Supervised learning

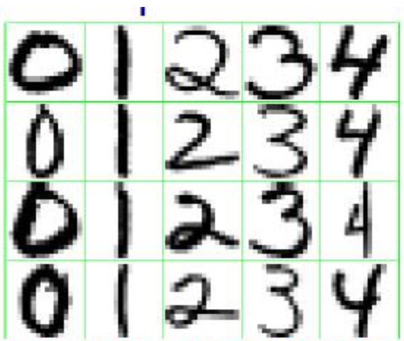
Supervised learning

Formal setup

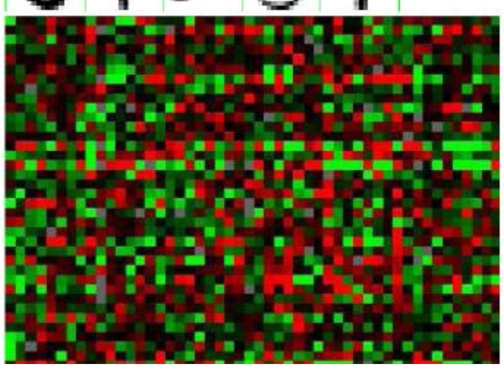
- Input data space $\mathcal{X}$
- Output (label, target) space $\mathcal{Y}$
- Unknown function $f : \mathcal{X} \to \mathcal{Y}$
- We are given a set of labeled examples $(\mathbf{x}_i, y_i)$, $i = 1, \ldots, N$, with $\mathbf{x}_i \in \mathcal{X}$, $y_i \in \mathcal{Y}$.
- Finite $\mathcal{Y} \Rightarrow$ 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;
$\mathcal{Y} = \{\text{desease present/absent}\}$

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:

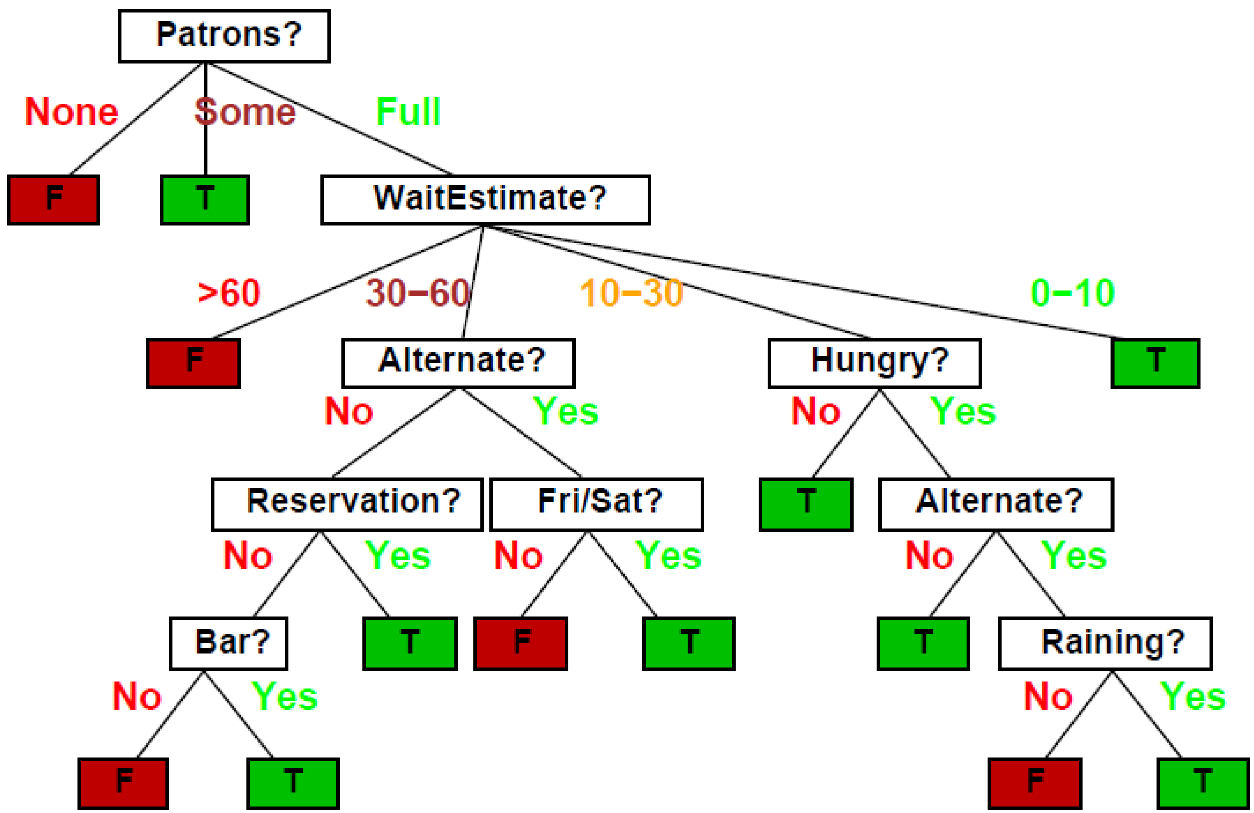
Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*Wait*
X_1	T	F	F	T	Some	\$\$\$	F	T	French	0–10	T
X_2	T	F	F	T	Full	\$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	\$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	\$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	\$\$\$	F	T	French	>60	F
X_6	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

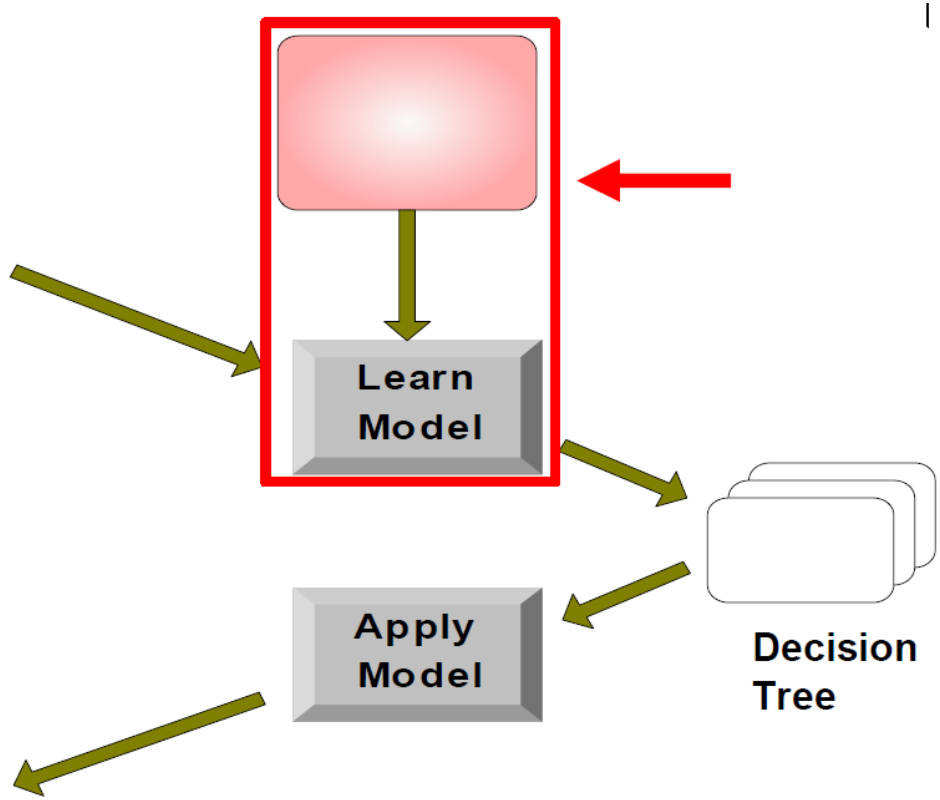
One possible representation for hypotheses

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



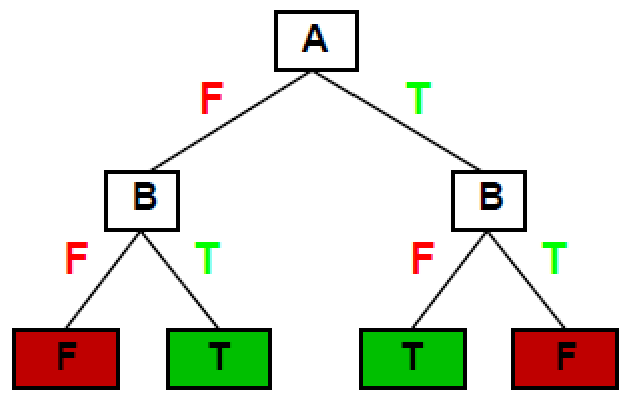
Tid	Attrib1	Attrib2	Attrib3	Class
11	No	Small	55K	?
12	Yes	Medium	80K	?
13	Yes	Large	110K	?
14	No	Small	95K	?
15	No	Large	67K	?

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

Decision tree learning

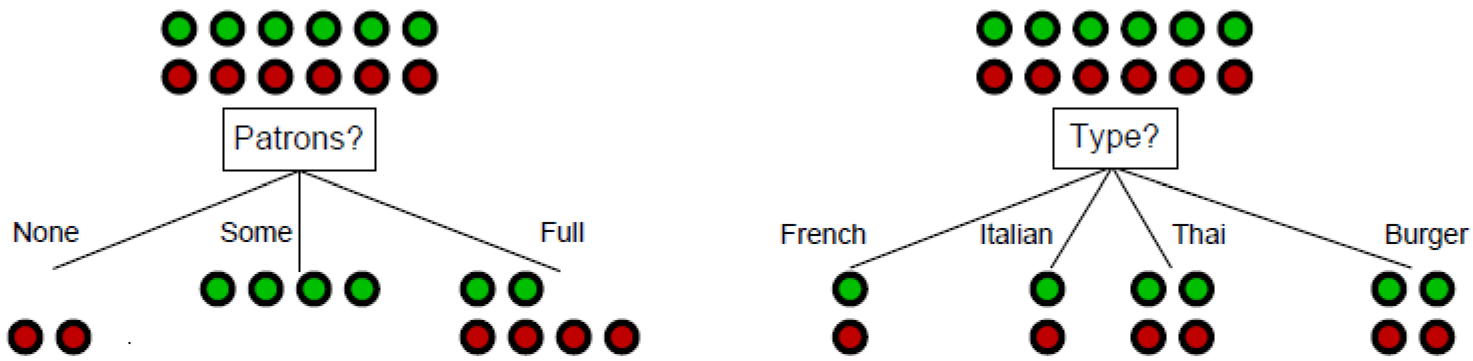
Aim: find a small tree consistent with the training examples

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 ← CHOOSE-ATTRIBUTE(attributes, examples)
        tree ← a new decision tree with root test best
        for each value v_i of best do
            examples_i ← {elements of examples with best = v_i}
            subtree ← 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):

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

- 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):

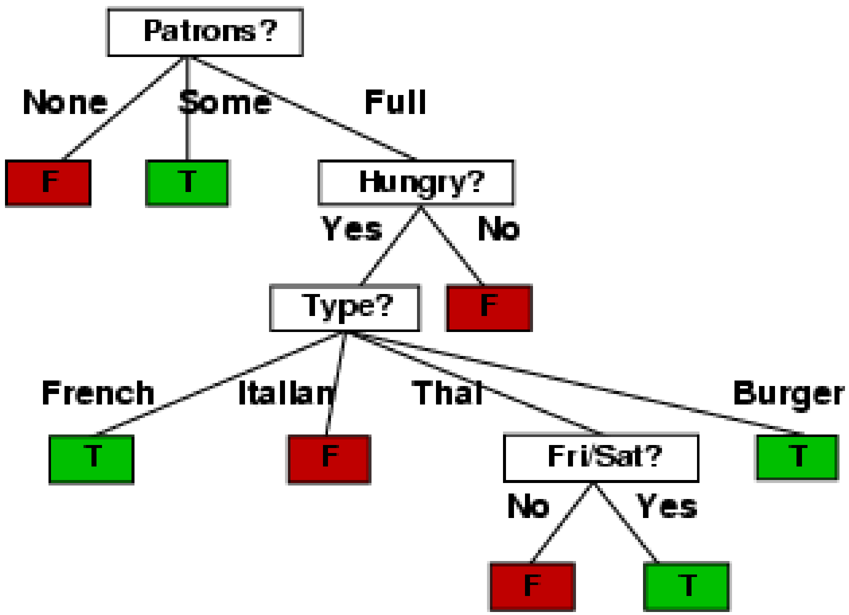
$$IG(Patrons) = 1 - [\frac{2}{12} I(0,1) + \frac{4}{12} I(1,0) + \frac{6}{12} I(\frac{2}{6}, \frac{4}{6})] = .541 \text{ bits}$$

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

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

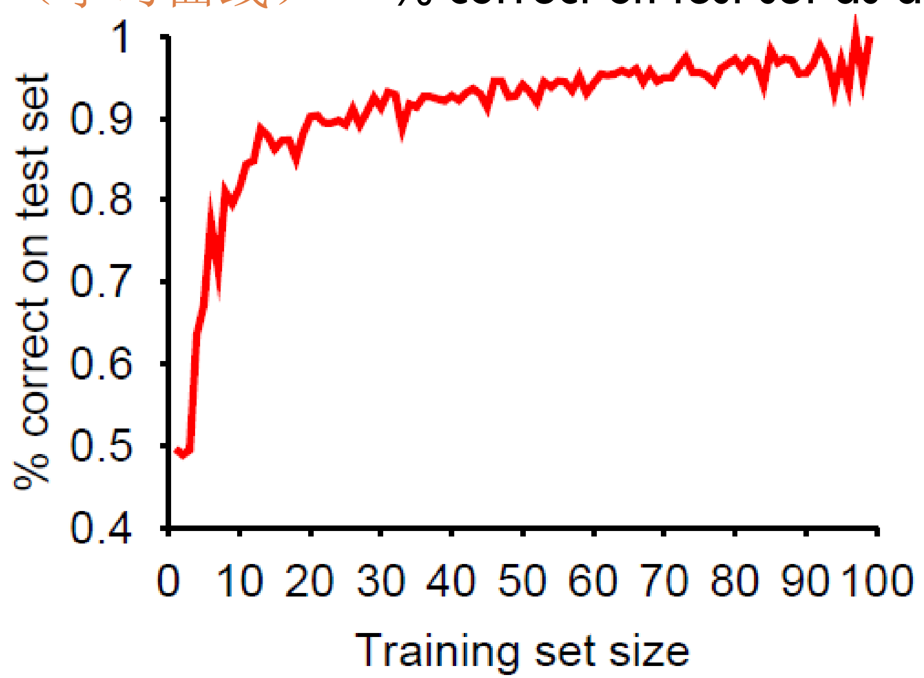
Performance measurement

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

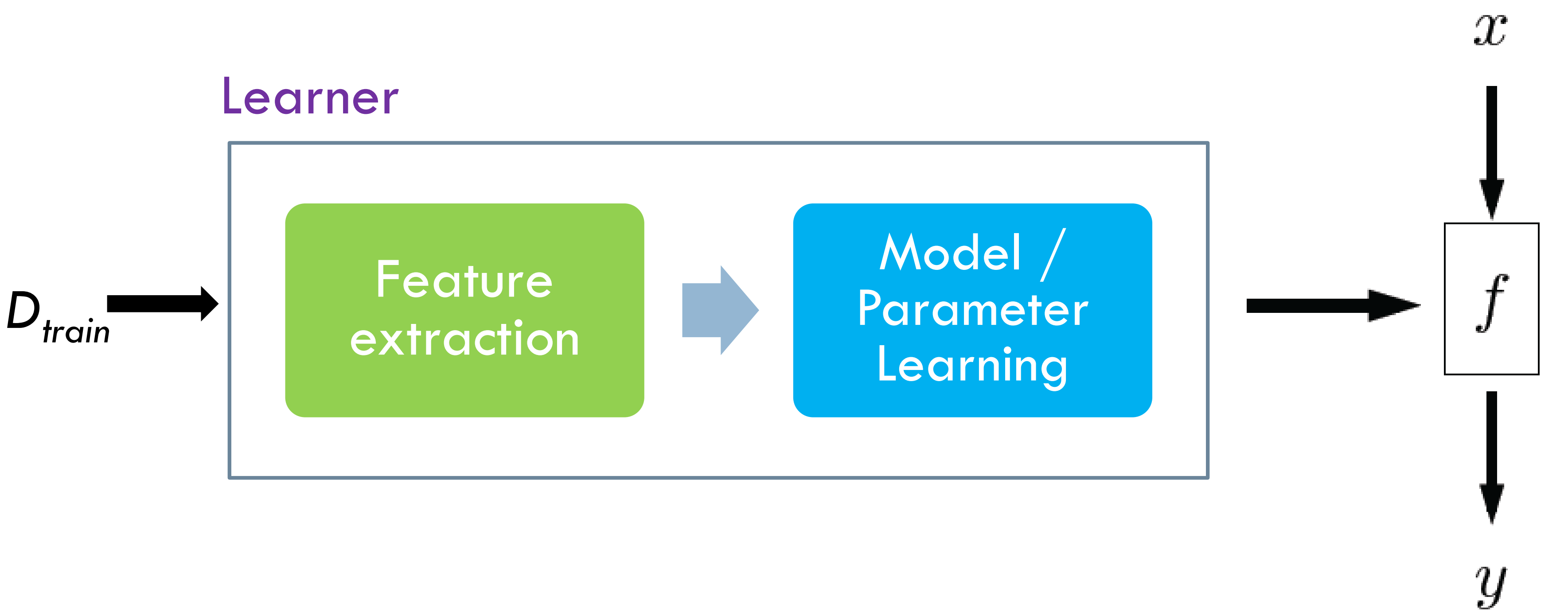
- Simple depth-first construction.
- Uses Information Gain

K nearest neighbor classifier 最近邻模型

Section 20.4

Linear predictions
线性预测

Learning Framework



Focus of this part

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

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

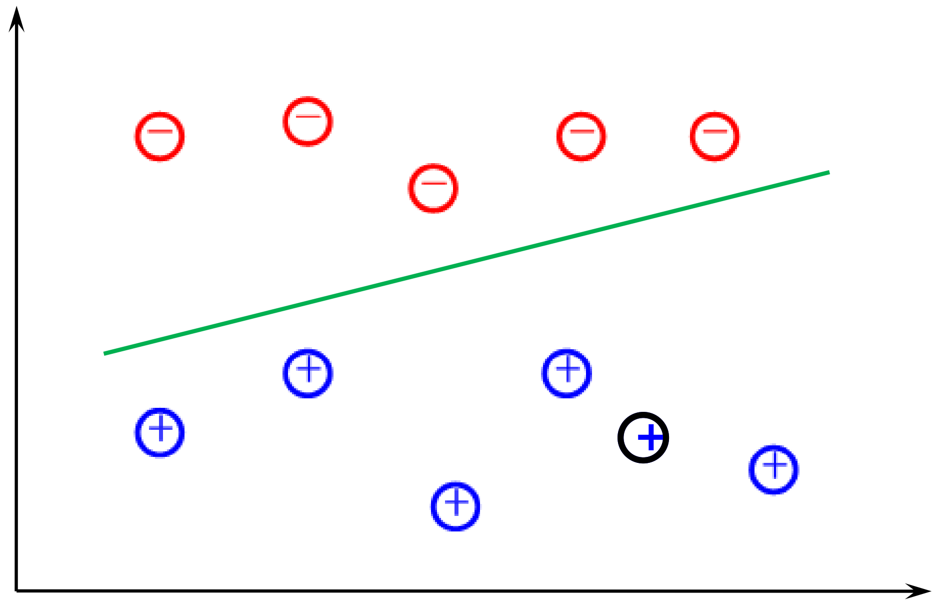
- Regression (e.g., predicting housing price):

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

Classification

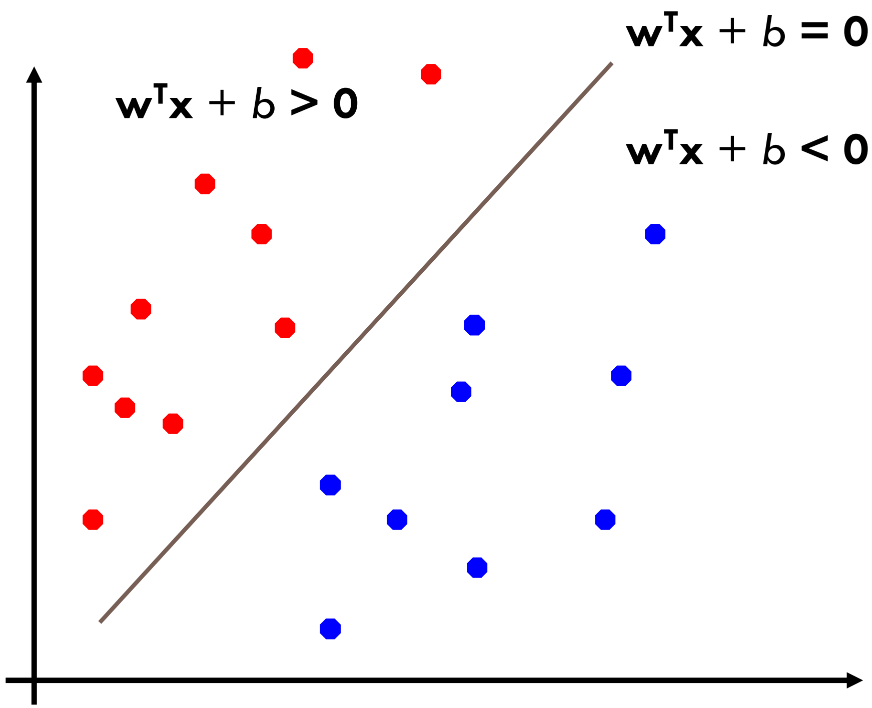
Classification

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



Linear Classifiers

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



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

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

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

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

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

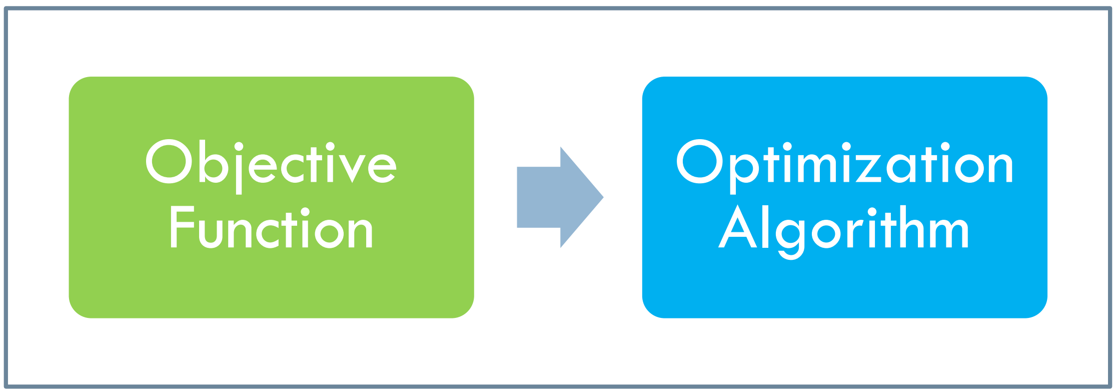
Unfortunately, this is a hard problem..

Alternate loss functions:

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

Learning as Optimization

Parameter Learning



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

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

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

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

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

- $X^+ = (X^\top X)^{-1}X^\top$ is 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;
```

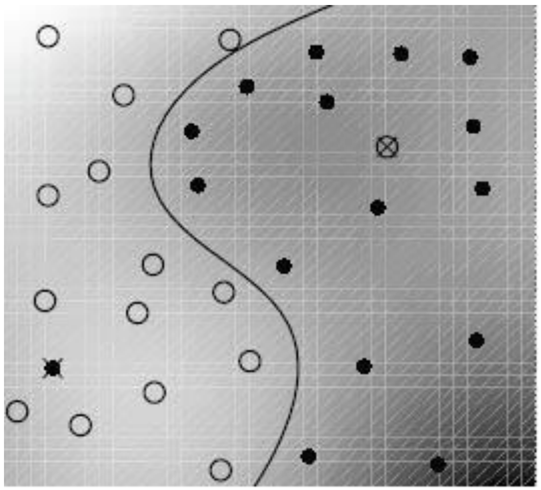
- Prediction for $\mathbf{x}_0$

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

General linear classification

Basis (nonlinear) functions （基函数）

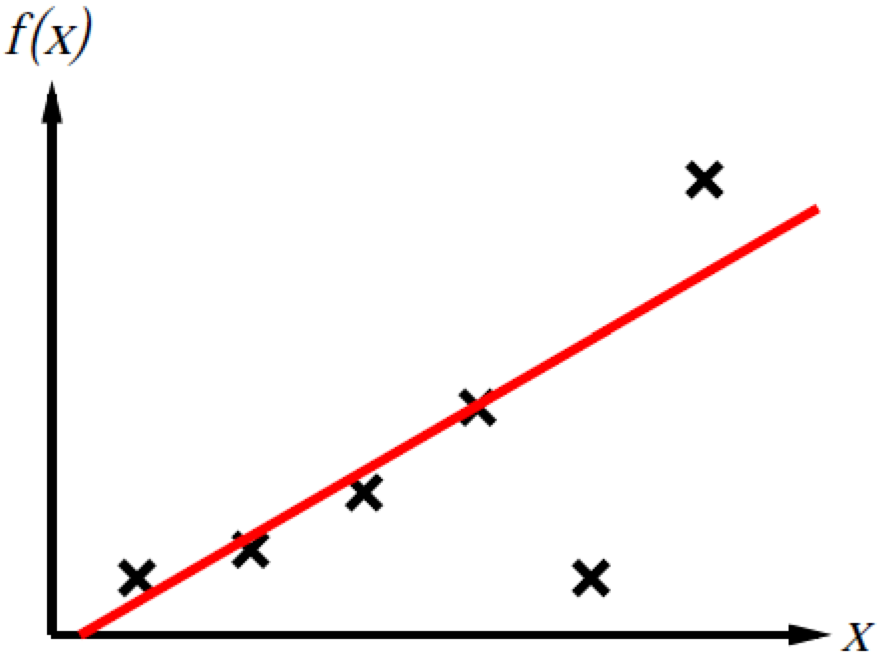
$$f(\mathbf{x}, \mathbf{w}) = b + w_1\phi_1(\mathbf{x}) + w_2\phi_2(\mathbf{x}) + \cdots + w_m\phi_m(\mathbf{x})$$



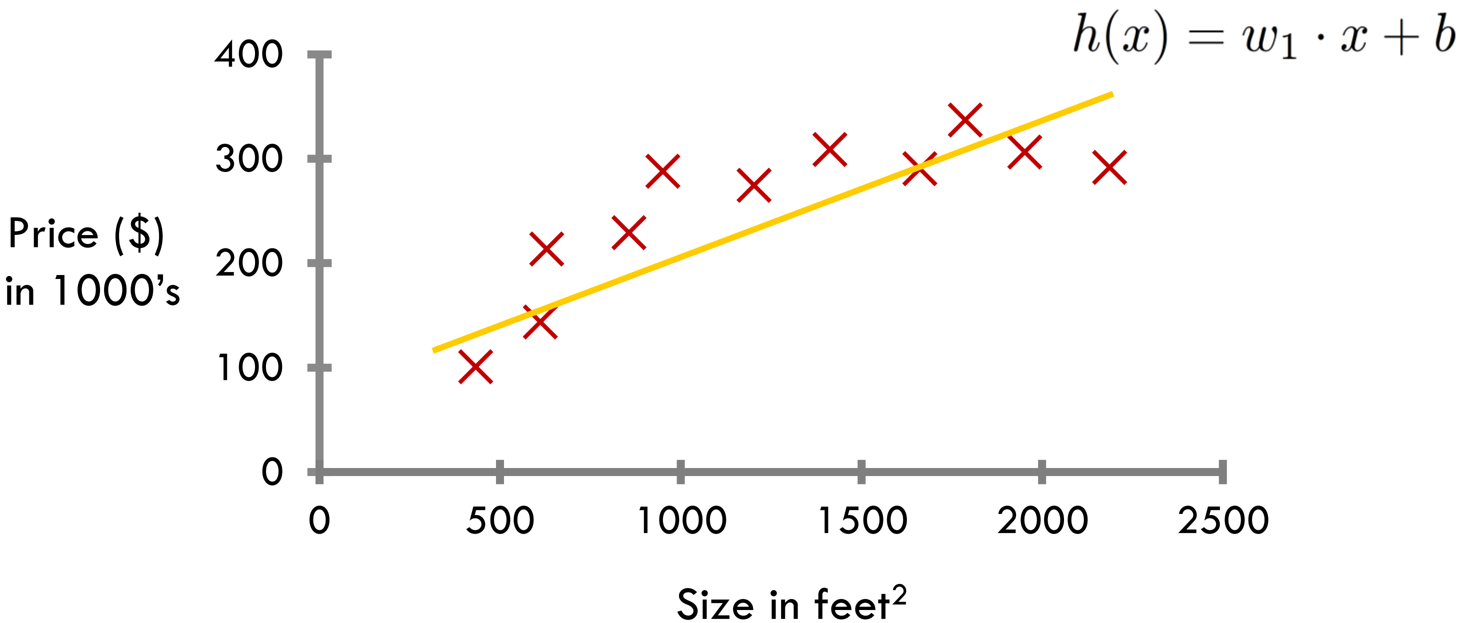
Regression（回归）

Regression

= learning from continuously labeled data.



Linear Regression

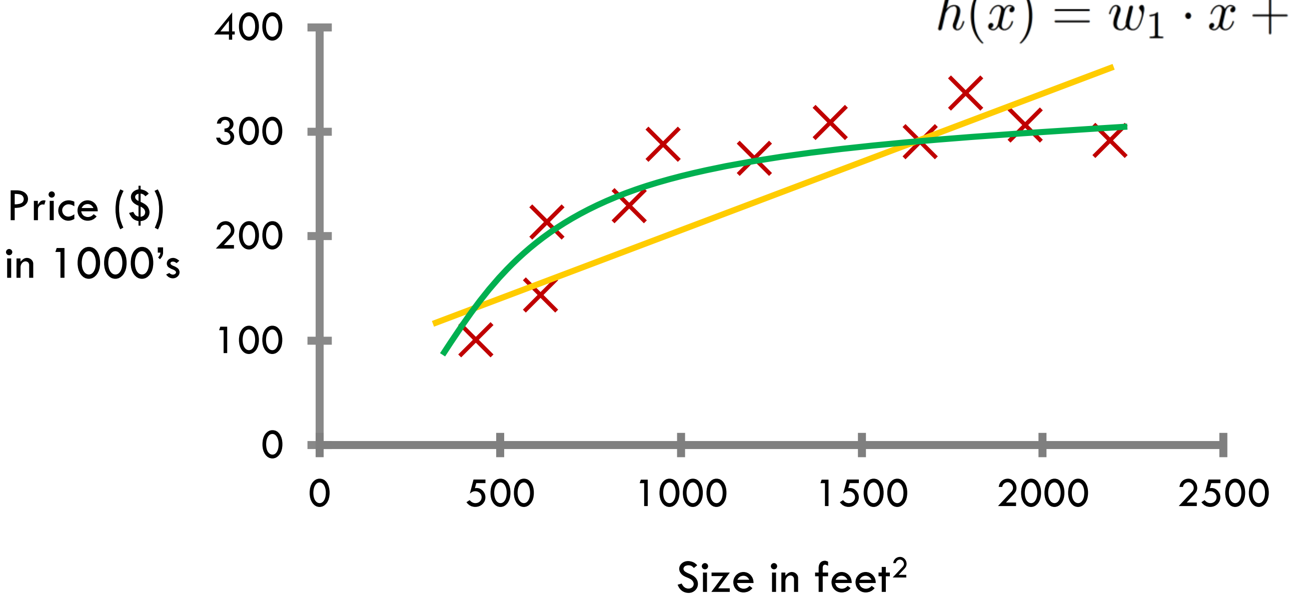


$$
\begin{aligned}
Loss &= \min_{\mathbf{w},b} \sum_i L_2(h(x_i), y_i) \\
&= \min_{\mathbf{w},b} \sum_i (y_i - w_1 \cdot x_i - b)^2
\end{aligned}
$$

Least Squares

General Linear/Polynomial Regression

$$h(x) = w_1 \cdot x + w_2 \cdot x^2 + b$$

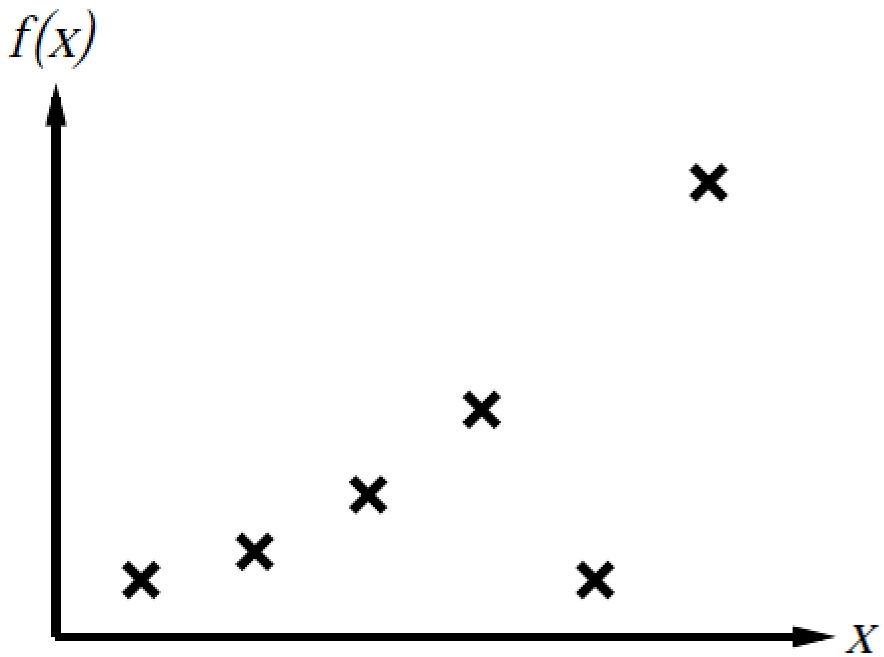


$$\begin{aligned} Loss &= \min_{\mathbf{w},b} \sum_i L_2(h(x_i), y_i) \\ &= \min_{\mathbf{w},b} \sum_i (y_i - w_1 \cdot x_i - w_2 \cdot x_i^2 - b)^2 \end{aligned}$$

Least Squares

Model complexity and overfitting

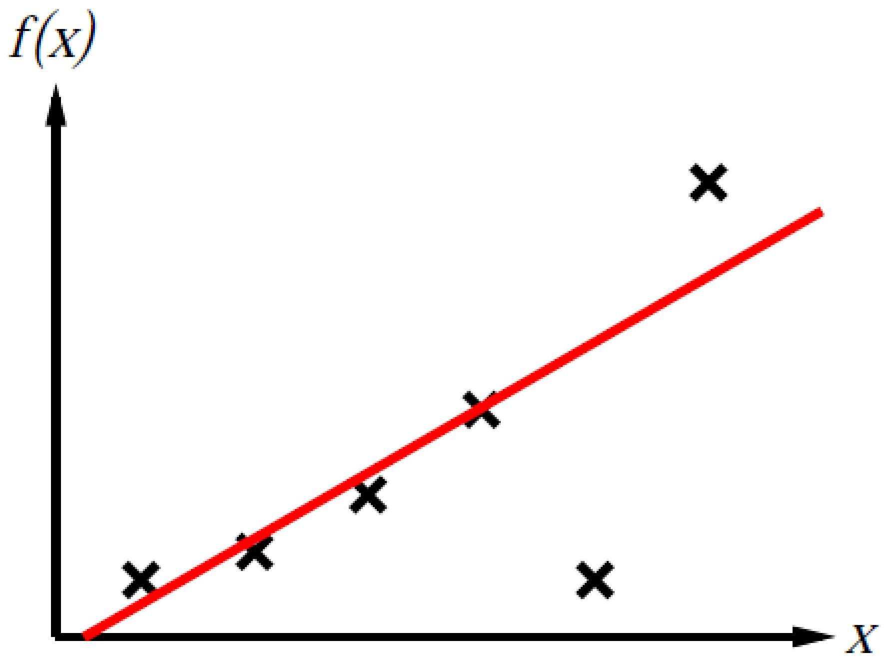
E.g., curve fitting（曲线拟合）:



Model complexity and overfitting

E.g., curve fitting（曲线拟合）：

$$f(x) = w_1 \cdot x + b$$



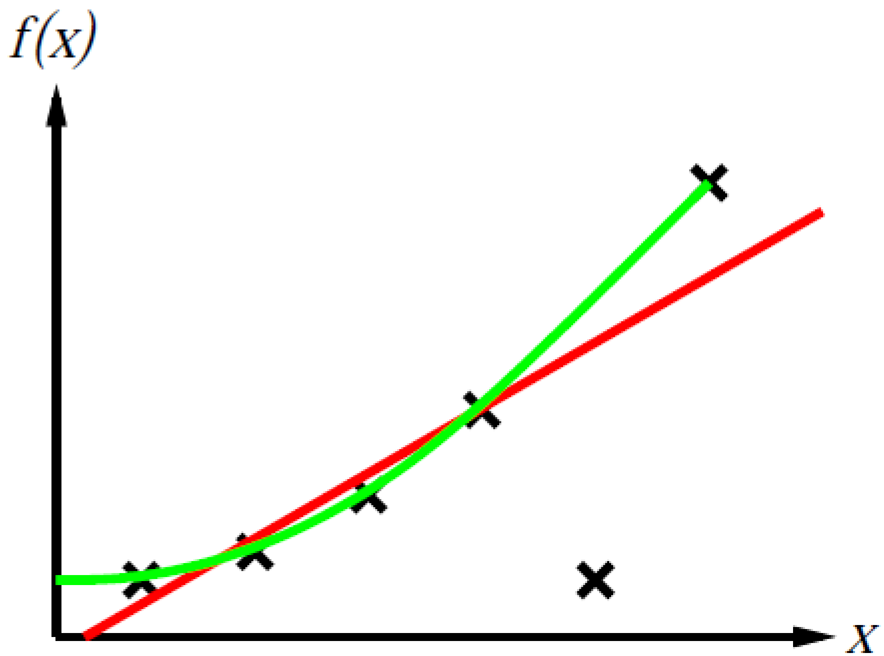
Underfitting

High **Bias**

Model complexity and overfitting

E.g., curve fitting（曲线拟合）：

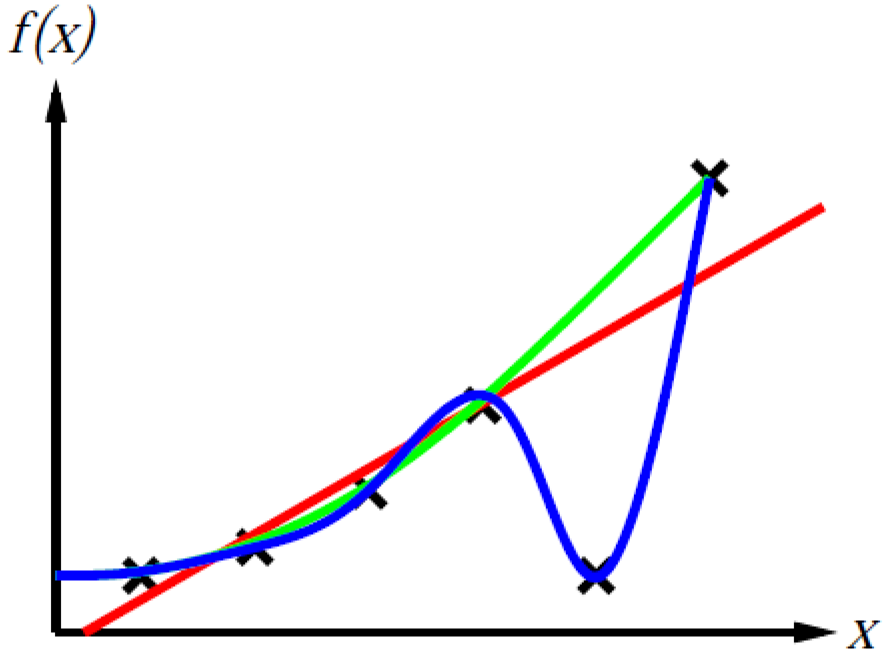
$$f(x) = w_1 \cdot x + w_2 \cdot x^2 + b$$



Model complexity and overfitting

E.g., curve fitting（曲线拟合）：

$$f(x) = w_1 \cdot x + w_2 \cdot x^2 + w_3 \cdot x^3 + w_4 \cdot x^4 + w_5 \cdot x^5 + b$$



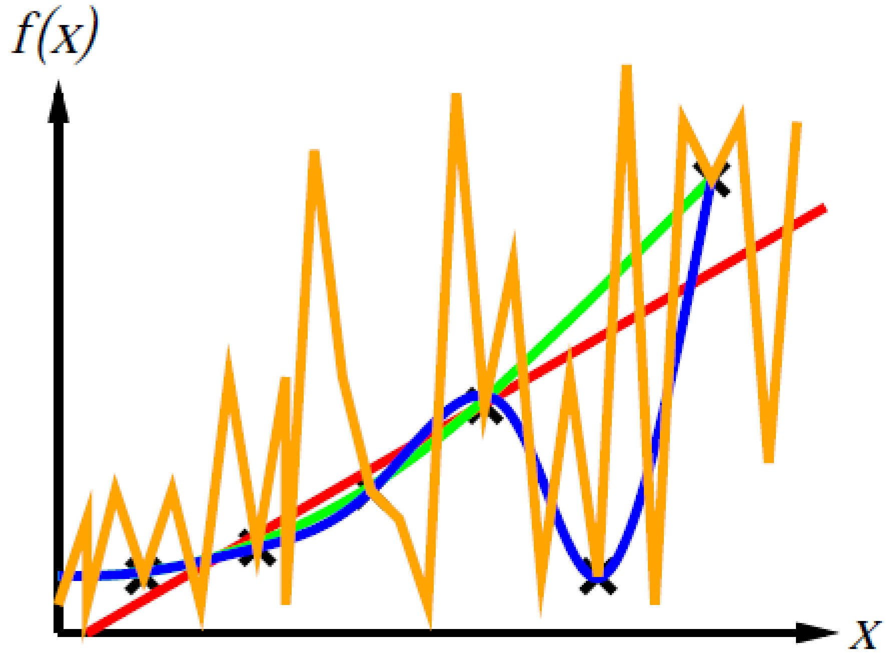
Overfitting

High **Variance**

Model complexity and overfitting

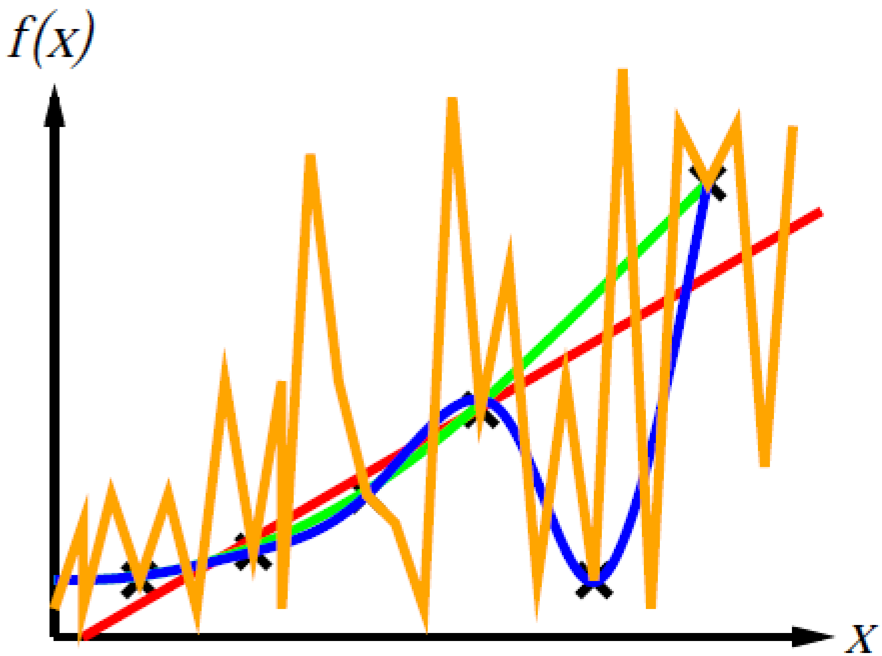
E.g., curve fitting（曲线拟合）：

$$f(x) = w_1 \cdot x + w_2 \cdot x^2 + \ldots + w_n \cdot x^n + b$$



Model complexity and overfitting

E.g., curve fitting（曲线拟合）：

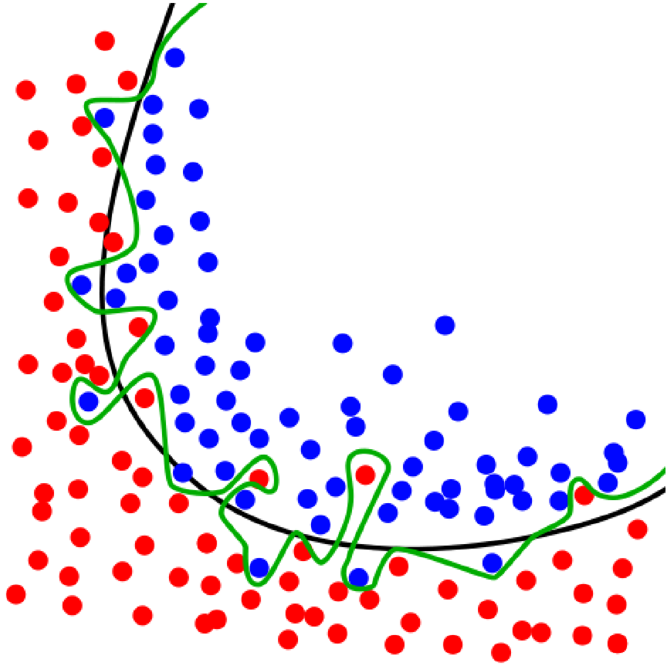


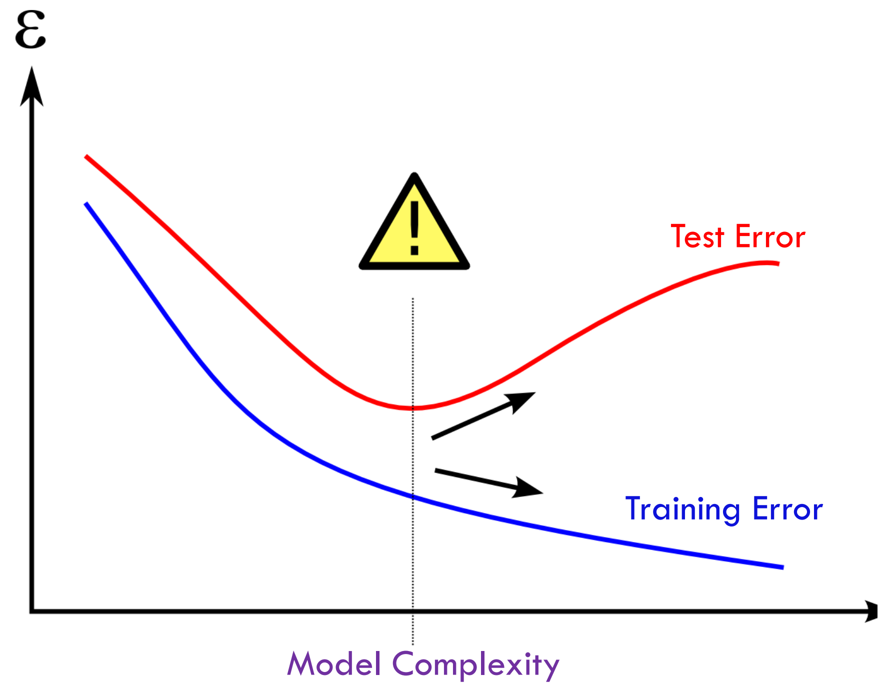
Ockham's razor（奥卡姆剃刀原则）：maximize a combination of consistency and simplicity
优先选择与数据一致的最简单的假设

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: small values for parameters

- "Simpler" hypothesis
- Less prone to overfitting

$$L_p - norm: \|\boldsymbol{v}\|_p = \left(\sum_i |v_i|^p\right)^{1/p}$$

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

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?

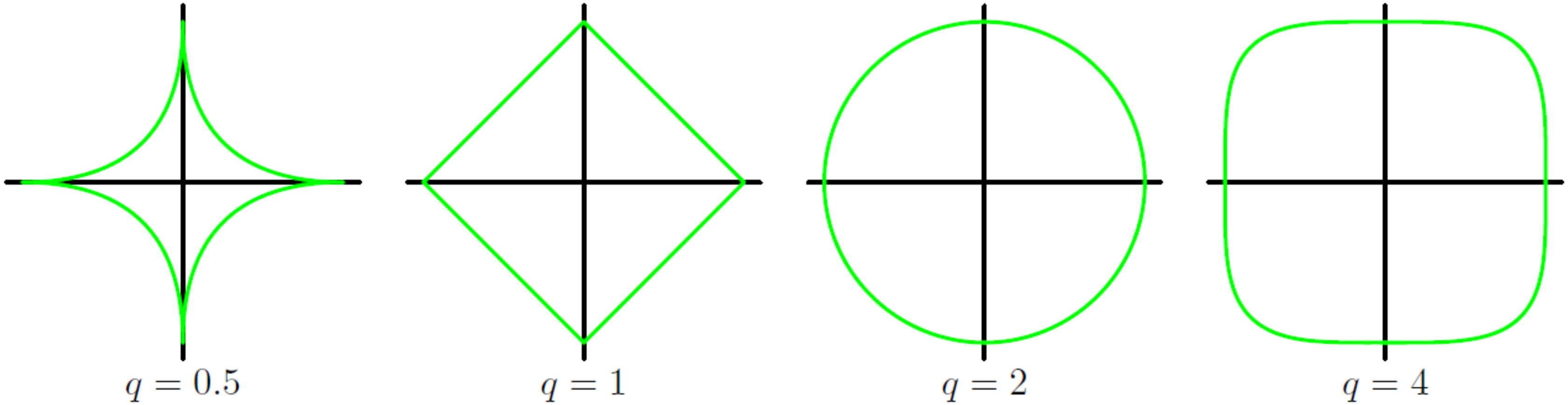
Regularization

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

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

When λ sufficiently large, equivalent to:

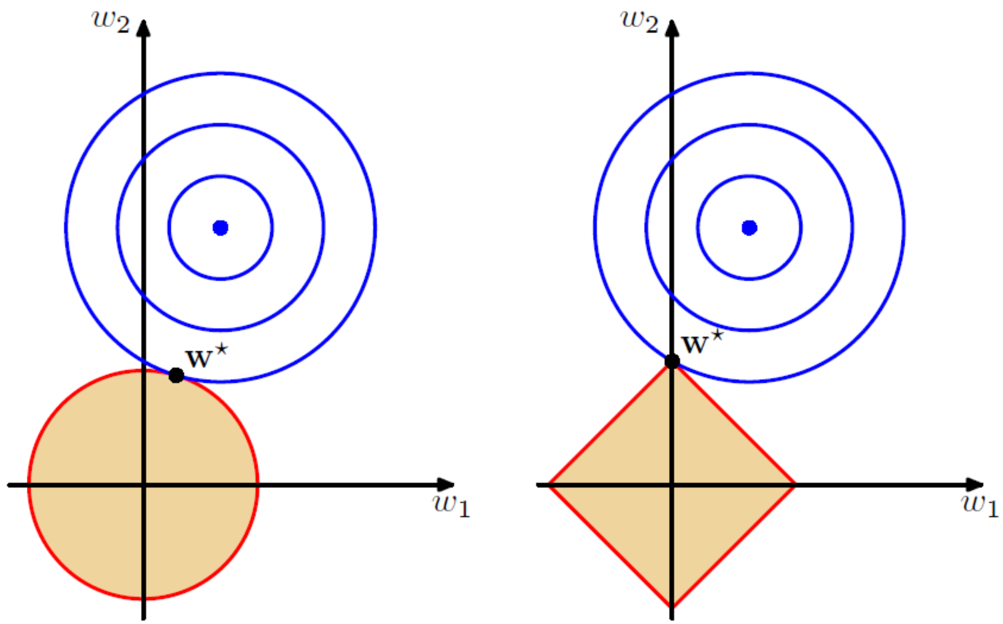
$$\min_{\mathbf{w}} \; Loss \text{ subject to } \sum_i |w_i|^q \leq \eta$$



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



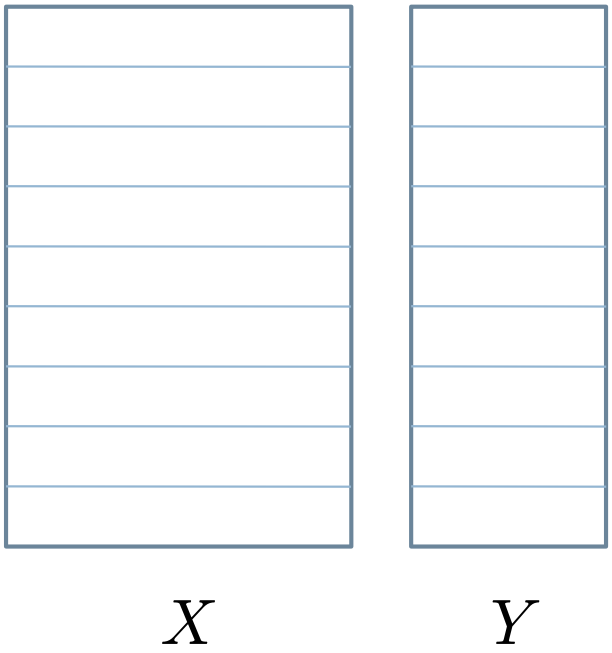
More than two classes?

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 ($d \times k$) for a model $f_W : X \to Y$
- 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

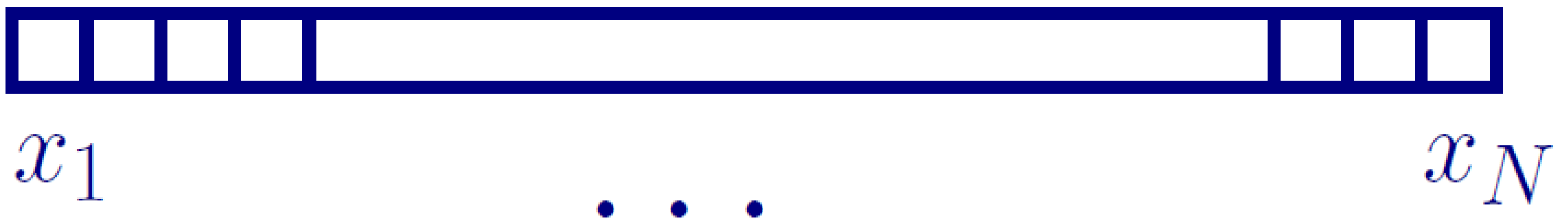
Cross-validation（交叉验证）

- 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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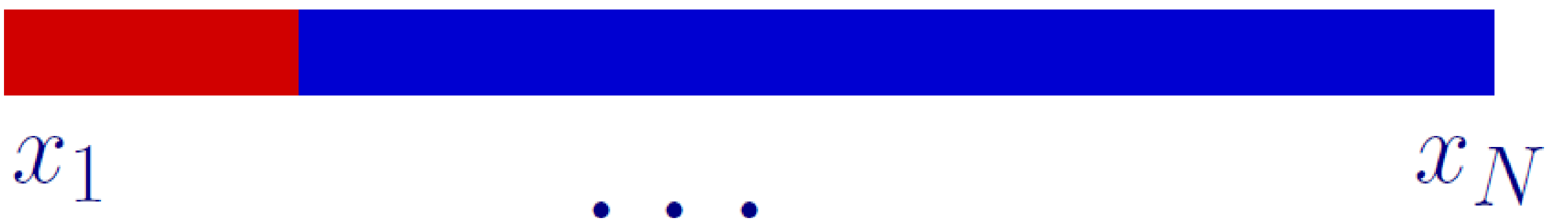

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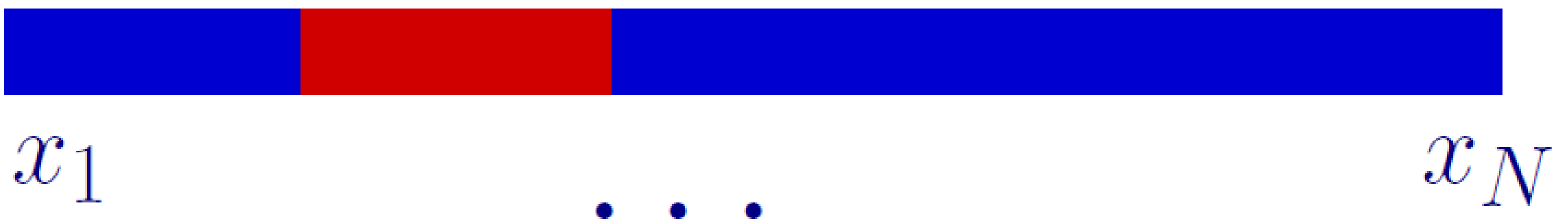

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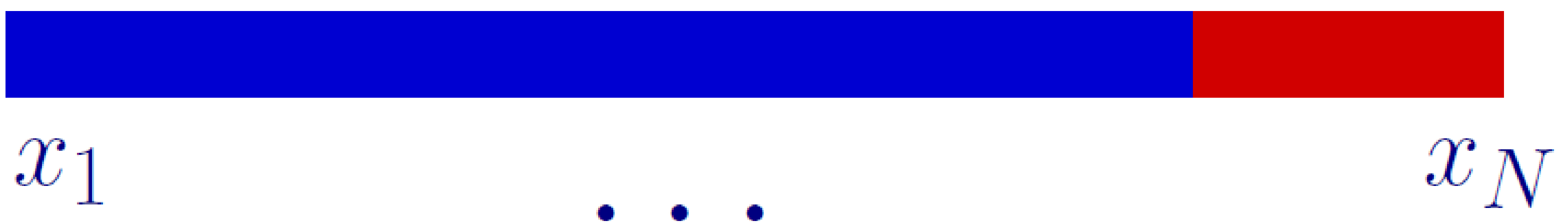
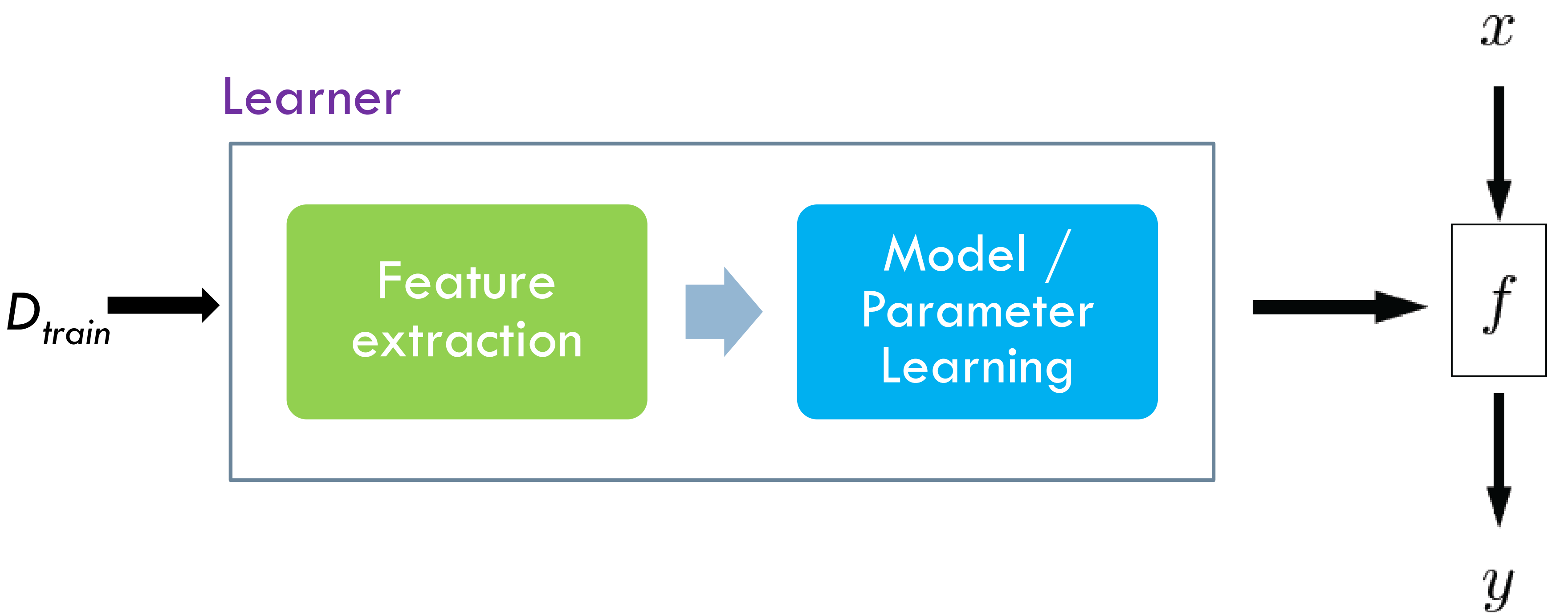


Learning Framework



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

作业

- 试证明对于不含冲突数据（即特征向量完全相同但标记不同）的训练集，必存在与训练集一致（即训练误差为0）的决策树。