Learning from Observations

Chapter 18

Outline

- Introduction to machine learning
- Supervised learning（监督学习）
  - Decision tree learning（决策树学习）
  - Linear predictions （线性预测）
  - Support vector machines （支持向量机）

  …
- Unsupervised learning （无监督学习）

Learning

Learning is essential for unknown environments,

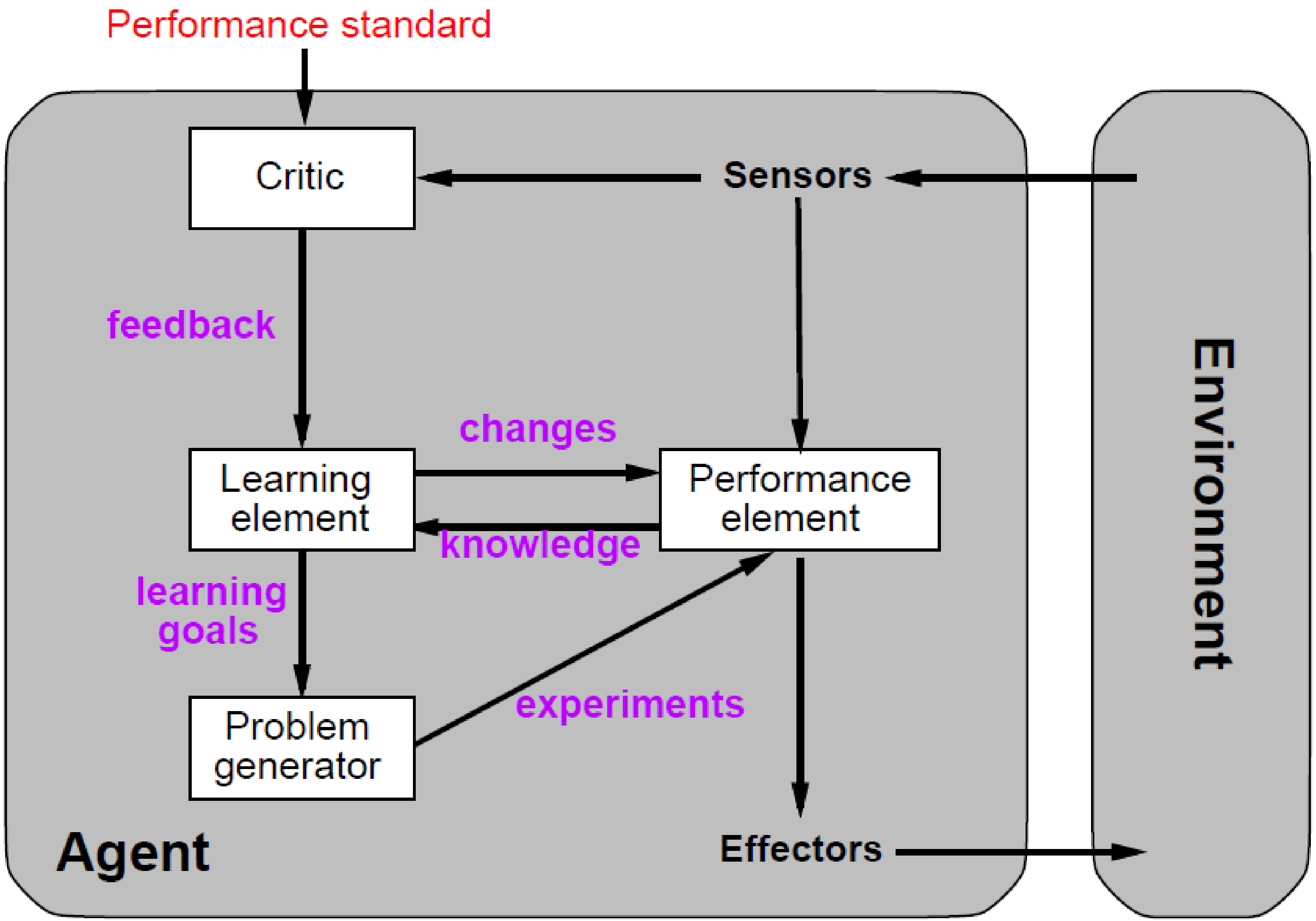
- i.e., when designer lacks omniscience（全知）

Learning is useful as a system construction method,

- i.e., expose the agent to reality rather than trying to write it down

Learning modifies the agent's decision mechanisms to improve performance

Learning agents



Learning element

Design of a learning element is affected by

- Which components of the performance element are to be learned
- What feedback is available to learn these components
- What representation is used for the components

Machine learning

Machine learning is an interdisciplinary field focusing on both the mathematical foundations and practical applications of systems that learn, reason and act.

机器学习是一个交叉学科的领域，着重于研究具有学习、推理和行动的系统所需要的数学基础以及实际应用

Other related terms: Pattern Recognition（模式识别）, Neural Networks（神经网络）, Data Mining（数据挖掘）, Statistical Modeling（统计模型） …

Using ideas from: Statistics, Computer Science, Engineering, Applied Mathematics, Cognitive Science（认知科学）, Psychology（心理学）, Computational Neuroscience（计算神经学）, Economics

The goal of these lectures: to introduce important concepts, models and algorithms in machine learning.

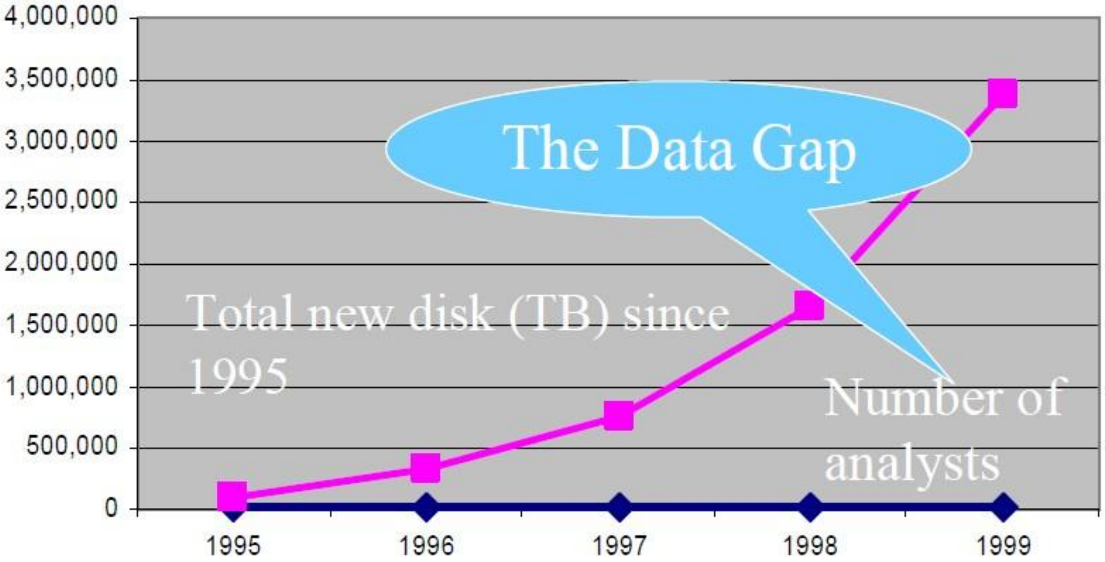
Why machine learning?

- □ Solve classification problems
- □ Learn models of data (“data fitting”)
- □ Understand and improve efficiency of human learning
- □ Discover new things or structures that are unknown to humans (“data mining”)

…

Why machine learning?

- Large amounts of data
  - Web data
  - Medical data
  - Biological data…
- Expensive to analyze by hand
- Computers become cheaper and more powerful



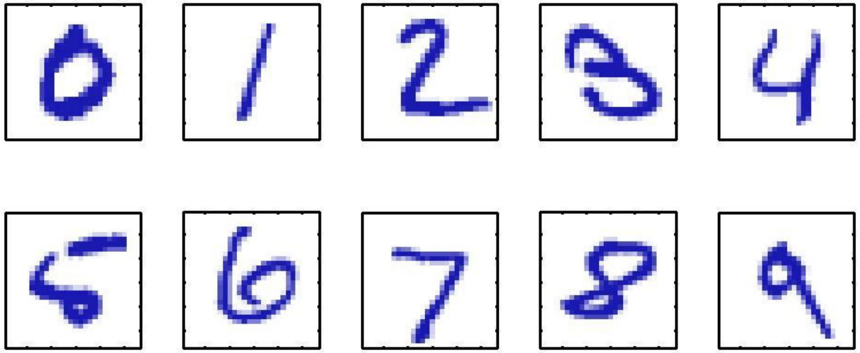
From: R. Grossman, C. Kamath, V. Kumar, "Data Mining for Scientific and Engineering Applications"

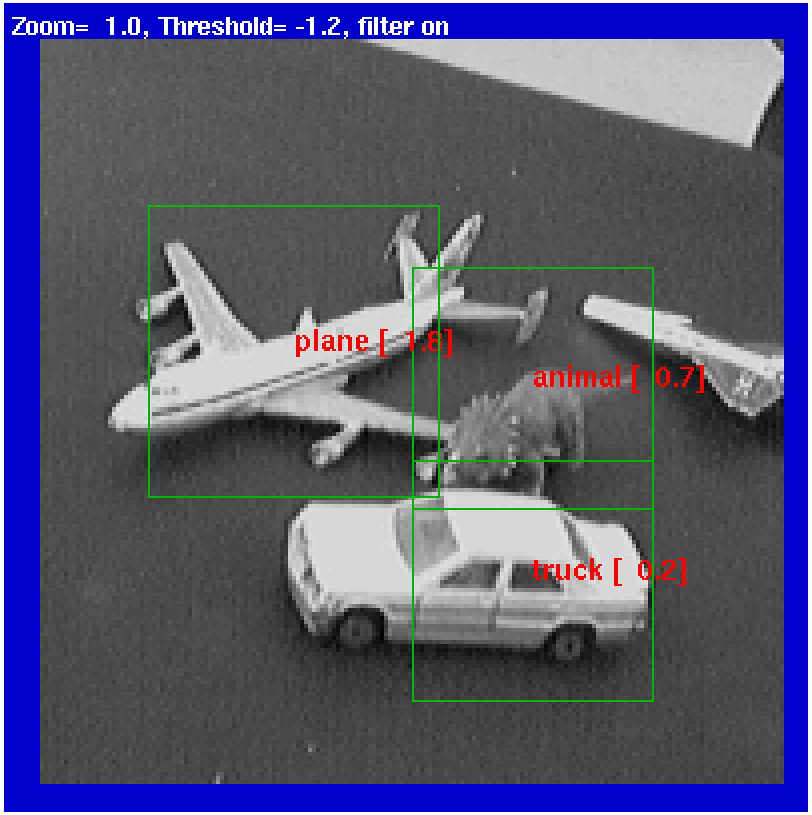
What is machine learning useful for?

Automatic speech recognition
自动语音识别

Now most **Speech Recognizers or Translators** are able to learn — the more you play/use them, the smarter they become

Computer vision: e.g. object, face and handwriting recognition





Zoom= 1.0, Threshold= -1.2, filter on

Information retrieval—信息检索

- Reading, digesting, and categorizing a vast text database is too much for human

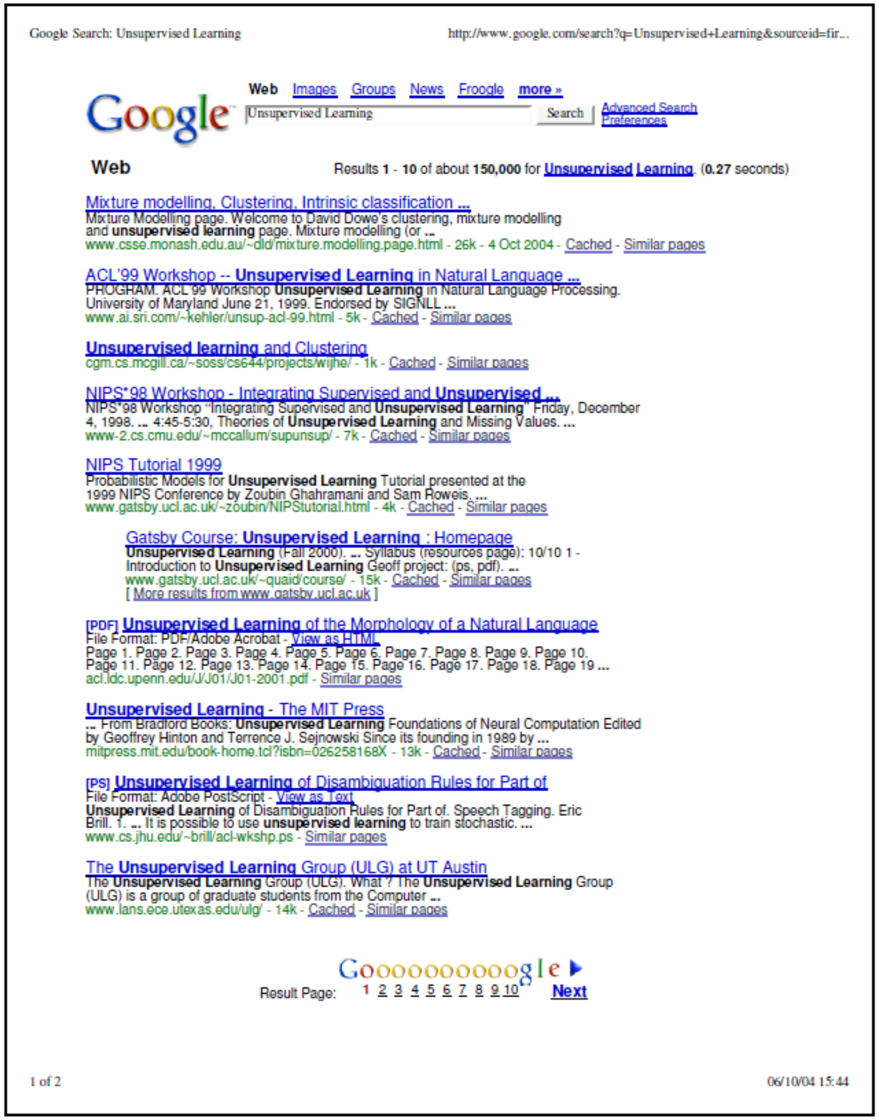
Web Pages

Retrieval（检索）

Categorization（分类）

Clustering（聚类）

Relations between pages



Google Search: Unsupervised Learning http://www.google.com/search?q=Unsupervised+Learning&sourceid=fir...

Unsupervised Learning

Web Results **1** - **10** of about **150,000** for **Unsupervised Learning**. (**0.27** seconds)

Mixture modelling, Clustering, Intrinsic classification ...
Mixture Modelling page. Welcome to David Dowe's clustering, mixture modelling and **unsupervised learning** page. Mixture modelling (or ...
www.csse.monash.edu.au/~dld/mixture.modelling.page.html - 26k - 4 Oct 2004 - Cached - Similar pages

ACL'99 Workshop -- **Unsupervised Learning** in Natural Language ...
PROGRAM. ACL'99 Workshop **Unsupervised Learning** in Natural Language Processing. University of Maryland June 21, 1999. Endorsed by SIGNLL ...
www.ai.sri.com/~kehler/unsup-acl-99.html - 5k - Cached - Similar pages

Unsupervised learning and Clustering
cgm.cs.mcgill.ca/~soss/cs644/projects/wijhe/ - 1k - Cached - Similar pages

NIPS*98 Workshop - Integrating Supervised and **Unsupervised** ...
NIPS*98 Workshop "Integrating Supervised and **Unsupervised Learning**" Friday, December 4, 1998. ... 4:45-5:30, Theories of **Unsupervised Learning** and Missing Values. ...
www-2.cs.cmu.edu/~mccallum/supunsup/ - 7k - Cached - Similar pages

NIPS Tutorial 1999
Probabilistic Models for **Unsupervised Learning** Tutorial presented at the 1999 NIPS Conference by Zoubin Ghahramani and Sam Roweis. ...
www.gatsby.ucl.ac.uk/~zoubin/NIPStutorial.html - 4k - Cached - Similar pages

> Gatsby Course: **Unsupervised Learning** : Homepage
> **Unsupervised Learning** (Fall 2000). ... Syllabus (resources page): 10/10 1 - Introduction to **Unsupervised Learning** Geoff project: (ps, pdf). ...
> www.gatsby.ucl.ac.uk/~quaid/course/ - 15k - Cached - Similar pages
> [More results from www.gatsby.ucl.ac.uk]

[PDF] **Unsupervised Learning** of the Morphology of a Natural Language
File Format: PDF/Adobe Acrobat - View as HTML
Page 1. Page 2. Page 3. Page 4. Page 5. Page 6. Page 7. Page 8. Page 9. Page 10. Page 11. Page 12. Page 13. Page 14. Page 15. Page 16. Page 17. Page 18. Page 19 ...
acl.ldc.upenn.edu/J/J01/J01-2001.pdf - Similar pages

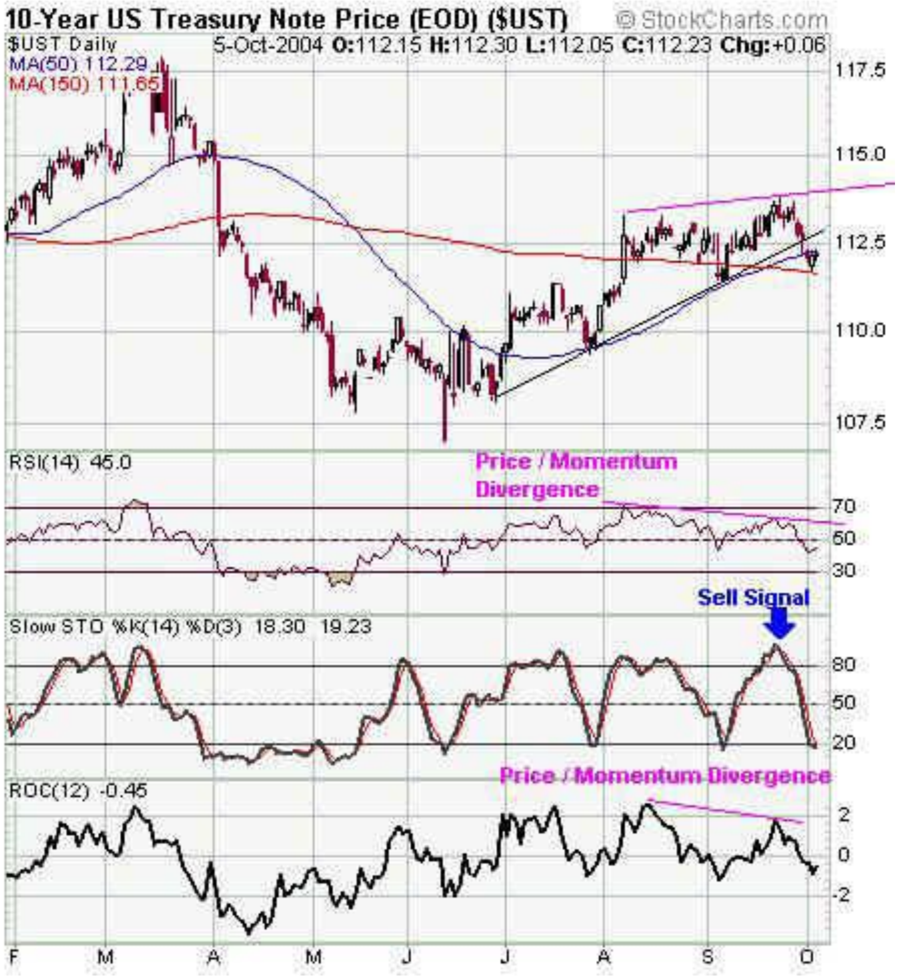
Unsupervised Learning - The MIT Press
... From Bradford Books: **Unsupervised Learning** Foundations of Neural Computation Edited by Geoffrey Hinton and Terrence J. Sejnowski Since its founding in 1989 by ...
mitpress.mit.edu/book-home.tcl?isbn=026258168X - 13k - Cached - Similar pages

[PS] **Unsupervised Learning** of Disambiguation Rules for Part of
File Format: Adobe PostScript - View as Text
Unsupervised Learning of Disambiguation Rules for Part of. Speech Tagging. Eric Brill. 1. ... It is possible to use **unsupervised learning** to train stochastic. ...
www.cs.jhu.edu/~brill/acl-wkshp.ps - Similar pages

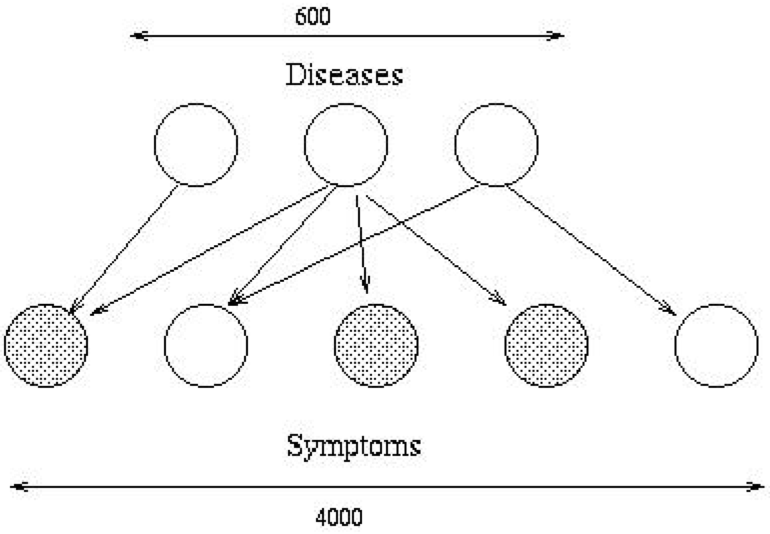
The **Unsupervised Learning** Group (ULG) at UT Austin
The **Unsupervised Learning** Group (ULG). What ? The **Unsupervised Learning** Group (ULG) is a group of graduate students from the Computer ...
www.lans.ece.utexas.edu/ulg/ - 14k - Cached - Similar pages

1 of 2 06/10/04 15:44

Financial prediction

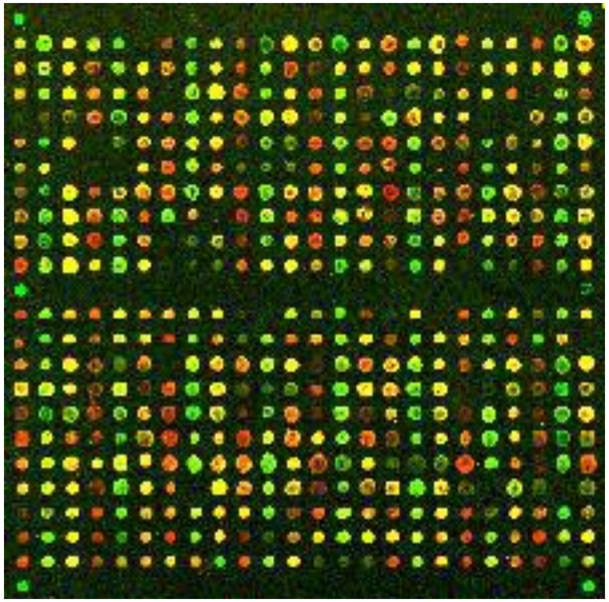


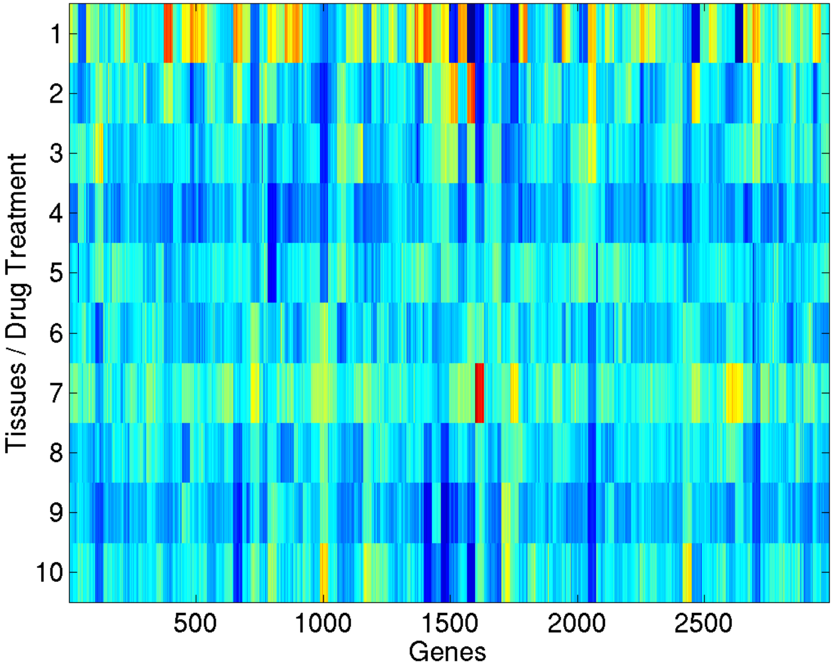
Medical diagnosis（医学诊断）



(image from Kevin Murphy)

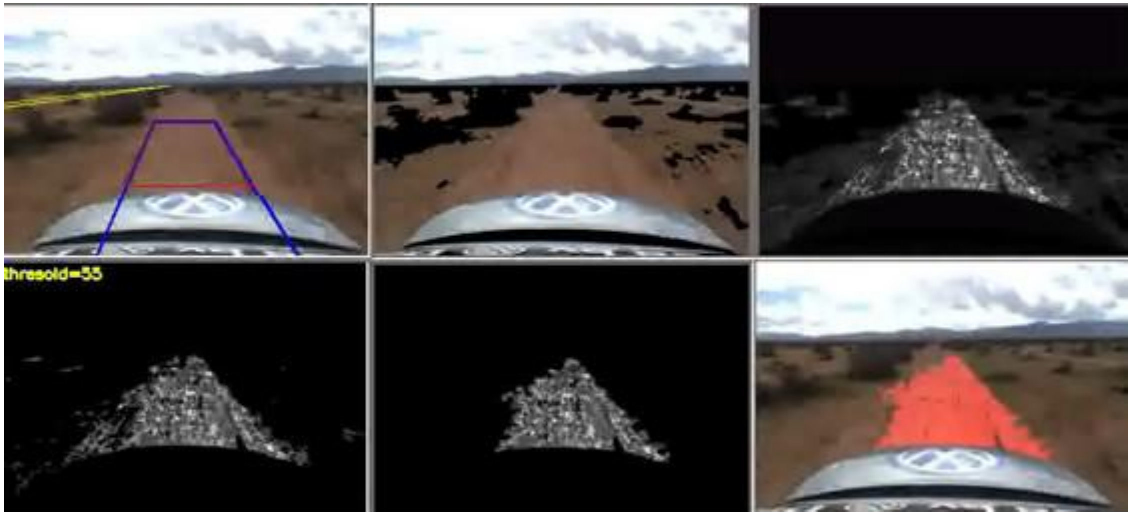
Bioinformatics（生物信息学）





e.g. modeling gene microarray（微阵列）data, protein structure prediction

Robotics



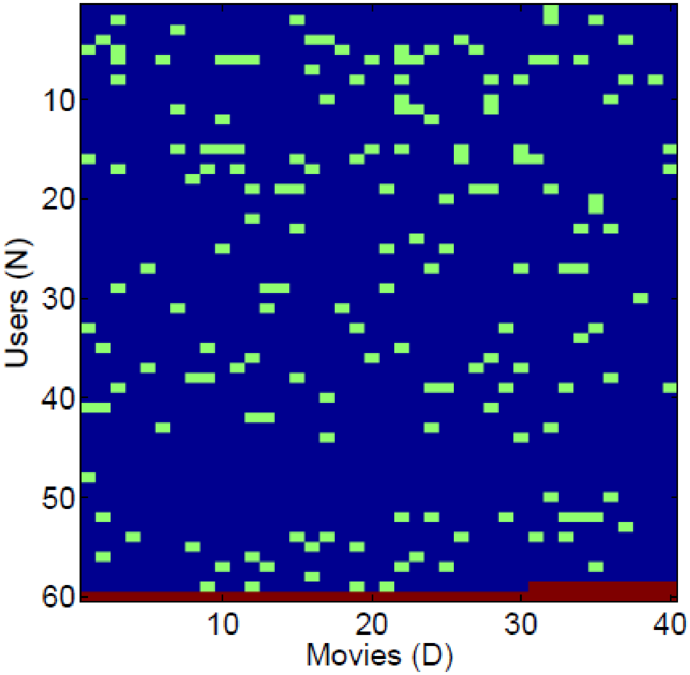
Movie recommendation systems

The Netflix Prize seeks to substantially improve the accuracy of predictions about how much someone is going to love a movie based on their movie preferences. Improve it enough and you win one (or more) Prizes. Winning the Netflix Prize improves our ability to connect people to the movies they love.

Read the Rules to see what is required to win the Prizes. If you are interested in joining the quest, you should register a team.

You should also read the frequently-asked questions about the Prize. And check out how various teams are doing on the Leaderboard.

Good luck and thanks for helping!



Challenge: to improve the accuracy of movie preference predictions Netflix $1m Prize.

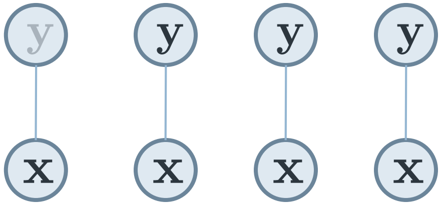
Types of Learning

Imagine an agent or machine which experiences a series of sensory inputs:

$x_1, x_2, x_3, x_4, \ldots$

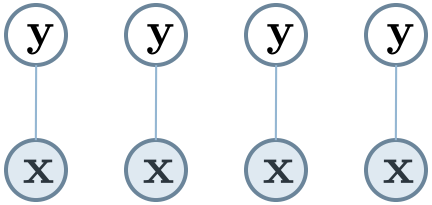
Supervised learning（监督学习）：

The machine is also given desired outputs $y_1, y_2, \ldots,$ and its goal is to learn to produce the correct output given a new input.

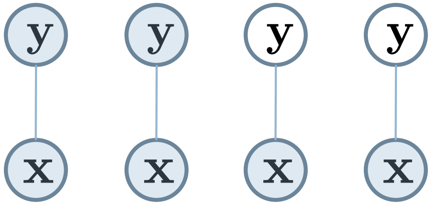


Unsupervised learning（无监督学习）：

outputs $y_1, y_2, \ldots$ Not given, the agent still wants to build a model of x that can be used for reasoning, decision making, predicting things, communicating etc.



Semi-supervised learning （半监督学习）



Representing “objects” in machine learning

- An example or instance, *x*, represents a specific object
- *x* often represented by a d-dimensional feature vector $x = (x_1, \ldots, x_d) \in R^d$
- Each dimension is called a feature or attribute
- Continuous or discrete
- *x* is a point in the *d*-dimensional feature space
- Abstraction of object. Ignores any other aspects (e.g., two people having the same weight and height may be considered identical)

Feature vector representation

- Text document
  - Vocabulary of size d (~100,000)
  - "bag of words": counts of each vocabulary entry
  - Often remove stopwords: the, of, at, in, …
  - Special "out-of-vocabulary" (OOV) entry catches all unknown words

Feature vector representation

- Image
  - Pixels, Color histogram
- Software
  - Execution profile: the number of times each line is executed
- Bank account
  - Credit rating, balance, #deposits in last day, week, month, year, #withdrawals, …
- You and me
  - Medical test1, test2, test3, …

Key Ingredients

Data

The data set D consists of N data points:

$D = \{x_1, x_2 \ldots, x_N\}$

Predictions （预测）

We are generally interested in predicting something based on the observed data set.

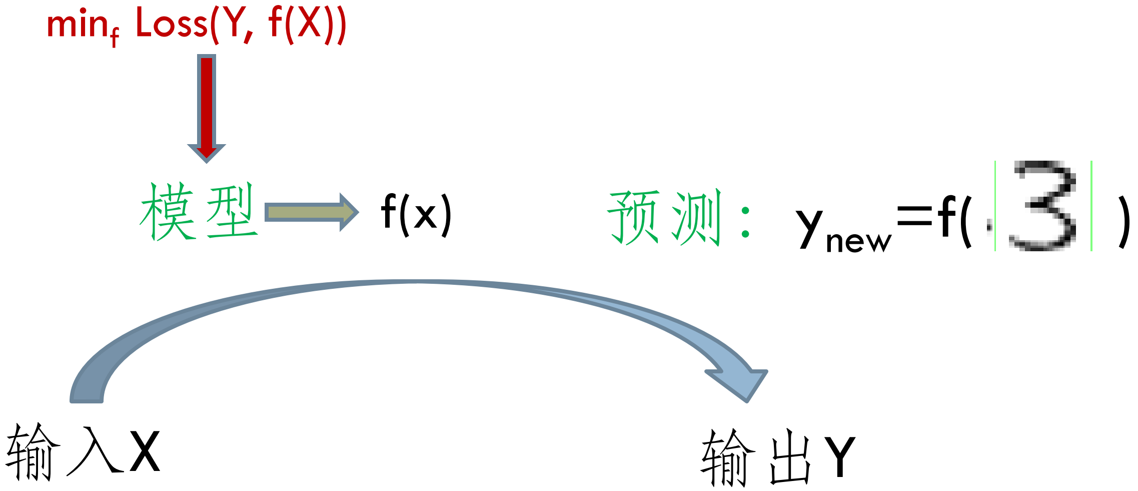
Given D what can we say about x_{N+1}?

Model

To make predictions, we need to make some assumptions. We can often express these assumptions in the form of a model, with some parameters （参数）

Given data D, we learn the model parameters , from which we can predict new data points.

Key Ingredients



$\min_f$ Loss(Y, f(X))

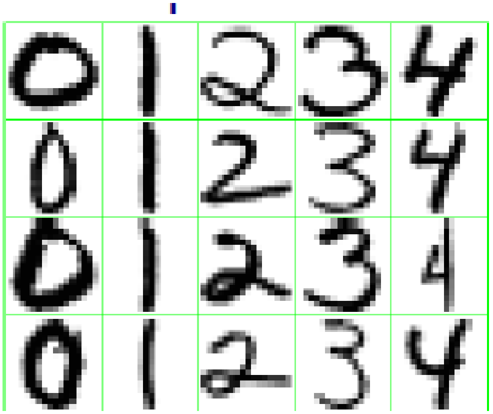
模型 → f(x)

预测： $y_{new}=f(3)$

输入X

输出Y

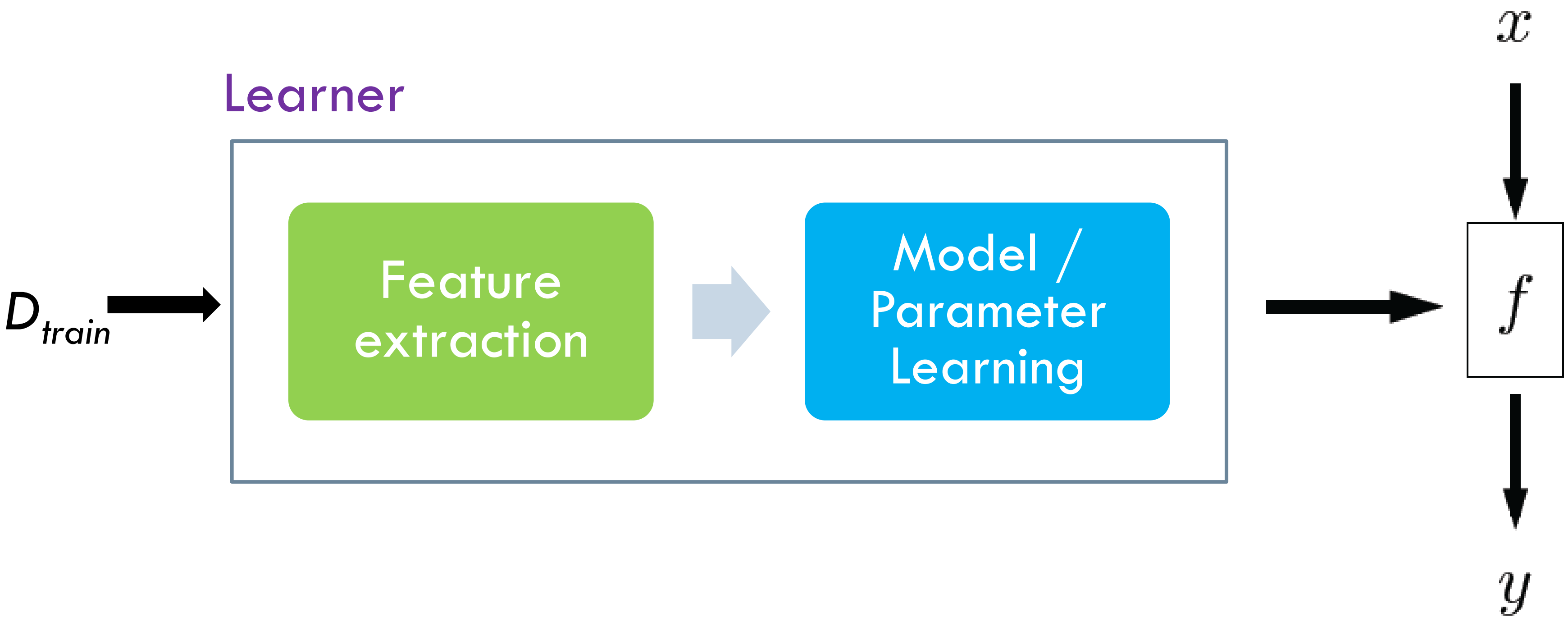
数据 →



digits recognition;

$\mathcal{Y} = \{0, \ldots, 9\}$

Learning Framework



Supervised learning

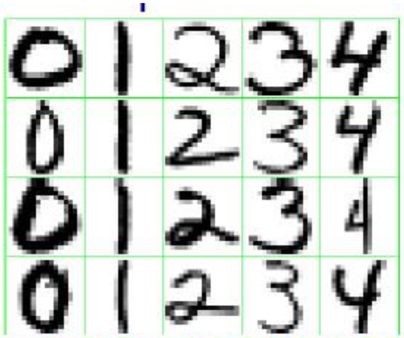
Supervised learning

Formal setup

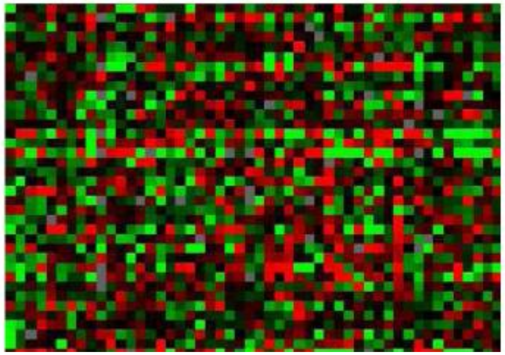
- Input data space $\mathcal{X}$
- Output (label, target) space $\mathcal{Y}$
- Unknown function $f : \mathcal{X} \rightarrow \mathcal{Y}$
- We are given a set of labeled examples $(\mathbf{x}_i, y_i)$, $i = 1, \ldots, N$, with $\mathbf{x}_i \in \mathcal{X}$, $y_i \in \mathcal{Y}$.
- Finite $\mathcal{Y} \Rightarrow$ classification
- Continuous $\mathcal{Y} \Rightarrow$ regression

Classification （分类）

- We are given a set of N observations $\{(\mathbf{x}_i, y_i)\}_{i=1..N}$
- Need to map x $\in \mathcal{X}$ to a label y $\in \mathcal{Y}$
- Examples:



digits recognition; $\mathcal{Y} = \{0, \ldots, 9\}$



prediction from microarray data; $\mathcal{Y} = \{\text{desease present}/\text{absent}\}$

Decision Trees
决策树

Section 18.3

Learning decision trees

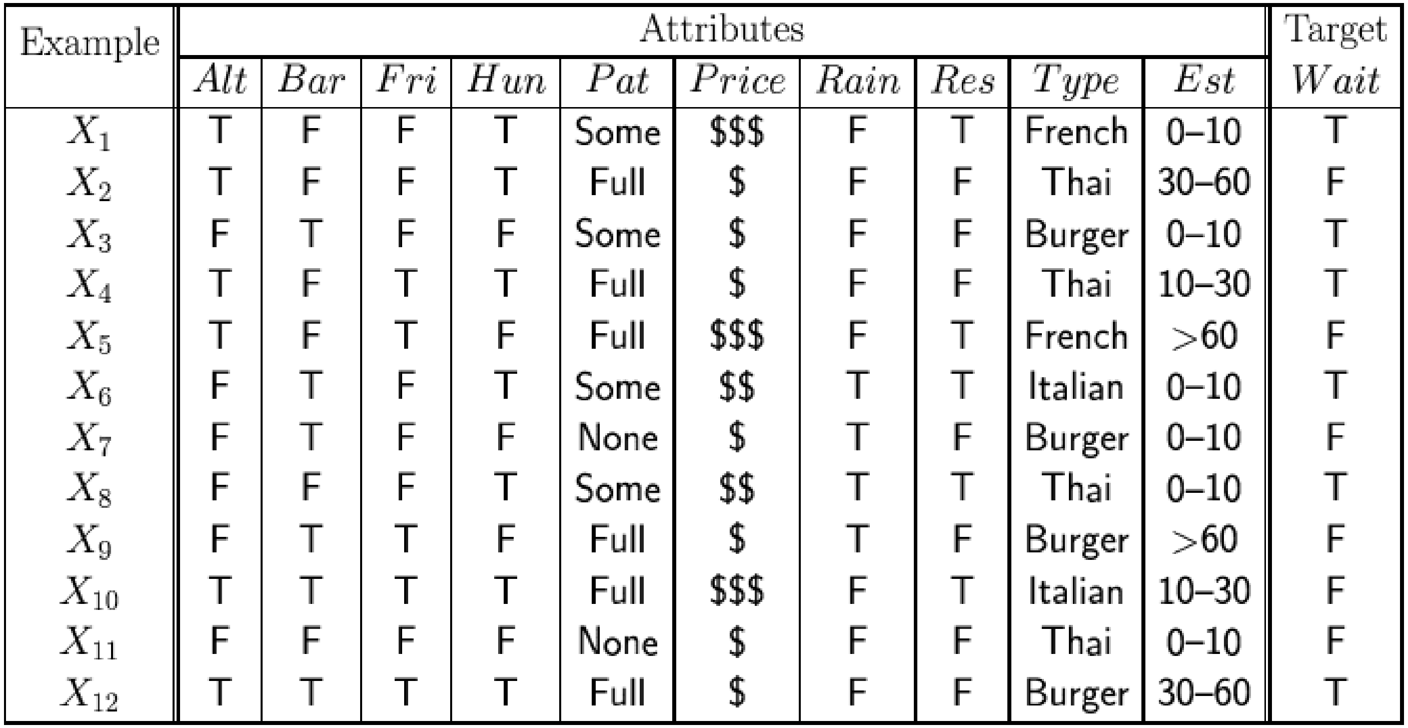
Problem: decide whether to wait for a table at a restaurant, based on the following attributes（属性）：

1. Alternate（别的选择）: is there an alternative restaurant nearby?
2. Bar: is there a comfortable bar area to wait in?
3. Fri/Sat: is today Friday or Saturday?
4. Hungry: are we hungry?
5. Patrons（顾客）: number of people in the restaurant (None, Some, Full)
6. Price: price range ($, $$, $$$)
7. Raining: is it raining outside?
8. Reservation（预约）: have we made a reservation?
9. Type: kind of restaurant (French, Italian, Thai, Burger)
10. WaitEstimate: estimated waiting time (0-10, 10-30, 30-60, >60)

Attribute-based representations

Examples described by attribute values（属性） (Boolean, discrete, continuous)

E.g., situations where I will/won't wait for a table:



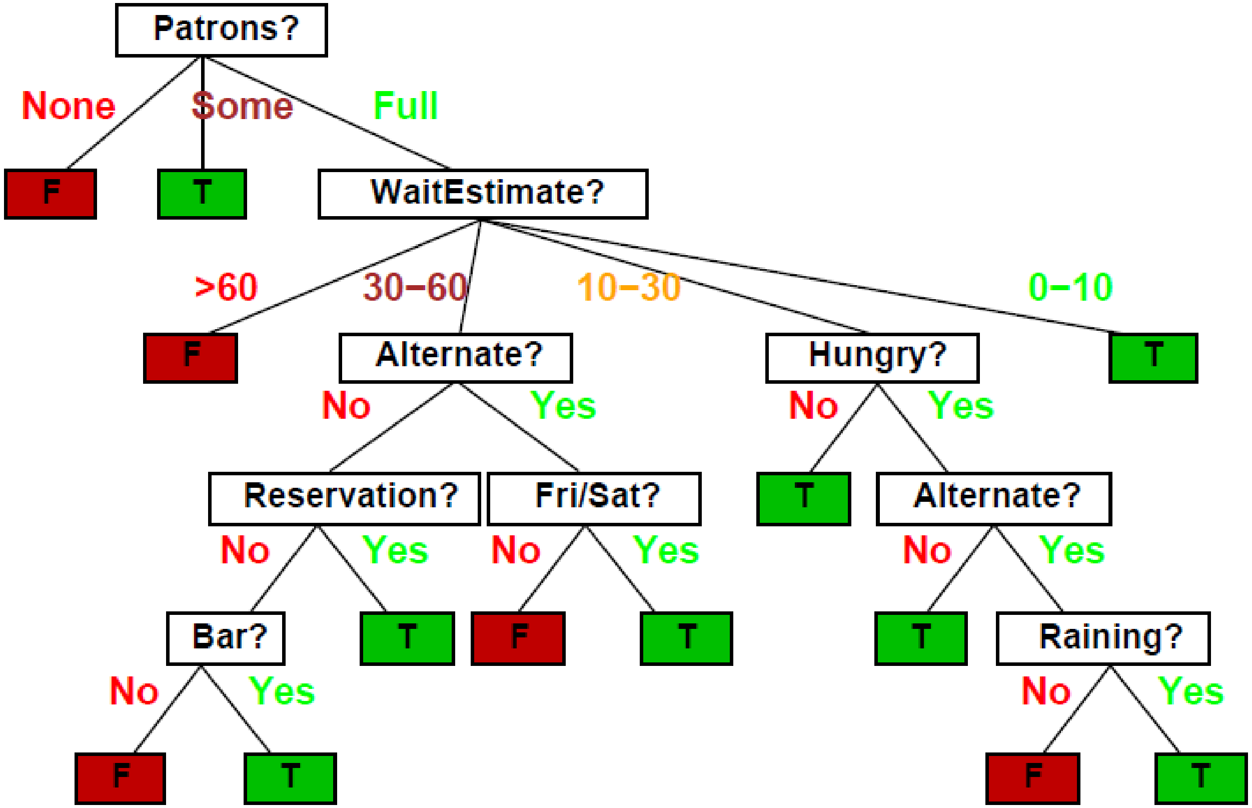
Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	\$\$\$	F	T	French	0–10	T
X_2	T	F	F	T	Full	\$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	\$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	\$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	\$\$\$	F	T	French	>60	F
X_6	F	T	F	T	Some	\$\$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	\$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	\$\$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	\$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	\$\$\$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	\$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	\$	F	F	Burger	30–60	T

Classification（分类） of examples is positive (T) or negative (F)

Decision trees

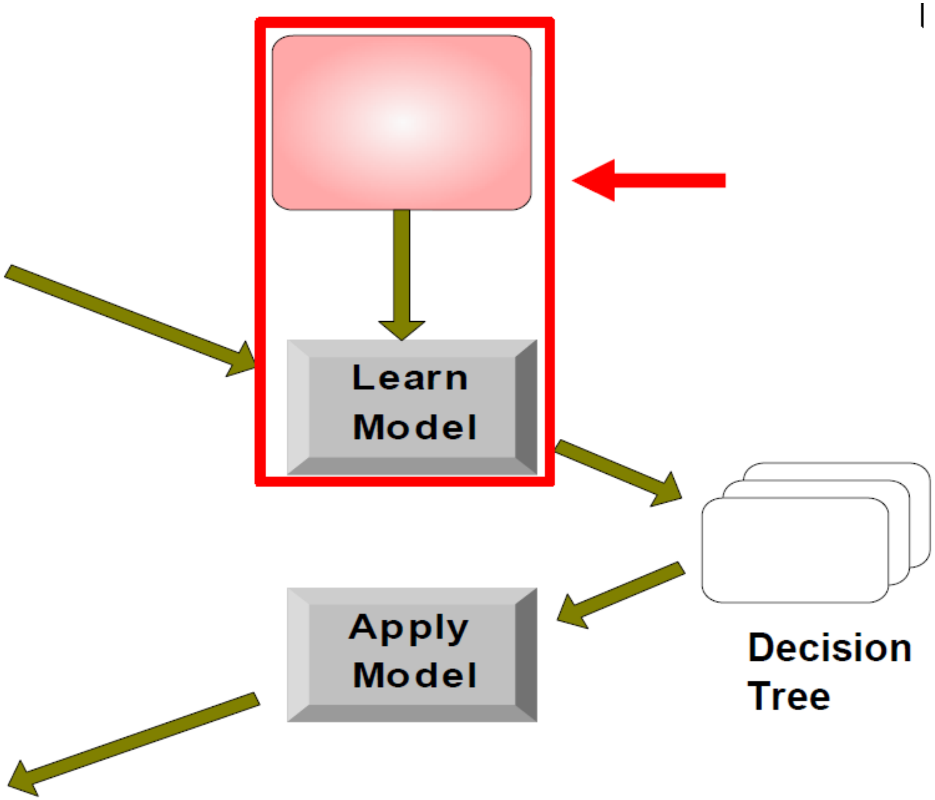
One possible representation for hypotheses

E.g., here is the "true" tree for deciding whether to wait:



Decision Tree Learning

Tid	Attrib1	Attrib2	Attrib3	Class
1	Yes	Large	125K	No
2	No	Medium	100K	No
3	No	Small	70K	No
4	Yes	Medium	120K	No
5	No	Large	95K	Yes
6	No	Medium	60K	No
7	Yes	Large	220K	No
8	No	Small	85K	Yes
9	No	Medium	75K	No
10	No	Small	90K	Yes



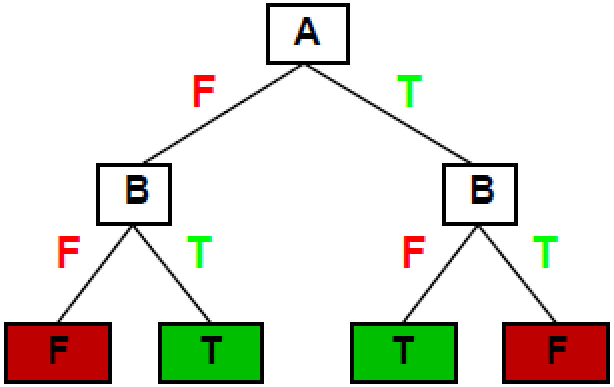
Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

Expressiveness（表达能力）

Decision trees can express any function of the input attributes.

E.g., for Boolean functions, truth table row → path to leaf（函数真值表的每行对应于树中的一条路径）：

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



Trivially, there is a consistent decision tree for any training set with one path to leaf for each example (unless *f* nondeterministic in *x*) but it probably won't generalize to new examples

Prefer to find more compact decision trees

Hypothesis spaces（假设空间）

How many distinct decision trees with *n* Boolean attributes?

= number of Boolean functions

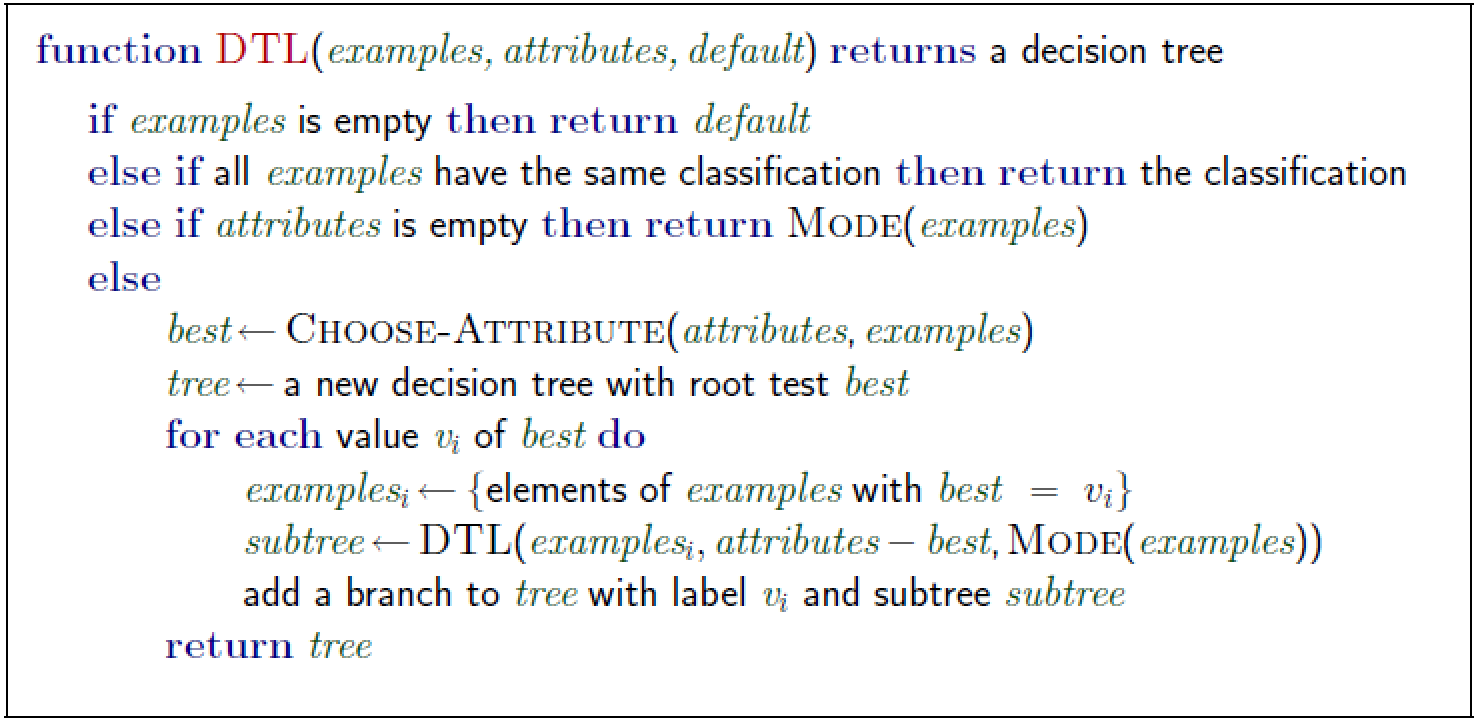
= number of distinct truth tables with 2^n rows = 2^{2^n}

- E.g., with 6 Boolean attributes, there are 18,446,744,073,709,551,616 trees

Decision tree learning

Aim: find a small tree consistent with the training examples

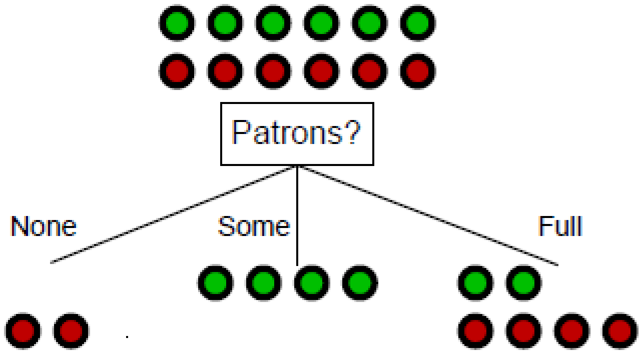
Idea: (recursively) choose "most significant" attribute as root of (sub)tree

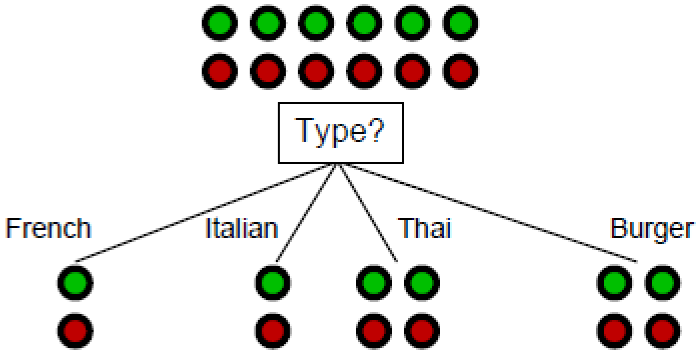


```
function DTL($examples$, $attributes$, $default$) returns a decision tree
    if $examples$ is empty then return $default$
    else if all $examples$ have the same classification then return the classification
    else if $attributes$ is empty then return MODE($examples$)
    else
        $best \leftarrow$ CHOOSE-ATTRIBUTE($attributes$, $examples$)
        $tree \leftarrow$ a new decision tree with root test $best$
        for each value $v_i$ of $best$ do
            $examples_i \leftarrow$ {elements of $examples$ with $best = v_i$}
            $subtree \leftarrow$ DTL($examples_i$, $attributes - best$, MODE($examples$))
            add a branch to $tree$ with label $v_i$ and subtree $subtree$
        return $tree$
```

Choosing an attribute

Idea: a good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative"





Patrons? is a better choice

Using information theory（信息论）

To implement `Choose-Attribute` in the DTL algorithm

Information Content 信息量(Entropy熵):

$$I(P(v_1), \ldots, P(v_n)) = \sum_{i=1}^{n} -P(v_i) \log_2 P(v_i)$$

For a training set containing *p* positive examples and *n* negative examples:

$$I(\frac{p}{p+n}, \frac{n}{p+n}) = -\frac{p}{p+n}\log_2 \frac{p}{p+n} - \frac{n}{p+n}\log_2 \frac{n}{p+n}$$

Information gain（信息增益）

A chosen attribute *A* divides the training set *E* into subsets E_1, … , E_v according to their values for *A*, where *A* has v distinct values.

$$remainder(A) = \sum_{i=1}^{v} \frac{p_i + n_i}{p+n} I\left(\frac{p_i}{p_i + n_i}, \frac{n_i}{p_i + n_i}\right)$$

Information Gain (IG) or reduction in entropy from the attribute test:

$$IG(A) = I\left(\frac{p}{p+n}, \frac{n}{p+n}\right) - remainder(A)$$

Choose the attribute with the largest IG

Information gain

For the training set, $p = n = 6$, $I(6/12, 6/12) = 1$ bit

Consider the attributes *Patrons* and *Type* (and others too):

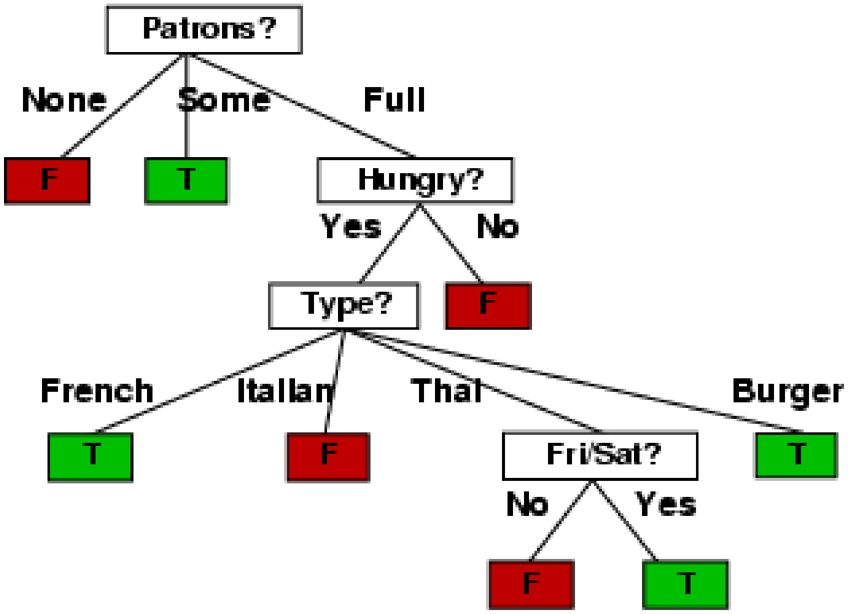
$$IG(Patrons) = 1 - [\frac{2}{12}I(0,1) + \frac{4}{12}I(1,0) + \frac{6}{12}I(\frac{2}{6},\frac{4}{6})] = .541\,\text{bits}$$

$$IG(Type) = 1 - [\frac{2}{12}I(\frac{1}{2},\frac{1}{2}) + \frac{2}{12}I(\frac{1}{2},\frac{1}{2}) + \frac{4}{12}I(\frac{2}{4},\frac{2}{4}) + \frac{4}{12}I(\frac{2}{4},\frac{2}{4})] = 0\,\text{bits}$$

Patrons has the highest IG of all attributes and so is chosen by the DTL algorithm as the root

Example contd.

Decision tree learned from the 12 examples:



Substantially simpler than “true” tree---a more complex hypothesis isn’t justified by small amount of data

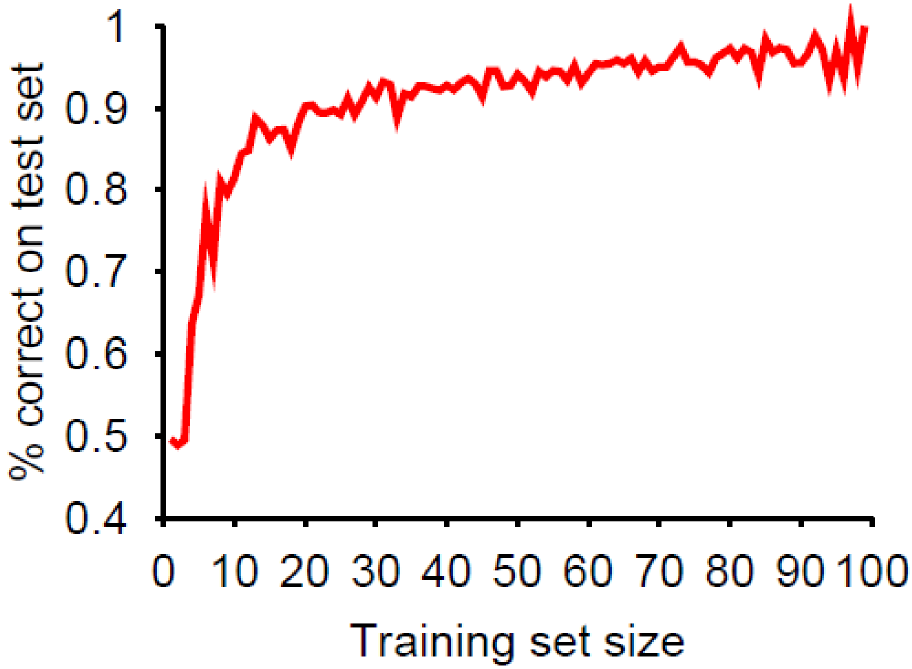
Performance measurement

How do we know that $h \approx f$?

1. Use theorems of computational/statistical learning theory
2. Try h on a new test set（测试集） of examples

(use same distribution over example space as training set)

Learning curve（学习曲线） = % correct on test set as a function of training set size



Comments on decision tree based classification

Advantages:

- Inexpensive to construct
- Extremely fast at classifying unknown records
- Easy to interpret for small-sized trees
- Accuracy is comparable to other classification techniques for many simple data sets

Example: C4.5

- Simple depth-first construction.
- Uses Information Gain
- You can download the software from:

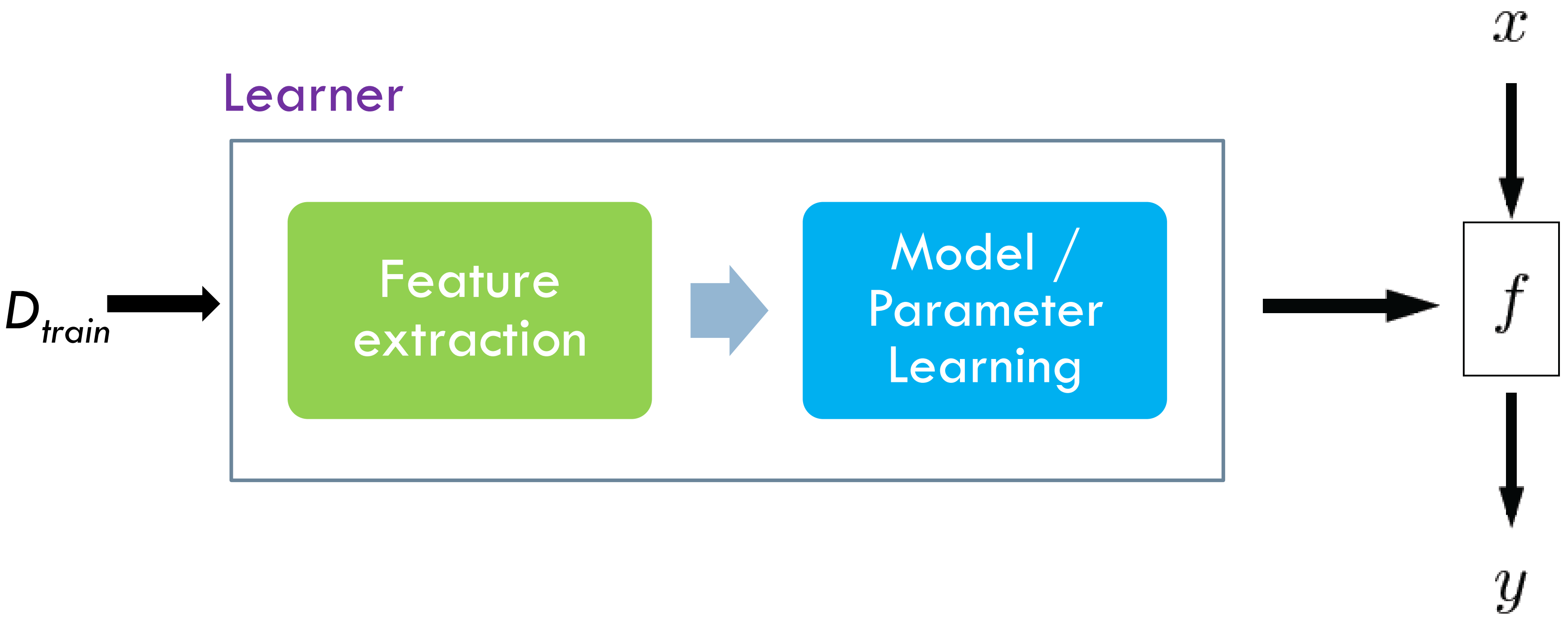
  http://www.cse.unsw.edu.au/~quinlan/c4.5r8.tar.gz

K nearest neighbor classifier 最近邻模型

Section 20.4

Linear predictions
线性预测

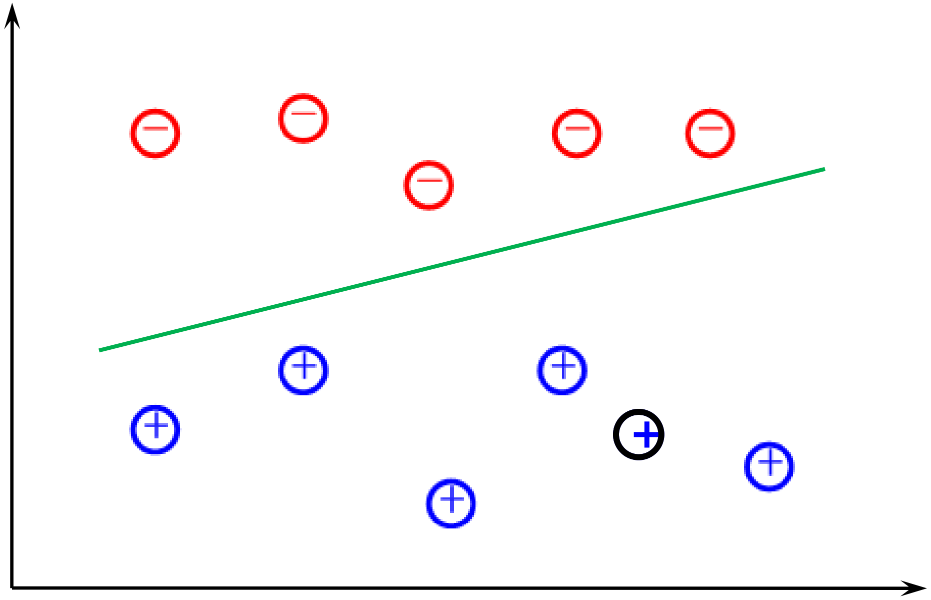
Learning Framework



Classification

Classification

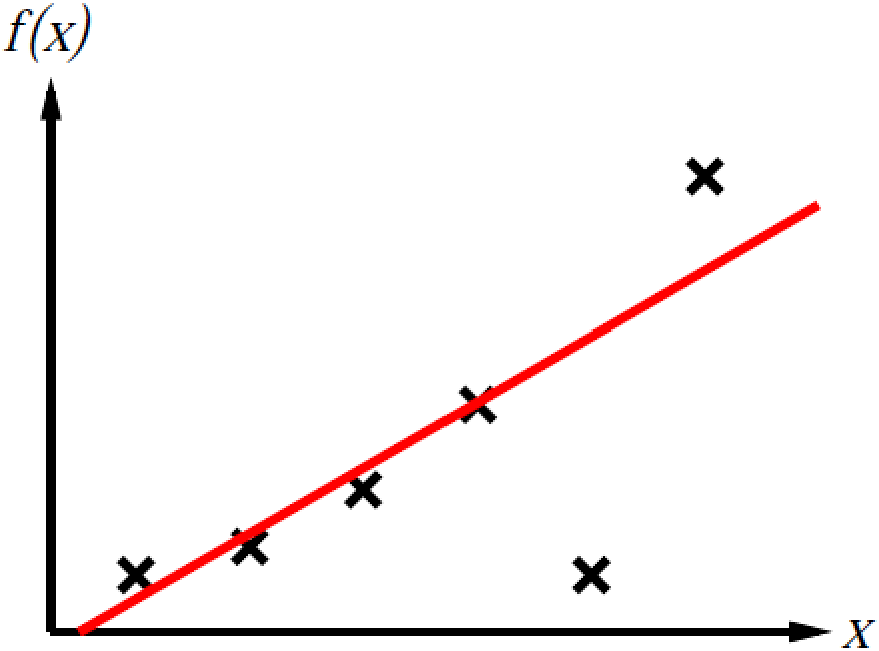
= learning from data with finite discrete labels. Dominant problem in Machine Learning



Regression（回归）

Regression

= learning from continuously labeled data.



Focus of this part

- □ Binary classification (e.g., predicting spam or not spam):

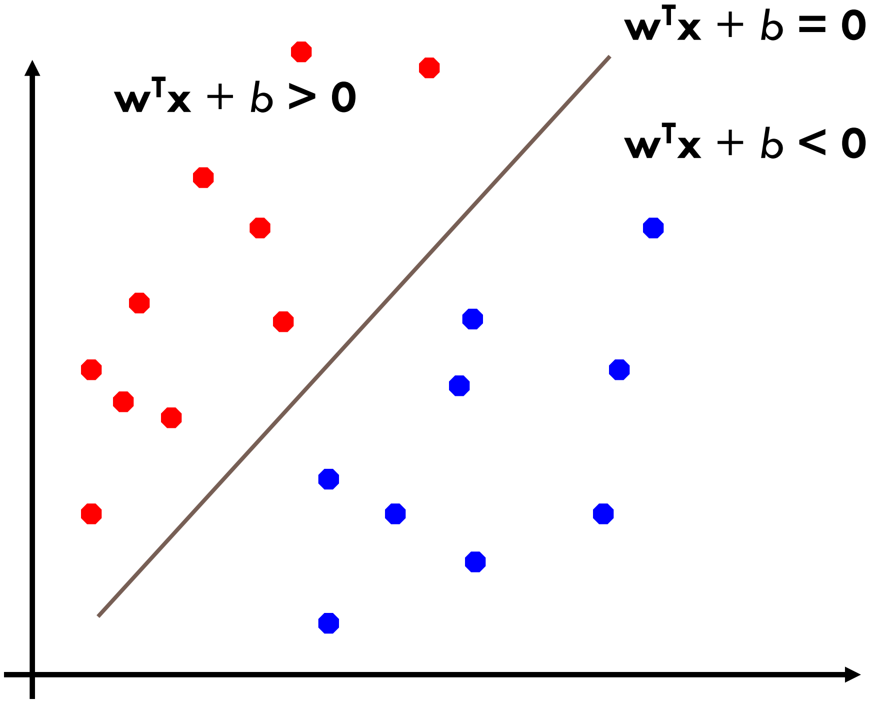
$$x \longrightarrow \boxed{f} \longrightarrow y \in \{-1, +1\}$$

- □ Regression (e.g., predicting housing price):

$$x \longrightarrow \boxed{f} \longrightarrow y \in \mathbb{R}$$

Linear Classifiers

Binary classification can be viewed as the task of separating classes in feature space（特征空间）：


$\mathbf{w}^T\mathbf{x} + b = 0$
$\mathbf{w}^T\mathbf{x} + b > 0$
$\mathbf{w}^T\mathbf{x} + b < 0$

Decide $\hat{y} = 1$ if $\mathbf{w}^T\mathbf{x} + b > 0$,
otherwise $\hat{y} = -1$

$$\hat{y} = h(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$$

Roadmap

Linear Prediction

Loss Minimization

Linear Classifiers

$$h(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$$

- □ Need to find **w** (direction) and *b* (location) of the boundary
- □ Want to minimize the expected zero/one loss（损失）for classifier *h*: $\mathcal{X} \rightarrow \mathcal{Y}$, which is

$$L(h(\mathbf{x}), y) = \begin{cases} 0 & \text{if } h(\mathbf{x}) = y, \\ 1 & \text{if } h(\mathbf{x}) \neq y. \end{cases}$$

Gold standard (ideal case)

Linear Classifiers → Loss Minimization

Ideally we want to find a classifier

$h(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^T\mathbf{x} + b)$ to minimize the 0/1 loss

$$\min_{\mathbf{w},b} \sum_i L_{0/1}(h(\mathbf{x}_i), y_i)$$

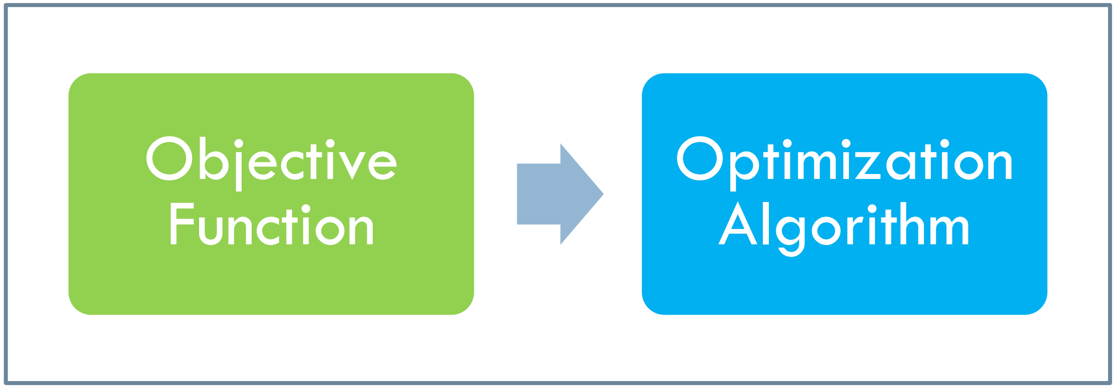
Unfortunately, this is a hard problem..

Alternate loss functions:

$$\begin{aligned} L_2(h(\mathbf{x}), y) &= (y - \mathbf{w}^\top \mathbf{x} - b)^2 = (1 - y(\mathbf{w}^\top \mathbf{x} + b))^2 \\ L_1(h(\mathbf{x}), y) &= |y - \mathbf{w}^\top \mathbf{x} - b| = |1 - y(\mathbf{w}^\top \mathbf{x} + b)| \\ L_{hinge}(h(\mathbf{x}), y) &= (1 - y(\mathbf{w}^\top \mathbf{x} + b))_+ \end{aligned}$$

Learning as Optimization

Parameter Learning



Objective Function

Optimization Algorithm

Least Squares Classification

Least squares loss function:

$$L_2(h(\mathbf{x}), y) = (y - \mathbf{w}^\top \mathbf{x} - b)^2$$

The goal:

to learn a classifier *h*(**x**) = sign(**w**ᵀ**x** + *b*) to minimize the least squares loss

$$\begin{aligned} Loss &= \min_{\mathbf{w},b} \sum_i L_2(h(\mathbf{x}_i), y_i) \\ &= \min_{\mathbf{w},b} \sum_i (y_i - \mathbf{w}^\top \mathbf{x}_i - b)^2 \end{aligned}$$

Solving Least Squares Classification

Let

$$\mathbf{X} = \begin{bmatrix} 1 & x_{11} & \cdots & x_{1d} \\ \vdots & & \vdots & \\ 1 & x_{N1} & \cdots & x_{Nd} \end{bmatrix}, \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix}, \qquad \mathbf{w} = \begin{bmatrix} b \\ \vdots \\ w_d \end{bmatrix}$$

$$\begin{aligned} Loss = \min_{\mathbf{w}}(\mathbf{y} - X\mathbf{w})^2 &= \min_{\mathbf{w}}(X\mathbf{w} - \mathbf{y})^2 \\ &= \min_{\mathbf{w}}(X\mathbf{w} - \mathbf{y})^\top(X\mathbf{w} - \mathbf{y}) \end{aligned}$$

Solving for w

$$\begin{aligned}
\frac{\partial Loss}{\partial \mathbf{w}} = 2(X\mathbf{w} - \mathbf{y})^\top X &= 0 \\
X^\top X\mathbf{w} - X^\top \mathbf{y} &= 0 \\
\mathbf{w}^* &= (X^\top X)^{-1} X^\top \mathbf{y}
\end{aligned}$$

Note: $d(\mathbf{Ax}+\mathbf{b})^T\mathbf{C}(\mathbf{Dx}+\mathbf{e}) = ((\mathbf{Ax}+\mathbf{b})^T\mathbf{CD} + (\mathbf{Dx}+\mathbf{e})^T\mathbf{C}^T\mathbf{A})\, d\mathbf{x}$

$d(\mathbf{Ax}+\mathbf{b})^T(\mathbf{Ax}+\mathbf{b}) = (2(\mathbf{Ax}+\mathbf{b})^T\mathbf{A})\, d\mathbf{x}$

- □ $X^+ = (X^\top X)^{-1} X^\top$ called the *Moore-Penrose* pseudoinverse （伪逆） of X
- □ Least squares classification in Matlab

```
% X(i: ,) is the i-th example, y(i) is the i-th label
wLSQ = pinv([ones(size(X, 1), 1) X])*y;
```

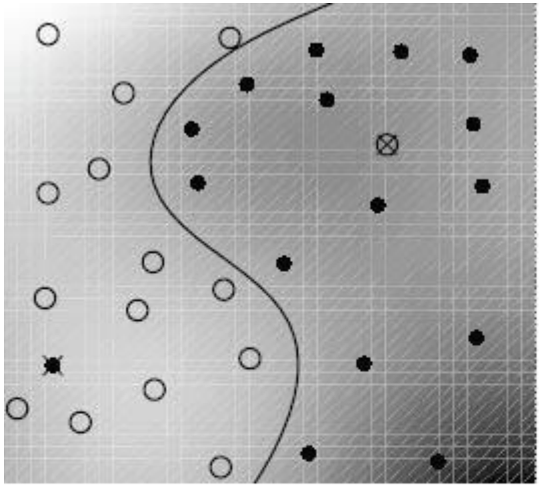
- □ Prediction for $\mathbf{x}_0$

$$\hat{y} = \operatorname{sign}\left(\mathbf{w}^{*\top}\begin{bmatrix}1\\ \mathbf{x}_0\end{bmatrix}\right) = \operatorname{sign}\left(\mathbf{y}^\top X^{+\top}\begin{bmatrix}1\\ \mathbf{x}_0\end{bmatrix}\right)$$

General linear classification

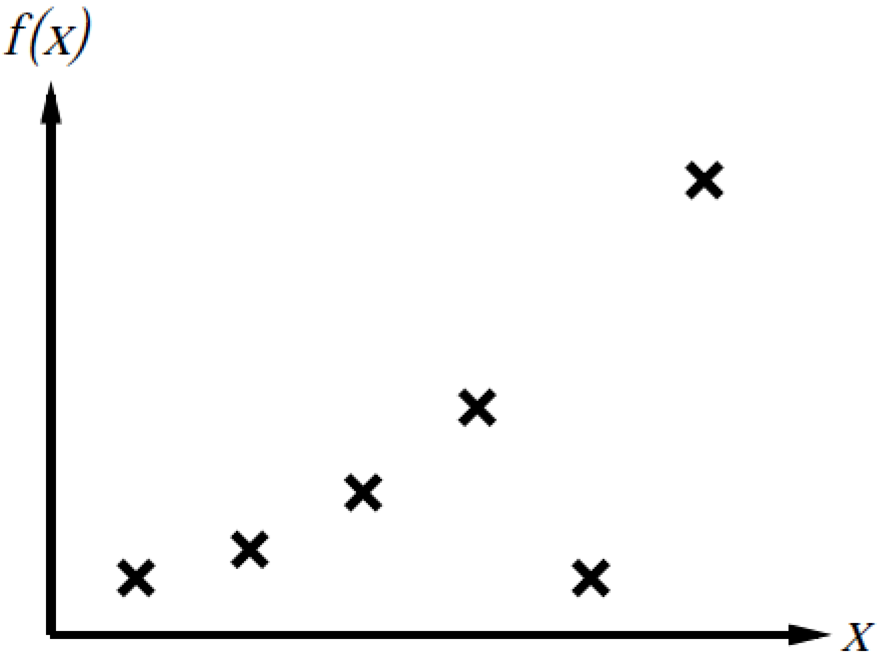
Basis (nonlinear) functions （基函数）

$$f(\mathbf{x},\mathbf{w}) = b + w_1\phi_1(\mathbf{x}) + w_2\phi_2(\mathbf{x}) + \cdots + w_m\phi_m(\mathbf{x})$$



Model complexity and overfitting

E.g., curve fitting（曲线拟合）：



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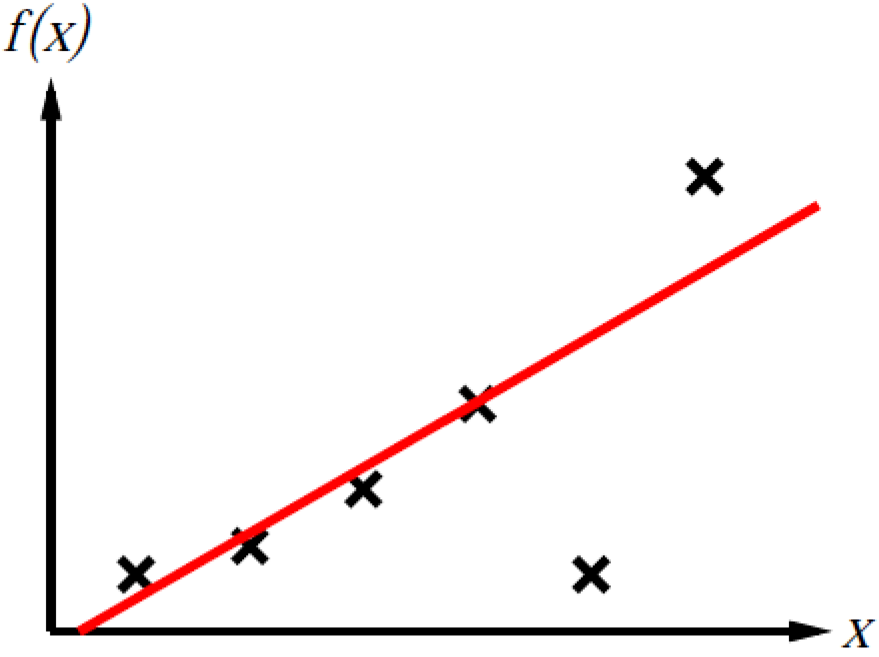

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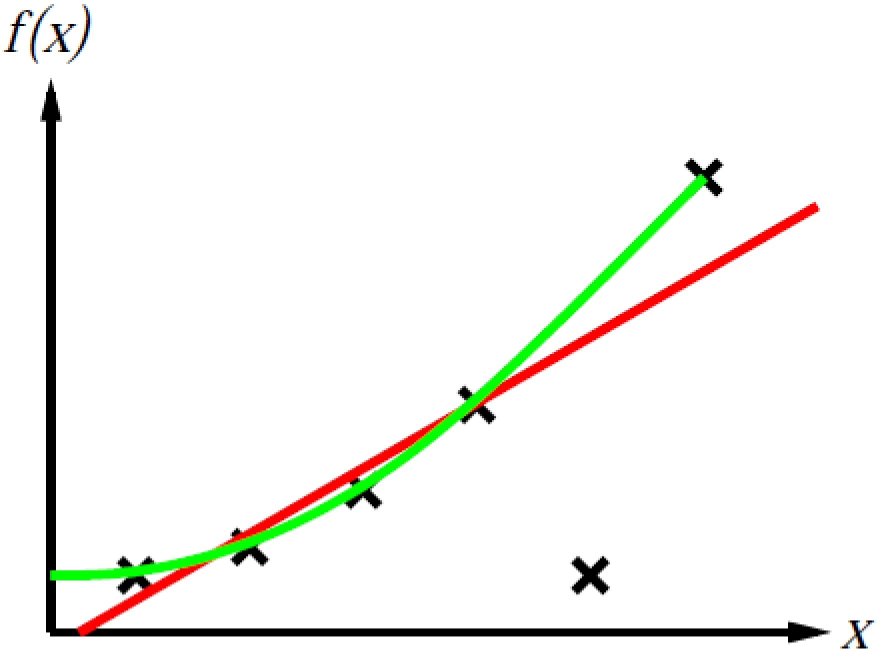

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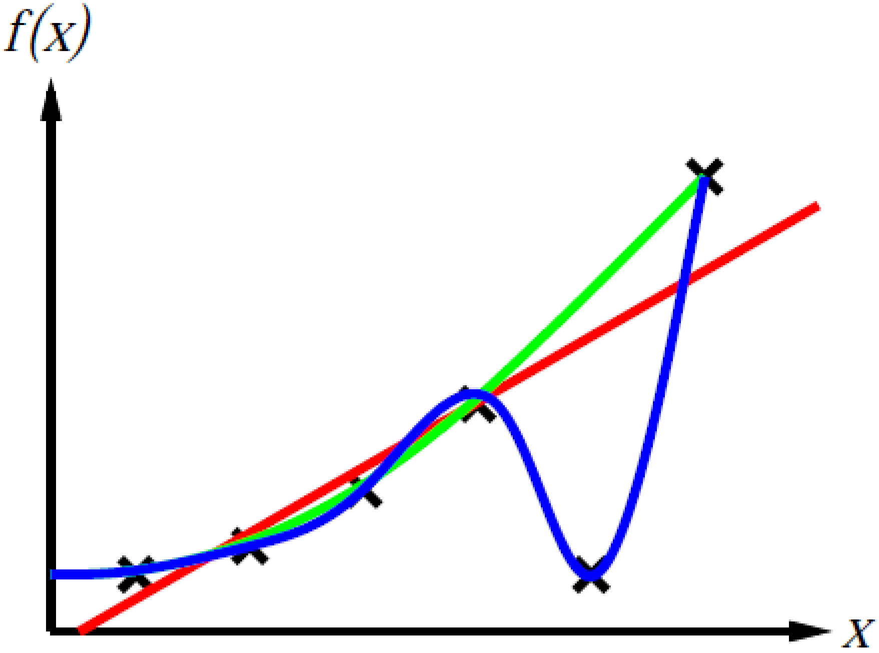

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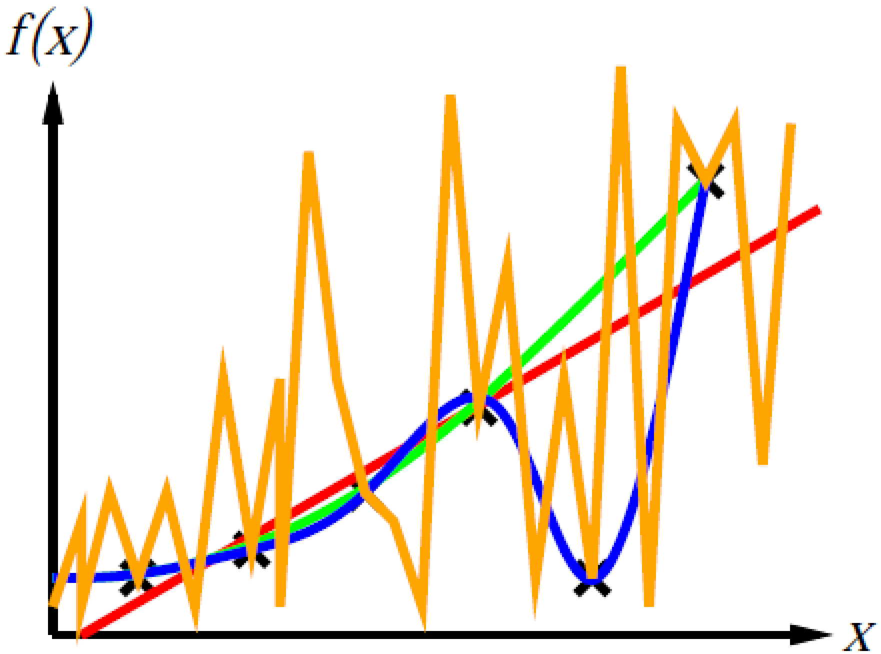

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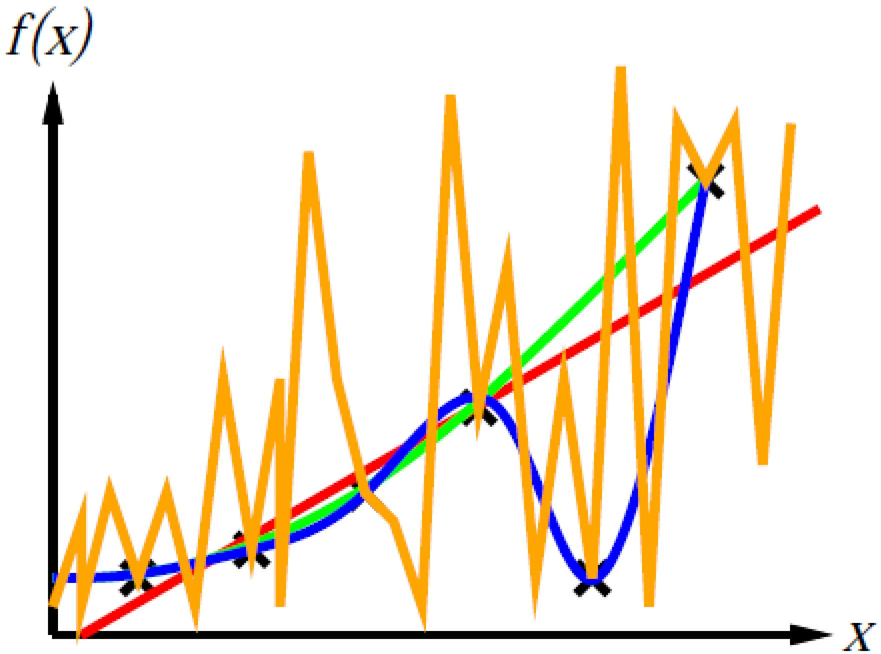


Ockham‘s razor（奥卡姆剃刀原则）: maximize a combination of consistency and simplicity
优先选择与数据一致的最简单的假设

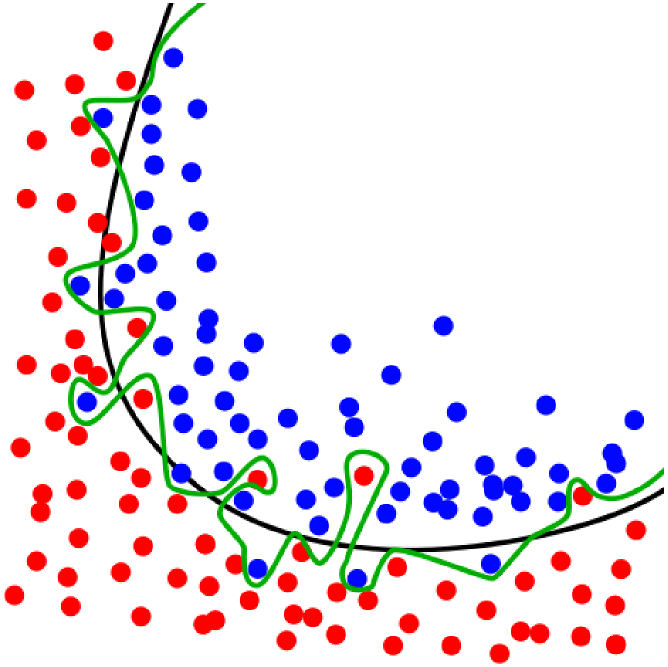
Prediction Errors

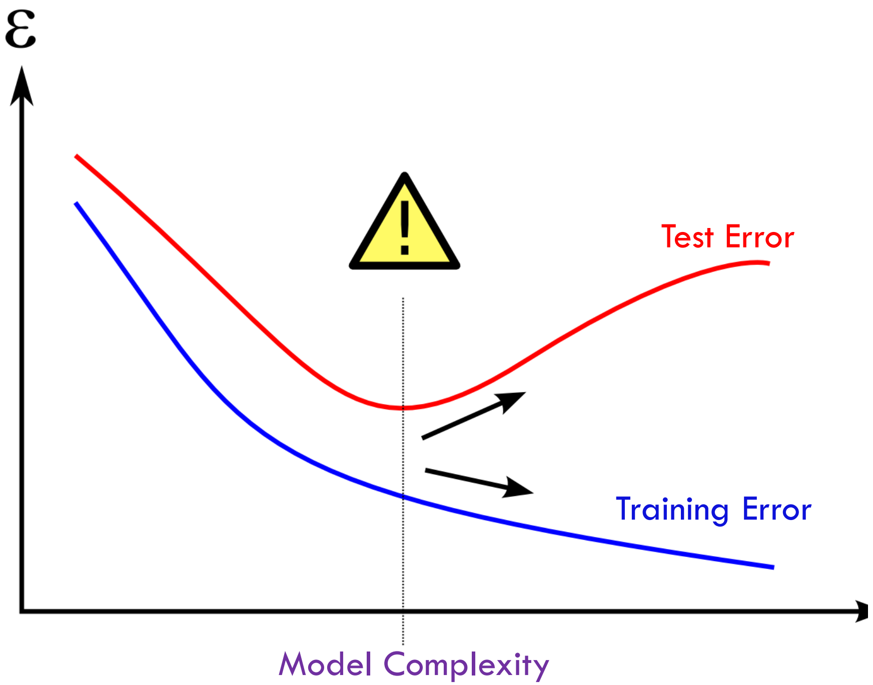
- Training errors (apparent errors) — 训练误差
  - Errors committed on the training set

- Test errors — 测试误差
  - Errors committed on the test set

- Generalization errors — 泛化误差
  - Expected error of a model over random selection of records from same distribution（未知记录上的期望误差）

Model complexity and overfitting





Underfitting: when model is too simple, both training and test errors are large

Overfitting: when model is too complex, training error is small but test error is large

Incorporating Model Complexity

- Rationale: Ockham's Razor
  - Given two models of similar generalization errors, one should prefer the simpler model over the more complex model
  - A complex model has a greater chance of being fitted accidentally by errors in data
  - Therefore, one should include model complexity when evaluating a model

Regularization（规范化）

Intuition: should penalize not the parameters, but the number of bits required to encode the parameters

$$\mathbf{w}^* = \arg\min_{\mathbf{w}} \; Loss + \lambda \cdot penalty(\mathbf{w})$$

L2 regularization $$\mathbf{w}^* = \arg\min_{\mathbf{w}} \; Loss + \lambda \|\mathbf{w}\|^2$$

L1 regularization $$\mathbf{w}^* = \arg\min_{\mathbf{w}} \; Loss + \lambda |\mathbf{w}|$$

Regularization parameter

- □ Solving L2-regularized LS

$$\min_{\mathbf{w}} (X\mathbf{w} - \mathbf{y})^2 + \lambda \|\mathbf{w}\|^2$$

Solution?

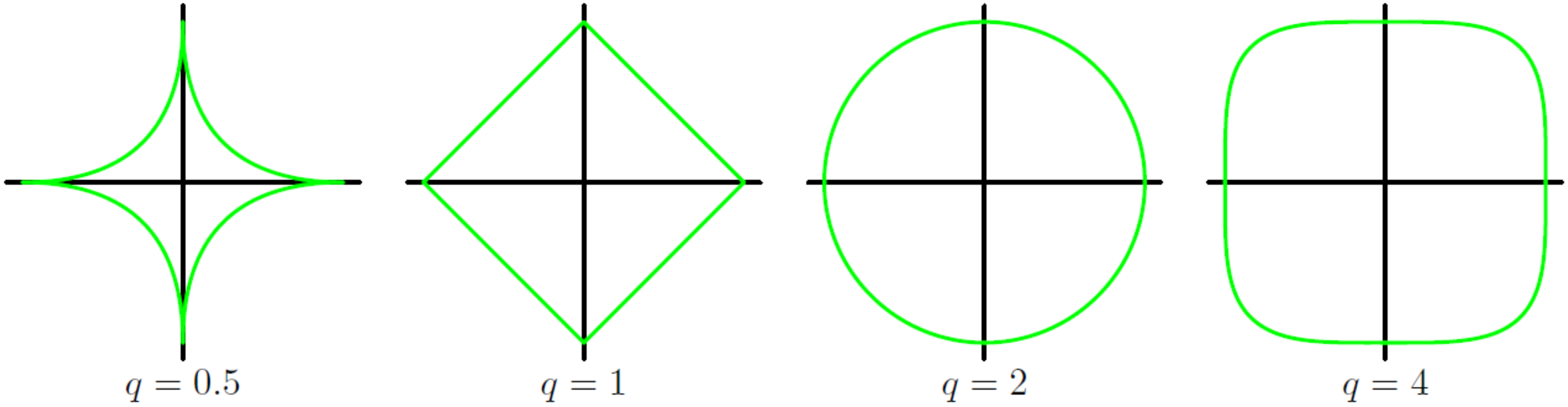
Regularization

$$\begin{aligned}\mathbf{w}^* &= \arg\min_{\mathbf{w}} \; Loss + \lambda \cdot penalty(\mathbf{w}) \\ &= \arg\min_{\mathbf{w}} \; Loss + \lambda R_q\end{aligned}$$

$$R_q = \sum_i |w_i|^q$$

When λ sufficiently large, equivalent to:

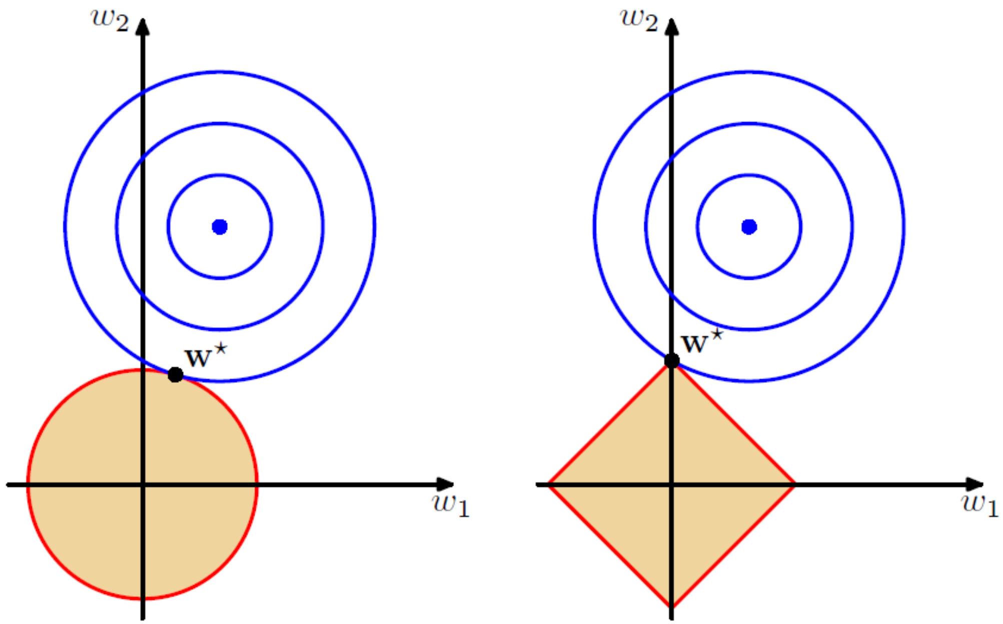
$$\min_{\mathbf{w}} \; Loss \text{ subject to } \sum_i |w_i|^q \cdot \; \eta$$



Contours of the regularization term for various value of q

L-2 and L-1 regularization

- L-2: easy to optimize, closed form solution
- L-1: sparsity



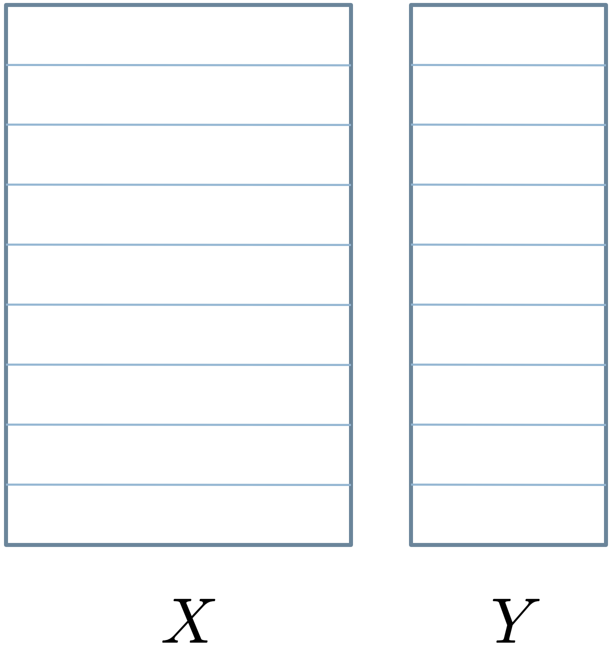
More than two classes?

Given

- $N \times d$ data matrix X
- $N\times\ k$ label matrix Y
- $N =$ # training instances
- $d =$ # features
- $k =$ # targets

Assume

- $k < d$



More than two classes

- Learn:
  - parameters W $(N \times d)$ for a model $f_W : X \mapsto Y$
- Objective $\min_{W} tr\left((XW - Y)(XW - Y)^\top\right)$
  - A convex quadratic, so just solve for a critical point:

$$\frac{d}{dW} = 2X^\top(XW - Y) = 0$$

  - Thus $$\begin{aligned} X^\top XW &= X^\top Y \\ W &= (X^\top X)^{-1}X^\top Y = X^\dagger Y \end{aligned}$$

Comments on least squares classification

- Not the best thing to do for classification
- But
  - Easy to train, closed form solution（闭式解）
  - Ready to connect with many classical learning principles

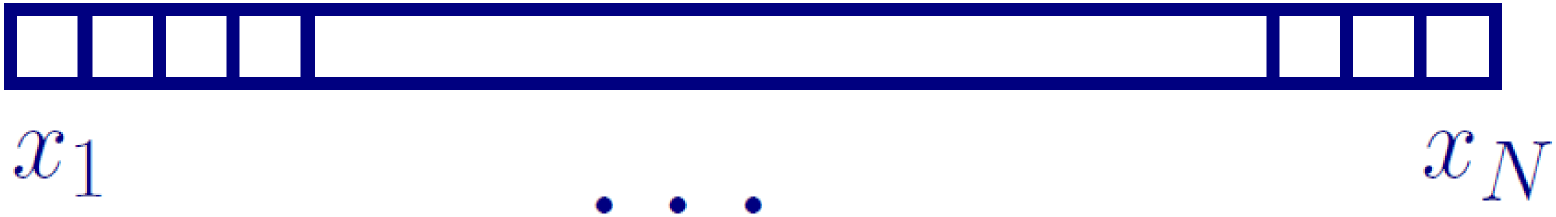
Cross-validation（交叉验证）

- The basic idea: if a model overfits (is too sensitive to data) it will be unstable. I.e. removal part of the data will change the fit significantly.

- We can hold out（取出） part of the data, fit the model to the rest, and then test on the heldout set.

Cross-validation

- The improved holdout method: k-fold *cross-validation*
  - Partition data into k roughly equal parts;
  - Train on all but j-th part, test on j-th part



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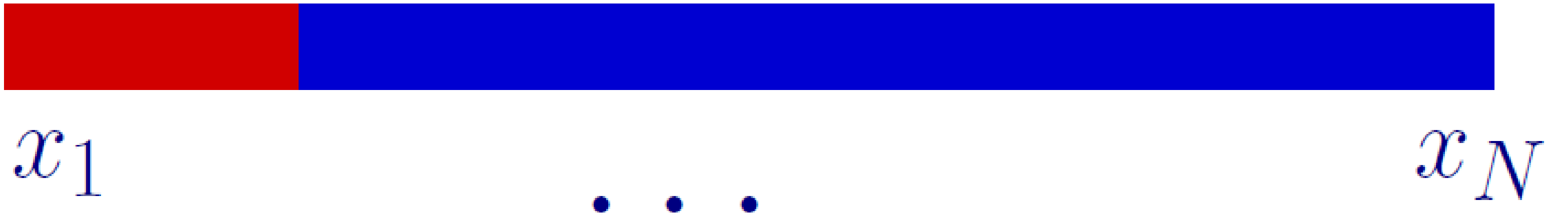

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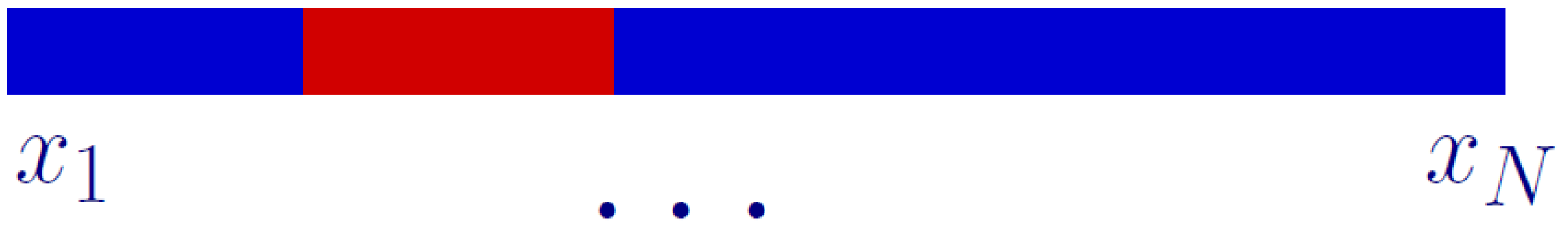

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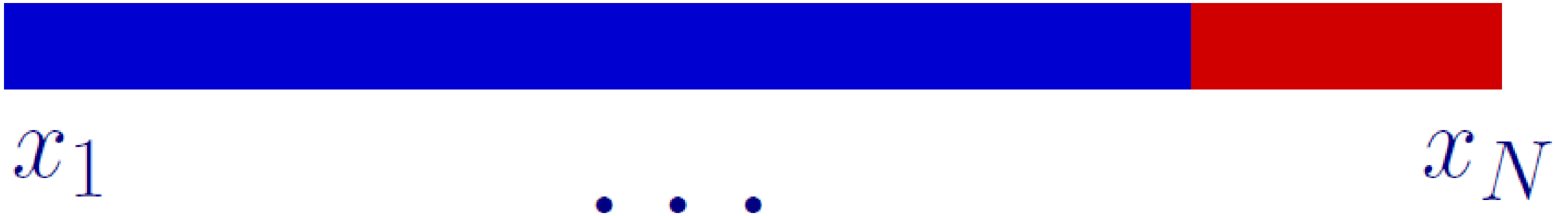
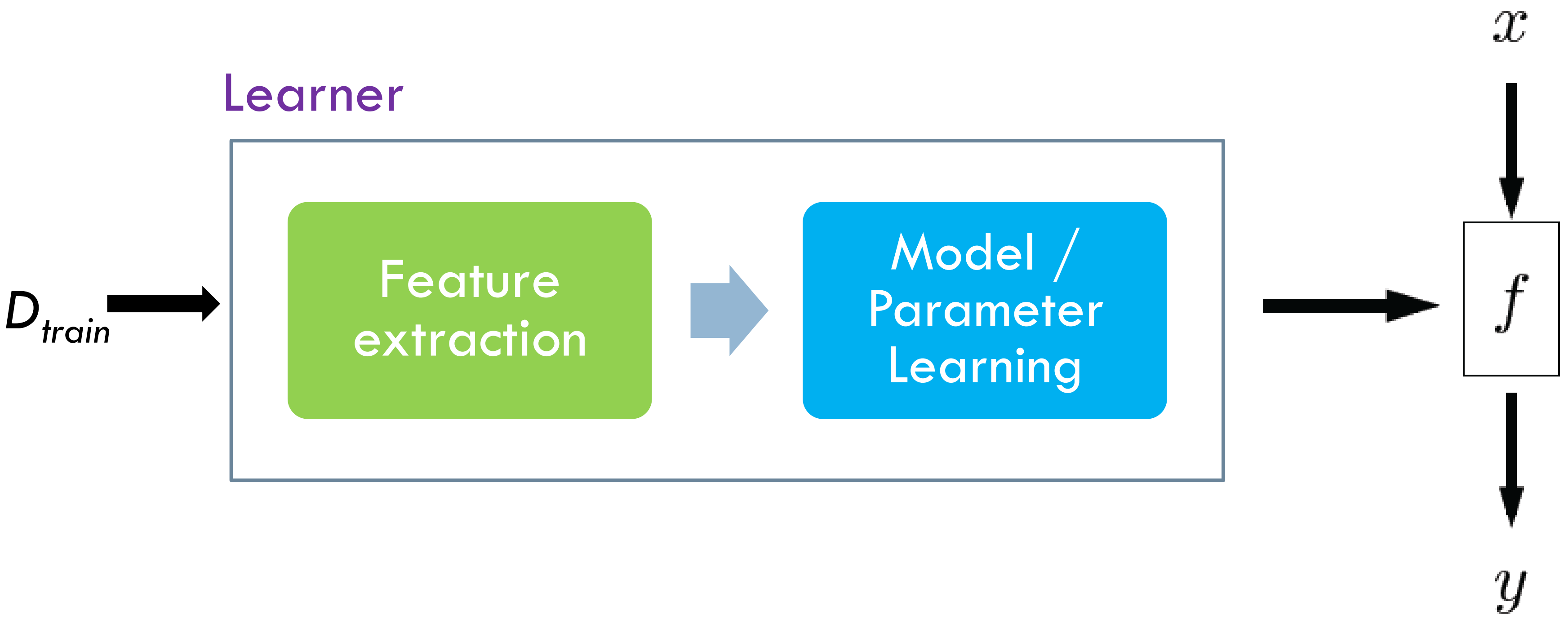


Learning Framework



Model/parameter learning paradigm

- Choose a model class
  - NB, kNN, decision tree, loss/regularization combination
- Model selection
  - Cross validation
- Training
  - Optimization
- Testing

Summary

Supervised learning

- Classification
  - Naïve Bayes model
  - Decision tree
  - Least squares classification
- Regression
  - Least squares regression