster centre.

K-Means Example

Number of clusters: $K = 2$



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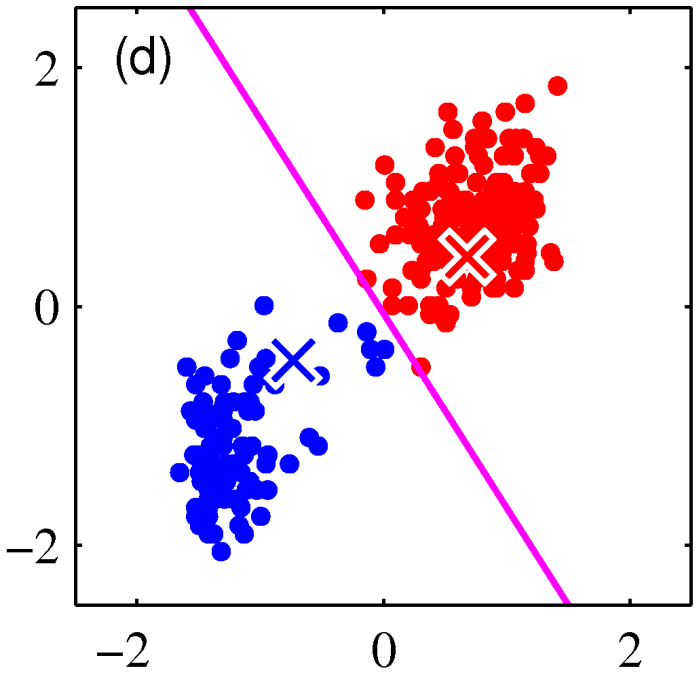
Re-compute each cluster centre to be the mean of the points previously assigned.

K-Means Example

Number of clusters: $K = 2$



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K-Means Example

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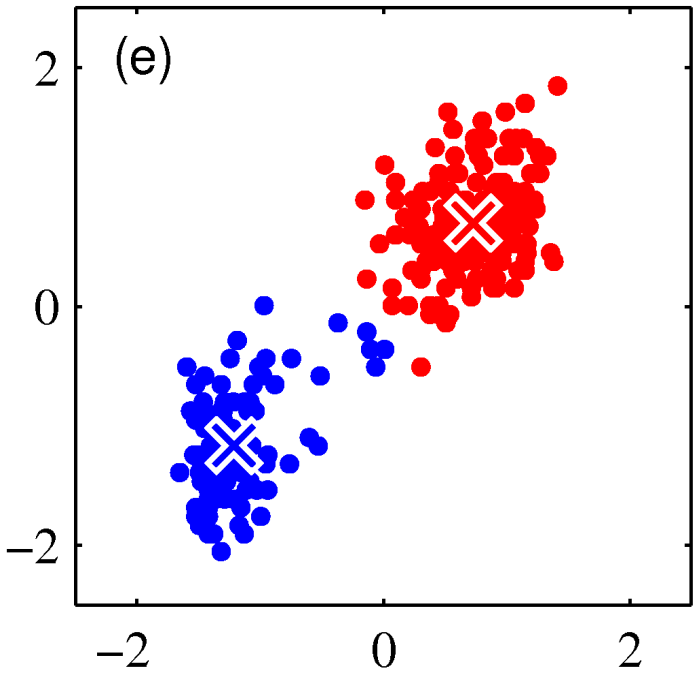
Number of clusters: $K = 2$



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Re-compute each cluster centre to be the mean of the points previously assigned.

K-Means Example

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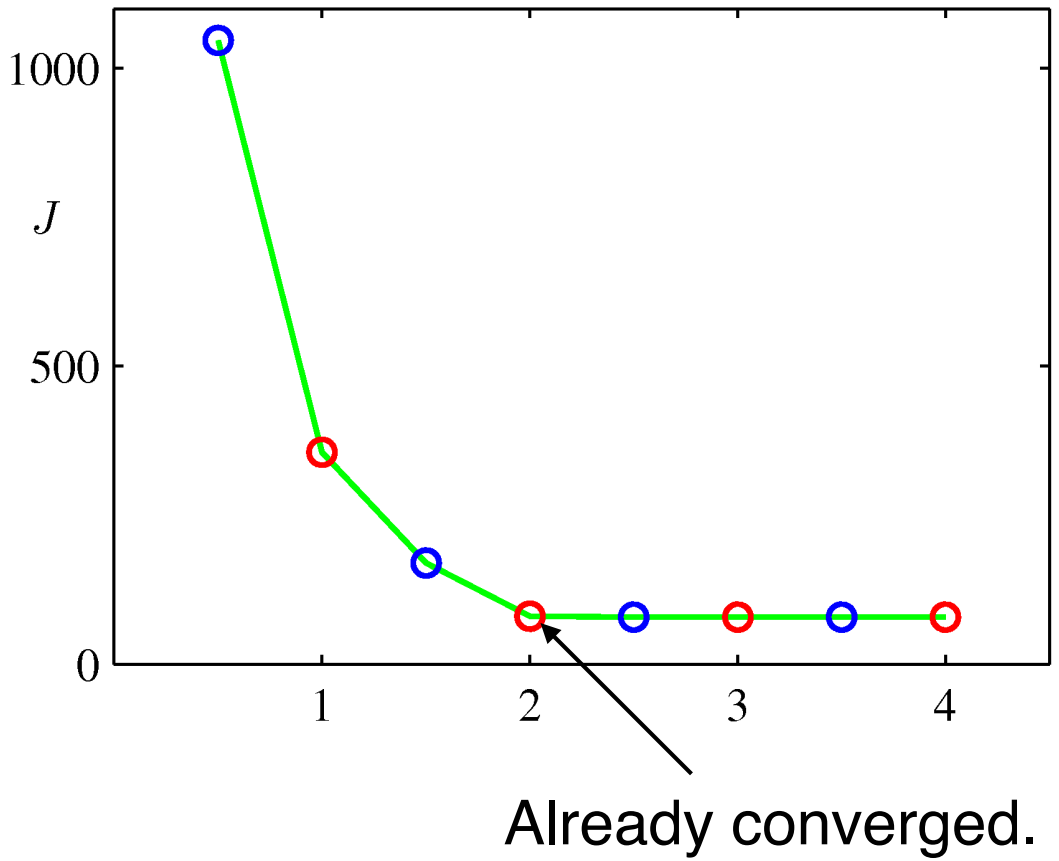
Plot of the cost function for each iteration.



EM for Gaussian Mixtures

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Likelihood function:

$$\ln\, p(\mathbf{X}|\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k) \right\}$$

Conditions to be satisfied at maximum likelihood:

$$0 = \frac{\partial \ln\, p(\mathbf{X}|\boldsymbol{\pi},\boldsymbol{\mu},\boldsymbol{\Sigma})}{\partial \boldsymbol{\mu}_k}$$

$$0 = -\sum_{n=1}^{N} \underbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j,\boldsymbol{\Sigma}_j)}}_{\gamma(z_{nk})} \boldsymbol{\Sigma}_k(\mathbf{x}_n - \boldsymbol{\mu}_k)$$

$$\boldsymbol{\mu}_k = \frac{1}{N_k}\sum_{n=1}^{N} \gamma(z_{nk})\mathbf{x}_n \qquad N_k = \sum_{n=1}^{N} \gamma(z_{nk})$$

N_k is the effective number of points assigned to cluster k.

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Exam: what to expect?

- Numerical questions, e.g., what is probability of X … given … Y
- Theoretical on the main concepts, e.g., why should I regularise logistic regression
- Maths will be simple; no need to memorise equations
- Pros vs Cons for different methods
- In Dim Red, what does each method preserve in low D?
- Check the exercises in Bishop, Ullman, and Murphy's books
- Check the questions here: https://www.analyticsvidhya.com/blog/2016/09/40-interview-questions-asked-at-startups-in-machine-learning-data-science/
- For deep learning, see these: https://www.analyticsvidhya.com/blog/2017/01/must-know-questions-deep-learning/