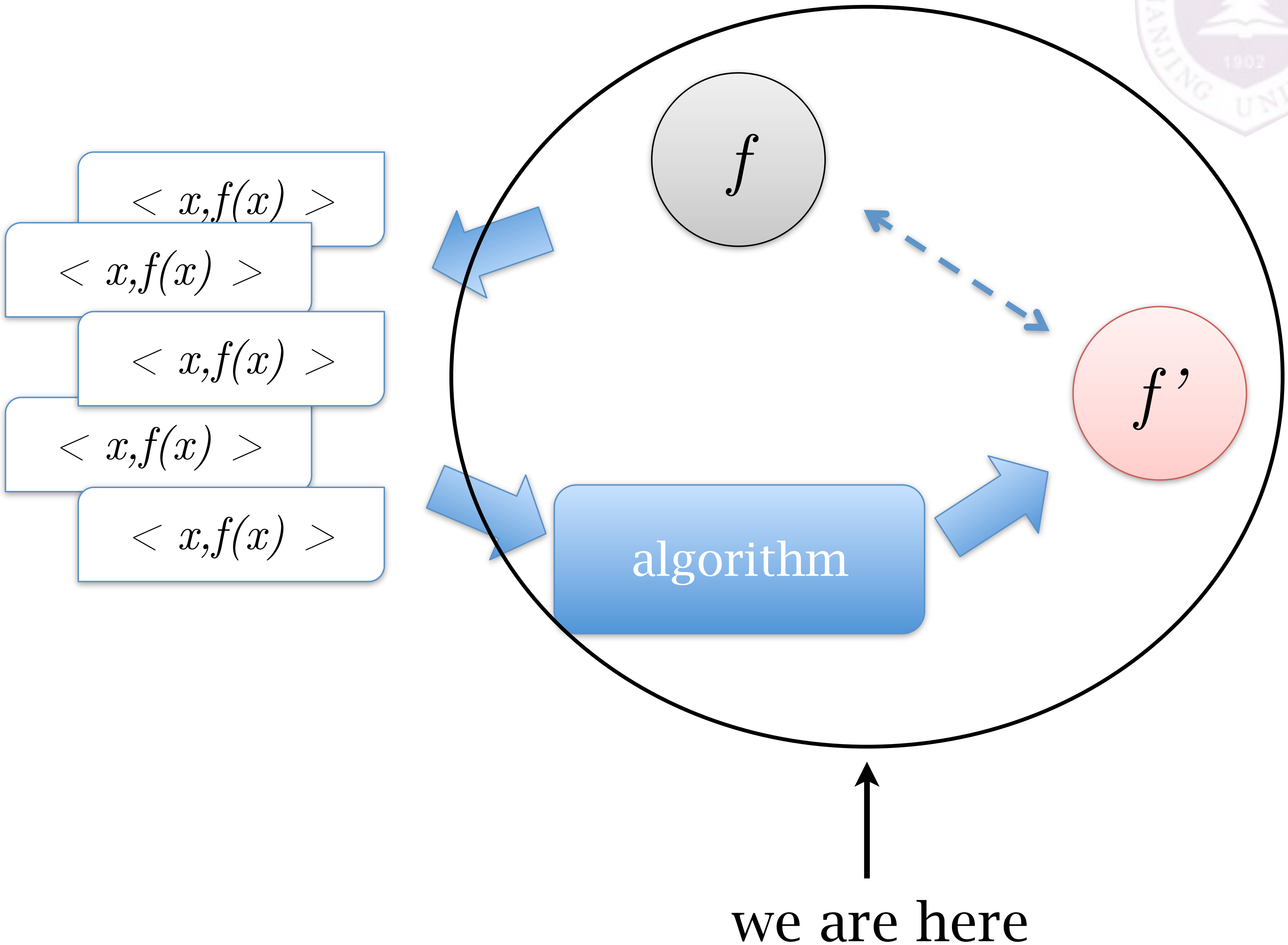
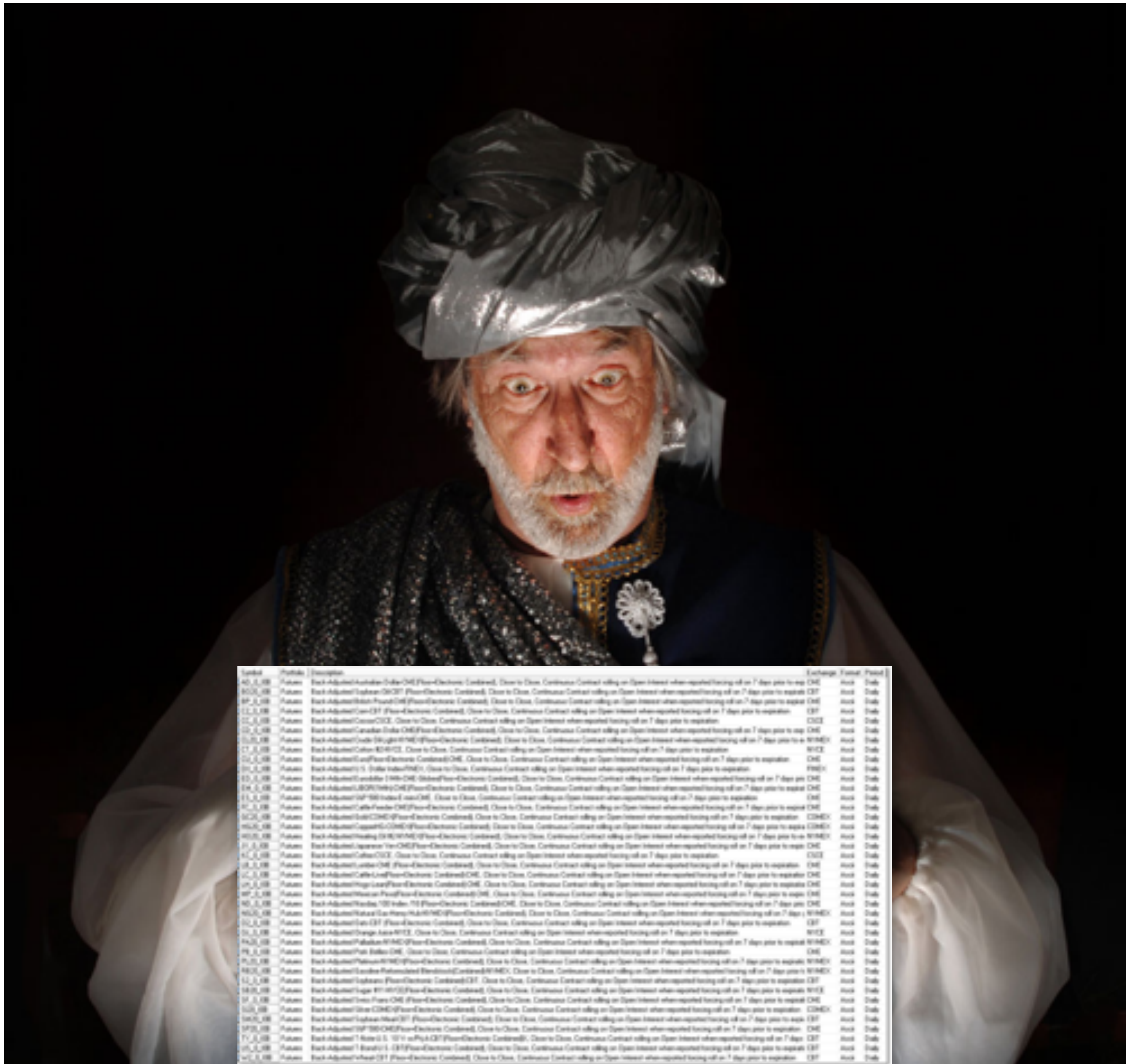
Lecture 3:
Supervised Learning

http://cs.nju.edu.cn/yuy/course_dm12.ashx

Position

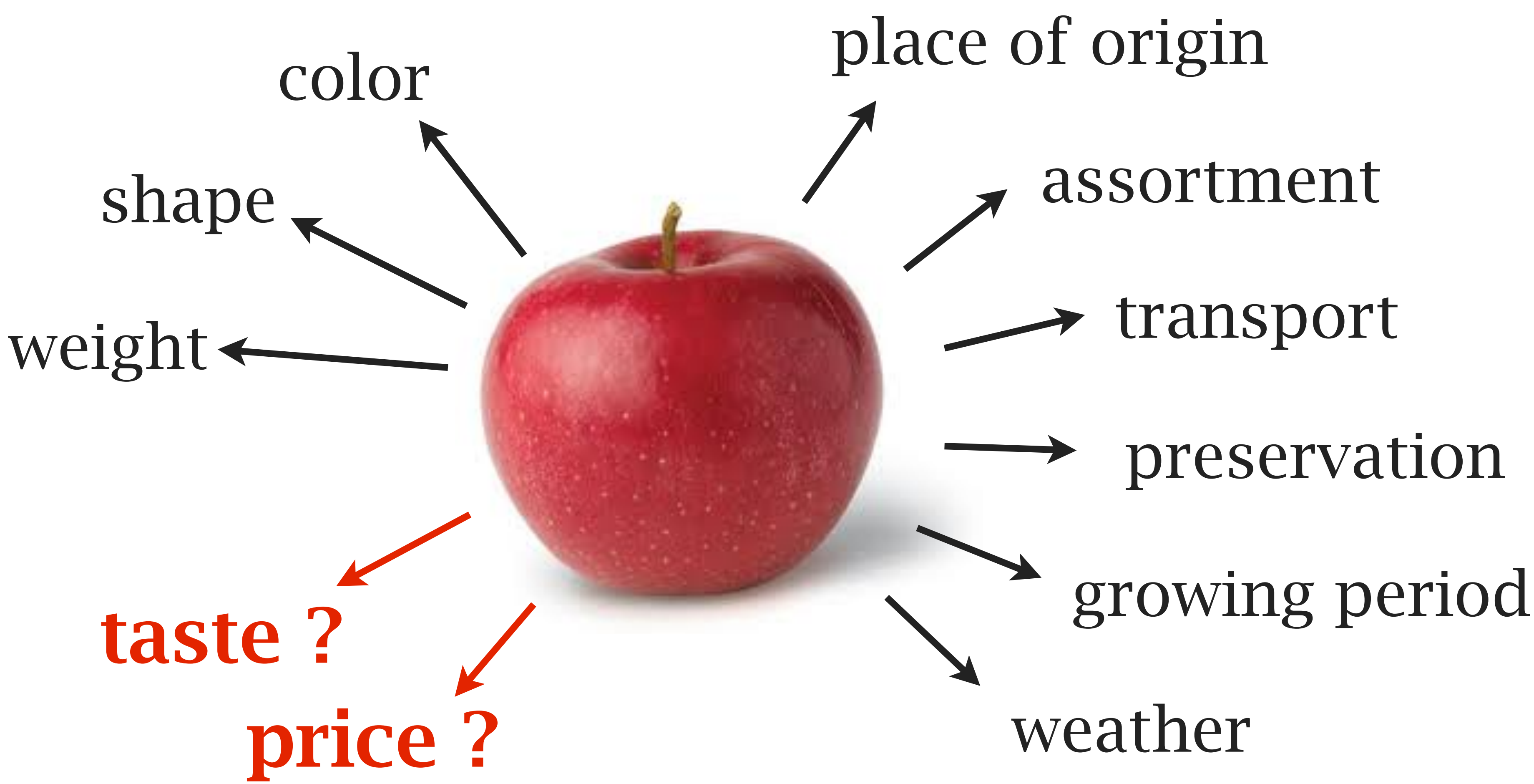


The desire of prediction



Predictive modeling

Find a relation between a set of variables (features) to target variables (labels).



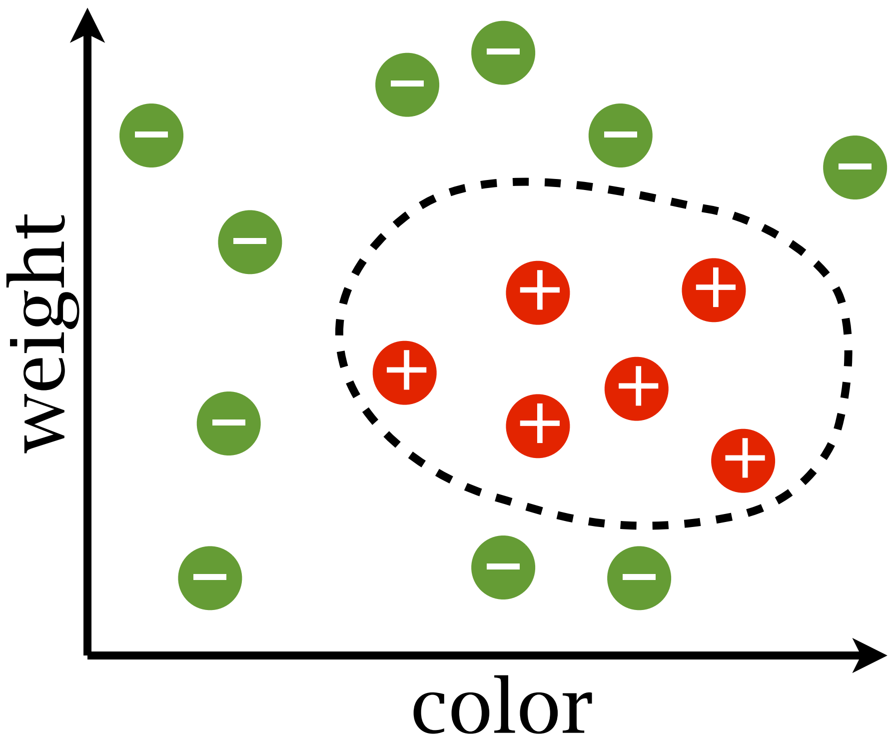
Supervised learning/inductive learning

Find a relation between a set of variables (features) to target variables (labels) *from finite examples*.

tasks
- Classification: label is a nominal feature
- Regression: label is a numerical feature
- Ranking: label is a ordinal feature
- ...

Classification

Features: color, weight
Label: taste is sweet (positive/+) or not (negative/-)



(color, weight) → sweet ?

$\mathcal{X} \quad \to \{-1, +1\}$

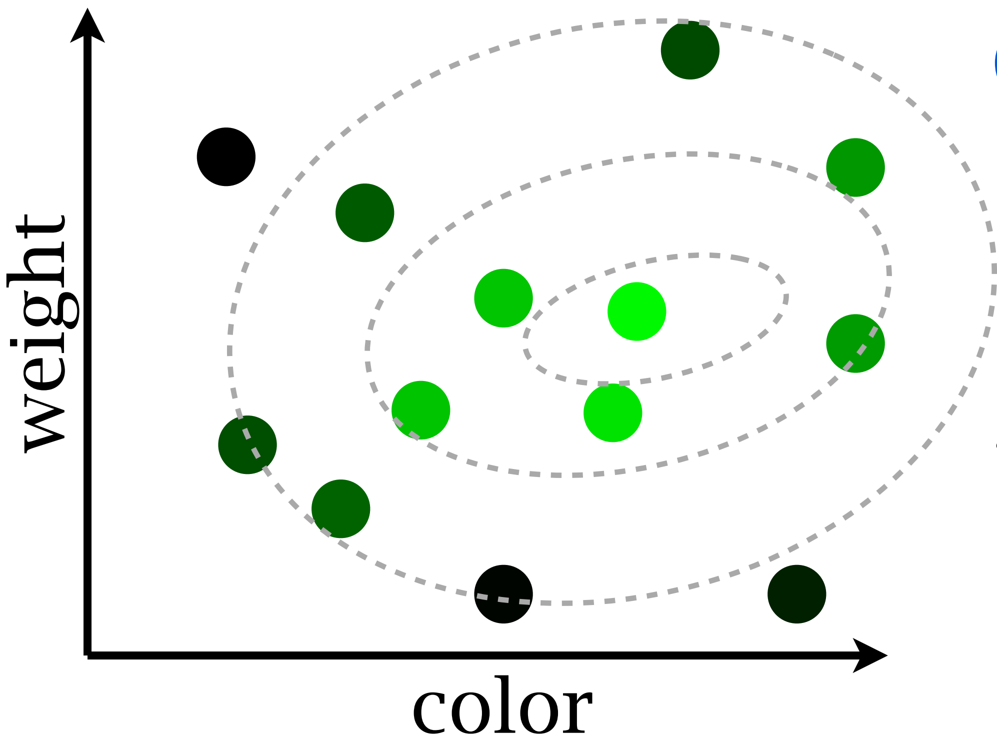
ground-truth function f

examples/training data:
$\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)\}$

$y_i = f(\boldsymbol{x}_i)$

Regression

Features: color, weight
Label: sweetness [0,1]



(color, weight) → sweetness

$\mathcal{X} \rightarrow [-1, +1]$

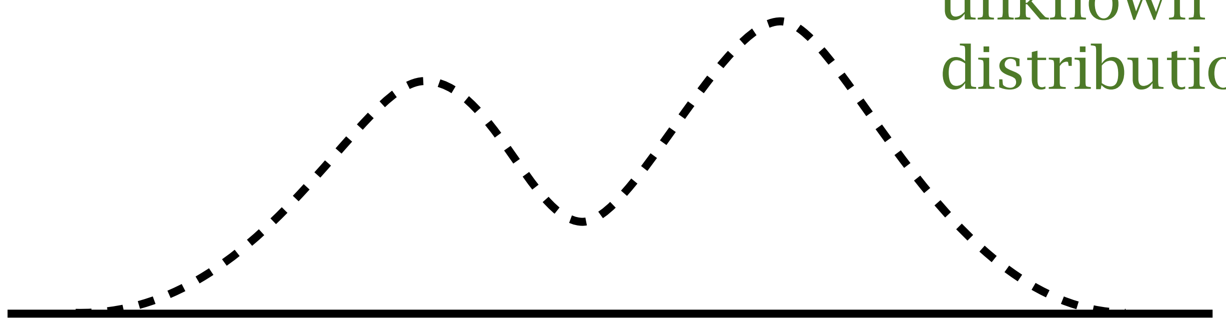
ground-truth function f

examples/training data:
$\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)\}$

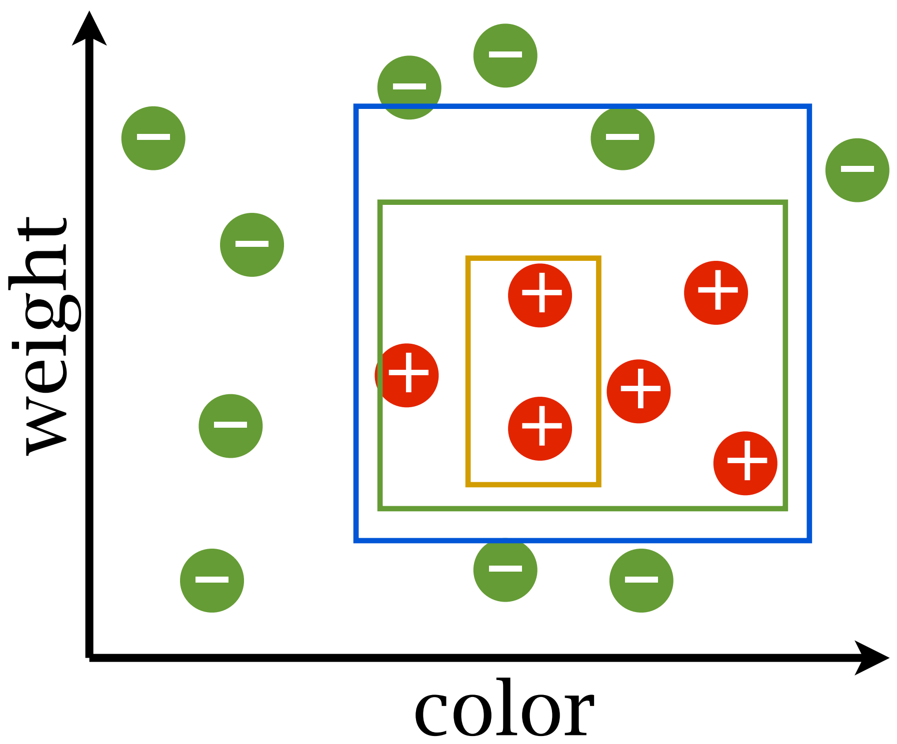
$y_i = f(\boldsymbol{x}_i)$

I.I.D. assumption

all training examples and future (test) examples are drawn *independently* from an *identical distribution*



Hypothesis class

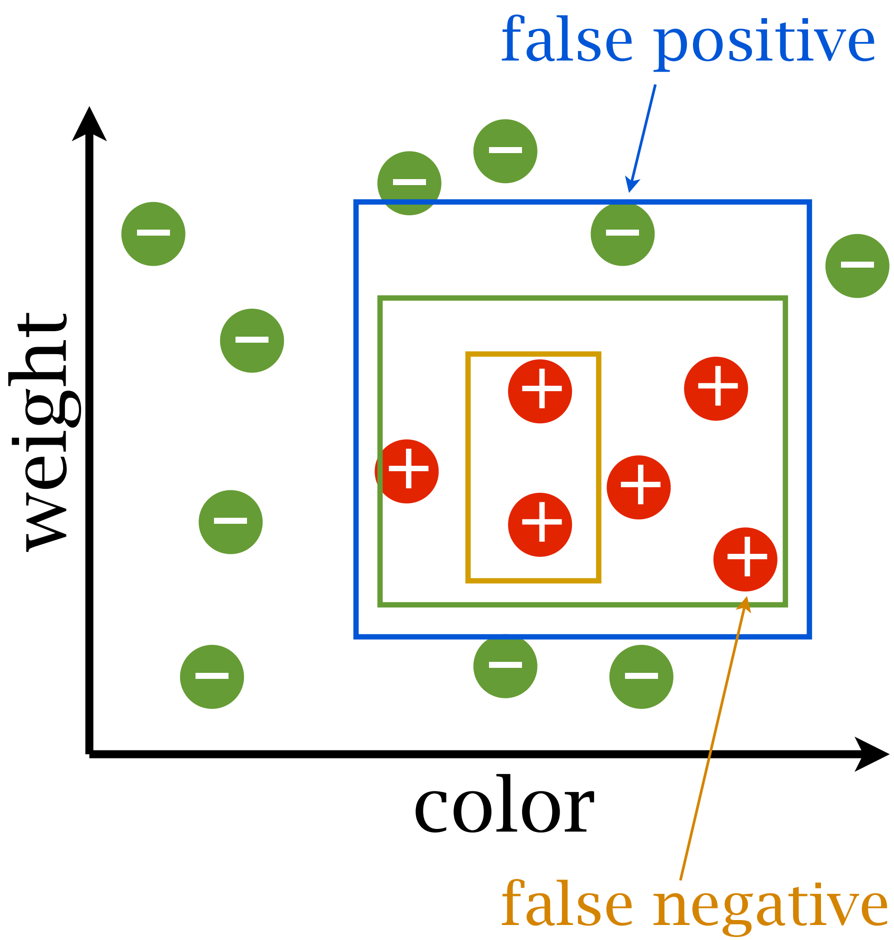


box hypothesis class $\mathcal{H}$ contains all boxes

$h \in \mathcal{H}$ is a hypothesis

$$h(\boldsymbol{x}) = \begin{cases} +1, \text{if } x \text{ is inside the box} \\ -1, \text{if } x \text{ is outside the box} \end{cases}$$

Training and generalization errors



training error

$$\epsilon_t = \frac{1}{m}\sum_{i=1}^{m} I(h(\boldsymbol{x}_i) \neq y_i)$$

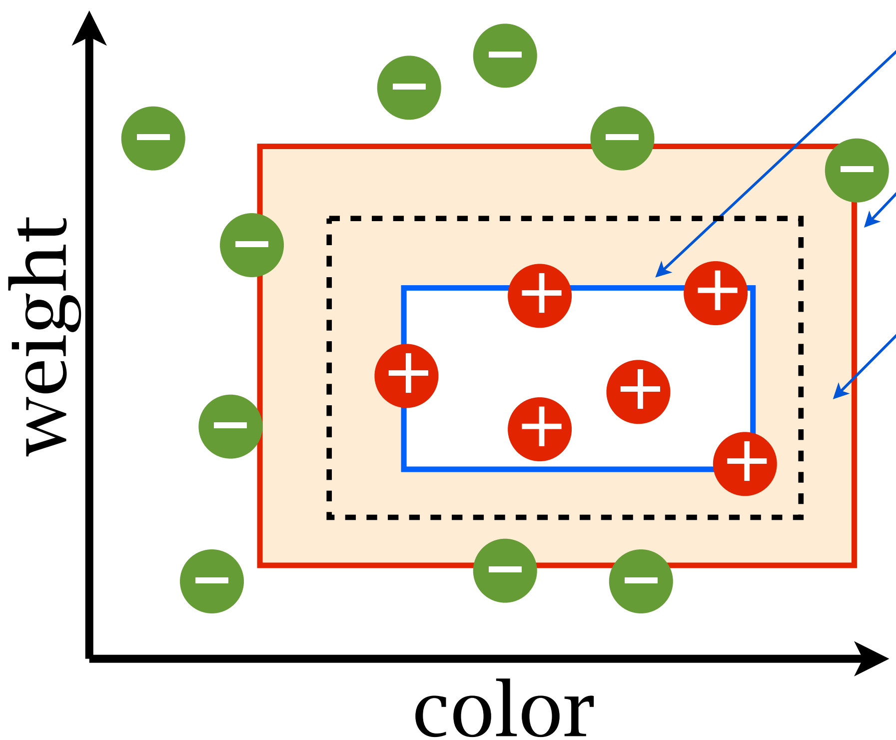
generalization error

$$\epsilon_g = \mathbb{E}_x[I(h(\boldsymbol{x}) \neq f(\boldsymbol{x}))]$$

$$= \int_{\mathcal{X}} p(x) I(h(\boldsymbol{x}) \neq f(\boldsymbol{x}))]\mathrm{d}x$$

find a hypothesis minimizes the generalization error

S, G, and the version space algorithm



S: most specific hypothesis

G: most general hypothesis

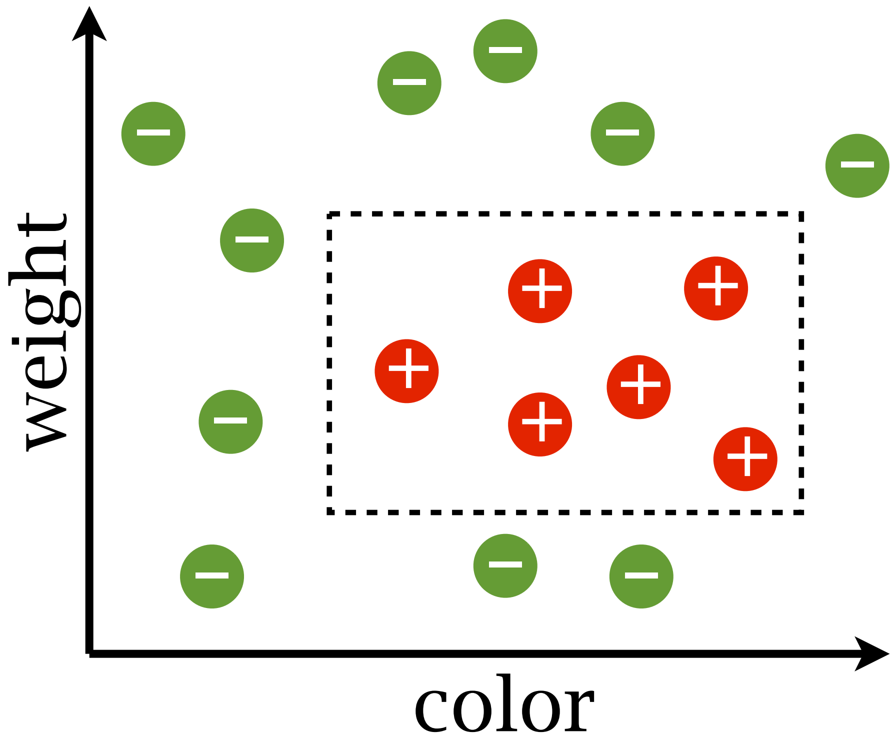
version space: consistent hypotheses [Mitchell, 1997]

a conceptual algorithm:

1. for every example, remove the conflict boxes
2. find S in remaining boxes
3. find G in remaining boxes
4. output the mean of S and G

Generalization error

assume i.i.d. examples, and the ground-truth hypothesis is a box



the error of picking a consistent hypothesis:

with probability at least $1-\delta$

$$\epsilon_g < \frac{1}{m} \cdot \left(\ln |\mathcal{H}| + \ln \frac{1}{\delta}\right)$$

smaller generalization error:

- more examples
- smaller hypothesis space

Generalization error

for one *h*

What is the probability of h is consistent, $\epsilon_g(h) \geq \epsilon$

assume *h* is ***bad***: $\epsilon_g(h) \geq \epsilon$

h is consistent with 1 example:

$$P \leq 1 - \epsilon$$

h is consistent with ***m*** example:

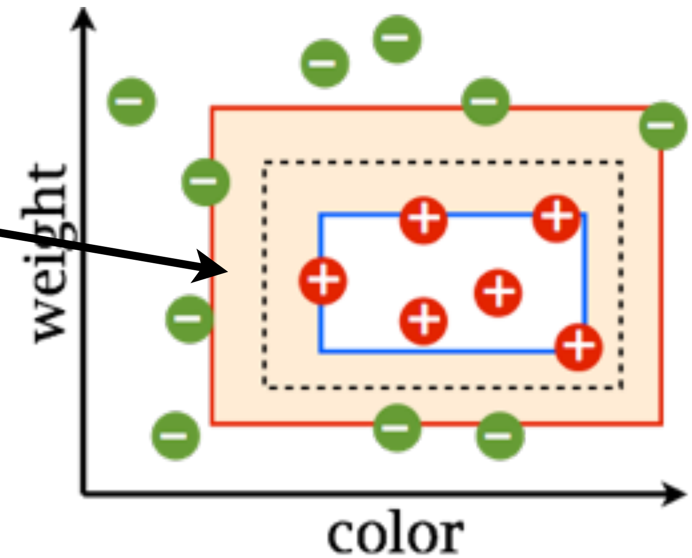
$$P \leq (1 - \epsilon)^m$$

Generalization error

h is consistent with $\boldsymbol{m}$ example:

$$P \leq (1-\epsilon)^m$$

There are $\boldsymbol{k}$ consistent hypotheses



Probability of choosing a bad one:

h_1 is chosen and h_1 is bad $P \leq (1-\epsilon)^m$

h_2 is chosen and h_2 is bad $P \leq (1-\epsilon)^m$

...

h_k is chosen and h_k is bad $P \leq (1-\epsilon)^m$

overall:

$\exists h$: h can be chosen (consistent) but is bad

Generalization error

h_1 is chosen and h_1 is bad $P \leq (1-\epsilon)^m$
h_2 is chosen and h_2 is bad $P \leq (1-\epsilon)^m$
...
h_k is chosen and h_k is bad $P \leq (1-\epsilon)^m$

overall:

$\exists h$: h can be chosen (consistent) but is bad

Union bound: $P(A \cup B) \leq P(A) + P(B)$

$$P(\exists h \text{ is consistent but bad}) \leq k \cdot (1-\epsilon)^m \leq |\mathcal{H}| \cdot (1-\epsilon)^m$$

Generalization error

$$P(\exists h \text{ is consistent but bad}) \leq k \cdot (1-\epsilon)^m \leq |\mathcal{H}| \cdot (1-\epsilon)^m$$

$$\Downarrow$$

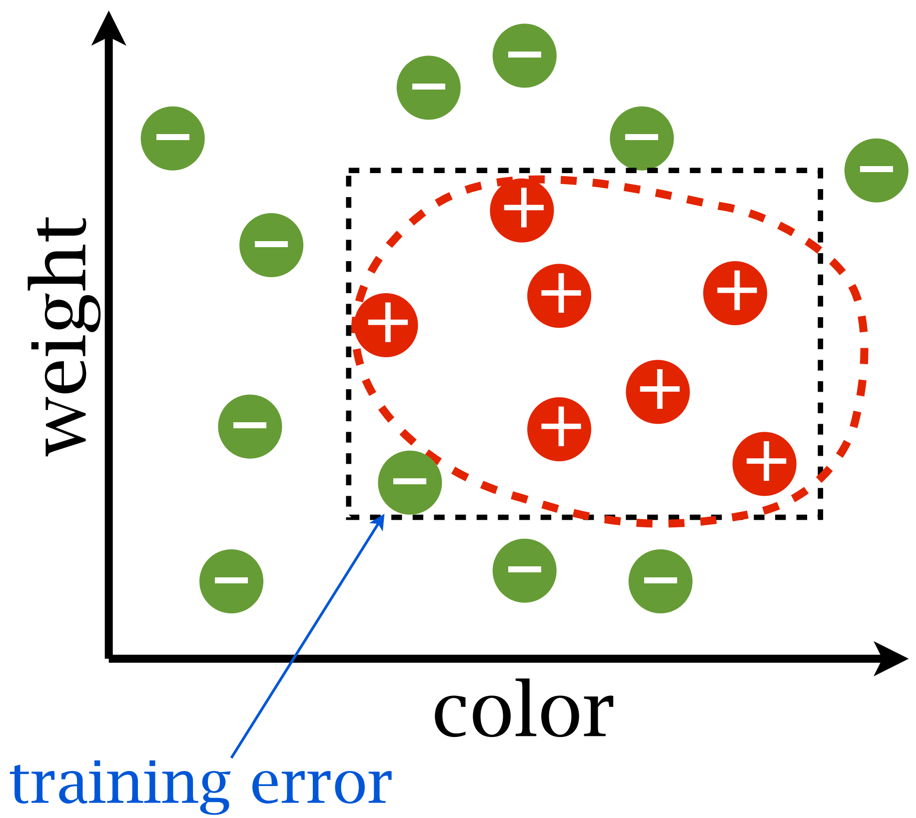
$$P(\epsilon_g \geq \epsilon) \leq \underbrace{|\mathcal{H}| \cdot (1-\epsilon)^m}_{\delta}$$

$$\text{with probability at least } 1-\delta$$

$$\epsilon_g < \frac{1}{m} \cdot (\ln|\mathcal{H}| + \ln\frac{1}{\delta})$$

Inconsistent hypothesis

What if the ground-truth hypothesis
is NOT a box: non-zero training error



with probability at least $1-\delta$

$$\epsilon_g < \epsilon_t + \sqrt{\frac{1}{m}(\ln|\mathcal{H}| + \ln\frac{1}{\delta})}$$

smaller generalization error:

- more examples
- smaller hypothesis space
- **smaller training error**

Hoeffding's inequality

X be an i.i.d. random variable

$X_1, X_2, \ldots, X_m$ be m samples $\qquad X_i \in [b-a]$

$$\frac{1}{m}\sum_{i=1}^{m} X_i - \mathbb{E}[X] \leftarrow \text{ difference between sum and expectation}$$

$$P(\frac{1}{m}\sum_{i=1}^{m} X_i - \mathbb{E}[X] \geq \epsilon) \leq \exp\left(-\frac{2\epsilon^2 m}{(b-a)^2}\right)$$

Generalization error

$$\text{for one } h$$

$$X_i = I(h(x_i) \neq f(x_i)) \in [0, 1]$$

$$\frac{1}{m}\sum_{i=1}^{m} X_i \to \epsilon_t(h) \qquad\qquad \mathbb{E}[X_i] \to \epsilon_g(h)$$

$$P(\epsilon_t(h) - \epsilon_g(h) \geq \epsilon) \leq \exp\left(-2\epsilon^2 m\right)$$

$$P(\epsilon_t - \epsilon_g \geq \epsilon)$$

$$\leq P(\exists h \in |\mathcal{H}| : \epsilon_t(h) - \epsilon_g(h) \geq \epsilon) \leq \underbrace{|\mathcal{H}| \exp\left(-2\epsilon^2 m\right)}_{\delta}$$

$$\text{with probability at least } 1 - \delta$$

$$\epsilon_g < \epsilon_t + \sqrt{\frac{1}{2m} \cdot (\ln |\mathcal{H}| + \ln \frac{1}{\delta})}$$

Generalization error: Summary

assume i.i.d. examples

consistent hypothesis case:

with probability at least $1-\delta$

$$\epsilon_g < \frac{1}{m} \cdot (\ln |\mathcal{H}| + \ln \frac{1}{\delta})$$

inconsistent hypothesis case:

with probability at least $1-\delta$

$$\epsilon_g < \epsilon_t + \sqrt{\frac{1}{m}(\ln |\mathcal{H}| + \ln \frac{1}{\delta})}$$

generalization error:

- number of examples m
- training error ϵ_t
- hypothesis space complexity $\ln |\mathcal{H}|$

PAC-learning

Probably approximately correct (PAC):

with probability at least $1-\delta$

$$\epsilon_g < \epsilon_t + \sqrt{\frac{1}{2m} \cdot (\ln|\mathcal{H}| + \ln\frac{1}{\delta})}$$

Leslie Valiant
Turing Award (2010)
EATCS Award (2008)
Knuth Prize (1997)
Nevanlinna Prize (1986)

PAC-learnable: [Valiant, 1984]

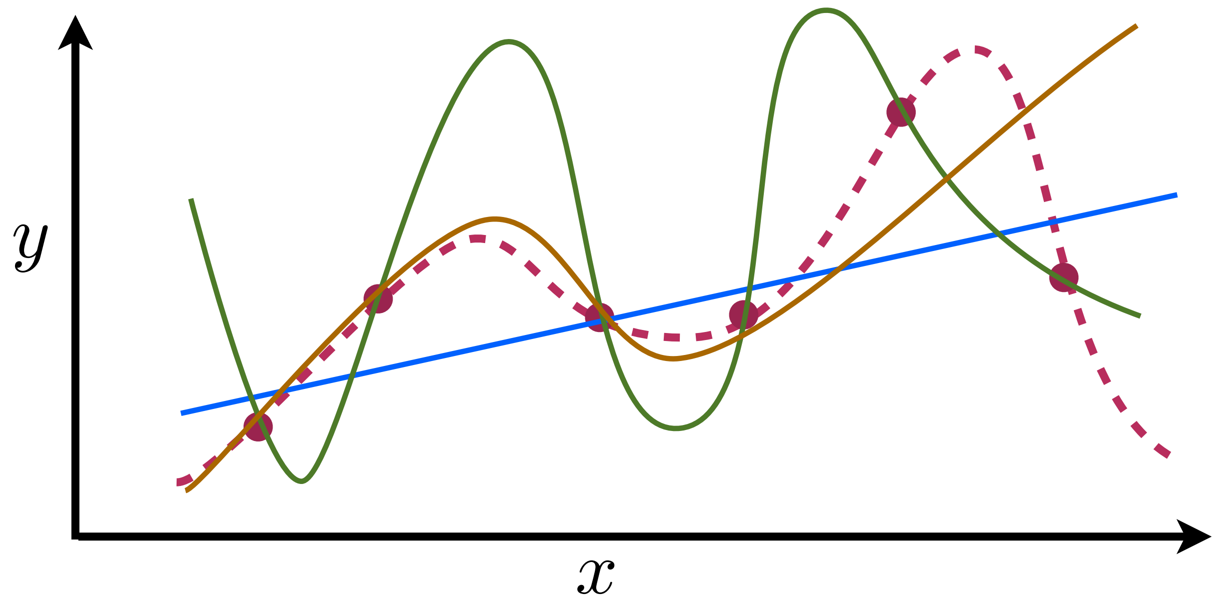
A concept class $\mathcal{C}$ is PAC-learnable if exists a learning algorithm A such that for all $f \in \mathcal{C}$, $\epsilon > 0, \delta > 0$ and distribution D

$$P_D(\epsilon_g \leq \epsilon) \geq 1-\delta$$

using $m = poly(1/\epsilon, 1/\delta)$ examples and polynomial time.

Overfitting and underfitting

training error v.s. hypothesis space size



linear functions: high training error, small space

$$\{y = a + bx \mid a, b \in \mathbb{R}\}$$

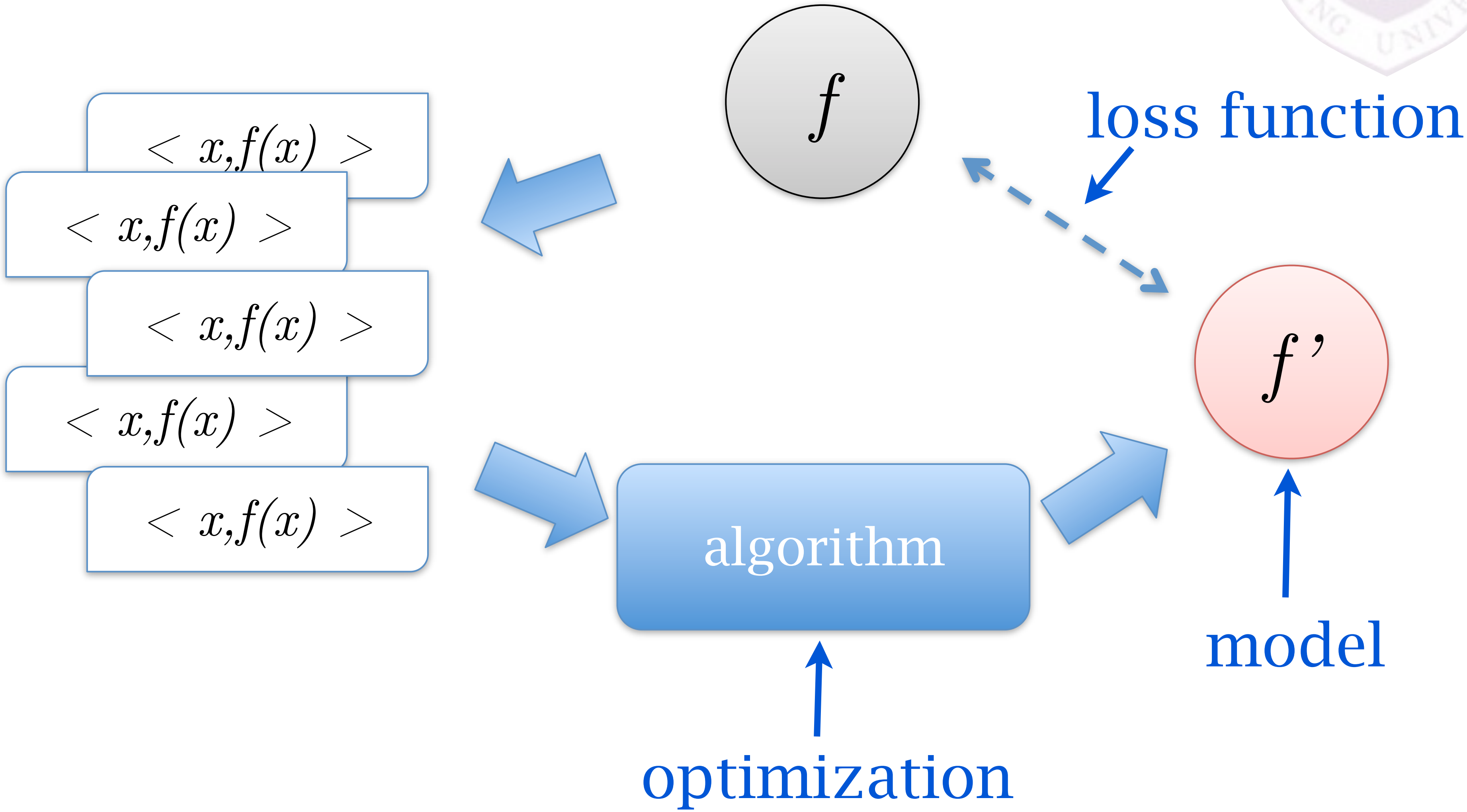
higher polynomials: moderate training error, moderate space

$$\{y = a + bx + cx^2 + dx^3 \mid a, b, c, d \in \mathbb{R}\}$$

even higher order: no training error, large space

$$\{y = a + bx + cx^2 + dx^3 + ex^4 + fx^5 \mid a, b, c, d, e, f \in \mathbb{R}\}$$

Dimensions of modeling



习题

监督学习的目标是否是最小化训练误差?

PAC-learning泛化界对于任意的潜在分布是否都成立?

以下两个多项式函数空间，哪一个的复杂度更高?

$$\mathcal{F}_1 = \{y = a + bx + cx^2 \mid a, b, c \in \mathbb{R}\}$$

$$\mathcal{F}_2 = \{y = a + ax + bx^2 + bx^3 + (a+b)x^4 \mid a, b \in \mathbb{R}\}$$

解释过配(overfitting)和欠配(underfitting)现象。