C19 Machine Learning

8 Lectures
2 Tutorial Sheets

Hilary Term 2015
A. Zisserman

Overview:

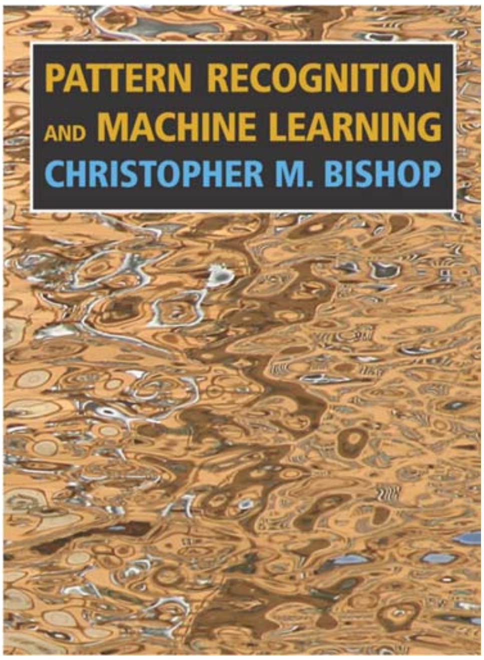
- Supervised classification
  - perceptron, support vector machine, loss functions, kernels, random forests, neural networks and deep learning
- Supervised regression
  - ridge regression, lasso regression, SVM regression
- Unsupervised learning (Frank Wood)
  - graphical models, sequential Monte Carlo, PCA, Gaussian Mixture Models, probabilistic PCA, hidden Markov models

Recommended book

- **Pattern Recognition and Machine Learning**

Christopher Bishop, Springer, 2006.

  - Excellent on classification and regression



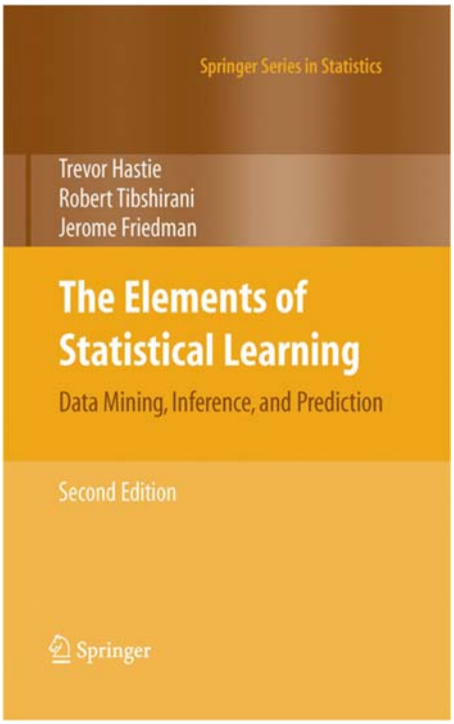
Textbooks 2

- **Elements of Statistical Learning**

Hastie, Tibshirani, Friedman,

Springer, 2009, second edition

- Good explanation of algorithms
- pdf available online


Springer Series in Statistics
Trevor Hastie
Robert Tibshirani
Jerome Friedman
The Elements of Statistical Learning
Data Mining, Inference, and Prediction
Second Edition
Springer

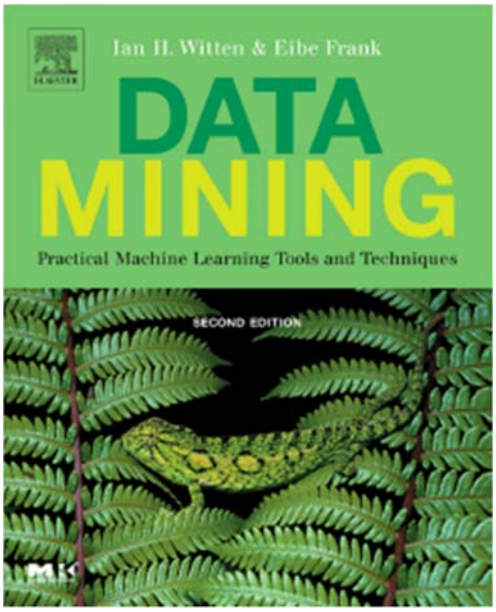
One more book for background reading …

- Data Mining: Practical Machine Learning Tools and Techniques (Second Edition)

Ian Witten & Eibe Frank,

Morgan Kaufmann, 2005.

- Very readable and practical guide


Ian H. Witten & Eibe Frank
DATA MINING
Practical Machine Learning Tools and Techniques
SECOND EDITION

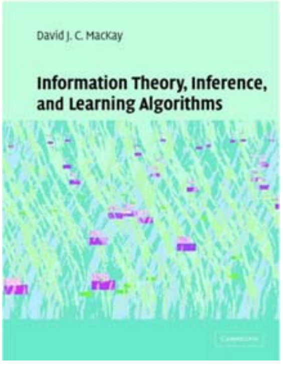
Web resources

- On line book:

Information Theory, Inference, and Learning Algorithms.

David J. C. MacKay, CUP, 2003

  - Covers some of the course material though at an advanced level



- Further reading (www addresses) and the lecture notes are on

http://www.robots.ox.ac.uk/~az/lectures/ml

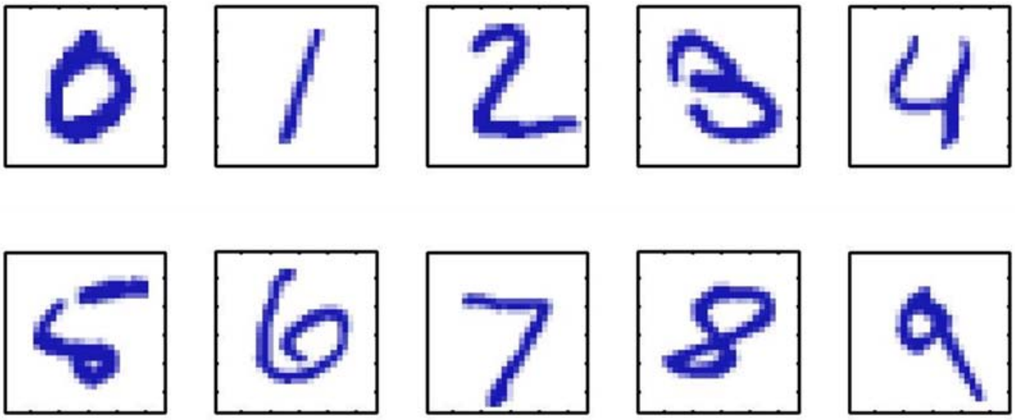
Introduction: What is Machine Learning?

Algorithms that can improve their performance using training data

- Typically the algorithm has a (large) number of parameters whose values are learnt from the data

- Can be applied in situations where it is very challenging (= impossible) to define rules by hand, e.g.:
  - Face detection
  - Speech recognition
  - Stock prediction

Example 1: hand-written digit recognition



Images are 28 x 28 pixels

Represent input image as a vector $\mathbf{x} \in \mathbb{R}^{784}$

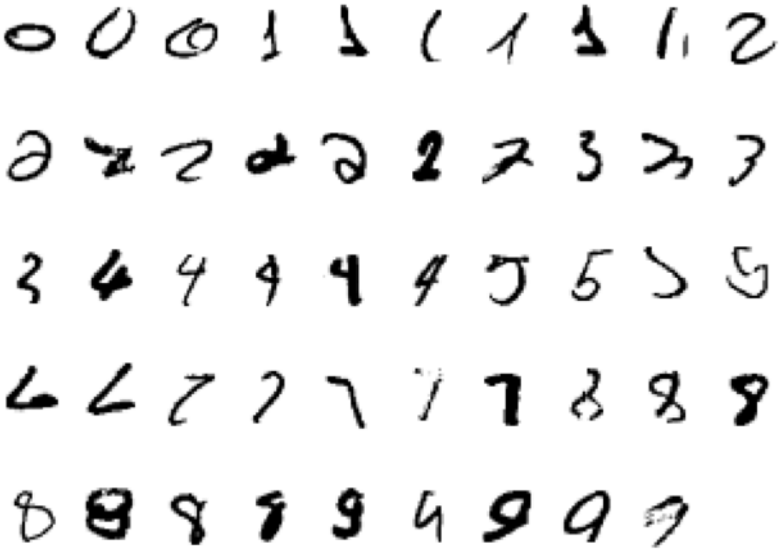
Learn a classifier $f(\mathbf{x})$ such that,

$$f : \mathbf{x} \rightarrow \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$$

How to proceed …

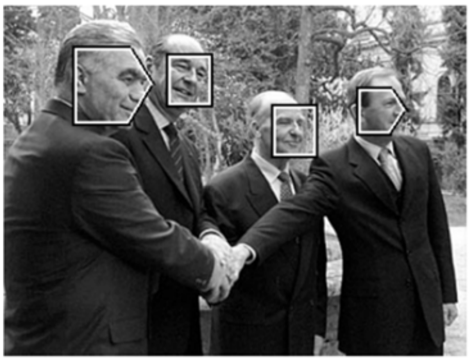
As a supervised classification problem

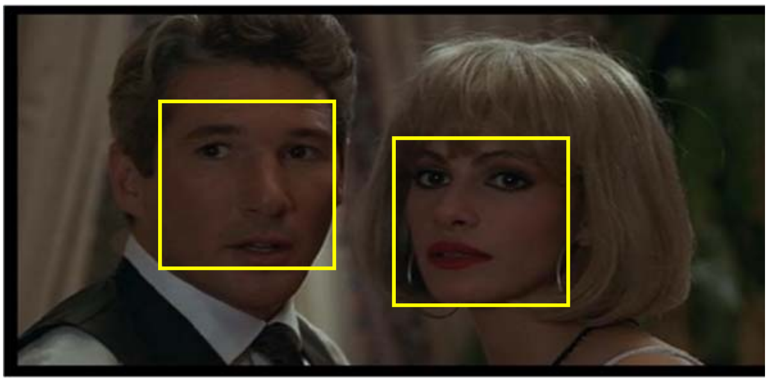
Start with training data, e.g. 6000 examples of each digit



- Can achieve testing error of 0.4%
- One of first commercial and widely used ML systems (for zip codes & checks)

Example 2: Face detection



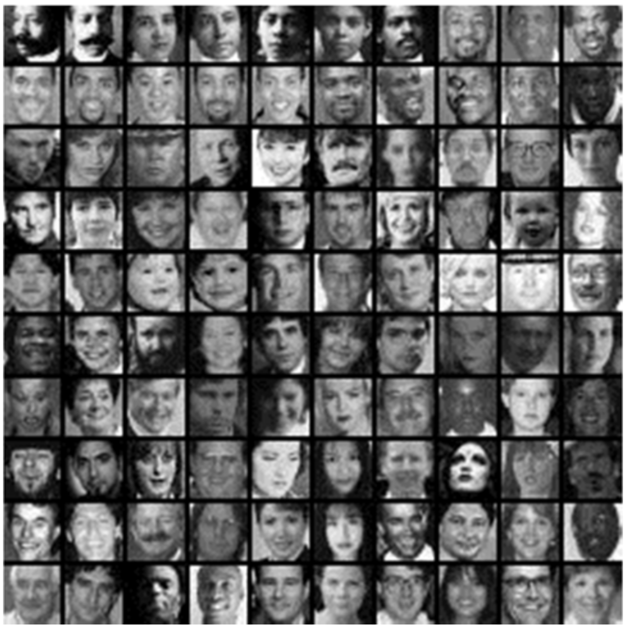


- Again, a supervised classification problem
- Need to classify an image window into three classes:
  - non-face
  - frontal-face
  - profile-face

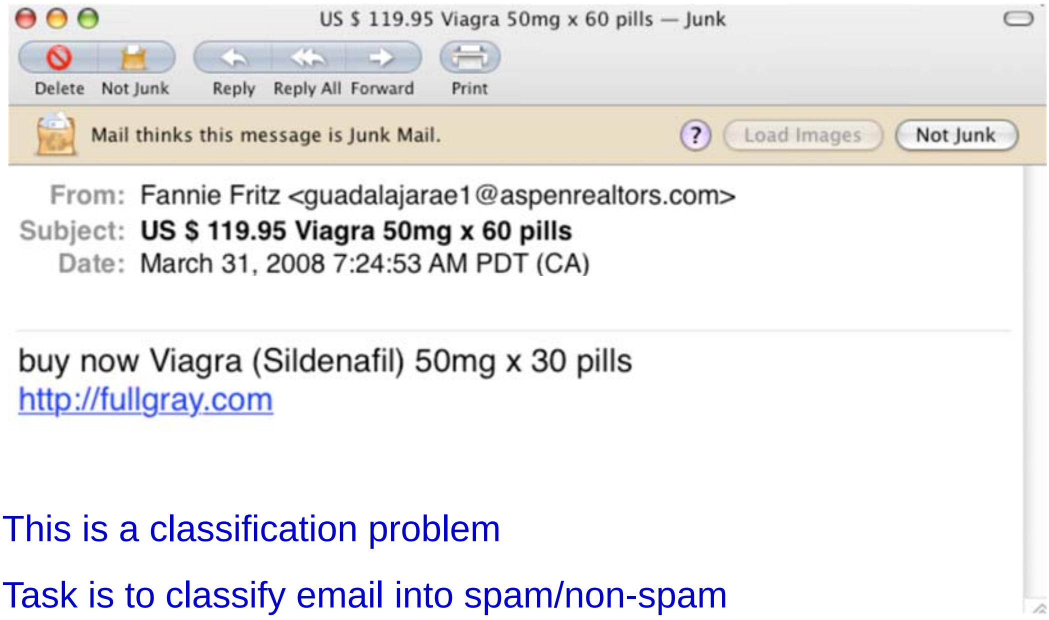
Classifier is learnt from labelled data

Training data for frontal faces

- 5000 faces
  - All near frontal
  - Age, race, gender, lighting
- 10^8 non faces
- faces are normalized
  - scale, translation



Example 3: Spam detection



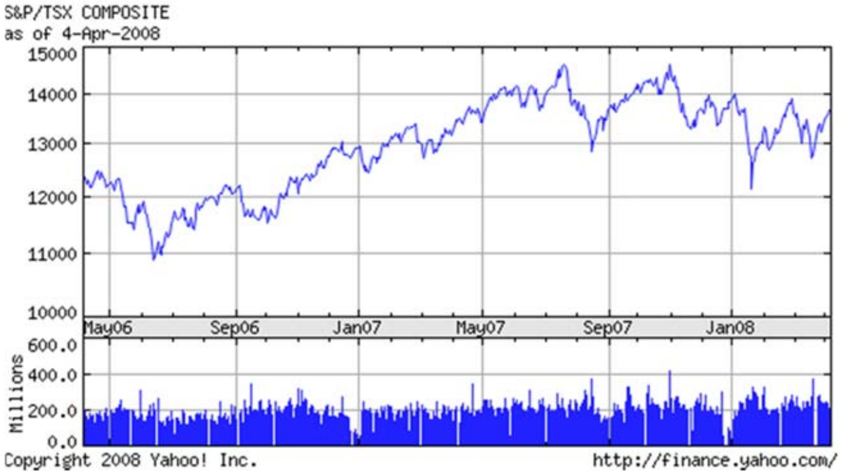
Mail thinks this message is Junk Mail.

From: Fannie Fritz <guadalajarae1@aspenrealtors.com>
Subject: **US $ 119.95 Viagra 50mg x 60 pills**
Date: March 31, 2008 7:24:53 AM PDT (CA)

buy now Viagra (Sildenafil) 50mg x 30 pills
http://fullgray.com

- This is a classification problem
- Task is to classify email into spam/non-spam
- Data x_i is word count, e.g. of viagra, outperform, “you may be surprized to be contacted” …
- Requires a learning system as “enemy” keeps innovating

Example 4: Stock price prediction



Copyright 2008 Yahoo! Inc. http://finance.yahoo.com/

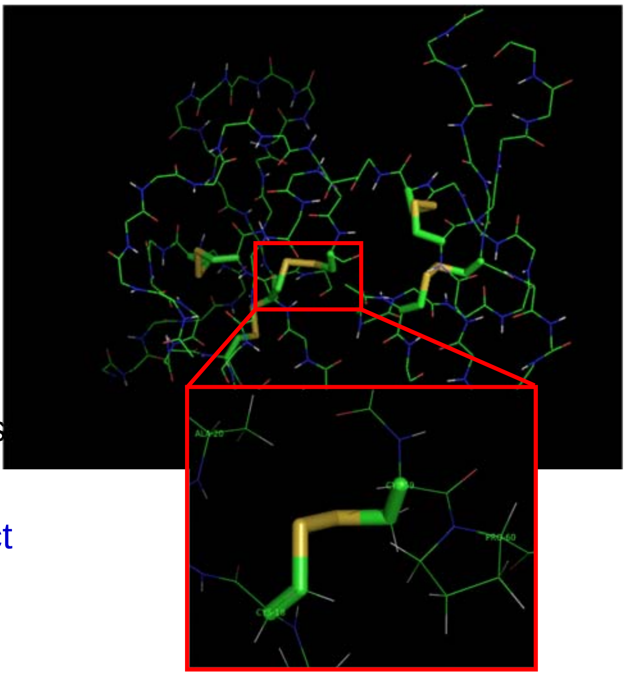
- Task is to predict stock price at future date
- This is a regression task, as the output is continuous

Example 5: Computational biology

x

y

AVITGACERDLQCG
KGTCCAVSLWIKSV
RVCTPVGTSGEDCH
PASHKIPFSGQRMH
HTCPCAPNLACVQT
SPKKFKCLSK



Protein Structure and Disulfide Bridges

Regression task: given sequence predict 3D structure

Protein: 1IMT

Web examples: Machine translation

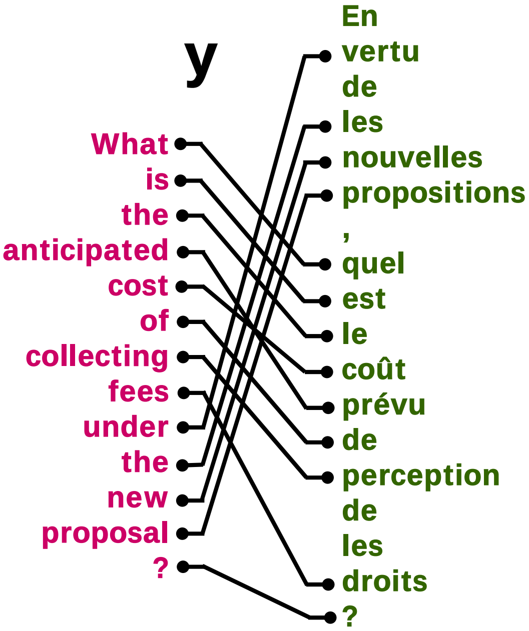
Use of aligned text

x

y

What is the anticipated cost of collecting fees under the new proposal?

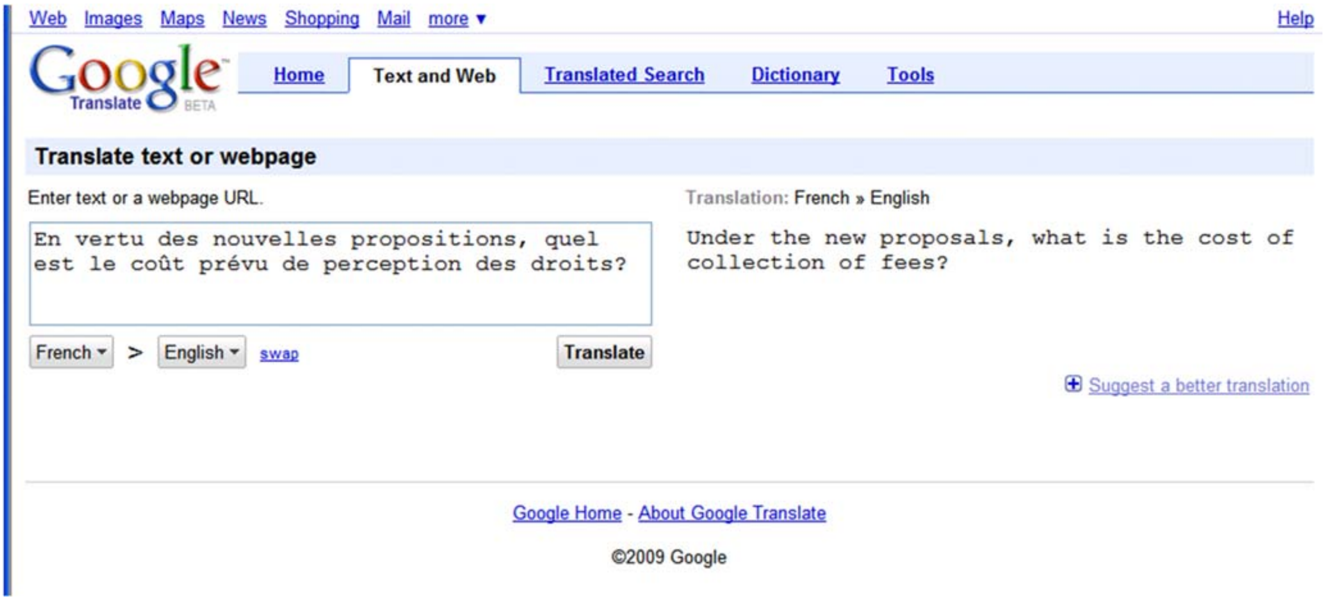
En vertu des nouvelles propositions, quel est le coût prévu de perception des droits?



What
is
the
anticipated
cost
of
collecting
fees
under
the
new
proposal
?

En
vertu
de
les
nouvelles
propositions
,
quel
est
le
coût
prévu
de
perception
de
les
droits
?

e.g. Google translate



Translate text or webpage

Enter text or a webpage URL.

En vertu des nouvelles propositions, quel est le coût prévu de perception des droits?

French ▾ > English ▾ swap

Translate

Translation: French » English

Under the new proposals, what is the cost of collection of fees?

⊞ Suggest a better translation

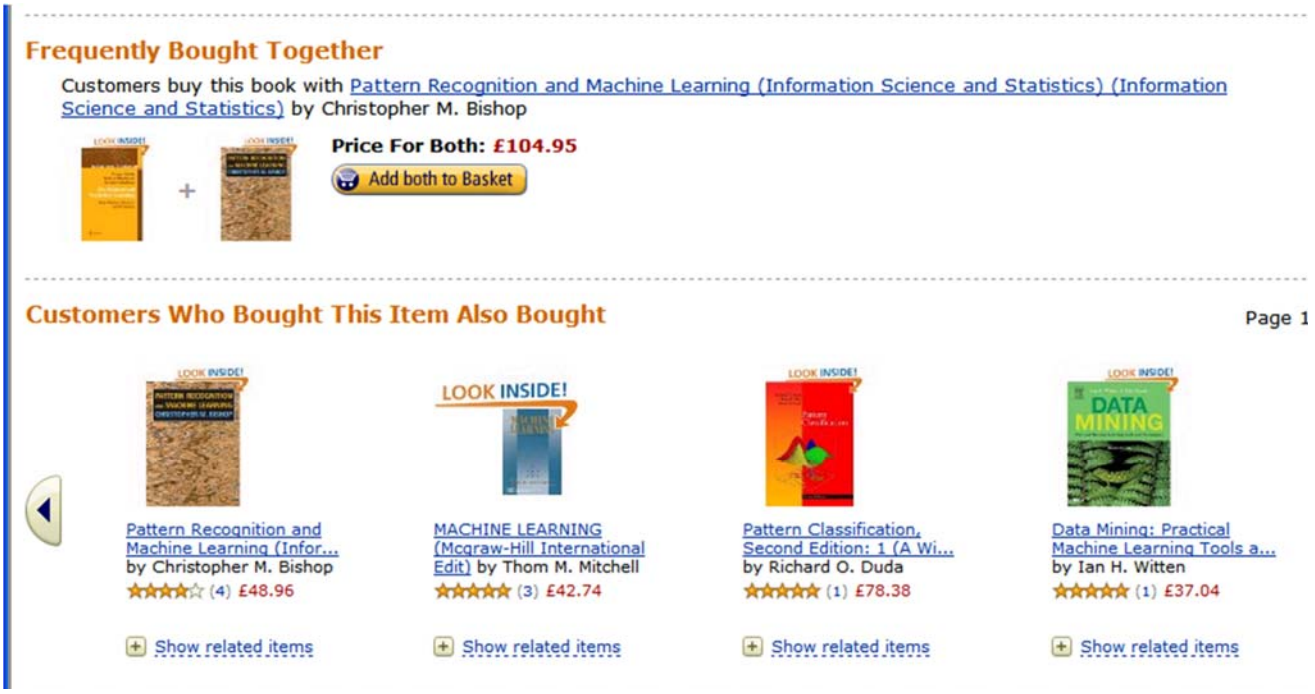
Google Home - About Google Translate

©2009 Google

What is the anticipated cost of collecting fees under the new proposal?

Web examples: Recommender systems

People who bought Hastie …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Price For Both: £104.95

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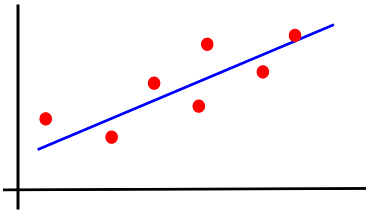
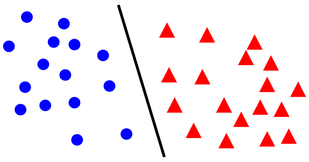
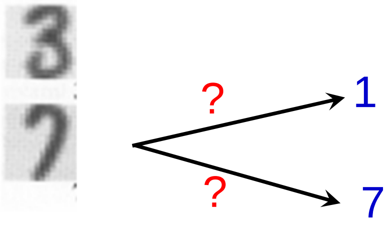
Three canonical learning problems

1. Regression - supervised
   - estimate parameters, e.g. of weight vs height

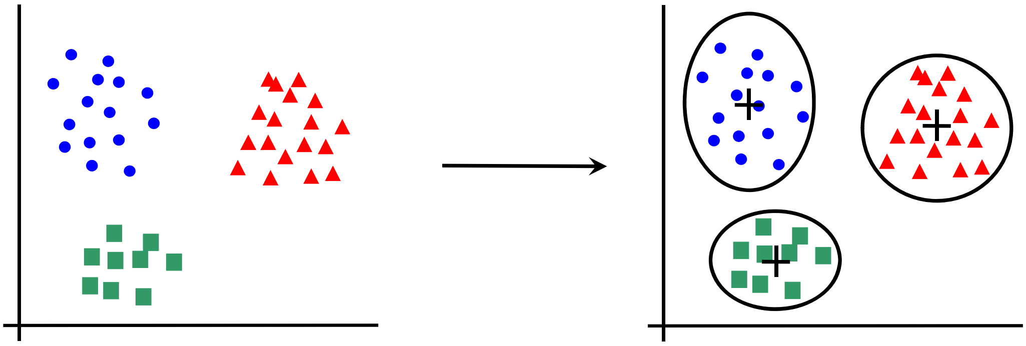


2. Classification - supervised
   - estimate class, e.g. handwritten digit classification

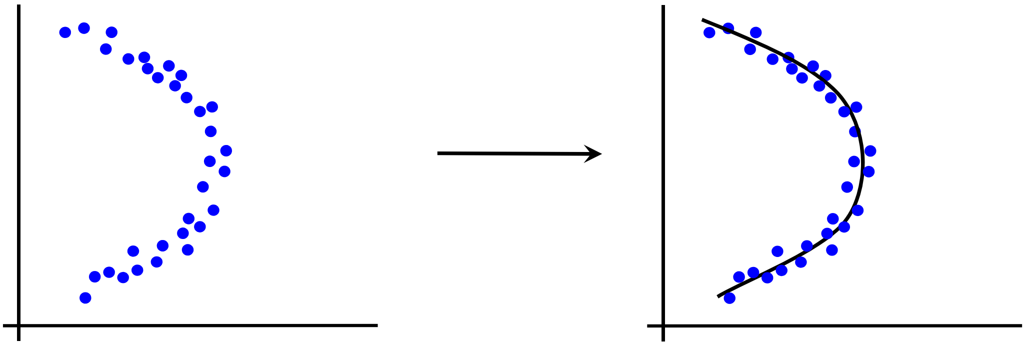




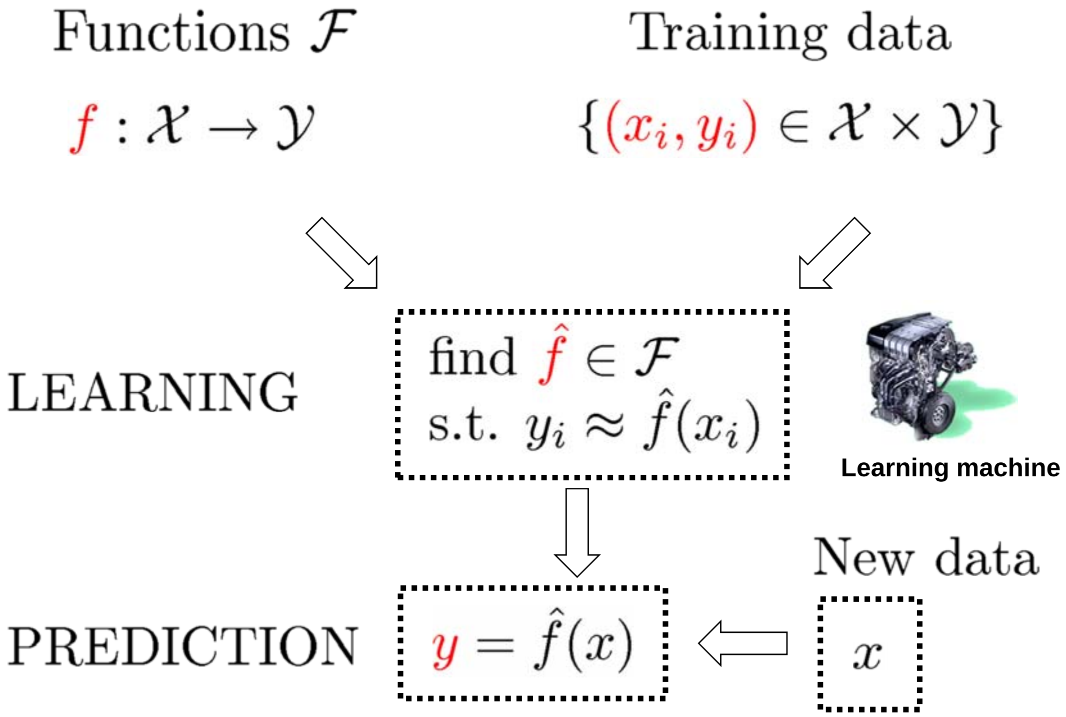
3. Unsupervised learning – model the data
   - clustering



- dimensionality reduction



Supervised Learning: Overview



Functions $\mathcal{F}$

$f : \mathcal{X} \to \mathcal{Y}$

Training data

$\{(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}\}$

LEARNING

find $\hat{f} \in \mathcal{F}$ s.t. $y_i \approx \hat{f}(x_i)$

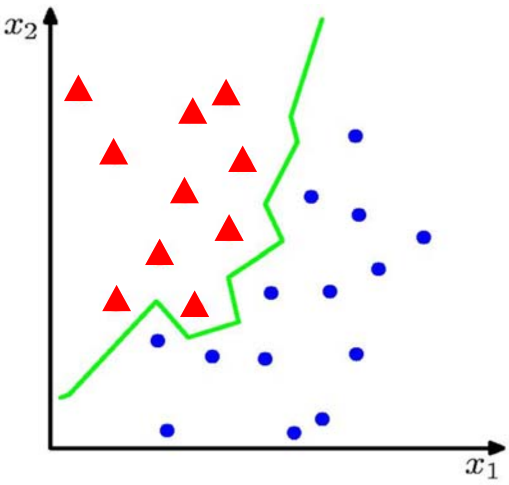
New data

PREDICTION

$y = \hat{f}(x)$

x

Classification



- Suppose we are given a training set of N observations

$$(x_1, \dots, x_N) \text{ and } (y_1, \dots, y_N), x_i \in \mathbb{R}^d, y_i \in \{-1, 1\}$$

- Classification problem is to estimate f(x) from this data such that

$$f(x_i) = y_i$$

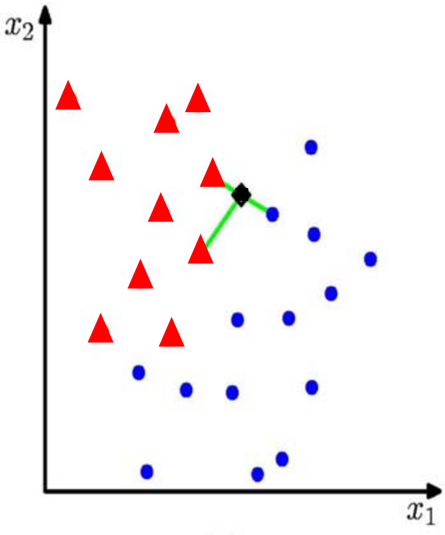
K Nearest Neighbour (K-NN) Classifier

Algorithm

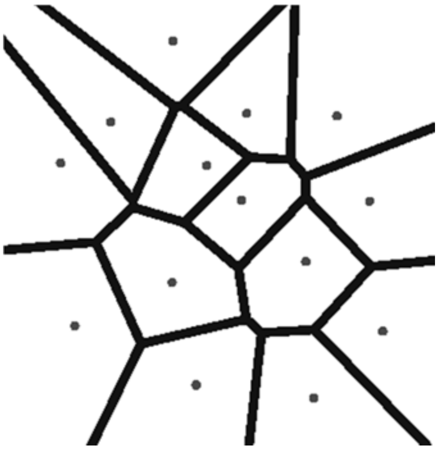
- For each test point, x, to be classified, find the K nearest samples in the training data
- Classify the point, x, according to the majority vote of their class labels

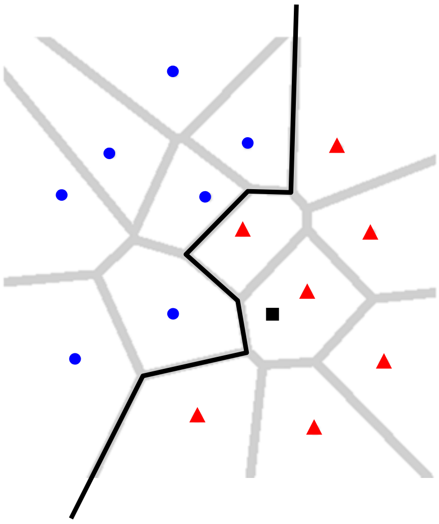
e.g. K = 3

- applicable to multi-class case



K = 1





Voronoi diagram:

- partitions the space into regions
- boundaries are equal distance from training points

Classification boundary:

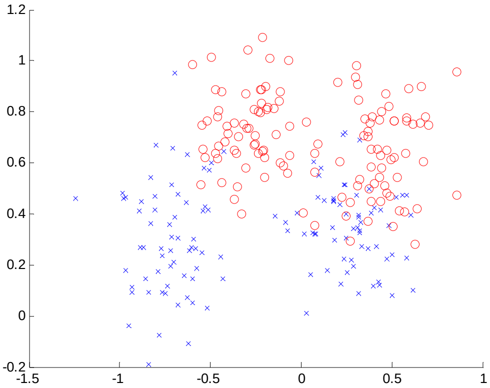
- non-linear

A sampling assumption: training and test data

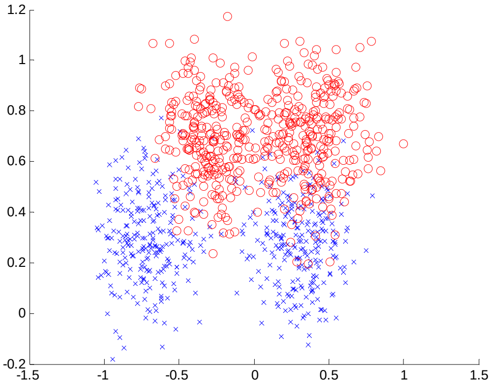
- Assume that the training examples are drawn independently from the set of all possible examples.

- This makes it very unlikely that a strong regularity in the training data will be absent in the test data.

- Measure classification error as $= \frac{1}{N}\sum_{i=1}^{N} \underbrace{[\mathbf{y}_i \neq f(\mathbf{x}_i)]}_{\text{loss function}}$ The “risk”



Training data

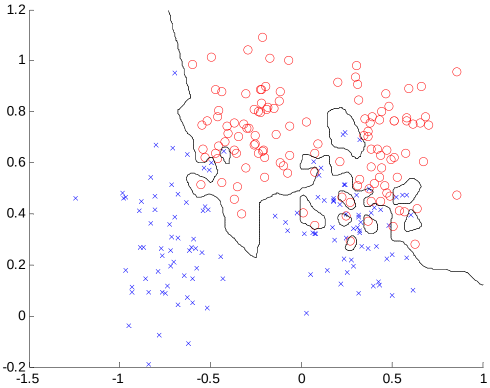


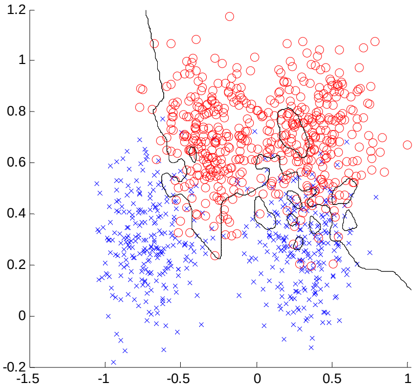
Testing data

K = 1

Training data

Testing data



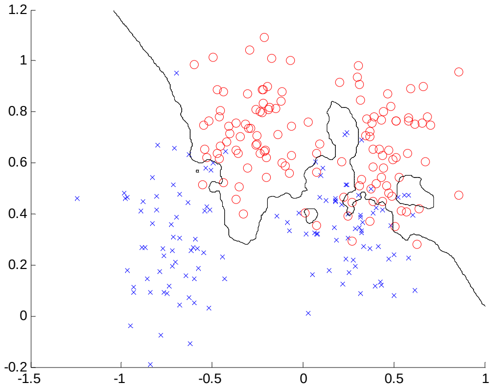


error = 0.0

error = 0.15

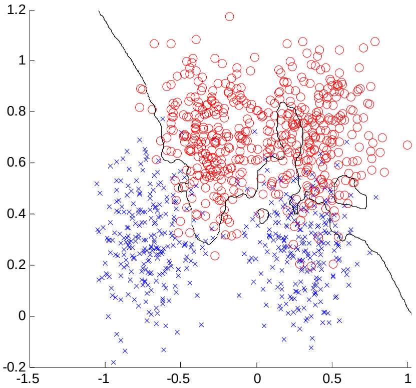
K = 3

Training data



error = 0.0760

Testing data



error = 0.1340

Generalization

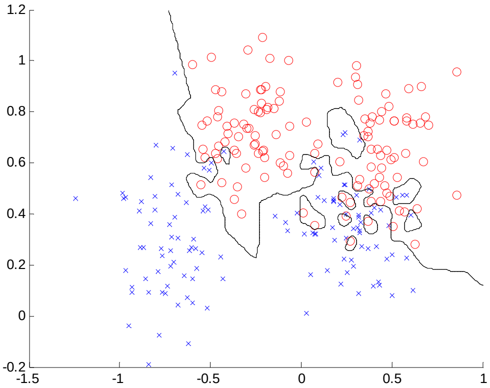
- The real aim of supervised learning is to do well on test data that is not known during learning

- Choosing the values for the parameters that minimize the loss function on the training data is not necessarily the best policy

- We want the learning machine to model the true regularities in the data and to ignore the noise in the data.

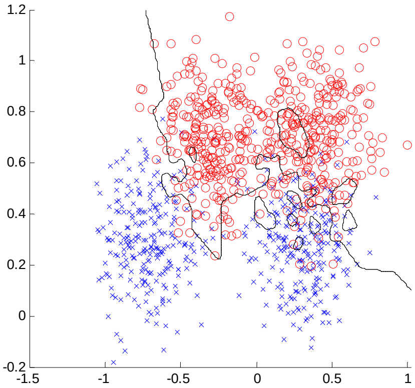
K = 1

Training data



error = 0.0

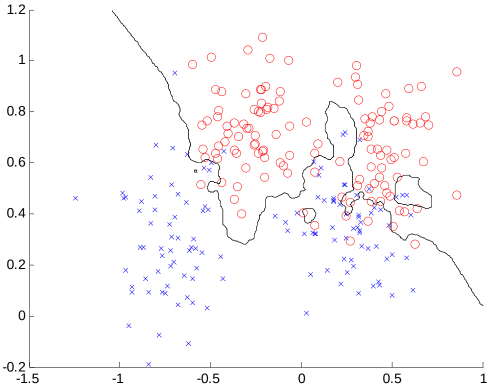
Testing data



error = 0.15

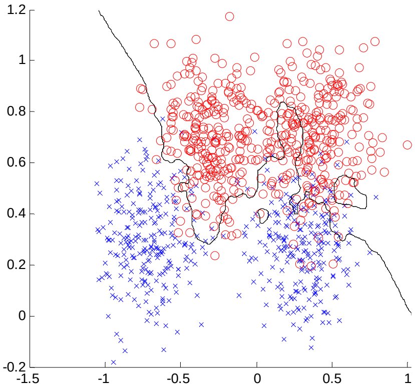
K = 3

Training data



error = 0.0760

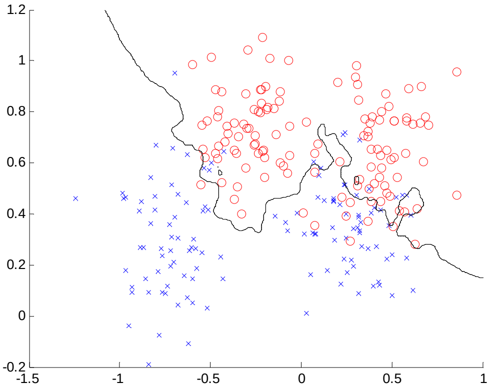
Testing data



error = 0.1340

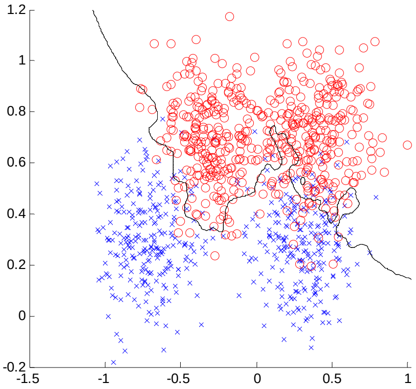
K = 7

Training data



error = 0.1320

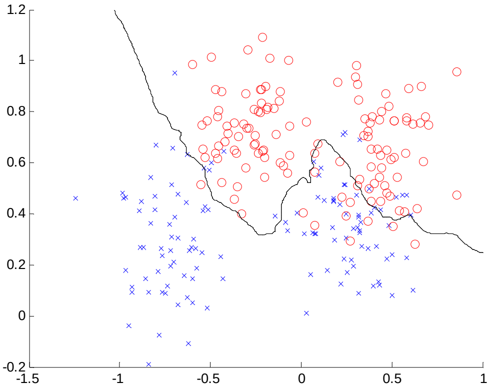
Testing data



error = 0.1110

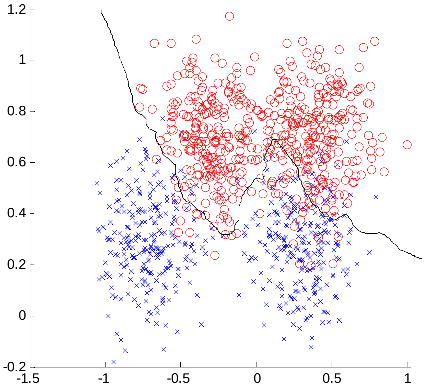
K = 21

Training data



error = 0.1120

Testing data



error = 0.0920

Properties and training

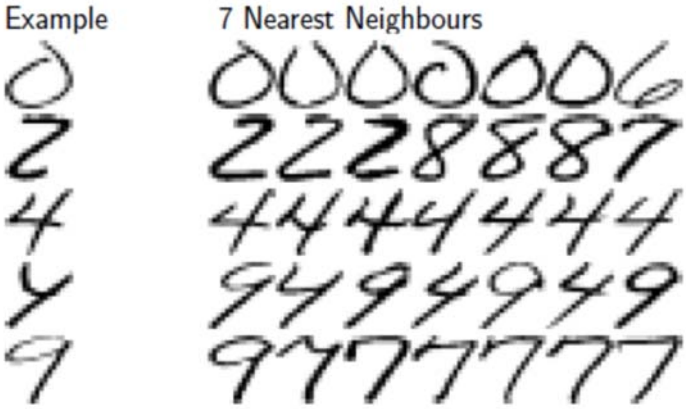
As K increases:

- Classification boundary becomes smoother
- Training error can increase

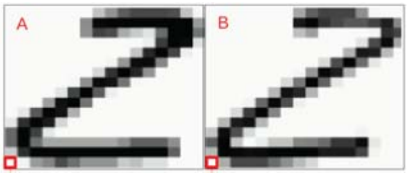
Choose (learn) K by cross-validation

- Split training data into training and validation
- Hold out validation data and measure error on this

Example: hand written digit recognition



- MNIST data set
- Distance = raw pixel distance between images
- 60K training examples
- 10K testing examples
- K-NN gives 5% classification error

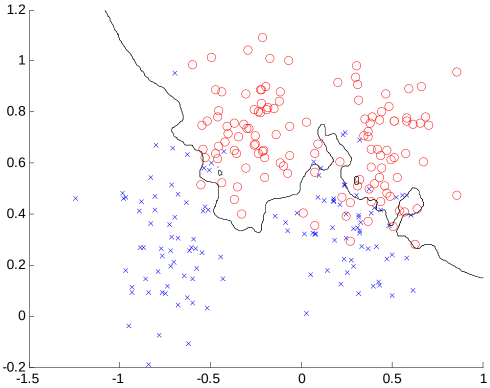


$$D(\mathbf{A},\mathbf{B}) = \sum_{ij} \sqrt{\left(a_{ij} - b_{ij}\right)^2}$$

Summary

Advantages:

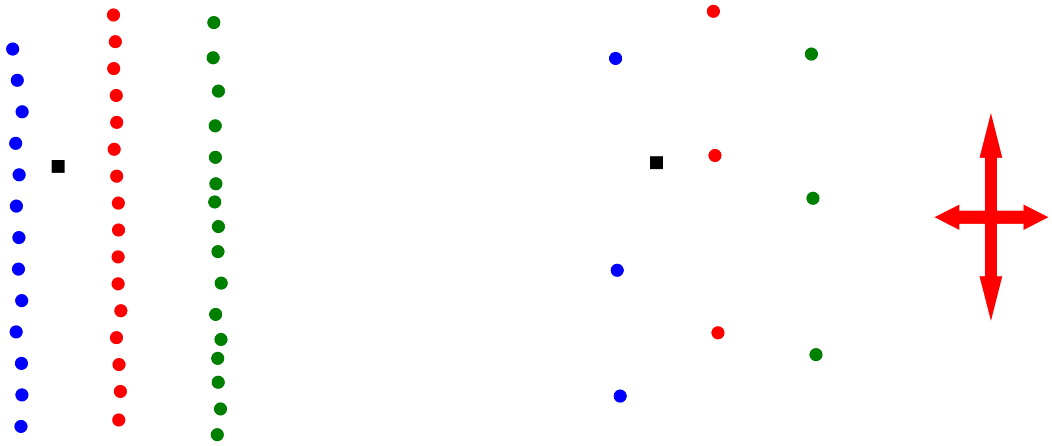
- K-NN is a simple but effective classification procedure
- Applies to multi-class classification
- Decision surfaces are non-linear
- Quality of predictions automatically improves with more training data
- Only a single parameter, K; easily tuned by cross-validation



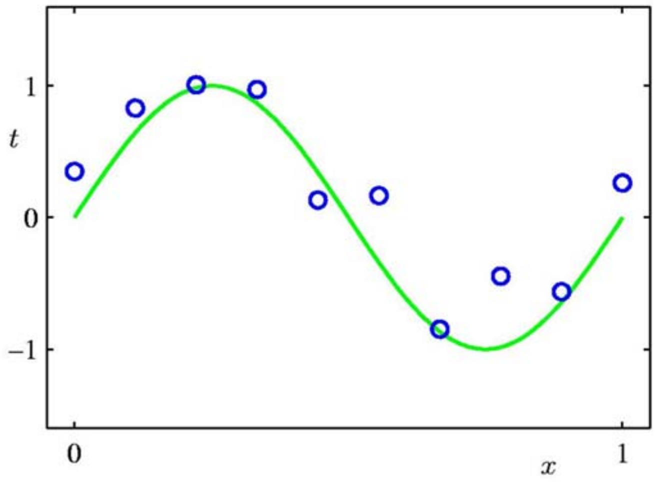
Summary

Disadvantages:

- What does nearest mean? Need to specify a distance metric.
- Computational cost: must store and search through the entire training set at test time. Can alleviate this problem by thinning, and use of efficient data structures like KD trees.



Regression



- Suppose we are given a training set of N observations

$$(x_1, \ldots, x_N) \text{ and } (y_1, \ldots, y_N), x_i, y_i \in \mathbb{R}$$

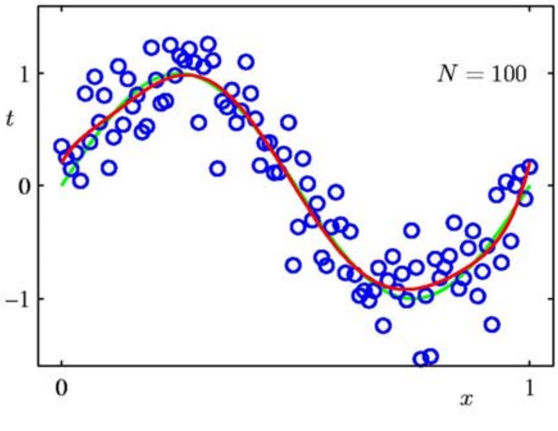
- Regression problem is to estimate y(x) from this data

K-NN Regression

Algorithm

- For each test point, x, find the K nearest samples x_i in the training data and their values y_i
- Output is mean of their values $f(\mathbf{x}) = \frac{1}{K} \sum_{i=1}^{K} y_i$

- Again, need to choose (learn) K



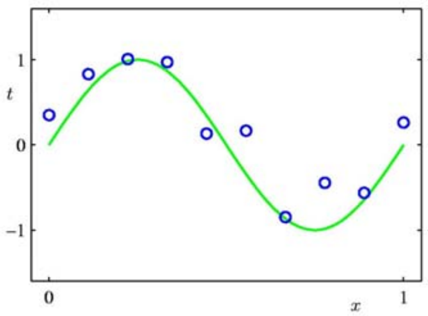
Regression example: polynomial curve fitting

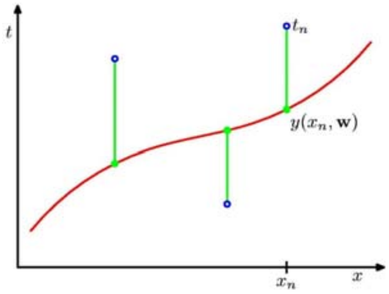
- The green curve is the true function (which is not a polynomial)

- The data points are uniform in x but have noise in y.

- We will use a loss function that measures the squared error in the prediction of y(x) from x. The loss for the red polynomial is the sum of the squared vertical errors.

from Bishop





$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\{y(x_i,\mathbf{w}) - \underset{\uparrow}{t_i}\}^2$$

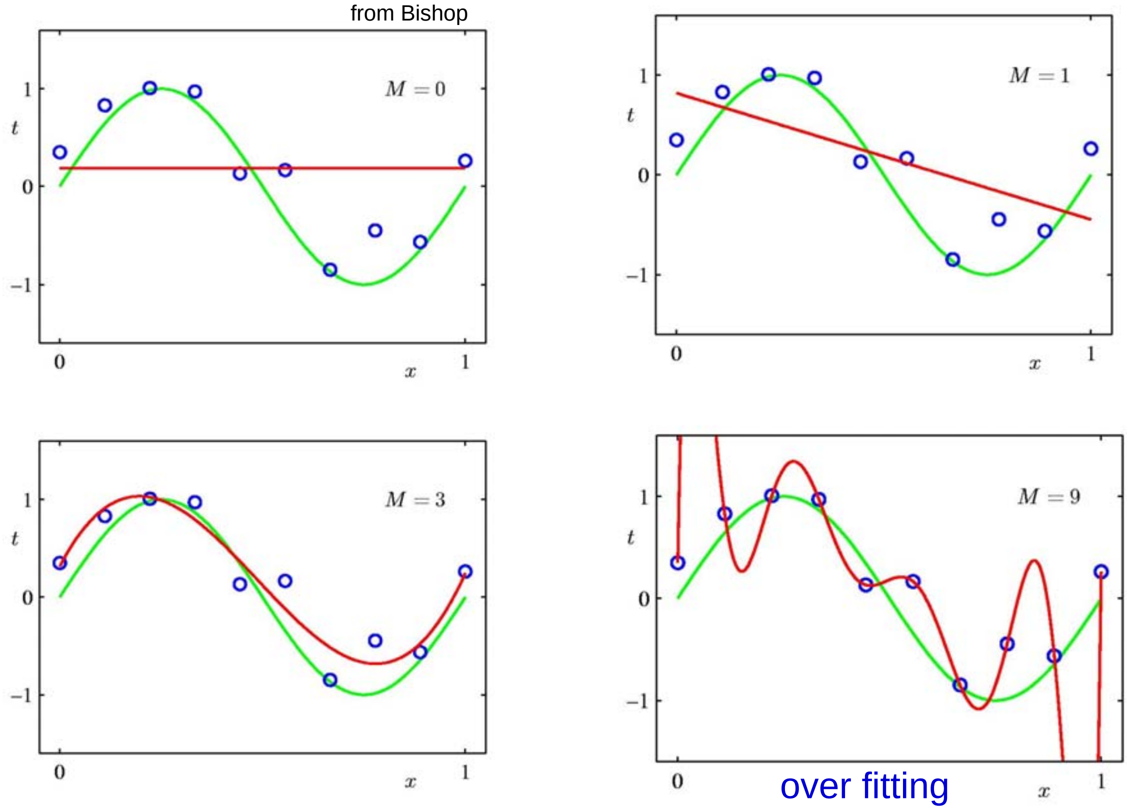
target value

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

polynomial regression

Some fits to the data: which is best?

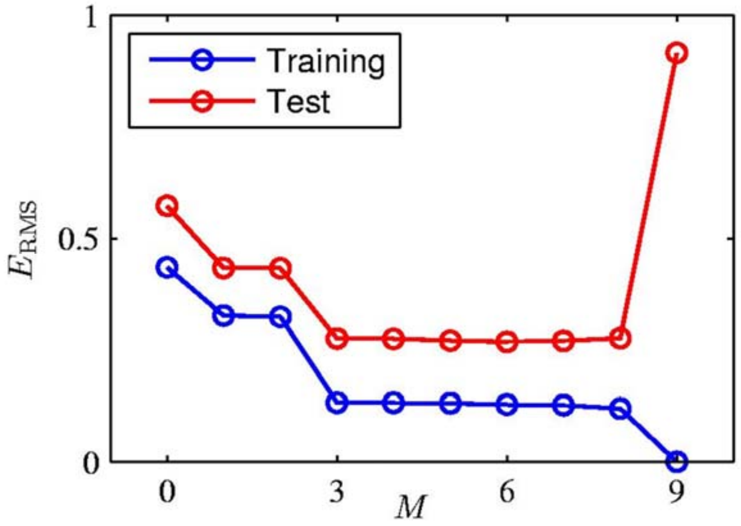
from Bishop



over fitting

Over-fitting

- test data: a different sample from the same true function



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

- training error goes to zero, but test error increases with M

Trading off goodness of fit against model complexity

- If the model has as many degrees of freedom as the data, it can fit the training data perfectly

- But the objective in ML is generalization

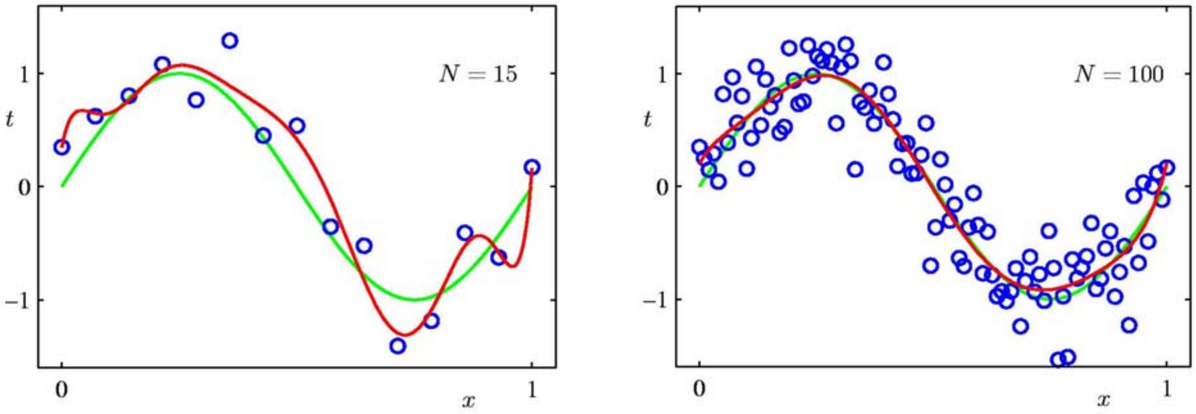
- Can expect a model to generalize well if it explains the training data surprisingly well given the complexity of the model.

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

How to prevent over fitting? I

- Add more data than the model “complexity”
- For 9th order polynomial:

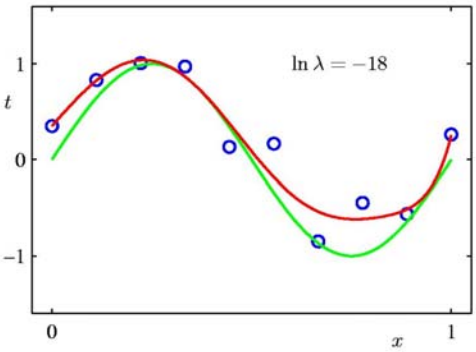


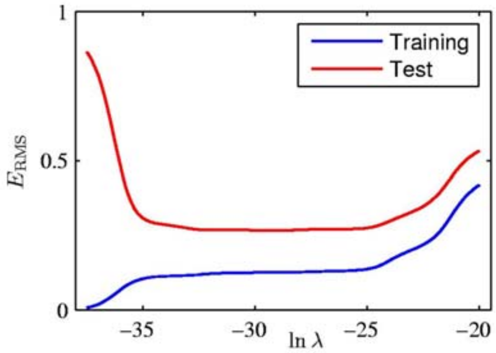
How to prevent over fitting? II

- Regularization: penalize large coefficient values

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\underbrace{\{y(x_i,\mathbf{w}) - t_i\}^2}_{\text{loss function}} + \underbrace{\frac{\lambda}{2}\|\mathbf{w}\|^2}_{\text{regularization}}$$

"ridge" regression





In practice use validation data to choose λ (not test)

- cf with KNN classification as K increases
- we will return to regularization for regression later

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

Summary: How to set parameters?

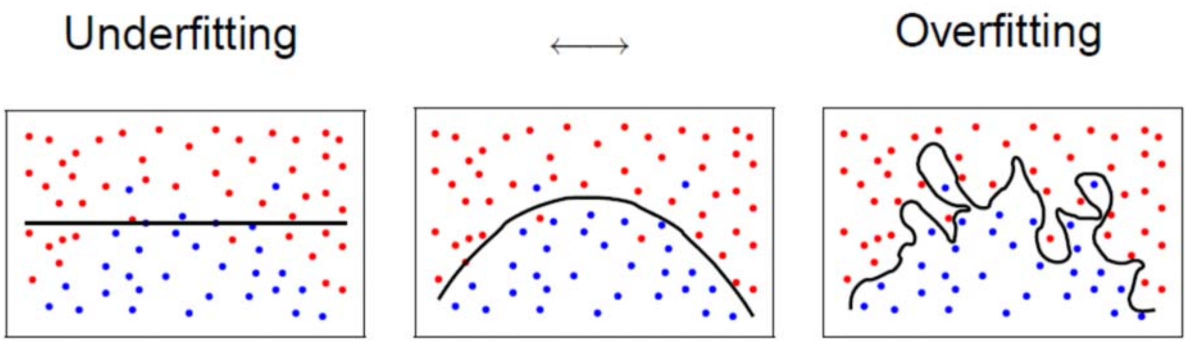
Use a validation set:

Divide the total dataset into three subsets:

- Training data is used for learning the parameters of the model.
- Validation data is not used for learning but is used for deciding what type of model and what amount of regularization works best.
- Test data is used to get a final, unbiased estimate of how well the learning machine works. We expect this estimate to be worse than on the validation data.

We could then re-divide the total dataset to get another unbiased estimate of the true error rate.

Generalization Problem in Classification



• Again, need to control the complexity of the (discriminant) function

What comes next?

- Learning by optimizing a cost function:

$$\widetilde{E}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N}\underbrace{\{y(x_i,\mathbf{w}) - t_i\}^2}_{\text{loss function}} + \underbrace{\frac{\lambda}{2}\|\mathbf{w}\|^2}_{\text{regularization}}$$

- In general Minimize with respect to $f \in \mathcal{F}$

$$\sum_{i=1}^{N} l\left(f(x_i), y_i\right) + \lambda R\left(f\right)$$

- choose loss function for: classification, regression, clustering …
- choose regularization function

Background reading

- Bishop, chapter 1

- Hastie et al, chapter 2

- Witten & Frank, chapter 1 for example applications

- More on web page:
  http://www.robots.ox.ac.uk/~az/lectures/ml