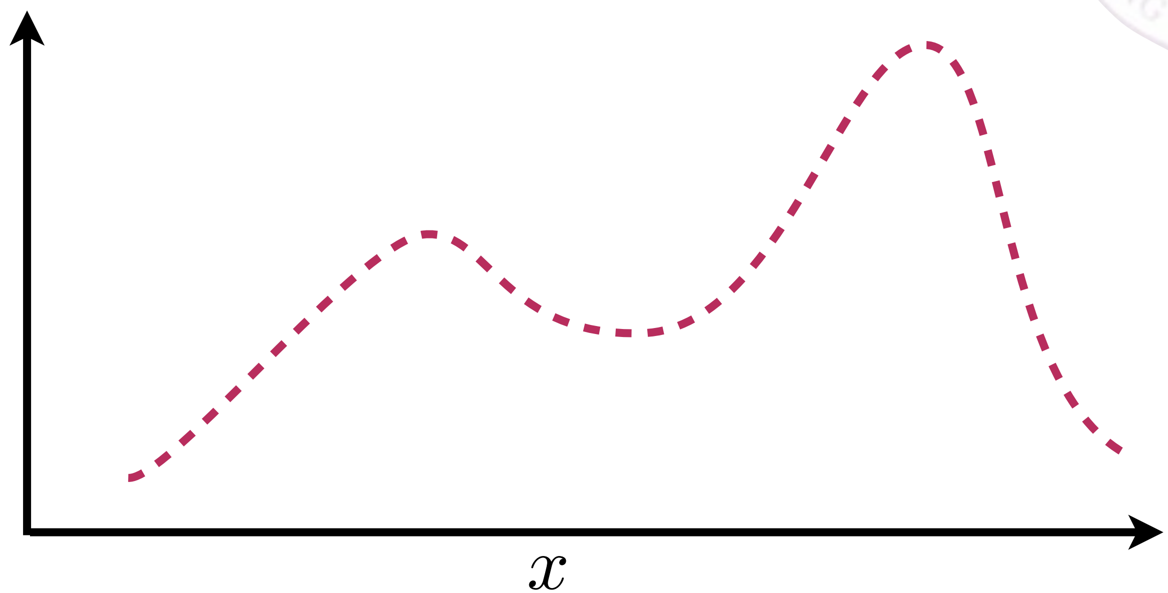
Lecture 4: Machine Learning II

Principle of Learning

http://cs.nju.edu.cn/yuy/course_dm13ms.ashx

The core of all the problems

infinite samples

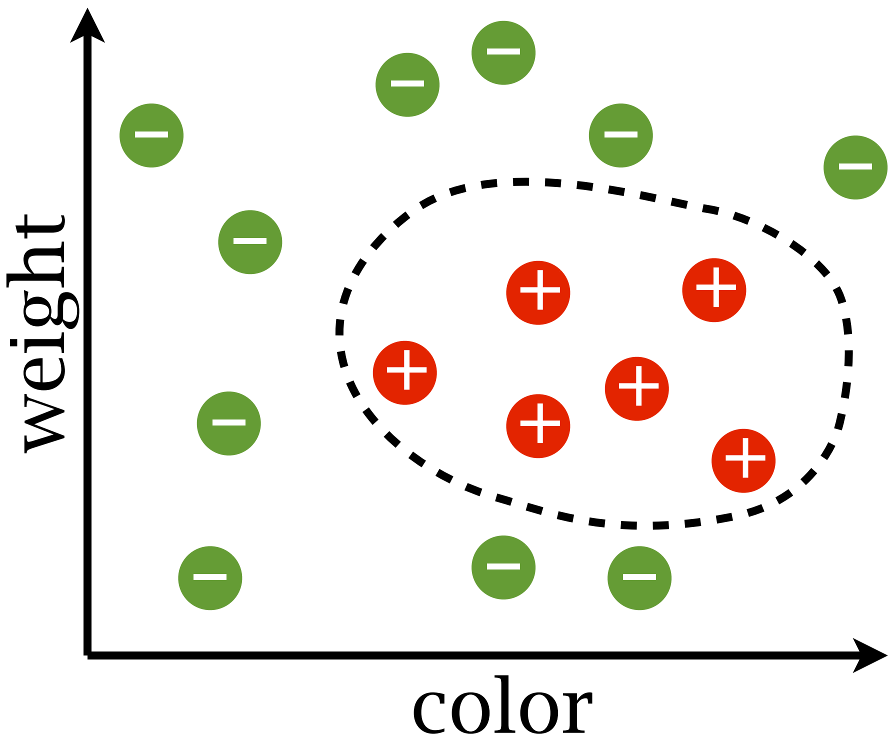


v.s.

finite samples

Classification

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



(color, weight) $\rightarrow$ sweet ?

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

ground-truth function f

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

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

learning: find an f' that is <u>close</u> to f

Classification

what can be observed:

on examples/training data:

$$\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)\} \quad y_i = f(\boldsymbol{x}_i)$$

e.g. training error

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

what is expected:

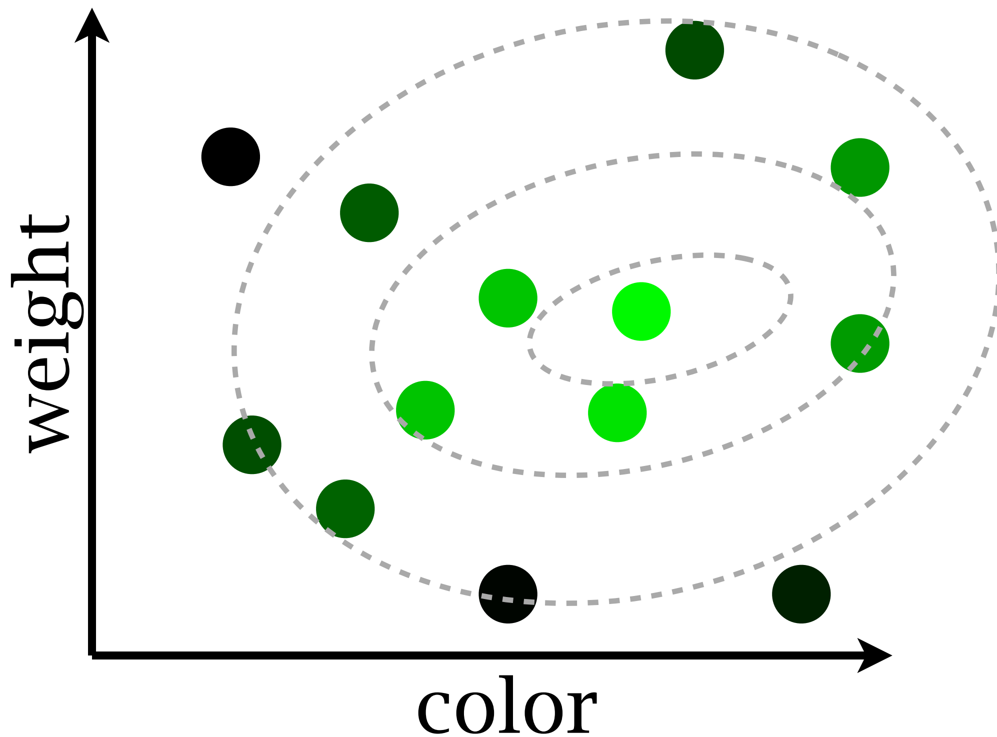
over the whole distribution: generalization error

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

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

Regression

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



(color, weight) $\rightarrow$ price

$\mathcal{X} \rightarrow [0, +1]$

ground-truth function f

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

learning: find an f' that is close to f

Regression

what can be observed:

on examples/training data:

$\{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_m, y_m)\} \quad y_i = f(\boldsymbol{x}_i)$

e.g. training mean square error/MSE

$$\epsilon_t = \frac{1}{m}\sum_{i=1}^{m}(h(\boldsymbol{x}_i) - y_i)^2$$

what is expected:

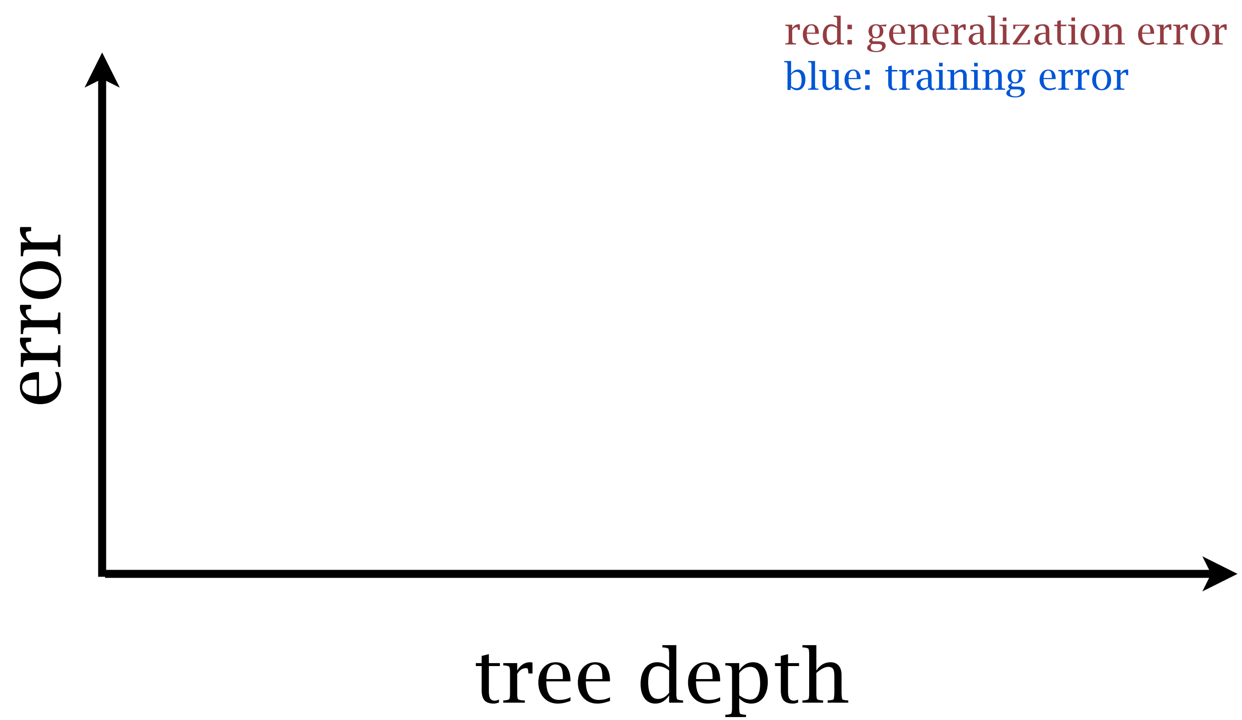
over the whole distribution: generalization MSE

$$\epsilon_g = \mathbb{E}_x(h(\boldsymbol{x}) \neq f(\boldsymbol{x}))^2$$

$$= \int_{\mathcal{X}} p(x)(h(\boldsymbol{x}) - f(\boldsymbol{x}))^2 \mathrm{d}x$$

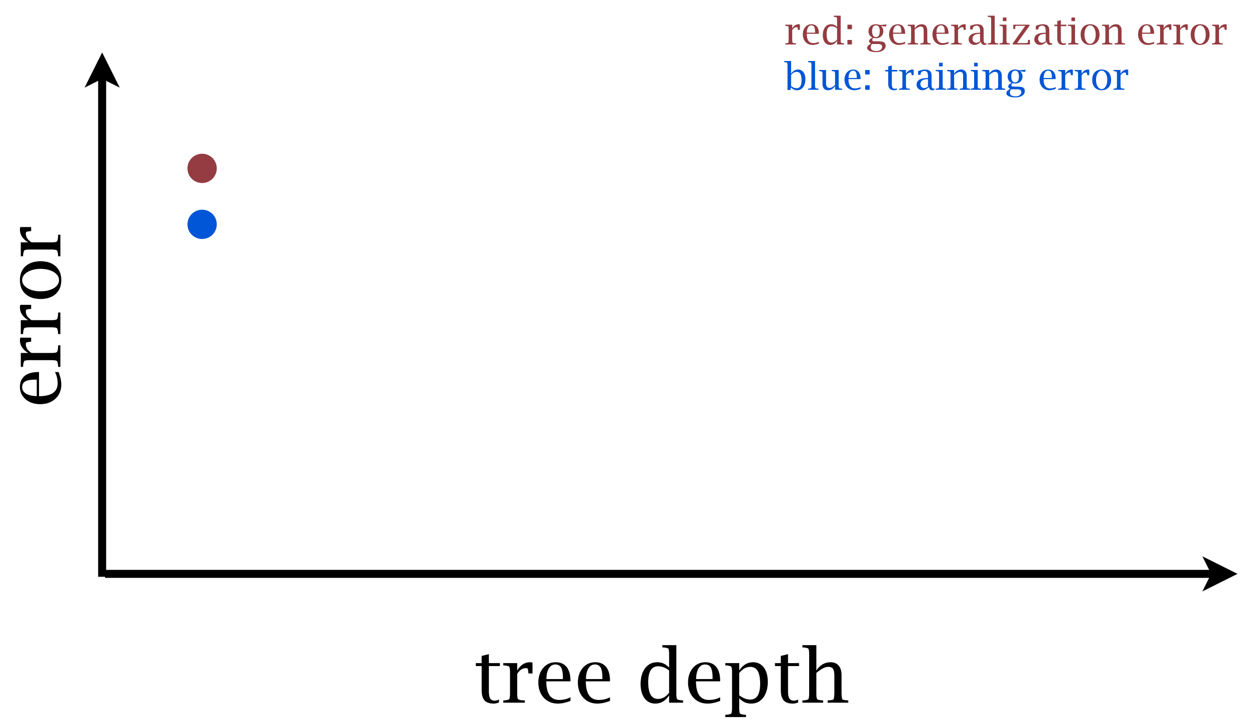
The overfitting phenomena

-- the divergence between infinite and finite samples



The overfitting phenomena

-- the divergence between infinite and finite samples



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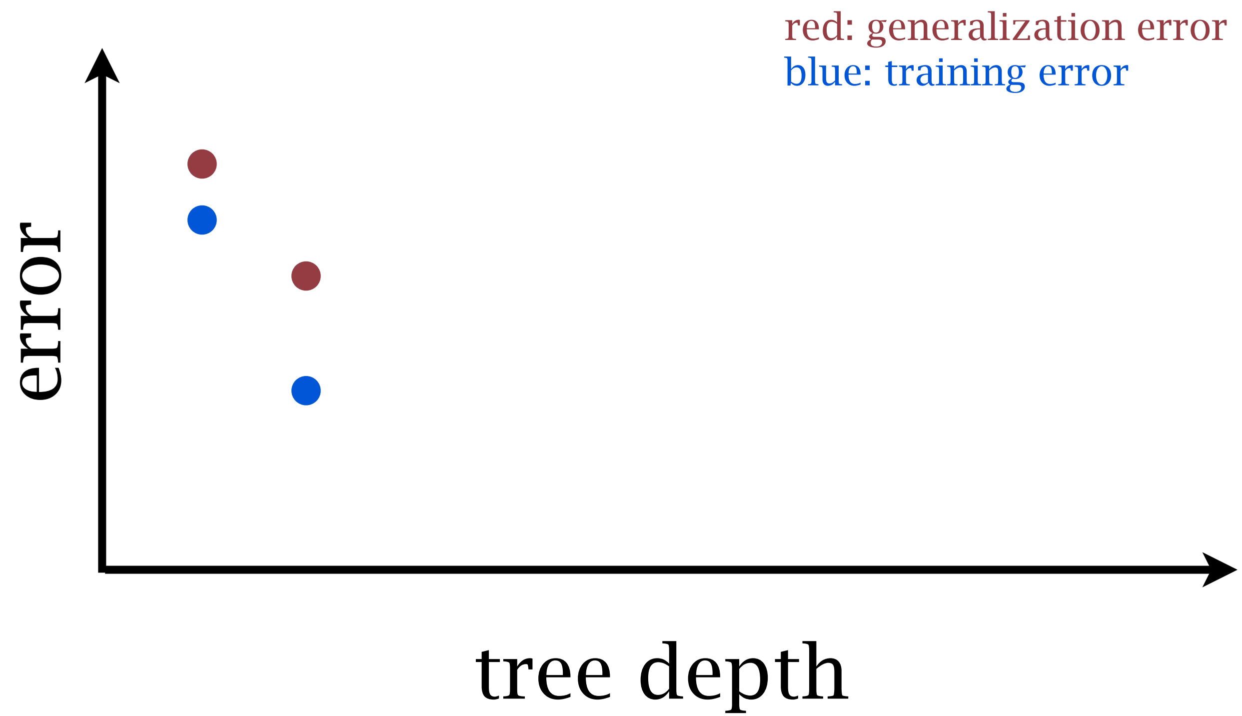

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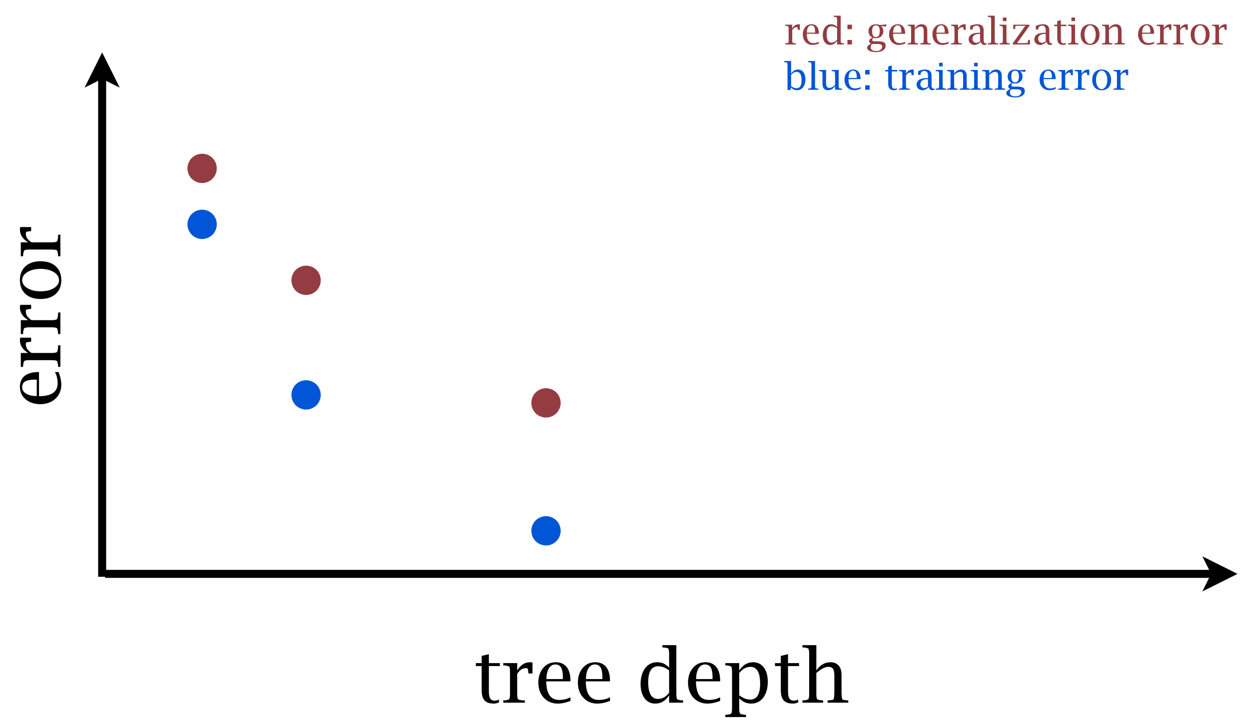

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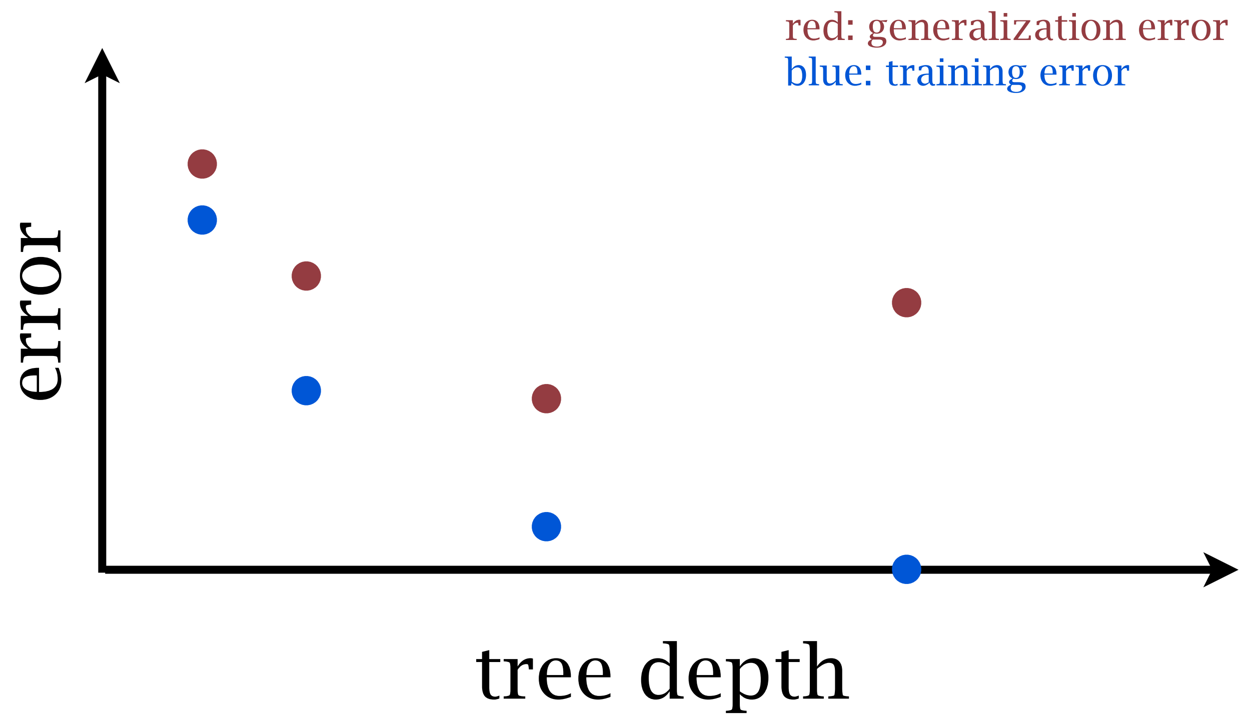

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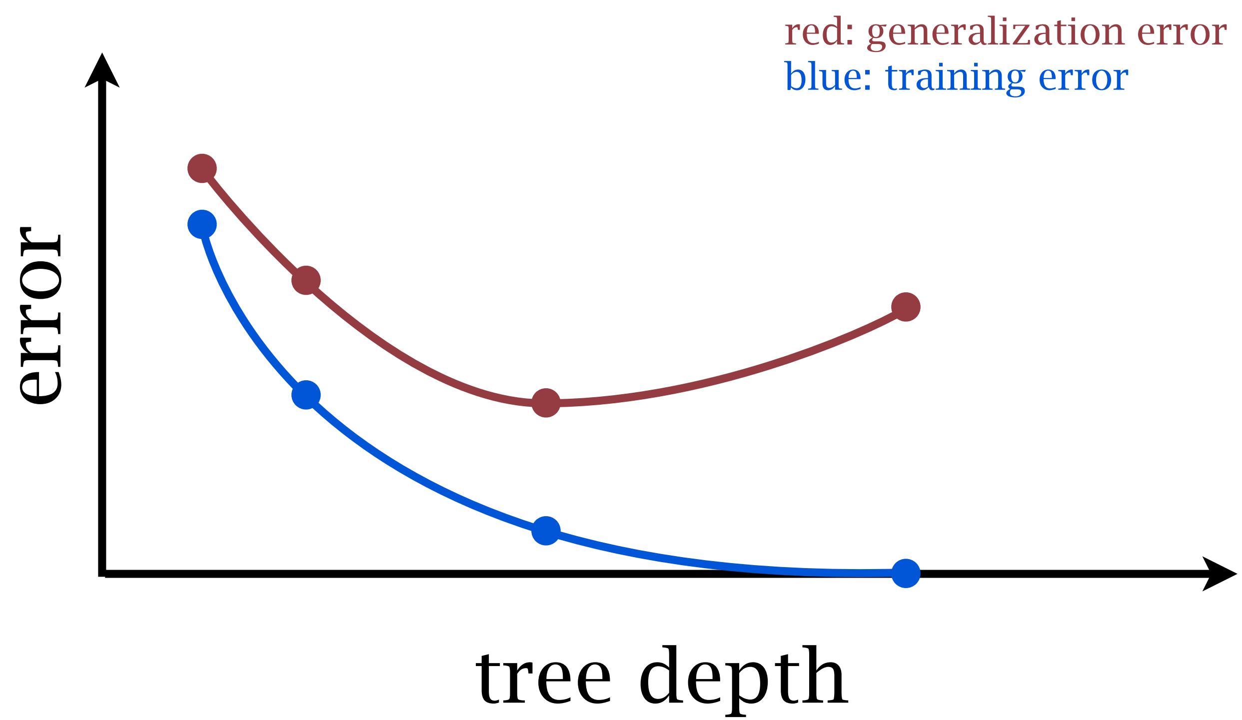

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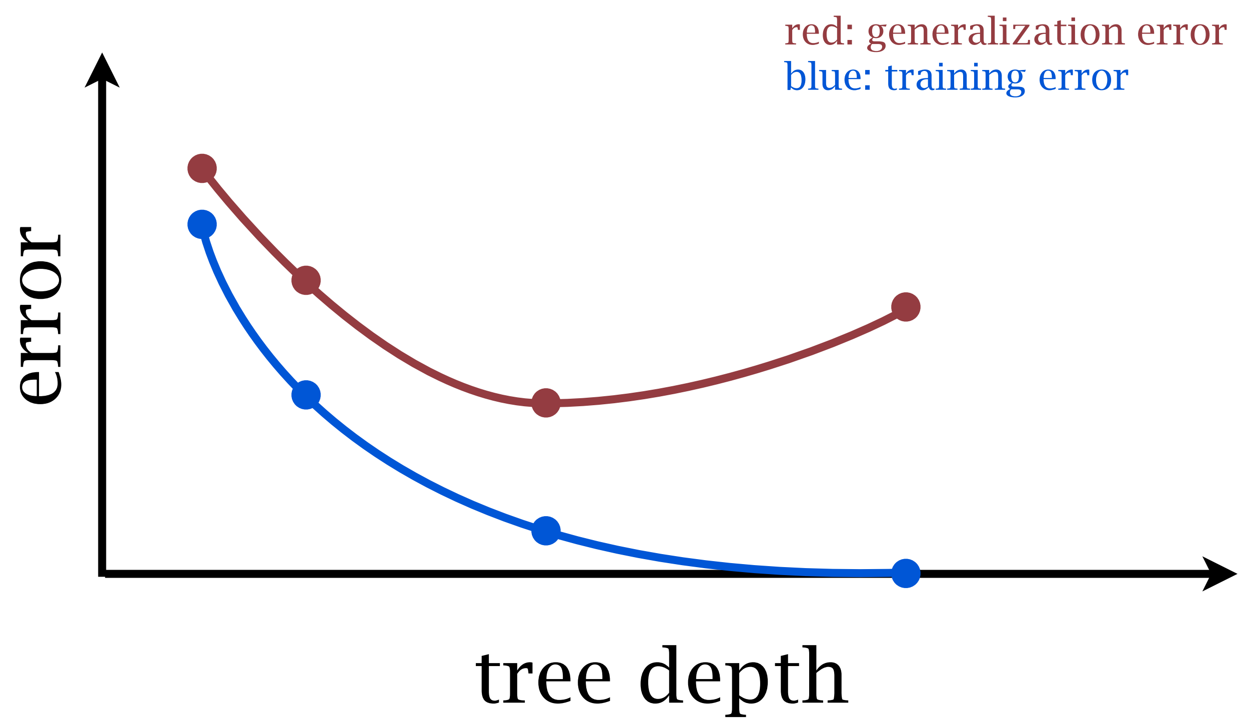
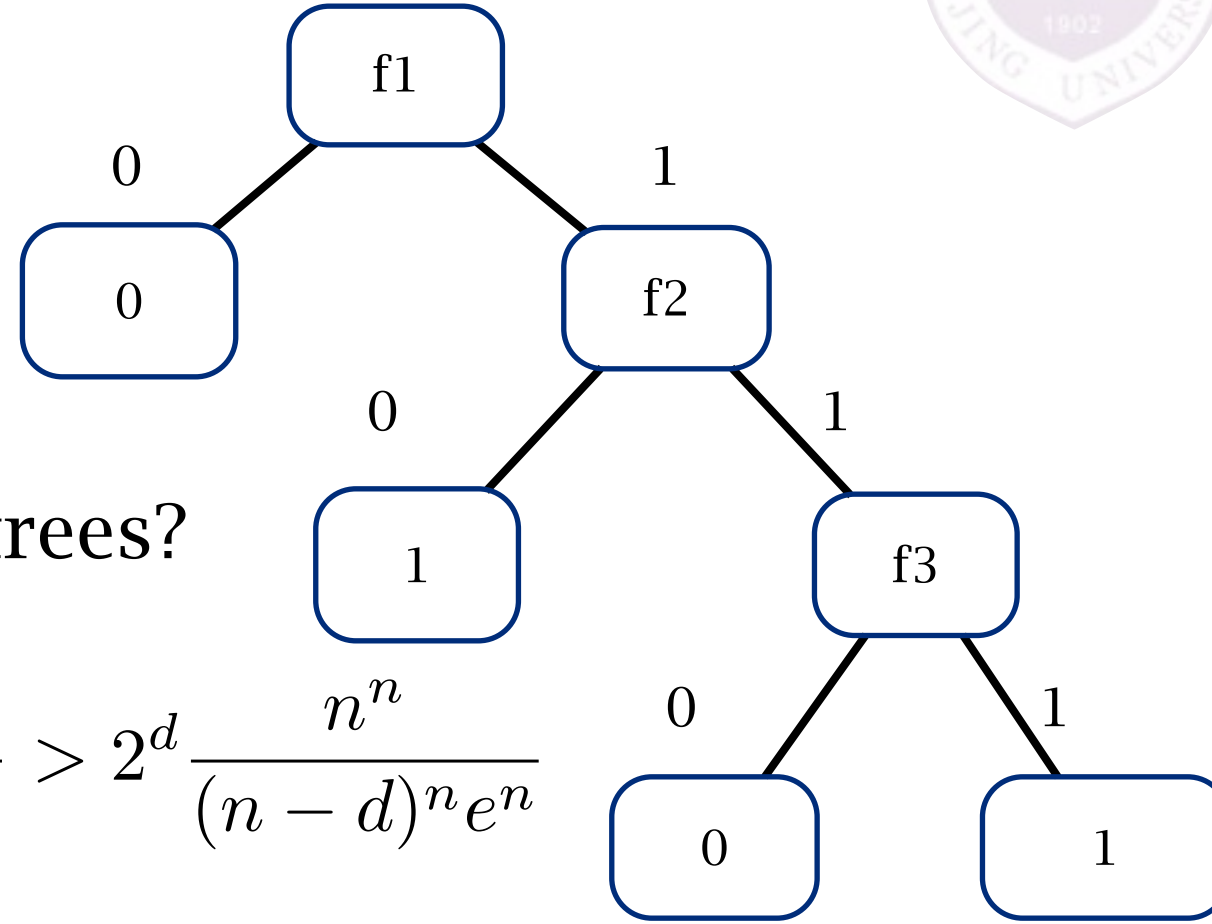


why tree depth?

Tree depth and the possibilities

features: n
feature type: binary
depth: $d<n$



How many different trees?

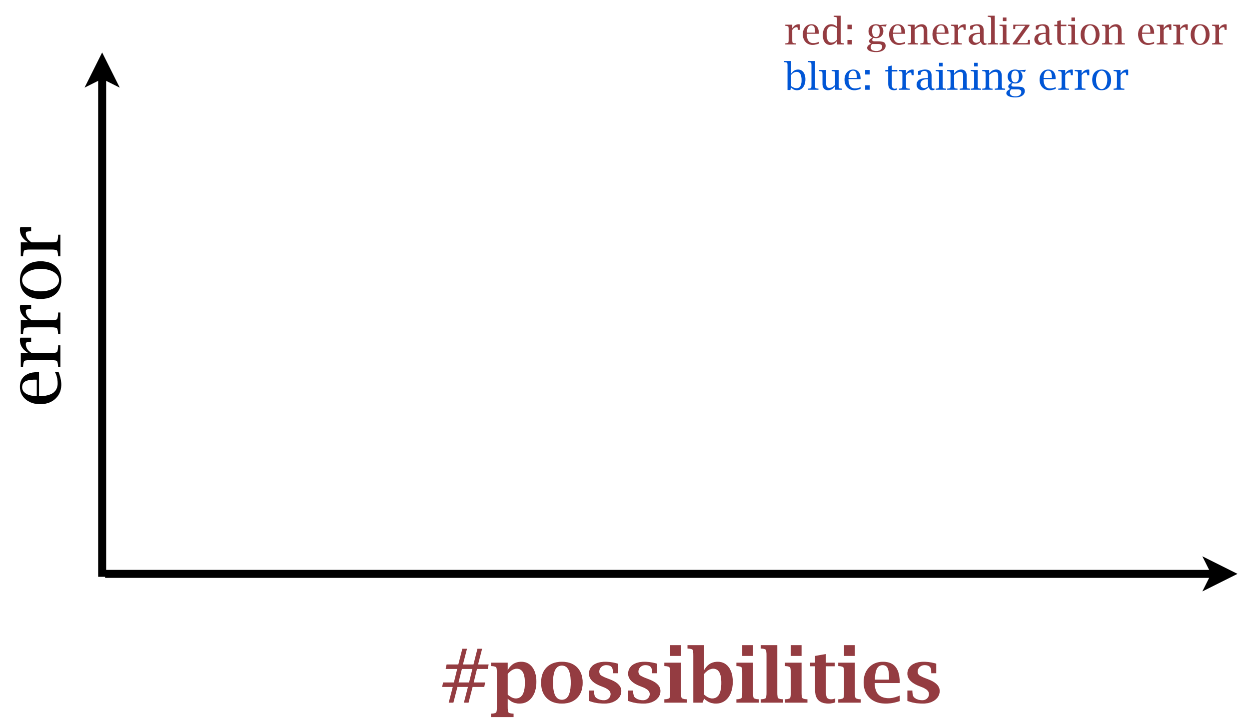
one-branch: $2^d \frac{n!}{(n-d)!} > 2^d \frac{n^n}{(n-d)^n e^n}$

full-tree: $2^{2^d} \prod_{i=0}^{d-1} \frac{(n-i)!}{(n-d-i)!}$

the possibility of trees grows very fast with d

The overfitting phenomena

-- the divergence between infinite and finite samples



The overfitting phenomena

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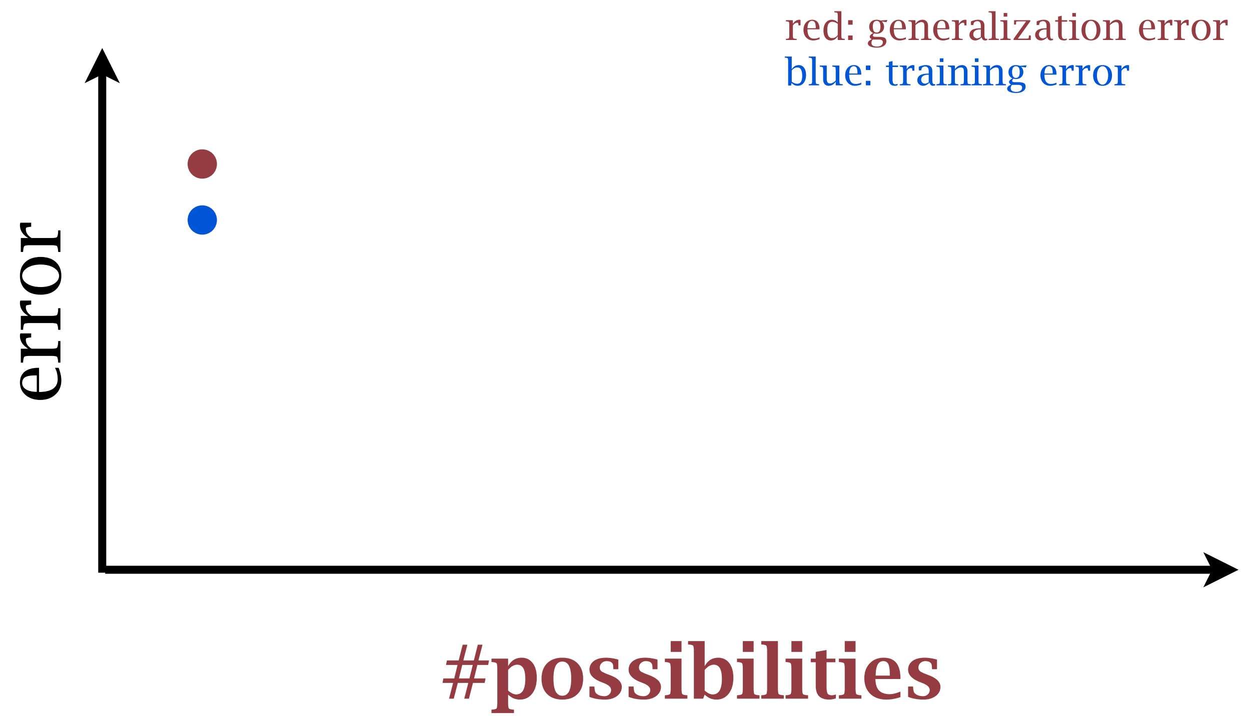

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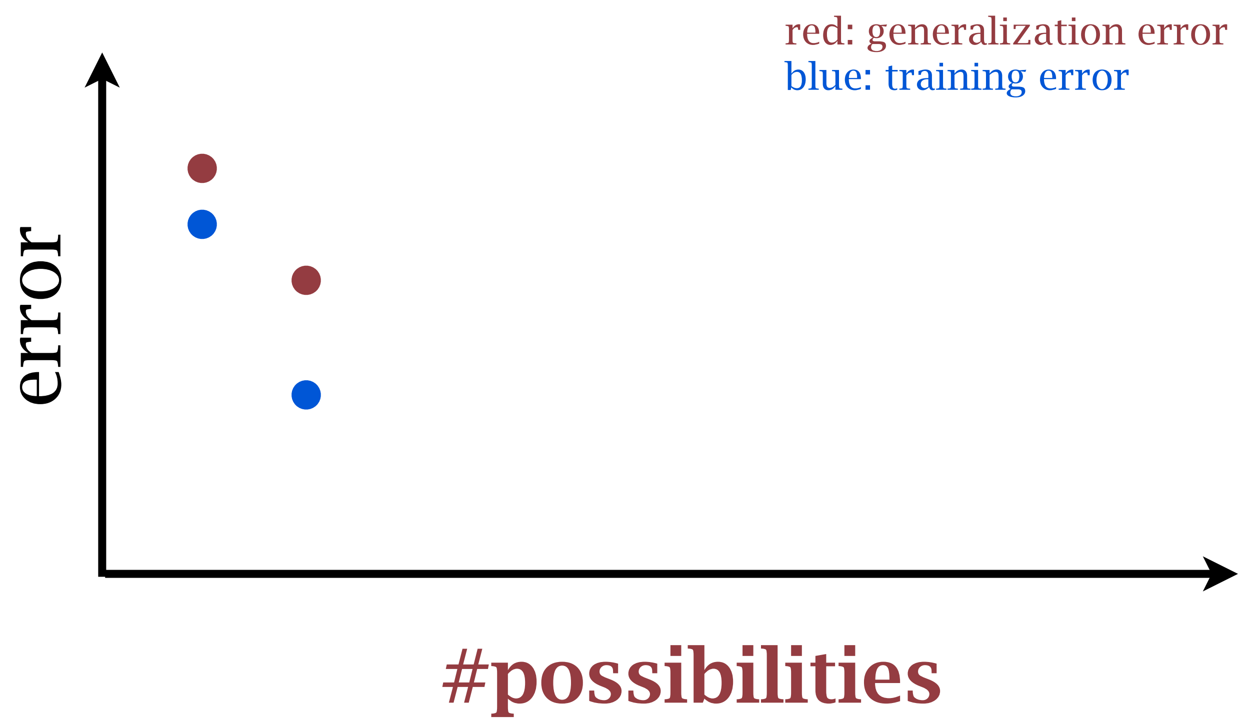

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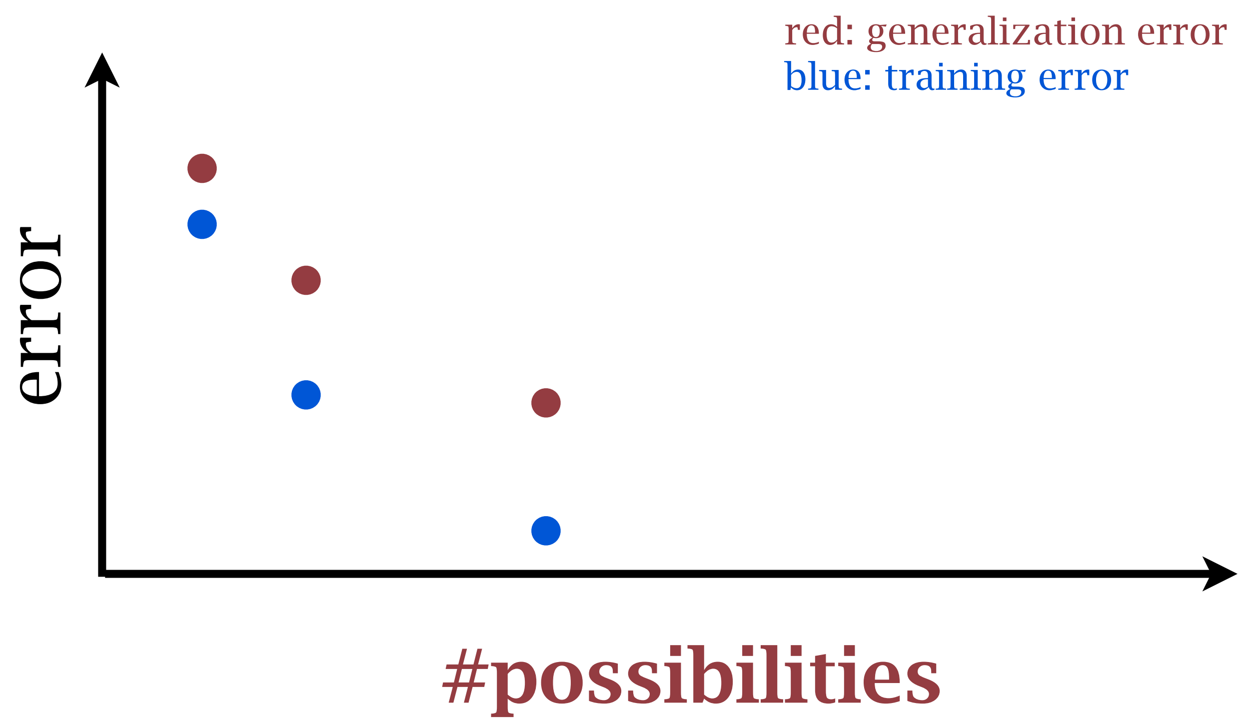

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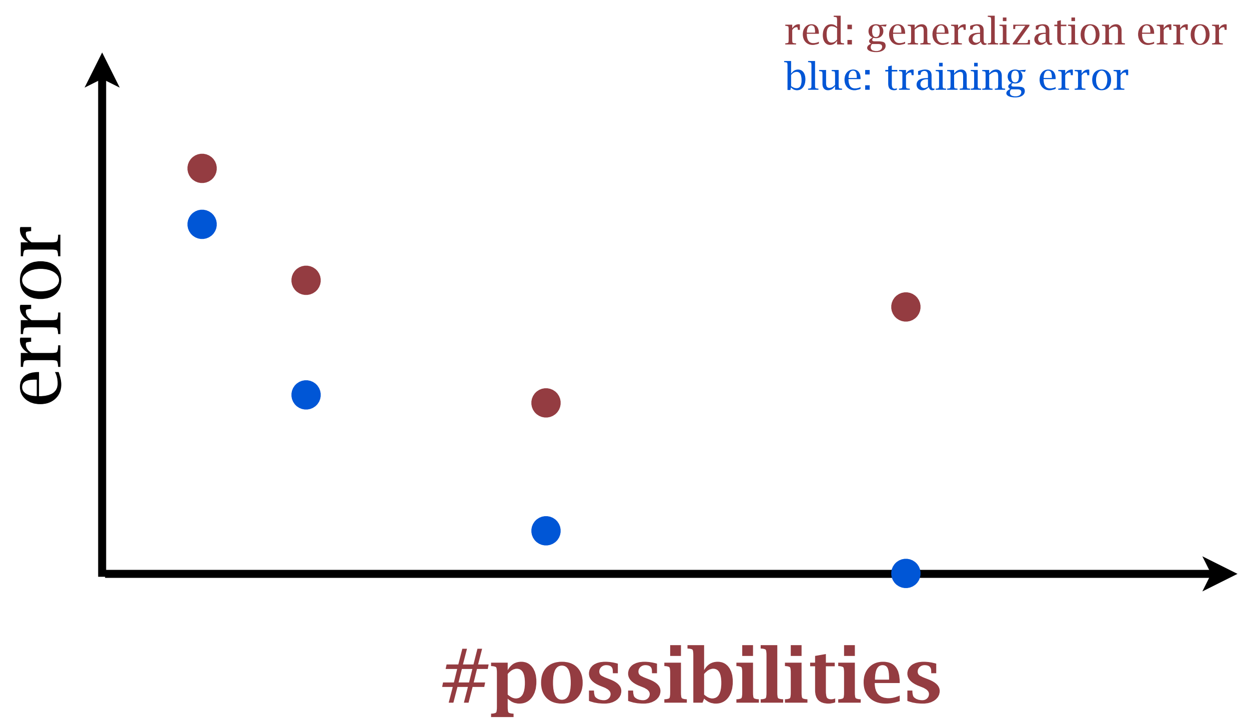

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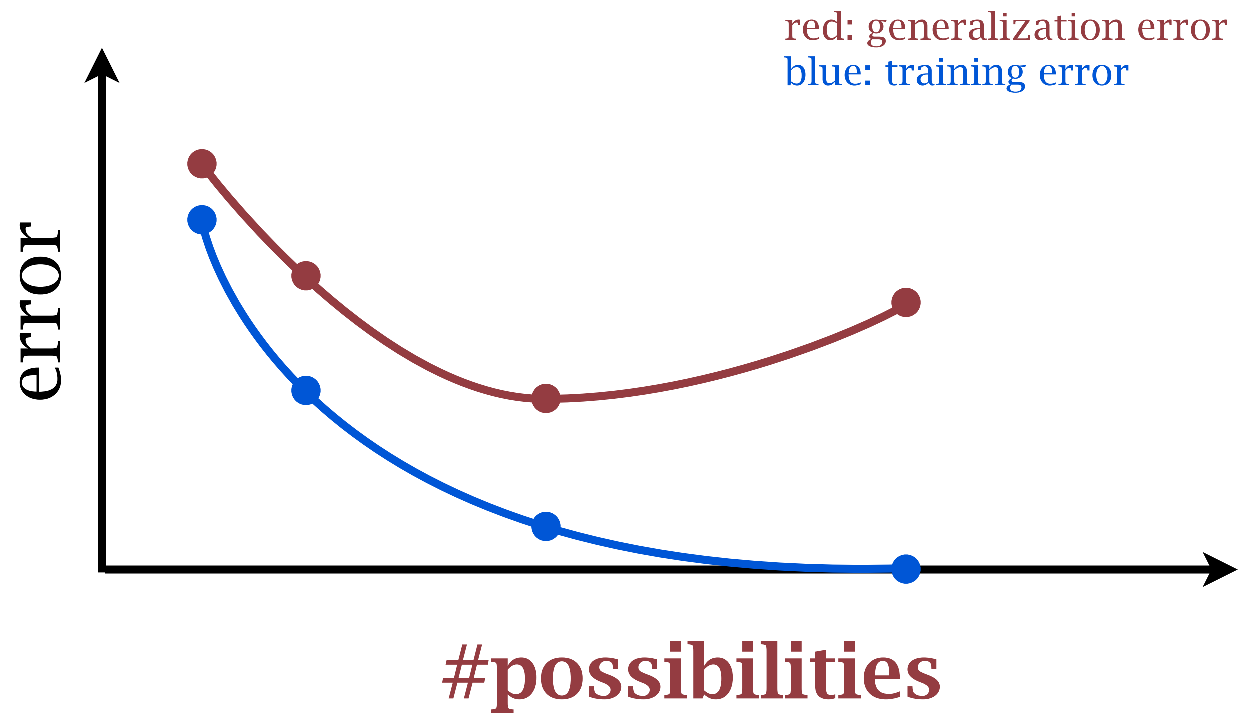

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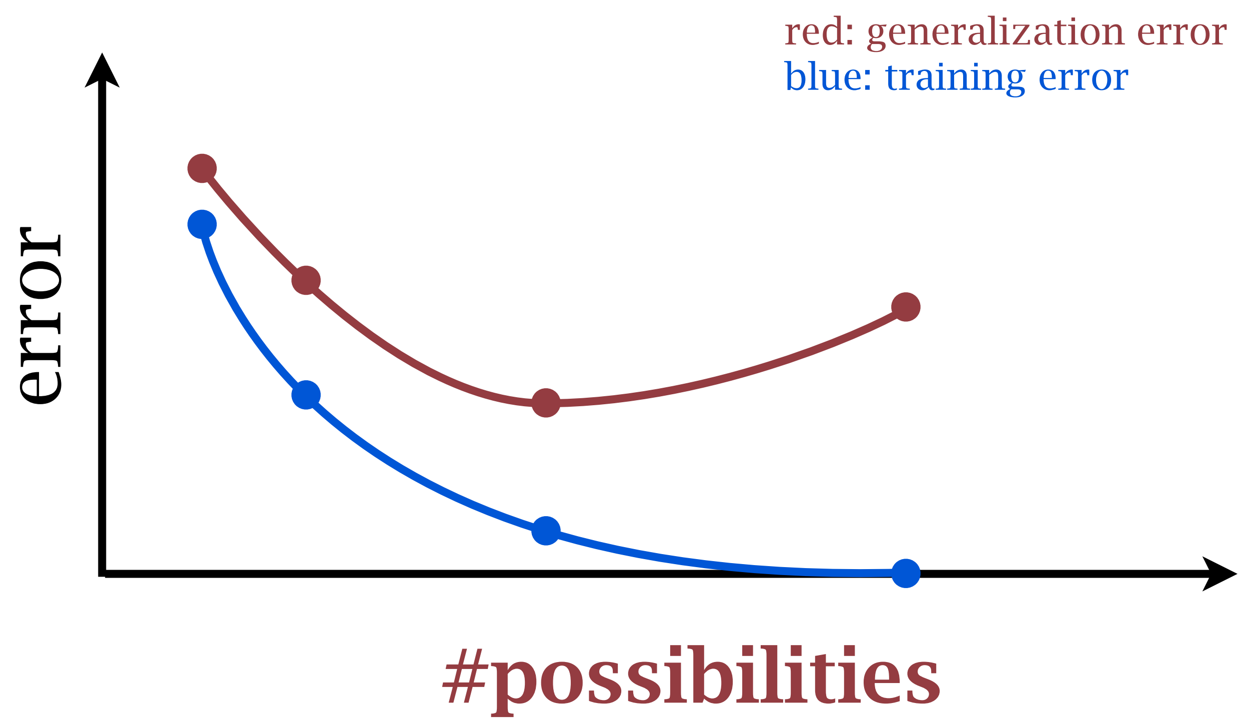
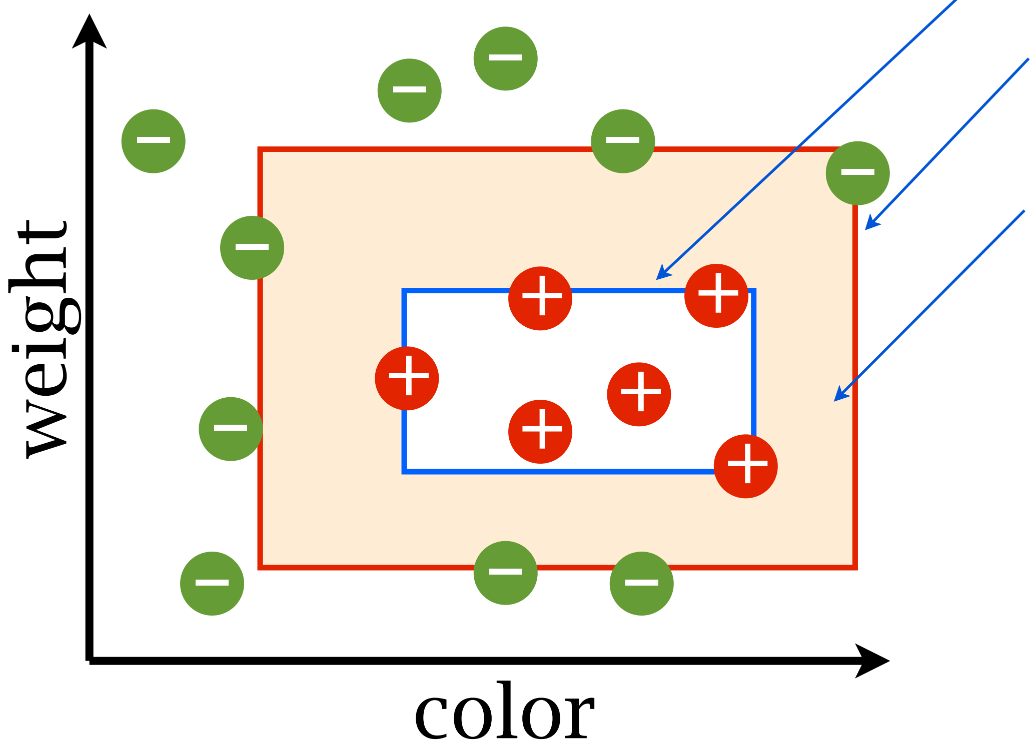


why #possibilities?

The version space algorithm

an abstract view of learning algorithms



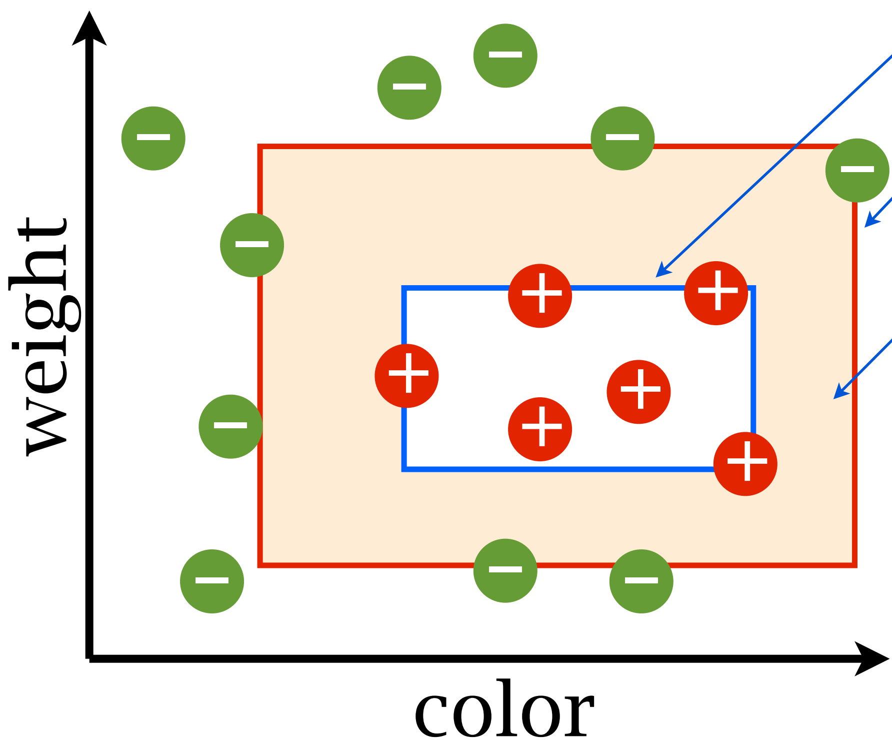
S: most specific hypothesis

G: most general hypothesis

version space: consistent hypotheses [Mitchell, 1997]

The version space algorithm

an abstract view of learning algorithms



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

The version space algorithm

an abstract view of learning algorithms

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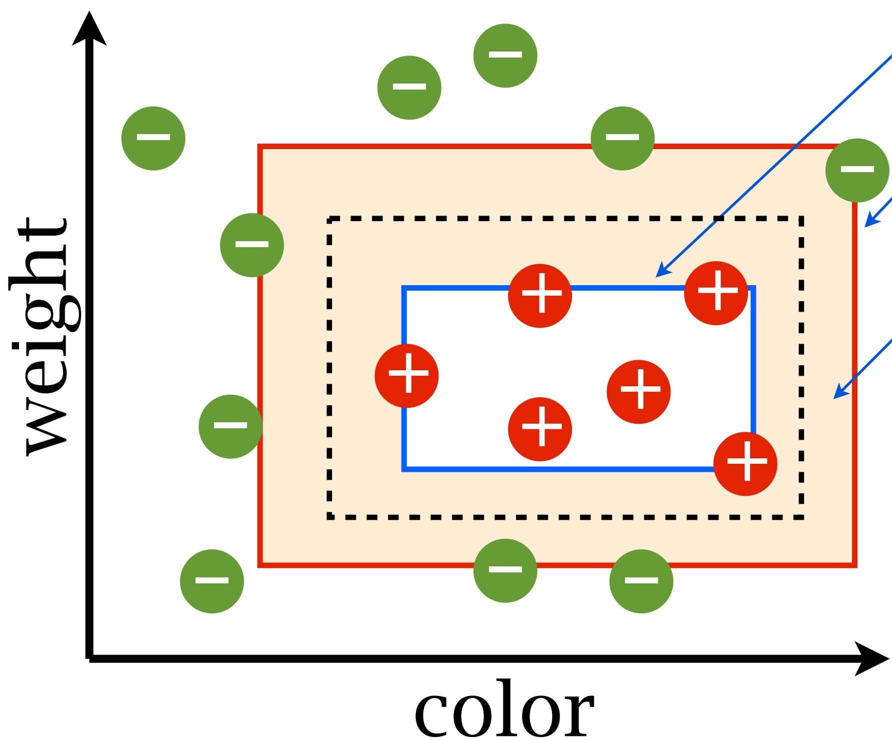

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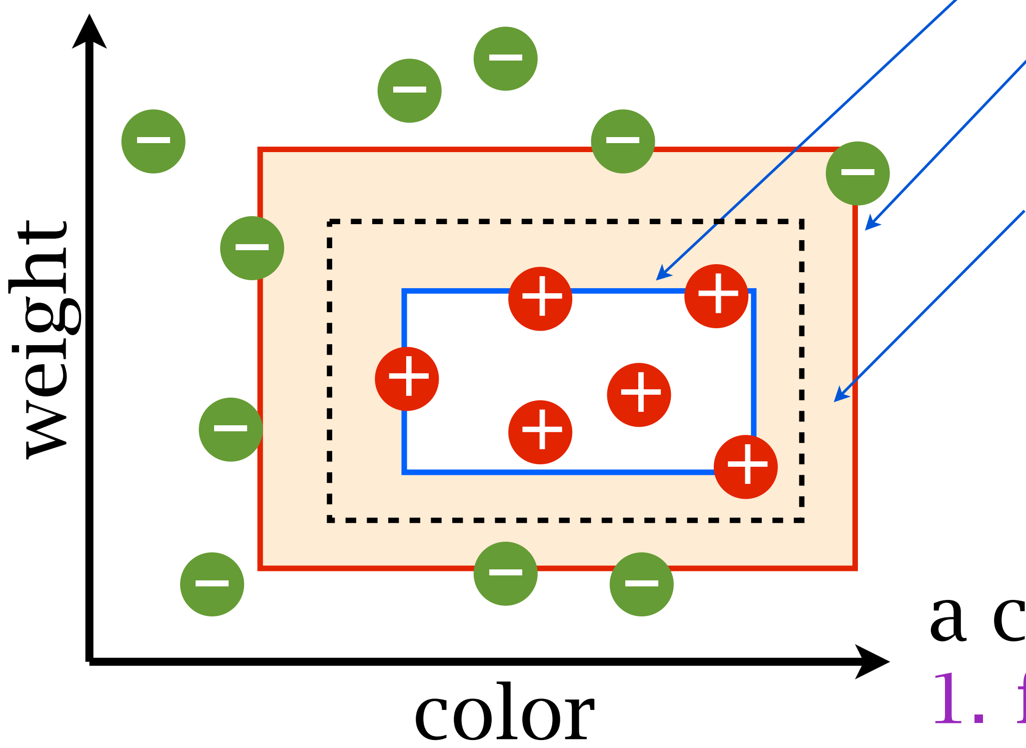

S: most specific hypothesis

G: most general hypothesis

version space: consistent hypotheses [Mitchell, 1997]

selection a hypothesis according to learner's bias

a conceptual algorithm:

1. for every example, remove the conflict boxes
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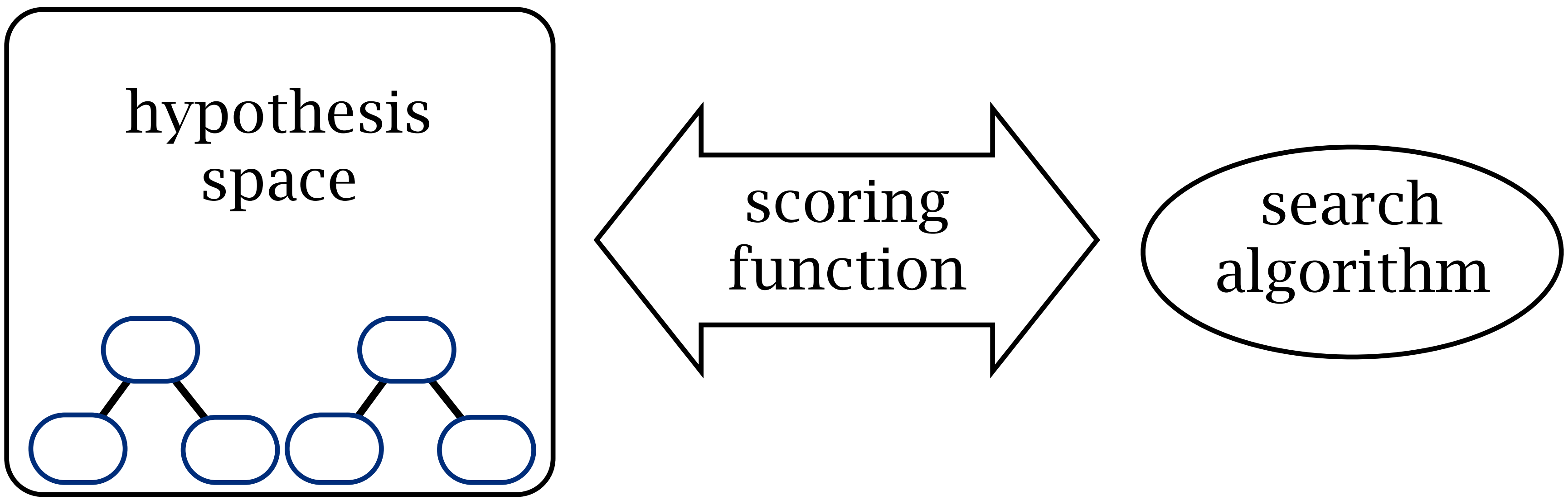
The version space algorithm

an abstract view of learning algorithms

three components of a learning algorithm

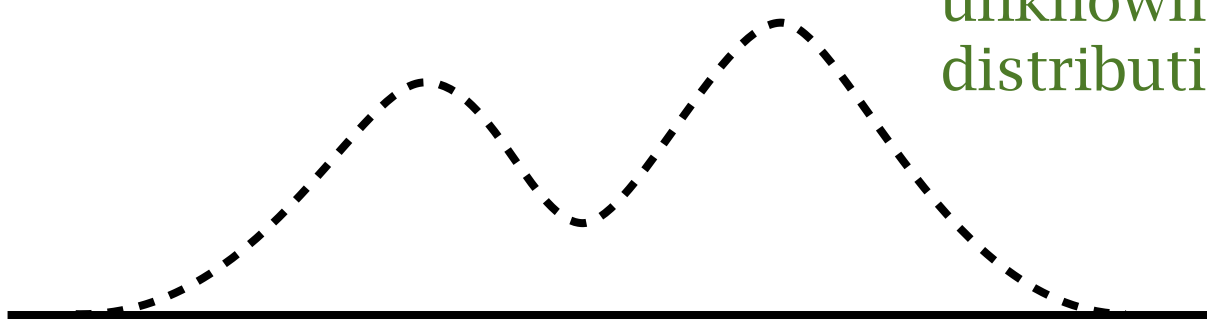


#possibility ≈ hypothesis space size

Theories

The i.i.d. assumption:

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



bias-variance dilemma (regression)

generalization bound (classification)

Bias-variance dilemma

Suppose we have 100 training examples
but there can be different 100 training examples

Start from the expected training MSE:

$$E_D[\epsilon_t] = E_D\left[\frac{1}{m}\sum_{i=1}^{m}(h(\boldsymbol{x}_i) - y_i)^2\right] = \frac{1}{m}\sum_{i=1}^{m} E_D\left[(h(\boldsymbol{x}_i) - y_i)^2\right]$$

(assume no noise)

$$= E_D\left[(h(\boldsymbol{x}) - f(\boldsymbol{x}))^2\right]$$

$$= E_D\left[(h(\boldsymbol{x}) - E_D[h(\boldsymbol{x})] + E_D[h(\boldsymbol{x})] - f(\boldsymbol{x}))^2\right]$$

$$= E_D\left[(h(\boldsymbol{x}) - E_D[h(\boldsymbol{x})])^2\right] + E_D\left[(E_D[h(\boldsymbol{x})] - f(\boldsymbol{x}))^2\right]$$

$$+ E_D\left[2(h(\boldsymbol{x}) - E_D[h(\boldsymbol{x})])(E_D[h(\boldsymbol{x})] - f(\boldsymbol{x}))\right]$$

$$= E_D\left[(h(\boldsymbol{x}) - E_D[h(\boldsymbol{x})])^2\right] + E_D\left[(E_D[h(\boldsymbol{x})] - f(\boldsymbol{x}))^2\right]$$

variance bias^2

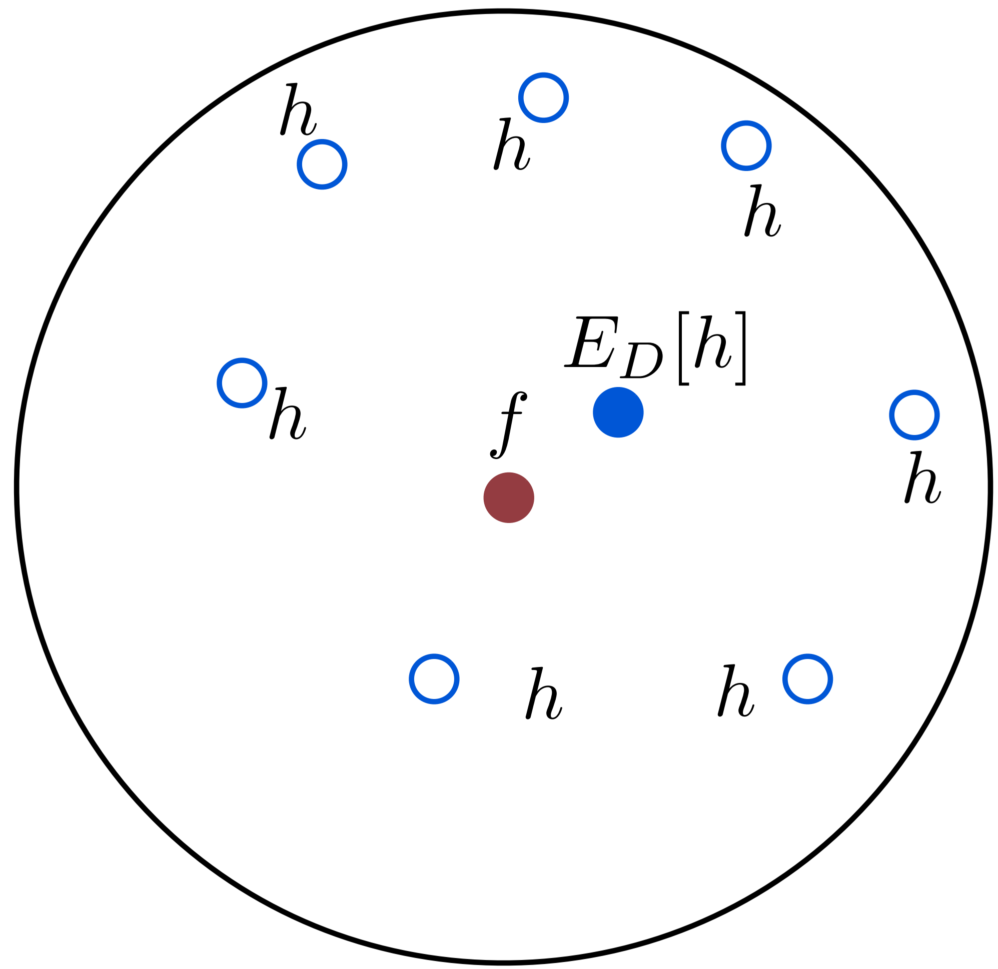
Bias-variance dilemma

$$E_D\left[(h(\boldsymbol{x}) - E_D[h(\boldsymbol{x})])^2\right]$$

variance

$$E_D\left[(E_D[h(\boldsymbol{x})] - f(\boldsymbol{x}))^2\right]$$

bias^2

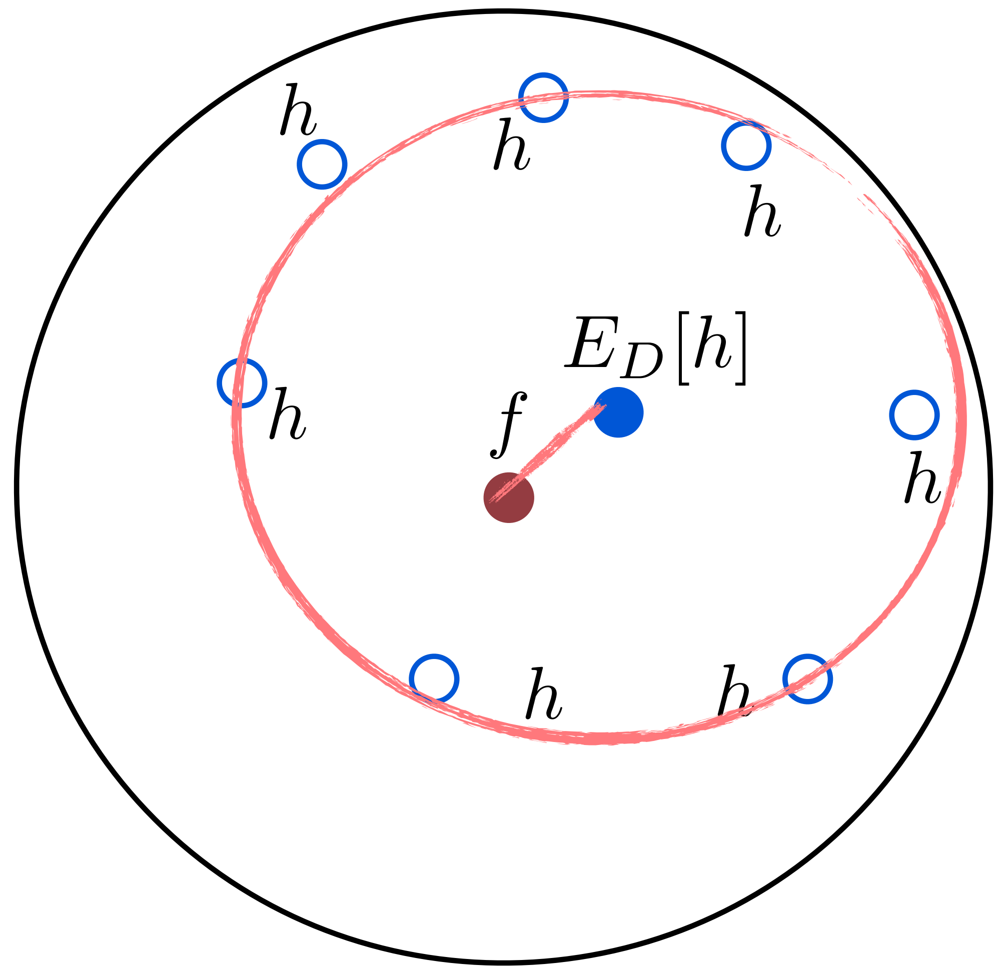


hypothesis space

Bias-variance dilemma

$$E_D\left[(h(\boldsymbol{x}) - E_D[h(\boldsymbol{x})])^2\right] \qquad E_D\left[(E_D[h(\boldsymbol{x})] - f(\boldsymbol{x}))^2\right]$$

variance bias^2



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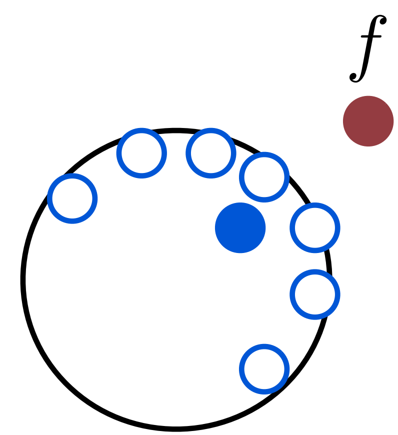
bias^2

smaller hypothesis space
=>
smaller variance
but higher bias



hypothesis space

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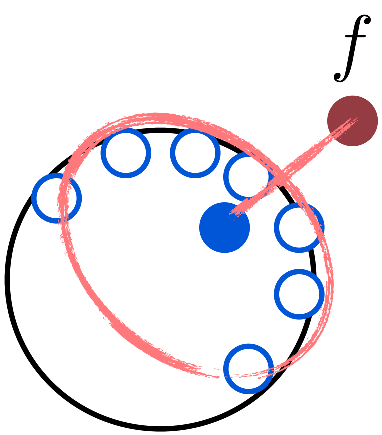

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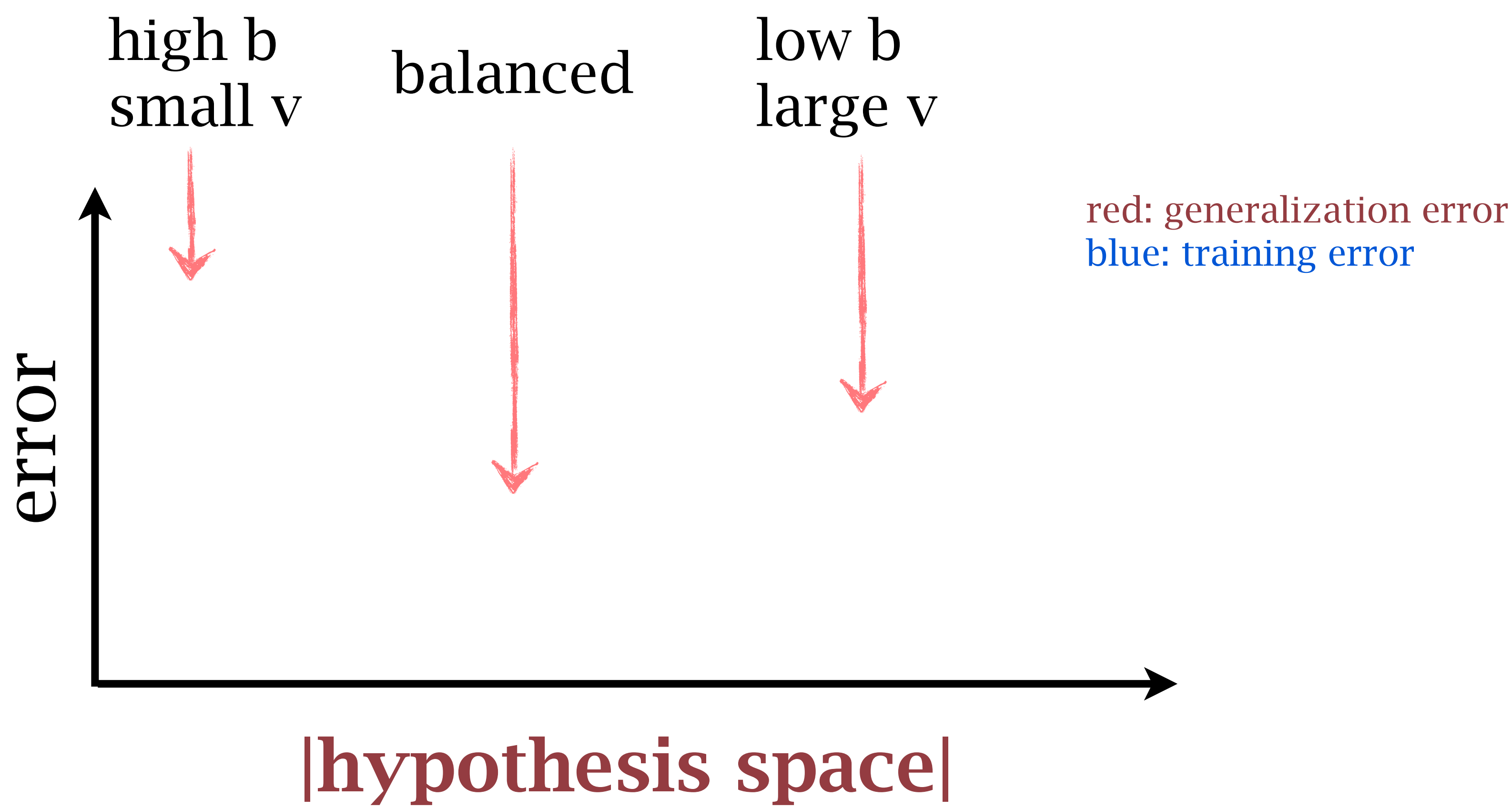

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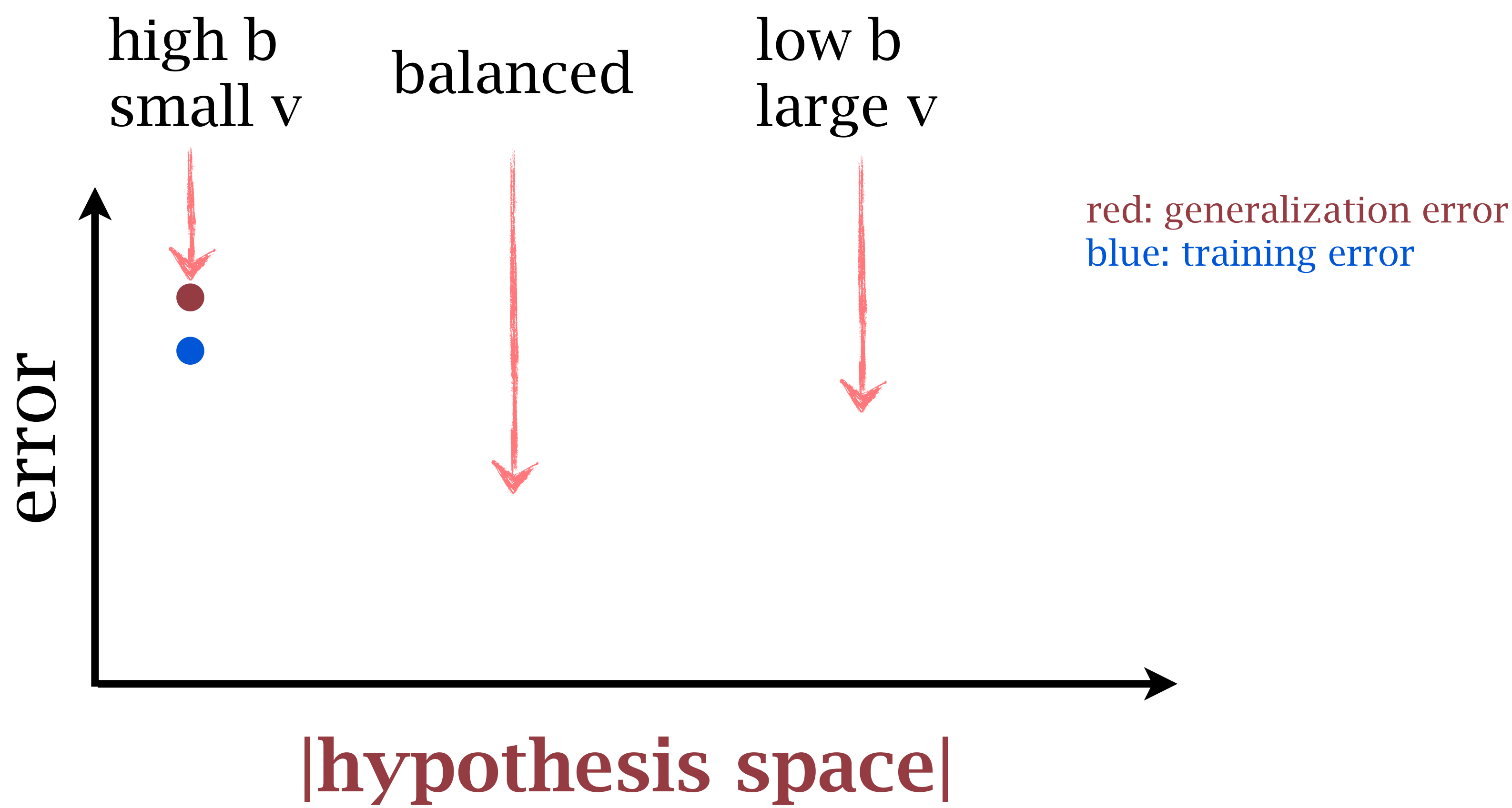

Bias-variance dilemma

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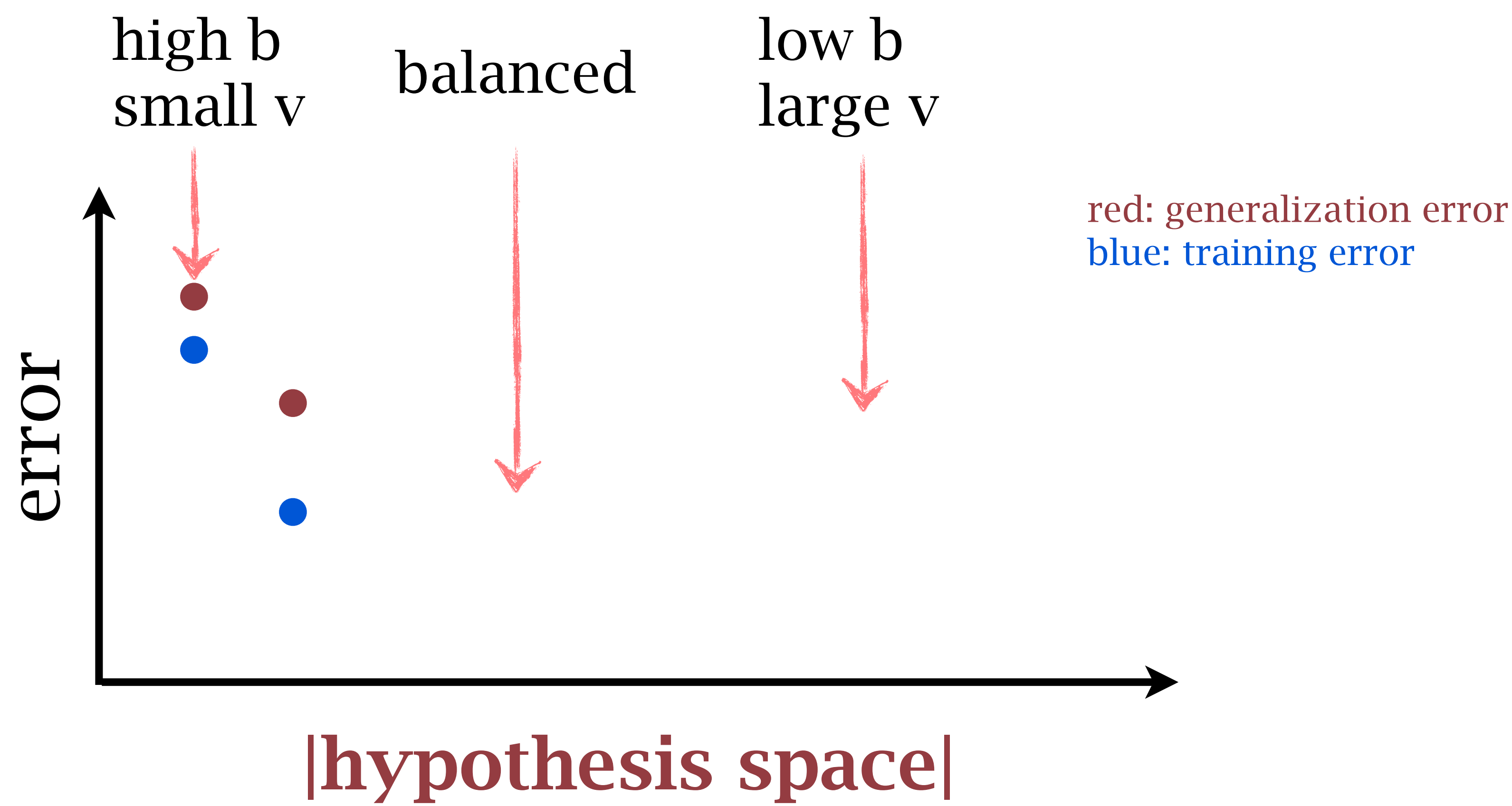
variance　　　　　　　　bias^2



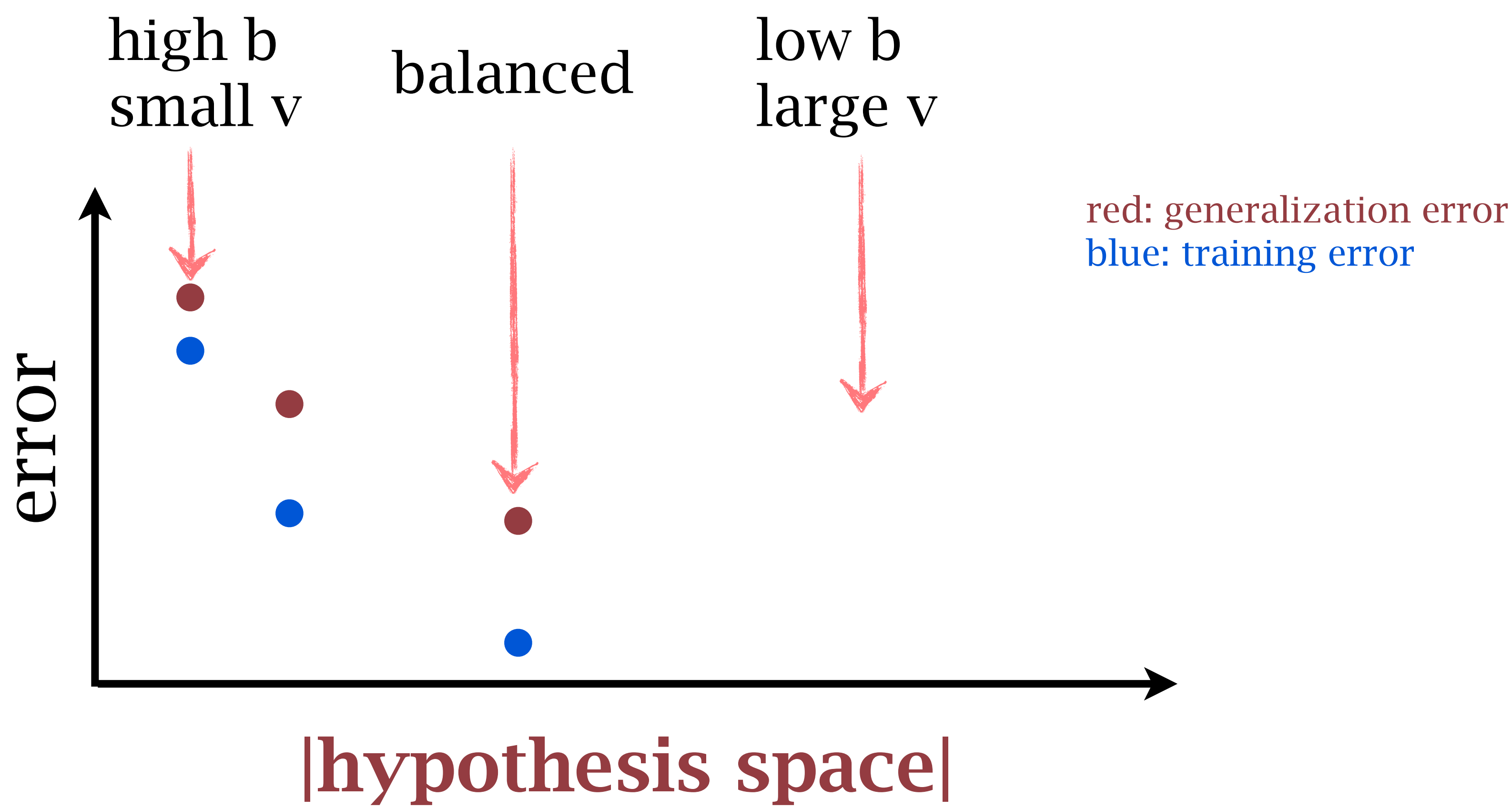
Bias-variance dilemma

$$E_D\left[\left(h(\boldsymbol{x}) - E_D[h(\boldsymbol{x})]\right)^2\right]$$

variance

$$E_D\left[\left(E_D[h(\boldsymbol{x})] - f(\boldsymbol{x})\right)^2\right]$$

bias^2



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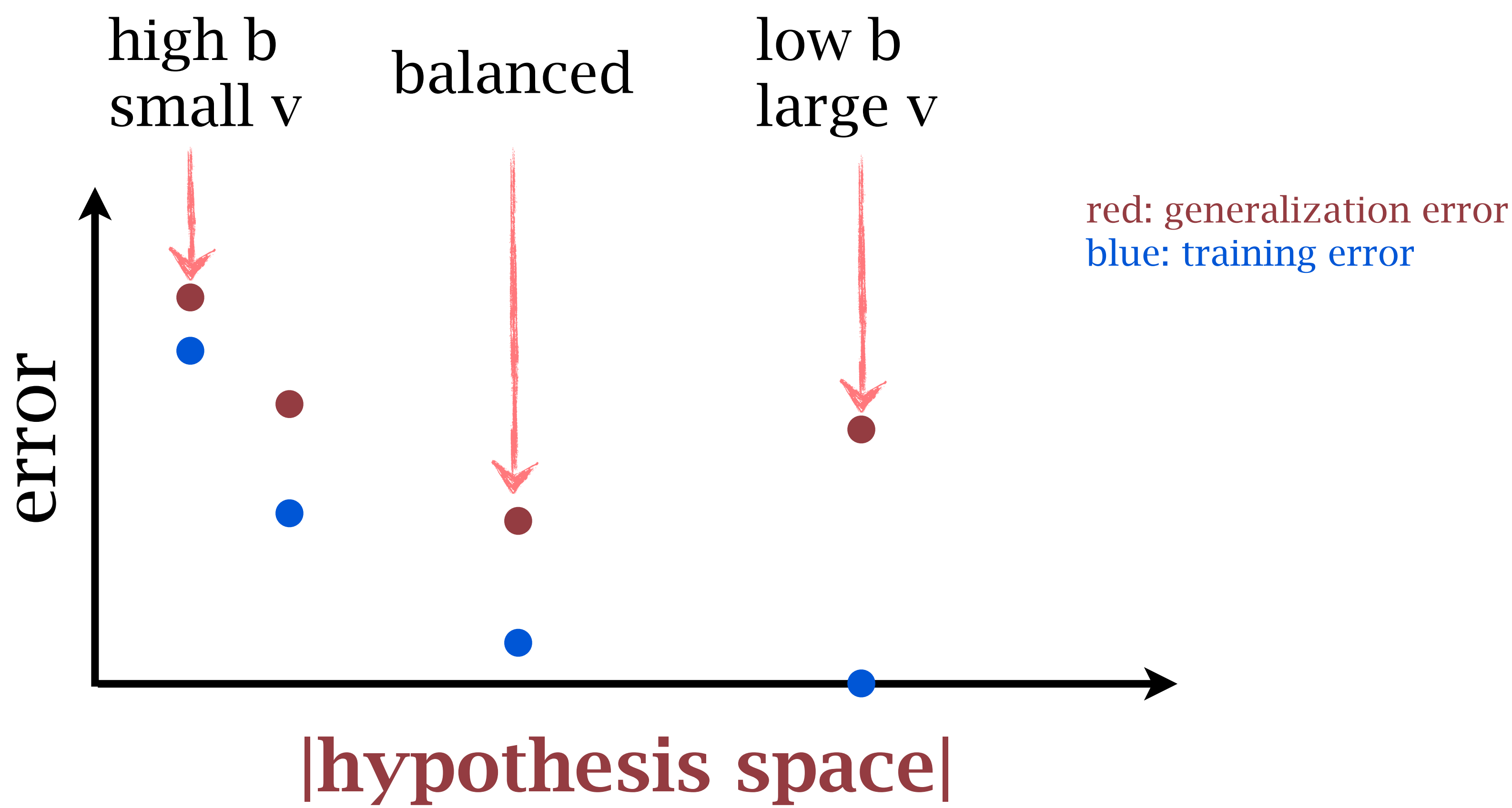

Bias-variance dilemma

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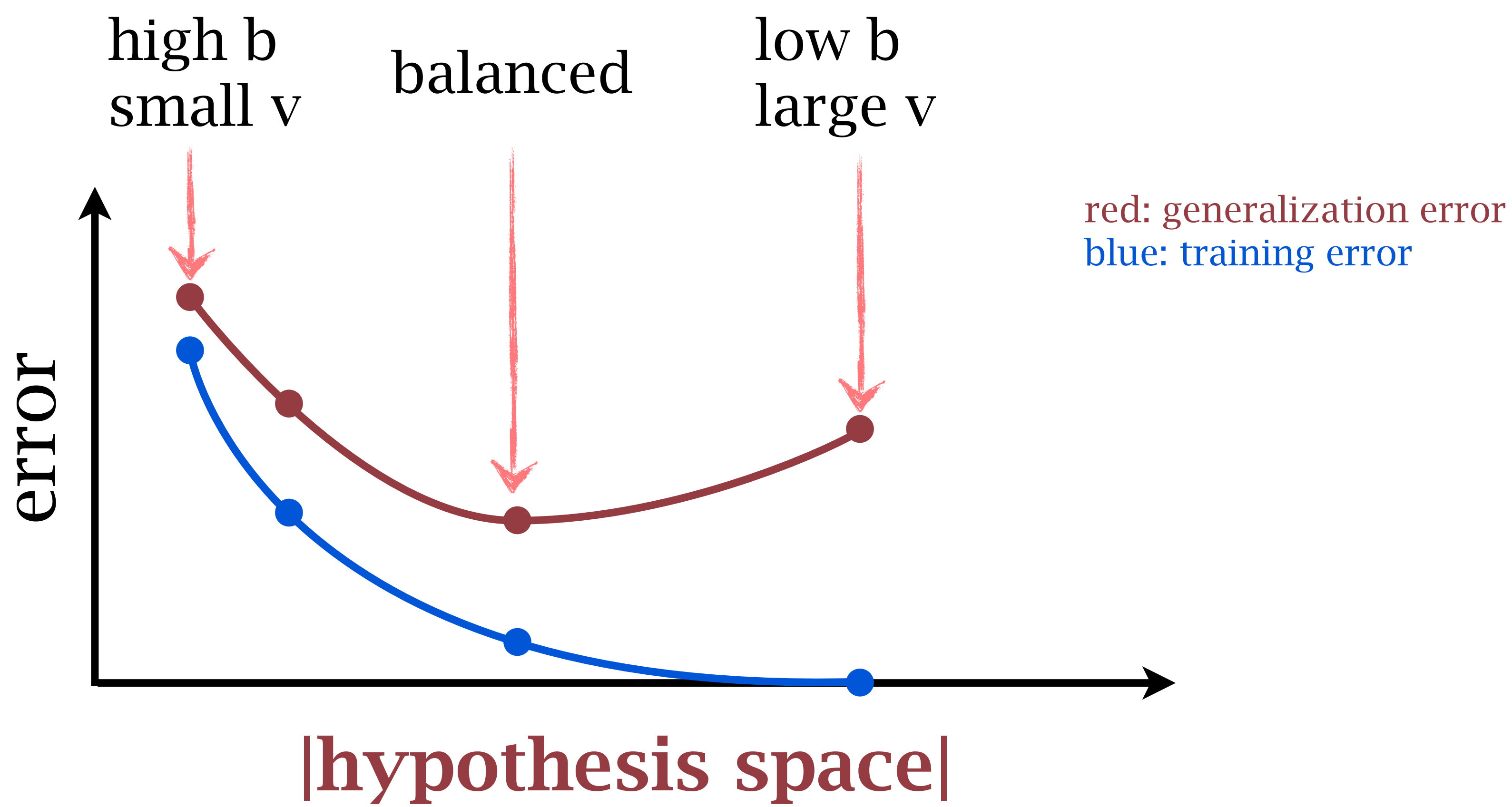
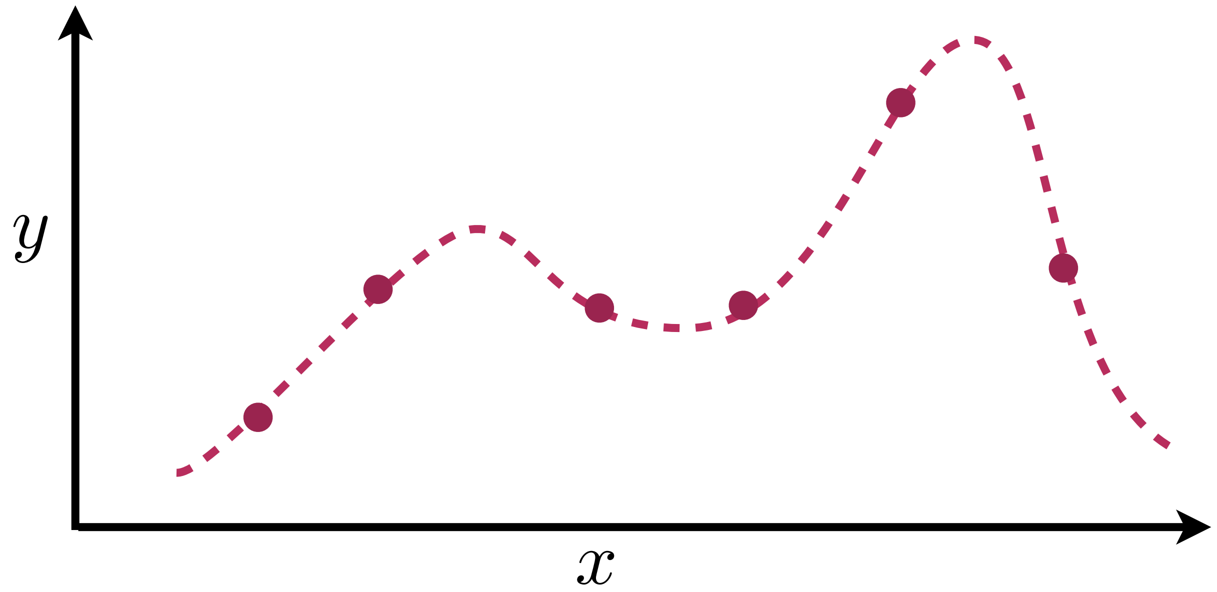
bias^2



Overfitting and underfitting

training error v.s. hypothesis space size



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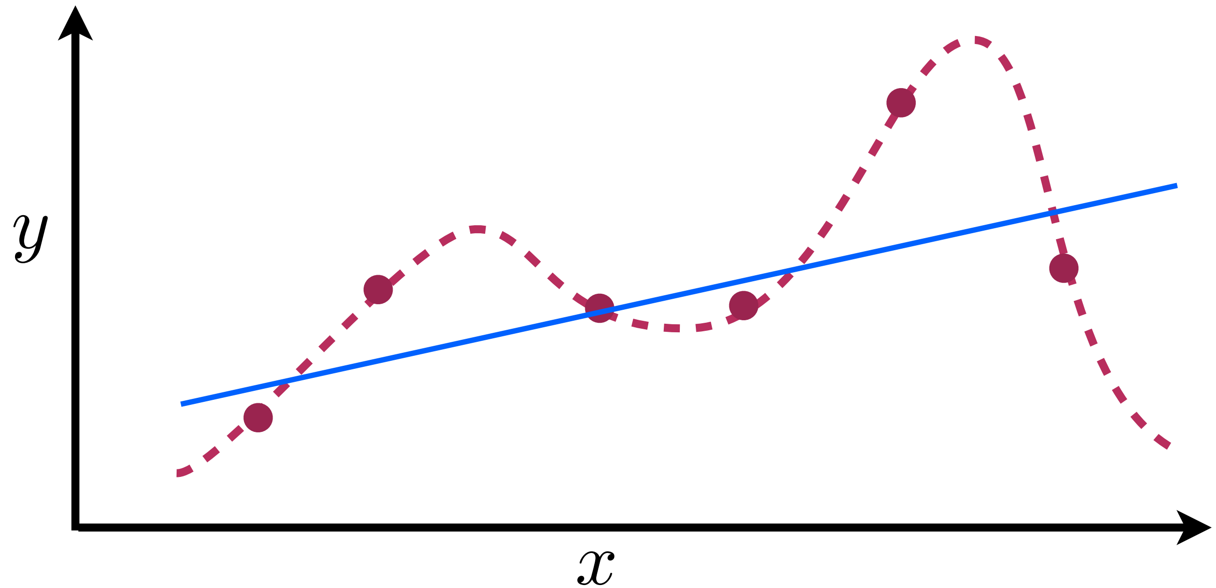
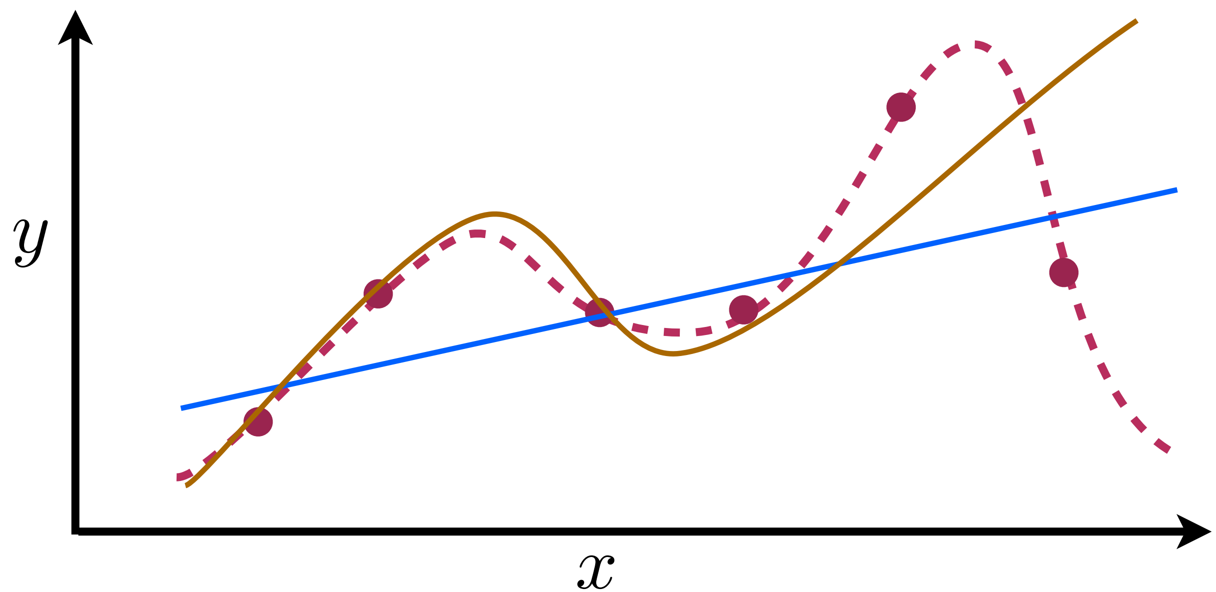


linear functions: high training error, small space

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

Overfitting and underfitting

training error v.s. hypothesis space size



linear functions: high training error, small space

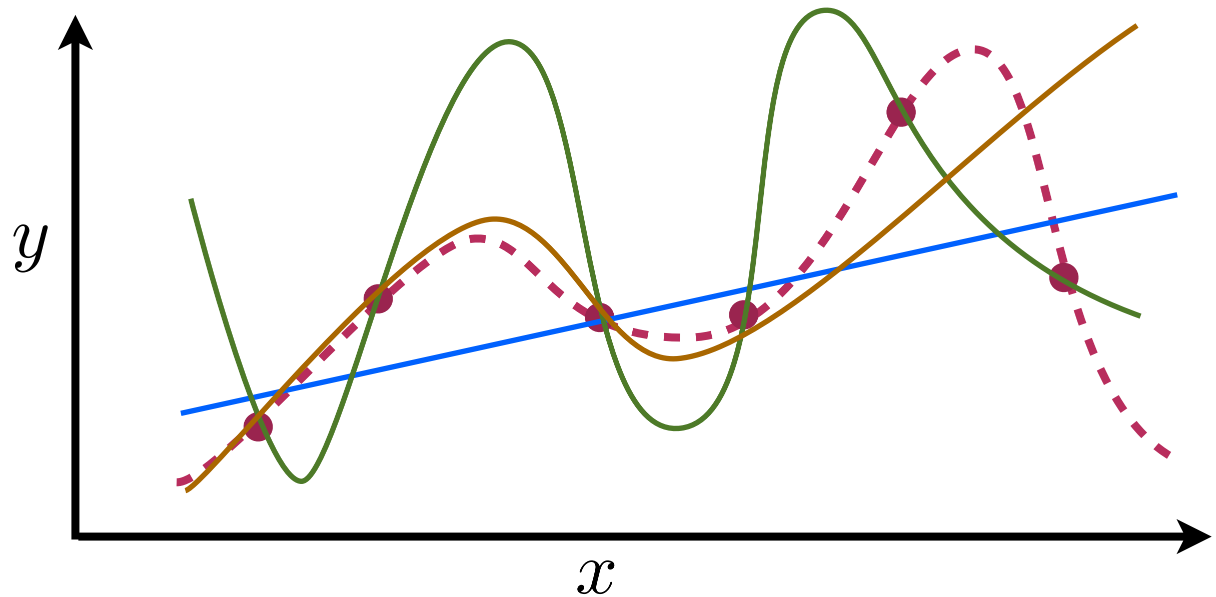
$$\{y = a + bx \mid a, b \in \mathbb{R}\}$$

higher polynomials: moderate training error, moderate space

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

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

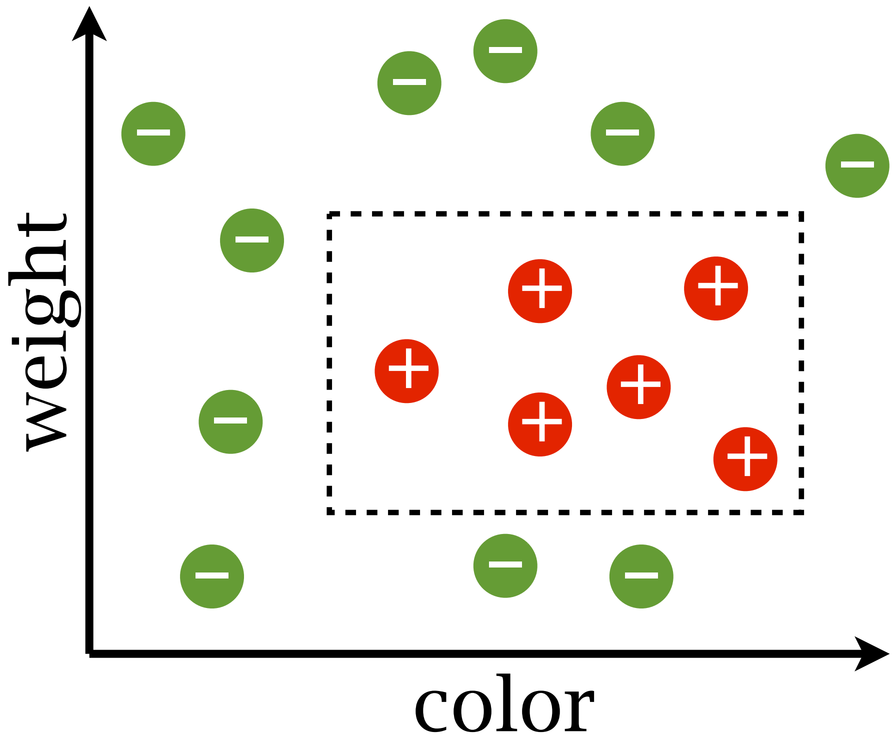
$$\{y = a + bx + cx^2 + dx^3 \mid a, b, c, d \in \mathbb{R}\}$$

even higher order: no training error, large space

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

Generalization error

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



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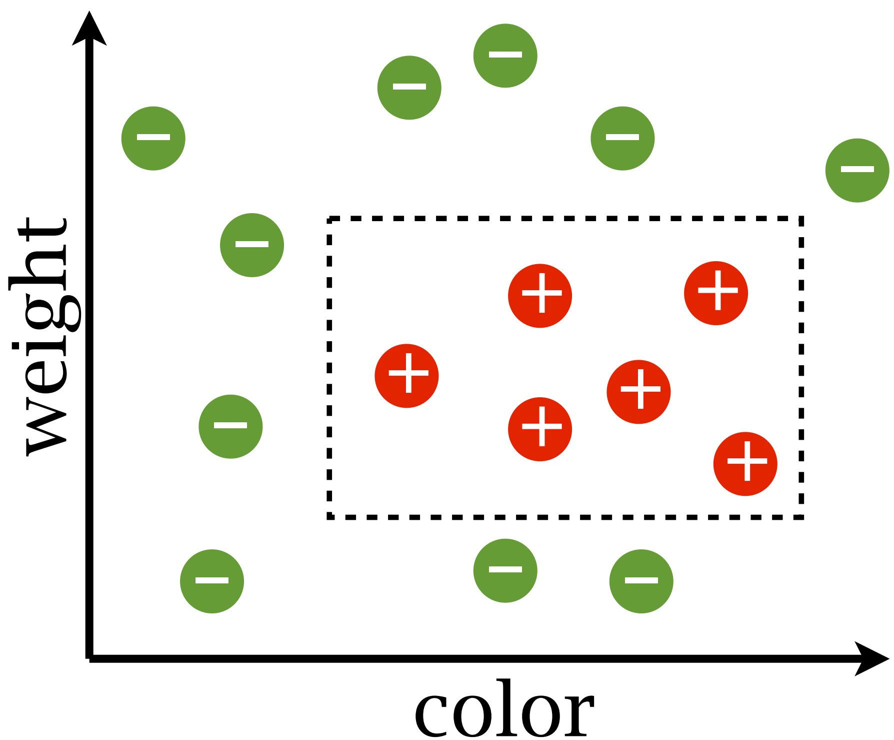


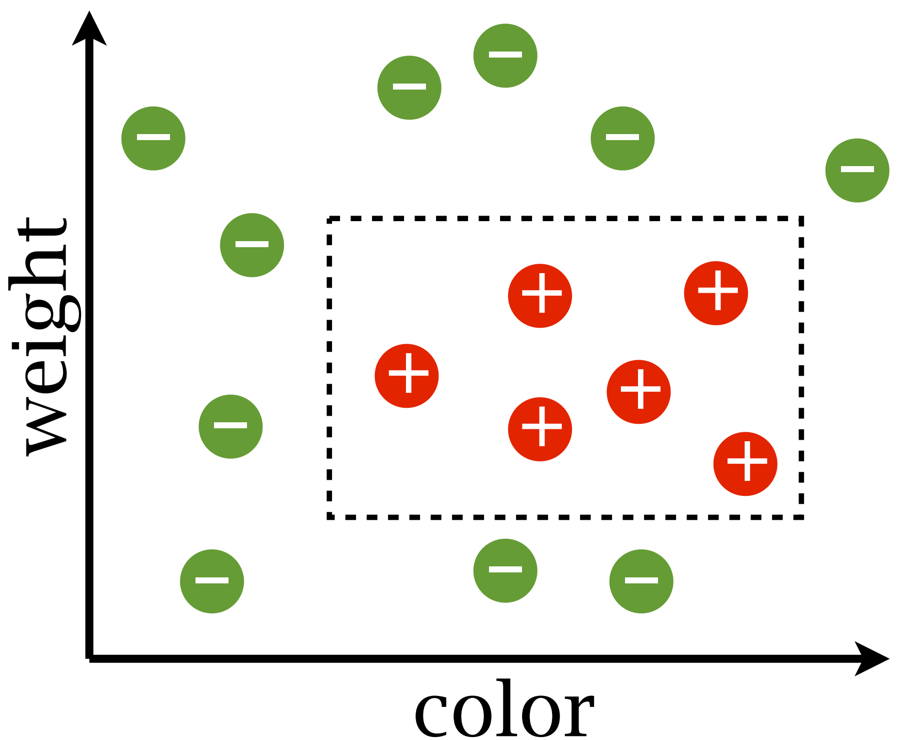
the error of picking a consistent hypothesis:

with probability at least $1 - \delta$

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

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 $1-\delta$

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

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***: $\epsilon_g(h) \geq \epsilon$

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:

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:

$$P \leq 1 - \epsilon$$

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:

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:

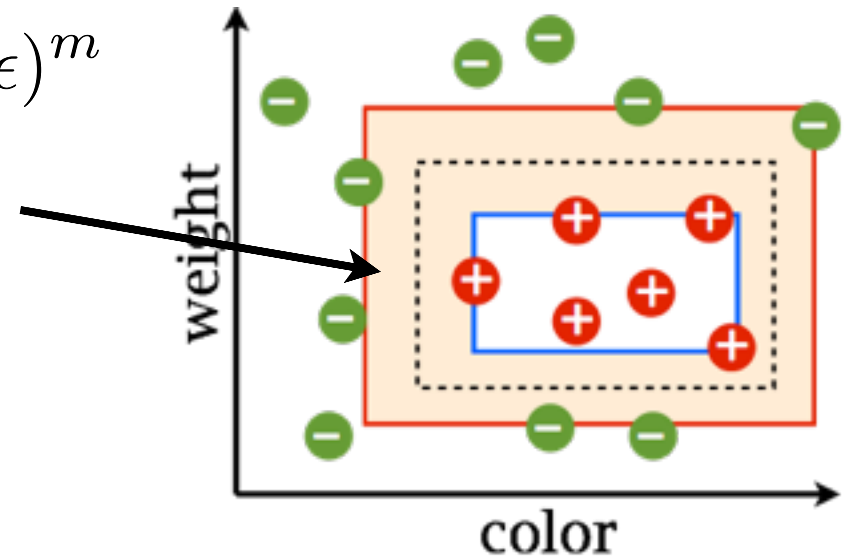
$$P \leq (1 - \epsilon)^m$$

Generalization error

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

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

There are ***k*** consistent hypotheses



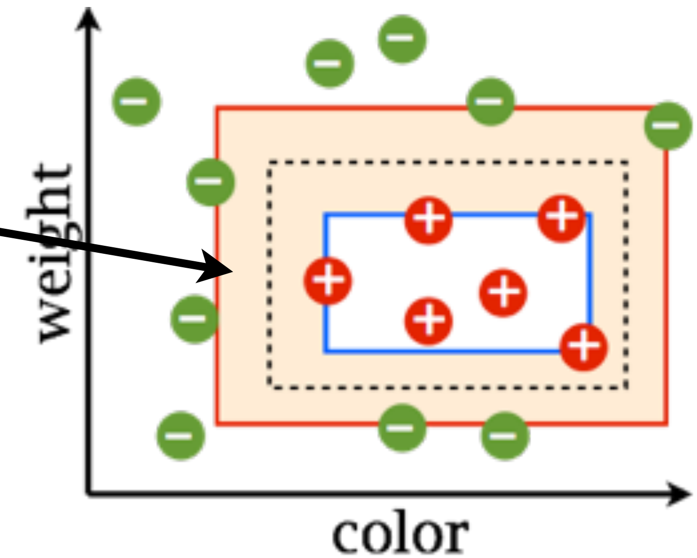
...

Generalization error

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

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

There are ***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 $P \leq (1-\epsilon)^m$

...

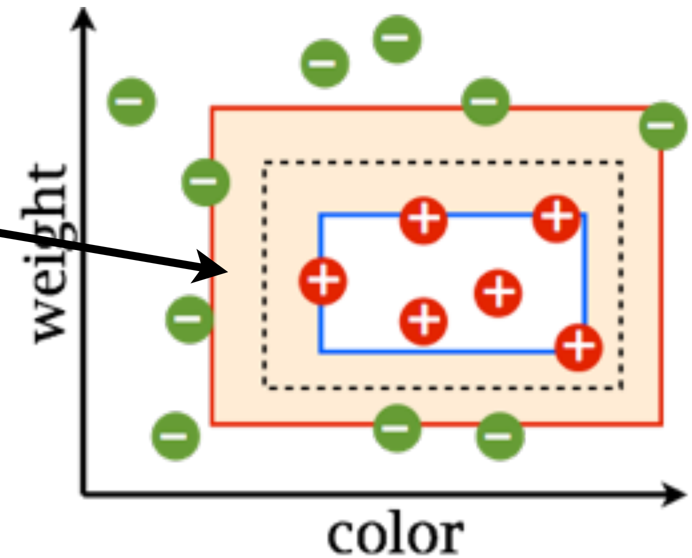
h_k is chosen and h_k is bad $P \leq (1-\epsilon)^m$

Generalization error

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

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

There are $\boldsymbol{k}$ consistent hypotheses



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overall:

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

Generalization error

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

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

Generalization error

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

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

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

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

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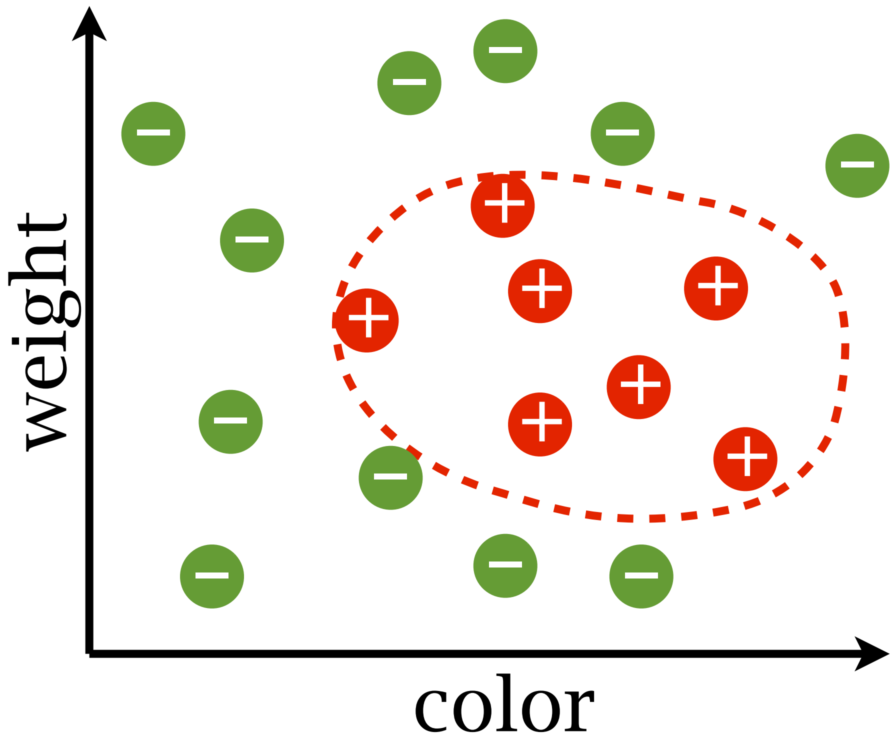
Inconsistent hypothesis

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



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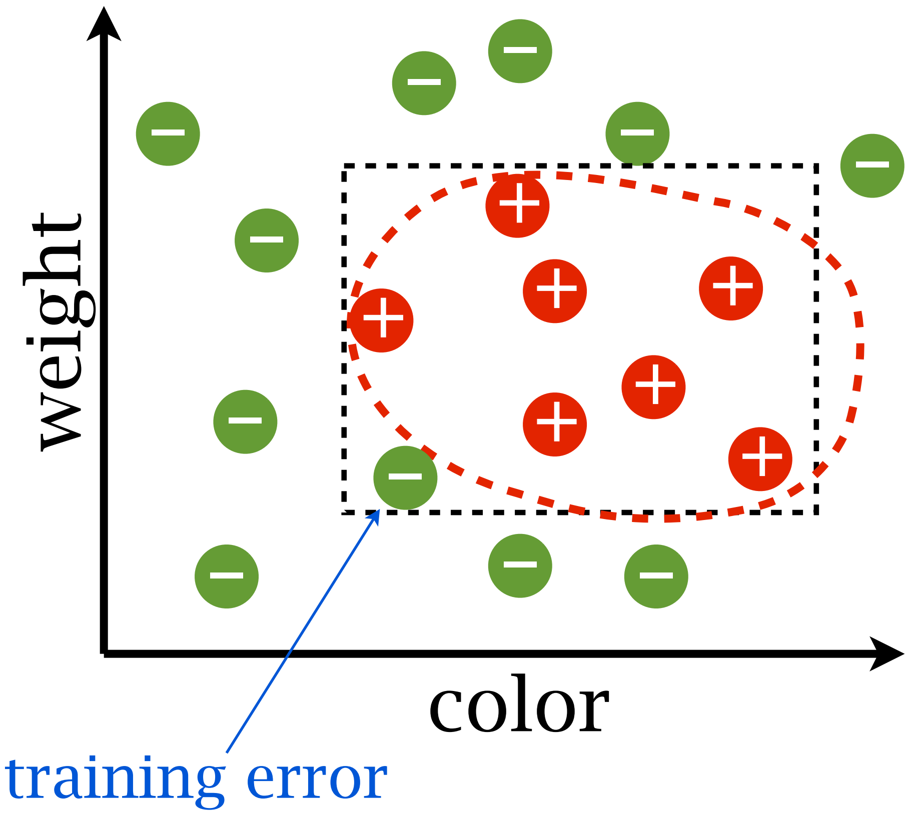

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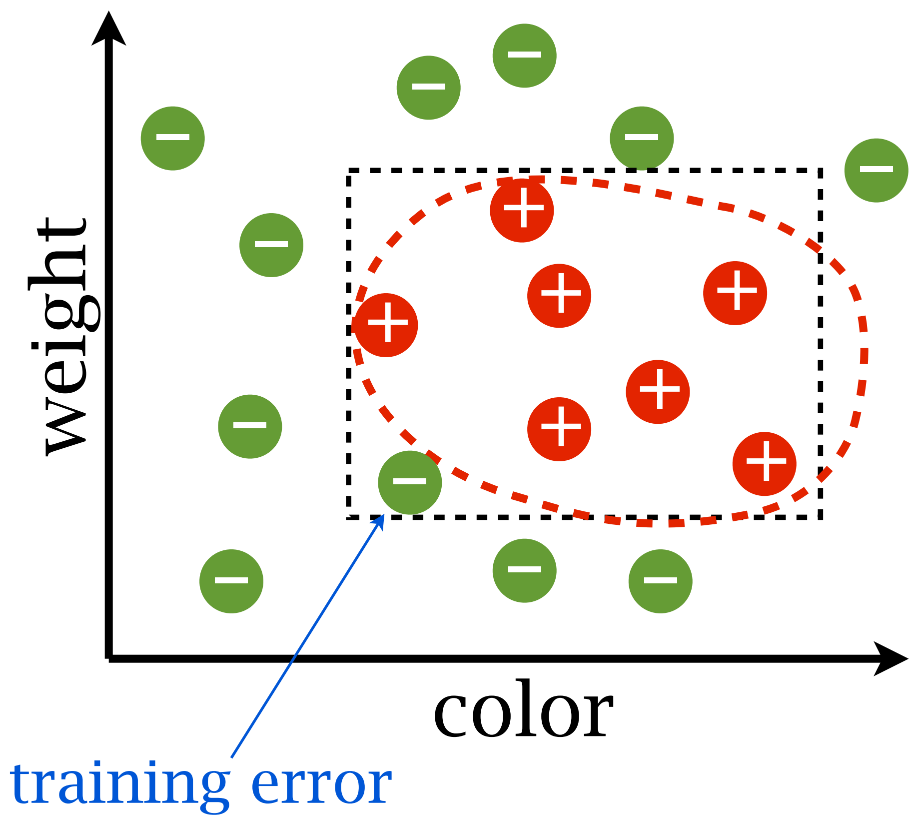

with probability at least $1 - \delta$

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

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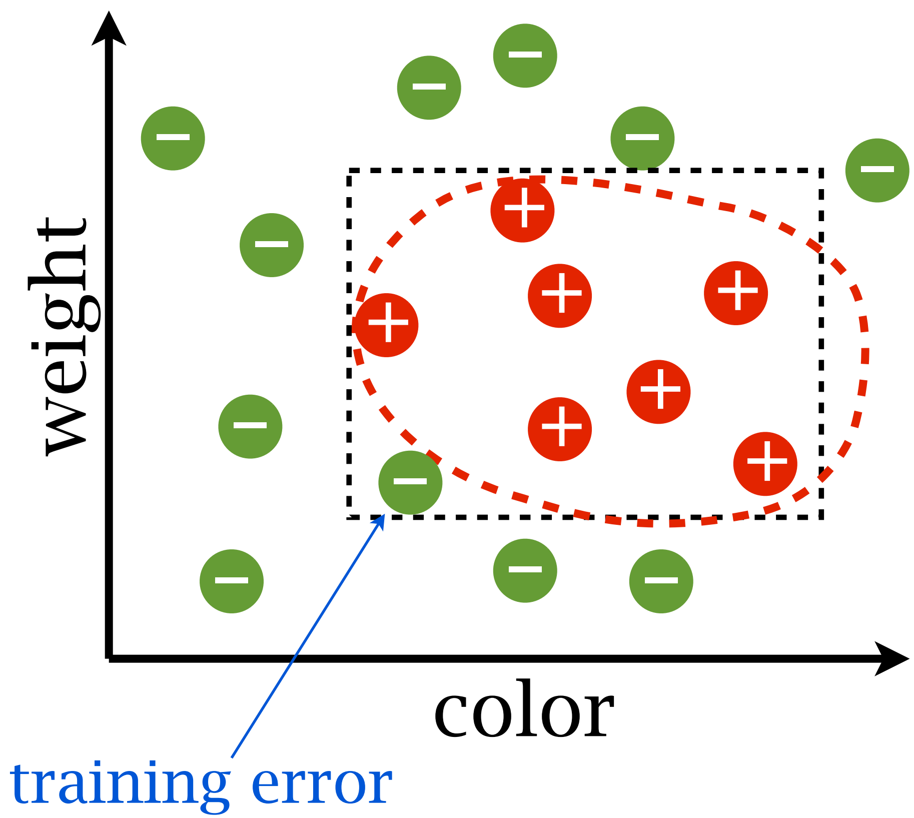

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smaller generalization error:
- more examples
- smaller hypothesis space
- **smaller training error**

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

$$\text{for one } h$$

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

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

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

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

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

Generalization error

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

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

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:

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

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

inconsistent hypothesis case:

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

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

generalization error:

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

PAC-learning

Probably approximately correct (PAC):

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

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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.

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

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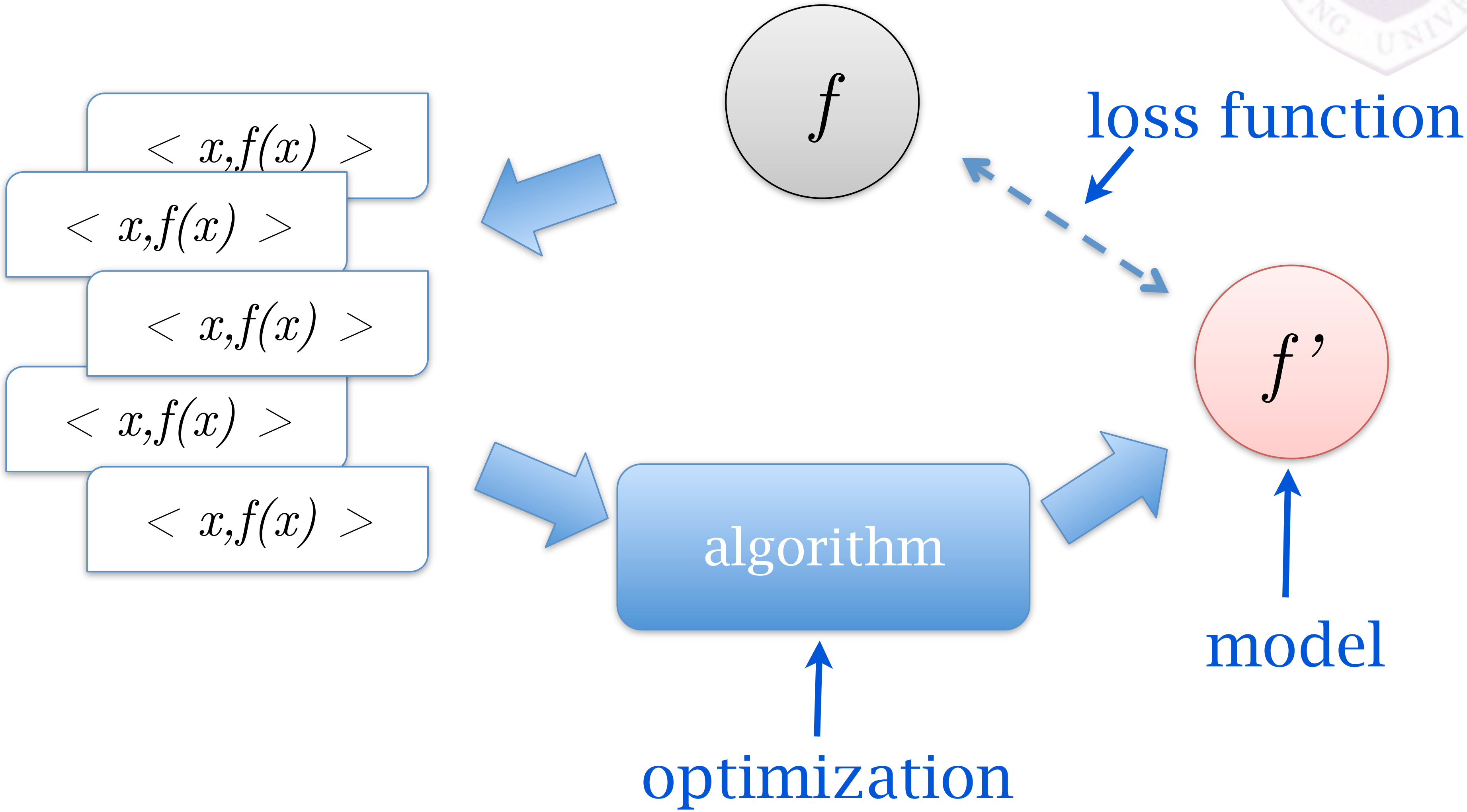
Dimensions of modeling



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。

解释 Bias-Variance 困境