Outline of the Course

1. The Learning Problem *(April 3)*
2. Is Learning Feasible? *(April 5)*
3. The Linear Model I *(April 10)*
4. Error and Noise *(April 12)*
5. Training versus Testing *(April 17)*
6. Theory of Generalization *(April 19)*
7. The VC Dimension *(April 24)*
8. Bias-Variance Tradeoff *(April 26)*
9. The Linear Model II *(May 1)*
10. Neural Networks *(May 3)*
11. Overfitting *(May 8)*
12. Regularization *(May 10)*
13. Validation *(May 15)*
14. Support Vector Machines *(May 17)*
15. Kernel Methods *(May 22)*
16. Radial Basis Functions *(May 24)*
17. Three Learning Principles *(May 29)*
18. Epilogue *(May 31)*

- theory; mathematical
- technique; practical
- analysis; conceptual

Learning From Data

Yaser S. Abu-Mostafa
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Lecture 1: The Learning Problem

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Tuesday, April 3, 2012

The learning problem - Outline

- Example of machine learning
- Components of Learning
- A simple model
- Types of learning
- Puzzle

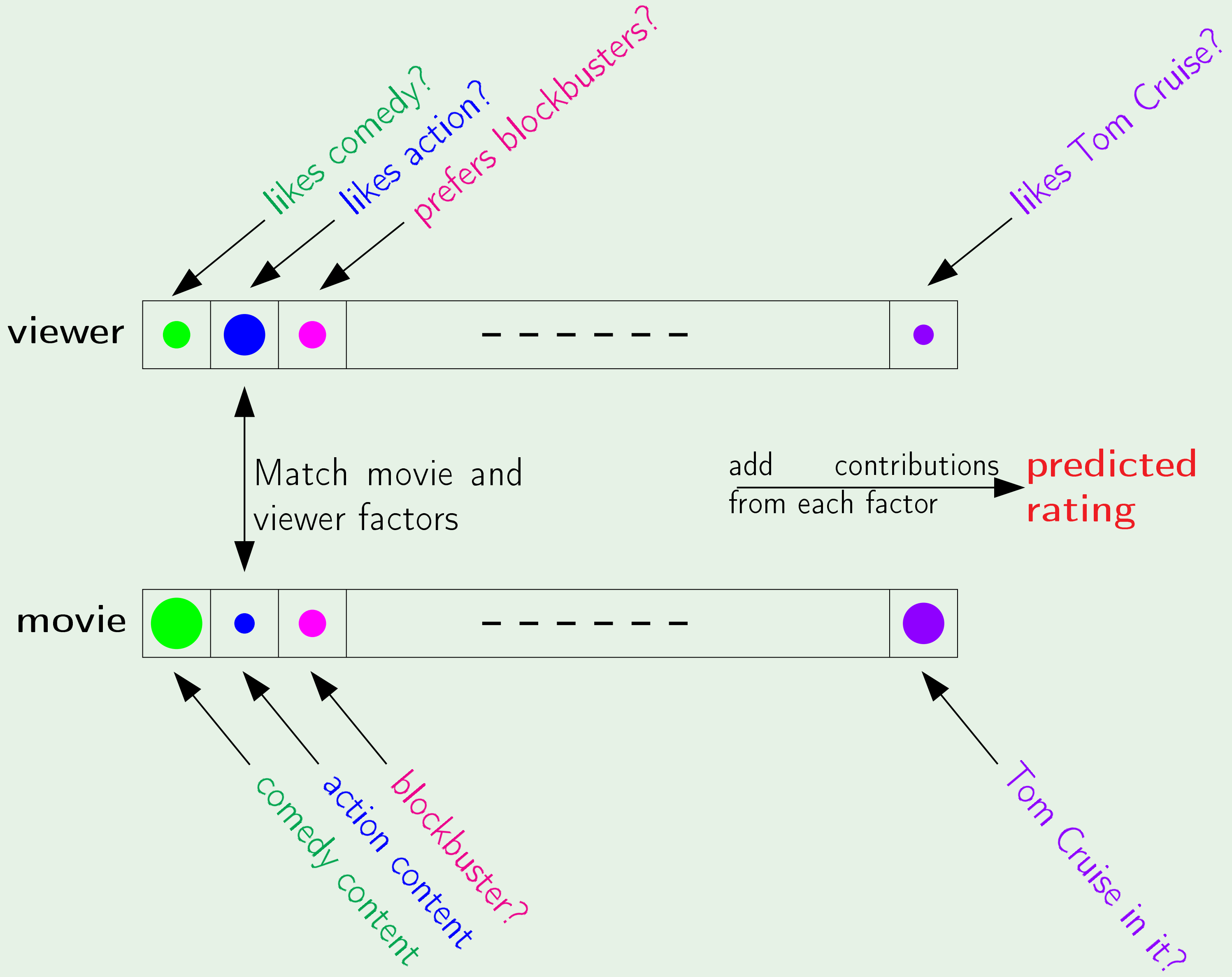
Example: Predicting how a viewer will rate a movie

10% improvement = **1 million dollar prize**

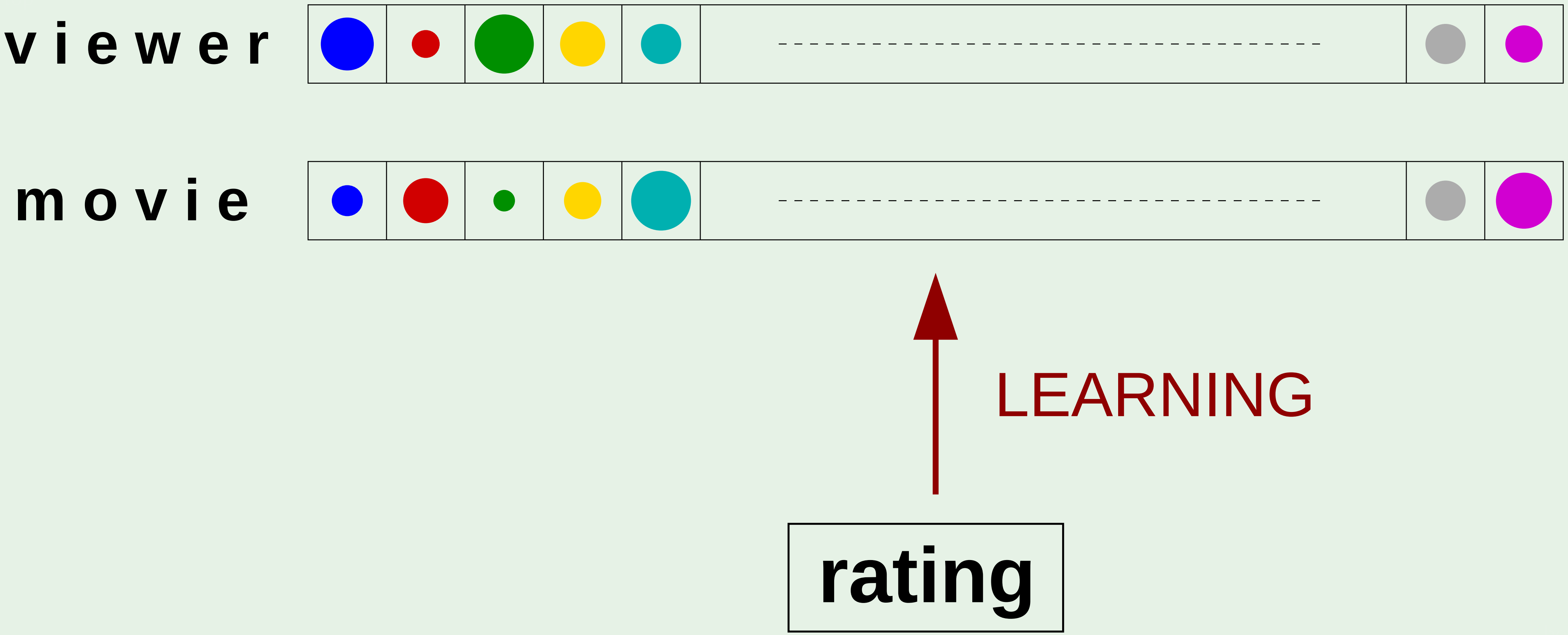
The essence of machine learning:

- A pattern exists.
- We cannot pin it down mathematically.
- We have data on it.

Movie rating - a solution



The learning approach



Components of learning

Metaphor: Credit approval

Applicant information:

age	23 years
gender	male
annual salary	$30,000
years in residence	1 year
years in job	1 year
current debt	$15,000
...	...

Approve credit?

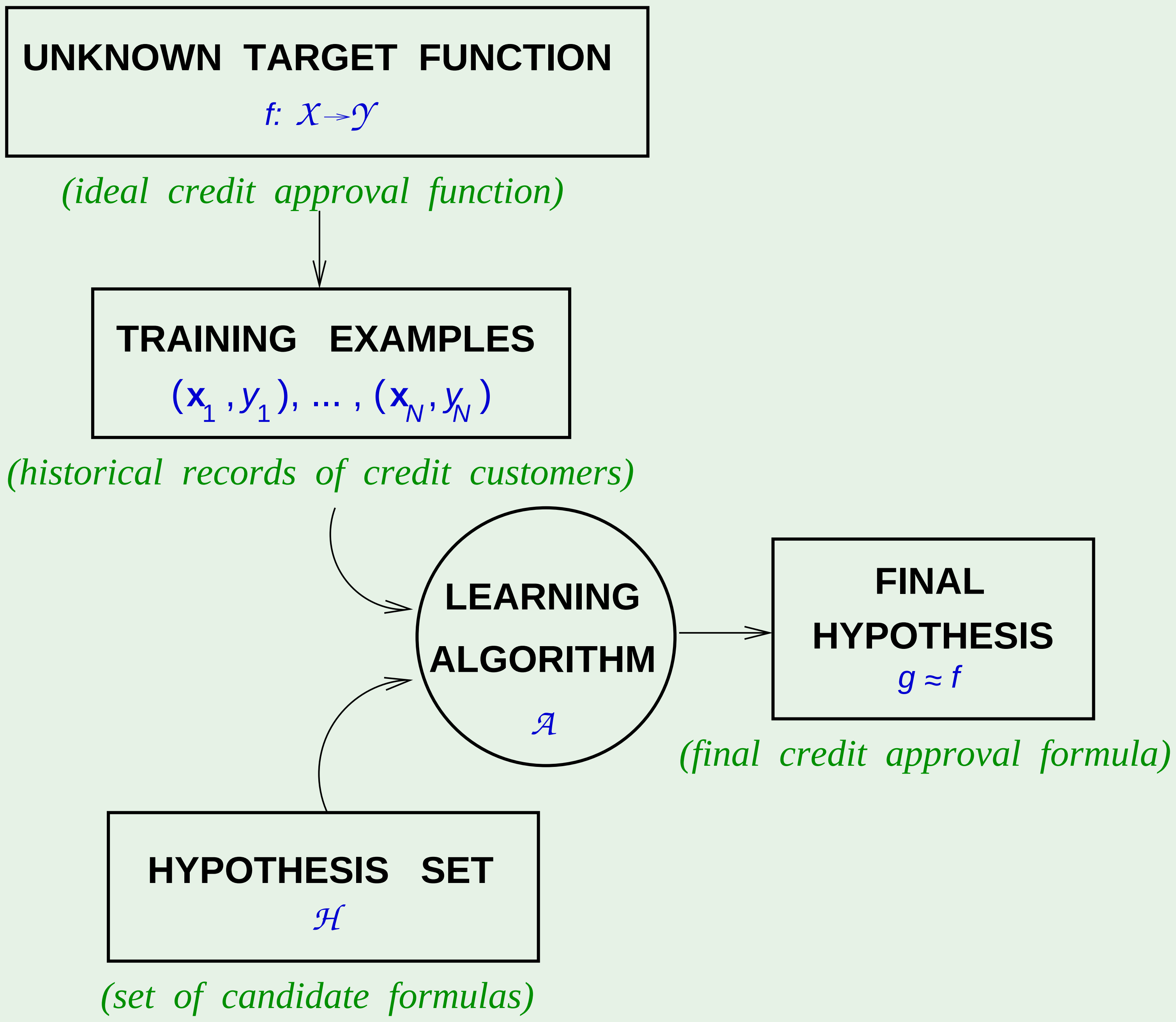
Components of learning

Formalization:

- Input: $\mathbf{x}$ *(customer application)*
- Output: y *(good/bad customer?)*
- Target function: $f : \mathcal{X} \to \mathcal{Y}$ *(ideal credit approval formula)*
- Data: $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_N, y_N)$ *(historical records)*

$$\downarrow \quad \downarrow \quad \downarrow$$

- Hypothesis: $g : \mathcal{X} \to \mathcal{Y}$ *(formula to be used)*


UNKNOWN TARGET FUNCTION
$f: \mathcal{X} \to \mathcal{Y}$
(ideal credit approval function)
TRAINING EXAMPLES
$(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$
(historical records of credit customers)
LEARNING ALGORITHM
$\mathcal{A}$
FINAL HYPOTHESIS
$g \approx f$
(final credit approval formula)
HYPOTHESIS SET
$\mathcal{H}$
(set of candidate formulas)

Solution components

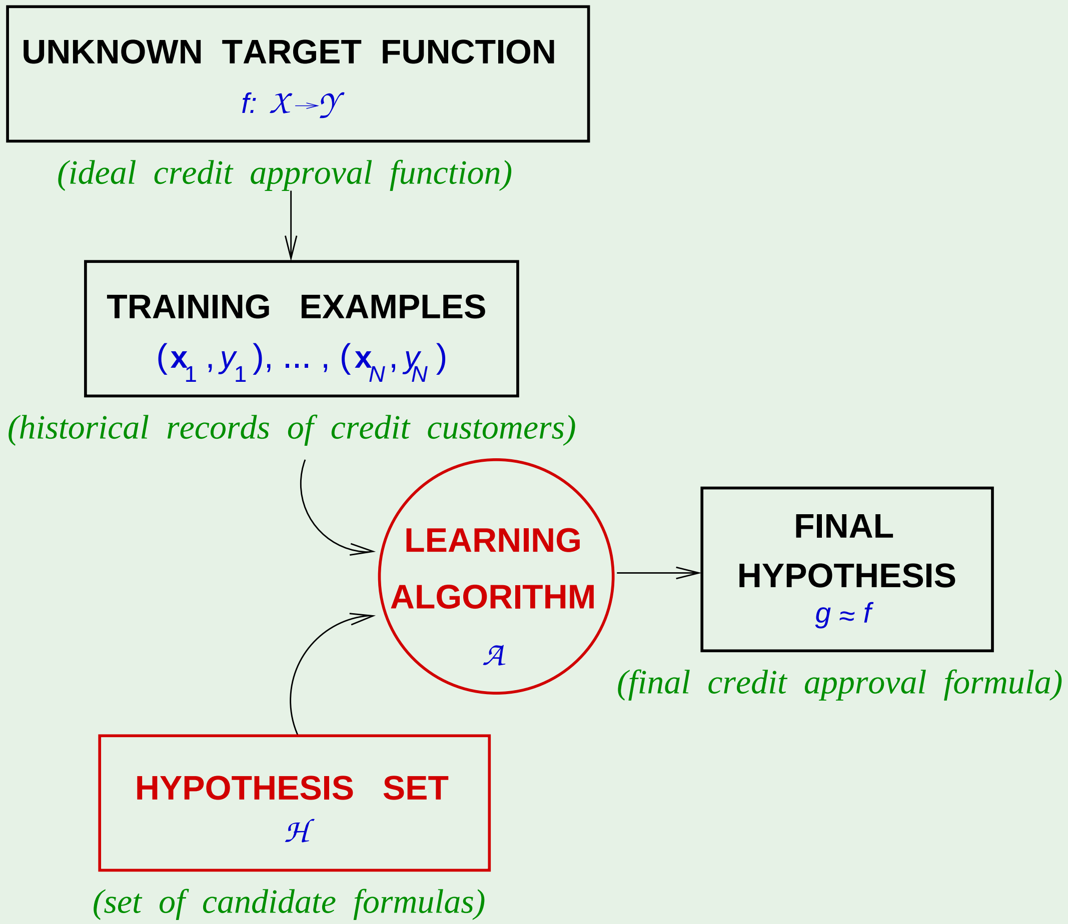
The 2 solution components of the learning problem:

- The Hypothesis Set

  $\mathcal{H} = \{h\} \qquad g \in \mathcal{H}$

- The Learning Algorithm

Together, they are referred to as the *learning model*.



A simple hypothesis set - the 'perceptron'

For input $\mathbf{x} = (x_1, \cdots, x_d)$ 'attributes of a customer'

$$\text{Approve credit if } \sum_{i=1}^{d} w_i x_i > \text{threshold},$$

$$\text{Deny credit if } \sum_{i=1}^{d} w_i x_i < \text{threshold}.$$

This linear formula $h \in \mathcal{H}$ can be written as

$$h(\mathbf{x}) = \text{sign}\left(\left(\sum_{i=1}^{d} w_i x_i\right) - \text{threshold}\right)$$

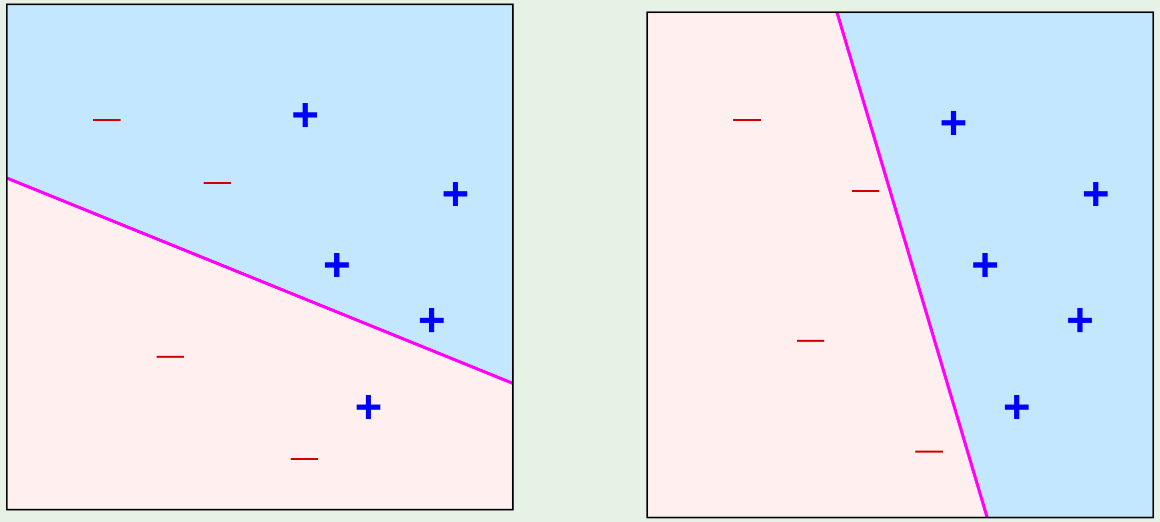
$$h(\mathbf{x}) = \text{sign}\left(\left(\sum_{i=1}^{d} w_i \; x_i\right) + \qquad w_0 \qquad\right)$$

Introduce an artificial coordinate $x_0 = 1$:

$$h(\mathbf{x}) = \text{sign}\left(\sum_{i=0}^{d} w_i \; x_i\right)$$

In vector form, the perceptron implements

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



'linearly separable' data

A simple learning algorithm - PLA

The perceptron implements

$$h(\mathbf{x}) = \text{sign}(\mathbf{w}^\intercal \mathbf{x})$$

Given the training set:

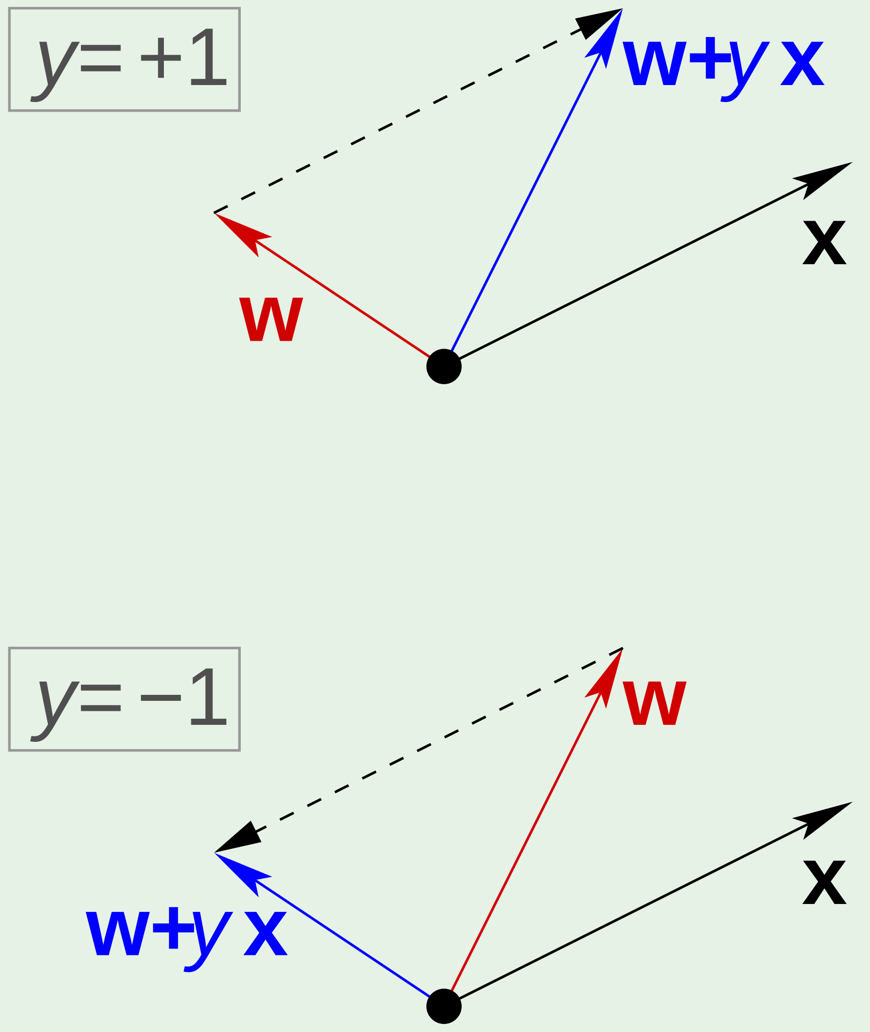
$$(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_N, y_N)$$

pick a misclassified point:

$$\text{sign}(\mathbf{w}^\intercal \mathbf{x}_n) \neq y_n$$

and update the weight vector:

$$\boxed{\mathbf{w} \leftarrow \mathbf{w} + y_n \mathbf{x}_n}$$



Iterations of PLA

- One iteration of the PLA:

$$\mathbf{w} \leftarrow \mathbf{w} + y\mathbf{x}$$

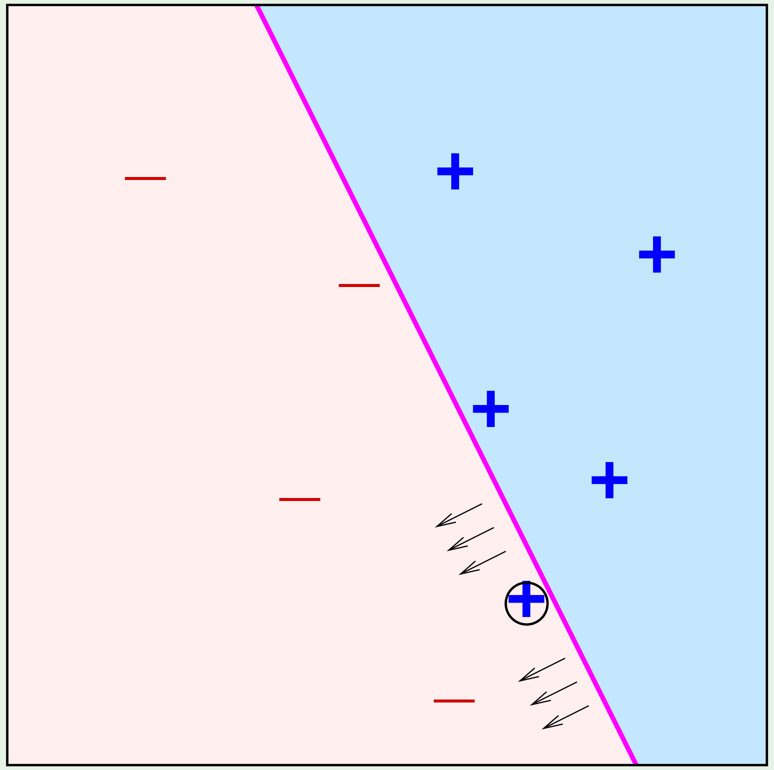
where $(\mathbf{x}, y)$ is a misclassified training point.

- At iteration $t = 1, 2, 3, \cdots$, pick a misclassified point from

$$(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_N, y_N)$$

and run a PLA iteration on it.

- That's it!



The learning problem - Outline

- Example of machine learning
- Components of learning
- A simple model
- Types of learning
- Puzzle

Basic premise of learning

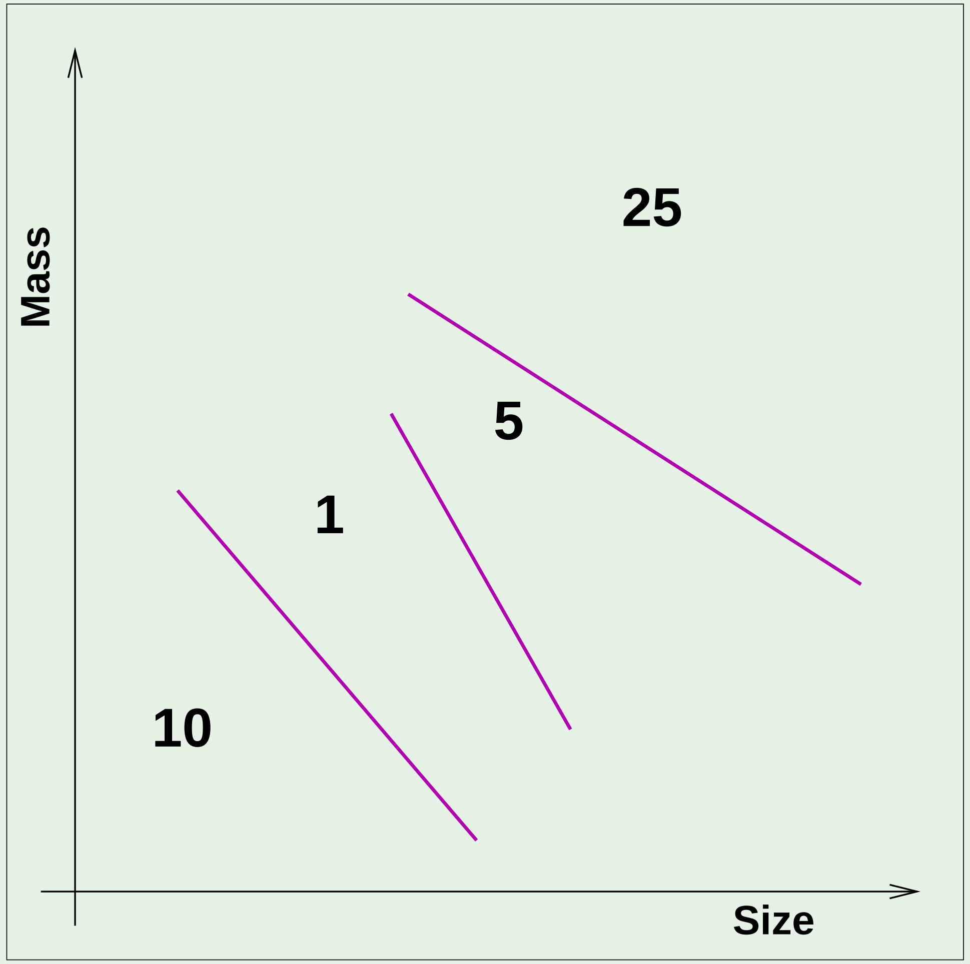
"using a set of observations to uncover an underlying process"

broad premise $\Longrightarrow$ many variations

- **Supervised Learning**
- **Unsupervised Learning**
- **Reinforcement Learning**

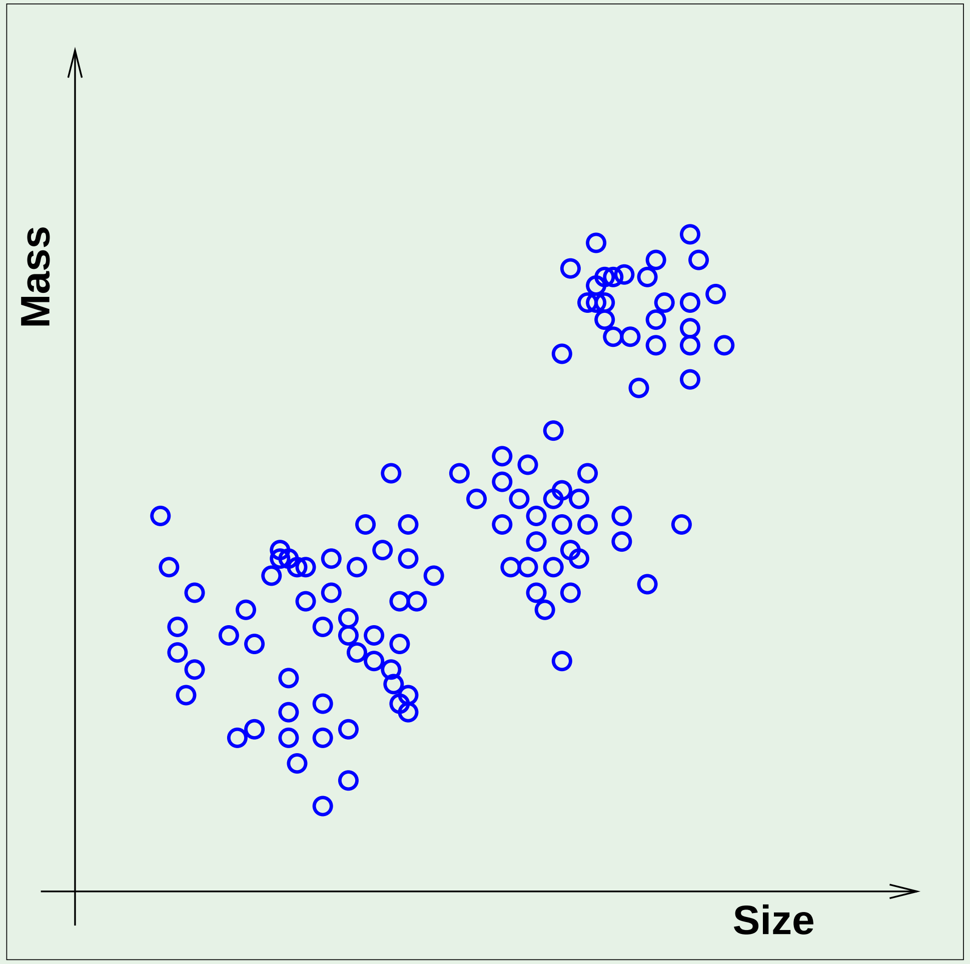
Supervised learning

Example from vending machines – **coin recognition**



Unsupervised learning

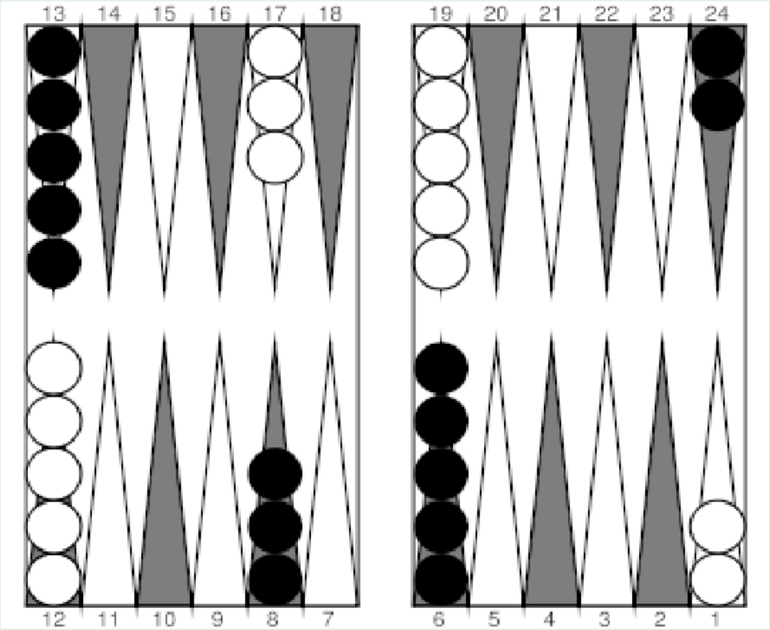
Instead of (input,correct output), we get (input, ?)



Reinforcement learning

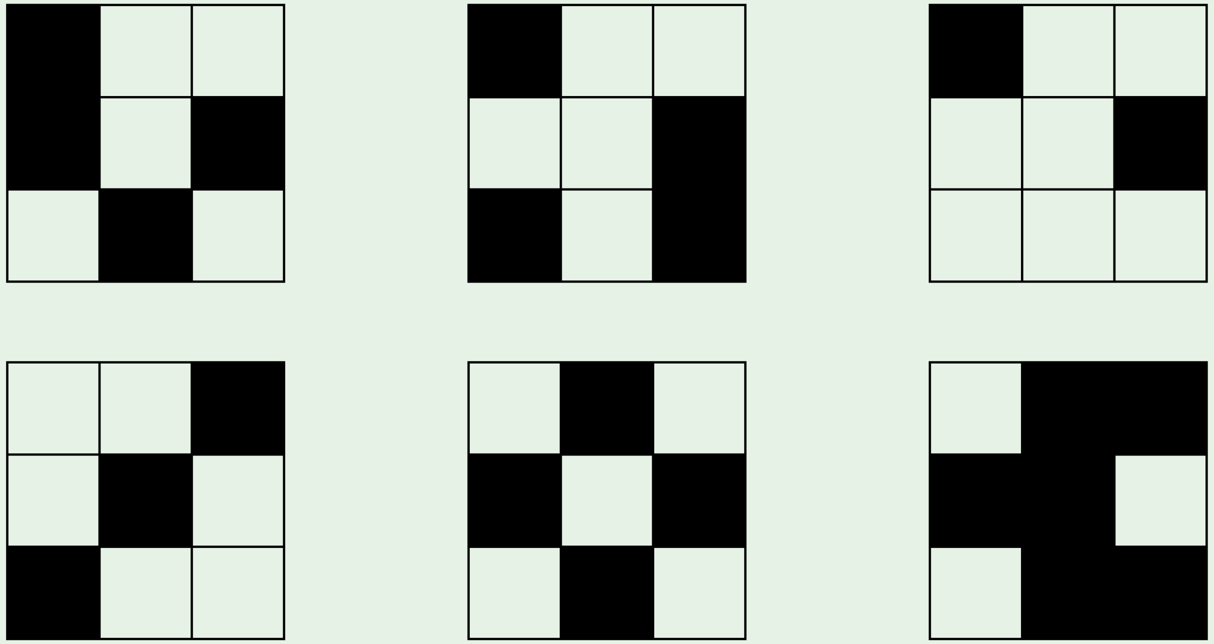
Instead of (input, correct output),

we get (input, *some* output, grade for this output)



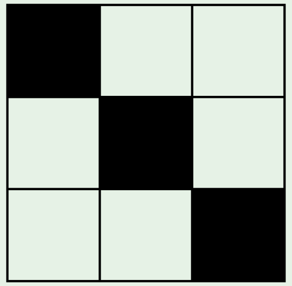
The world champion was a neural network!

A Learning puzzle



$f = -1$

$f = +1$

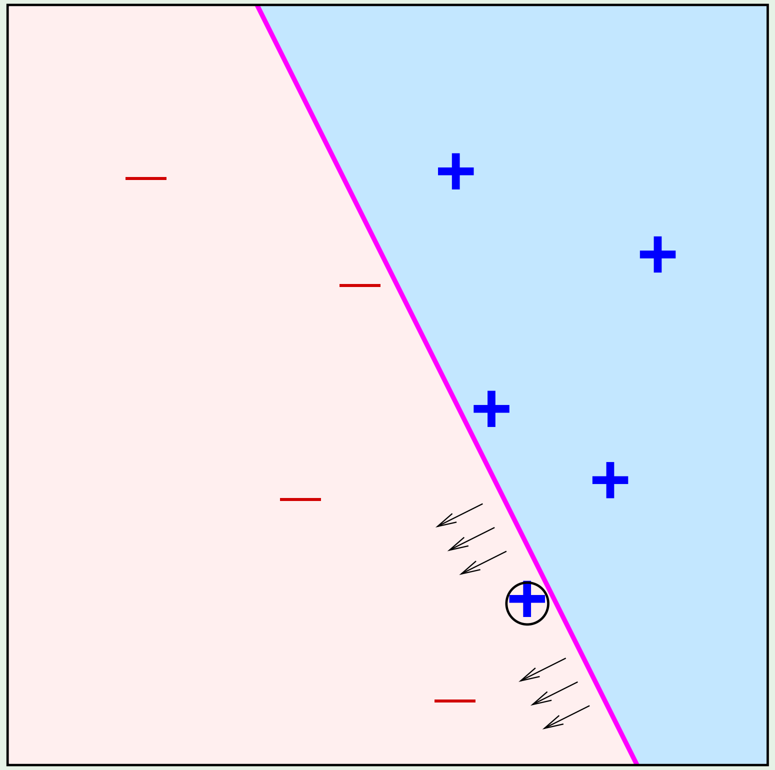


$f = ?$

Review of Lecture 1

- **Learning is used when**
  - A pattern exists
  - We cannot pin it down mathematically
  - We have data on it
- **Focus on supervised learning**
  - Unknown target function $y = f(\mathbf{x})$
  - Data set $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$
  - Learning algorithm picks $g \approx f$ from a hypothesis set $\mathcal{H}$

Example: Perceptron Learning Algorithm



- **Learning an unknown function?**
  - Impossible ☹. The function can assume any value outside the data we have.
  - So what now?

Learning From Data

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Lecture 2: Is Learning Feasible?

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Feasibility of learning - Outline

- Probability to the rescue
- Connection to learning
- Connection to *real* learning
- A dilemma and a solution

A related experiment

- Consider a 'bin' with red and green marbles.

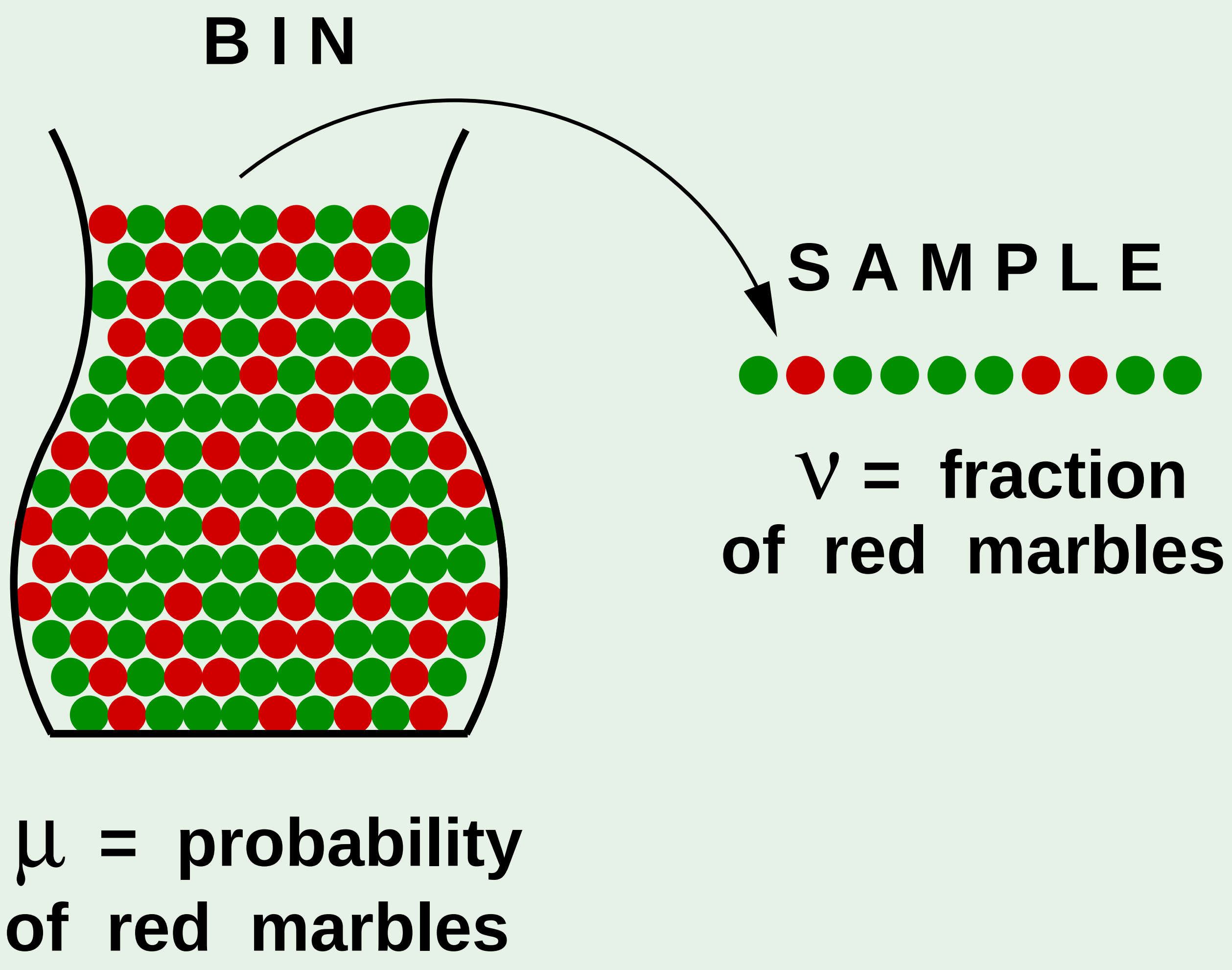
$$\mathbb{P}[\text{ picking a red marble }] = \mu$$

$$\mathbb{P}[\text{ picking a green marble }] = 1 - \mu$$

- The value of μ is unknown to us.

- We pick N marbles independently.

- The fraction of red marbles in sample $= \nu$



Does ν say anything about μ?

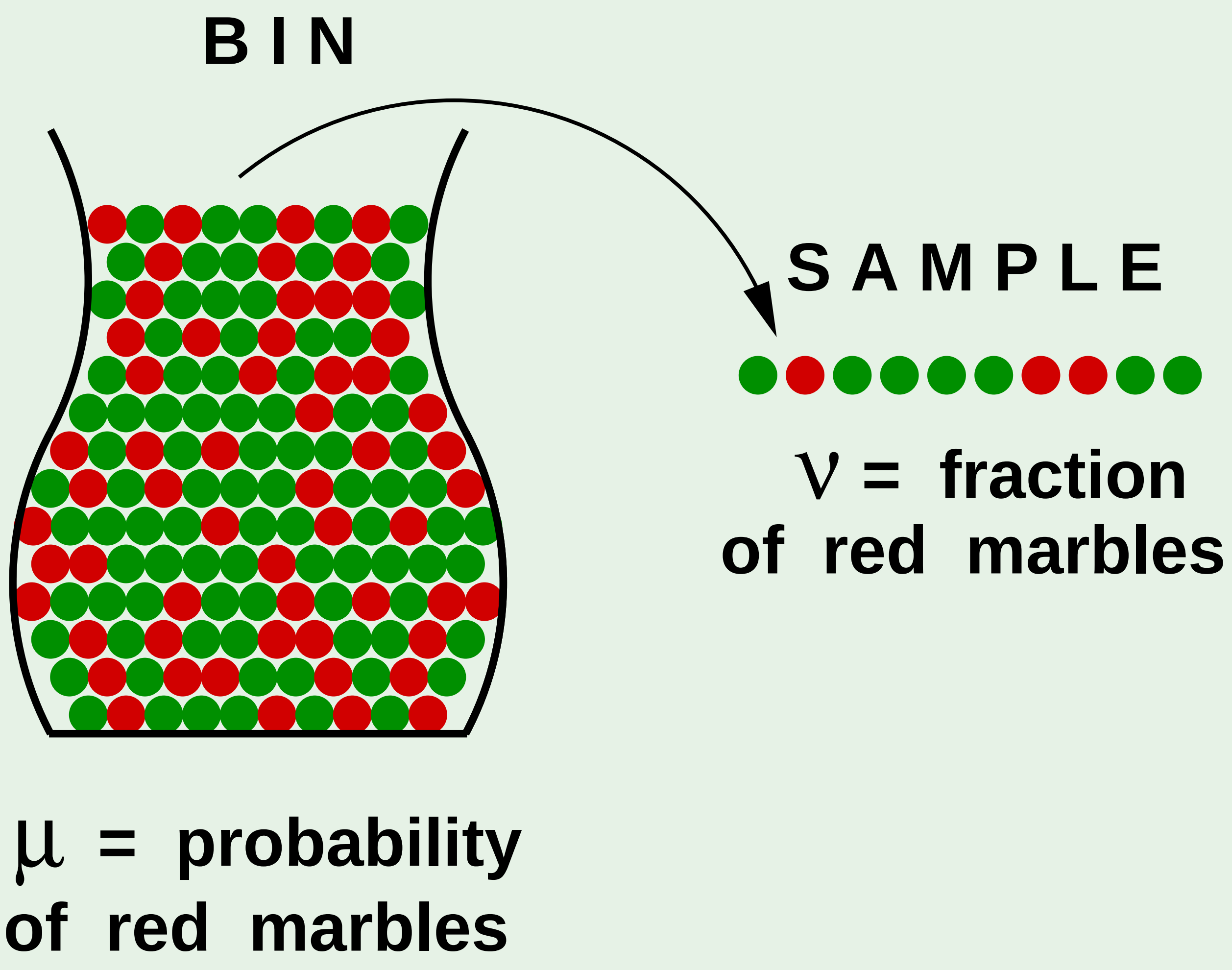
No!

Sample can be mostly green while bin is mostly red.

Yes!

Sample frequency ν is likely close to bin frequency μ.

possible versus **probable**



What does ν say about μ?

In a big sample (large N), ν is probably close to μ (within ϵ).

Formally,

$$\mathbb{P}\left[\,|\nu - \mu| > \epsilon\,\right] \leq 2e^{-2\epsilon^2 N}$$

This is called **Hoeffding's Inequality**.

In other words, the statement "$\mu = \nu$" is P.A.C.

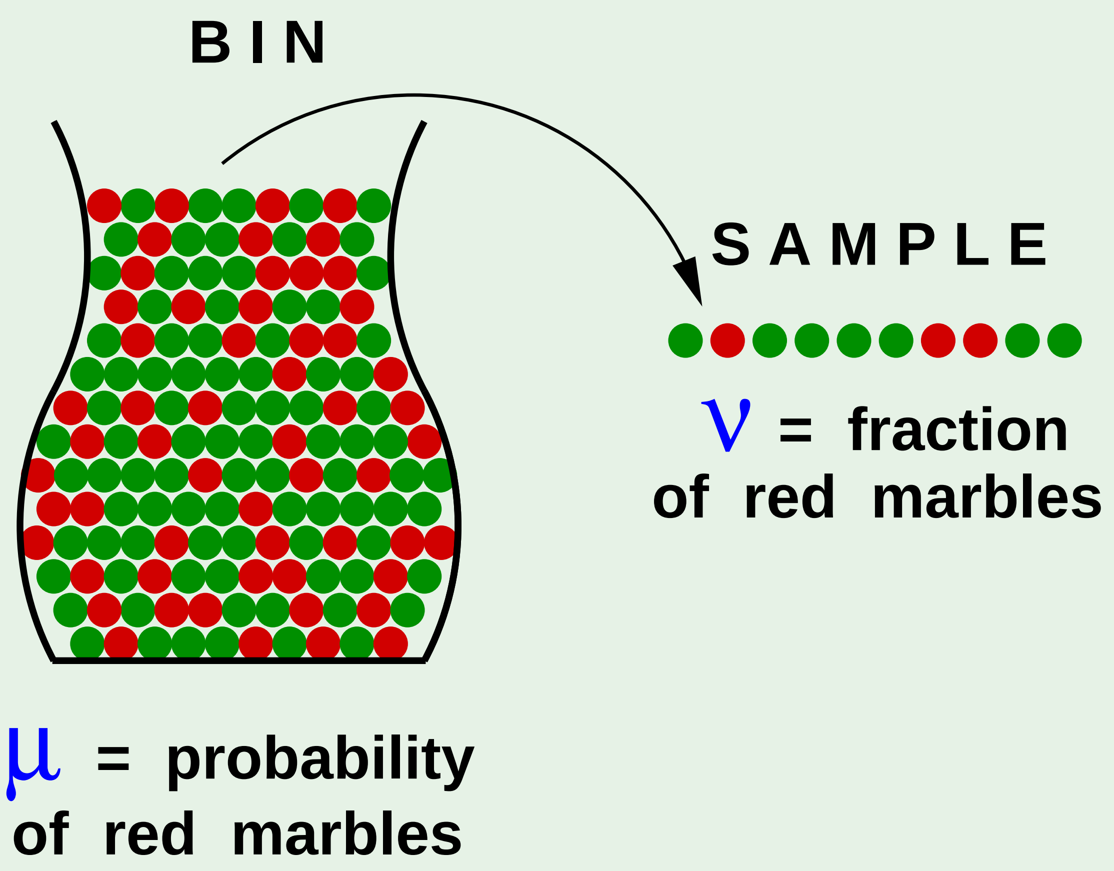
$$\mathbb{P}\left[|\nu - \mu| > \epsilon\right] \le 2e^{-2\epsilon^2 N}$$

- Valid for all N and ϵ

- Bound does not depend on μ

- Tradeoff: N, ϵ, and the bound.

- $\nu \approx \mu \implies \mu \approx \nu$ ☺



Connection to learning

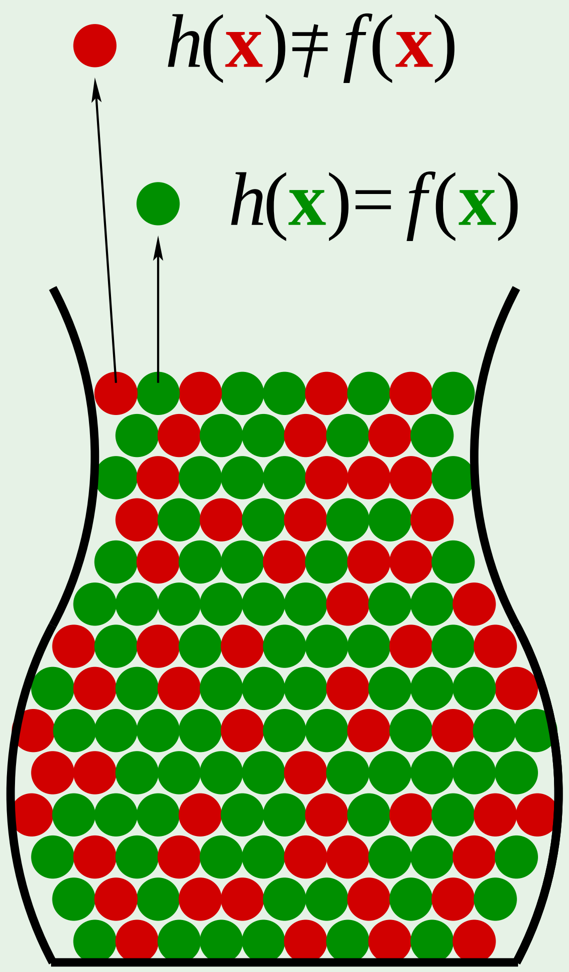
Bin: The unknown is a number μ

Learning: The unknown is a function $f : \mathcal{X} \to \mathcal{Y}$

Each marble ● is a point $\mathbf{x} \in \mathcal{X}$

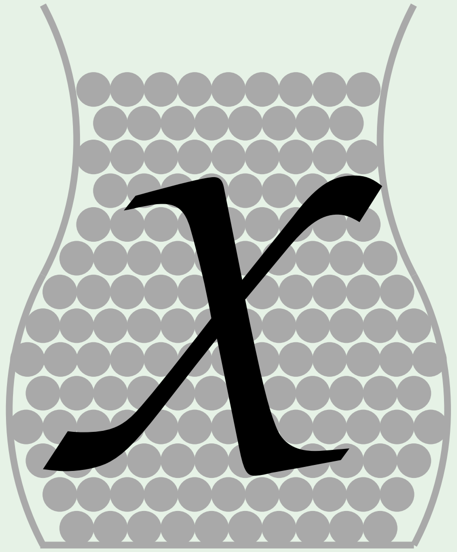
● : Hypothesis got it right $h(\mathbf{x}) = f(\mathbf{x})$

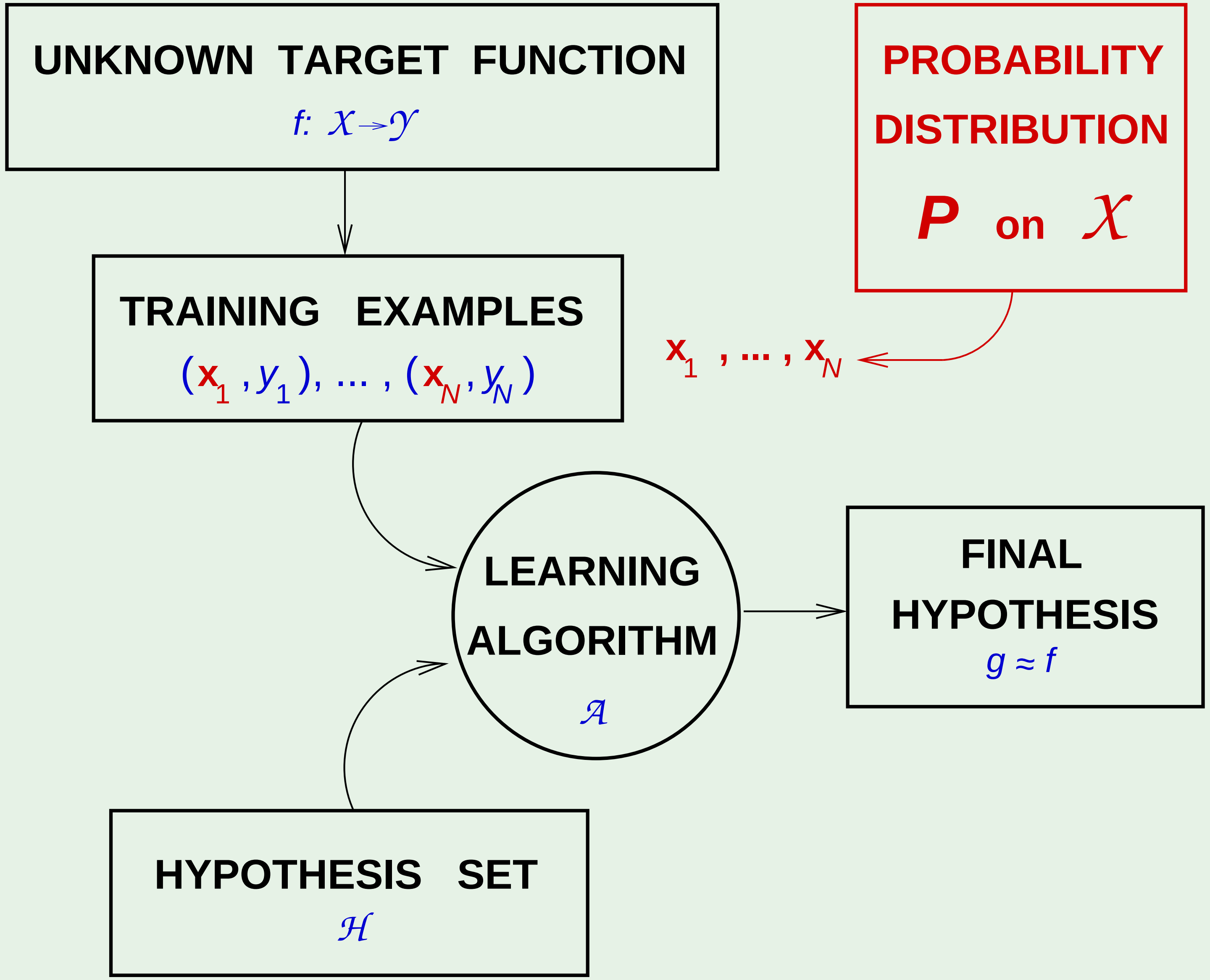
● : Hypothesis got it wrong $h(\mathbf{x}) \neq f(\mathbf{x})$



Back to the learning diagram

The bin analogy:





Are we done?

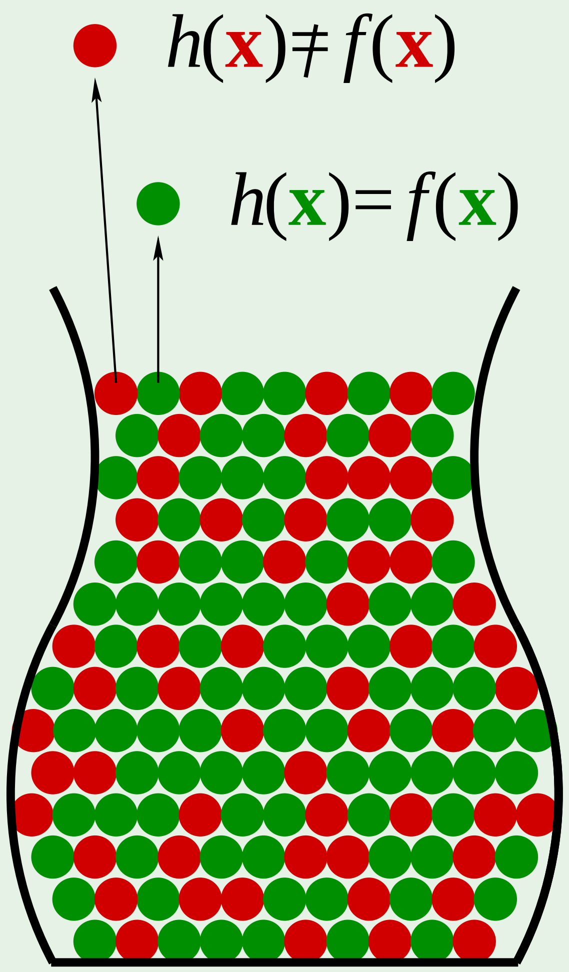
Not so fast! h is fixed.

For <u>this</u> h, ν generalizes to μ.

'**verification**' of h, not **learning**

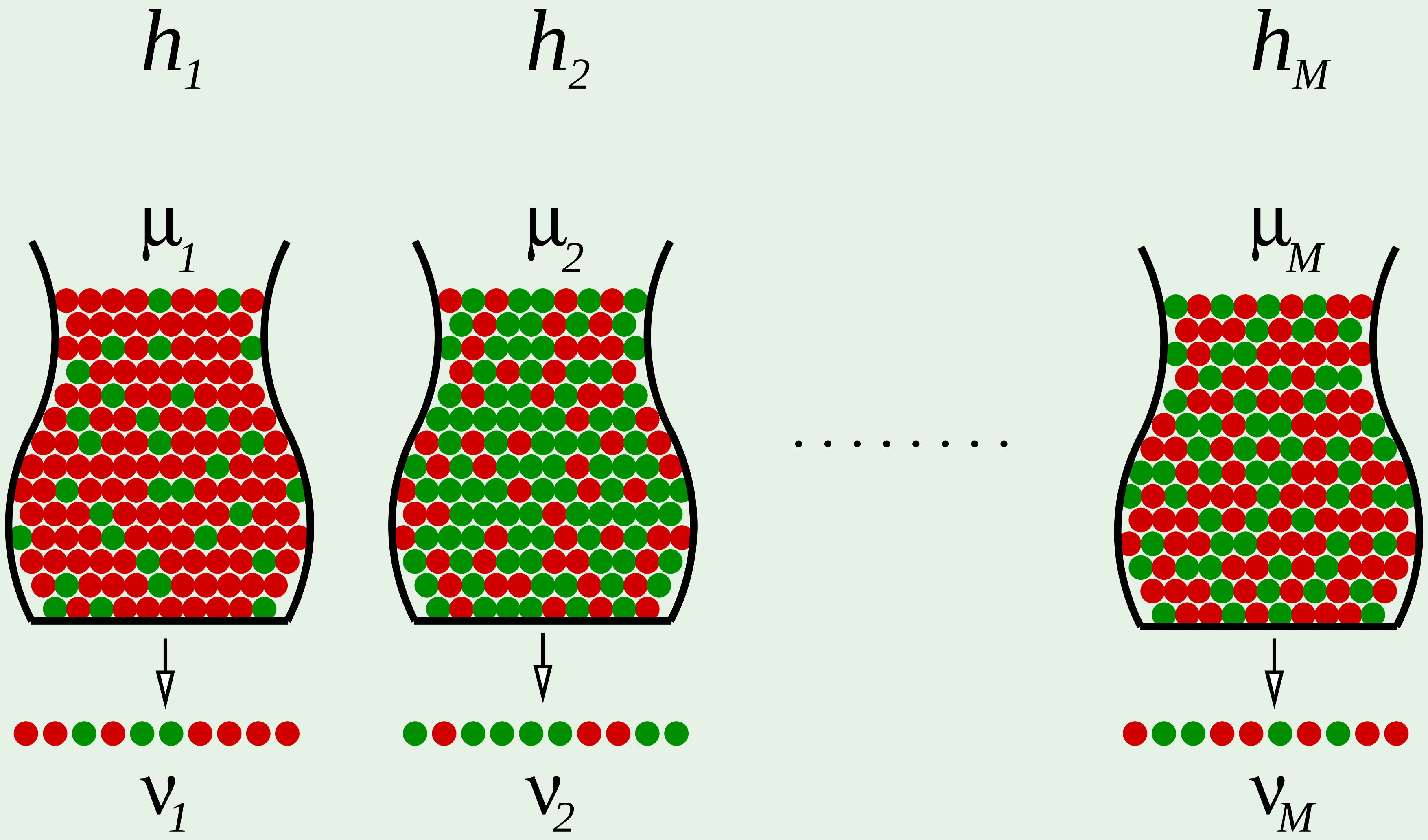
No guarantee ν will be small.

We need to **choose** from multiple h's.



Multiple bins

Generalizing the bin model to more than one hypothesis:



Notation for learning

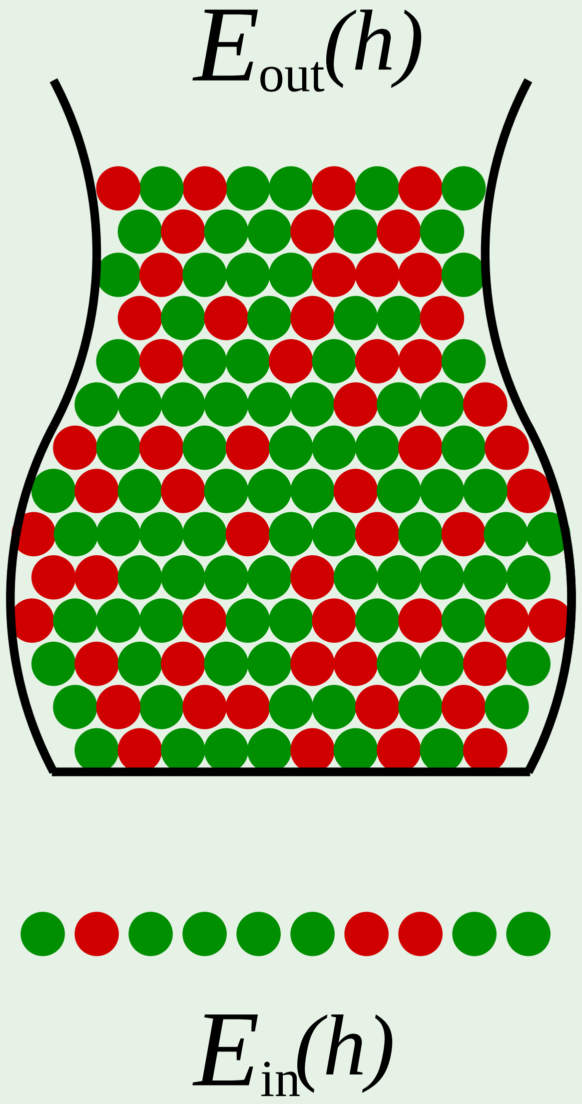
Both μ and ν depend on which hypothesis h

ν is 'in sample' denoted by $E_{\text{in}}(h)$

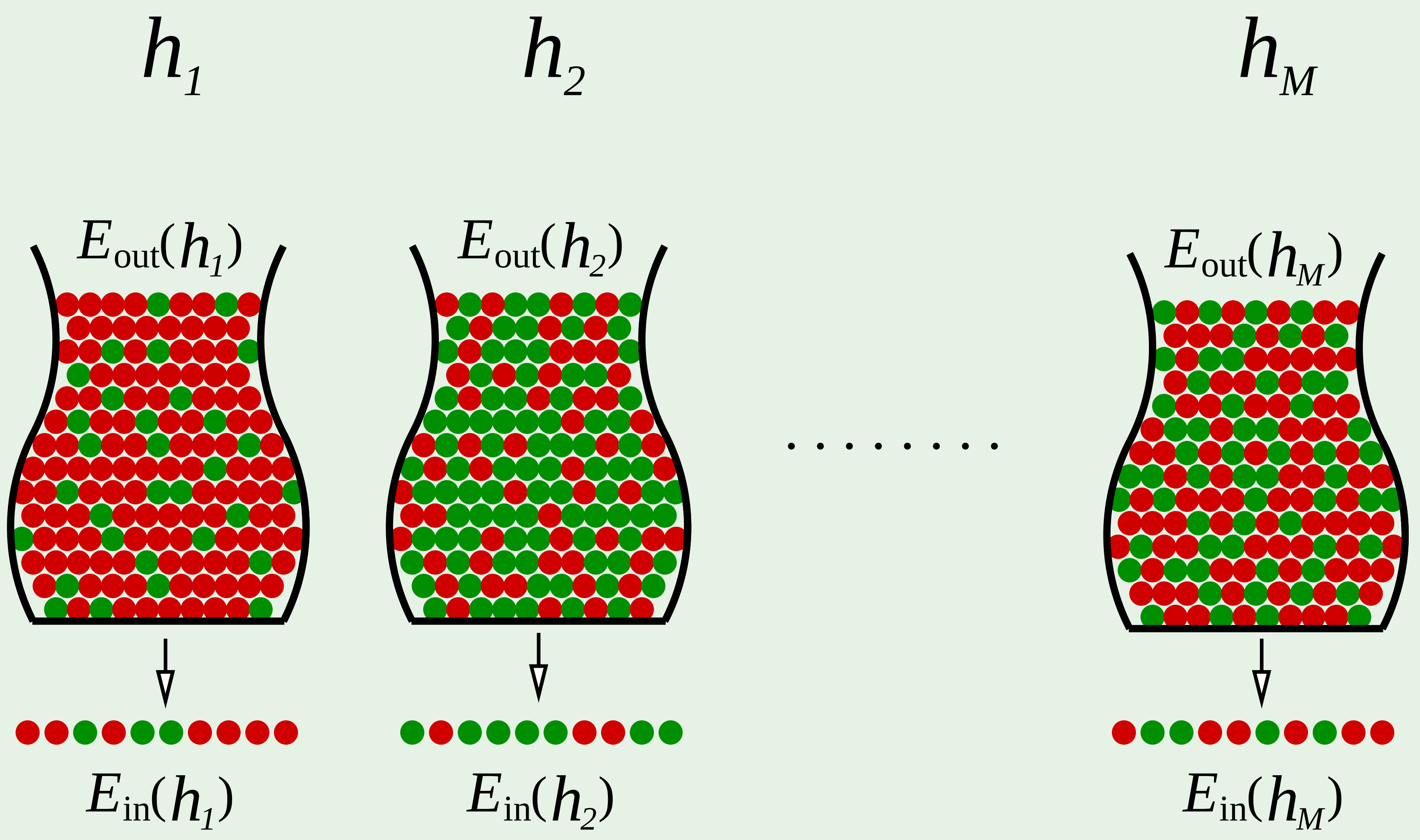
μ is 'out of sample' denoted by $E_{\text{out}}(h)$

The Hoeffding inequality becomes:

$$\mathbb{P}\left[\,|E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon\,\right] \;\leq\; 2e^{-2\epsilon^2 N}$$



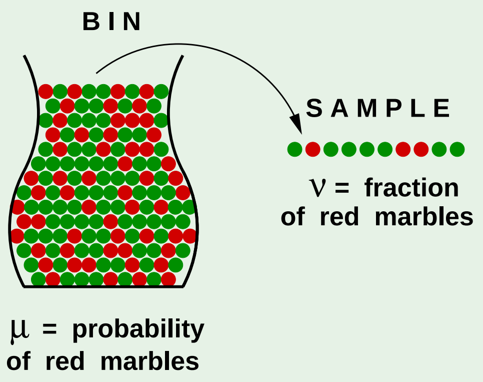
Notation with multiple bins

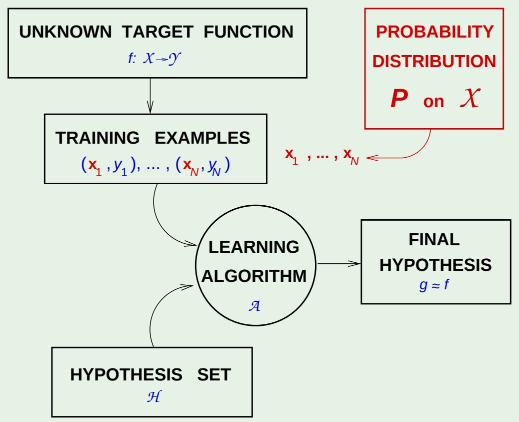


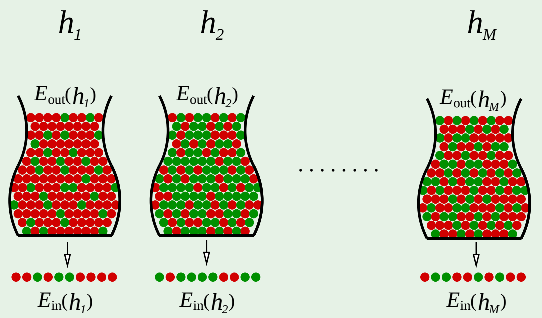
Are we done already? ☺

Not so fast!! Hoeffding doesn't apply to multiple bins.

What?







Coin analogy

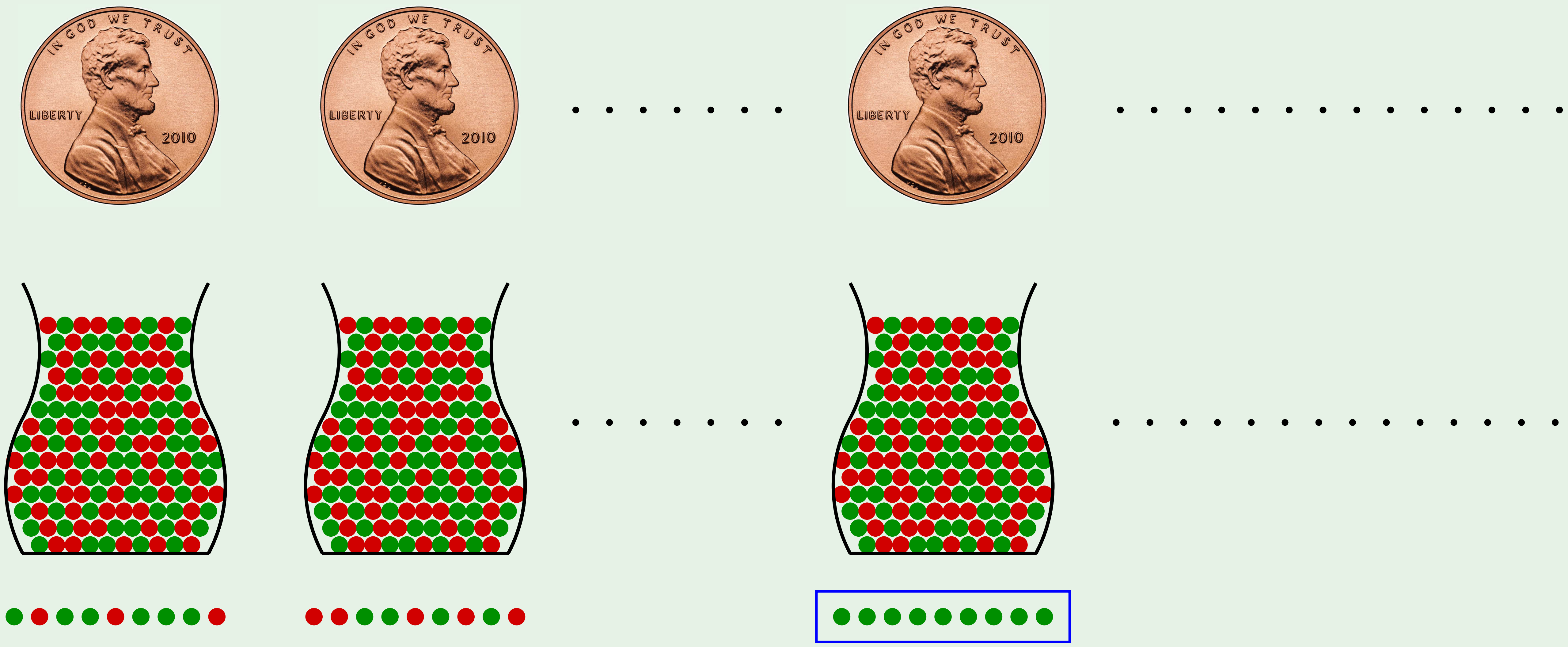
Question: If you toss a fair coin 10 times, what is the probability that you will get 10 heads?

Answer: $\approx 0.1\%$

Question: If you toss 1000 fair coins 10 times each, what is the probability that <u>some</u> coin will get 10 heads?

Answer: $\approx 63\%$

From coins to learning



BINGO ?

A simple solution

$$
\begin{aligned}
\mathbb{P}[\ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\ ] \ \leq\ \mathbb{P}[\quad & |E_{\text{in}}(h_1) - E_{\text{out}}(h_1)| > \epsilon \\
\textbf{or}\ & |E_{\text{in}}(h_2) - E_{\text{out}}(h_2)| > \epsilon \\
& \cdots \\
\textbf{or}\ & |E_{\text{in}}(h_M) - E_{\text{out}}(h_M)| > \epsilon\ ] \\
\leq\ \sum_{m=1}^{M} \mathbb{P}\left[|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon\right]
\end{aligned}
$$

The final verdict

$$\mathbb{P}[\ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\ ] \ \leq \ \sum_{m=1}^{M} \mathbb{P}\left[|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon\right]$$

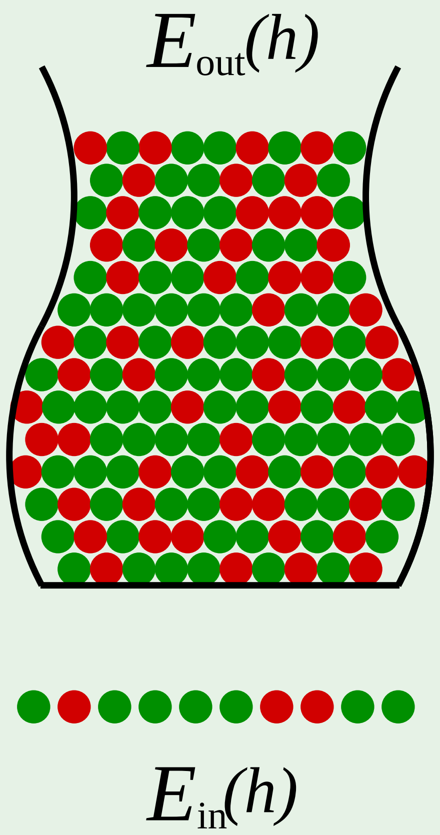
$$\leq \ \sum_{m=1}^{M} 2e^{-2\epsilon^2 N}$$

$$\mathbb{P}[|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon] \leq 2{\color{red}M}e^{-2\epsilon^2 N}$$

Review of Lecture 2

Is Learning feasible?

Yes, in a **probabilistic** sense.



$$\mathbb{P}\left[\,|E_{\text{in}}(h) - E_{\text{out}}(h)| > \epsilon\,\right] \leq 2e^{-2\epsilon^2 N}$$

Since g has to be one of $h_1, h_2, \cdots, h_M$, we conclude that

If:

$$|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon$$

Then:

$$|E_{\text{in}}(h_1) - E_{\text{out}}(h_1)| > \epsilon \quad \textbf{or}$$

$$|E_{\text{in}}(h_2) - E_{\text{out}}(h_2)| > \epsilon \quad \textbf{or}$$

$$\cdots$$

$$|E_{\text{in}}(h_M) - E_{\text{out}}(h_M)| > \epsilon$$

This gives us an added M factor.

Learning From Data

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Lecture 3: **Linear Models I**

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Outline

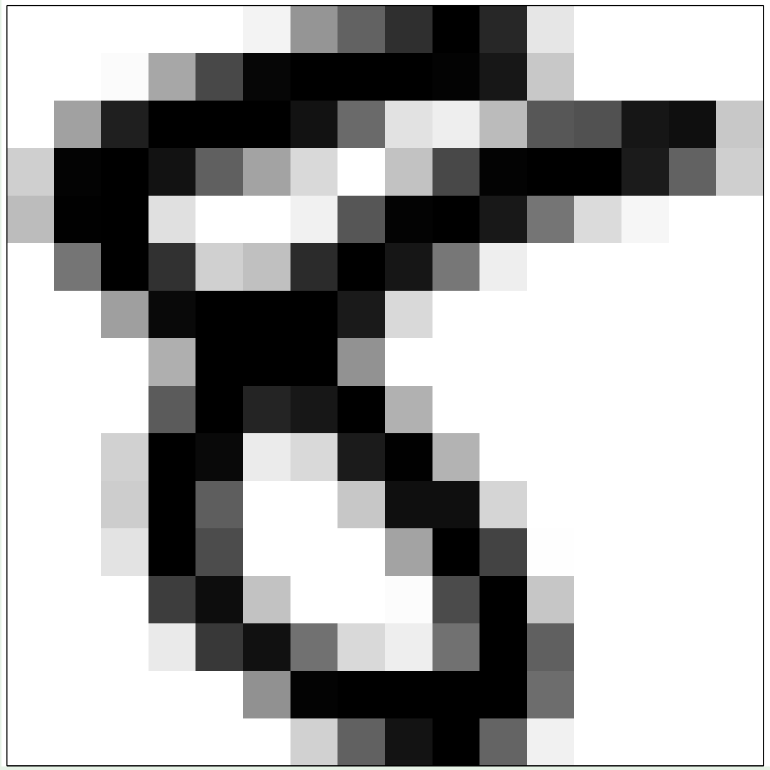
- Input representation
- Linear Classification
- Linear Regression
- Nonlinear Transformation

A real data set

Input representation

'raw' input $\mathbf{x} = (x_0, x_1, x_2, \cdots, x_{256})$

linear model: $(w_0, w_1, w_2, \cdots, w_{256})$



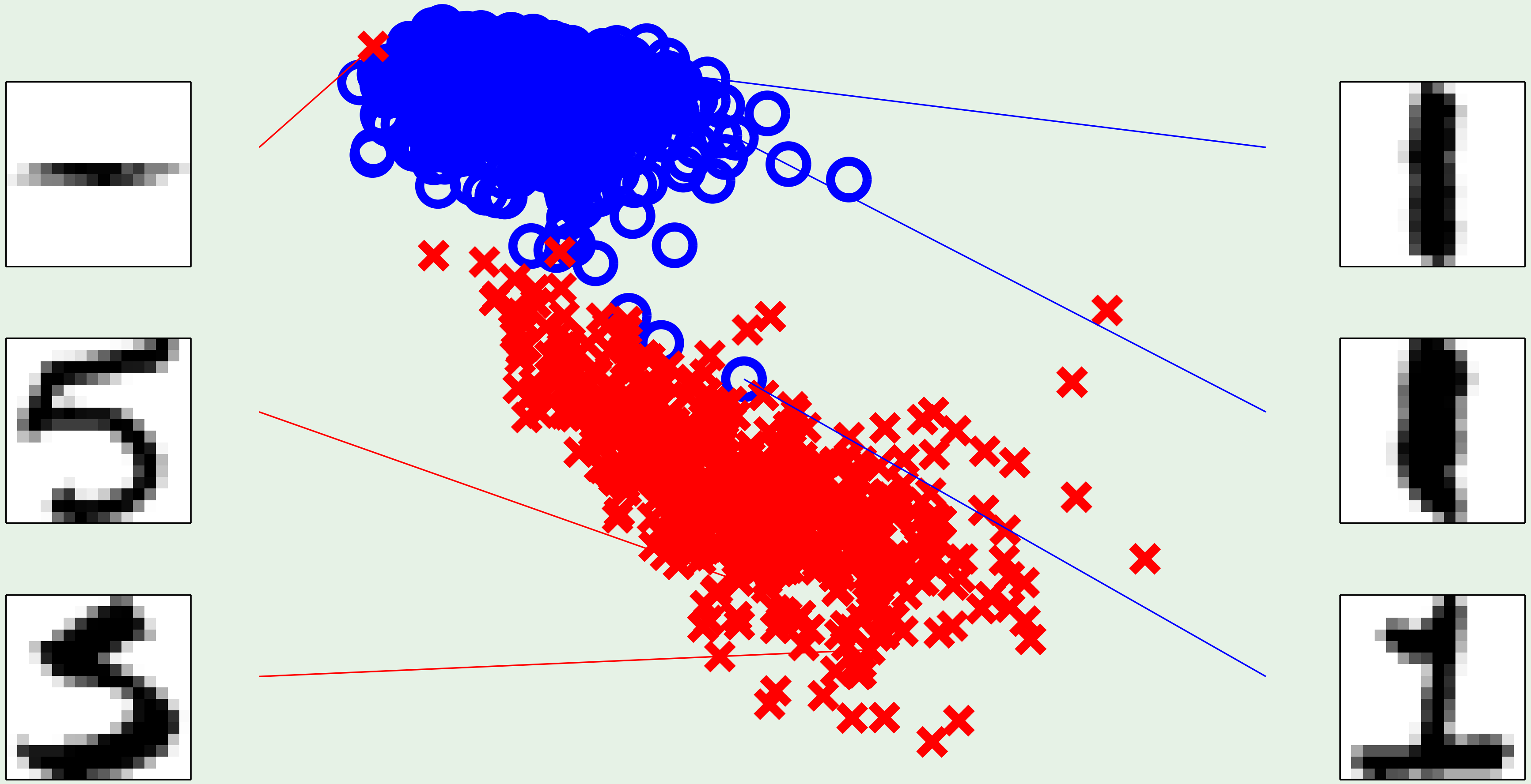
Features: Extract useful information, e.g.,

intensity and symmetry $\mathbf{x} = (x_0, x_1, x_2)$

linear model: (w_0, w_1, w_2)

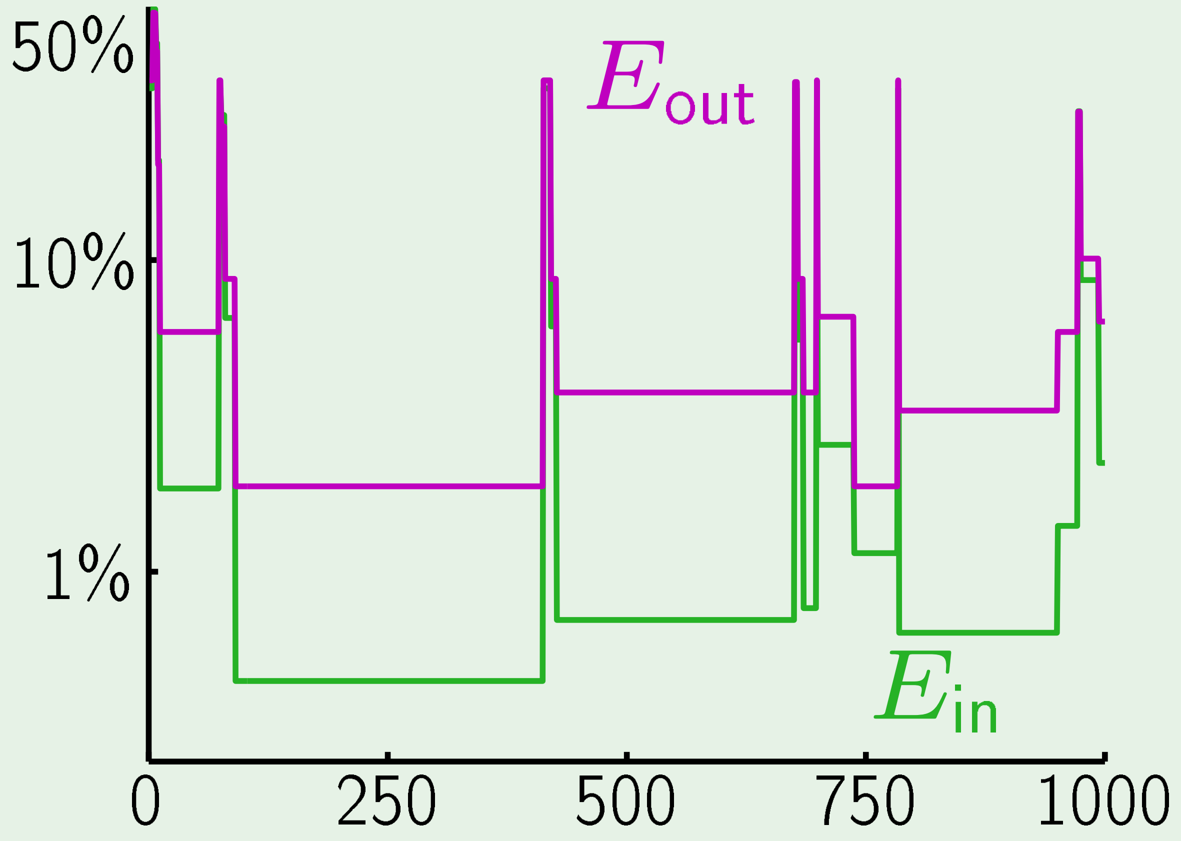
Illustration of features

$\mathbf{x} = (x_0, x_1, x_2)$ $\quad x_1$: intensity $\quad x_2$: symmetry

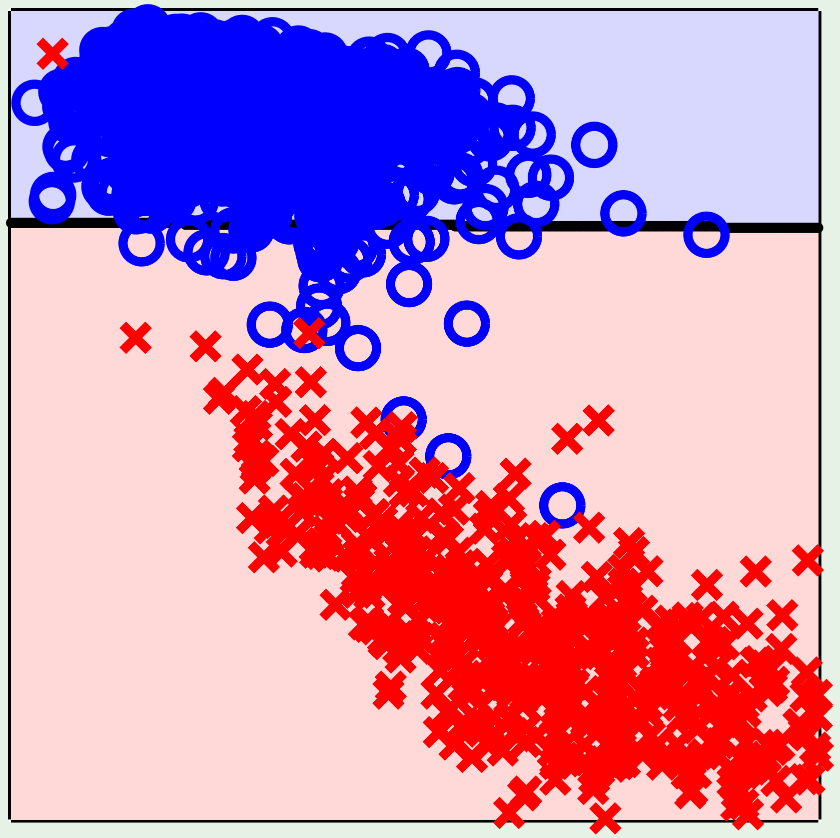


What PLA does

Evolution of E_{in} and E_{out}

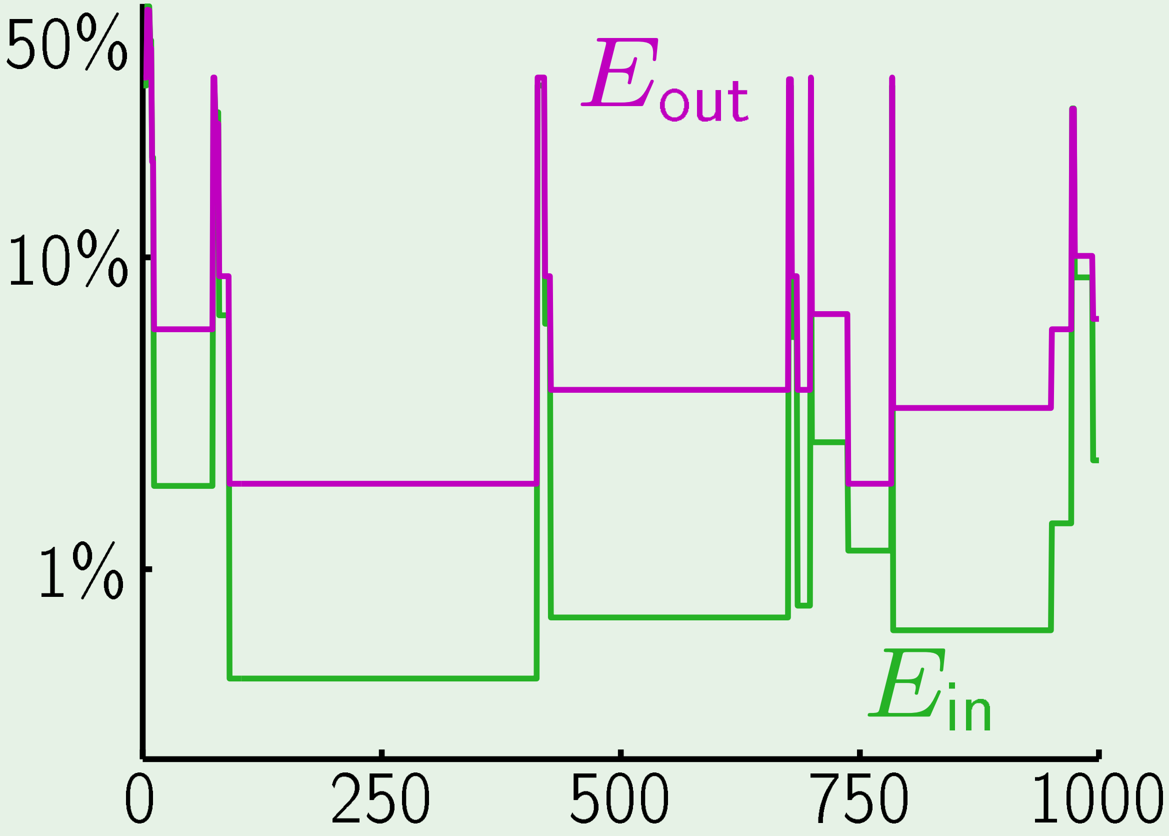


Final perceptron boundary

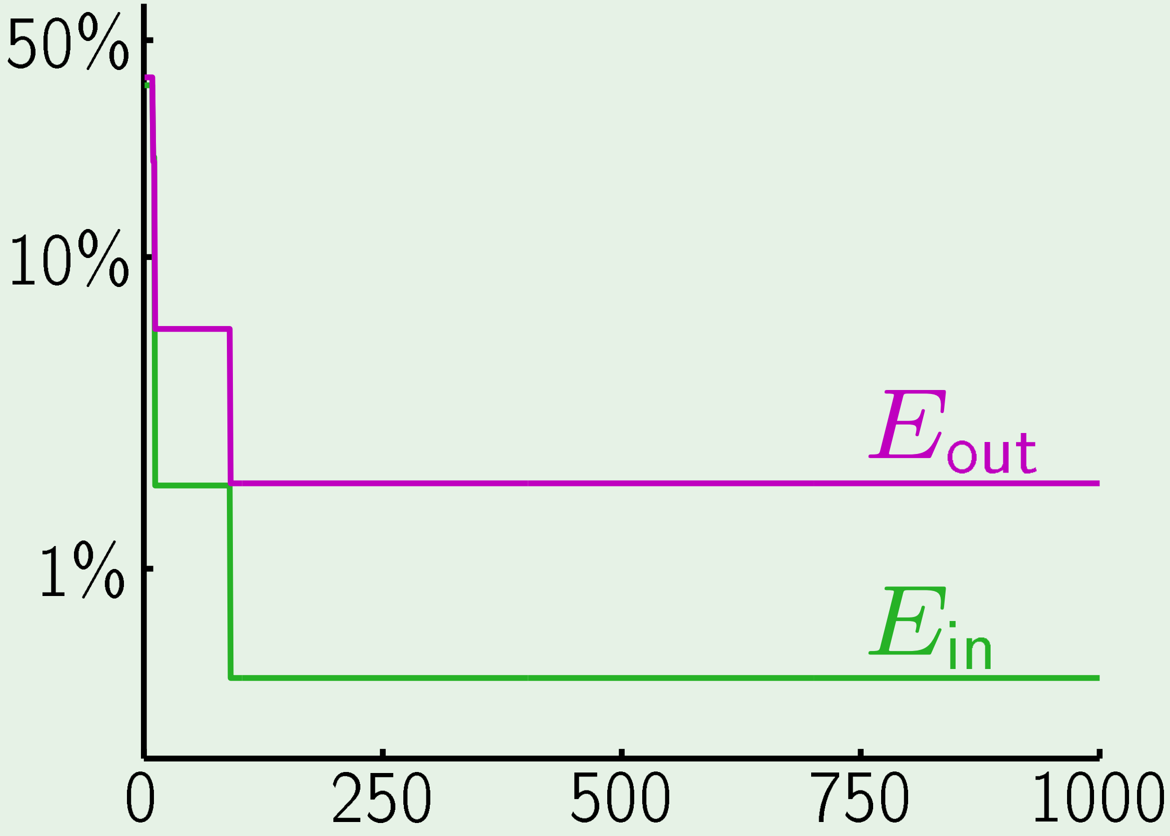


The 'pocket' algorithm

PLA:

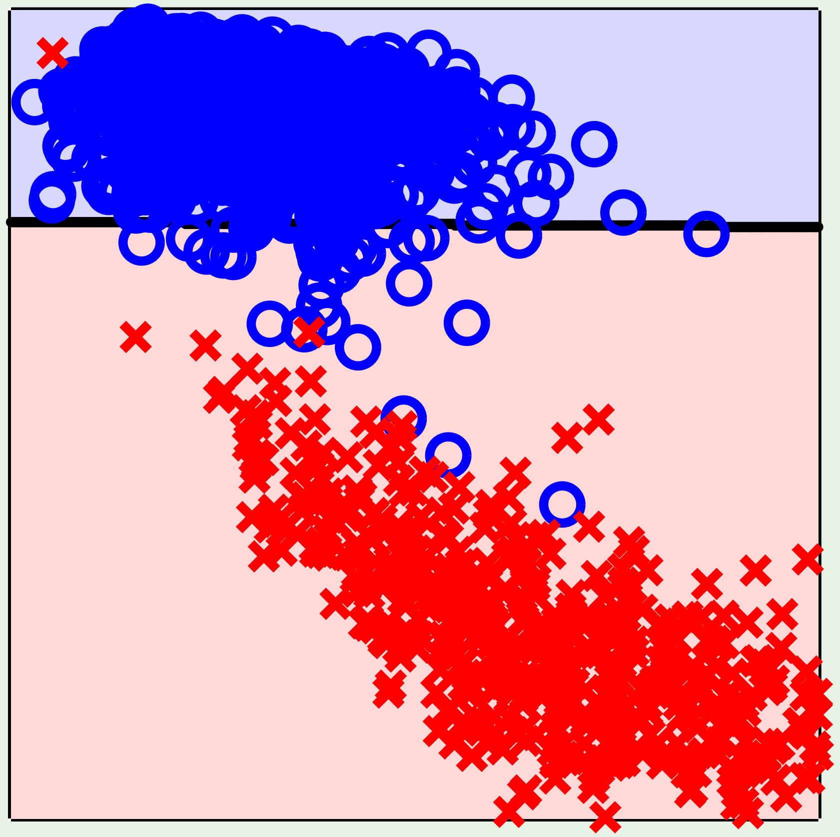


Pocket:

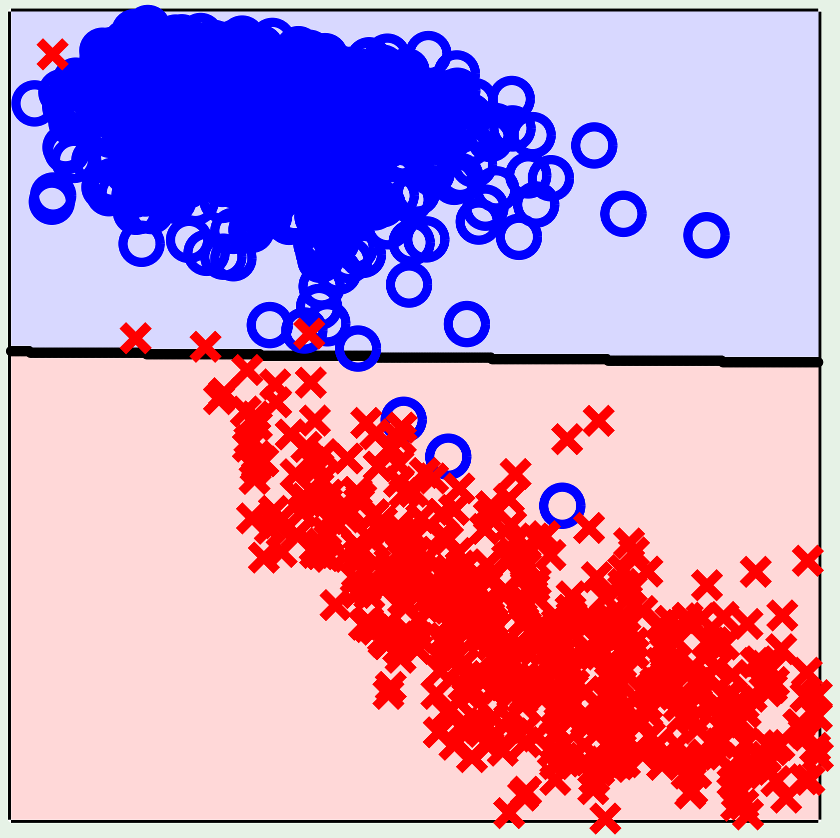


Classification boundary - PLA versus Pocket

PLA:



Pocket:



Outline

- Input representation
- Linear Classification
- Linear Regression **regression ≡ real-valued output**
- Nonlinear Transformation

Credit again

Classification: Credit approval (yes/no)

Regression: Credit line (dollar amount)

Input: $\mathbf{x} =$

age	23 years
annual salary	$30,000
years in residence	1 year
years in job	1 year
current debt	$15,000
...	...

Linear regression output: $h(\mathbf{x}) = \sum_{i=0}^{d} w_i \, x_i = \mathbf{w}^{\intercal}\mathbf{x}$

The data set

Credit officers decide on credit lines:

$$(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \cdots, (\mathbf{x}_N, y_N)$$

$y_n \in \mathbb{R}$ is the credit line for customer $\mathbf{x}_n$.

Linear regression tries to replicate that.

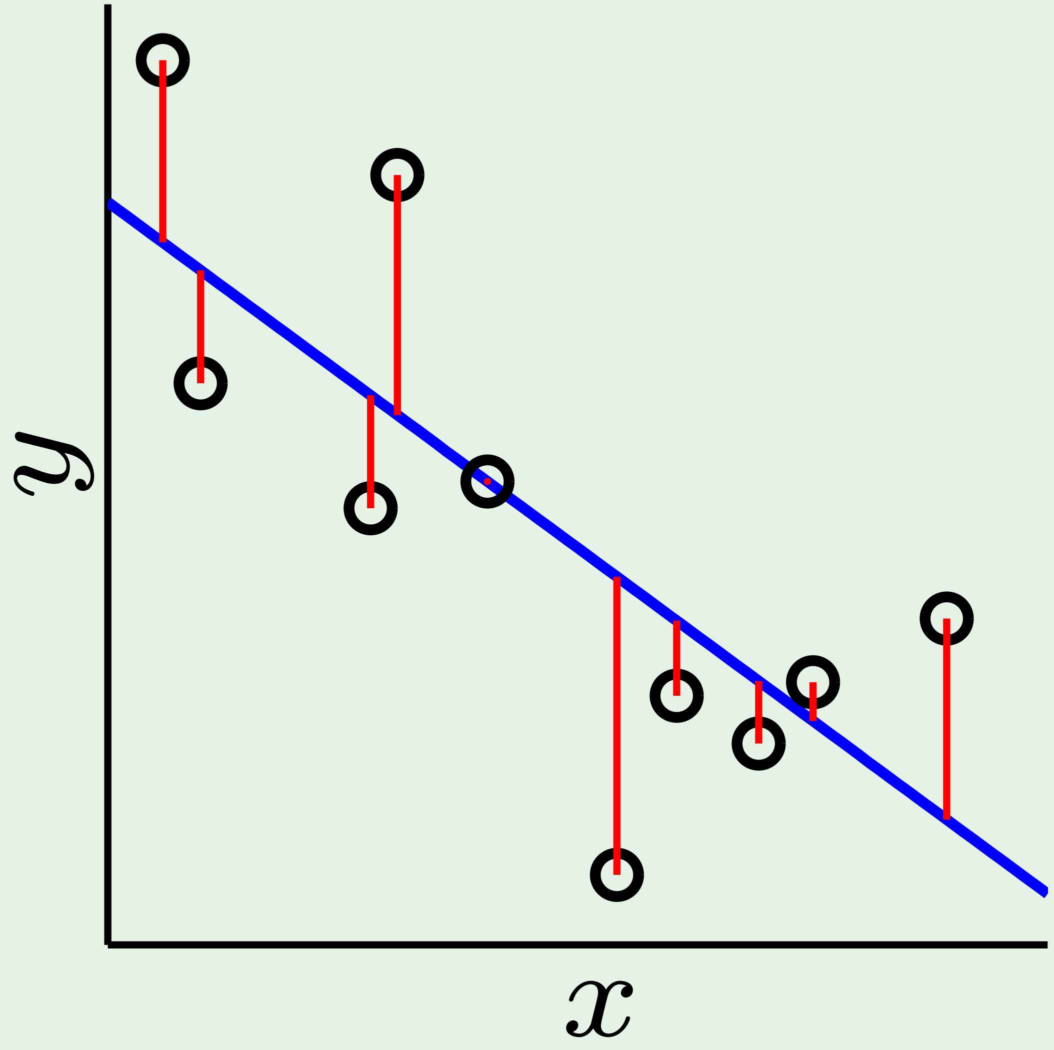
How to measure the error

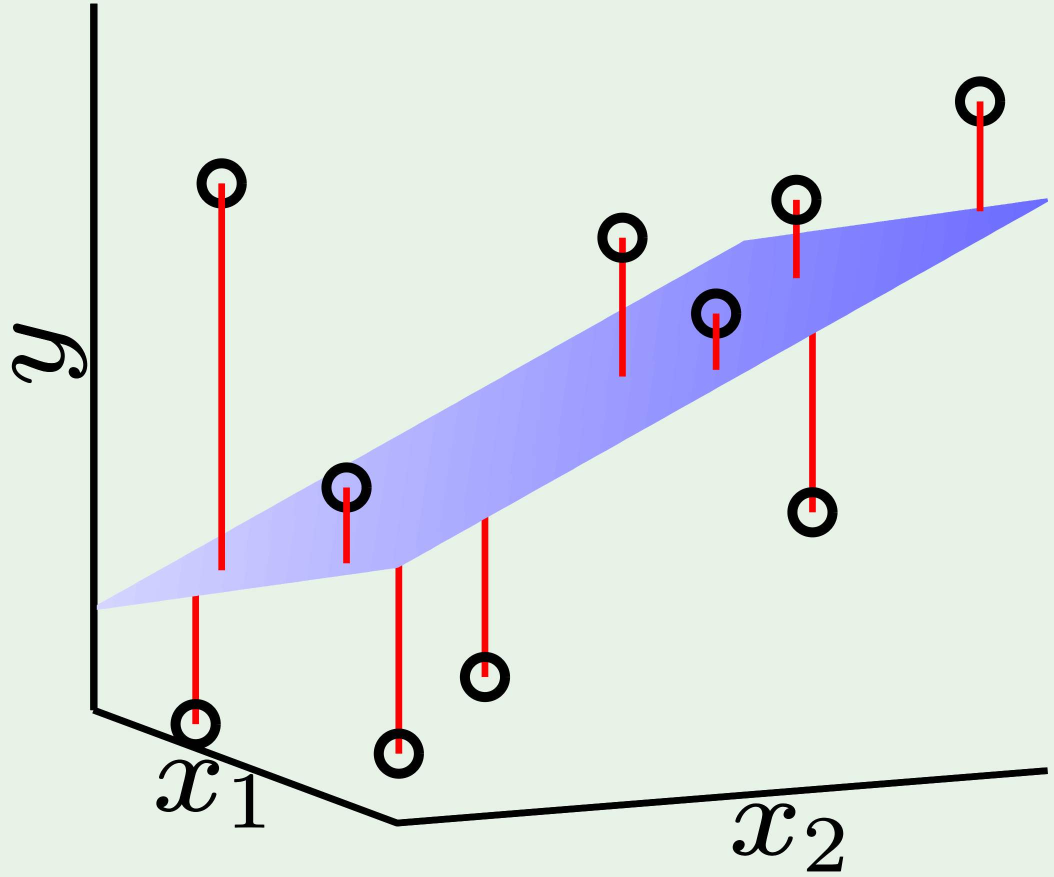
How well does $h(\mathbf{x}) = \mathbf{w}^{\intercal}\mathbf{x}$ approximate $f(\mathbf{x})$?

In linear regression, we use squared error $(h(\mathbf{x}) - f(\mathbf{x}))^2$

in-sample error: $E_{\text{in}}(h) = \frac{1}{N}\sum_{n=1}^{N}(h(\mathbf{x}_n) - y_n)^2$

Illustration of linear regression





The expression for E_{in}

$$
\begin{aligned}
E_{\text{in}}(\mathbf{w}) &= \frac{1}{N}\sum_{n=1}^{N}\left(\mathbf{w}^{\intercal}\mathbf{x}_n - y_n\right)^2 \\
&= \frac{1}{N}\|\mathrm{X}\mathbf{w} - \mathbf{y}\|^2
\end{aligned}
$$

where $\mathrm{X} = \begin{bmatrix} \text{—}\mathbf{x}_1{}^{\intercal}\text{—} \\ \text{—}\mathbf{x}_2{}^{\intercal}\text{—} \\ \vdots \\ \text{—}\mathbf{x}_N{}^{\intercal}\text{—} \end{bmatrix}, \qquad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}$

Minimizing E_{in}

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\|\mathrm{X}\mathbf{w} - \mathbf{y}\|^2$$

$$\nabla E_{\text{in}}(\mathbf{w}) = \frac{2}{N}\mathrm{X}^\top(\mathrm{X}\mathbf{w} - \mathbf{y}) = \mathbf{0}$$

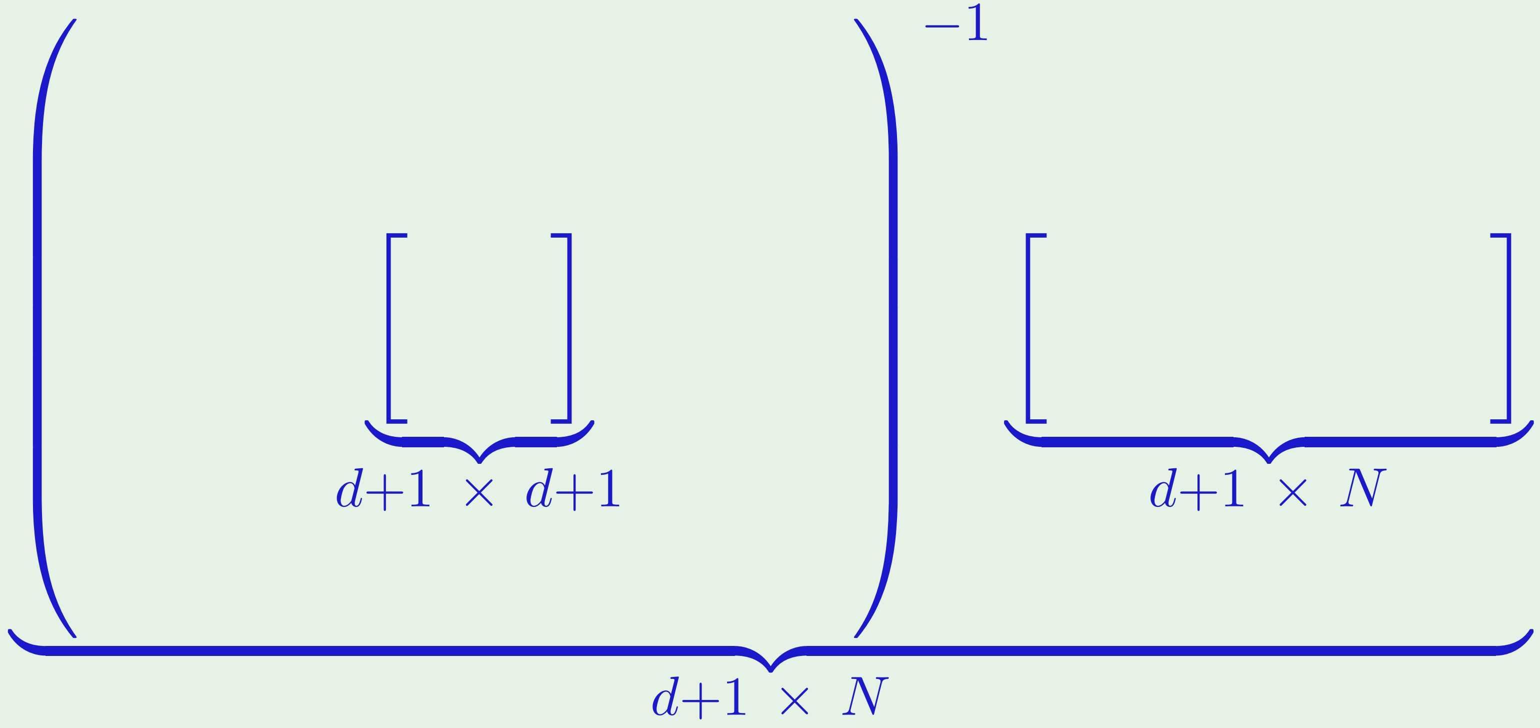
$$\mathrm{X}^\top\mathrm{X}\mathbf{w} = \mathrm{X}^\top\mathbf{y}$$

$$\mathbf{w} = \mathrm{X}^\dagger\mathbf{y} \quad \text{where} \quad \mathrm{X}^\dagger = (\mathrm{X}^\top\mathrm{X})^{-1}\mathrm{X}^\top$$

$\mathrm{X}^\dagger$ is the '**pseudo-inverse**' of X

The pseudo-inverse

$$\mathrm{X}^{\dagger} = (\mathrm{X}^{\intercal}\mathrm{X})^{-1}\mathrm{X}^{\intercal}$$



The linear regression algorithm

1: Construct the matrix X and the vector $\mathbf{y}$ from the data set $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$ as follows

$$\underbrace{\mathrm{X} = \begin{bmatrix} \text{—}\mathbf{x}_1^\top\text{—} \\ \text{—}\mathbf{x}_2^\top\text{—} \\ \vdots \\ \text{—}\mathbf{x}_N^\top\text{—} \end{bmatrix}}_{\text{input data matrix}}, \qquad \underbrace{\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\text{target vector}}.$$

2: Compute the pseudo-inverse $\mathrm{X}^\dagger = (\mathrm{X}^\top \mathrm{X})^{-1}\mathrm{X}^\top$.

3: Return $\mathbf{w} = \mathrm{X}^\dagger \mathbf{y}$.

Linear regression for classification

Linear regression learns a real-valued function $y = f(\mathbf{x}) \in \mathbb{R}$

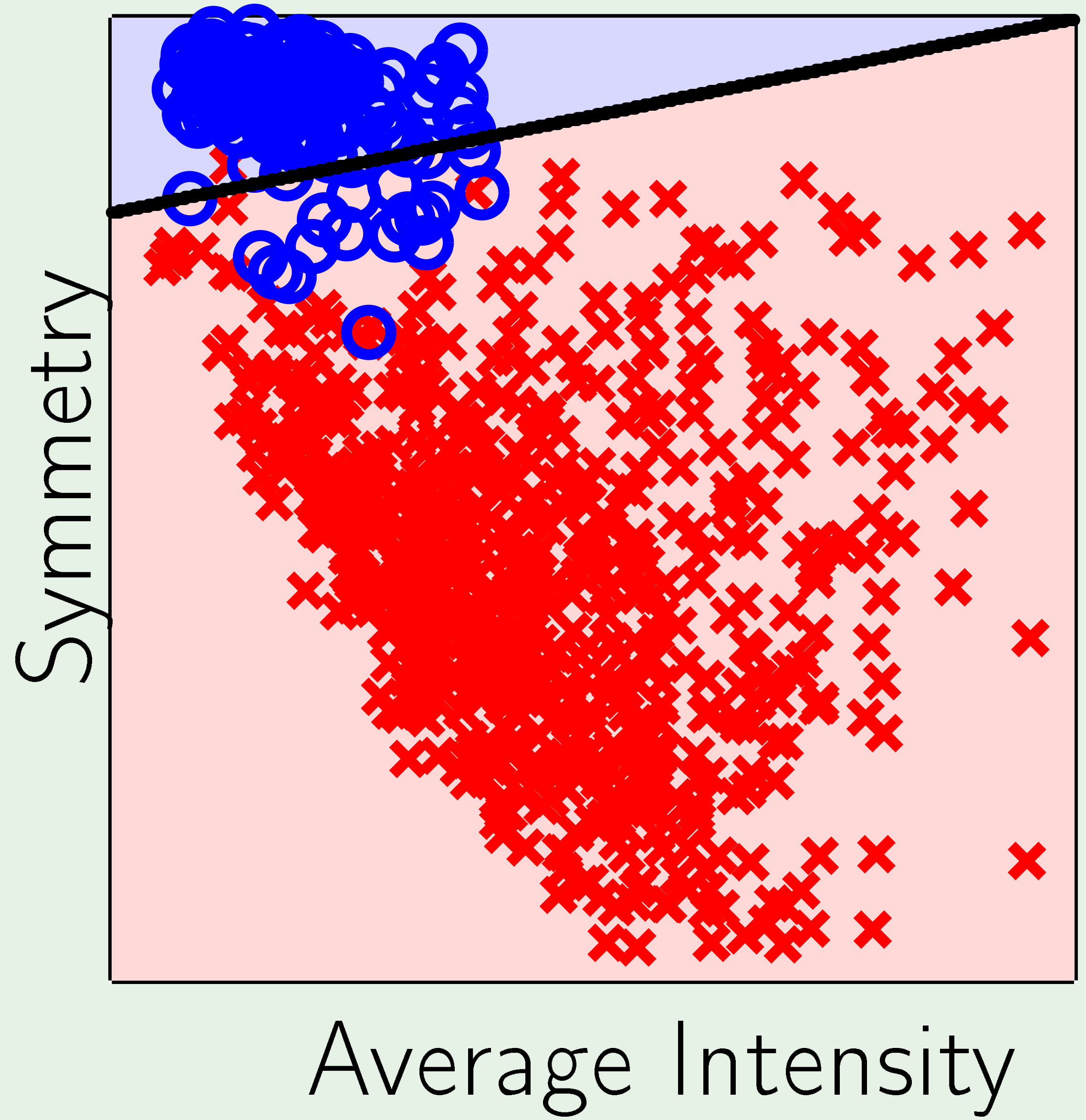
Binary-valued functions are also real-valued! $\pm 1 \in \mathbb{R}$

Use linear regression to get $\mathbf{w}$ where $\mathbf{w}^\intercal \mathbf{x}_n \approx y_n = \pm 1$

In this case, $\text{sign}(\mathbf{w}^\intercal \mathbf{x}_n)$ is likely to agree with $y_n = \pm 1$

Good initial weights for classification

Linear regression boundary

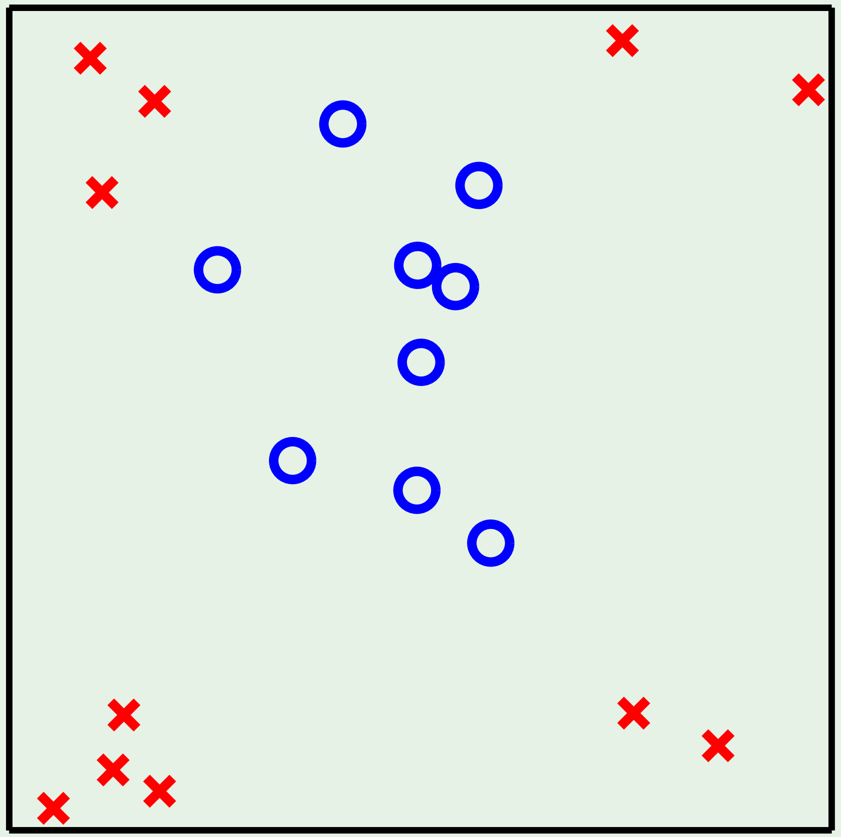


Outline

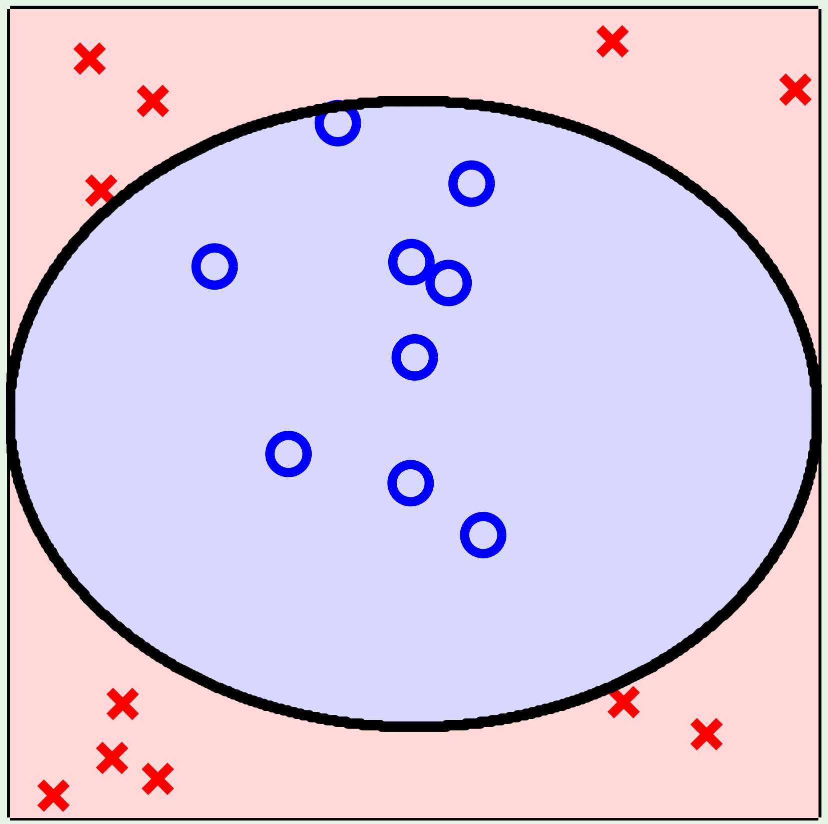
- Input representation
- Linear Classification
- Linear Regression
- Nonlinear Transformation

Linear is limited

Data:



Hypothesis:



Another example

Credit line is affected by 'years in residence'

but **not** in a linear way!

Nonlinear $[[x_i < 1]]$ and $[[x_i > 5]]$ are better.

Can we do that with linear models?

Linear in what?

Linear regression implements

$$\sum_{i=0}^{d} w_i \; x_i$$

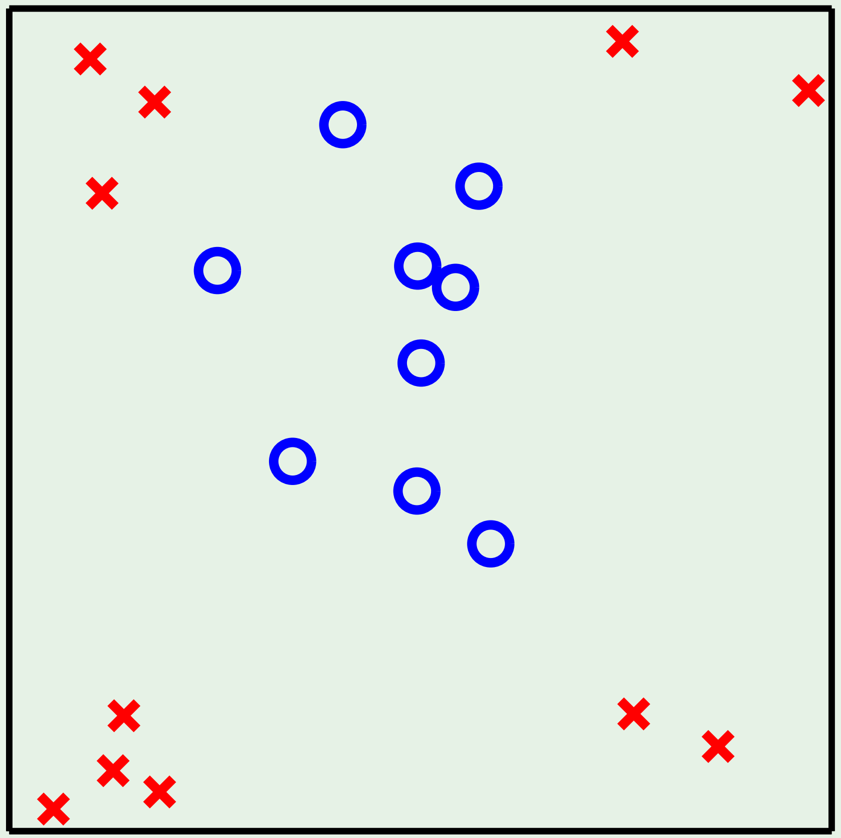
Linear classification implements

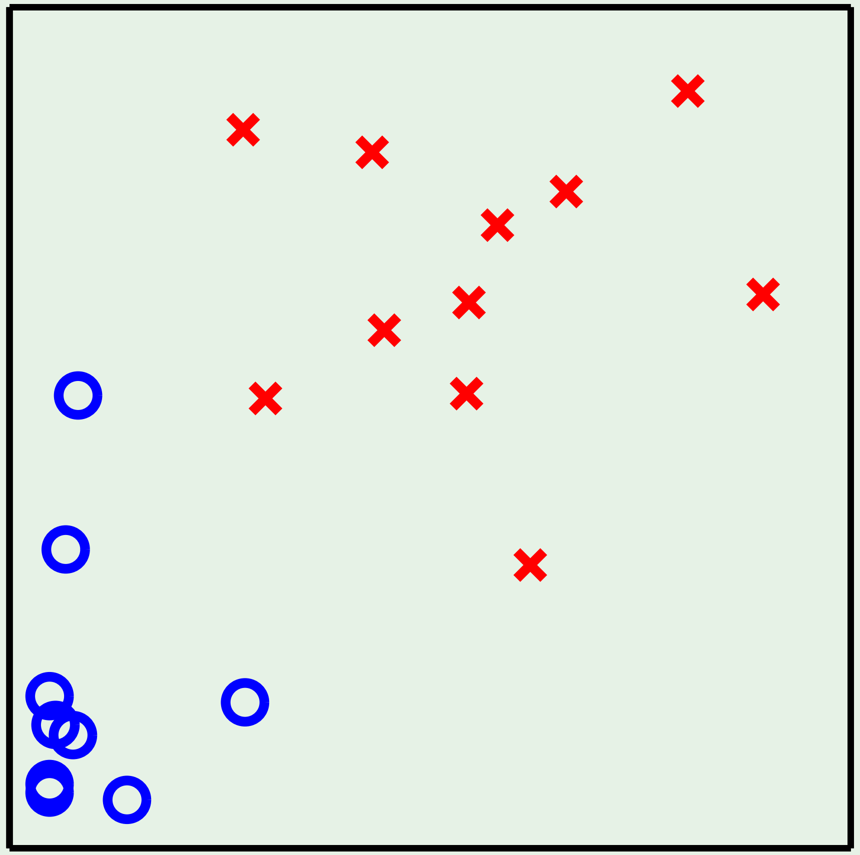
$$\text{sign}\left(\sum_{i=0}^{d} w_i \; x_i\right)$$

Algorithms work because of **linearity in the weights**

Transform the data nonlinearly

$$(x_1, x_2) \xrightarrow{\Phi} (x_1^2, x_2^2)$$





Review of Lecture 3

- Linear models use the 'signal':

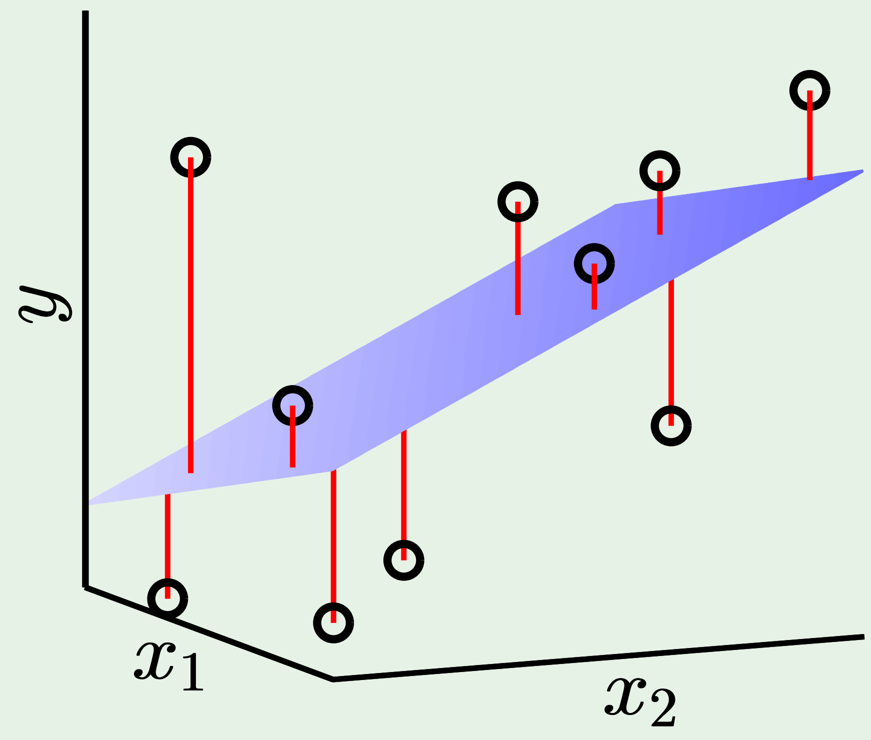
$$\sum_{i=0}^{d} w_i x_i = \mathbf{w}^\intercal \mathbf{x}$$

  - Classification: $h(\mathbf{x}) = \text{sign}(\mathbf{w}^\intercal \mathbf{x})$
  - Regression: $h(\mathbf{x}) = \mathbf{w}^\intercal \mathbf{x}$

- Linear regression algorithm:

$$\mathbf{w} = (\mathrm{X}^\intercal \mathrm{X})^{-1} \mathrm{X}^\intercal \mathbf{y}$$

"one-step learning"



- Nonlinear transformation:
  - $\mathbf{w}^\intercal \mathbf{x}$ is linear in $\mathbf{w}$
  - Any $\mathbf{x} \xrightarrow{\Phi} \mathbf{z}$ preserves this linearity.
  - Example: $(x_1, x_2) \xrightarrow{\Phi} (x_1^2, x_2^2)$

Learning From Data

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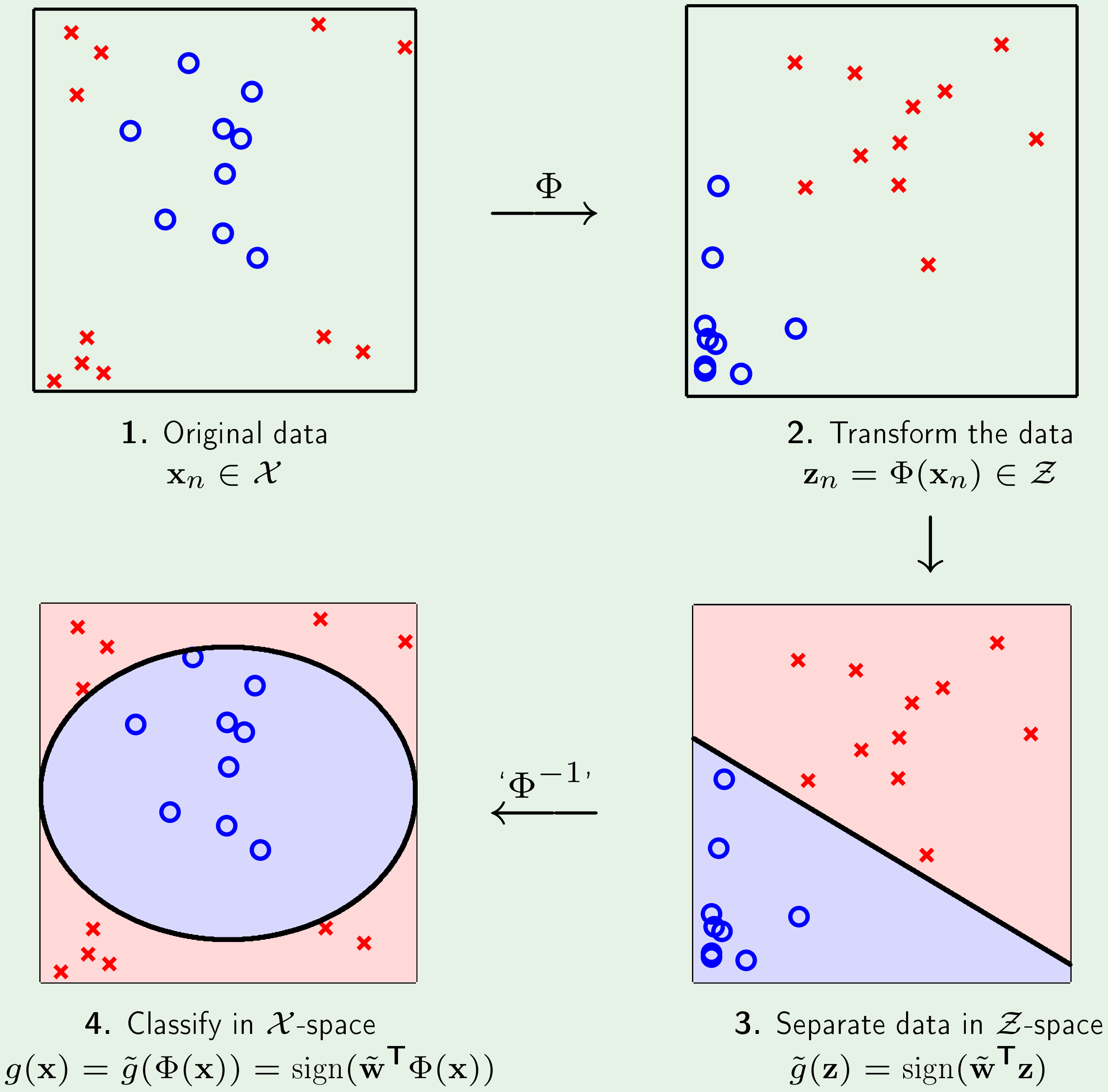
Lecture 4: Error and Noise

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Thursday, April 12, 2012

Outline

- Nonlinear transformation (continued)
- Error measures
- Noisy targets
- Preamble to the theory


Φ
1. Original data
$\mathbf{x}_n \in \mathcal{X}$
2. Transform the data
$\mathbf{z}_n = \Phi(\mathbf{x}_n) \in \mathcal{Z}$
3. Separate data in $\mathcal{Z}$-space
$\tilde{g}(\mathbf{z}) = \text{sign}(\tilde{\mathbf{w}}^{\mathsf{T}}\mathbf{z})$
'Φ^{-1}'
4. Classify in $\mathcal{X}$-space
$g(\mathbf{x}) = \tilde{g}(\Phi(\mathbf{x})) = \text{sign}(\tilde{\mathbf{w}}^{\mathsf{T}}\Phi(\mathbf{x}))$

What transforms to what

$$\mathbf{x} = (x_0, x_1, \cdots, x_d) \quad \xrightarrow{\Phi} \quad \mathbf{z} = (z_0, z_1, \cdots\cdots\cdots, z_{\tilde{d}})$$

$$\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N \quad \xrightarrow{\Phi} \quad \mathbf{z}_1, \mathbf{z}_2, \cdots, \mathbf{z}_N$$

$$y_1, y_2, \cdots, y_N \quad \xrightarrow{\Phi} \quad y_1, y_2, \cdots, y_N$$

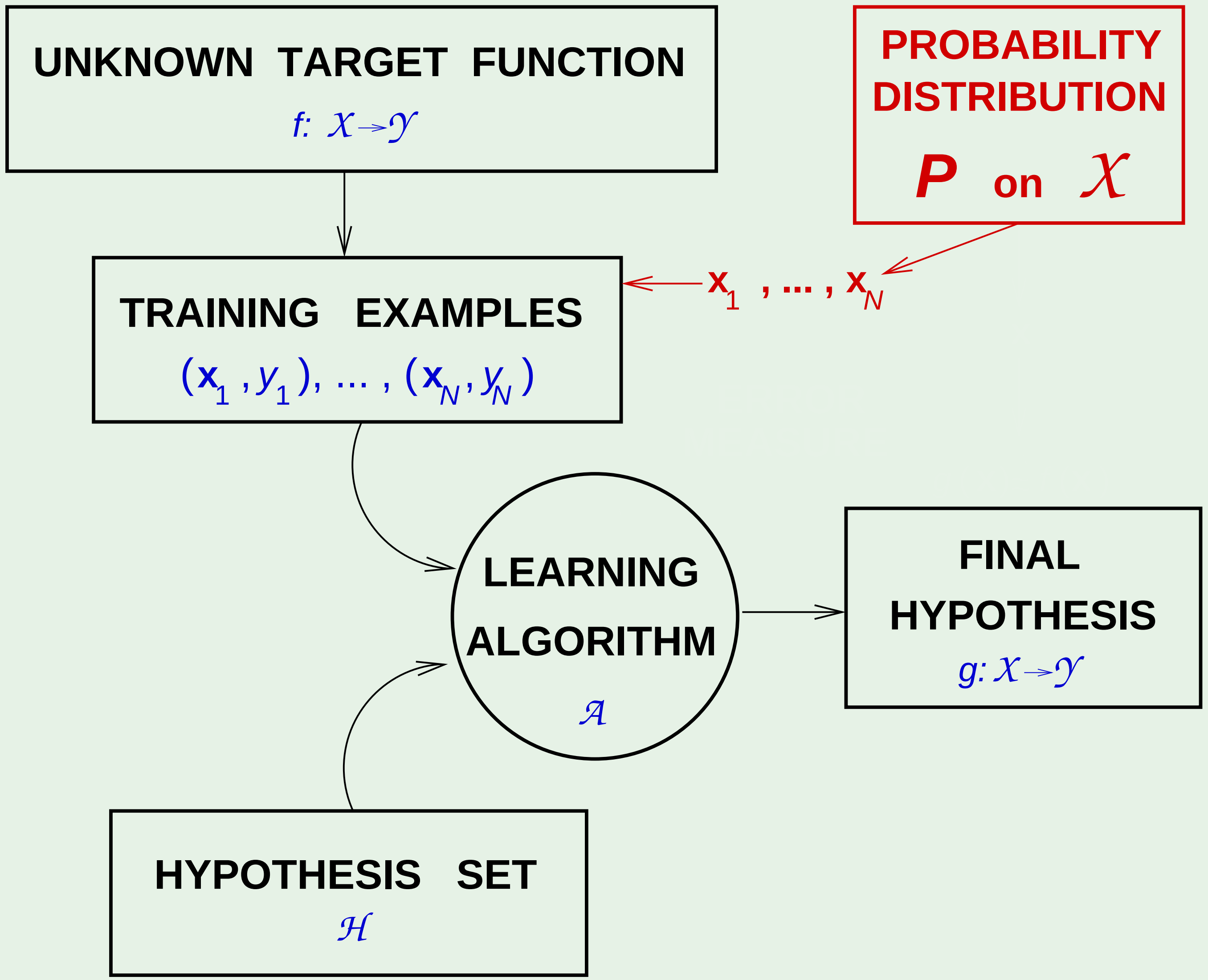
No weights in $\mathcal{X}$ $\qquad$ $\tilde{\mathbf{w}} = (w_0, w_1, \cdots\cdots\cdots, w_{\tilde{d}})$

$$g(\mathbf{x}) \quad = \quad \text{sign}(\tilde{\mathbf{w}}^\mathsf{T}\Phi(\mathbf{x}))$$

Outline

- Nonlinear transformation (continued)
- Error measures
- Noisy targets
- Preamble to the theory

The learning diagram - where we left it



Error measures

What does "$h \approx f$" mean?

Error measure: $E(h, f)$

Almost always *pointwise definition*: $\mathrm{e}\left(h(\mathbf{x}), f(\mathbf{x})\right)$

Examples:

Squared error: $\mathrm{e}\left(h(\mathbf{x}), f(\mathbf{x})\right) = \left(h(\mathbf{x}) - f(\mathbf{x})\right)^2$

Binary error: $\mathrm{e}\left(h(\mathbf{x}), f(\mathbf{x})\right) = [\![h(\mathbf{x}) \neq f(\mathbf{x})]\!]$

From pointwise to overall

Overall error $E(h, f)$ = average of pointwise errors $\mathrm{e}\left(h(\mathbf{x}), f(\mathbf{x})\right)$.

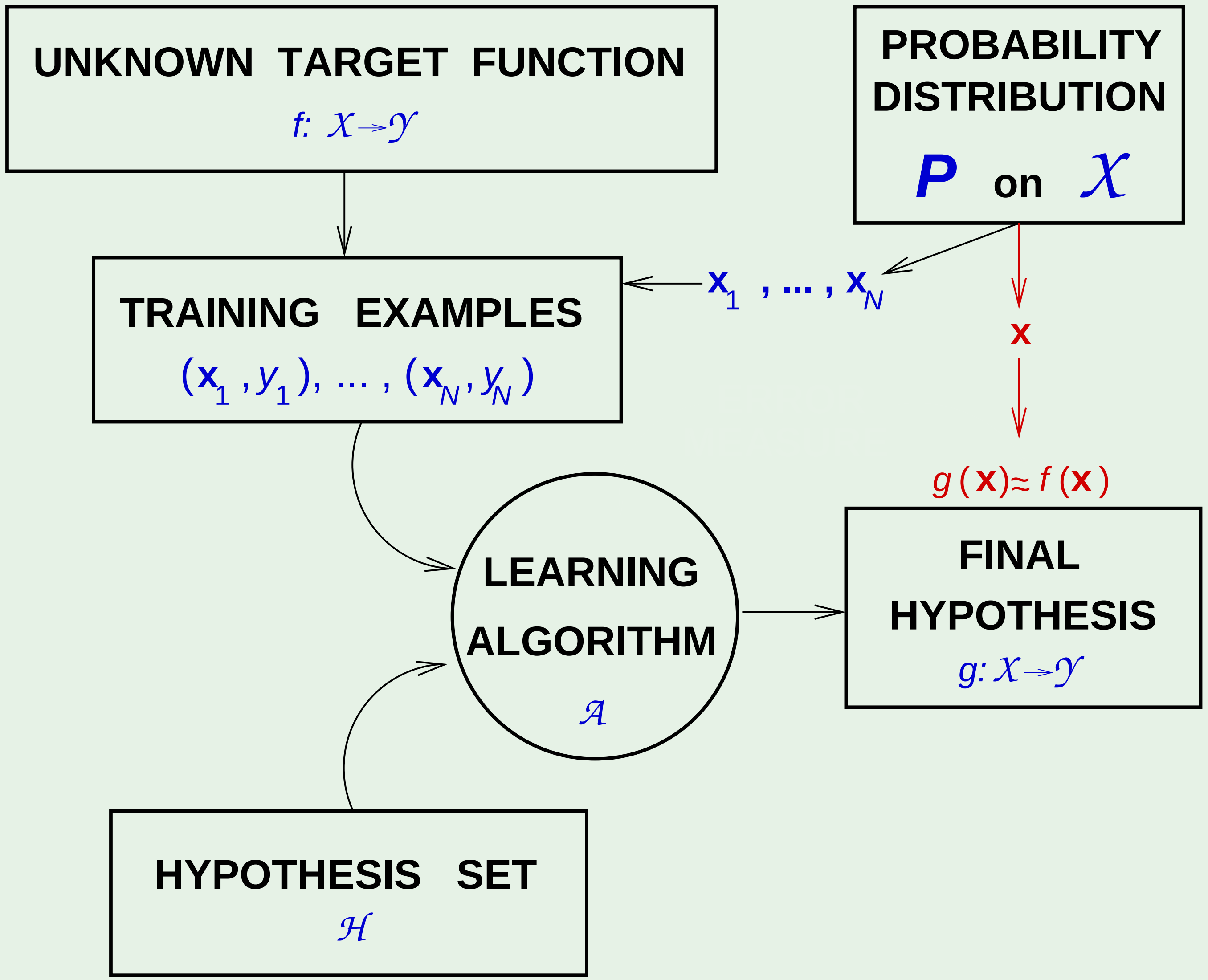
In-sample error:

$$E_{\text{in}}(h) = \frac{1}{N} \sum_{n=1}^{N} \mathrm{e}\left(h(\mathbf{x}_n), f(\mathbf{x}_n)\right)$$

Out-of-sample error:

$$E_{\text{out}}(h) = \mathbb{E}_{\mathbf{x}}\left[\mathrm{e}\left(h(\mathbf{x}), f(\mathbf{x})\right)\right]$$

The learning diagram - with pointwise error



How to choose the error measure

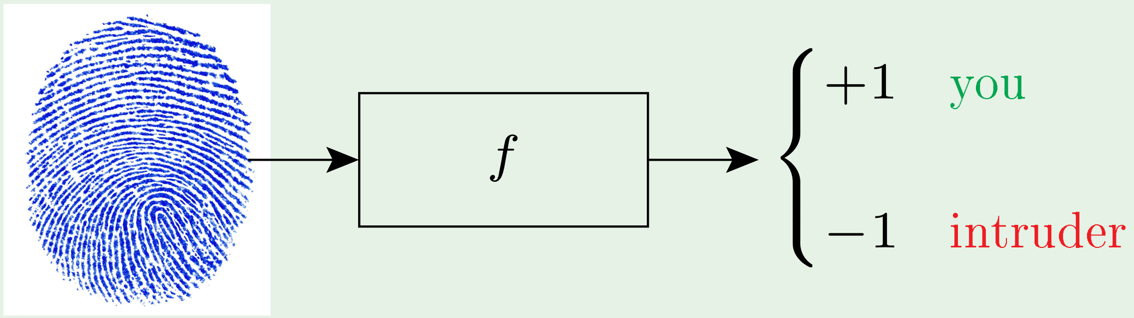
Fingerprint verification:

Two types of error:

false accept and *false reject*

How do we penalize each type?

		f	
		$+1$	-1
h	$+1$	no error	*false accept*
	-1	*false reject*	no error

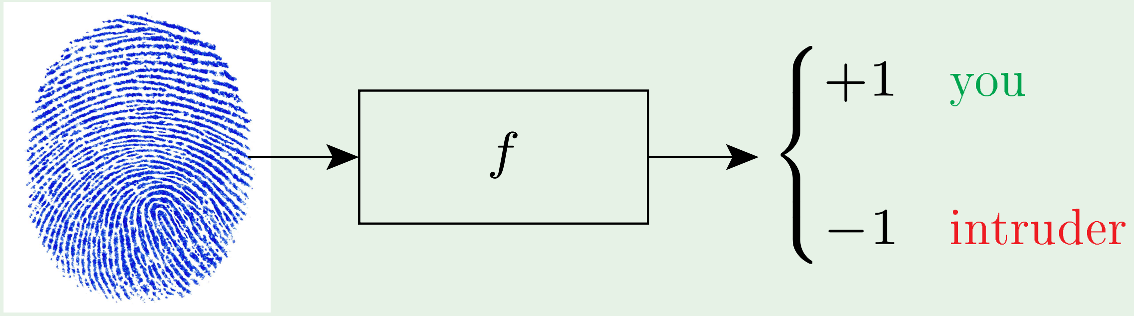


The error measure - for supermarkets

Supermarket verifies fingerprint for discounts

False reject is costly; customer gets annoyed!

False accept is minor; gave away a discount and intruder left their fingerprint ☺



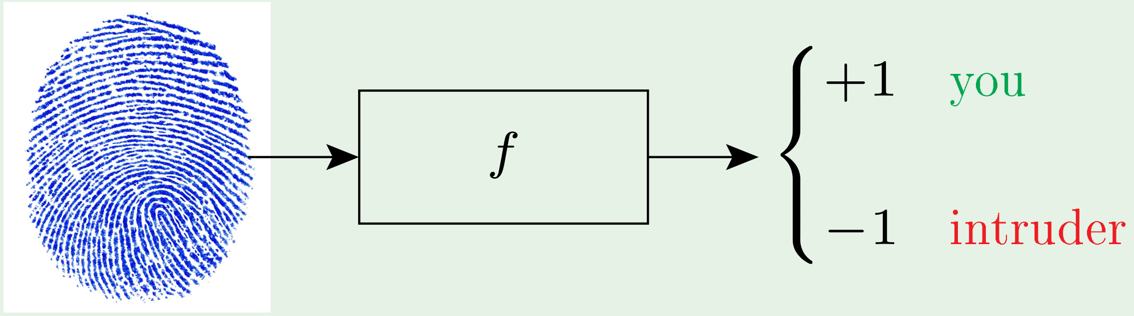
		f: $+1$	f: -1
h	$+1$	0	1
h	-1	10	0

The error measure - for the CIA

CIA verifies fingerprint for security

False accept is a disaster!

False reject can be tolerated
Try again; you are an employee ☺



		f	
		$+1$	-1
h	$+1$	0	1000
	-1	1	0

Take-home lesson

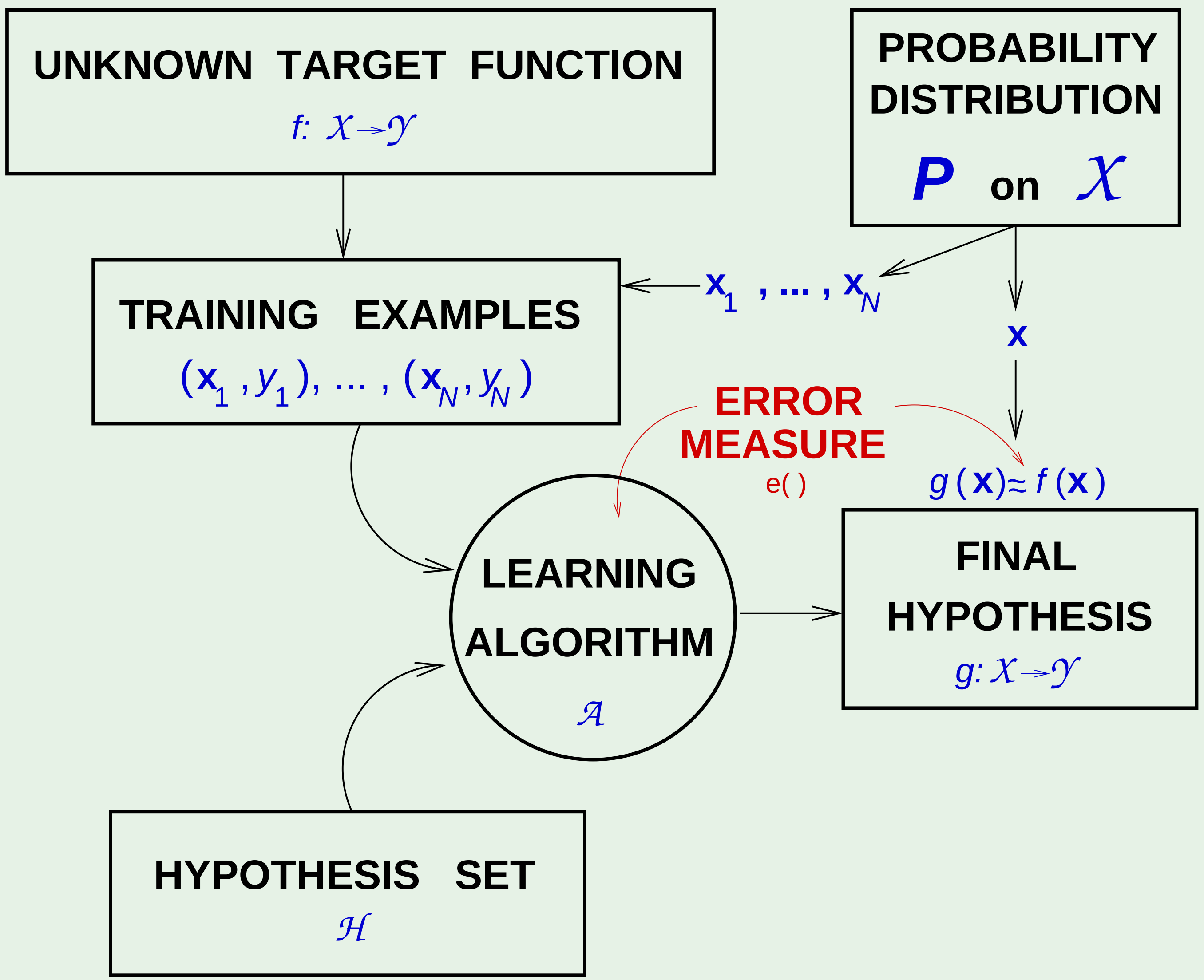
The error measure should be specified by the user.

Not always possible. Alternatives:

Plausible measures: squared error $\equiv$ Gaussian noise

Friendly measures: closed-form solution, convex optimization

The learning diagram - with error measure



Noisy targets

The 'target function' is not always a *function*

Consider the credit-card approval:

age	23 years
annual salary	$30,000
years in residence	1 year
years in job	1 year
current debt	$15,000
···	···

two 'identical' customers $\longrightarrow$ two different behaviors

Target 'distribution'

Instead of $y = f(\mathbf{x})$, we use target *distribution*:

$$P(y \mid \mathbf{x})$$

$(\mathbf{x}, y)$ is now generated by the joint distribution:

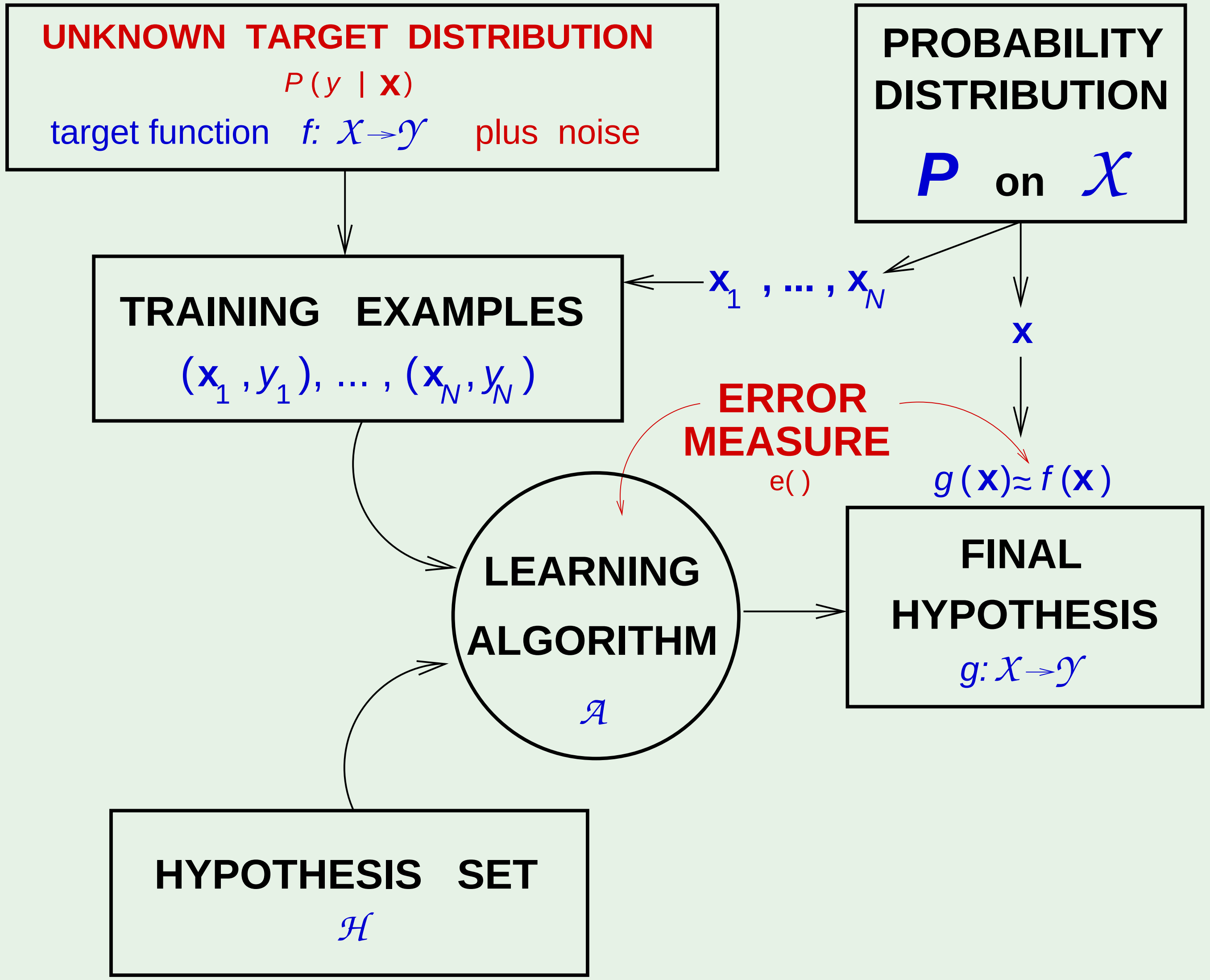
$$P(\mathbf{x})P(y \mid \mathbf{x})$$

Noisy target = deterministic target $f(\mathbf{x}) = \mathbb{E}(y|\mathbf{x})$ plus noise $y - f(\mathbf{x})$

Deterministic target is a special case of noisy target:

$$P(y \mid \mathbf{x}) \text{ is zero except for } y = f(\mathbf{x})$$

The learning diagram - including noisy target

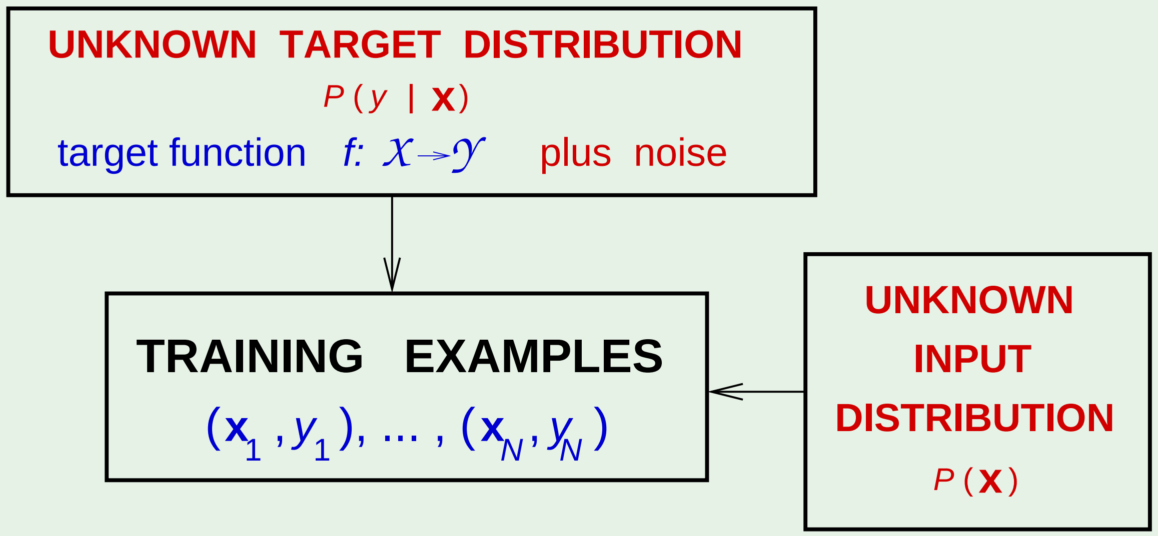


Distinction between $P(y|\mathbf{x})$ and $P(\mathbf{x})$

Both convey probabilistic aspects of $\mathbf{x}$ and y

The target distribution $P(y \mid \mathbf{x})$

is what we are trying to learn



The input distribution $P(\mathbf{x})$

quantifies relative importance of $\mathbf{x}$

Merging $P(\mathbf{x})P(y|\mathbf{x})$ as $P(\mathbf{x}, y)$

mixes the two concepts

Outline

- Nonlinear transformation (continued)
- Error measures
- Noisy targets
- Preamble to the theory

What we know so far

Learning is feasible. It is likely that

$$E_{\text{out}}(g) \approx E_{\text{in}}(g)$$

Is this learning?

We need $g \approx f$, which means

$$E_{\text{out}}(g) \approx 0$$

The 2 questions of learning

$E_{\text{out}}(g) \approx 0$ is achieved through:

$$\underbrace{E_{\text{out}}(g) \approx E_{\text{in}}(g)}_{\text{Lecture 2}} \qquad \text{and} \qquad \underbrace{E_{\text{in}}(g) \approx 0}_{\text{Lecture 3}}$$

Learning is thus split into 2 questions:

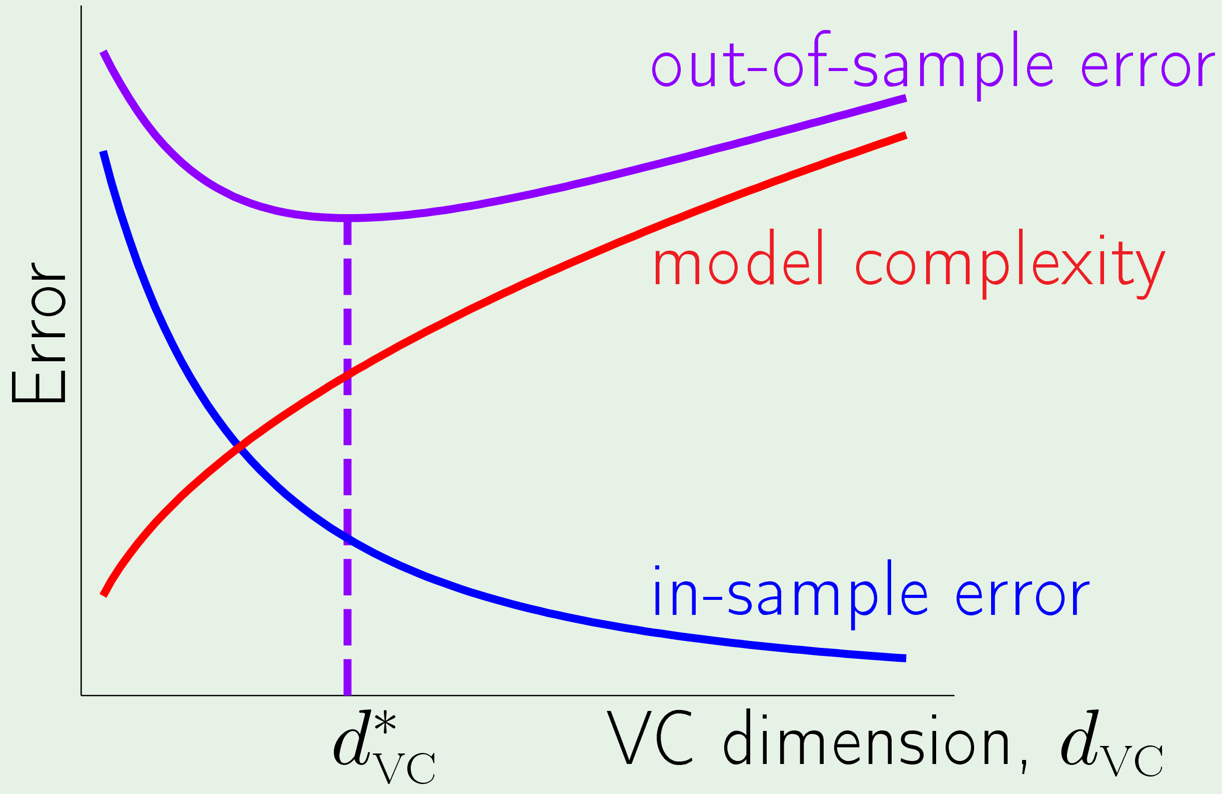
1. Can we make sure that $E_{\text{out}}(g)$ is close enough to $E_{\text{in}}(g)$?
2. Can we make $E_{\text{in}}(g)$ small enough?

What the theory will achieve

Characterizing the feasibility of learning for infinite M

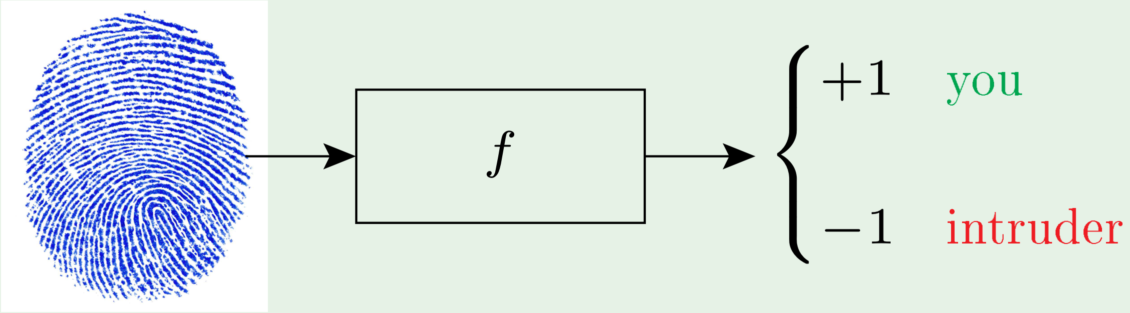
Characterizing the tradeoff:

Model complexity	$\uparrow$	E_{in}	$\downarrow$
Model complexity	$\uparrow$	$E_{\text{out}} - E_{\text{in}}$	$\uparrow$



Review of Lecture 4

- Error measures
  - User-specified $\mathrm{e}\left(h(\mathbf{x}), f(\mathbf{x})\right)$



  - In-sample:

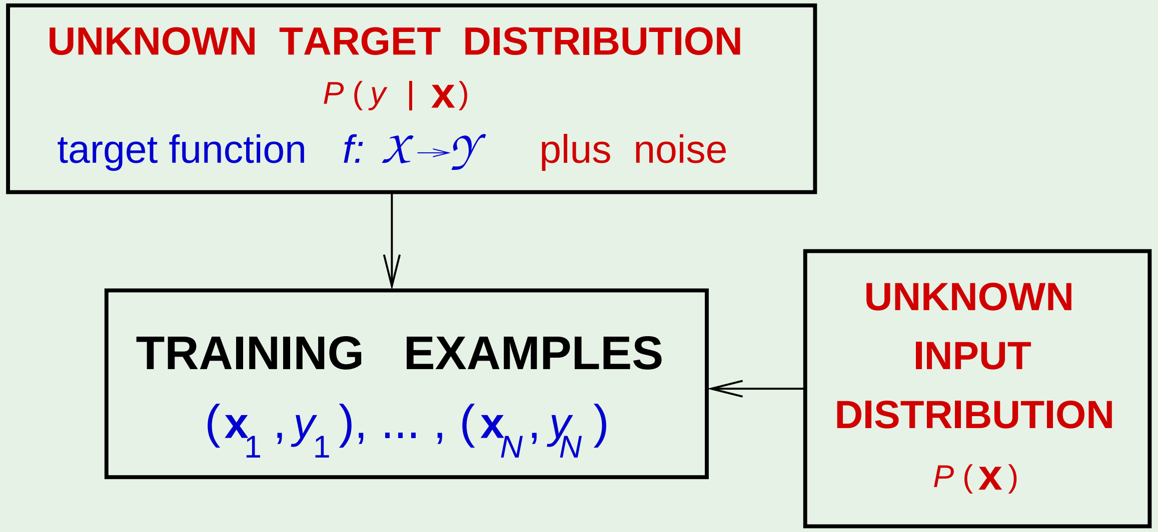
$$E_{\text{in}}(h) = \frac{1}{N}\sum_{n=1}^{N} \mathrm{e}\left(h(\mathbf{x}_n), f(\mathbf{x}_n)\right)$$

  - Out-of-sample

$$E_{\text{out}}(h) = \mathbb{E}_{\mathbf{x}}\left[\mathrm{e}\left(h(\mathbf{x}), f(\mathbf{x})\right)\right]$$

- Noisy targets

$$y = f(\mathbf{x}) \quad \longrightarrow \quad y \sim P(y \mid \mathbf{x})$$



  - $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$ generated by

$$P(\mathbf{x}, y) = P(\mathbf{x})P(y|\mathbf{x})$$

  - $E_{\text{out}}(h)$ is now $\mathbb{E}_{\mathbf{x},y}\left[\mathrm{e}\left(h(\mathbf{x}), y\right)\right]$

Learning From Data

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Lecture 5: Training versus Testing

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Tuesday, April 17, 2012

Outline

- From training to testing
- Illustrative examples
- Key notion: break point
- Puzzle

The final exam

Testing:

$$\mathbb{P}\left[\,|E_{\text{in}} - E_{\text{out}}| > \epsilon\,\right] \leq \quad 2 \;\; e^{-2\epsilon^2 N}$$

Training:

$$\mathbb{P}\left[\,|E_{\text{in}} - E_{\text{out}}| > \epsilon\,\right] \leq 2M e^{-2\epsilon^2 N}$$

Where did the M come from?

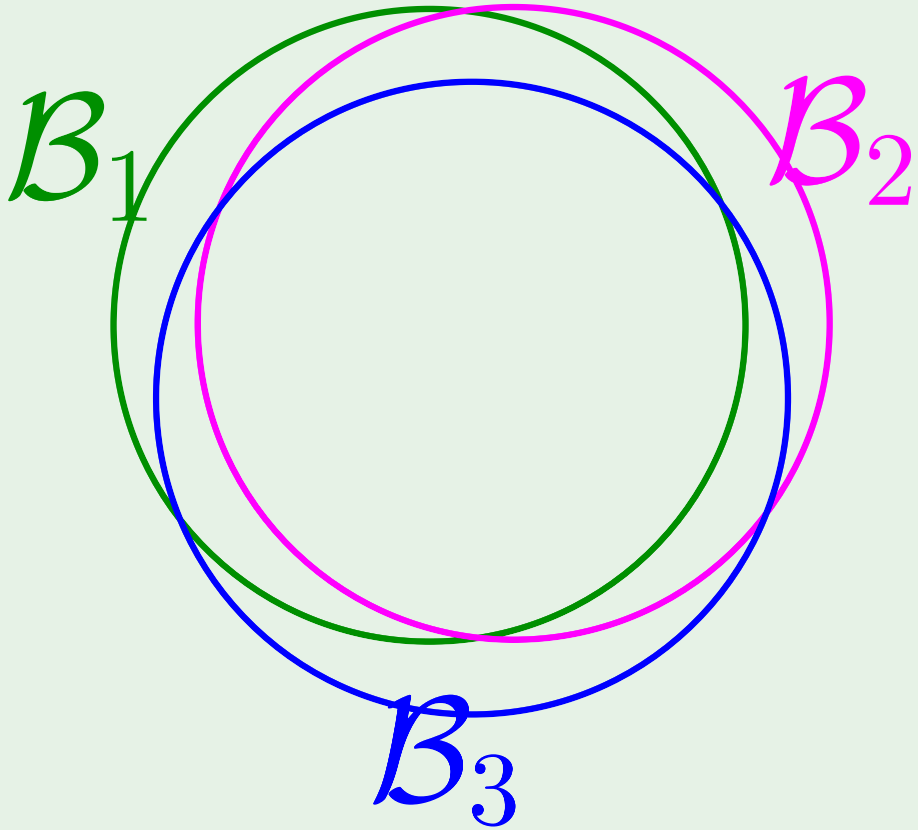
The $\mathcal{B}$ad events $\mathcal{B}_m$ are

$$\text{``}|E_{\text{in}}(h_m) - E_{\text{out}}(h_m)| > \epsilon\text{''}$$

The union bound:

$$\mathbb{P}[\mathcal{B}_1 \textbf{ or } \mathcal{B}_2 \textbf{ or } \cdots \textbf{ or } \mathcal{B}_M]$$

$$\le \underbrace{\mathbb{P}[\mathcal{B}_1] + \mathbb{P}[\mathcal{B}_2] + \cdots + \mathbb{P}[\mathcal{B}_M]}_{\text{no overlaps: } M \text{ terms}}$$



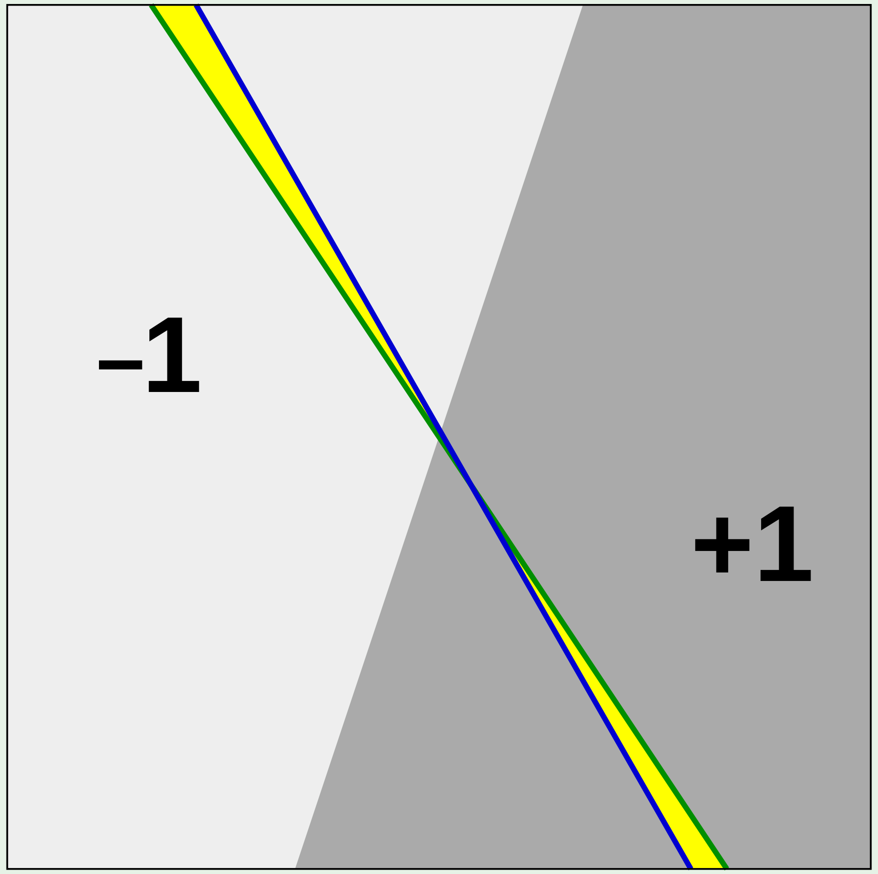
Can we improve on M?

Yes, bad events are *very* overlapping!

ΔE_{out}: change in $+1$ and -1 areas

ΔE_{in}: change in labels of data points

$$|E_{\text{in}}(h_1) - E_{\text{out}}(h_1)| \approx |E_{\text{in}}(h_2) - E_{\text{out}}(h_2)|$$

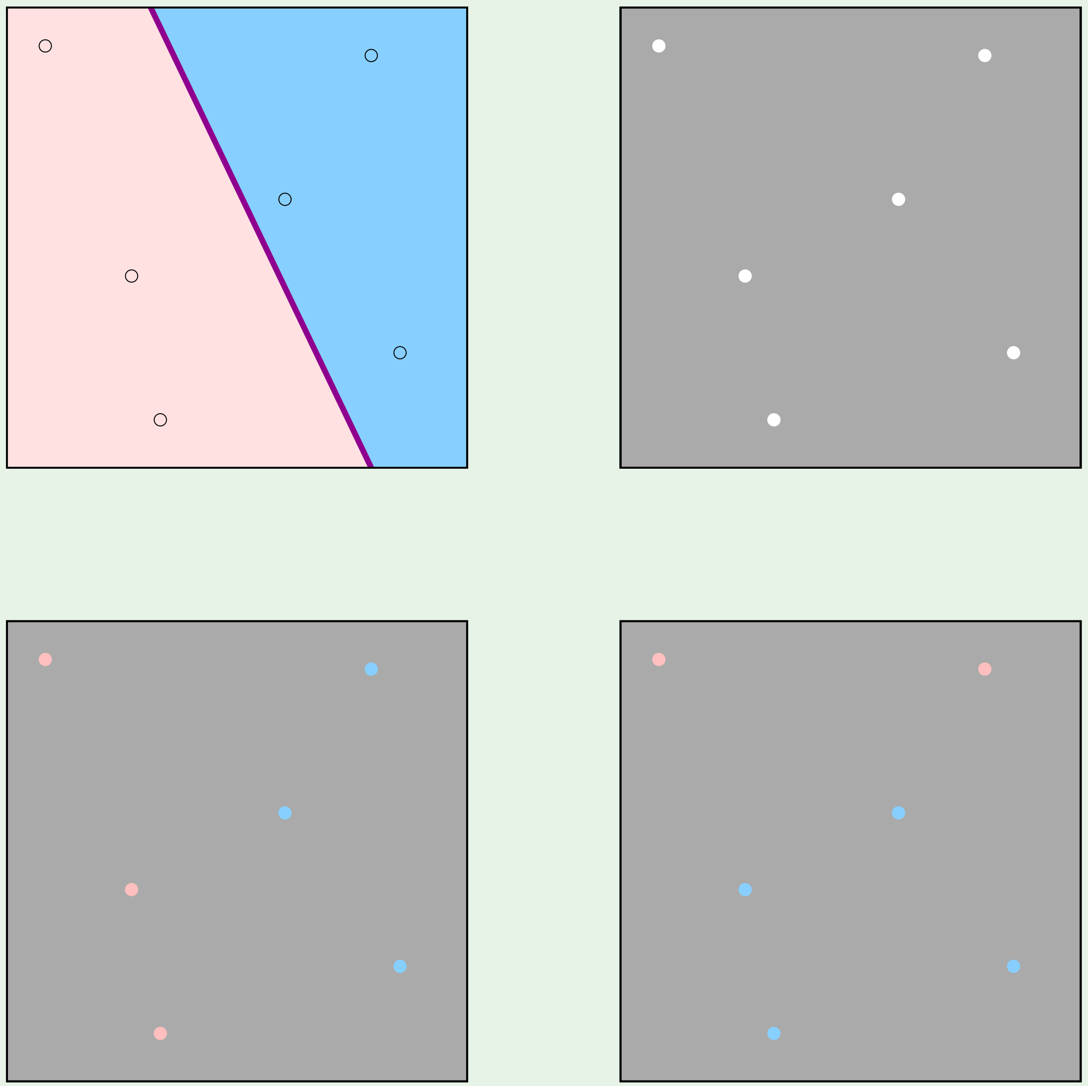


What can we replace M with?

Instead of the whole input space,

we consider a finite set of input points,

and count the number of *dichotomies*



Dichotomies: mini-hypotheses

A hypothesis $h : \mathcal{X} \rightarrow \{-1, +1\}$

A dichotomy $h : \{\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N\} \rightarrow \{-1, +1\}$

Number of hypotheses $|\mathcal{H}|$ can be infinite

Number of dichotomies $|\mathcal{H}(\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_N)|$ is at most 2^N

Candidate for replacing M

The growth function

The growth function counts the most dichotomies on any N points

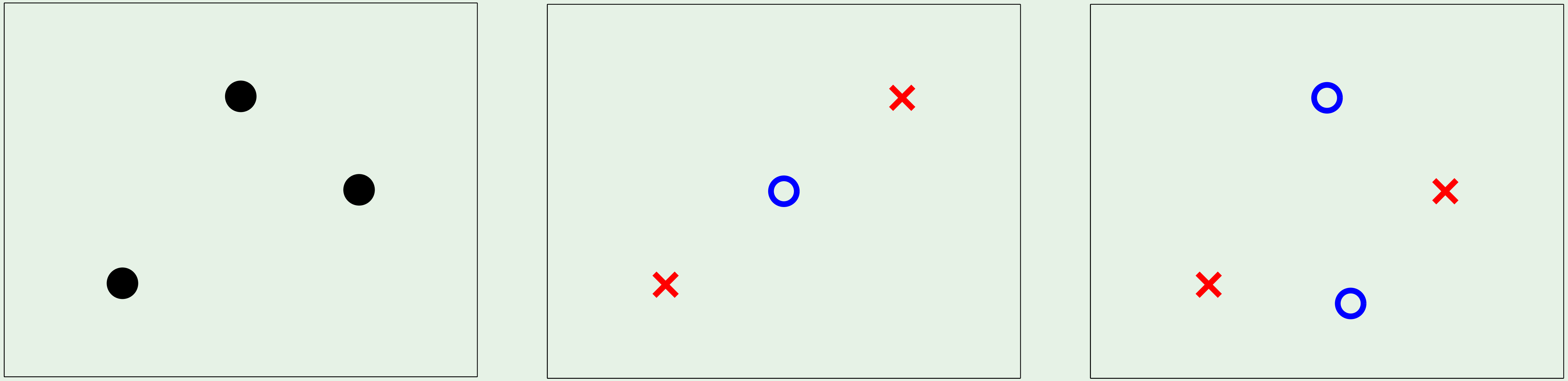
$$m_{\mathcal{H}}(N) = \max_{\mathbf{x}_1, \cdots, \mathbf{x}_N \in \mathcal{X}} |\mathcal{H}(\mathbf{x}_1, \cdots, \mathbf{x}_N)|$$

The growth function satisfies:

$$m_{\mathcal{H}}(N) \leq 2^N$$

Let's apply the definition.

Applying $m_{\mathcal{H}}(N)$ definition - perceptrons



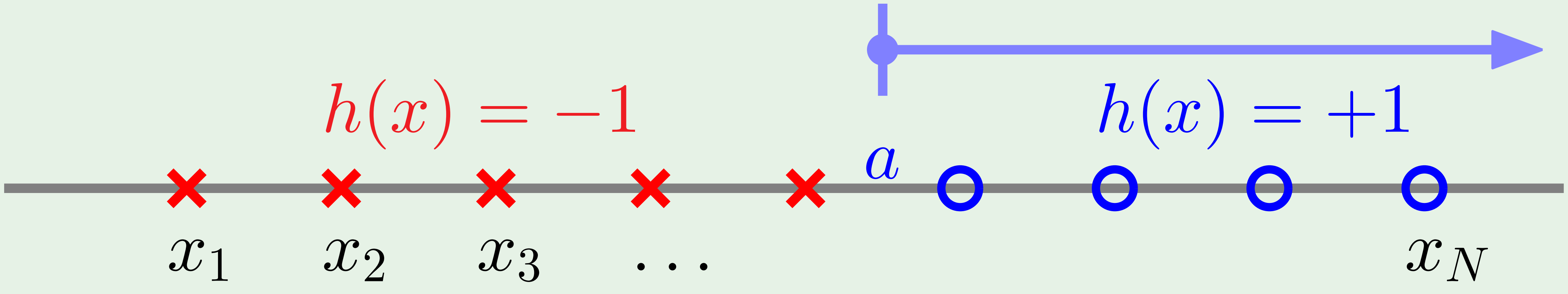
$N = 3$ $N = 3$ $N = 4$

$$m_{\mathcal{H}}(3) = 8 \qquad m_{\mathcal{H}}(4) = 14$$

Outline

- From training to testing
- Illustrative examples
- Key notion: break point
- Puzzle

Example 1: positive rays

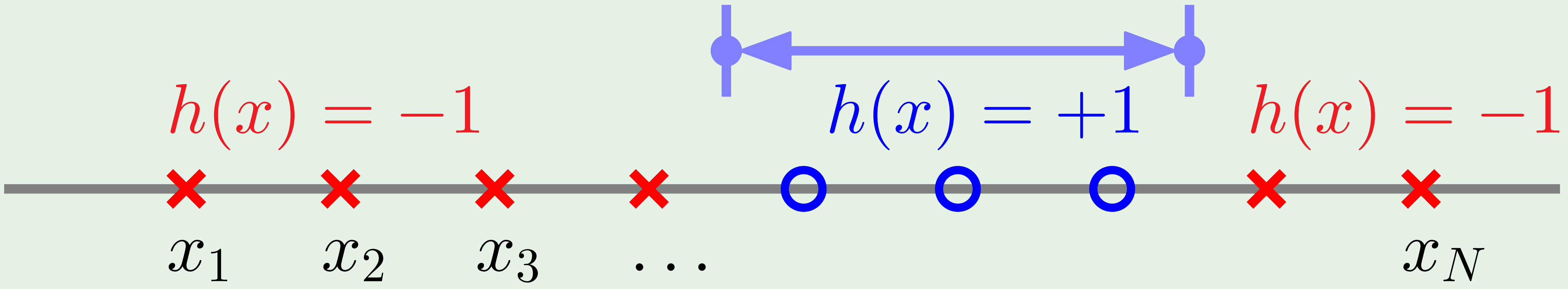


$\mathcal{H}$ is set of $h\colon \mathbb{R} \to \{-1, +1\}$

$h(x) = \text{sign}(x - a)$

$m_{\mathcal{H}}(N) = N + 1$

Example 2: positive intervals



$\mathcal{H}$ is set of $h\colon \mathbb{R} \to \{-1, +1\}$

Place interval ends in two of $N+1$ spots

$m_{\mathcal{H}}(N) = \binom{N+1}{2} + 1 = \frac{1}{2}N^2 + \frac{1}{2}N + 1$

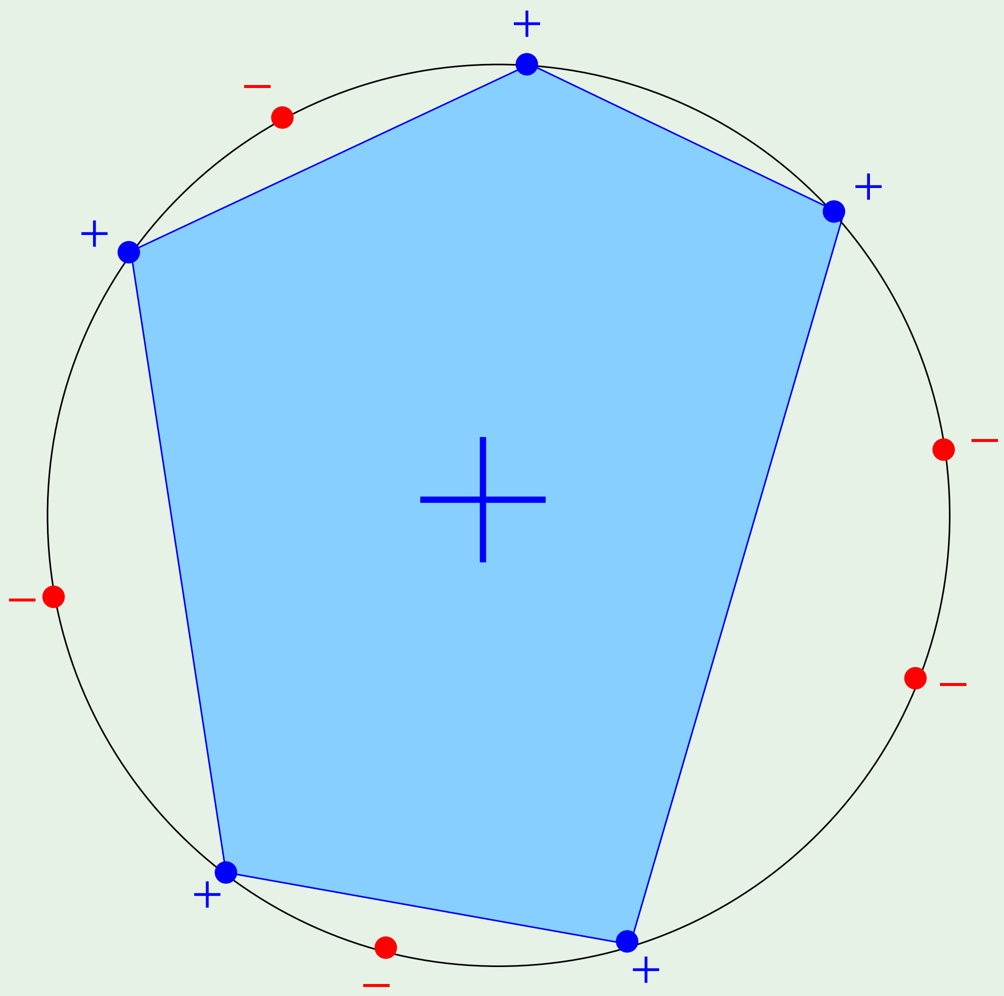
Example 3: convex sets

$\mathcal{H}$ is set of $h\colon \mathbb{R}^2 \to \{-1,+1\}$

$h(\mathbf{x}) = +1$ is convex

$m_{\mathcal{H}}(N) = 2^N$

The N points are 'shattered' by convex sets



The 3 growth functions

- $\mathcal{H}$ is positive rays:

$$m_{\mathcal{H}}(N) = N + 1$$

- $\mathcal{H}$ is positive intervals:

$$m_{\mathcal{H}}(N) = \tfrac{1}{2}N^2 + \tfrac{1}{2}N + 1$$

- $\mathcal{H}$ is convex sets:

$$m_{\mathcal{H}}(N) = 2^N$$

Back to the big picture

Remember this inequality?

$$\mathbb{P}\left[\,|E_{\text{in}} - E_{\text{out}}| > \epsilon\,\right] \leq 2M e^{-2\epsilon^2 N}$$

What happens if $m_{\mathcal{H}}(N)$ replaces M?

$m_{\mathcal{H}}(N)$ polynomial $\implies$ Good!

Just prove that $m_{\mathcal{H}}(N)$ is polynomial?

Outline

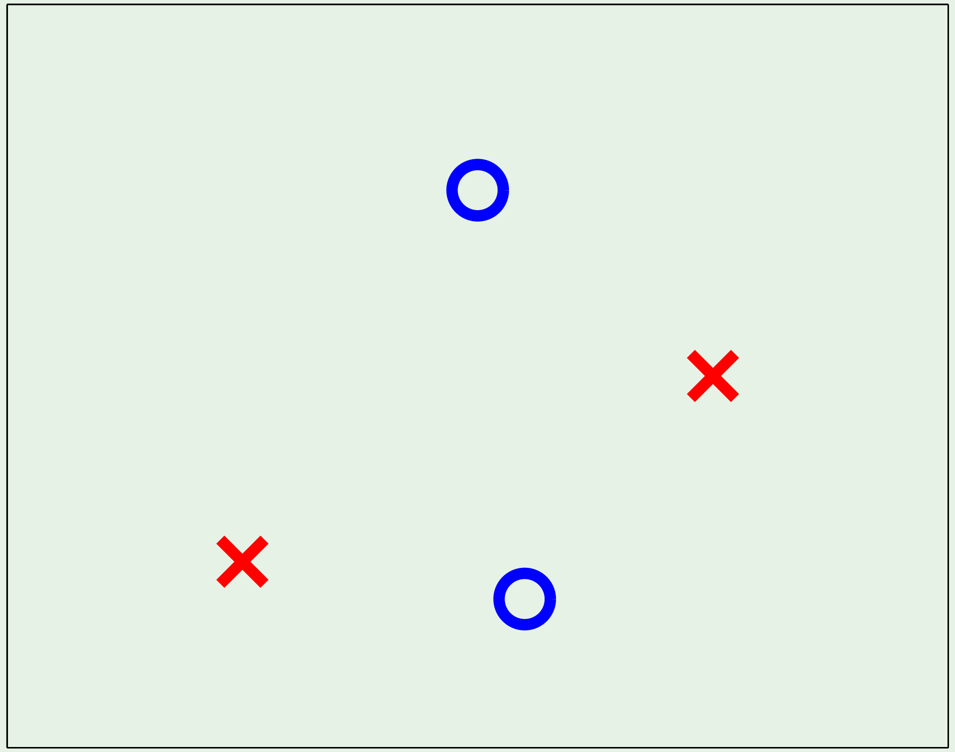
- From training to testing
- Illustrative examples
- Key notion: **break point**
- Puzzle

Break point of $\mathcal{H}$

Definition:

If no data set of size k can be shattered by $\mathcal{H}$, then k is a *break point* for $\mathcal{H}$

$$m_{\mathcal{H}}(k) \; < \; 2^k$$

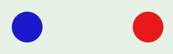


For 2D perceptrons, $k = 4$

A bigger data set cannot be shattered either

Break point - the 3 examples

- Positive rays $m_{\mathcal{H}}(N) = N + 1$

  break point $k =$ 2 

- Positive intervals $m_{\mathcal{H}}(N) = \frac{1}{2}N^2 + \frac{1}{2}N + 1$

  break point $k =$ 3 

- Convex sets $m_{\mathcal{H}}(N) = 2^N$

  break point $k =$'∞'

Main result

No break point $\Longrightarrow$ $m_{\mathcal{H}}(N) = 2^N$

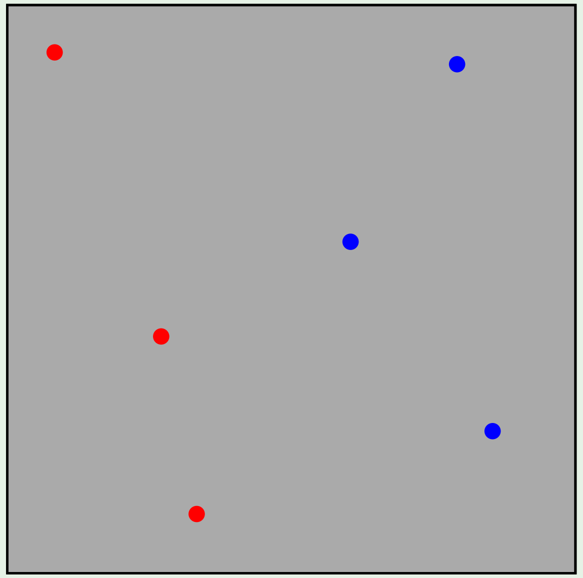
Any break point $\Longrightarrow$ $m_{\mathcal{H}}(N)$ is **polynomial** in N

Puzzle

$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
○	○	○
○	○	●
○	●	○
●	○	○

Review of Lecture 5

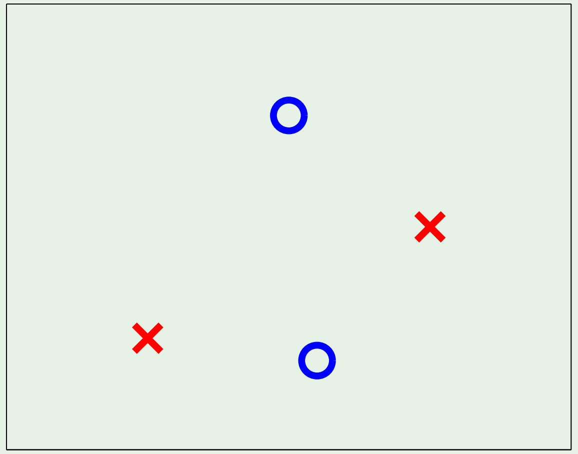
- Dichotomies



- Growth function

$$m_{\mathcal{H}}(N) = \max_{\mathbf{x}_1, \cdots, \mathbf{x}_N \in \mathcal{X}} |\mathcal{H}(\mathbf{x}_1, \cdots, \mathbf{x}_N)|$$

- Break point



- Maximum # of dichotomies

$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
○	○	○
○	○	●
○	●	○
●	○	○

Learning From Data

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Lecture 6: Theory of Generalization

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Thursday, April 19, 2012

Outline

- Proof that $m_{\mathcal{H}}(N)$ is polynomial

- Proof that $m_{\mathcal{H}}(N)$ can replace M

Bounding $m_{\mathcal{H}}(N)$

To show: $m_{\mathcal{H}}(N)$ is polynomial

We show: $m_{\mathcal{H}}(N) \leq \cdots \leq \cdots \leq$ a polynomial

Key quantity:

$B(N, k)$: Maximum number of dichotomies on N points, with break point k

Recursive bound on $B(N, k)$

Consider the following table:

$$B(N,k) = \alpha + 2\beta$$

		# of rows	$\mathbf{x}_1$	$\mathbf{x}_2$	$\dots$	$\mathbf{x}_{N-1}$	$\mathbf{x}_N$
	S_1	α	$+1$	$+1$	$\dots$	$+1$	$+1$
			-1	$+1$	$\dots$	$+1$	-1
			$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\dots$	-1	-1
			-1	$+1$	$\dots$	-1	$+1$
S_2	S_2^+	β	$+1$	-1	$\dots$	$+1$	$+1$
			-1	-1	$\dots$	$+1$	$+1$
			$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\dots$	$+1$	$+1$
			-1	-1	$\dots$	-1	$+1$
	S_2^-	β	$+1$	-1	$\dots$	$+1$	-1
			-1	-1	$\dots$	$+1$	-1
			$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\dots$	$+1$	-1
			-1	-1	$\dots$	-1	-1

Estimating α and β

Focus on $\mathbf{x}_1, \mathbf{x}_2, \cdots, \mathbf{x}_{N-1}$ columns:

$$\alpha + \beta \le B(N-1, k)$$

		# of rows	$\mathbf{x}_1$	$\mathbf{x}_2$	$\ldots$	$\mathbf{x}_{N-1}$	$\mathbf{x}_N$
			$+1$	$+1$	$\ldots$	$+1$	$+1$
			-1	$+1$	$\ldots$	$+1$	-1
	S_1	α	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\ldots$	-1	-1
			-1	$+1$	$\ldots$	-1	$+1$
			$+1$	-1	$\ldots$	$+1$	$+1$
			-1	-1	$\ldots$	$+1$	$+1$
	S_2^+	β	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\ldots$	$+1$	$+1$
S_2			-1	-1	$\ldots$	-1	$+1$
			$+1$	-1	$\ldots$	$+1$	-1
			-1	-1	$\ldots$	$+1$	-1
	S_2^-	β	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\ldots$	$+1$	-1
			-1	-1	$\ldots$	-1	-1

Estimating β by itself

Now, focus on the $S_2 = S_2^+ \cup S_2^-$ rows:

$$\beta \;\leq\; B(N-1, k-1)$$

		# of rows	$\mathbf{x}_1$	$\mathbf{x}_2$	$\dots$	$\mathbf{x}_{N-1}$	$\mathbf{x}_N$
			$+1$	$+1$	$\dots$	$+1$	$+1$
			-1	$+1$	$\dots$	$+1$	-1
	S_1	α	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\dots$	-1	-1
			-1	$+1$	$\dots$	-1	$+1$
			$+1$	-1	$\dots$	$+1$	$+1$
			-1	-1	$\dots$	$+1$	$+1$
	S_2^+	β	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\dots$	$+1$	$+1$
S_2			-1	-1	$\dots$	-1	$+1$
			$+1$	-1	$\dots$	$+1$	-1
			-1	-1	$\dots$	$+1$	-1
	S_2^-	β	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\dots$	$+1$	-1
			-1	-1	$\dots$	-1	-1

Putting it together

$$B(N,k) = \alpha + 2\beta$$

$$\alpha + \beta \le B(N-1,k)$$

$$\beta \le B(N-1,k-1)$$

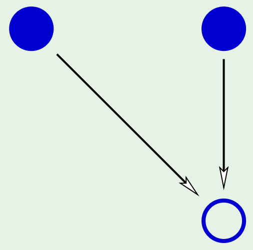
$$B(N,k) \le$$

$$B(N-1,k) + B(N-1,k-1)$$

		# of rows	$\mathbf{x}_1$	$\mathbf{x}_2$	$\dots$	$\mathbf{x}_{N-1}$	$\mathbf{x}_N$
S_1		α	$+1$	$+1$	$\dots$	$+1$	$+1$
			-1	$+1$	$\dots$	$+1$	-1
			$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\dots$	-1	-1
			-1	$+1$	$\dots$	-1	$+1$
S_2	S_2^+	β	$+1$	-1	$\dots$	$+1$	$+1$
			-1	-1	$\dots$	$+1$	$+1$
			$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\dots$	$+1$	$+1$
			-1	-1	$\dots$	-1	$+1$
	S_2^-	β	$+1$	-1	$\dots$	$+1$	-1
			-1	-1	$\dots$	$+1$	-1
			$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
			$+1$	-1	$\dots$	$+1$	-1
			-1	-1	$\dots$	-1	-1

Numerical computation of $B(N, k)$ bound

$$B(N, k) \leq B(N-1, k) + B(N-1, k-1)$$



		k						
		1	2	3	4	5	6	..
	1	1	2	2	2	2	2	..
	2	1	3	4	4	4	4	..
	3	1	4	7	8	8	8	..
N	4	1	5	11	..	..	..	..
	5	1	6	:	.			
	6	1	7	:		.		
	:	:	:	:			.	

Analytic solution for $B(N,k)$ bound

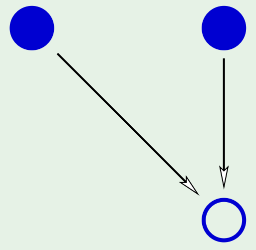
$$B(N,k) \leq B(N-1,k) + B(N-1,k-1)$$

Theorem:

$$B(N,k) \leq \sum_{i=0}^{k-1} \binom{N}{i}$$

1. Boundary conditions: easy

N \ k	1	2	3	4	5	6	..
1	1	2	2	2	2	2	..
2	1						
3	1						
4	1						
5	1						
6	1						
⋮	⋮						



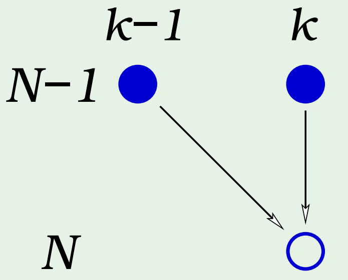
2. The induction step

$$\sum_{i=0}^{k-1}\binom{N}{i} = \sum_{i=0}^{k-1}\binom{N-1}{i} + \sum_{i=0}^{k-2}\binom{N-1}{i} \; ?$$

$$= 1 + \sum_{i=1}^{k-1}\binom{N-1}{i} + \sum_{i=1}^{k-1}\binom{N-1}{i-1}$$

$$= 1 + \sum_{i=1}^{k-1}\left[\binom{N-1}{i} + \binom{N-1}{i-1}\right]$$

$$= 1 + \sum_{i=1}^{k-1}\binom{N}{i} = \sum_{i=0}^{k-1}\binom{N}{i} \; \checkmark$$



It is polynomial!

For a given $\mathcal{H}$, the break point k is fixed

$$m_{\mathcal{H}}(N) \quad \leq \quad \underbrace{\sum_{i=0}^{k-1} \binom{N}{i}}_{\text{maximum power is } N^{k-1}}$$

Three examples

$$\sum_{i=0}^{k-1} \binom{N}{i}$$

- $\mathcal{H}$ is **positive rays**: (break point $k = 2$)

$$m_{\mathcal{H}}(N) = N + 1 \leq N + 1$$

- $\mathcal{H}$ is **positive intervals**: (break point $k = 3$)

$$m_{\mathcal{H}}(N) = \tfrac{1}{2}N^2 + \tfrac{1}{2}N + 1 \leq \tfrac{1}{2}N^2 + \tfrac{1}{2}N + 1$$

- $\mathcal{H}$ is **2D perceptrons**: (break point $k = 4$)

$$m_{\mathcal{H}}(N) = \ ? \ \leq \tfrac{1}{6}N^3 + \tfrac{5}{6}N + 1$$

Outline

- Proof that $m_{\mathcal{H}}(N)$ is polynomial

- Proof that $m_{\mathcal{H}}(N)$ can replace M

What we want

Instead of:

$$\mathbb{P}[\ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\ ] \ \leq\ 2 \quad M \quad e^{-2\epsilon^2 N}$$

We want:

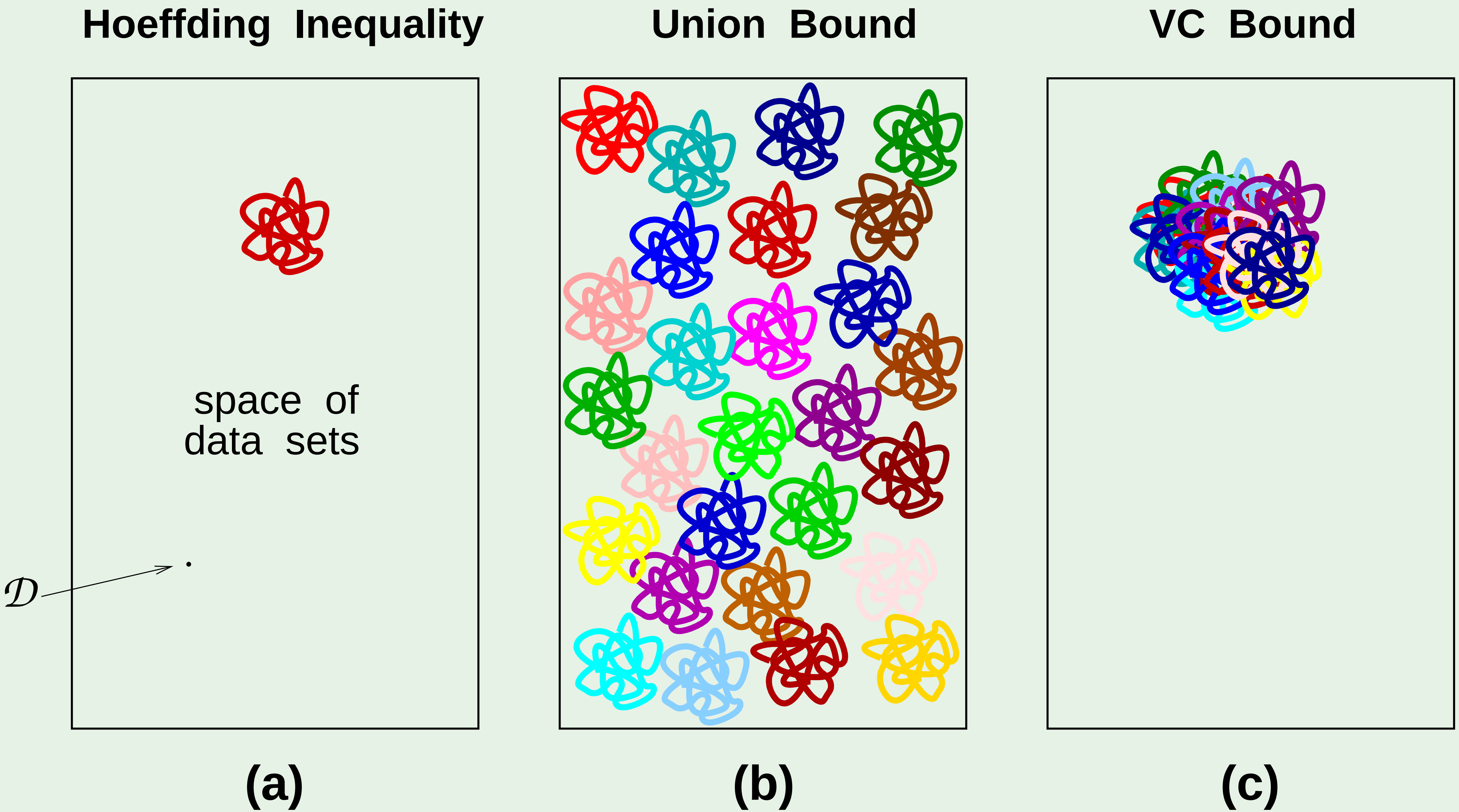
$$\mathbb{P}[\ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\ ] \ \leq\ 2\ \ m_{\mathcal{H}}(N)\ \ e^{-2\epsilon^2 N}$$

Pictorial proof ☺

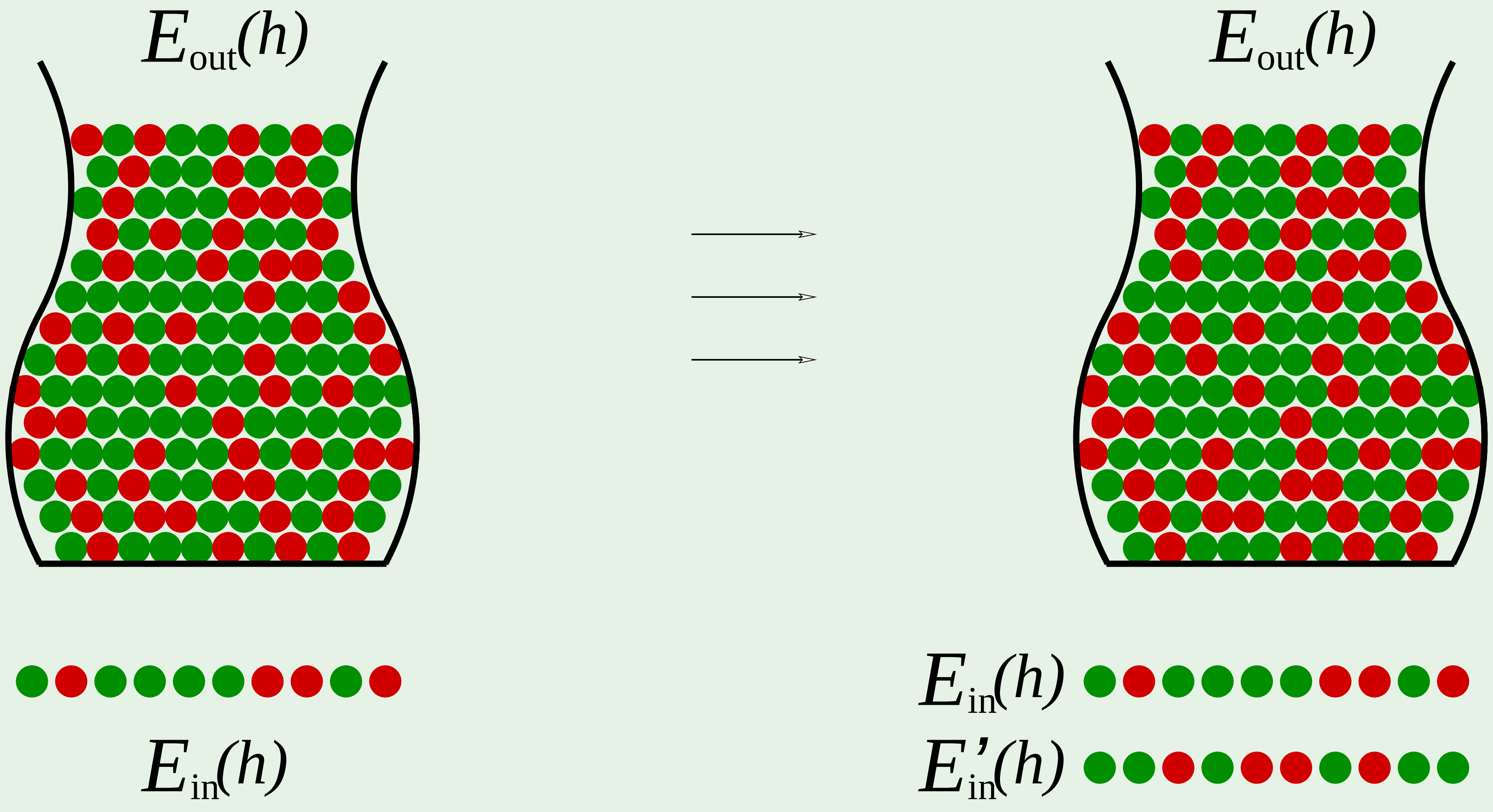
- How does $m_{\mathcal{H}}(N)$ relate to overlaps?

- What to do about E_{out}?

- Putting it together


Hoeffding Inequality
Union Bound
VC Bound
space of
data sets
$\mathcal{D}$
(a)
(b)
(c)

What to do about E_{out}



Putting it together

Not quite:

$$\mathbb{P}[\ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\ ] \ \leq\ 2\ \ m_{\mathcal{H}}(\ N\ )\ \ e^{-\,2\,\epsilon^2 N}$$

but rather:

$$\mathbb{P}[\ |E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\ ] \ \leq\ 4\ \ m_{\mathcal{H}}(2N)\ \ e^{-\,\frac{1}{8}\,\epsilon^2 N}$$

The Vapnik-Chervonenkis Inequality

Review of Lecture 6

- $m_{\mathcal{H}}(N)$ is polynomial

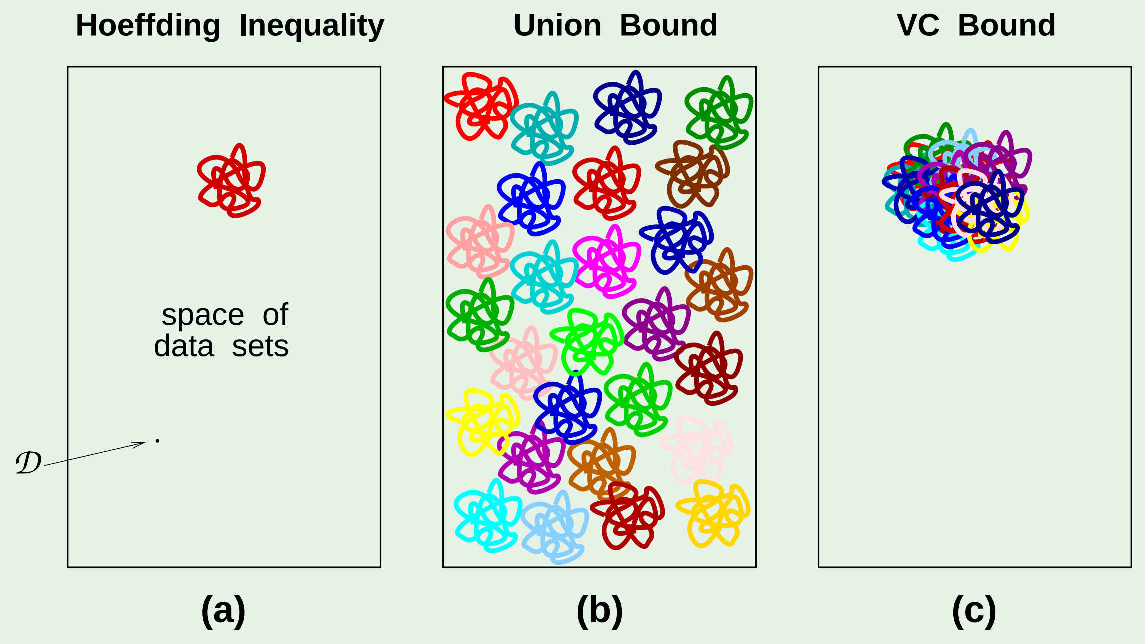
if $\mathcal{H}$ has a break point k

N \ k	1	2	3	4	5	6	..
1	1	2	2	2	2	2	..
2	1						
3	1						
4	1						
5	1						
6	1						
:	:						

$$m_{\mathcal{H}}(N) \leq \underbrace{\sum_{i=0}^{k-1} \binom{N}{i}}$$

maximum power is N^{k-1}

- The VC Inequality



$$\mathbb{P}\left[\,|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\,\right] \leq 2 \quad M \quad e^{-2\epsilon^2 N}$$

$$\downarrow \quad \downarrow \quad \downarrow$$

$$\mathbb{P}\left[\,|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\,\right] \leq 4 \quad \boxed{m_{\mathcal{H}}(2N)} \quad e^{-\frac{1}{8}\epsilon^2 N}$$

Learning From Data

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Lecture 7: The VC Dimension

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Tuesday, April 24, 2012

Outline

- The definition
- VC dimension of perceptrons
- Interpreting the VC dimension
- Generalization bounds

Definition of VC dimension

The VC dimension of a hypothesis set $\mathcal{H}$, denoted by $d_{\mathrm{VC}}(\mathcal{H})$, is

the largest value of N for which $m_{\mathcal{H}}(N) = 2^N$

"the most points $\mathcal{H}$ can shatter"

$N \leq d_{\mathrm{VC}}(\mathcal{H}) \implies \mathcal{H}$ can shatter N points

$k > d_{\mathrm{VC}}(\mathcal{H}) \implies k$ is a break point for $\mathcal{H}$

The growth function

In terms of a break point k:

$$m_{\mathcal{H}}(N) \le \sum_{i=0}^{k-1} \binom{N}{i}$$

In terms of the VC dimension d_{VC}:

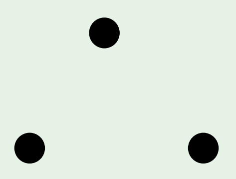
$$m_{\mathcal{H}}(N) \le \underbrace{\sum_{i=0}^{d_{\mathrm{VC}}} \binom{N}{i}}_{\text{maximum power is } N^{d_{\mathrm{VC}}}}$$

Examples

- $\mathcal{H}$ is positive rays:

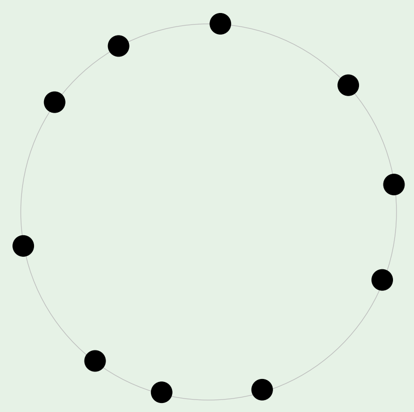
$$d_{\text{VC}} = 1$$

- $\mathcal{H}$ is 2D perceptrons:



$$d_{\text{VC}} = 3$$

- $\mathcal{H}$ is convex sets:



$$d_{\text{VC}} = \infty$$

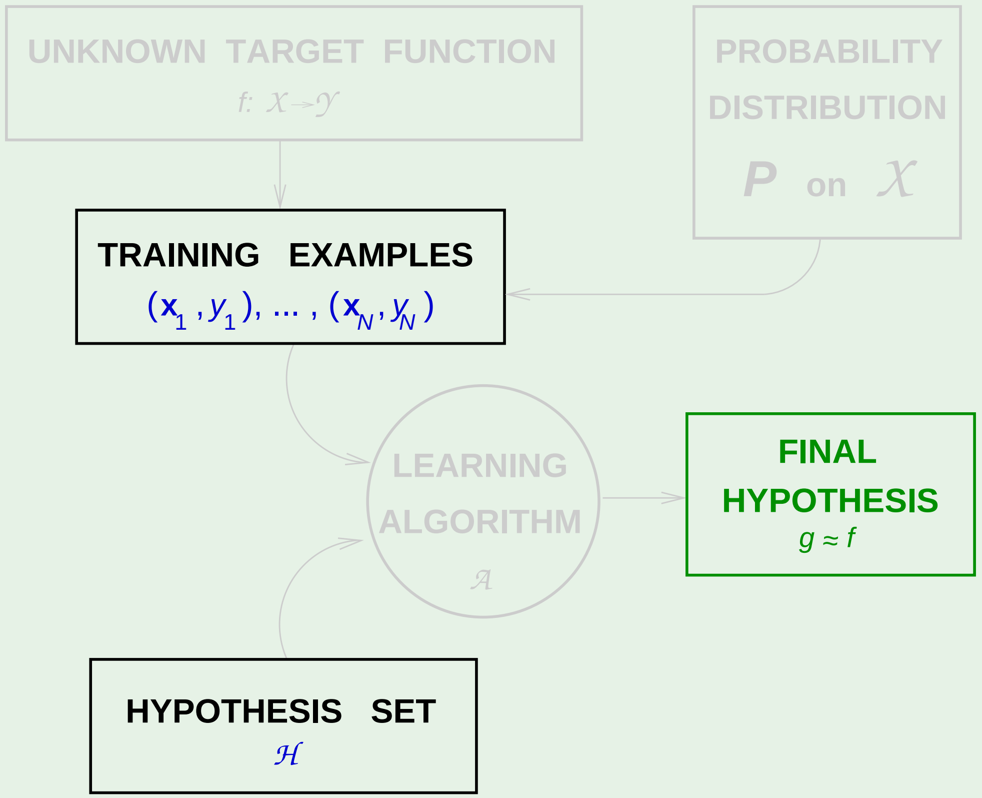
VC dimension and learning

$d_{\text{VC}}(\mathcal{H})$ is finite $\Longrightarrow$ $g \in \mathcal{H}$ will generalize

- Independent of the learning algorithm

- Independent of the input distribution

- Independent of the target function



VC dimension of perceptrons

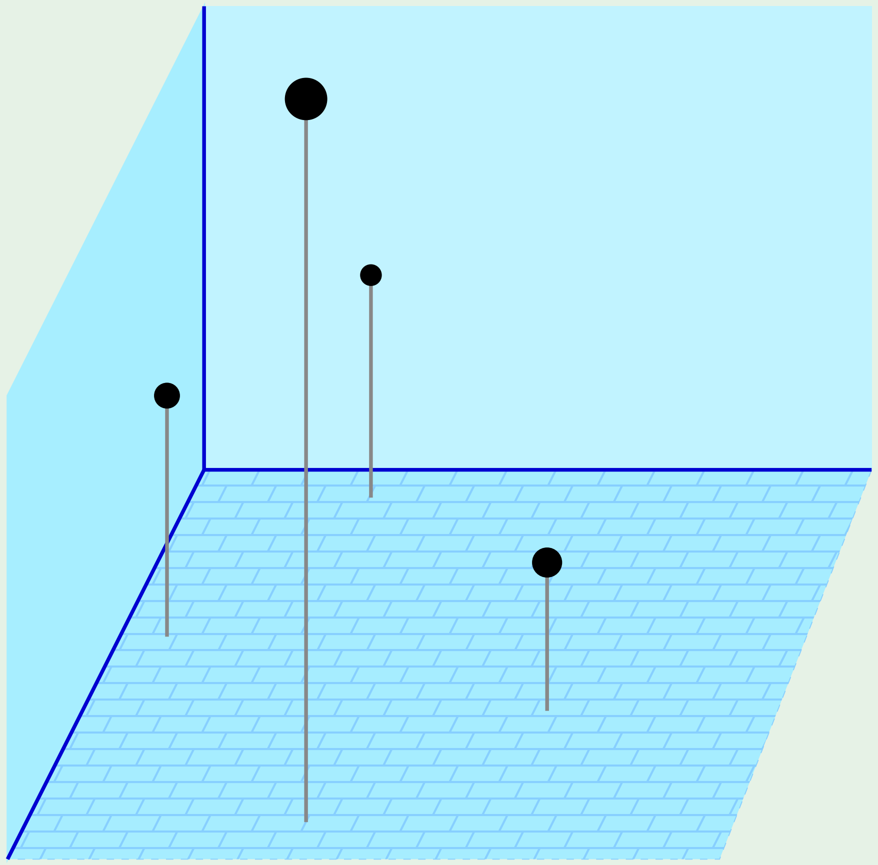
For $d = 2$, $d_{\text{VC}} = 3$

In general, $\boxed{d_{\text{VC}} = d + 1}$

We will prove two directions:

$$d_{\text{VC}} \leq d + 1$$

$$d_{\text{VC}} \geq d + 1$$



Here is one direction

A set of $N = d + 1$ points in $\mathbb{R}^d$ shattered by the perceptron:

$$\mathrm{X} = \begin{bmatrix} \text{—}\ \mathbf{x}_1^{\intercal}\ \text{—} \\ \text{—}\ \mathbf{x}_2^{\intercal}\ \text{—} \\ \text{—}\ \mathbf{x}_3^{\intercal}\ \text{—} \\ \vdots \\ \text{—}\ \mathbf{x}_{d+1}^{\intercal}\ \text{—} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 1 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & & 0 \\ & \vdots & & \ddots & 0 \\ 1 & 0 & \dots & 0 & 1 \end{bmatrix}$$

X is invertible

Can we shatter this data set?

For any $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_{d+1} \end{bmatrix} = \begin{bmatrix} \pm 1 \\ \pm 1 \\ \vdots \\ \pm 1 \end{bmatrix}$, can we find a vector $\mathbf{w}$ satisfying

$$\text{sign}(\mathrm{X}\mathbf{w}) = \mathbf{y}$$

Easy! Just make $\mathrm{X}\mathbf{w} = \mathbf{y}$

which means $\mathbf{w} = \mathrm{X}^{-1}\mathbf{y}$

We can shatter these $d+1$ points

This implies what?

[a] $d_{\mathrm{VC}} = d+1$

[b] $d_{\mathrm{VC}} \geq d+1$ ✓

[c] $d_{\mathrm{VC}} \leq d+1$

[d] No conclusion

Now, to show that $d_{\text{vc}} \leq d + 1$

We need to show that:

[a] There are $d + 1$ points we cannot shatter

[b] There are $d + 2$ points we cannot shatter

[c] We cannot shatter *any* set of $d + 1$ points

[d] We cannot shatter *any* set of $d + 2$ points ✓

Take any $d + 2$ points

For any $d + 2$ points,

$$\mathbf{x}_1, \cdots, \mathbf{x}_{d+1}, \mathbf{x}_{d+2}$$

More points than dimensions $\implies$ we must have

$$\mathbf{x}_j = \sum_{i \neq j} a_i \, \mathbf{x}_i$$

where not all the a_i's are zeros

So?

$$\mathbf{x}_j = \sum_{i \neq j} a_i \, \mathbf{x}_i$$

Consider the following dichotomy:

$\mathbf{x}_i$'s with non-zero a_i get $\quad y_i = \operatorname{sign}(a_i)$

and $\mathbf{x}_j$ gets $\quad y_j = -1$

No perceptron can implement such dichotomy!

Why?

$$\mathbf{x}_j = \sum_{i \neq j} a_i \, \mathbf{x}_i \implies \mathbf{w}^\intercal \mathbf{x}_j = \sum_{i \neq j} a_i \, \mathbf{w}^\intercal \mathbf{x}_i$$

If $y_i = \text{sign}(\mathbf{w}^\intercal \mathbf{x}_i) = \text{sign}(a_i)$, then $a_i \, \mathbf{w}^\intercal \mathbf{x}_i > 0$

This forces

$$\mathbf{w}^\intercal \mathbf{x}_j = \sum_{i \neq j} a_i \, \mathbf{w}^\intercal \mathbf{x}_i > 0$$

Therefore, $y_j = \text{sign}(\mathbf{w}^\intercal \mathbf{x}_j) = +1$

Putting it together

We proved $d_{\mathrm{VC}} \leq d+1$ and $d_{\mathrm{VC}} \geq d+1$

$$\boxed{d_{\mathrm{VC}} = d+1}$$

What is $d+1$ in the perceptron?

It is the number of parameters $w_0, w_1, \cdots, w_d$

Outline

- The definition
- VC dimension of perceptrons
- Interpreting the VC dimension
- Generalization bounds

1. Degrees of freedom

Parameters create degrees of freedom

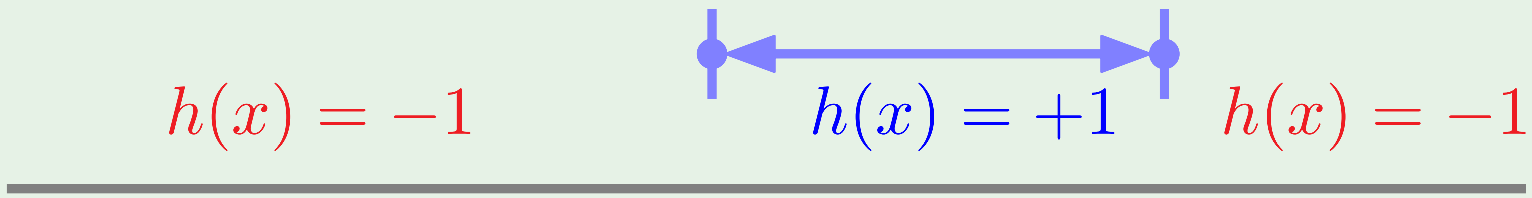
# of parameters: **analog** degrees of freedom

d_{VC}: equivalent **'binary'** degrees of freedom

The usual suspects

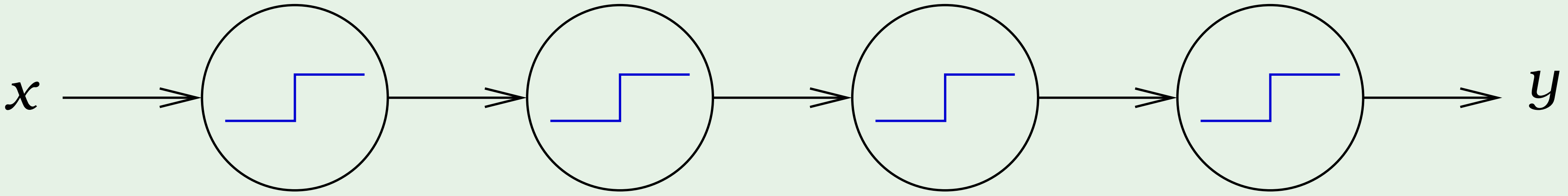
Positive rays ($d_{\text{VC}} = 1$):

Positive intervals ($d_{\text{VC}} = 2$):



Not just parameters

Parameters may not contribute degrees of freedom:



d_{VC} measures the **effective** number of parameters

2. Number of data points needed

Two small quantities in the VC inequality:

$$\mathbb{P}\left[|E_{\text{in}}(g) - E_{\text{out}}(g)| > \epsilon\right] \le \underbrace{4m_{\mathcal{H}}(2N)e^{-\frac{1}{8}\epsilon^2 N}}_{\delta}$$

If we want certain ϵ and δ, how does N depend on d_{VC}?

Let us look at $$N^{d}e^{-N}$$

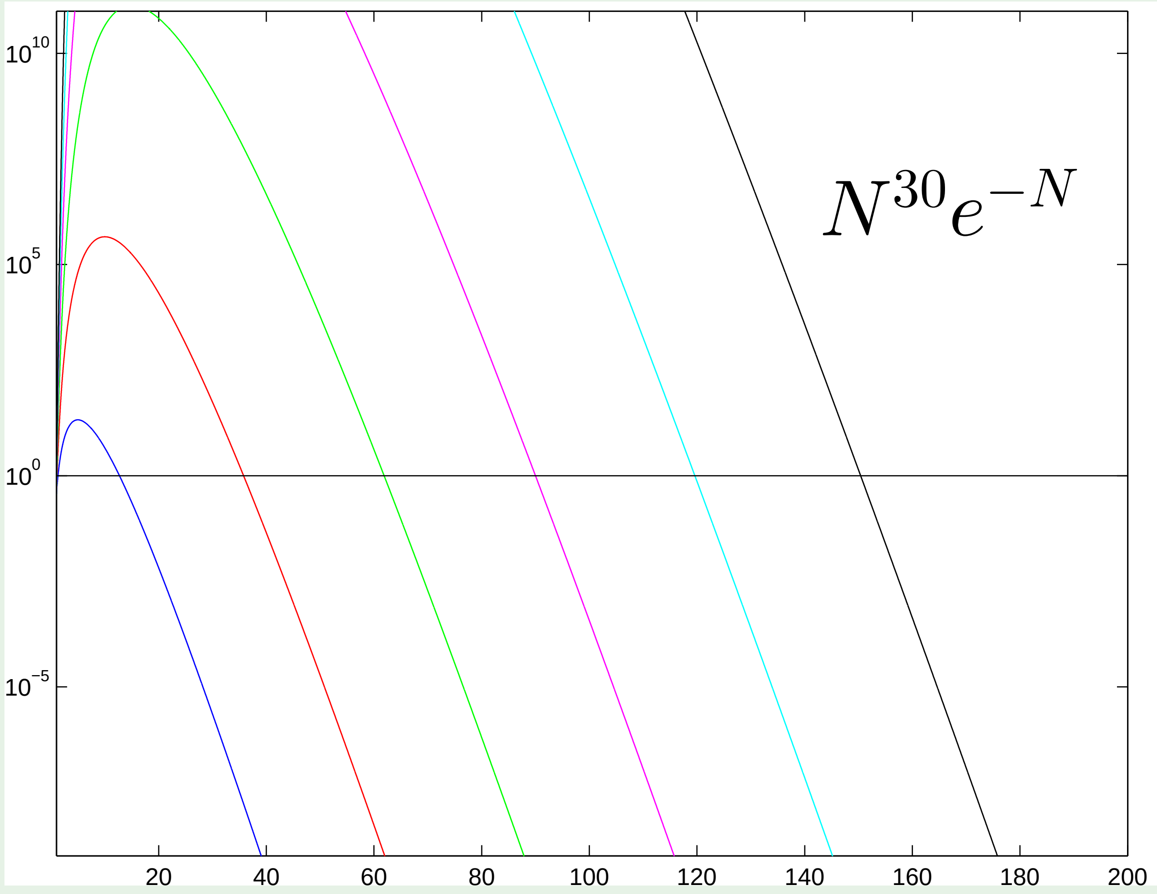
$N^{d} e^{-N}$

Fix $N^{d} e^{-N}$ = small value

How does N change with d?

Rule of thumb:

$$N \ \geq \ 10 \ d_{\mathrm{VC}}$$



Outline

- The definition
- VC dimension of perceptrons
- Interpreting the VC dimension
- Generalization bounds

Rearranging things

Start from the VC inequality:

$$\mathbb{P}[|E_{\text{out}} - E_{\text{in}})| > \epsilon] \;\leq\; \underbrace{4m_{\mathcal{H}}(2N)e^{-\frac{1}{8}\ {}^{2}N}}_{\delta}$$

Get ϵ in terms of δ:

$$\delta = 4m_{\mathcal{H}}(2N)e^{-\frac{1}{8}\epsilon^2 N} \implies \epsilon = \underbrace{\sqrt{\frac{8}{N}\ln\frac{4m_{\mathcal{H}}(2N)}{\delta}}}_{\Omega}$$

With probability $\geq 1 - \delta$, $\quad |E_{\text{out}} - E_{\text{in}}| \leq \Omega(N, \mathcal{H}, \delta)$

Generalization bound

With probability $\geq 1 - \delta$, $\quad E_{\text{out}} - E_{\text{in}} \leq \Omega$

$$\Longrightarrow$$

With probability $\geq 1 - \delta$,

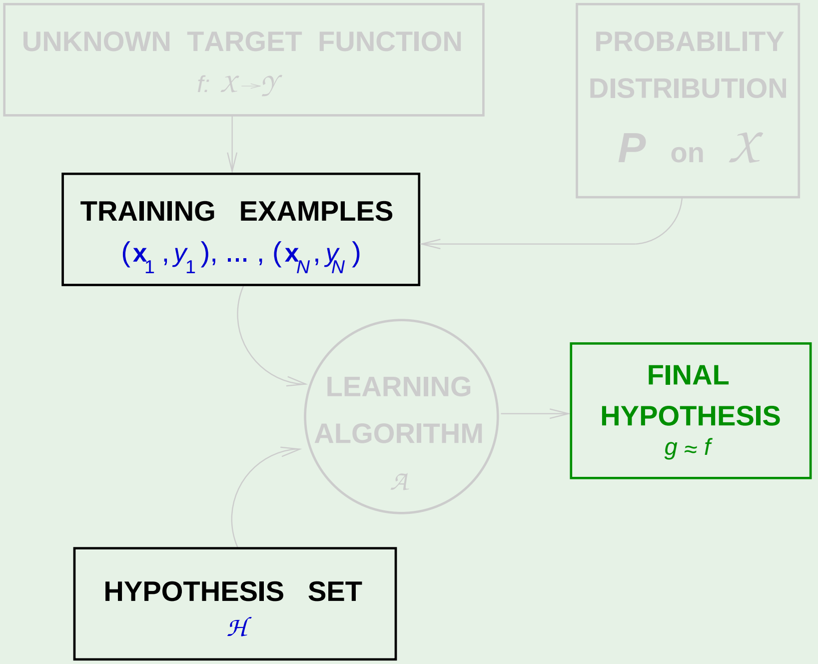
$$E_{\text{out}} \leq E_{\text{in}} + \Omega$$

Review of Lecture 7

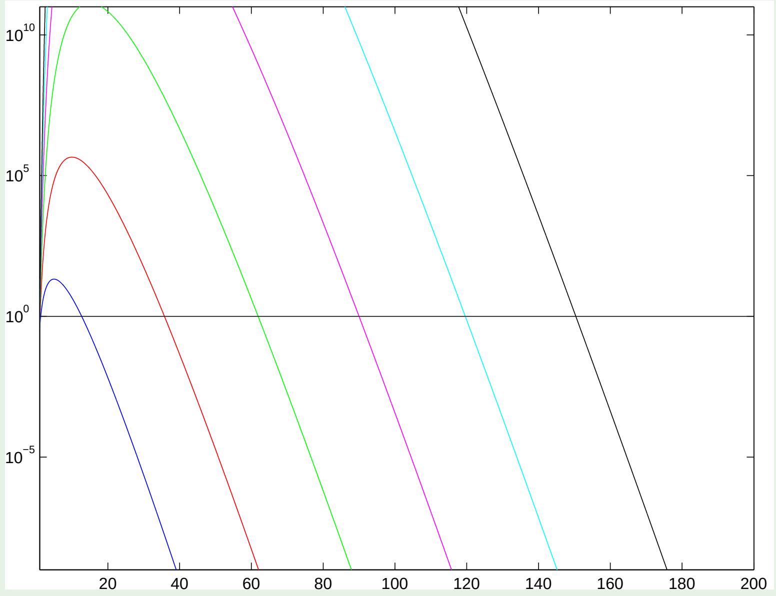
- VC dimension $d_{\text{VC}}(\mathcal{H})$

  most points $\mathcal{H}$ can shatter

- Scope of VC analysis



- Utility of VC dimension



$$N \propto d_{\text{VC}}$$

Rule of thumb: $N \geq 10\, d_{\text{VC}}$

- Generalization bound

$$E_{\text{out}} \leq E_{\text{in}} + \Omega$$

Learning From Data

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Lecture 8: Bias-Variance Tradeoff

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Thursday, April 26, 2012

Outline

- Bias and Variance

- Learning Curves

Approximation-generalization tradeoff

Small E_{out}: good approximation of f out of sample.

More complex $\mathcal{H} \Longrightarrow$ better chance of **approximating** f

Less complex $\mathcal{H} \Longrightarrow$ better chance of **generalizing** out of sample

Ideal $\mathcal{H} = \{f\}$ winning lottery ticket ☺

Quantifying the tradeoff

VC analysis was one approach: $E_{\text{out}} \leq E_{\text{in}} + \Omega$

Bias-variance analysis is another: decomposing E_{out} into

1. How well $\mathcal{H}$ can approximate f

2. How well we can zoom in on a good $h \in \mathcal{H}$

Applies to **real-valued targets** and uses **squared error**

Start with E_{out}

$$E_{\text{out}}(g^{(\mathcal{D})}) = \mathbb{E}_{\mathbf{x}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$$

$$\begin{aligned}\mathbb{E}_{\mathcal{D}}\left[E_{\text{out}}(g^{(\mathcal{D})})\right] &= \mathbb{E}_{\mathcal{D}}\left[\mathbb{E}_{\mathbf{x}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]\right] \\ &= \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]\right]\end{aligned}$$

Now, let us focus on:

$$\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$$

The average hypothesis

To evaluate $\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$

we define the 'average' hypothesis $\bar{g}(\mathbf{x})$:

$$\bar{g}(\mathbf{x}) = \mathbb{E}_{\mathcal{D}}\left[g^{(\mathcal{D})}(\mathbf{x})\right]$$

Imagine **many** data sets $\mathcal{D}_1, \mathcal{D}_2, \cdots, \mathcal{D}_K$

$$\bar{g}(\mathbf{x}) \approx \frac{1}{K}\sum_{k=1}^{K} g^{(\mathcal{D}_k)}(\mathbf{x})$$

Using $\bar{g}(\mathbf{x})$

$$\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right] = \mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x}) + \bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]$$

$$= \mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2 + \left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2\right.$$

$$\left. + \ 2 \ \left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right) \ \left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)\right]$$

$$= \mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right] + \left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2$$

Bias and variance

$$\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right] = \underbrace{\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right]}_{\mathsf{var}(\mathbf{x})} + \underbrace{\left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2}_{\mathsf{bias}(\mathbf{x})}$$

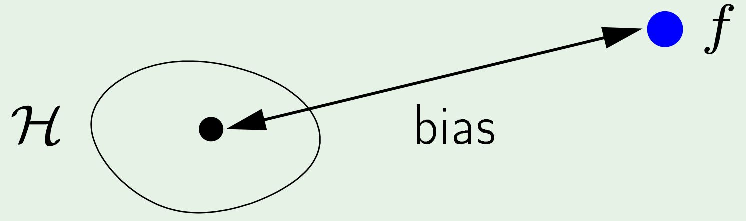
Therefore, $\mathbb{E}_{\mathcal{D}}\left[E_{\text{out}}(g^{(\mathcal{D})})\right] = \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]\right]$

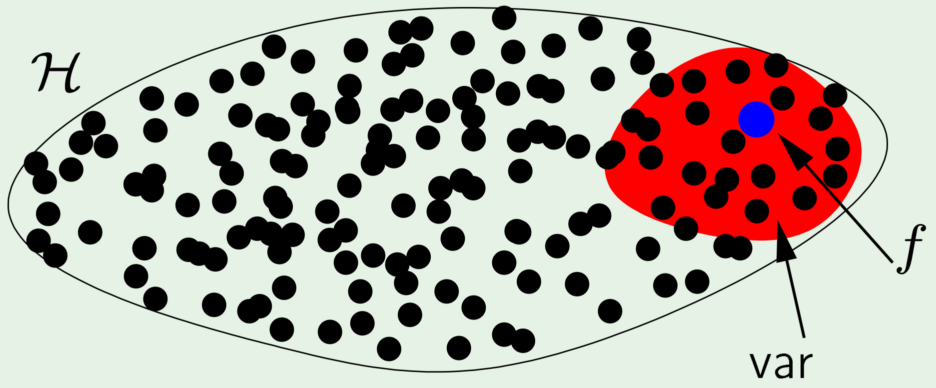
$$= \mathbb{E}_{\mathbf{x}}[\mathsf{bias}(\mathbf{x}) + \mathsf{var}(\mathbf{x})]$$

$$= \quad \mathsf{bias} \quad + \quad \mathsf{var}$$

The tradeoff

$$\text{bias} = \mathbb{E}_{\mathbf{x}}\left[\left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2\right] \qquad \text{var} = \mathbb{E}_{\mathbf{x}}\left[\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right]\right]$$





$$\downarrow \qquad \mathcal{H}\uparrow \qquad \uparrow$$

Example: sine target

$f : [-1, 1] \to \mathbb{R} \qquad f(x) = \sin(\pi x)$

Only two training examples! $\quad N = 2$

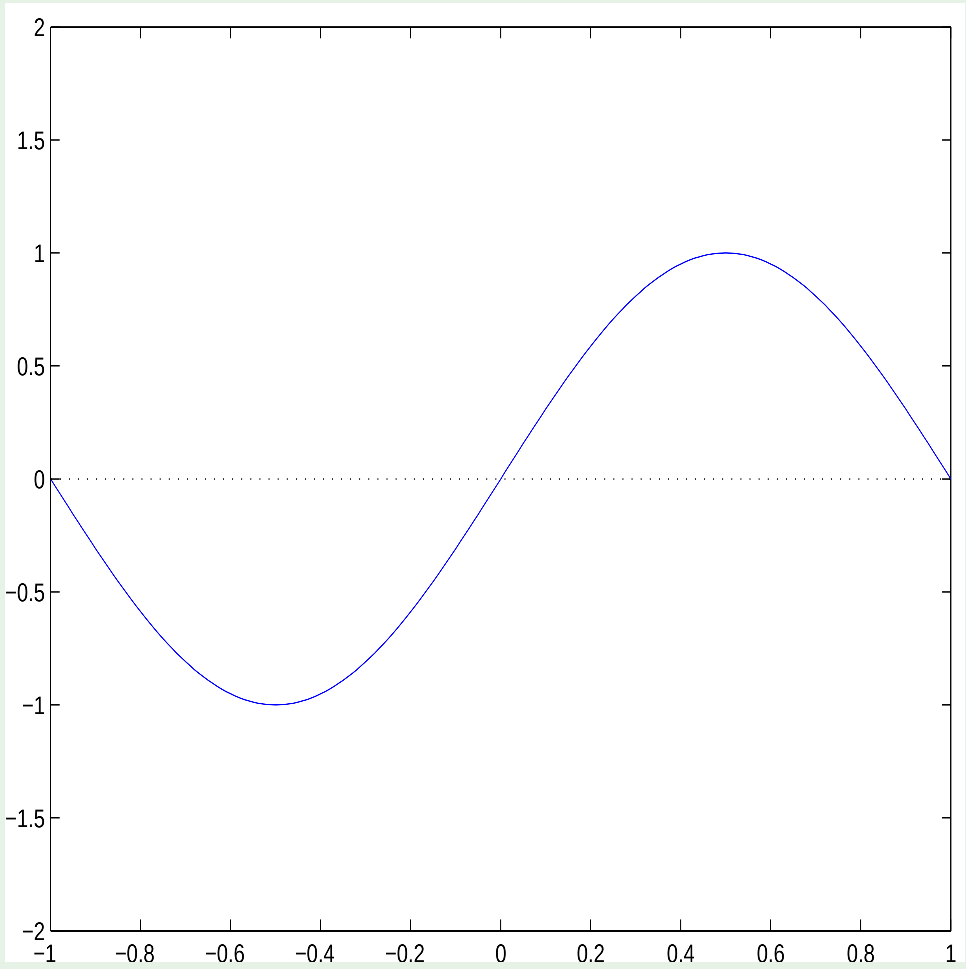
Two models used for learning:

$$\mathcal{H}_0: \quad h(x) = b$$

$$\mathcal{H}_1: \quad h(x) = ax + b$$

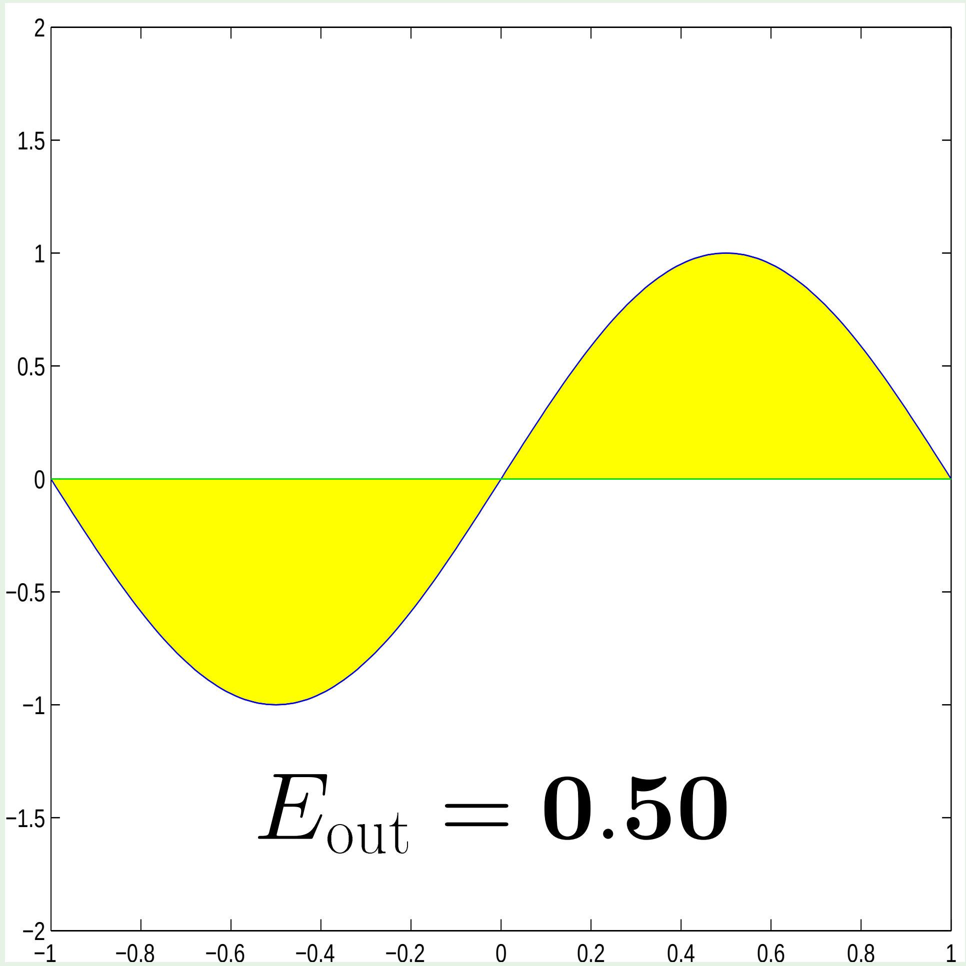
Which is better, $\mathcal{H}_0$ or $\mathcal{H}_1$?

f

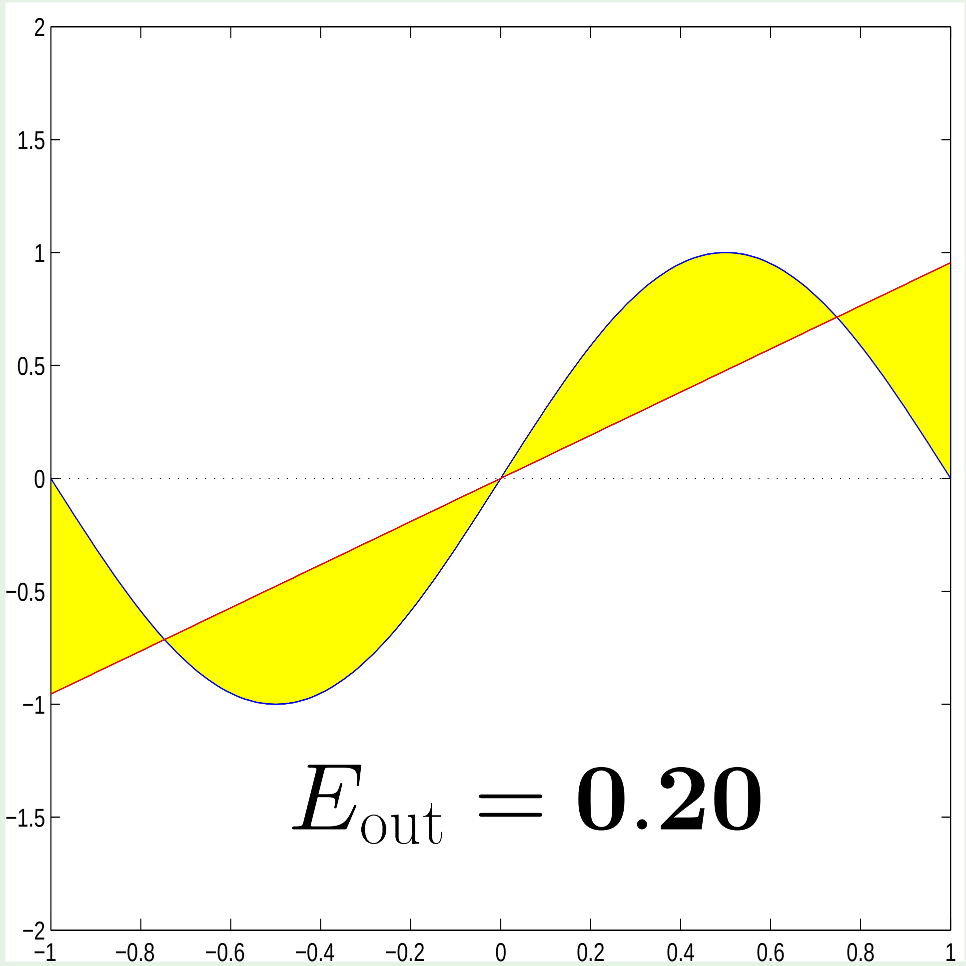


Approximation - $\mathcal{H}_0$ versus $\mathcal{H}_1$

$\mathcal{H}_0$

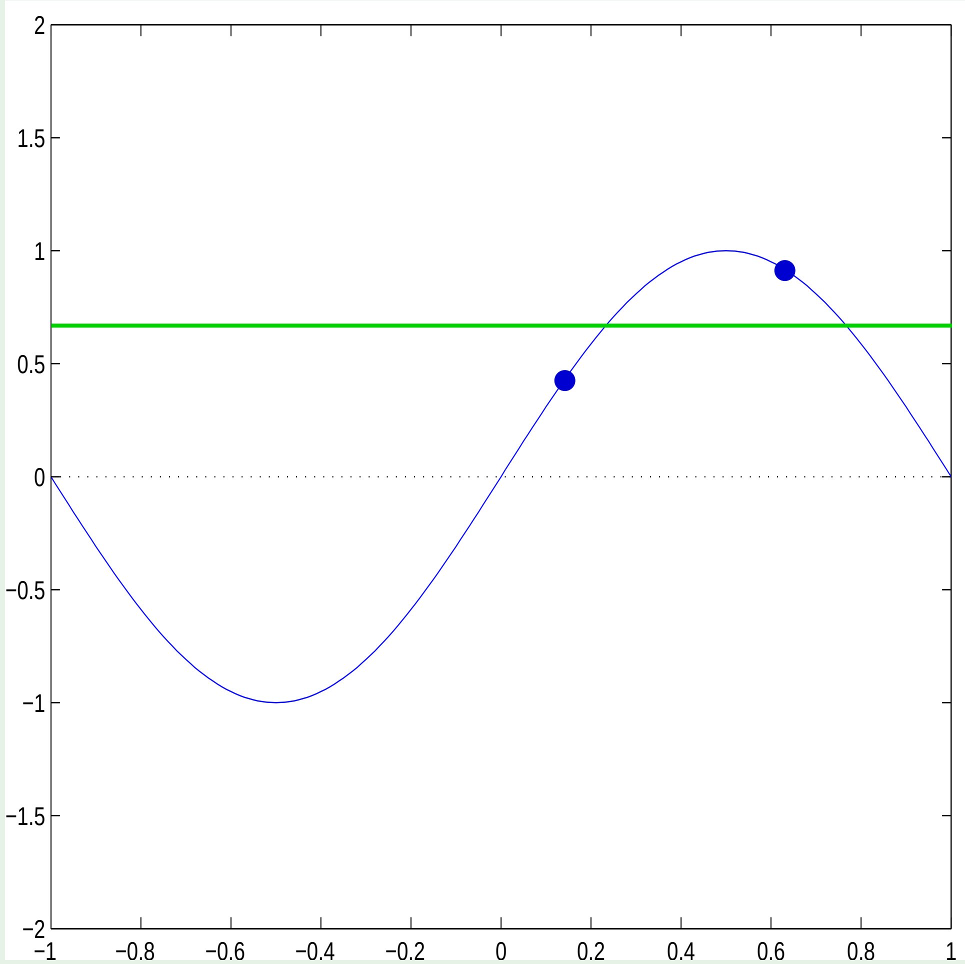


$\mathcal{H}_1$

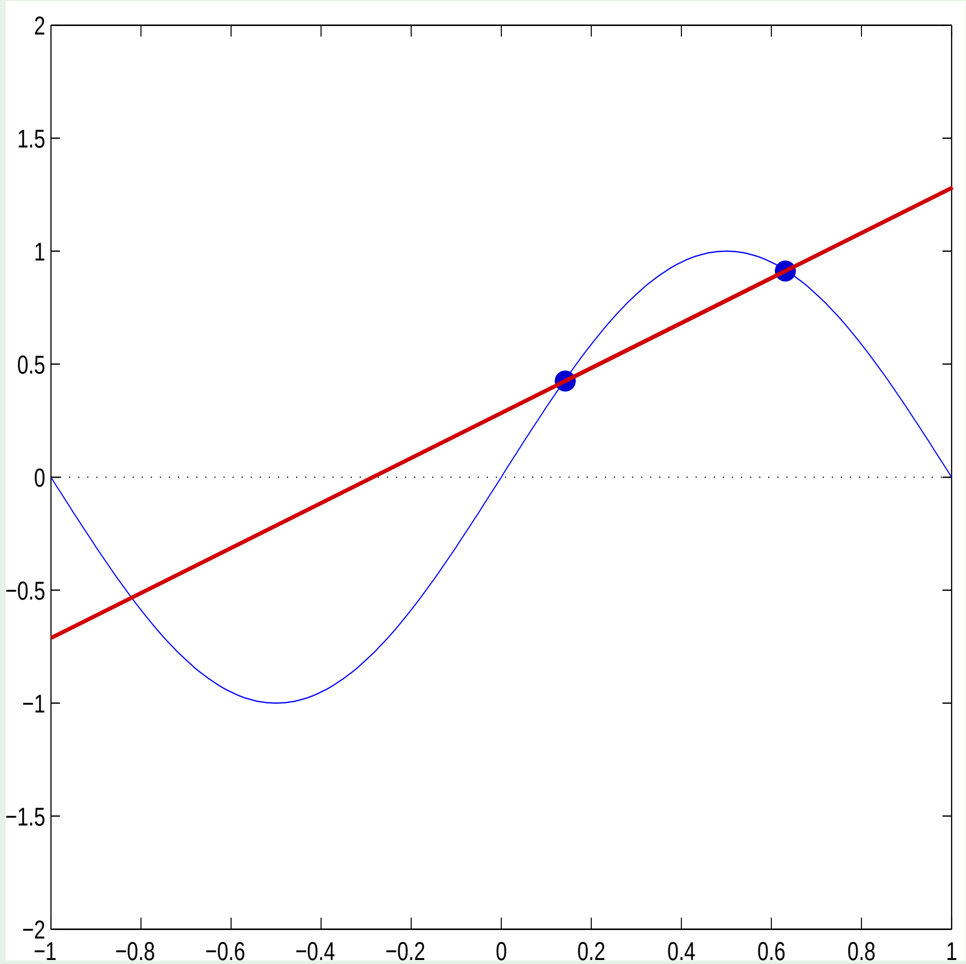


Learning - $\mathcal{H}_0$ versus $\mathcal{H}_1$

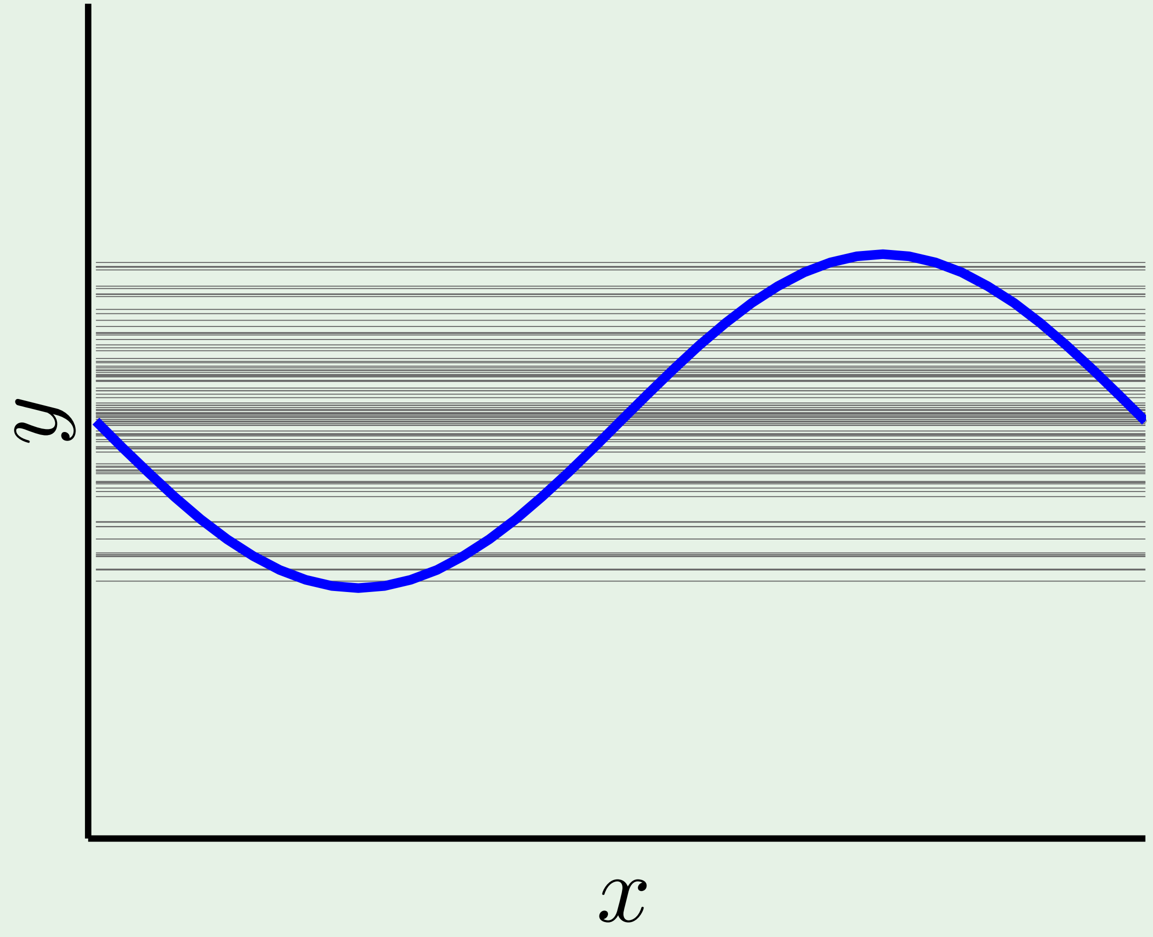
$\mathcal{H}_0$

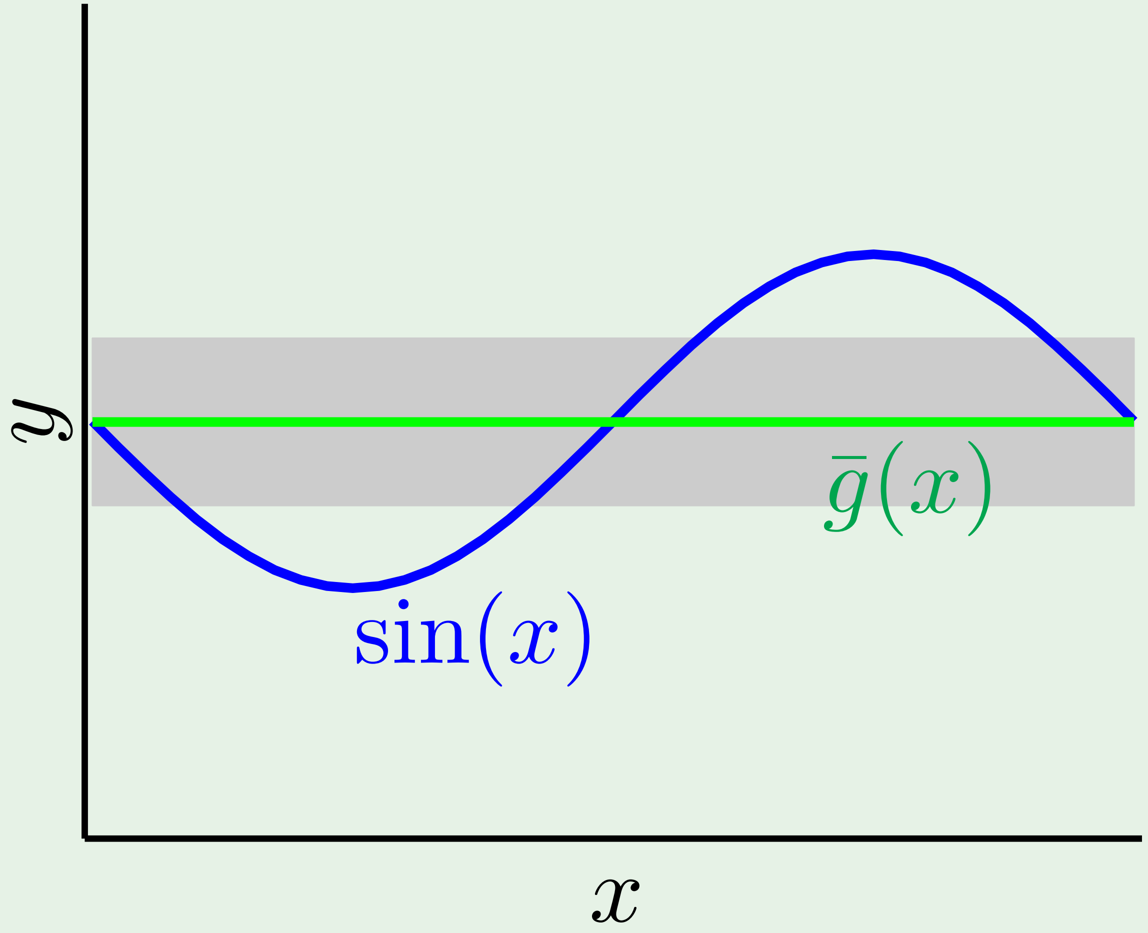


$\mathcal{H}_1$

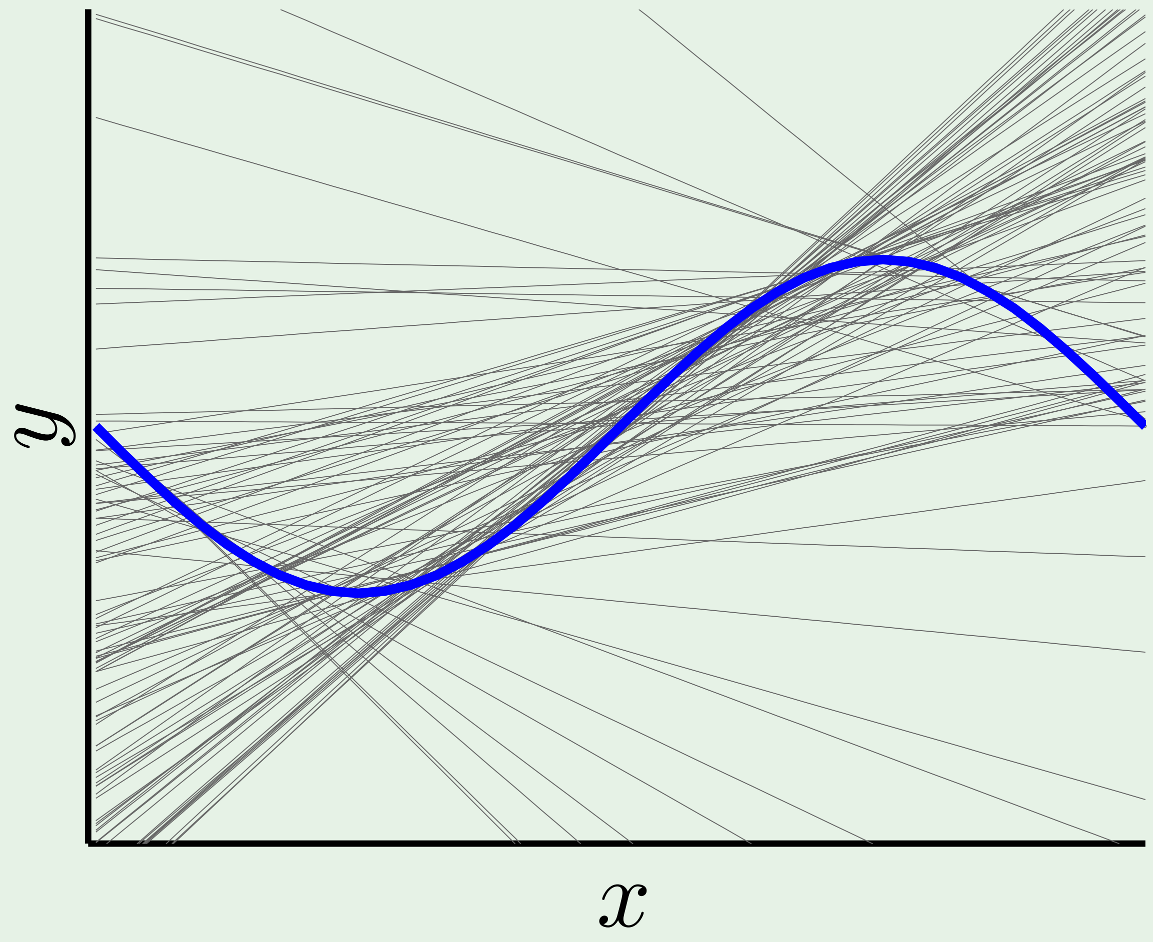


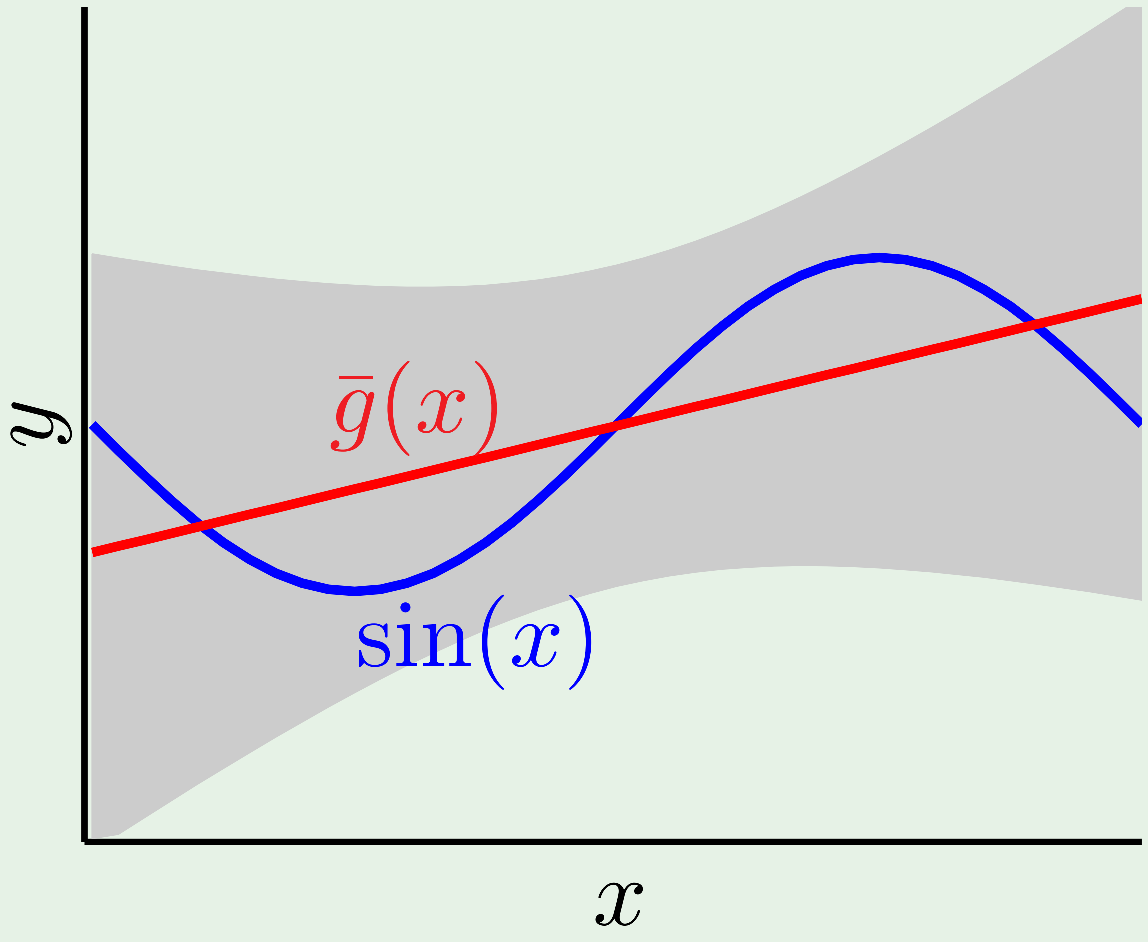
Bias and variance - $\mathcal{H}_0$





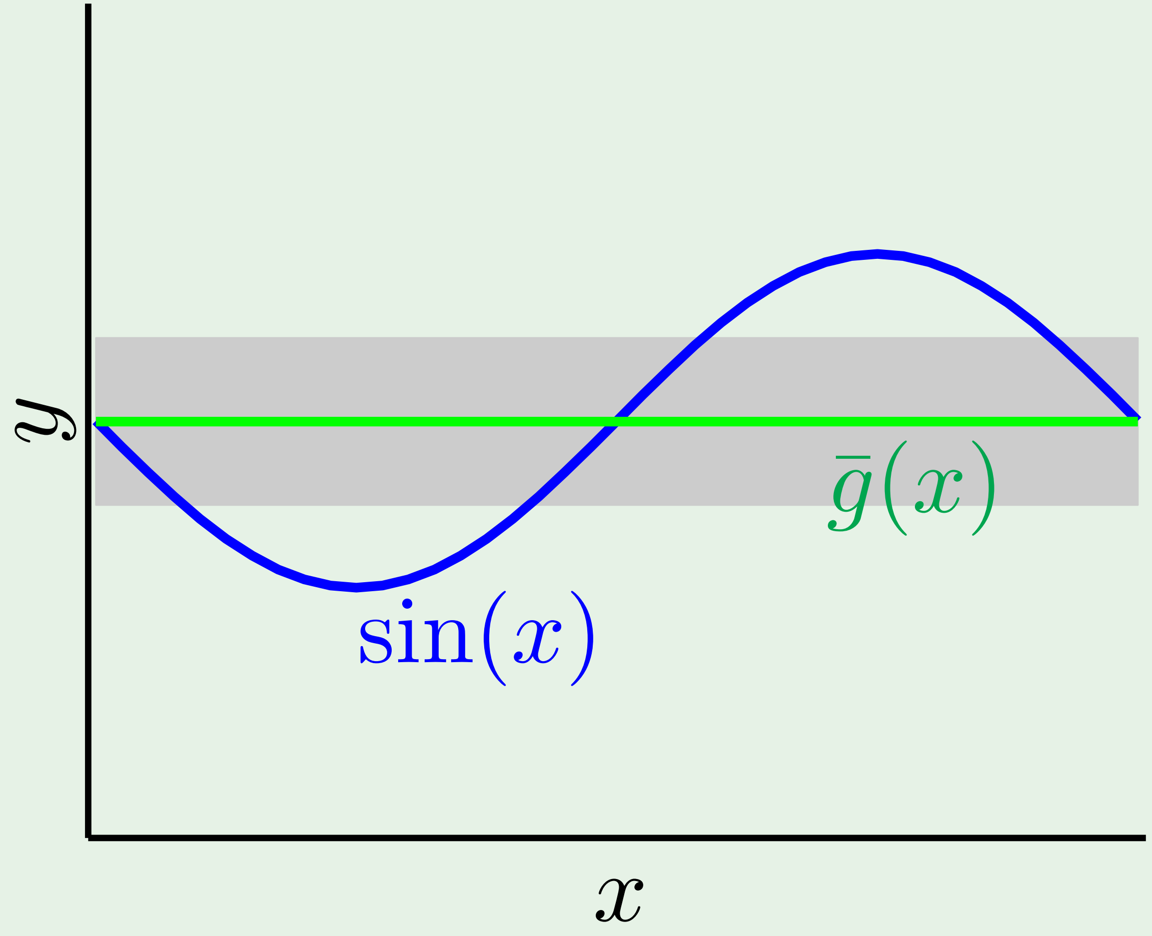
Bias and variance - $\mathcal{H}_1$





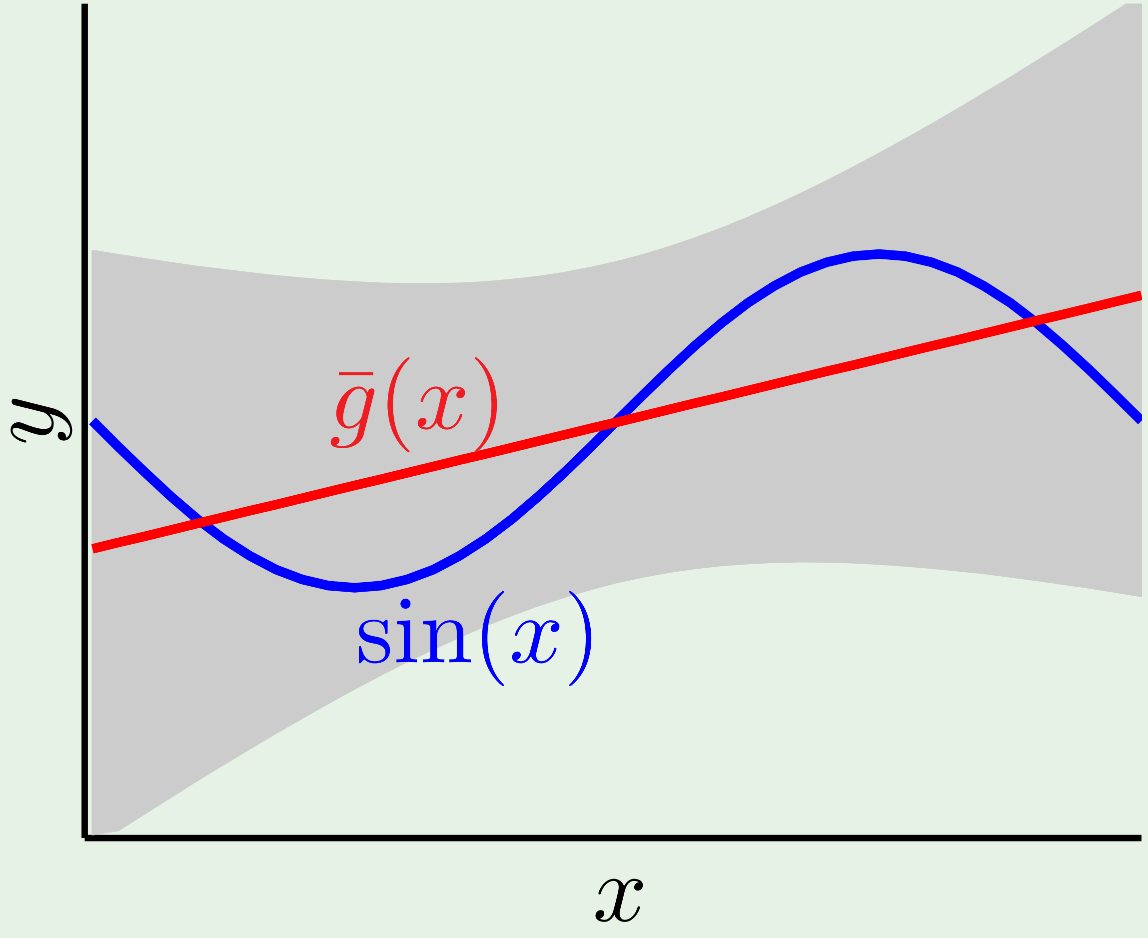
and the winner is ...

$\mathcal{H}_0$



bias = **0.50** var = **0.25**

$\mathcal{H}_1$



bias = **0.21** var = **1.69**

Lesson learned

Match the '**model complexity**'

to the **data resources**, not to the **target complexity**

Outline

- Bias and Variance

- Learning Curves

Expected E_{out} and E_{in}

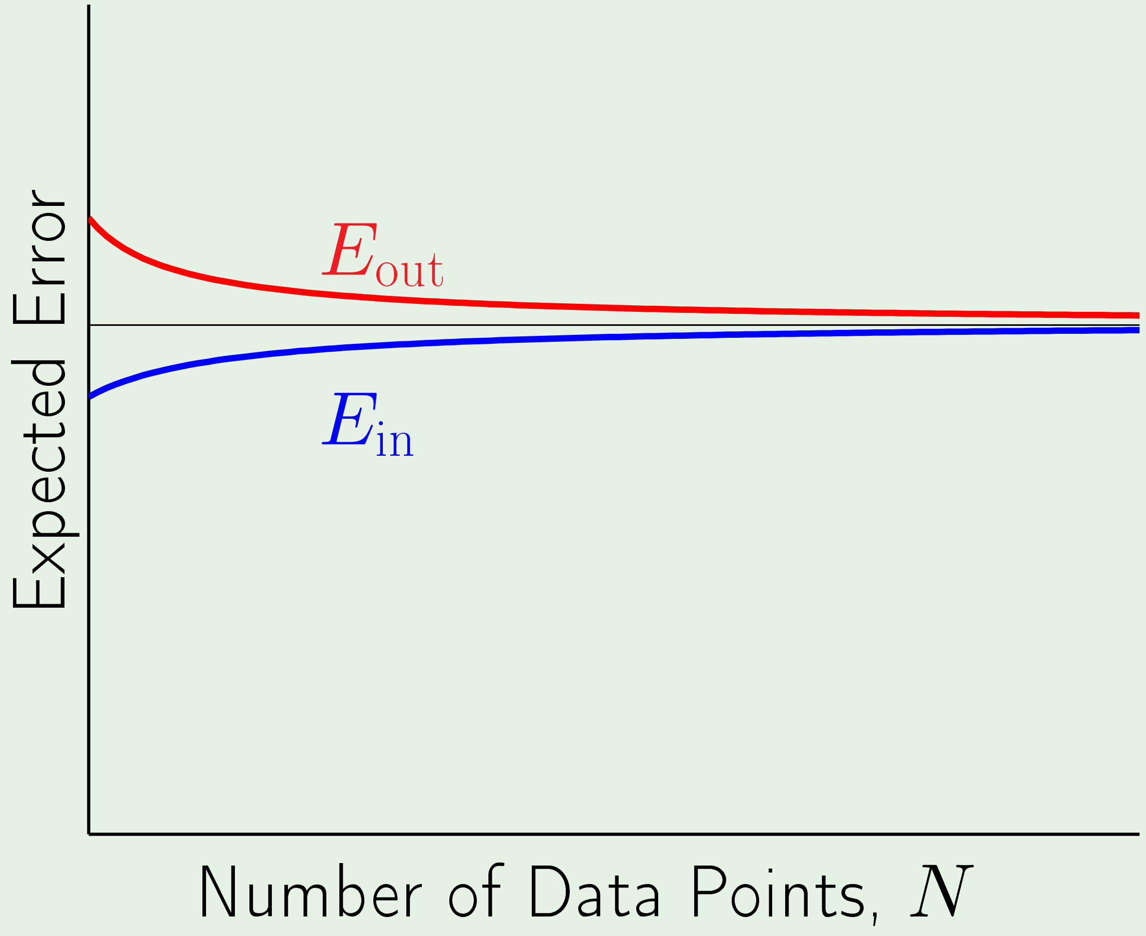
Data set $\mathcal{D}$ of size N

Expected out-of-sample error $\mathbb{E}_{\mathcal{D}}[E_{\text{out}}(g^{(\mathcal{D})})]$

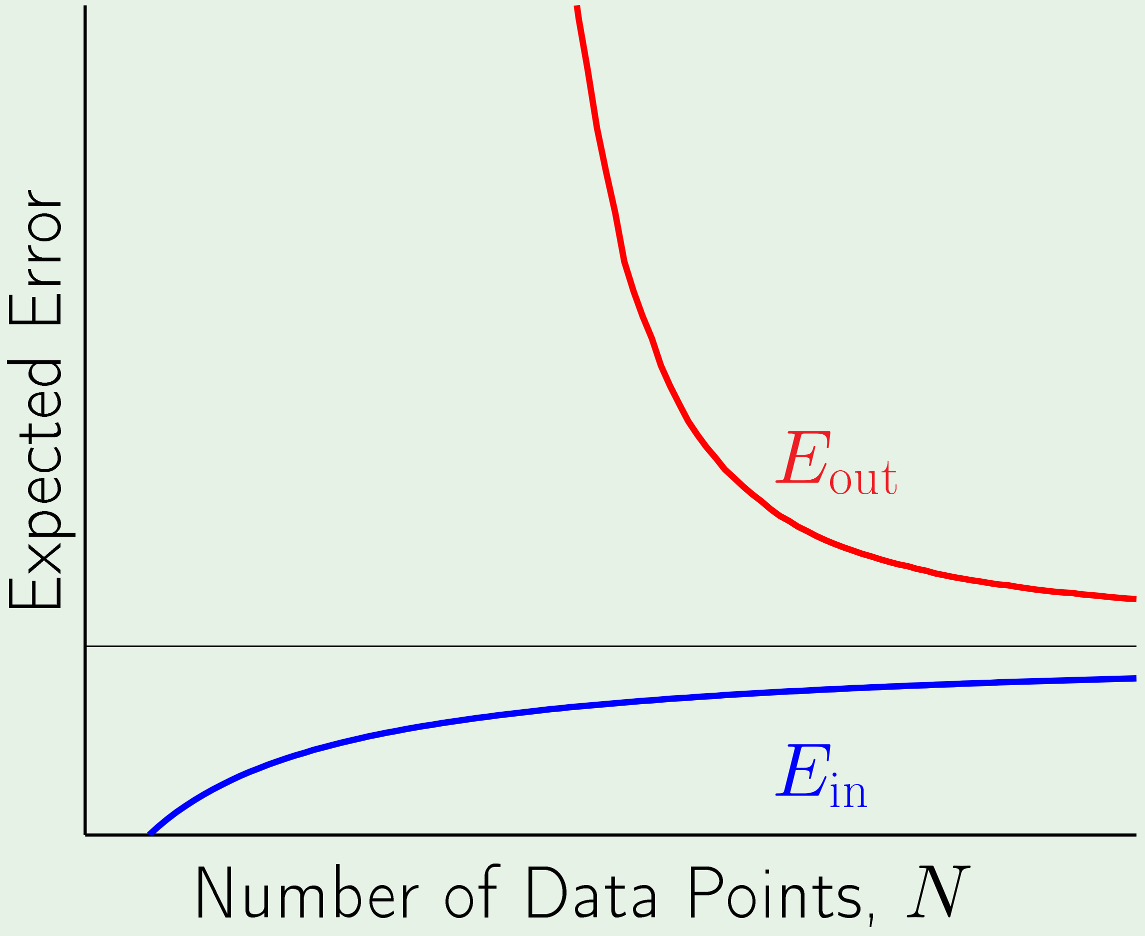
Expected in-sample error $\mathbb{E}_{\mathcal{D}}[E_{\text{in}}(g^{(\mathcal{D})})]$

How do they vary with N?

The curves

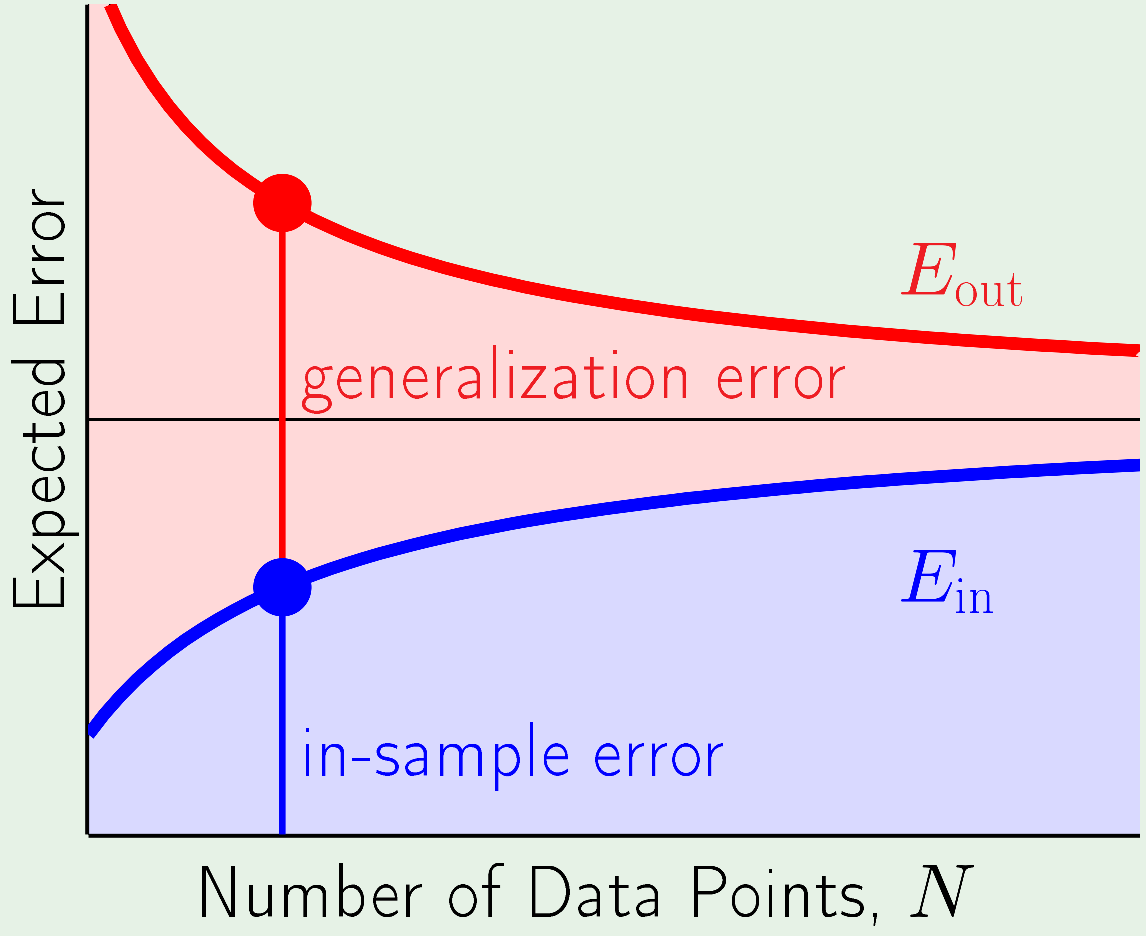


Simple Model

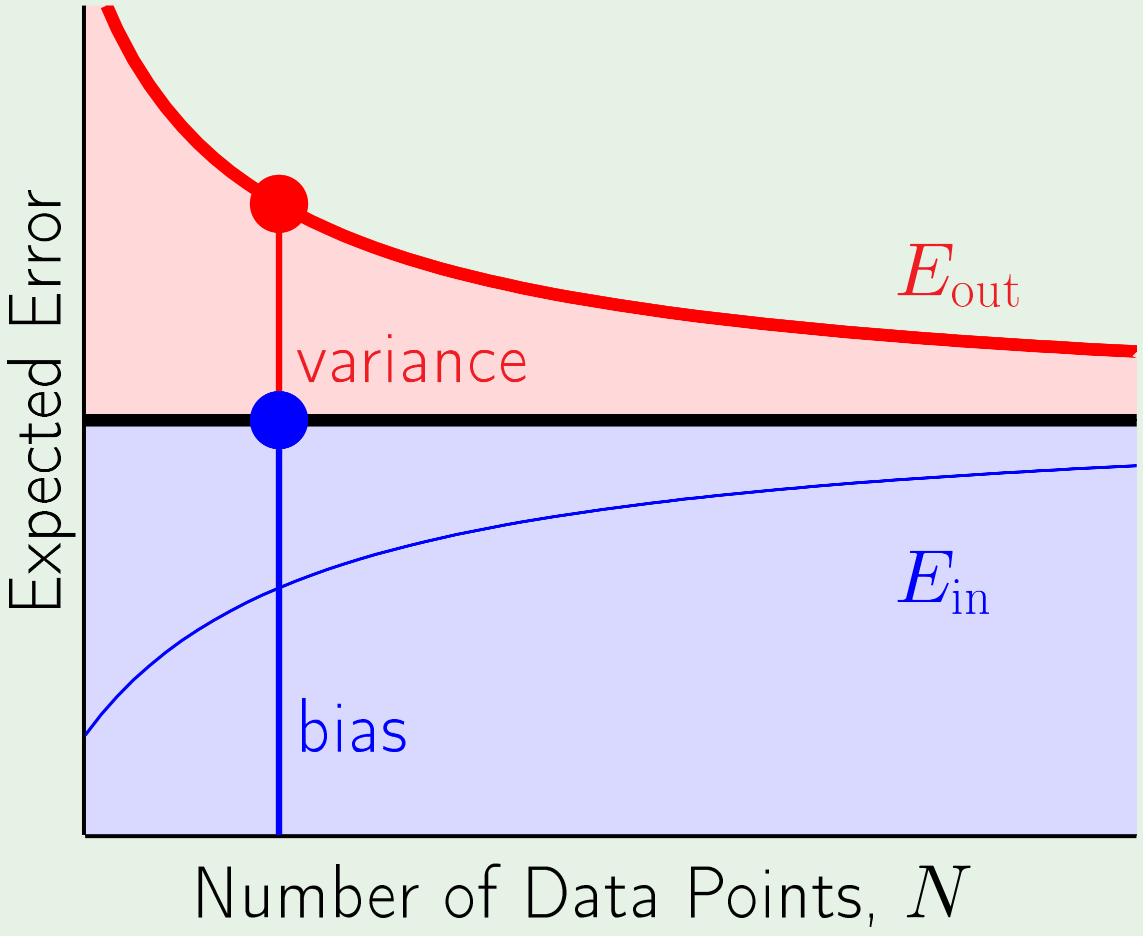


Complex Model

VC versus bias-variance



VC analysis



bias-variance

Linear regression case

Noisy target $y = \mathbf{w}^{*\intercal}\mathbf{x}$ + noise

Data set $\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\}$

Linear regression solution: $\mathbf{w} = (\mathrm{X}^\intercal \mathrm{X})^{-1}\mathrm{X}^\intercal \mathbf{y}$

In-sample error vector $= \mathrm{X}\mathbf{w} - \mathbf{y}$

'Out-of-sample' error vector $= \mathrm{X}\mathbf{w} - \mathbf{y}'$

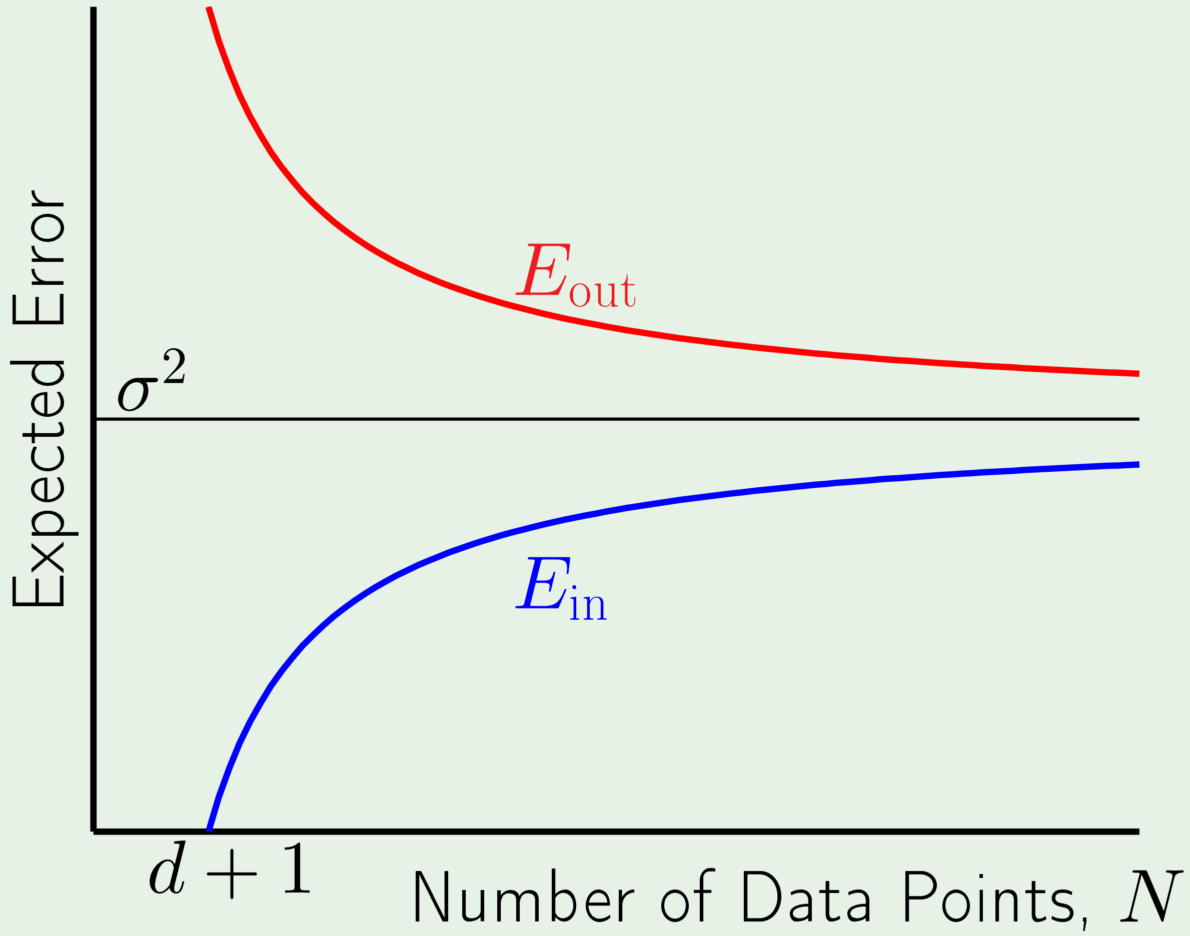
Learning curves for linear regression

Best approximation error $= \sigma^2$

Expected in-sample error $= \sigma^2 \left(1 - \frac{d+1}{N}\right)$

Expected out-of-sample error $= \sigma^2 \left(1 + \frac{d+1}{N}\right)$

Expected generalization error $= 2\sigma^2 \left(\frac{d+1}{N}\right)$

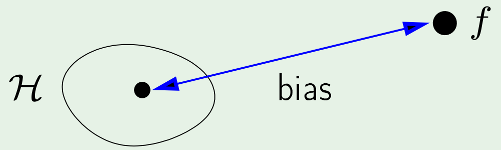


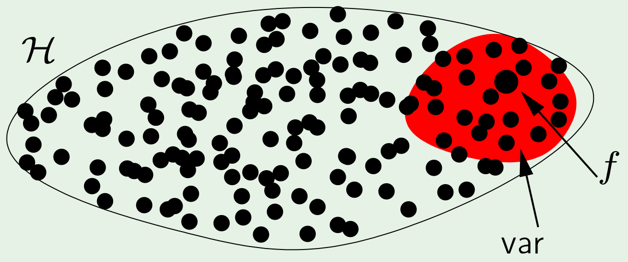
Review of Lecture 8

- Bias and variance

  Expected value of E_{out} w.r.t. $\mathcal{D}$

  $$= \text{bias} + \text{var}$$



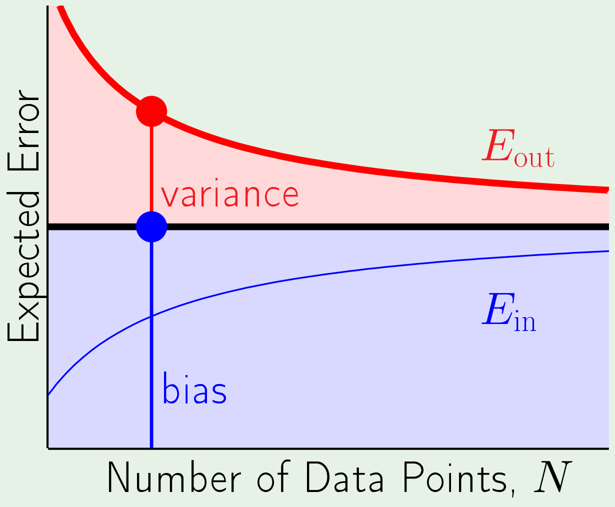


$$g^{(\mathcal{D})}(\mathbf{x}) \rightarrow \bar{g}(\mathbf{x}) \rightarrow f(\mathbf{x})$$

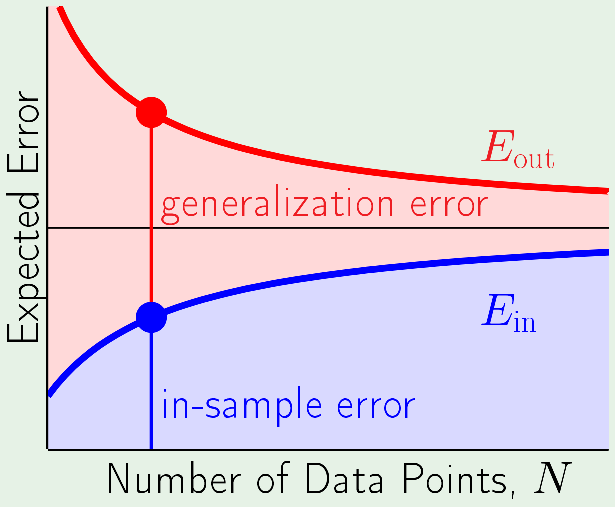
- Learning curves

  How E_{in} and E_{out} vary with N

B-V:



VC:



- $N \propto$ "VC dimension"

Learning From Data

Yaser S. Abu-Mostafa
California Institute of Technology

Lecture 9: The Linear Model II

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Tuesday, May 1, 2012

Where we are

- Linear classification ✓
- Linear regression ✓
- Logistic regression
- Nonlinear transforms ≈✓

Nonlinear transforms

$$\mathbf{x} = (x_0, x_1, \cdots, x_d) \quad \xrightarrow{\Phi} \quad \mathbf{z} = (z_0, z_1, \cdots\cdots\cdots\cdots, z_{\tilde{d}})$$

Each $z_i = \phi_i(\mathbf{x})$ $\qquad \mathbf{z} = \Phi(\mathbf{x})$

Example: $\mathbf{z} = (1, x_1, x_2, x_1 x_2, x_1^2, x_2^2)$

Final hypothesis $g(\mathbf{x})$ in $\mathcal{X}$ space:

$\operatorname{sign}\left(\tilde{\mathbf{w}}^\mathsf{T}\Phi(\mathbf{x})\right)$ or $\tilde{\mathbf{w}}^\mathsf{T}\Phi(\mathbf{x})$

The price we pay

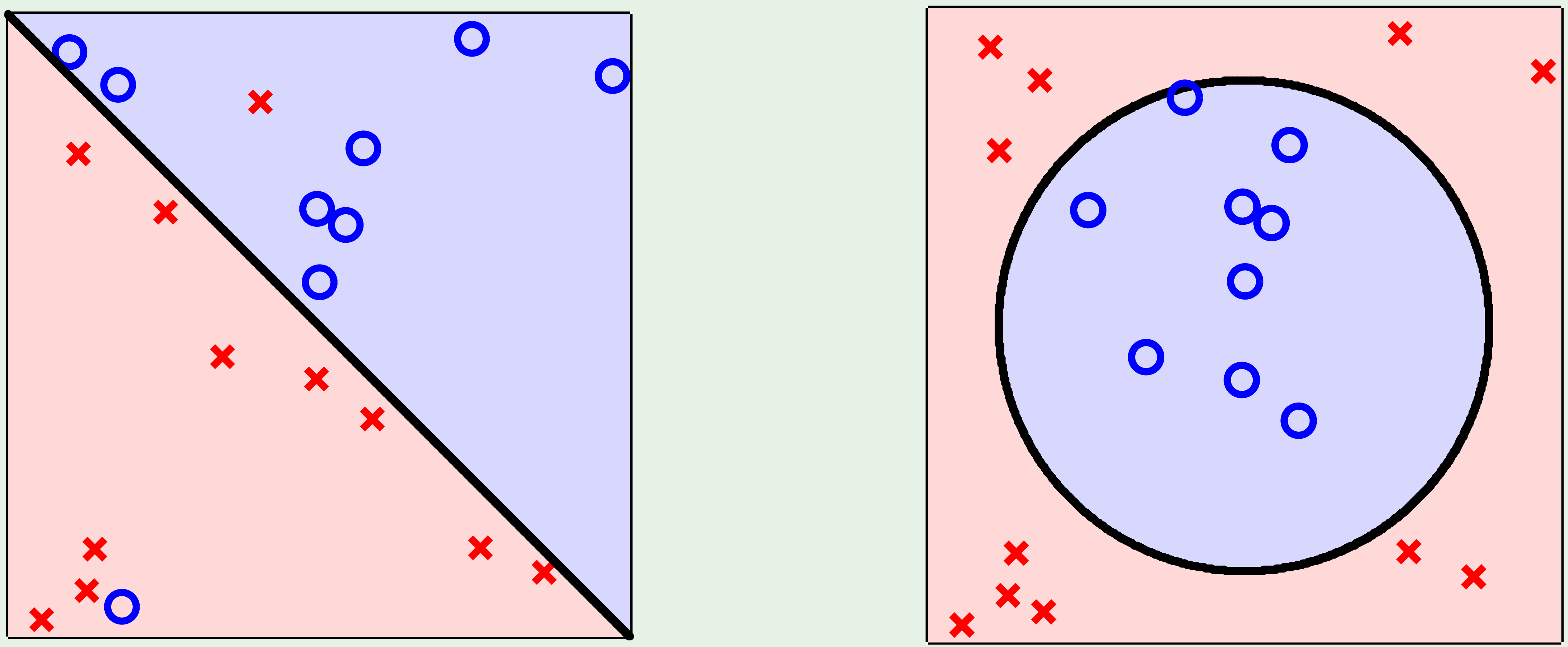
$$\mathbf{x} = (x_0, x_1, \cdots, x_d) \xrightarrow{\Phi} \mathbf{z} = (z_0, z_1, \cdots\cdots\cdots, z_{\tilde{d}})$$

$$\downarrow \qquad\qquad\qquad\qquad \downarrow$$

$$\mathbf{w} \qquad\qquad\qquad\qquad \tilde{\mathbf{w}}$$

$$d_{\mathrm{VC}} = d + 1 \qquad\qquad d_{\mathrm{VC}} \leq \tilde{d} + 1$$

Two non-separable cases

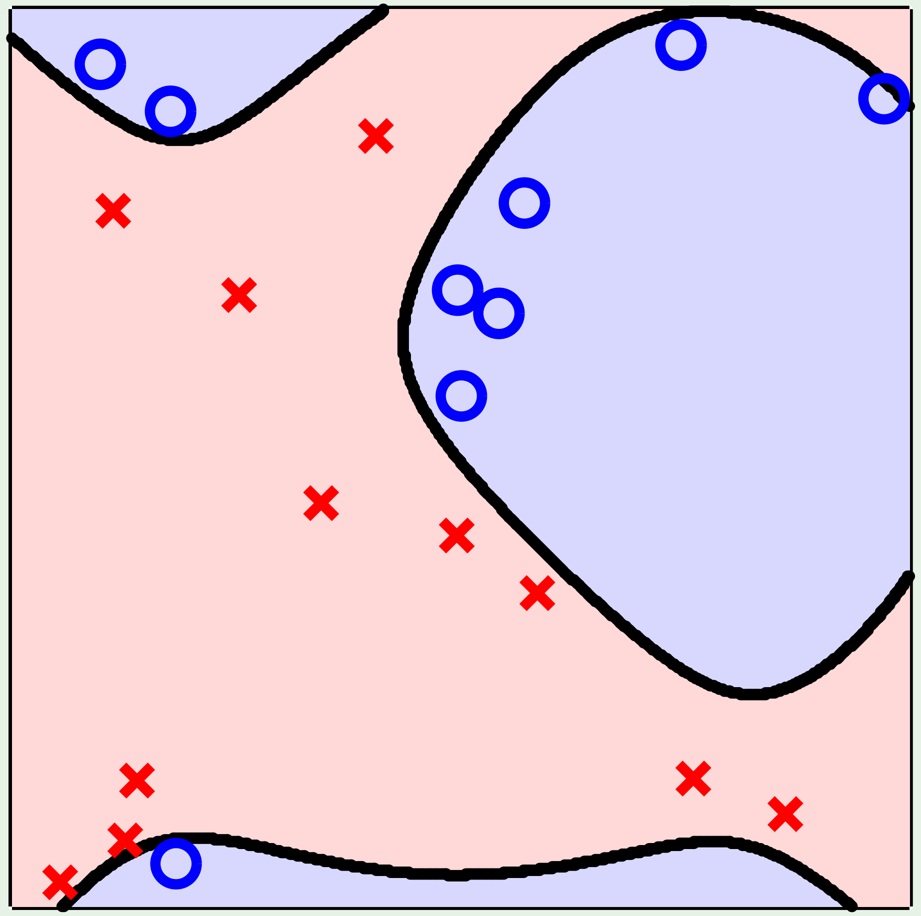


First case

Use a linear model in $\mathcal{X}$; accept $E_{\text{in}} > 0$

or

Insist on $E_{\text{in}} = 0$; go to high-dimensional $\mathcal{Z}$



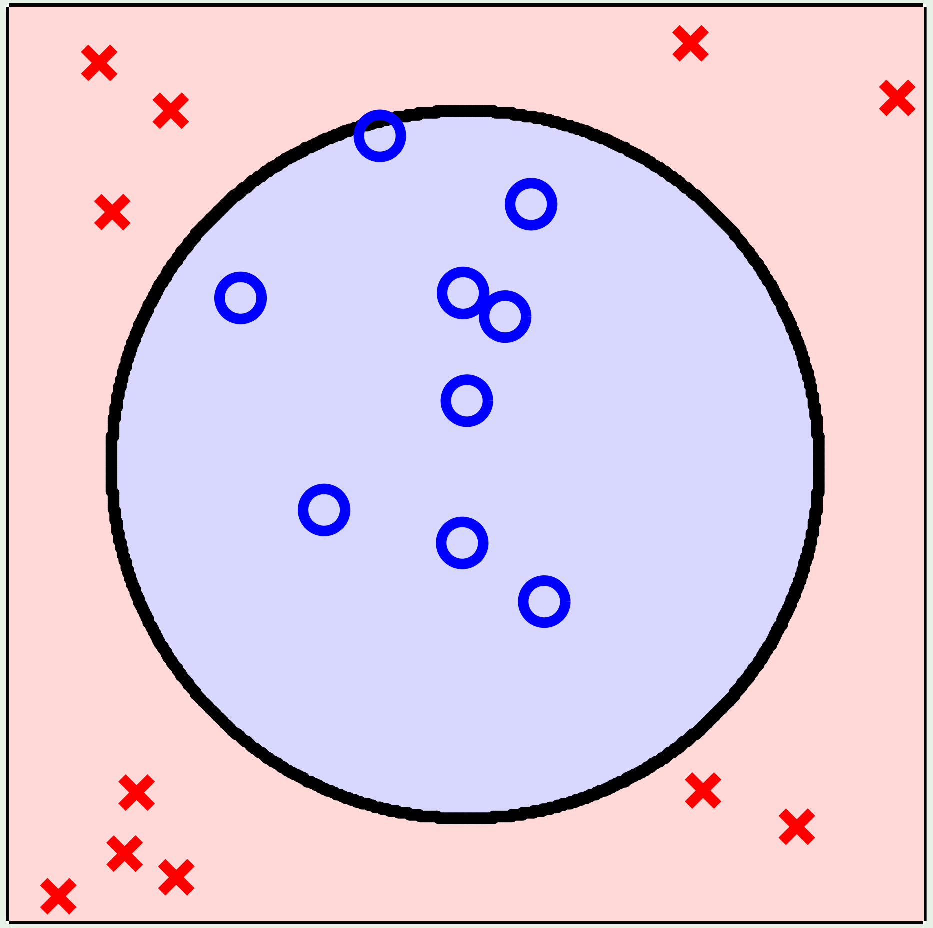
Second case

$\mathbf{z} = (1, x_1, x_2, x_1 x_2, x_1^2, x_2^2)$

Why not: $\mathbf{z} = (1, x_1^2, x_2^2)$

or better yet: $\mathbf{z} = (1, x_1^2 + x_2^2)$

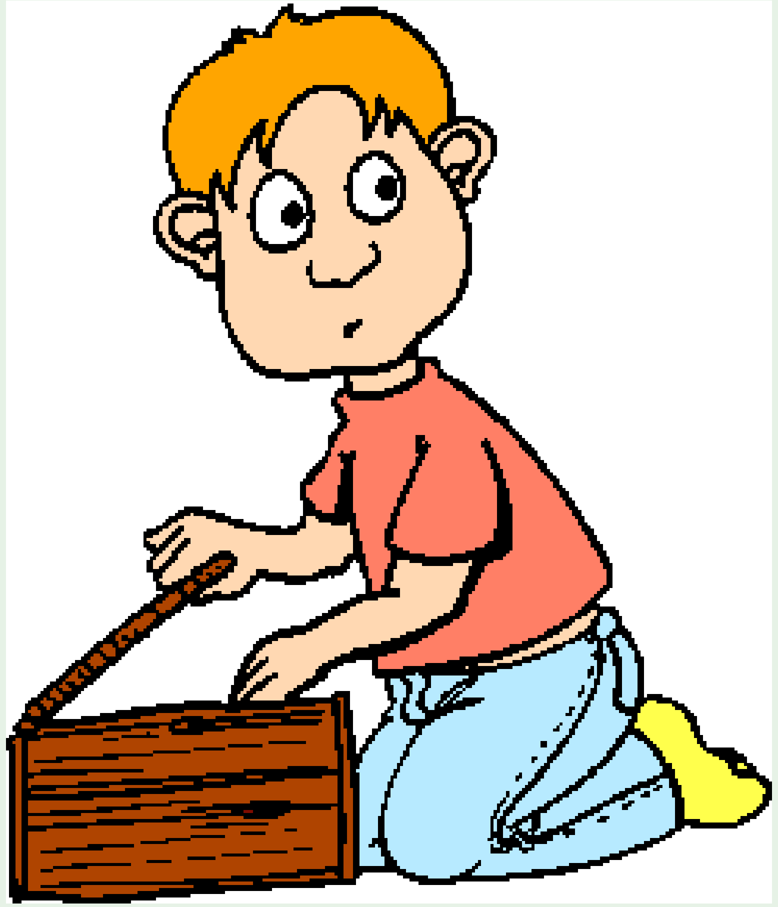
or even: $\mathbf{z} = (x_1^2 + x_2^2 - 0.6)$



Lesson learned

Looking at the data *before* choosing the model can be hazardous to your E_{out}

Data snooping



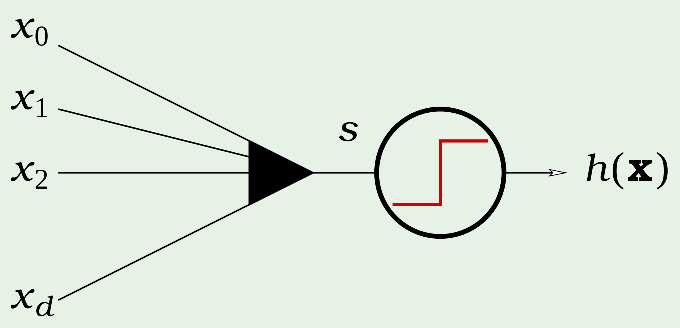
Logistic regression - Outline

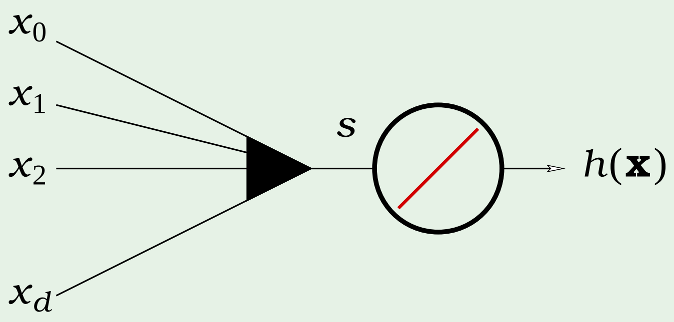
- The model
- Error measure
- Learning algorithm

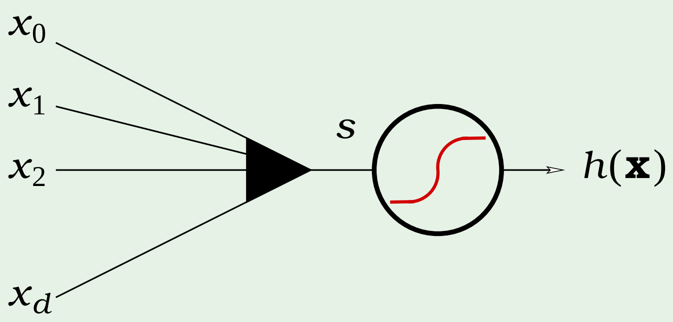
A third linear model

$$s = \sum_{i=0}^{d} w_i x_i$$

linear classification	linear regression	**logistic regression**
$h(\mathbf{x}) = \text{sign}(s)$	$h(\mathbf{x}) = s$	$h(\mathbf{x}) = \theta(s)$



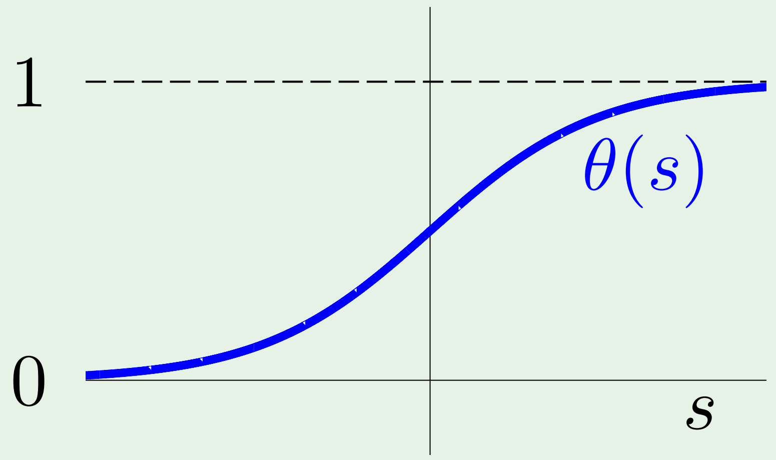




The logistic function θ

The formula:

$$\theta(s) = \frac{e^s}{1 + e^s}$$



soft threshold: uncertainty

sigmoid: flattened out 's'

Probability interpretation

$h(\mathbf{x}) = \theta(s)$ is interpreted as a probability

Example. Prediction of heart attacks

Input $\mathbf{x}$: cholesterol level, age, weight, etc.

$\theta(s)$: probability of a heart attack

The signal $s = \mathbf{w}^\intercal \mathbf{x}$ "risk score"

Genuine probability

Data $(\mathbf{x}, y)$ with binary y, generated by a noisy target:

$$P(y \mid \mathbf{x}) = \begin{cases} f(\mathbf{x}) & \text{for } y = +1; \\ 1 - f(\mathbf{x}) & \text{for } y = -1. \end{cases}$$

The target $f : \mathbb{R}^d \to [0, 1]$ is the probability

Learn $g(\mathbf{x}) = \theta(\mathbf{w}^{\intercal} \mathbf{x}) \approx f(\mathbf{x})$

Error measure

For each $(\mathbf{x}, y)$, y is generated by probability $f(\mathbf{x})$

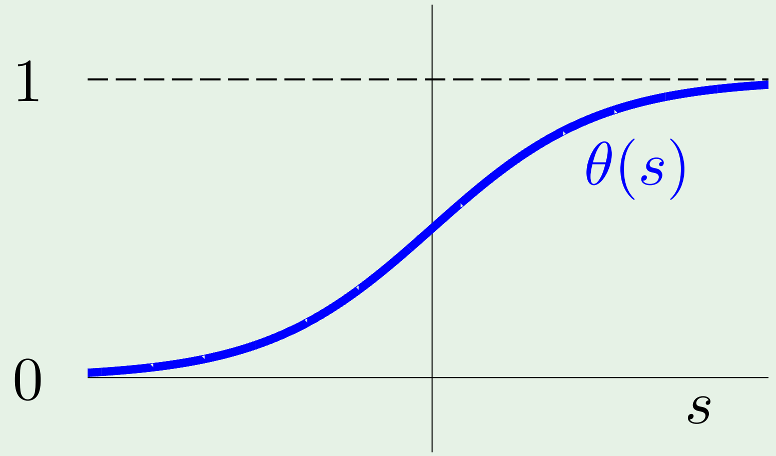
Plausible error measure based on **likelihood**:

If $h = f$, how likely to get y from $\mathbf{x}$?

$$P(y \mid \mathbf{x}) = \begin{cases} h(\mathbf{x}) & \text{for } y = +1; \\ 1 - h(\mathbf{x}) & \text{for } y = -1. \end{cases}$$

Formula for likelihood

$$P(y \mid \mathbf{x}) = \begin{cases} h(\mathbf{x}) & \text{for } y = +1; \\ 1 - h(\mathbf{x}) & \text{for } y = -1. \end{cases}$$



Substitute $h(\mathbf{x}) = \theta(\mathbf{w}^\intercal \mathbf{x})$, noting $\theta(-s) = 1 - \theta(s)$

$$P(y \mid \mathbf{x}) = \theta(y\ \mathbf{w}^\intercal \mathbf{x})$$

Likelihood of $\mathcal{D} = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)$ is

$$\prod_{n=1}^{N} P(y_n \mid \mathbf{x}_n) = \prod_{n=1}^{N} \theta(y_n \mathbf{w}^\intercal \mathbf{x}_n)$$

Maximizing the likelihood

Minimize

$$-\frac{1}{N}\ln\left(\prod_{n=1}^{N}\theta(y_n\,\mathbf{w}^{\mathsf{T}}\,\mathbf{x}_n)\right)$$

$$=\frac{1}{N}\sum_{n=1}^{N}\ln\left(\frac{1}{\theta(y_n\,\mathbf{w}^{\mathsf{T}}\,\mathbf{x}_n)}\right)$$

$$\left[\theta(s)=\frac{1}{1+e^{-s}}\right]$$

$$E_{\text{in}}(\mathbf{w})=\frac{1}{N}\sum_{n=1}^{N}\underbrace{\ln\left(1+e^{-y_n\mathbf{w}^{\mathsf{T}}\mathbf{x}_n}\right)}_{\mathrm{e}\left(h(\mathbf{x}_n),y_n\right)}$$

"cross-entropy" error

Logistic regression - Outline

- The model
- Error measure
- Learning algorithm

How to minimize E_{in}

For logistic regression,

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \ln\left(1 + e^{-y_n \mathbf{w}^{\mathsf{T}}\mathbf{x}_n}\right) \qquad \longleftarrow \textbf{iterative} \text{ solution}$$

Compare to linear regression:

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} (\mathbf{w}^{\mathsf{T}}\mathbf{x}_n - y_n)^2 \qquad \longleftarrow \text{closed-form solution}$$

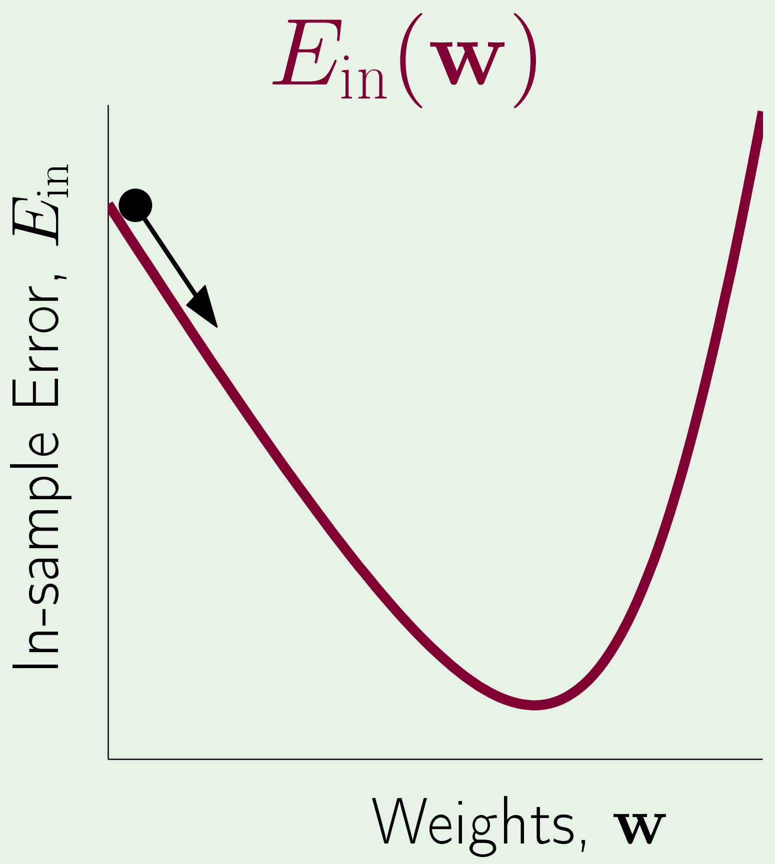
Iterative method: gradient descent

General method for nonlinear optimization

Start at $\mathbf{w}(0)$; take a step along steepest slope

Fixed step size: $\mathbf{w}(1) = \mathbf{w}(0) + \eta\, \hat{\mathbf{v}}$

What is the direction $\hat{\mathbf{v}}$?



Formula for the direction $\hat{\mathbf{v}}$

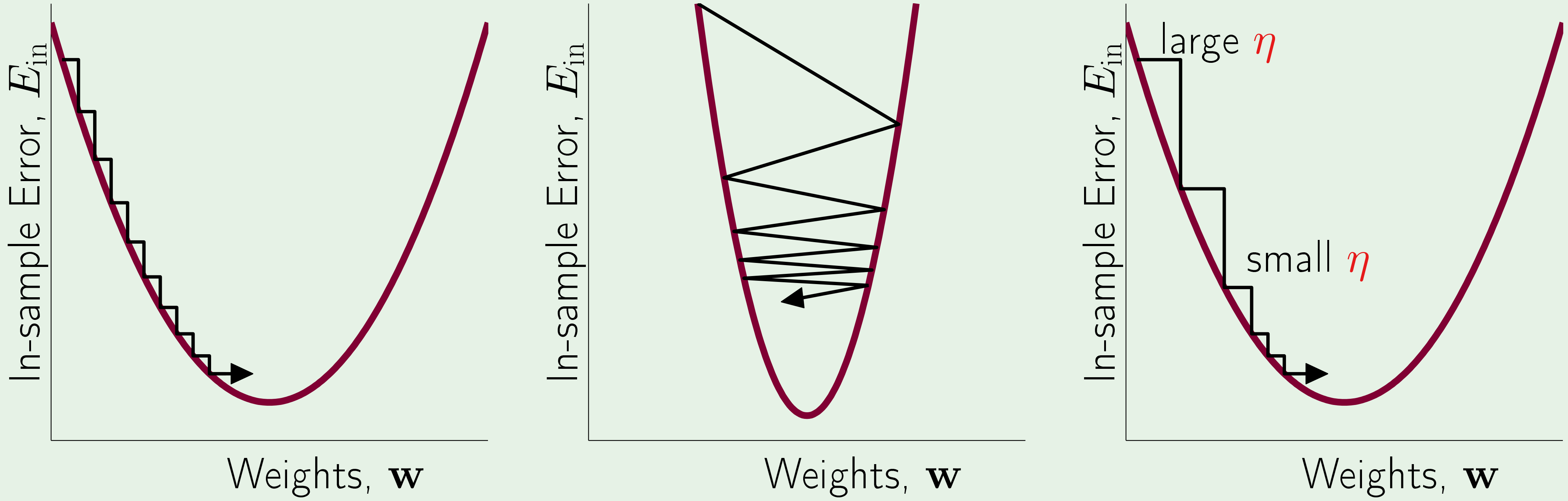
$$
\begin{aligned}
\Delta E_{\text{in}} &= E_{\text{in}}(\,\mathbf{w}(0) + \eta\hat{\mathbf{v}}\,) - E_{\text{in}}(\mathbf{w}(0)) \\
&= \eta \nabla E_{\text{in}}(\mathbf{w}(0))^{\mathrm{T}}\hat{\mathbf{v}} + O(\eta^2) \\
&\geq -\eta\|\nabla E_{\text{in}}(\mathbf{w}(0))\|
\end{aligned}
$$

Since $\hat{\mathbf{v}}$ is a unit vector,

$$
\hat{\mathbf{v}} = -\frac{\nabla E_{\text{in}}(\mathbf{w}(0))}{\|\nabla E_{\text{in}}(\mathbf{w}(0))\|}
$$

Fixed-size step?

How η affects the algorithm:



η too small — η too large — variable η – just right

η should increase with the slope

Easy implementation

Instead of

$$\Delta \mathbf{w} = \eta \, \hat{\mathbf{v}}$$

$$= -\eta \frac{\nabla E_{\text{in}}(\mathbf{w}(0))}{\|\nabla E_{\text{in}}(\mathbf{w}(0))\|}$$

Have

$$\Delta \mathbf{w} = -\eta \; \nabla E_{\text{in}}(\mathbf{w}(0))$$

Fixed **learning rate** η

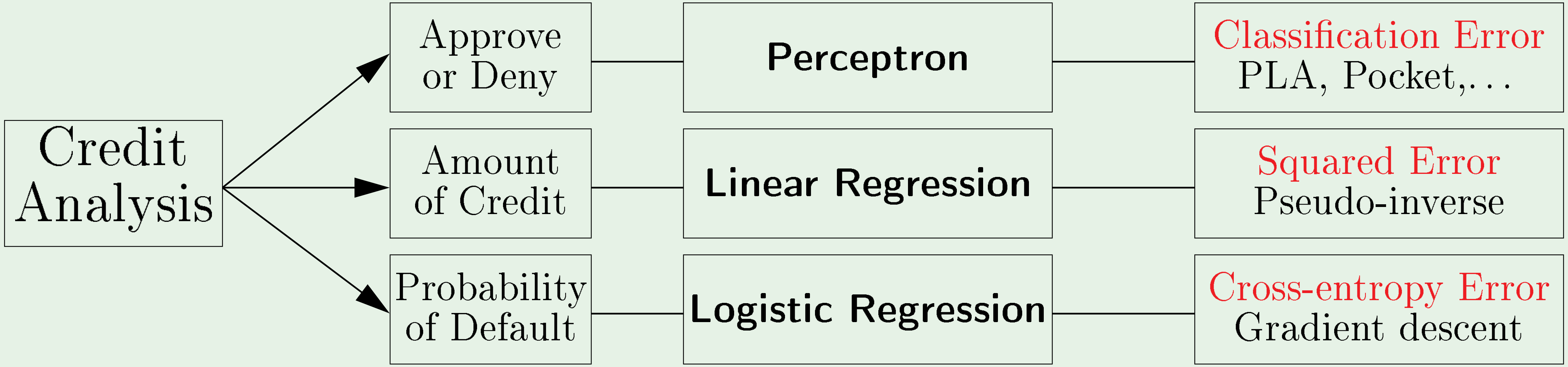
Logistic regression algorithm

Initialize the weights at $t = 0$ to $\mathbf{w}(0)$
for $t = 0, 1, 2, \ldots$ **do**
    Compute the gradient

$$\nabla E_{\text{in}} = -\frac{1}{N} \sum_{n=1}^{N} \frac{y_n \mathbf{x}_n}{1 + e^{y_n \mathbf{w}^{\intercal}(t) \mathbf{x}_n}}$$

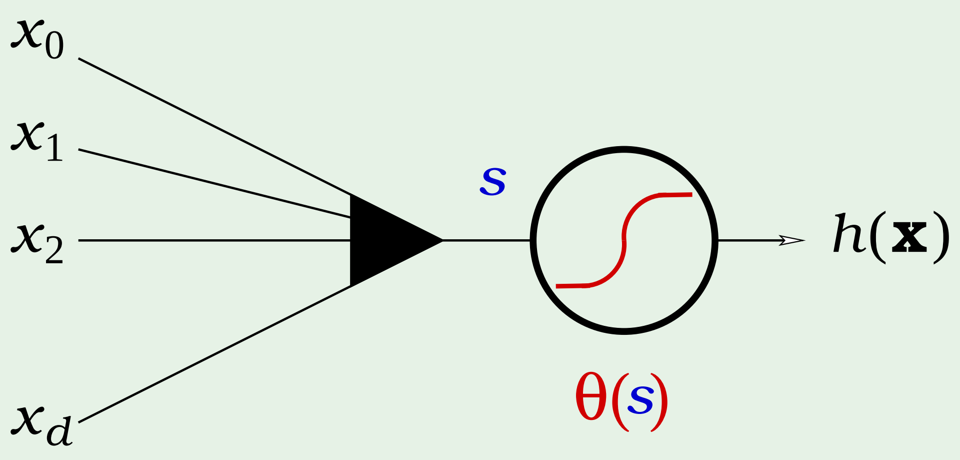
    Update the weights: $\mathbf{w}(t+1) = \mathbf{w}(t) - \eta \nabla E_{\text{in}}$
    Iterate to the next step until it is time to stop
Return the final weights $\mathbf{w}$

Summary of Linear Models



Review of Lecture 9

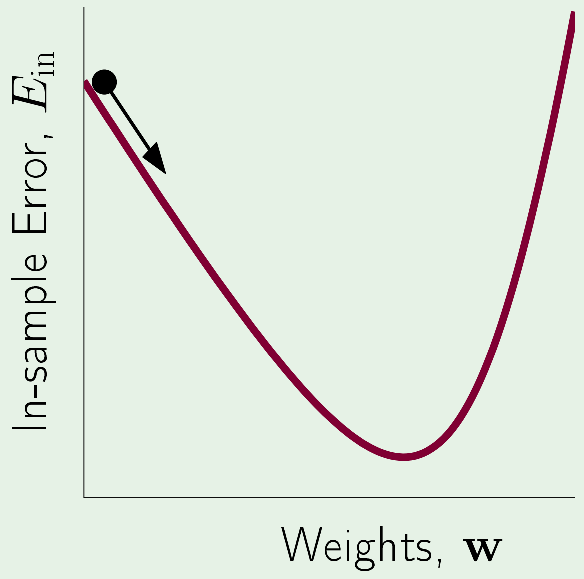
- Logistic regression



- Likelihood measure

$$\prod_{n=1}^{N} P(y_n \mid \mathbf{x}_n) = \prod_{n=1}^{N} \theta(y_n \mathbf{w}^{\mathsf{T}} \mathbf{x}_n)$$

- Gradient descent



- Initialize $\mathbf{w}(0)$
- For $t = 0, 1, 2, \cdots$ [to termination]

$$\mathbf{w}(t+1) = \mathbf{w}(t) - \eta \, \nabla E_{\text{in}}(\mathbf{w}(t))$$

- Return final $\mathbf{w}$

Learning From Data

Yaser S. Abu-Mostafa
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Lecture 10: Neural Networks

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Thursday, May 3, 2012

Outline

- Stochastic gradient descent
- Neural network model
- Backpropagation algorithm

Stochastic gradient descent

GD minimizes:

$$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} \underbrace{\mathbf{e}\left(h(\mathbf{x}_n), y_n\right)}_{\ln\left(1+e^{-y_n \mathbf{w}^{\mathsf{T}}\mathbf{x}_n}\right)}$$

$\longleftarrow$ in logistic regression

by iterative steps along $-\nabla E_{\text{in}}$:

$$\Delta\mathbf{w} = -\eta\,\nabla E_{\text{in}}(\mathbf{w})$$

∇E_{in} is based on all examples $(\mathbf{x}_n, y_n)$

"**batch**" GD

The stochastic aspect

Pick one $(\mathbf{x}_n, y_n)$ at a time. Apply GD to $\mathbf{e}\left(h(\mathbf{x}_n), y_n\right)$

"Average" direction: $$\mathbb{E}_n\left[-\nabla \mathbf{e}\left(h(\mathbf{x}_n), y_n\right)\right] = \frac{1}{N}\sum_{n=1}^{N} -\nabla \mathbf{e}\left(h(\mathbf{x}_n), y_n\right)$$

$$= -\nabla\, E_{\text{in}}$$

randomized version of GD

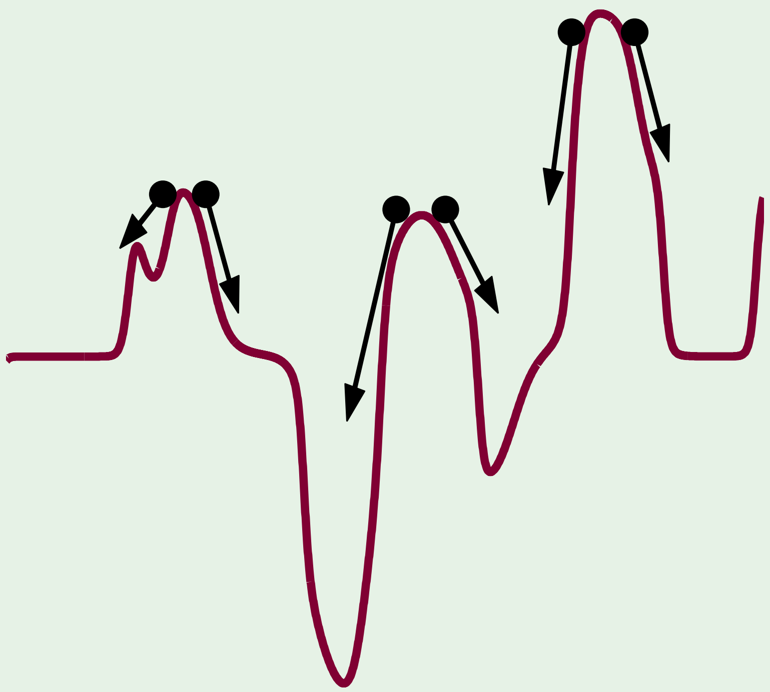
stochastic gradient descent (SGD)

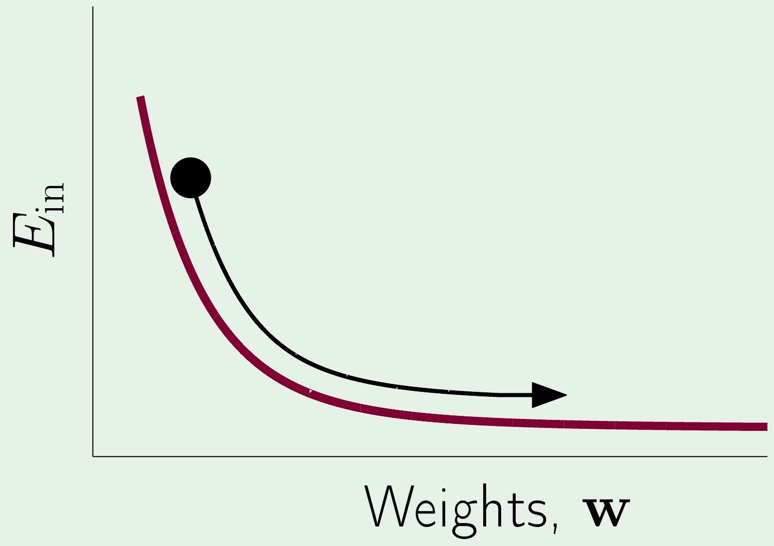
Benefits of SGD

1. cheaper computation

2. randomization

3. simple





Rule of thumb:

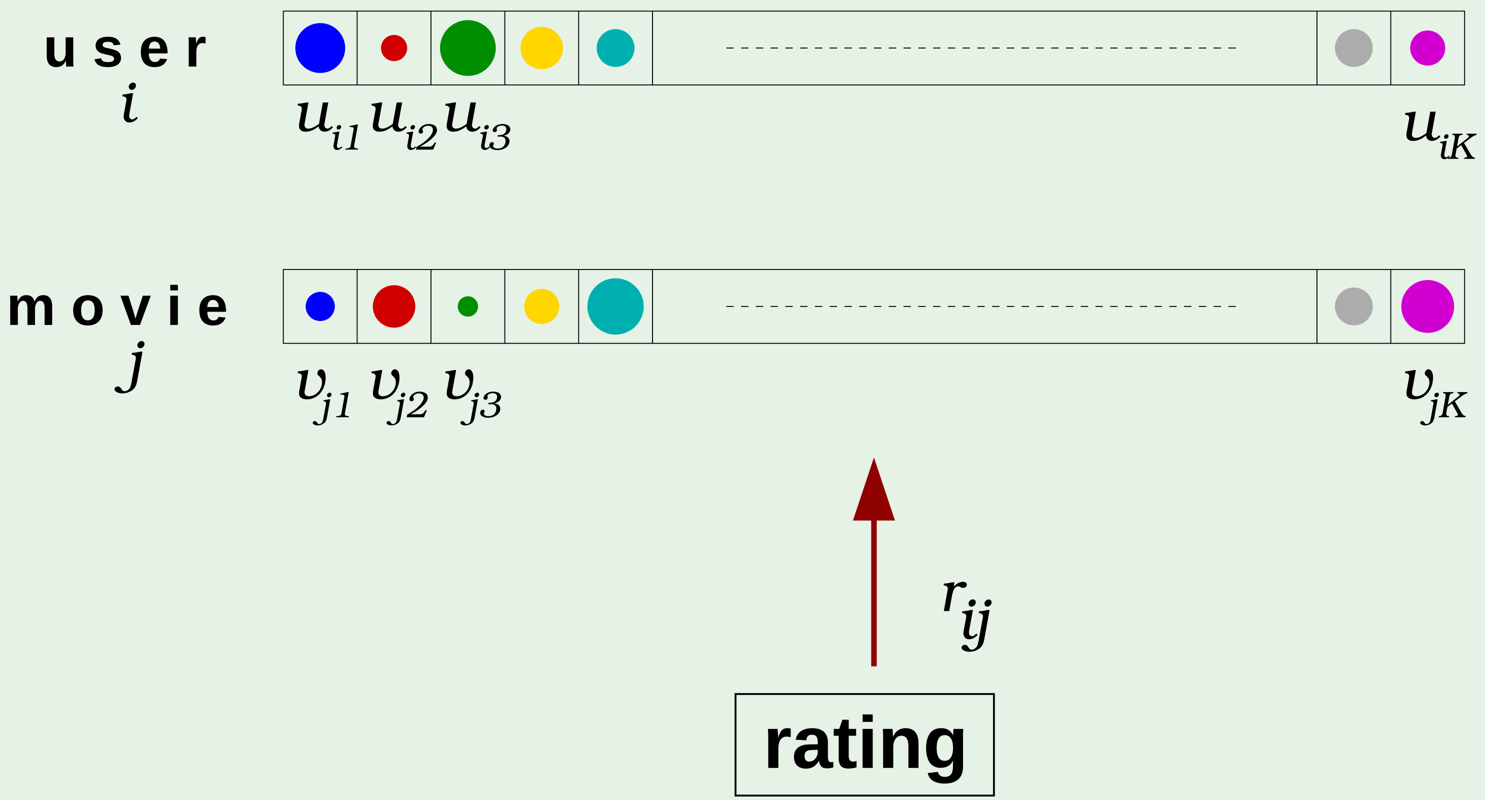
$\eta = 0.1$ works

randomization helps

SGD in action

Remember movie ratings?

$$\mathbf{e}_{ij} = \left(r_{ij} - \sum_{k=1}^{K} u_{ik} v_{jk} \right)^2$$

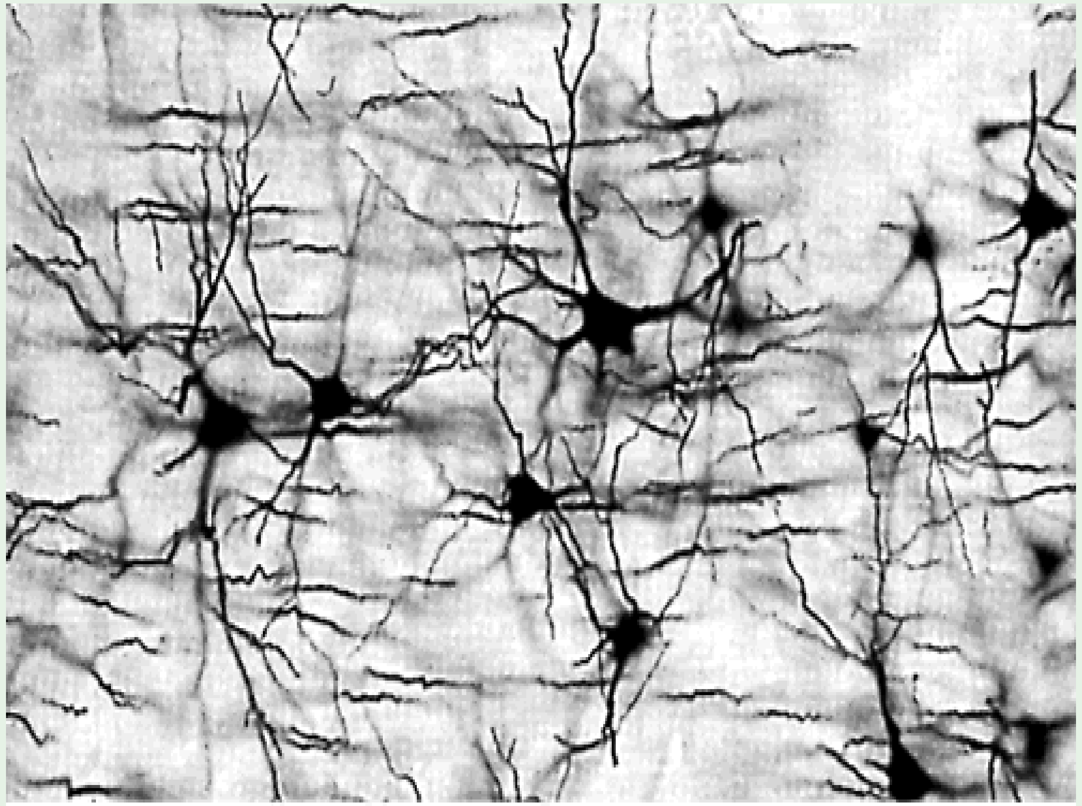


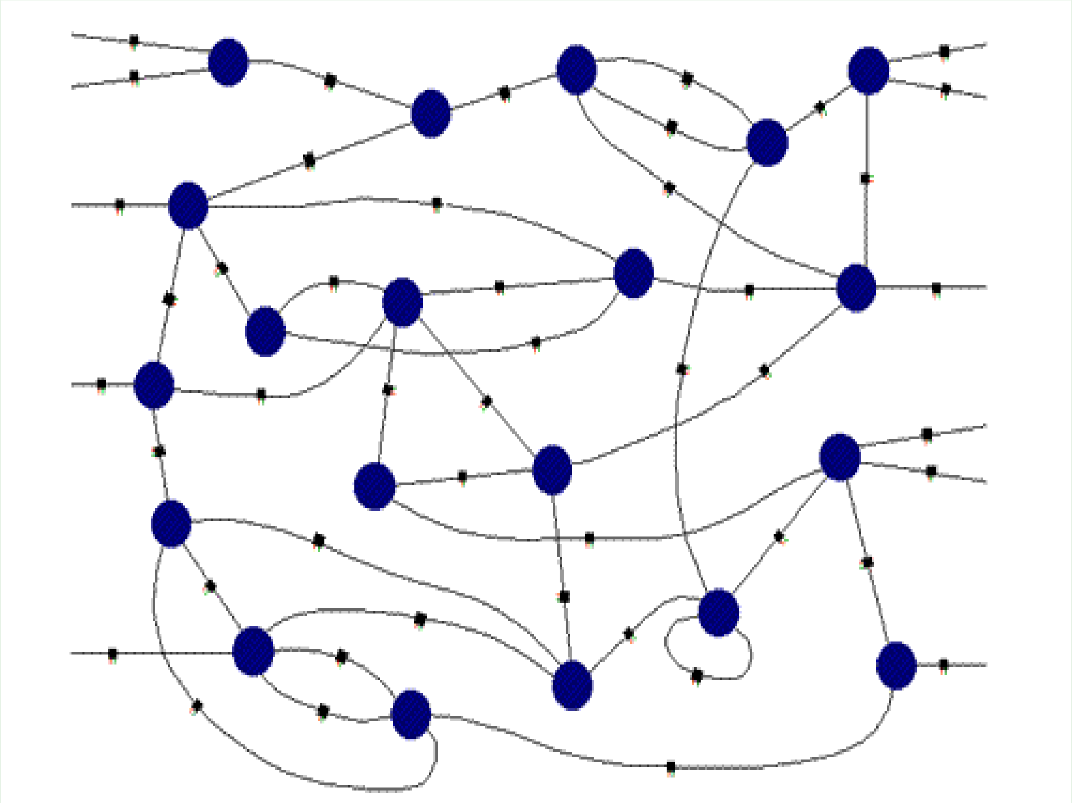
Outline

- Stochastic gradient descent
- Neural network model
- Backpropagation algorithm

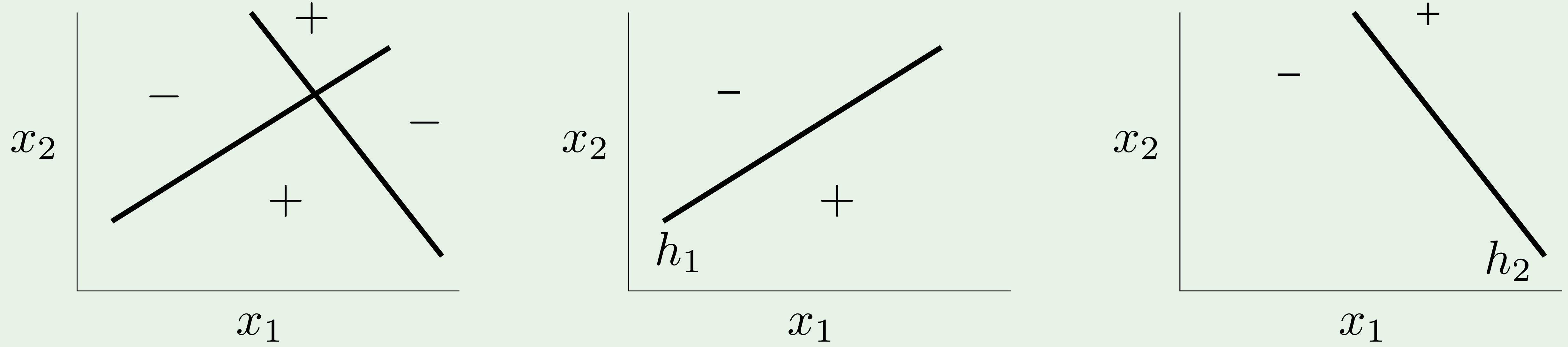
Biological inspiration

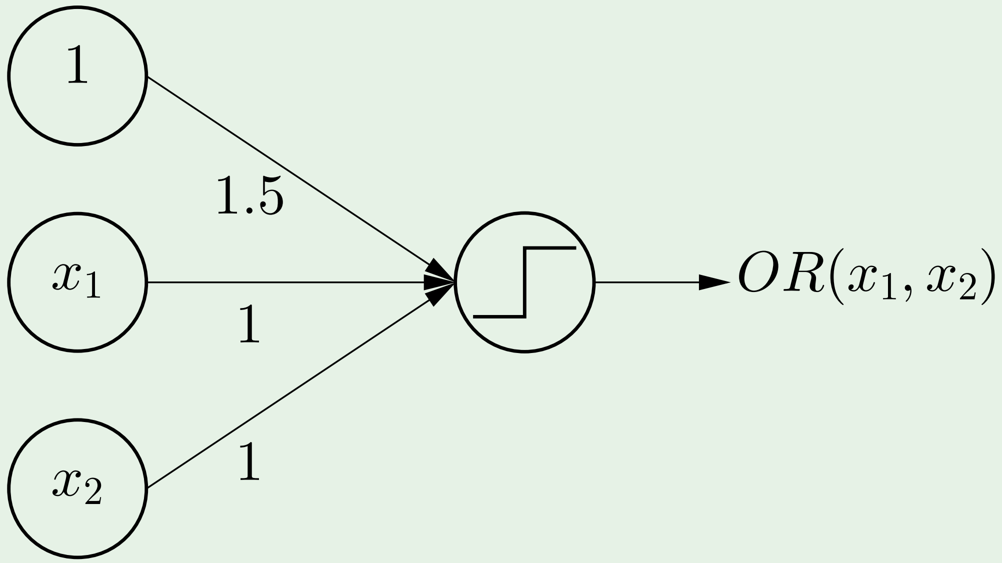
biological function $\longrightarrow$ biological structure

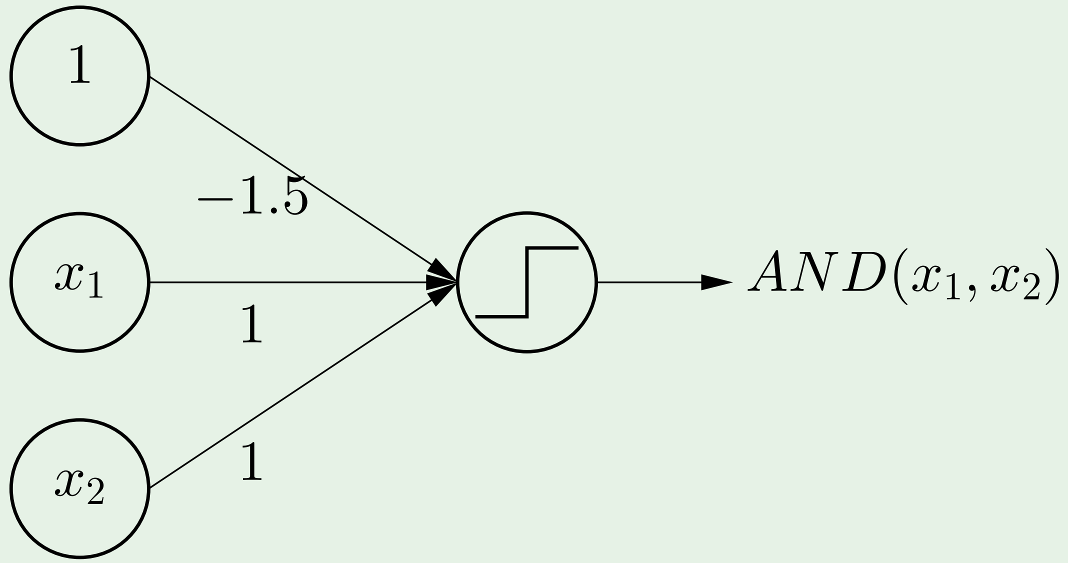




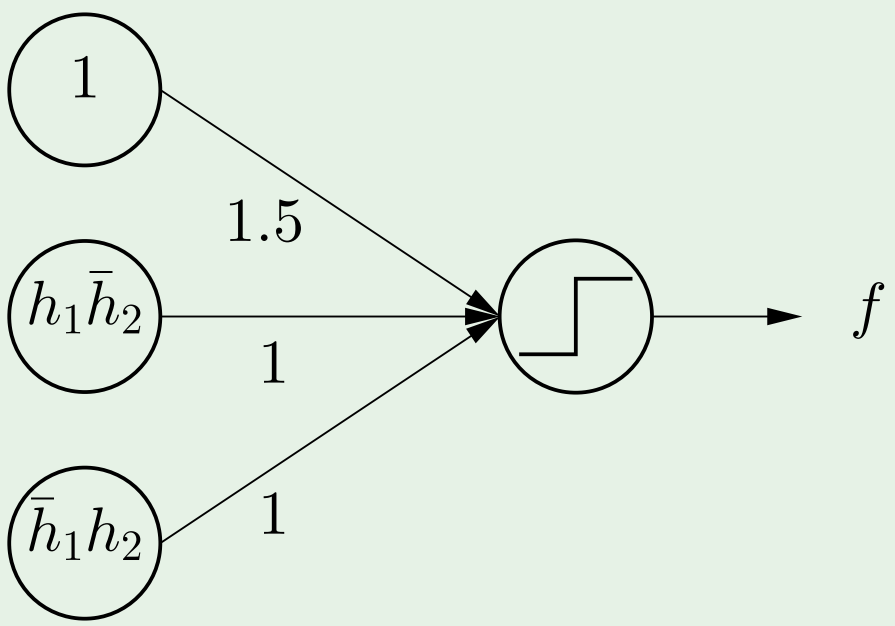
Combining perceptrons

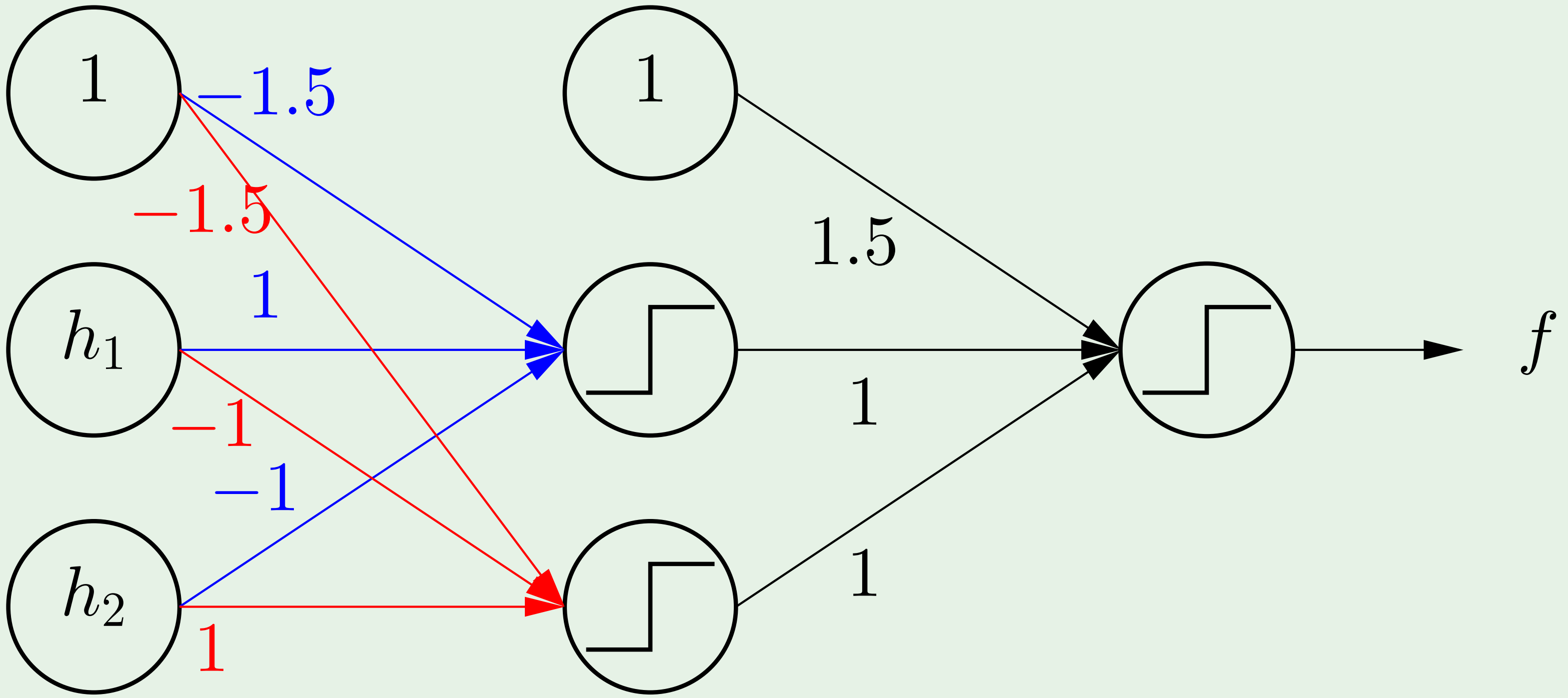




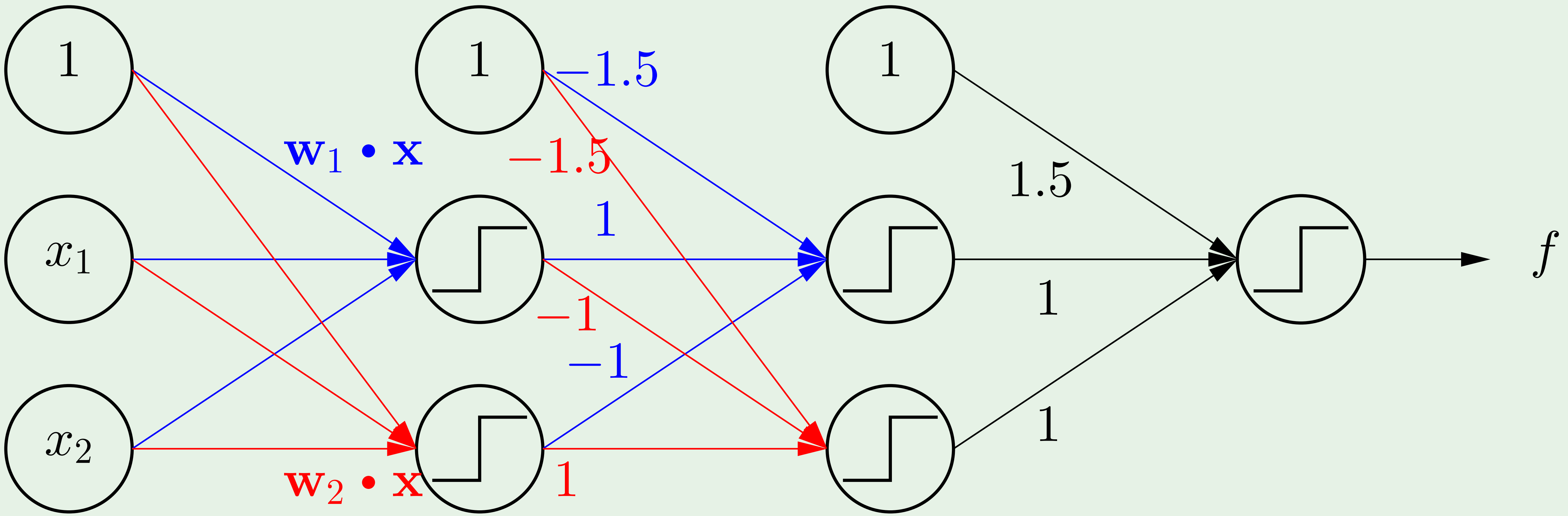


Creating layers



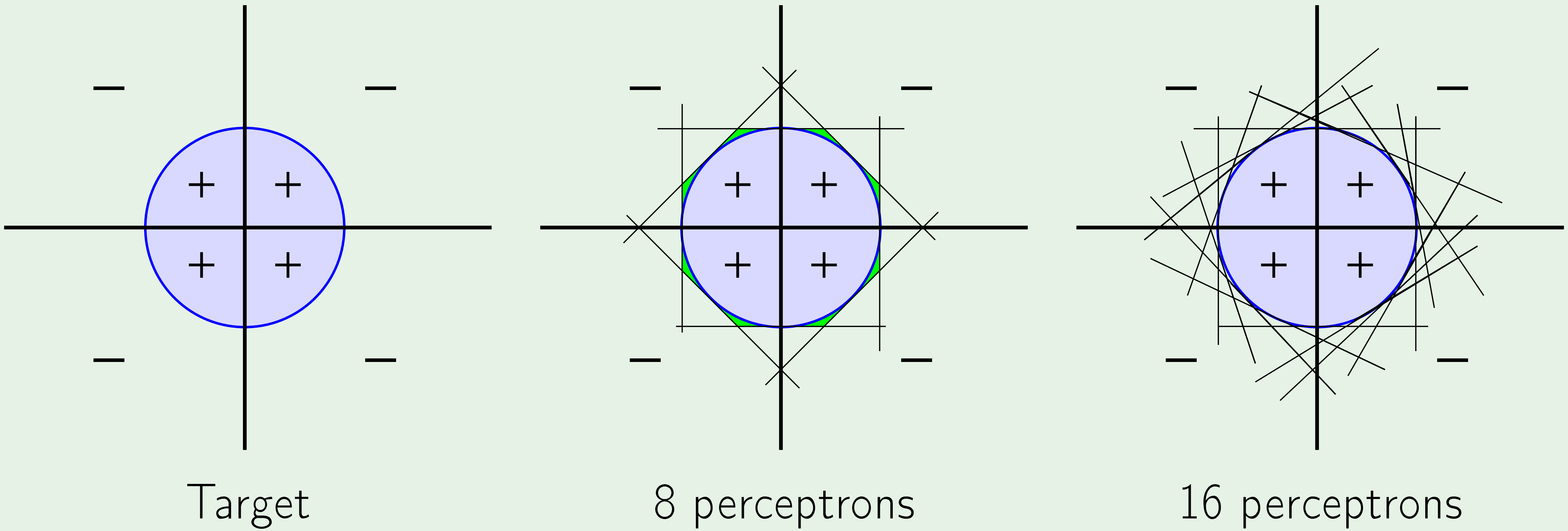


The multilayer perceptron



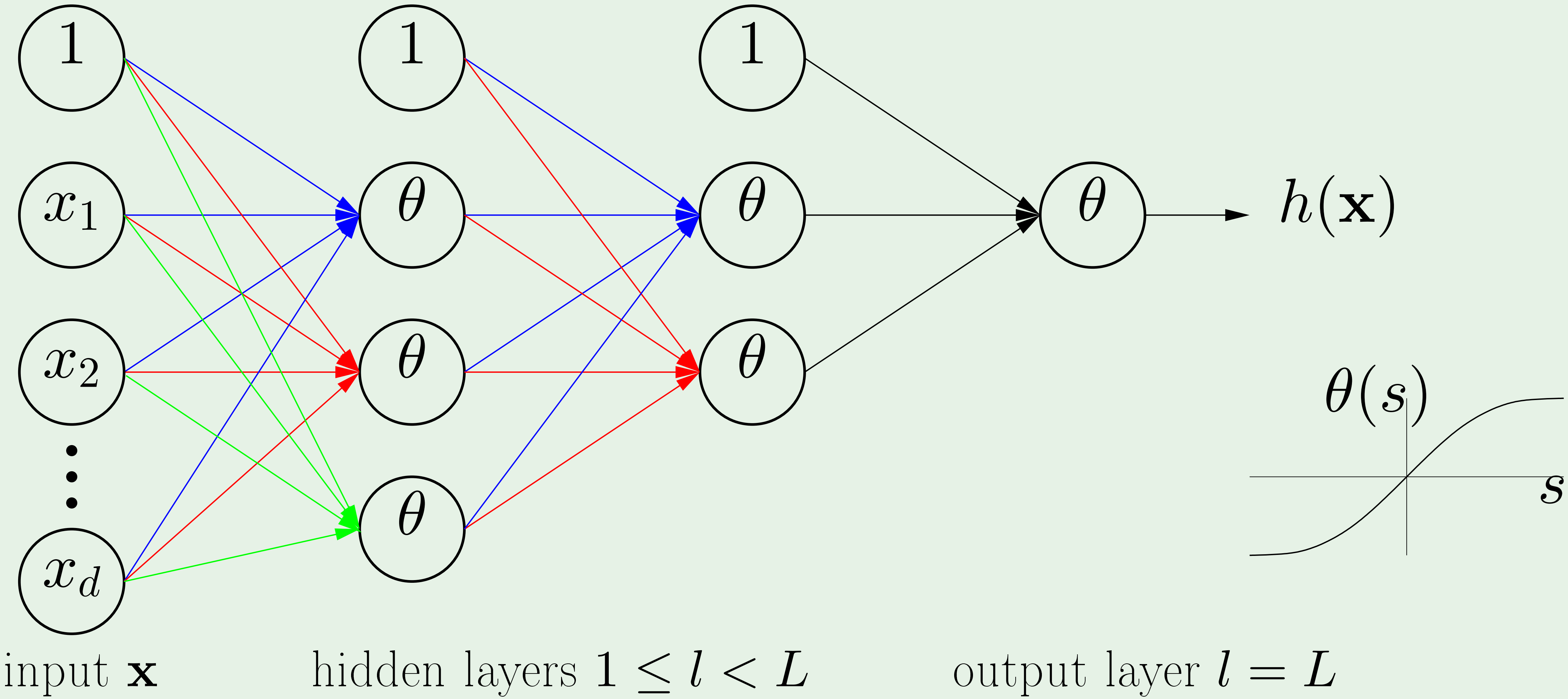
3 layers "feedforward"

A powerful model



2 red flags for **generalization** and **optimization**

The neural network

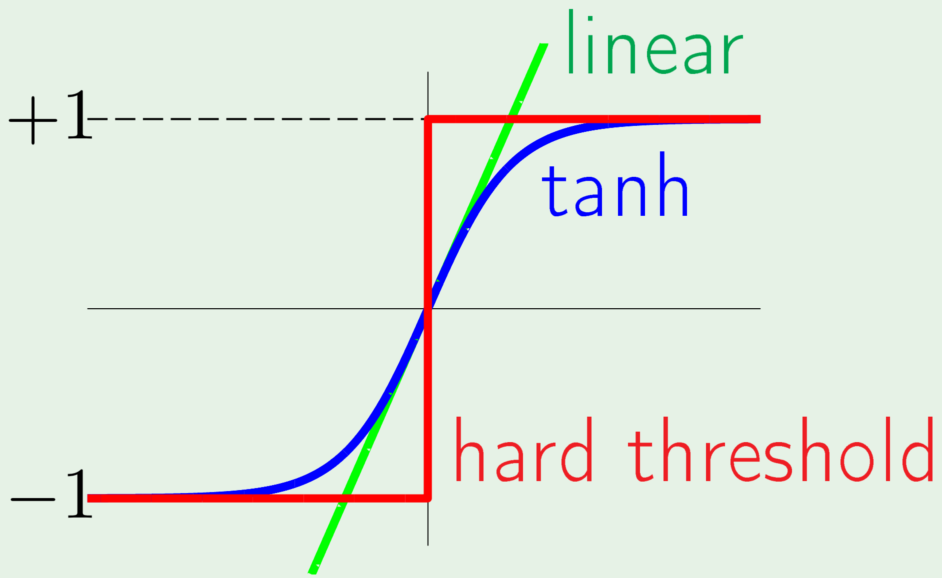


How the network operates

$$w_{ij}^{(l)} \quad \begin{cases} 1 \leq l \leq L & \text{layers} \\ 0 \leq i \leq d^{(l-1)} & \text{inputs} \\ 1 \leq j \leq d^{(l)} & \text{outputs} \end{cases}$$

$$x_j^{(l)} = \theta(s_j^{(l)}) = \theta\left(\sum_{i=0}^{d^{(l-1)}} w_{ij}^{(l)} \, x_i^{(l-1)}\right)$$

Apply $\mathbf{x}$ to $x_1^{(0)} \cdots x_{d^{(0)}}^{(0)} \rightarrow \rightarrow x_1^{(L)} = h(\mathbf{x})$



$$\theta(s) = \tanh(s) = \frac{e^s - e^{-s}}{e^s + e^{-s}}$$

Outline

- Stochastic gradient descent
- Neural network model
- Backpropagation algorithm

Applying SGD

All the weights $\mathbf{w} = \{w_{ij}^{(l)}\}$ determine $h(\mathbf{x})$

Error on example $(\mathbf{x}_n, y_n)$ is

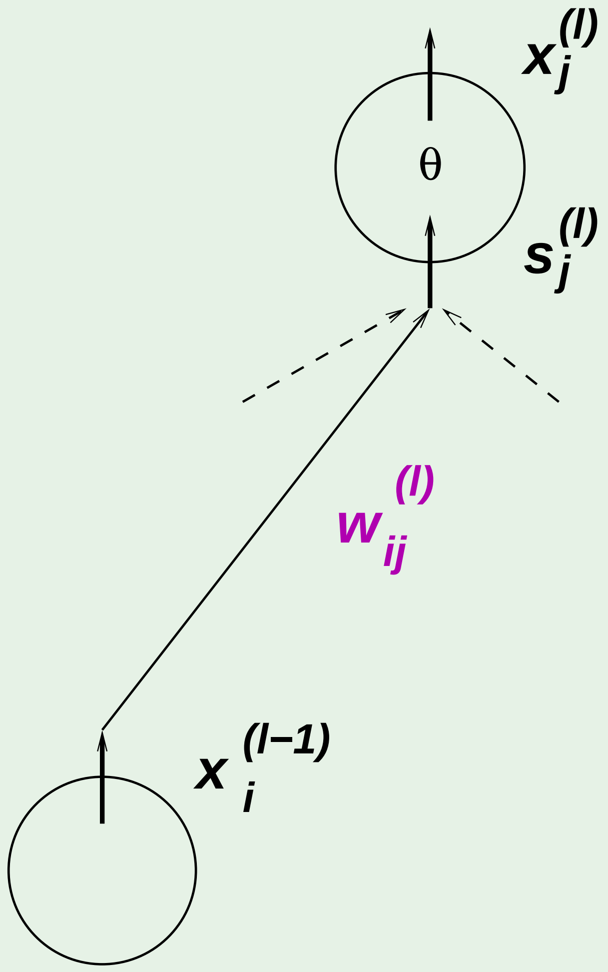
$$\mathbf{e}\left(h(\mathbf{x}_n), y_n\right) = \mathbf{e}(\mathbf{w})$$

To implement SGD, we need the gradient

$$\nabla \mathbf{e}(\mathbf{w}): \quad \frac{\partial\ \mathbf{e}(\mathbf{w})}{\partial\ w_{ij}^{(l)}} \quad \text{for all } i, j, l$$

Computing $\dfrac{\partial\ \mathrm{e}(\mathbf{w})}{\partial\ w_{ij}^{(l)}}$

We can evaluate $\dfrac{\partial\ \mathrm{e}(\mathbf{w})}{\partial\ w_{ij}^{(l)}}$ one by one: analytically or numerically



A trick for efficient computation:

$$\frac{\partial\ \mathrm{e}(\mathbf{w})}{\partial\ w_{ij}^{(l)}} = \frac{\partial\ \mathrm{e}(\mathbf{w})}{\partial\ s_j^{(l)}} \times \frac{\partial\ s_j^{(l)}}{\partial\ w_{ij}^{(l)}}$$

We have $\dfrac{\partial\ s_j^{(l)}}{\partial\ w_{ij}^{(l)}} = x_i^{(l-1)}$ We only need: $\dfrac{\partial\ \mathrm{e}(\mathbf{w})}{\partial\ s_j^{(l)}} = \delta_j^{(l)}$

δ for the final layer

$$\delta_j^{(l)} = \frac{\partial\ \mathrm{e}(\mathbf{w})}{\partial\ s_j^{(l)}}$$

For the final layer $l = L$ and $j = 1$:

$$\delta_1^{(L)} = \frac{\partial\ \mathrm{e}(\mathbf{w})}{\partial\ s_1^{(L)}}$$

$$\mathrm{e}(\mathbf{w}) = (\ x_1^{(L)} - \ y_n)^2$$

$$x_1^{(L)} = \theta(s_1^{(L)})$$

$$\theta'(s) = 1 - \theta^2(s)$$ for the tanh

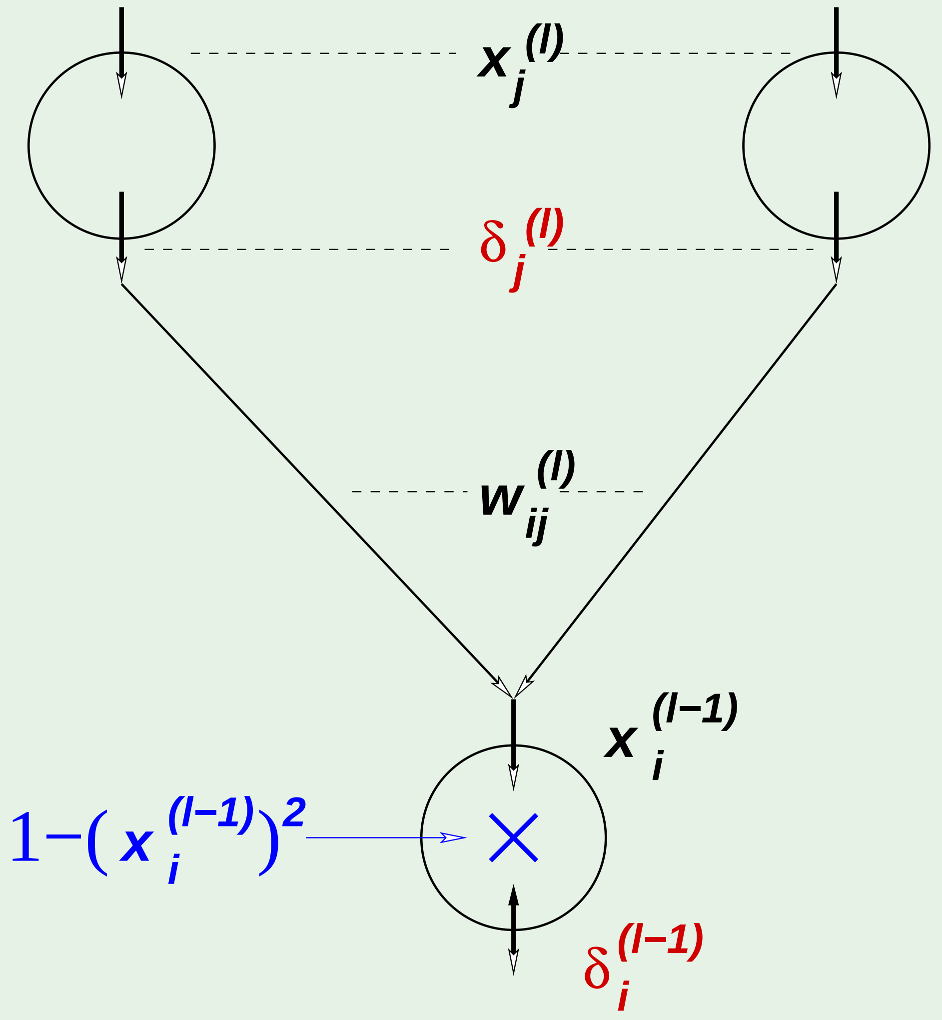
Back propagation of δ

$$\delta_i^{(l-1)} = \frac{\partial\, \mathbf{e}(\mathbf{w})}{\partial\, s_i^{(l-1)}}$$

$$= \sum_{j=1}^{d^{(l)}} \frac{\partial\, \mathbf{e}(\mathbf{w})}{\partial\, s_j^{(l)}} \times \frac{\partial\, s_j^{(l)}}{\partial\, x_i^{(l-1)}} \times \frac{\partial\, x_i^{(l-1)}}{\partial\, s_i^{(l-1)}}$$

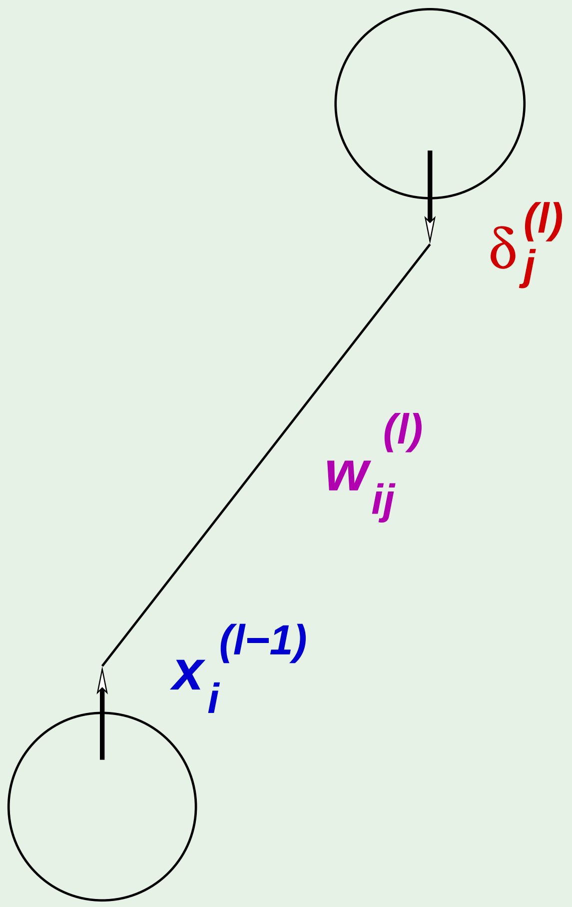
$$= \sum_{j=1}^{d^{(l)}} \delta_j^{(l)} \times w_{ij}^{(l)} \times \theta'(s_i^{(l-1)})$$

$$\delta_i^{(l-1)} = (1 - (x_i^{(l-1)})^2) \sum_{j=1}^{d^{(l)}} w_{ij}^{(l)}\, \delta_j^{(l)}$$



Backpropagation algorithm

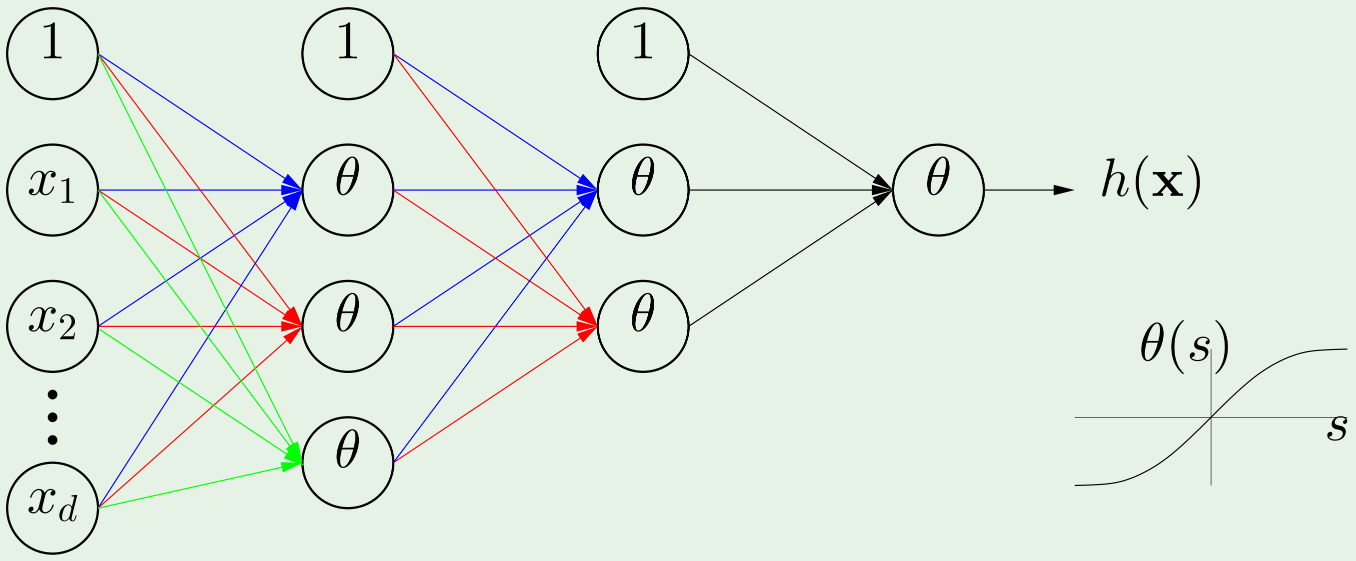
Initialize all weights $w_{ij}^{(l)}$ at random
for $t = 0, 1, 2, \ldots$ **do**
    Pick $n \in \{1, 2, \cdots, N\}$
    Forward: Compute all $x_j^{(l)}$
    Backward: Compute all $\delta_j^{(l)}$
    Update the weights: $w_{ij}^{(l)} \leftarrow w_{ij}^{(l)} - \eta\, x_i^{(l-1)} \delta_j^{(l)}$
    Iterate to the next step until it is time to stop
Return the final weights $w_{ij}^{(l)}$



Final remark: hidden layers

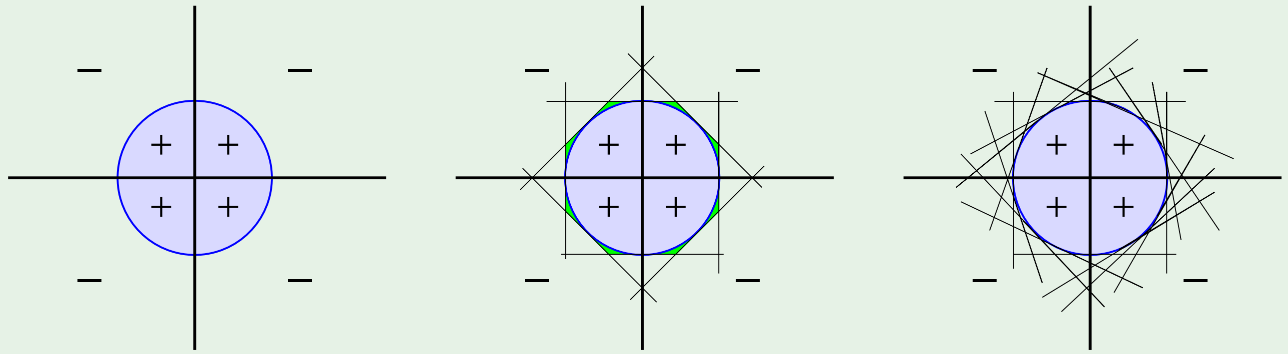
learned nonlinear transform

interpretation?



Review of Lecture 10

- Multilayer perceptrons

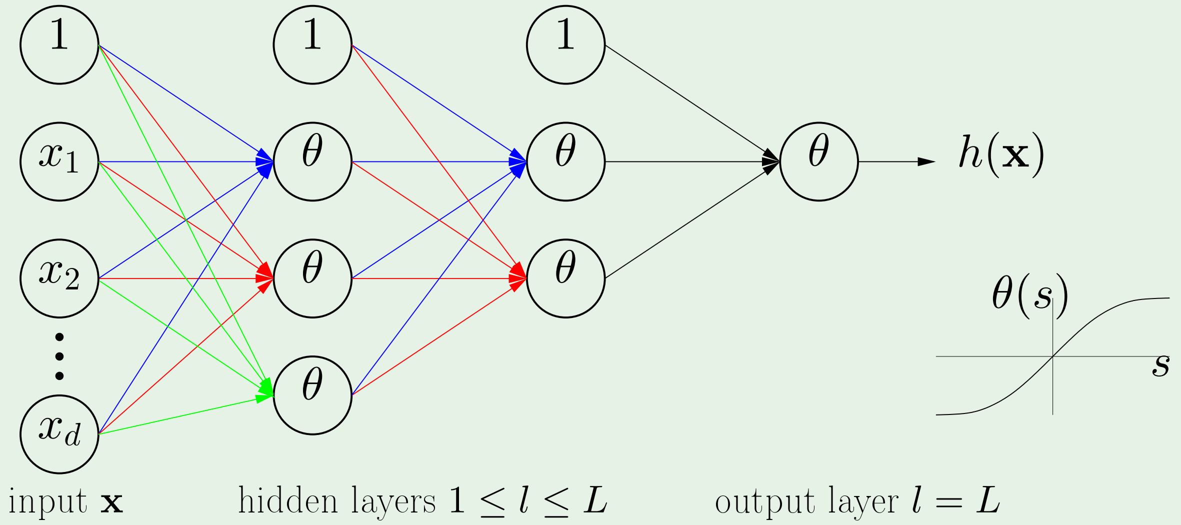


Logical combinations of perceptrons

- Neural networks

$$x_j^{(l)} = \theta\left(\sum_{i=0}^{d^{(l-1)}} w_{ij}^{(l)}\; x_i^{(l-1)}\right)$$

where $\theta(s) = \tanh(s)$



- Backpropagation

$$\Delta w_{ij}^{(l)} = -\eta\; x_i^{(l-1)} \delta_j^{(l)}$$

where

$$\delta_i^{(l-1)} = (1 - (x_i^{(l-1)})^2) \sum_{j=1}^{d^{(l)}} w_{ij}^{(l)}\; \delta_j^{(l)}$$

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Lecture 11: Overfitting

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Tuesday, May 8, 2012

Outline

- What is overfitting?
- The role of noise
- Deterministic noise
- Dealing with overfitting

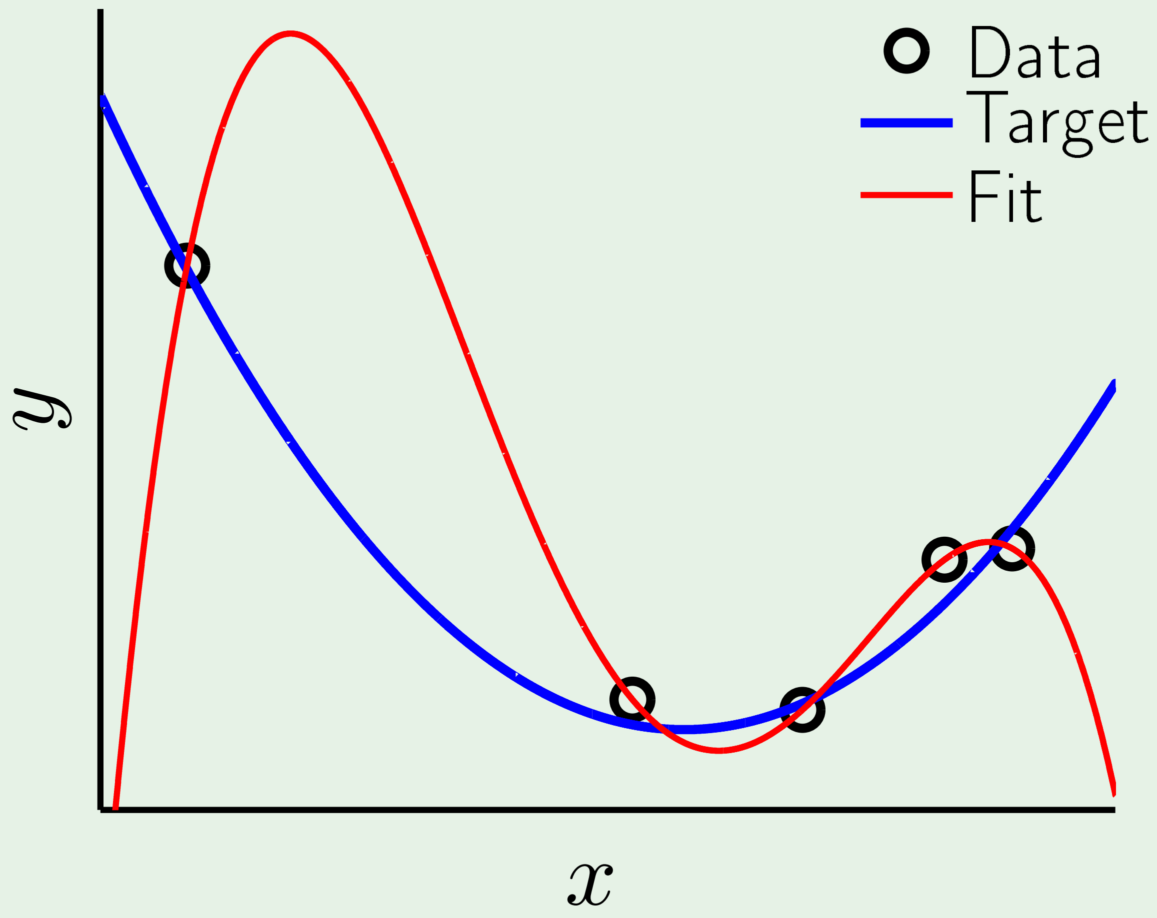
Illustration of overfitting

Simple target function

5 data points- **noisy**

4th-order polynomial fit

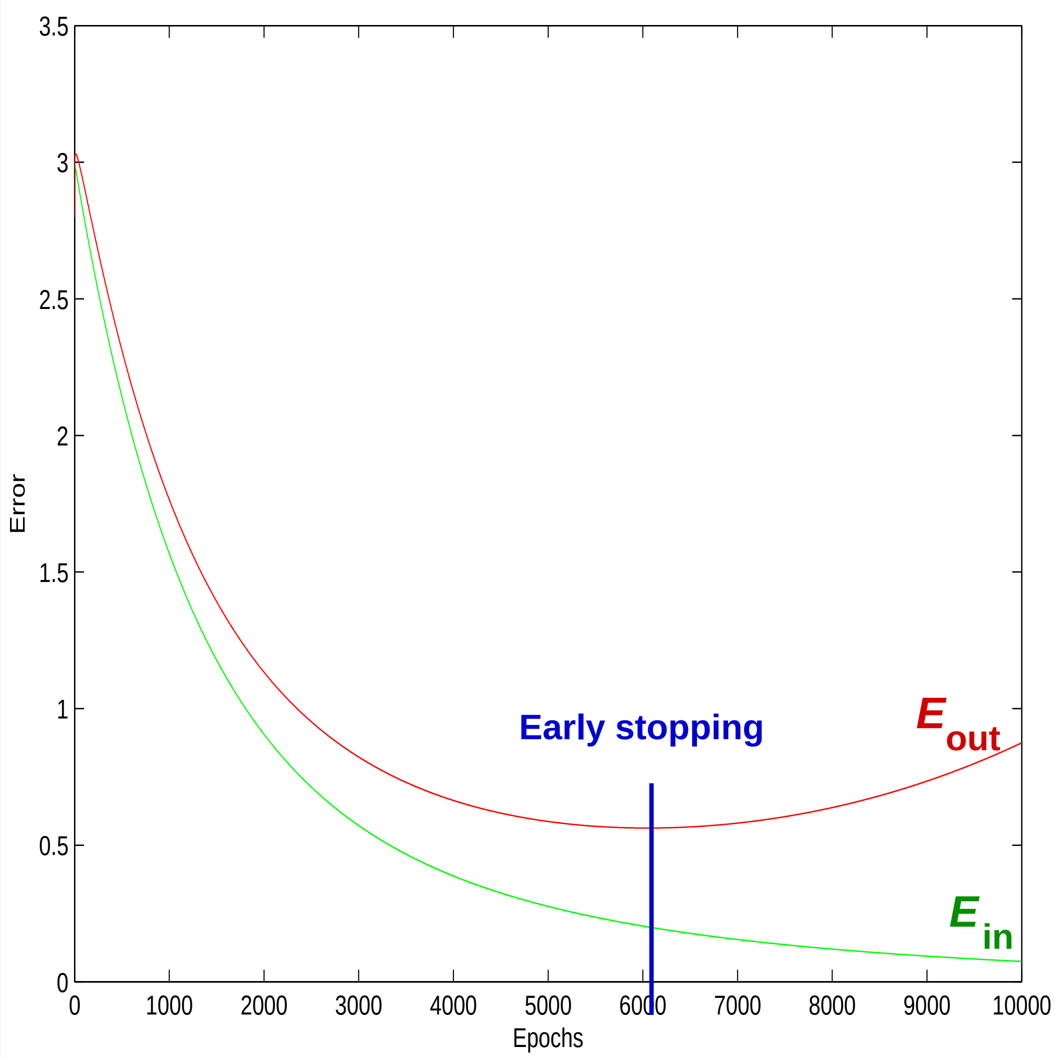
$$E_{\text{in}} = 0, \quad E_{\text{out}} \text{ is huge}$$



Overfitting versus bad generalization

Neural network fitting noisy data

Overfitting: $E_{\text{in}} \downarrow \qquad E_{\text{out}} \uparrow$



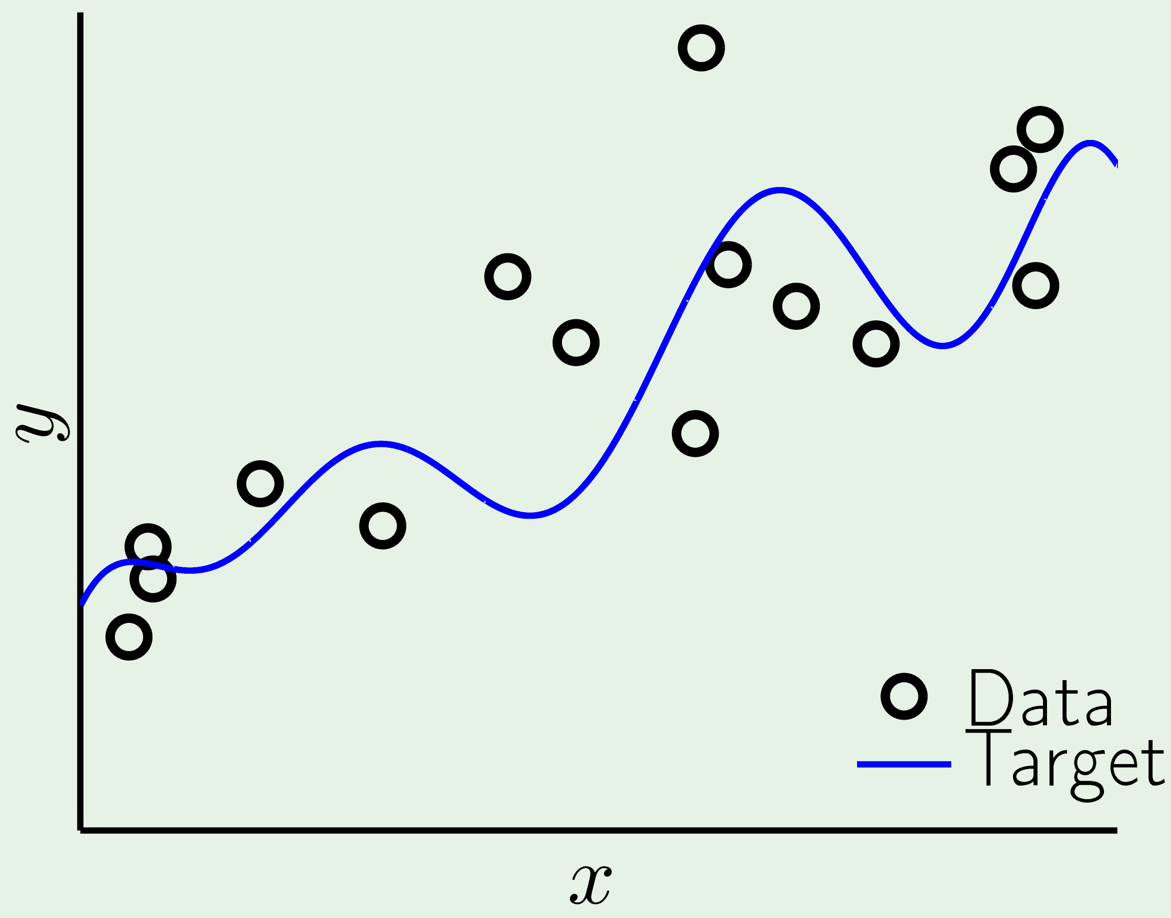
The culprit

Overfitting: "fitting the data more than is warranted"

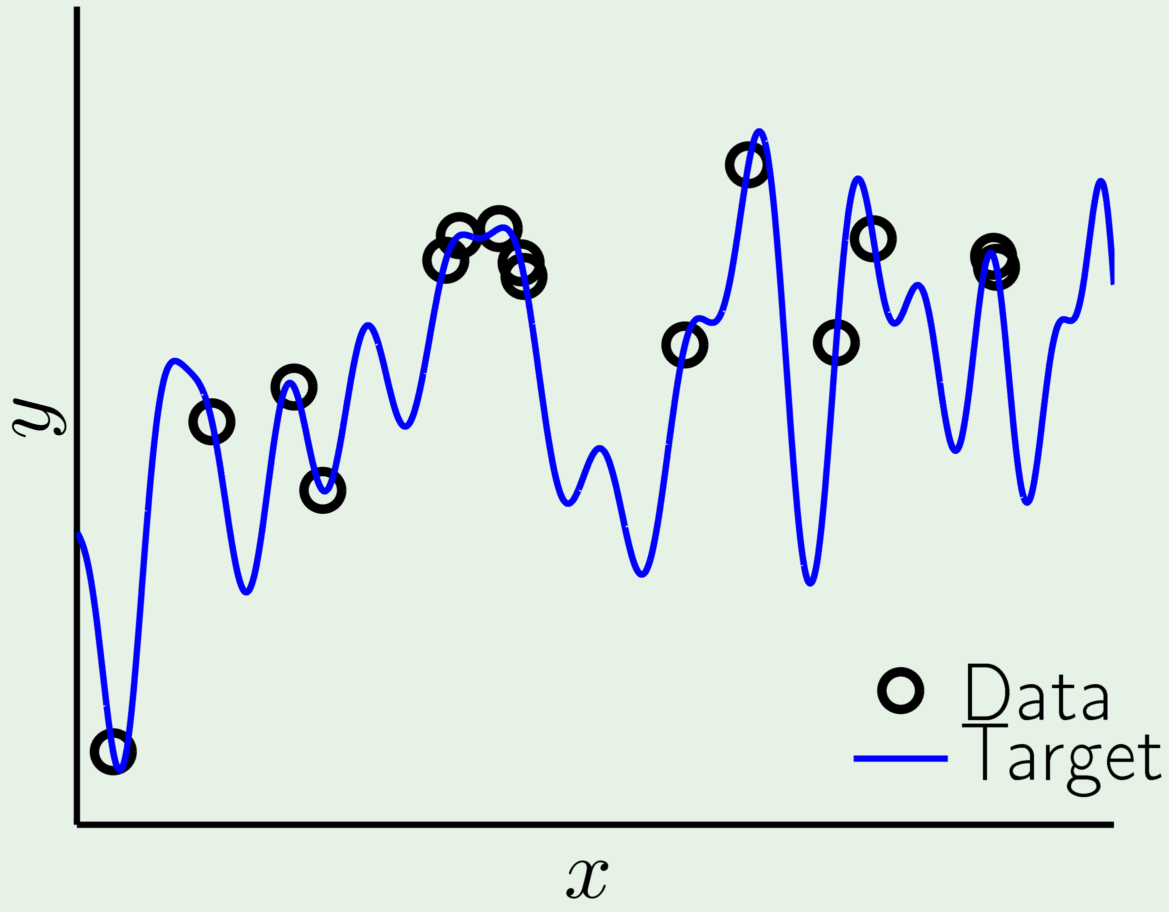
Culprit: fitting the noise - harmful

Case study

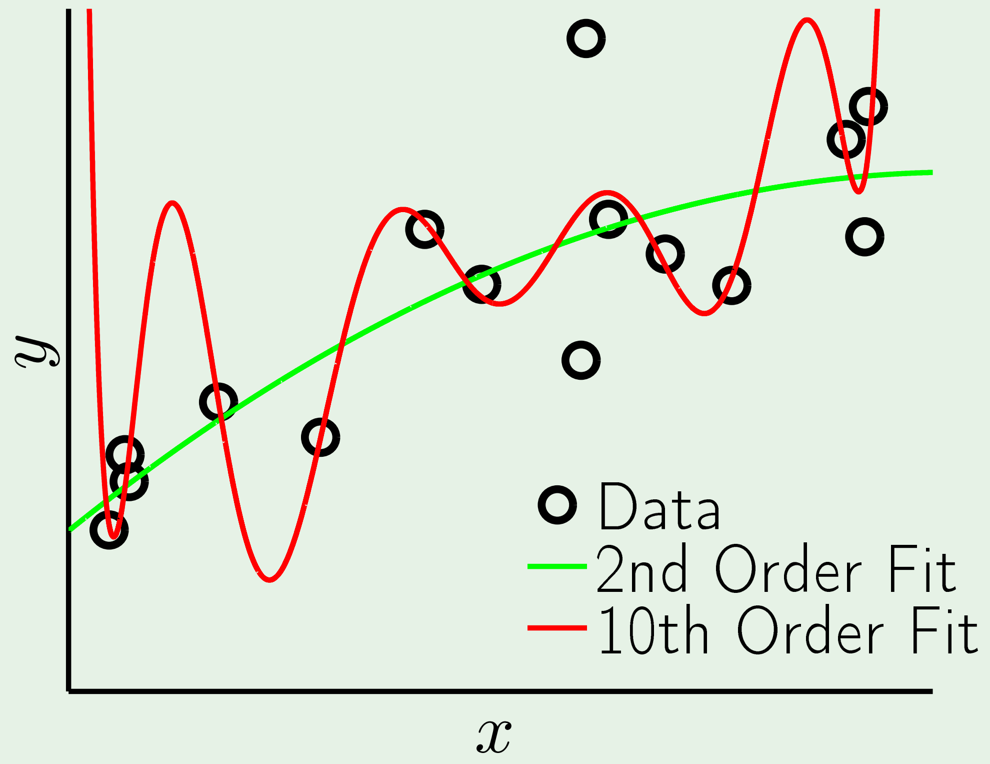
10th-order target + noise

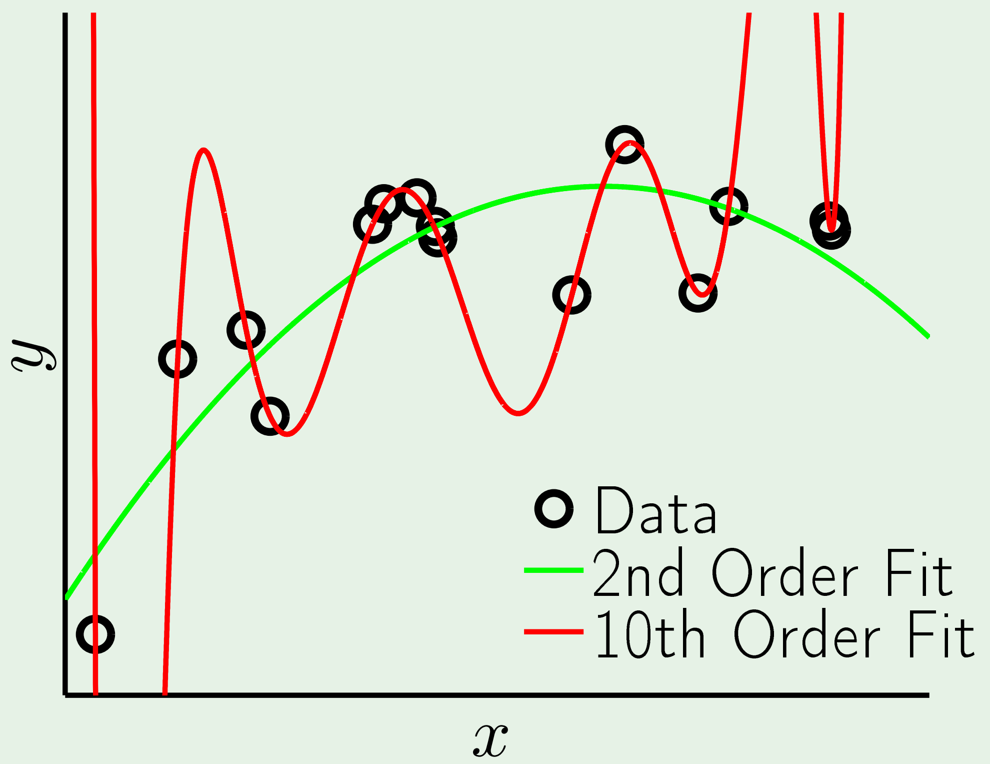


50th-order target



Two fits for each target





Noisy low-order target

	2nd Order	10th Order
E_{in}	0.050	0.034
E_{out}	0.127	**9.00**

Noiseless high-order target

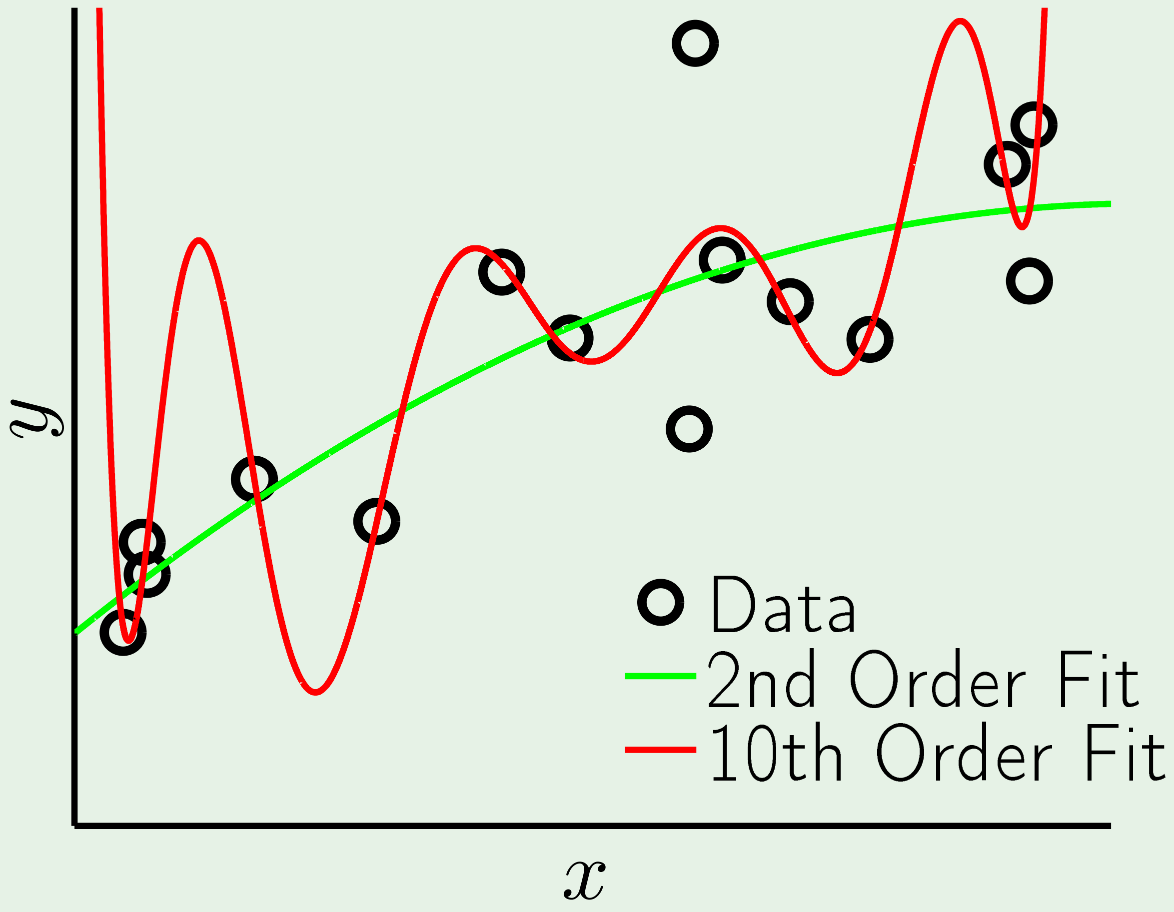
	2nd Order	10th Order
E_{in}	0.029	10^{-5}
E_{out}	0.120	**7680**

An irony of two learners

Two learners O and R

They <u>know</u> the target is 10th order

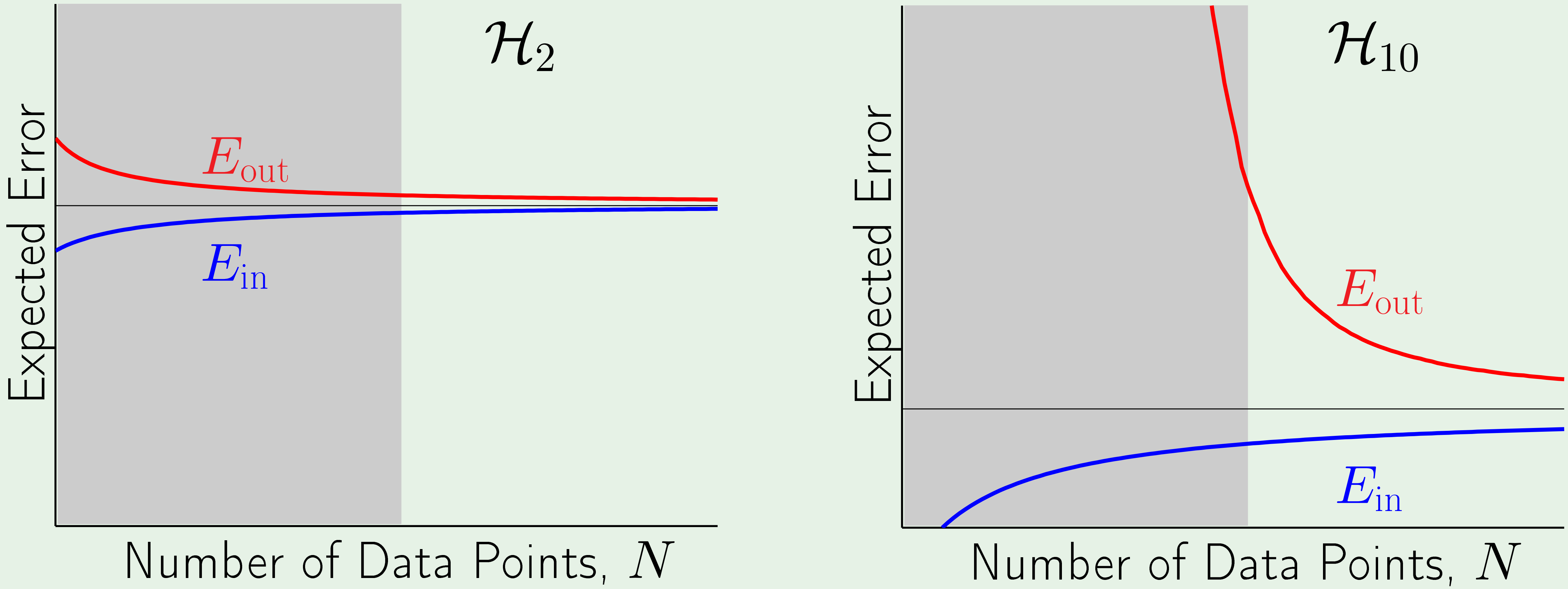
O chooses $\mathcal{H}_{10}$ R chooses $\mathcal{H}_2$



Learning a 10th-order target

We have seen this case

Remember learning curves?

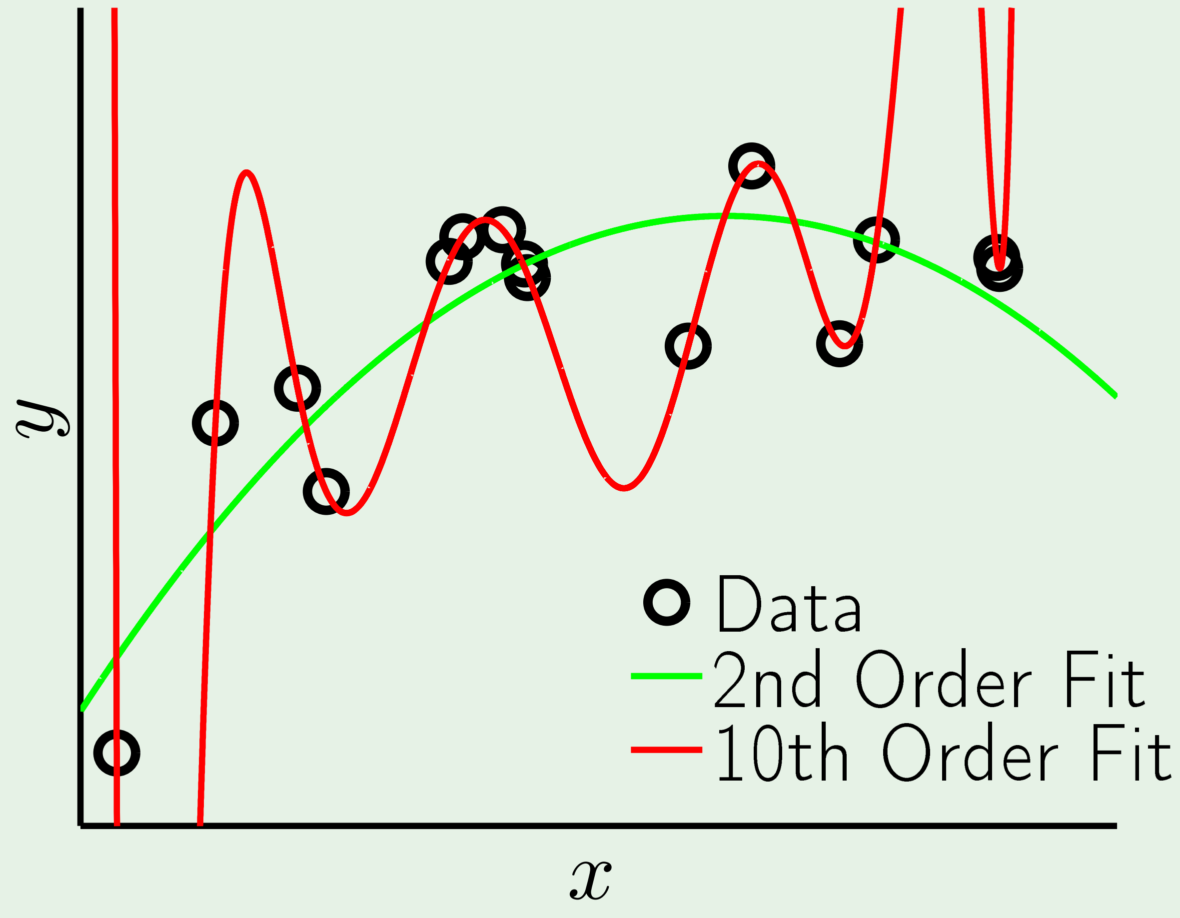


Even without noise

The two learners $\mathcal{H}_{10}$ and $\mathcal{H}_2$

They know there is no noise

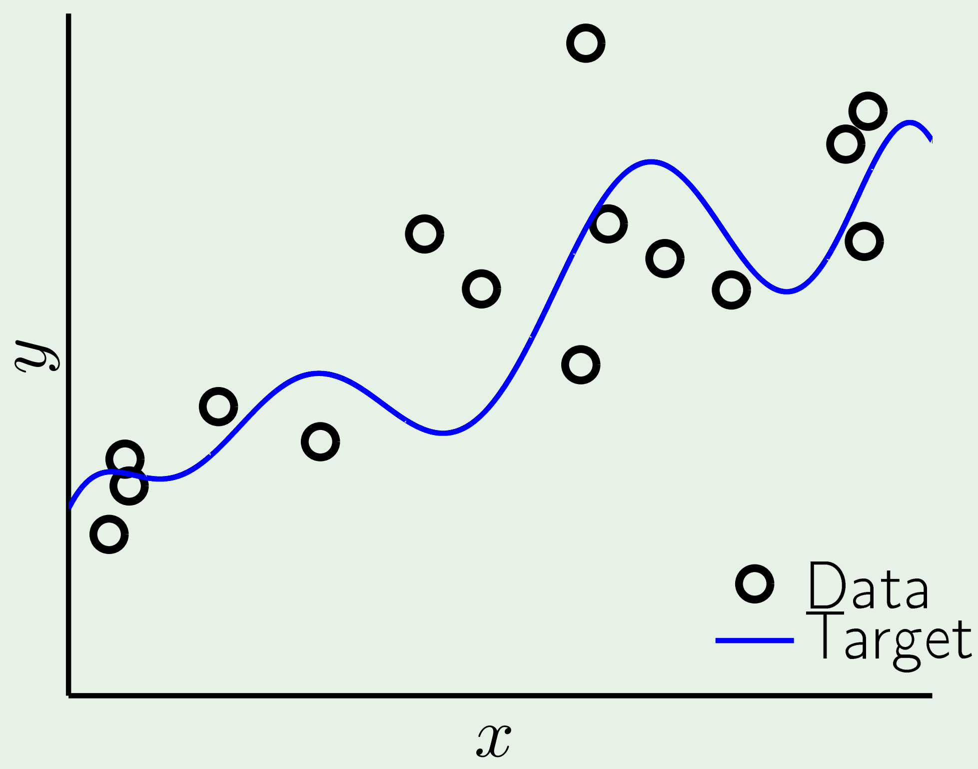
Is there really no noise?



Learning a 50th-order target

A detailed experiment

Impact of **noise level** and **target complexity**



$$y = f(x) + \underbrace{\epsilon(x)}_{\sigma^2} = \underbrace{\sum_{q=0}^{Q_f} \alpha_q \, x^q}_{\text{normalized}} + \epsilon(x)$$

noise level: σ^2

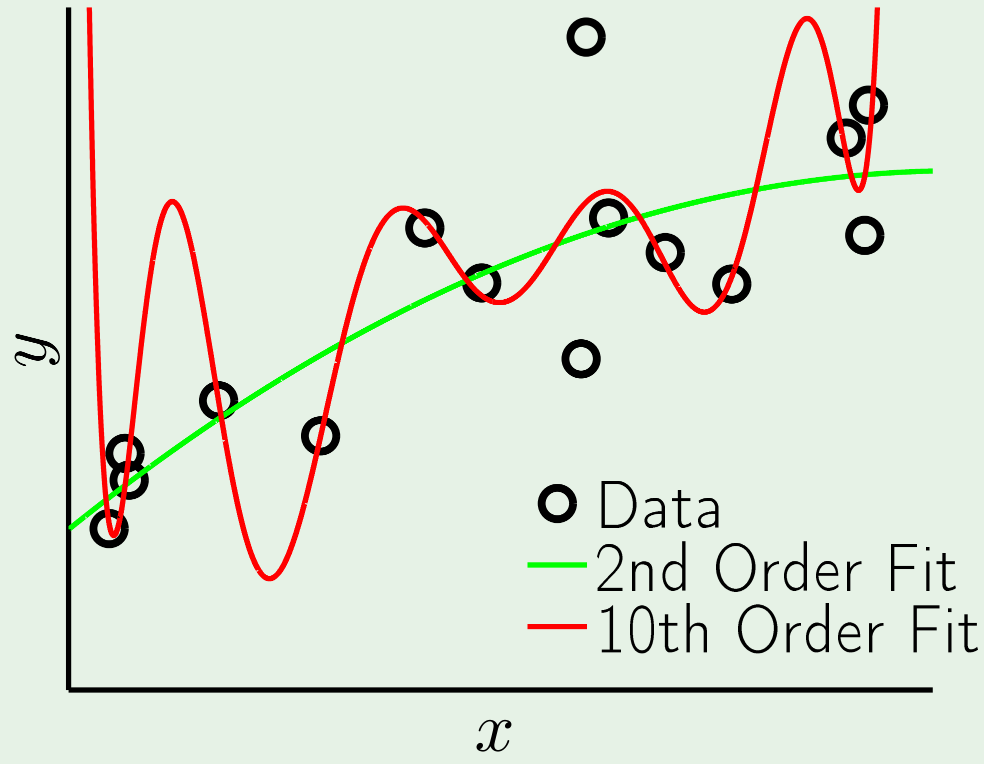
target complexity: Q_f

data set size: N

The overfit measure

We fit the data set $(x_1, y_1), \cdots, (x_N, y_N)$ using our two models:

$\mathcal{H}_2$: 2nd-order polynomials $\quad\quad$ $\mathcal{H}_{10}$: 10th-order polynomials

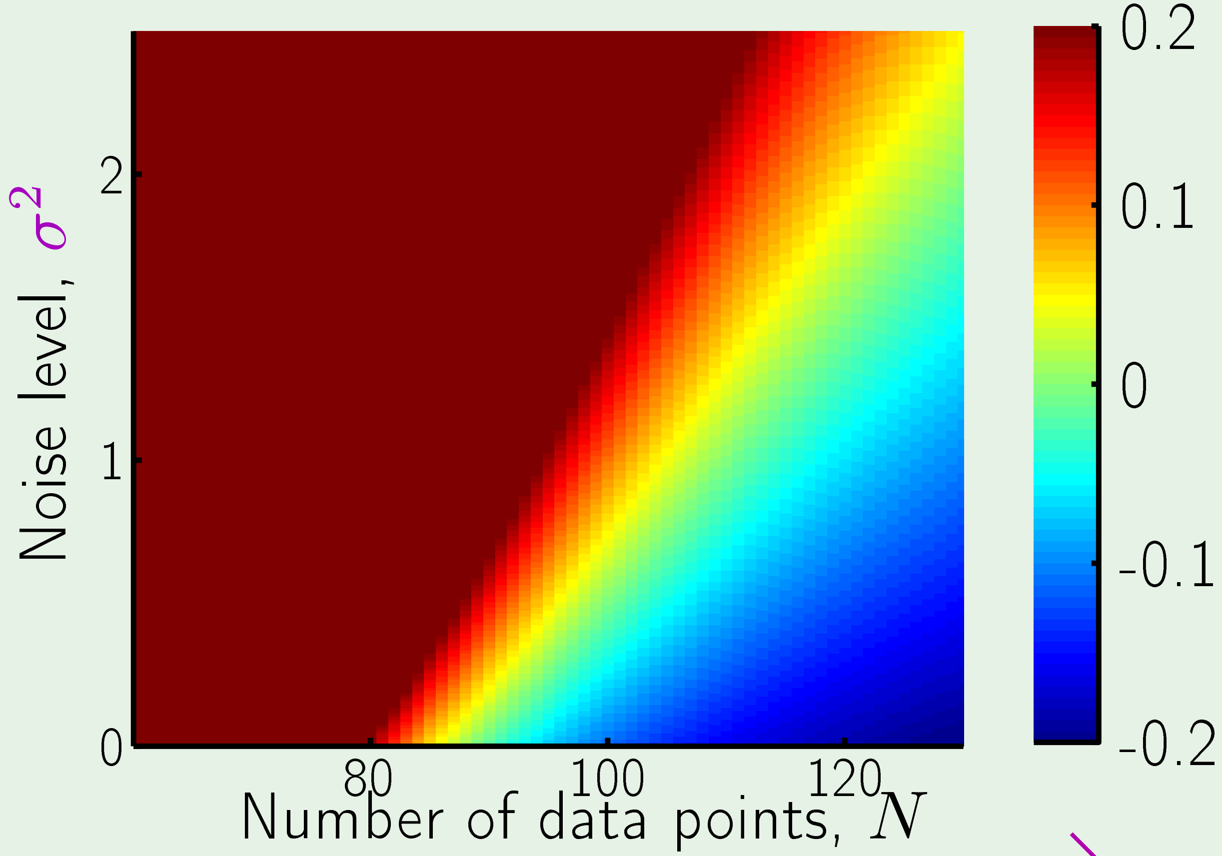


Compare out-of-sample errors of

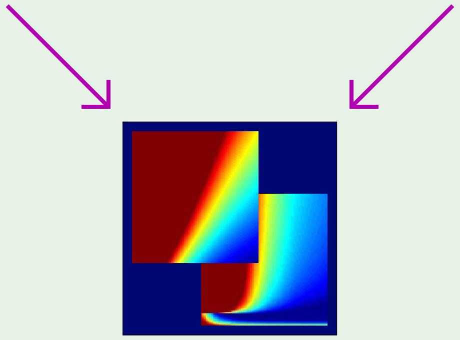
$$g_2 \in \mathcal{H}_2 \quad \text{and} \quad g_{10} \in \mathcal{H}_{10}$$

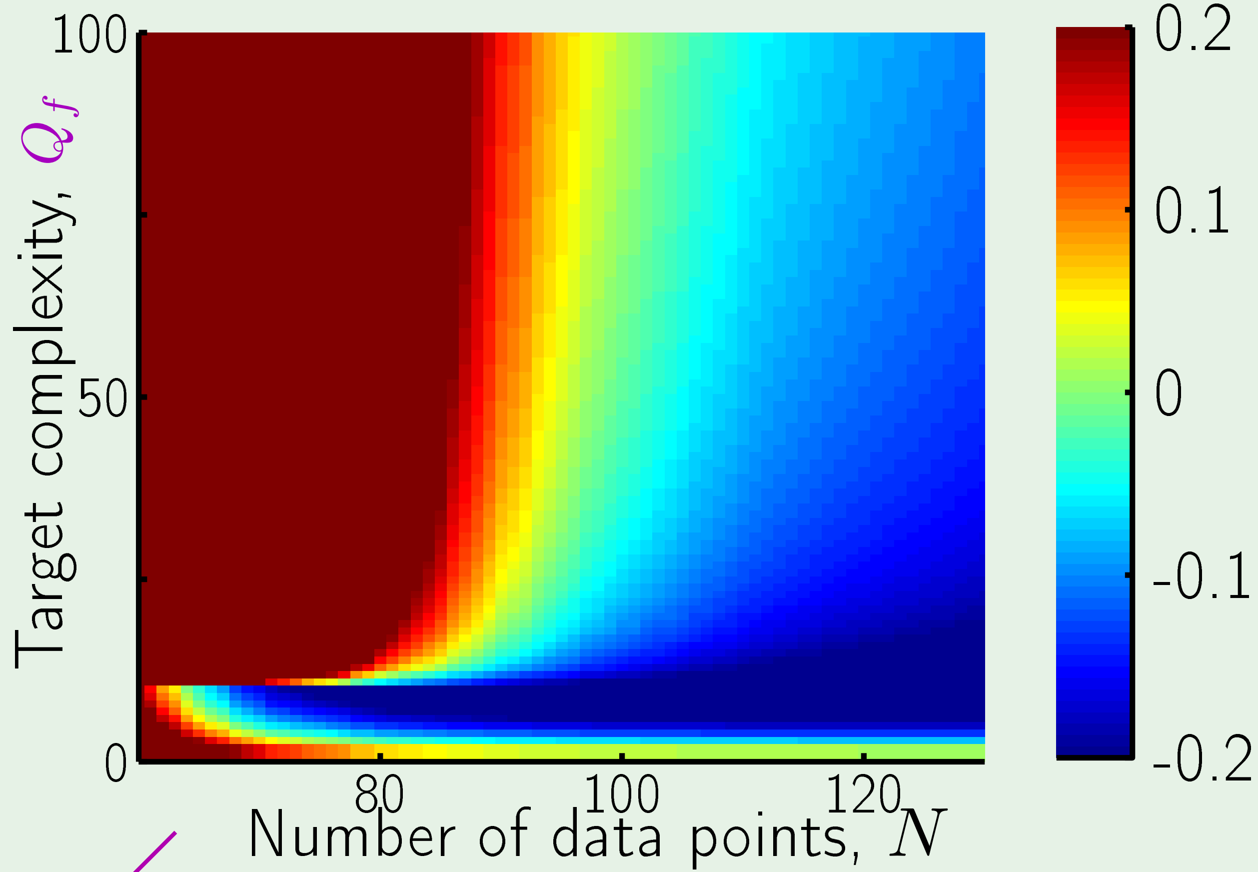
overfit measure: $E_{\text{out}}(g_{10}) - E_{\text{out}}(g_2)$

The results



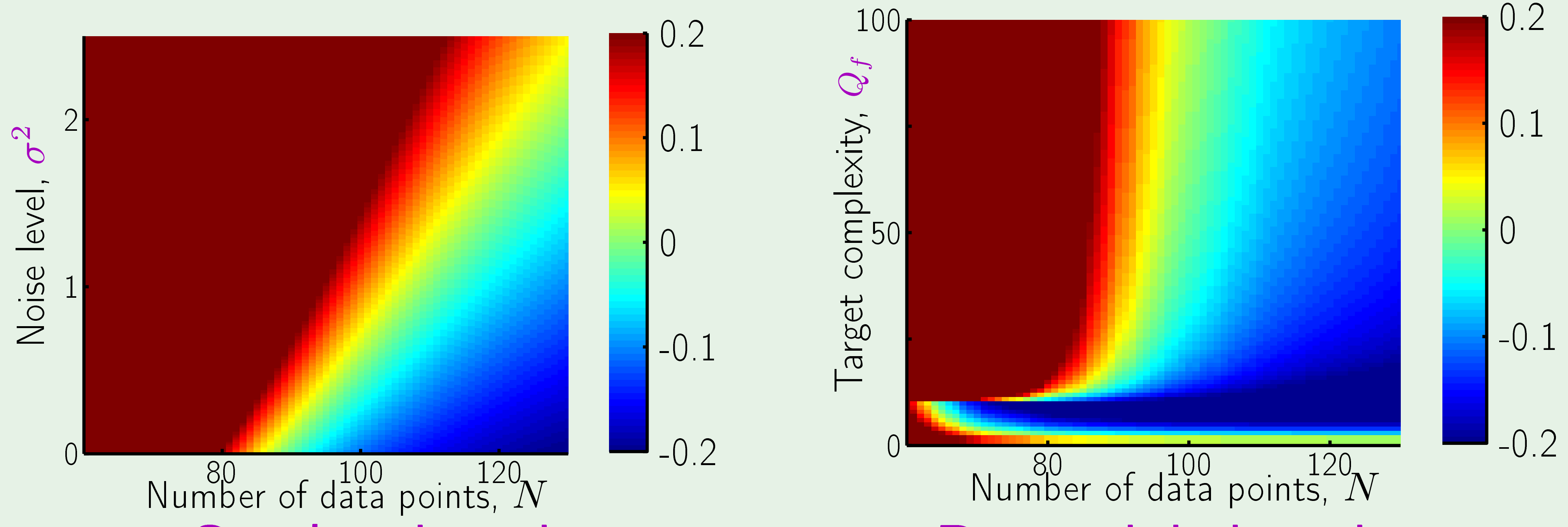
Impact of σ^2





Impact of Q_f

Impact of "noise"



Stochastic noise **Deterministic noise**

number of data points	↑	Overfitting	↓
stochastic noise	↑	Overfitting	↑
deterministic noise	↑	Overfitting	↑

Outline

- What is overfitting?
- The role of noise
- Deterministic noise
- Dealing with overfitting

Definition of deterministic noise

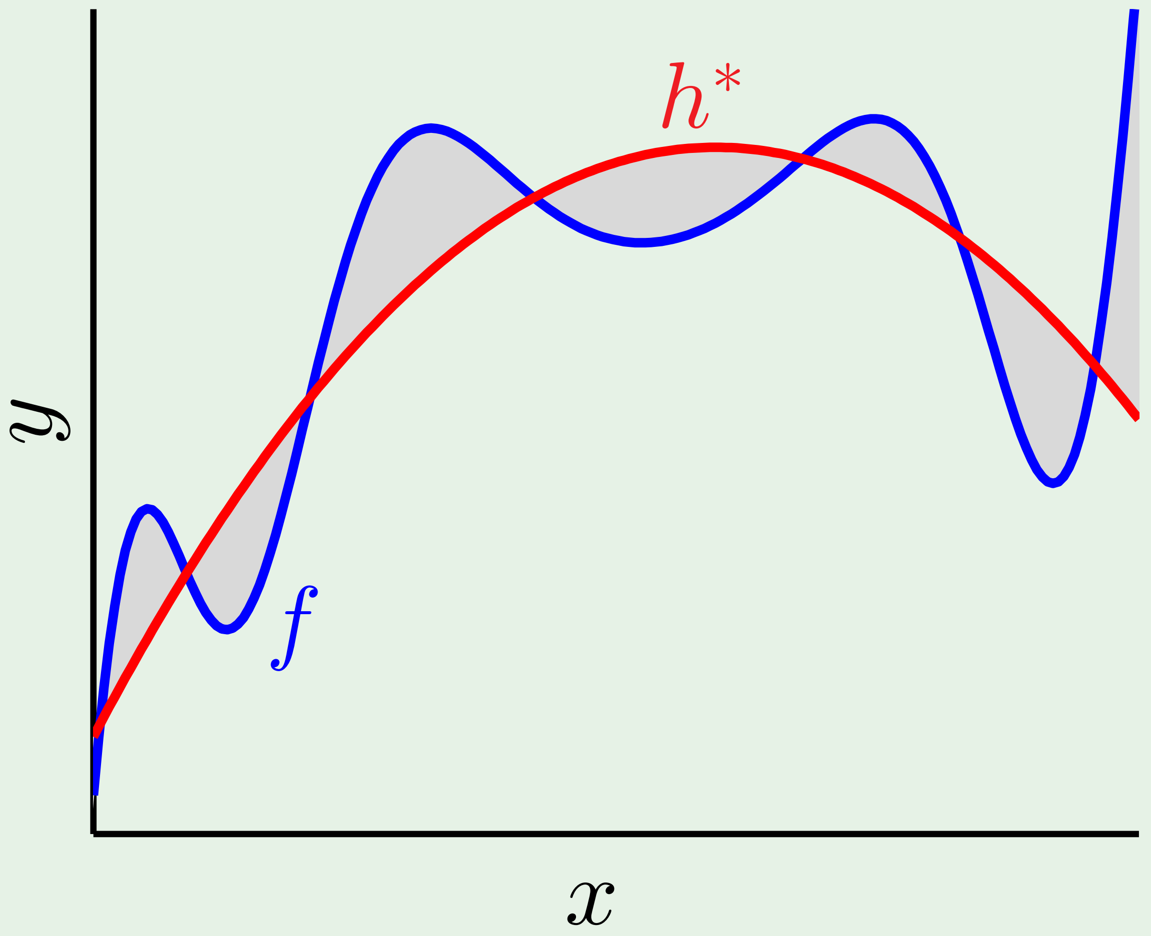
The part of f that $\mathcal{H}$ cannot capture: $f(\mathbf{x}) - h^*(\mathbf{x})$

Why "noise"?

Main differences with stochastic noise:

1. depends on $\mathcal{H}$

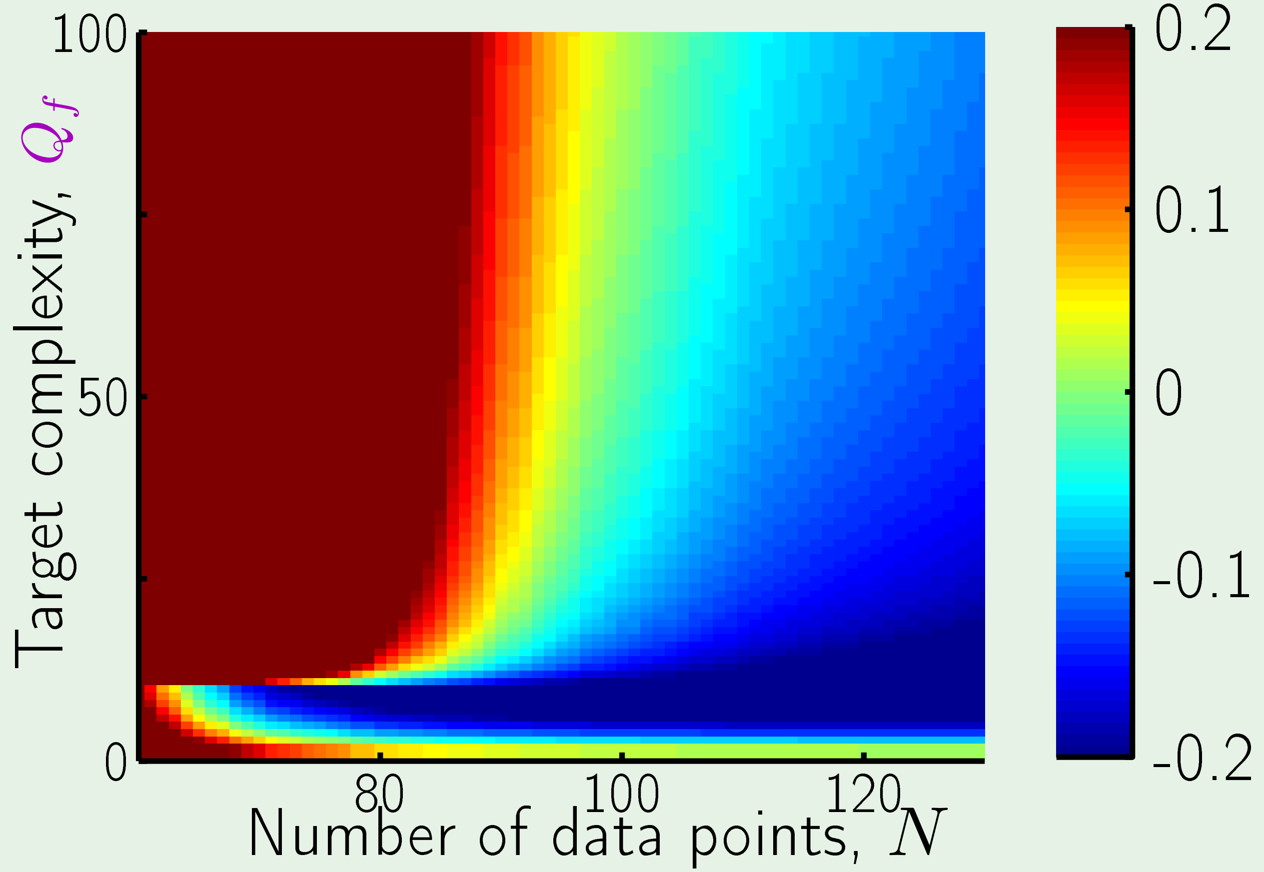
2. fixed for a given $\mathbf{x}$



Impact on overfitting

Deterministic noise and Q_f

Finite N: $\mathcal{H}$ tries to fit the noise



how much overfit

Noise and bias-variance

Recall the decomposition:

$$\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x})-f(\mathbf{x})\right)^2\right]=\underbrace{\mathbb{E}_{\mathcal{D}}\left[\left(g^{(\mathcal{D})}(\mathbf{x})-\bar{g}(\mathbf{x})\right)^2\right]}_{\textbf{var}(\mathbf{x})}+\underbrace{\left[\left(\bar{g}(\mathbf{x})-f(\mathbf{x})\right)^2\right]}_{\textbf{bias}(\mathbf{x})}$$

What if f is a noisy target?

$$y=f(\mathbf{x})+\epsilon(\mathbf{x}) \qquad \mathbb{E}\left[\epsilon(\mathbf{x})\right]=0$$

A noise term

$$\mathbb{E}_{\mathcal{D},\epsilon}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \quad y \quad\right)^2\right] = \mathbb{E}_{\mathcal{D},\epsilon}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - f(\mathbf{x}) - \epsilon(\mathbf{x})\right)^2\right]$$

$$= \mathbb{E}_{\mathcal{D},\epsilon}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x}) + \bar{g}(\mathbf{x}) - f(\mathbf{x}) - \epsilon(\mathbf{x})\right)^2\right]$$

$$= \mathbb{E}_{\mathcal{D},\epsilon}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2 + \left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2 + \left(\epsilon(\mathbf{x})\right)^2 \right.$$

$$\left. + \ \text{cross terms} \ \right]$$

Actually, two noise terms

$$\underbrace{\mathbb{E}_{\mathcal{D},\mathbf{x}}\left[\left(g^{(\mathcal{D})}(\mathbf{x}) - \bar{g}(\mathbf{x})\right)^2\right]}_{\text{var}} + \underbrace{\mathbb{E}_{\mathbf{x}}\left[\left(\bar{g}(\mathbf{x}) - f(\mathbf{x})\right)^2\right]}_{\text{bias}} + \underbrace{\mathbb{E}_{\epsilon,\mathbf{x}}\left[\left(\epsilon(\mathbf{x})\right)^2\right]}_{\sigma^2}$$

bias ↑ deterministic noise

σ^2 ↑ stochastic noise

Outline

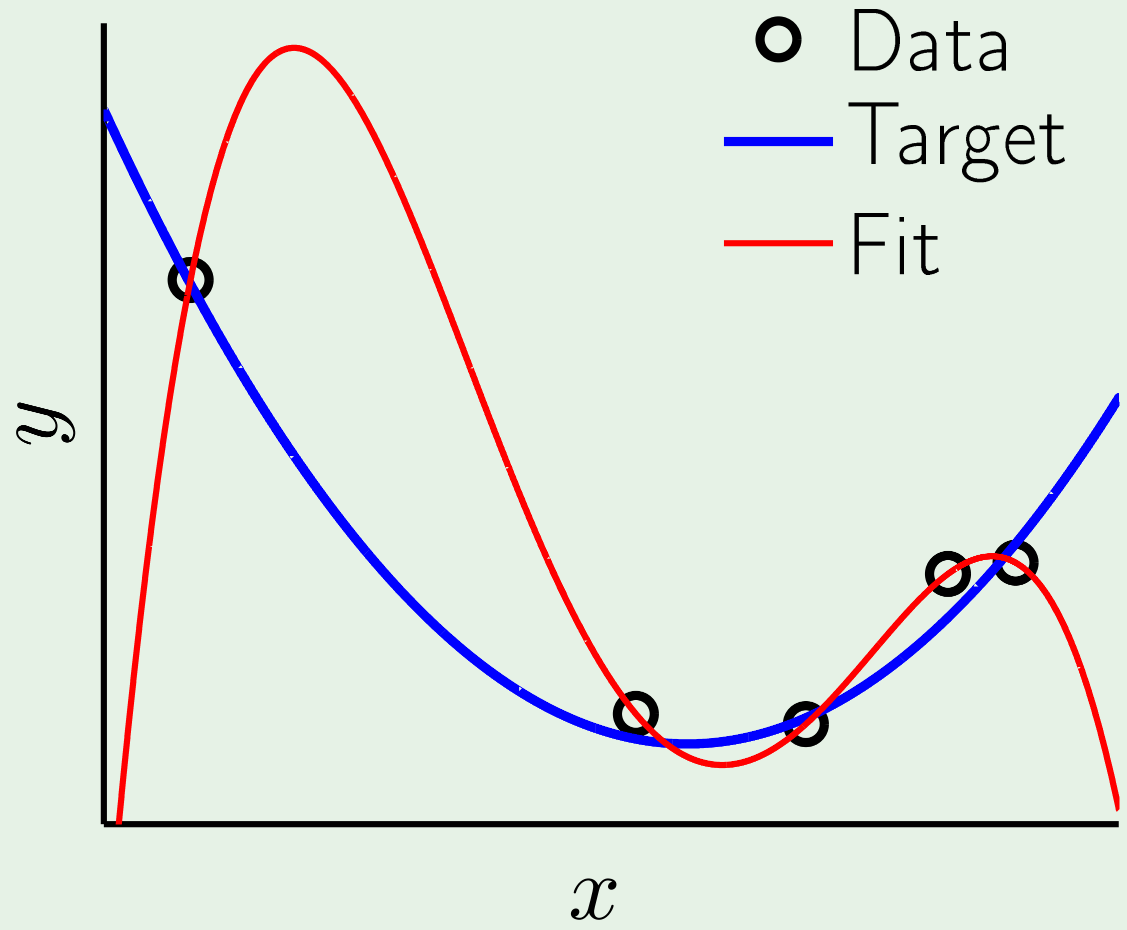
- What is overfitting?
- The role of noise
- Deterministic noise
- Dealing with overfitting

Two cures

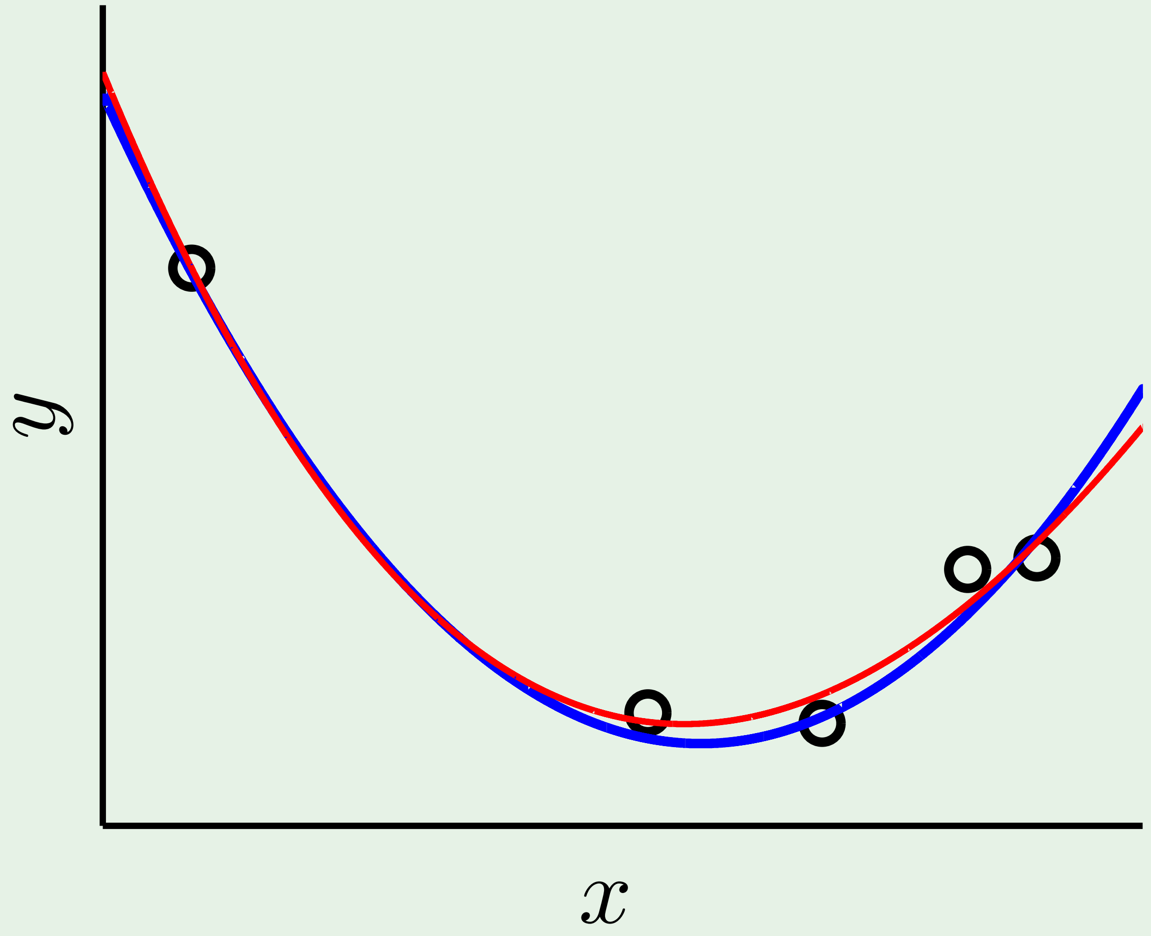
Regularization: Putting the brakes

Validation: Checking the bottom line

Putting the brakes



free fit

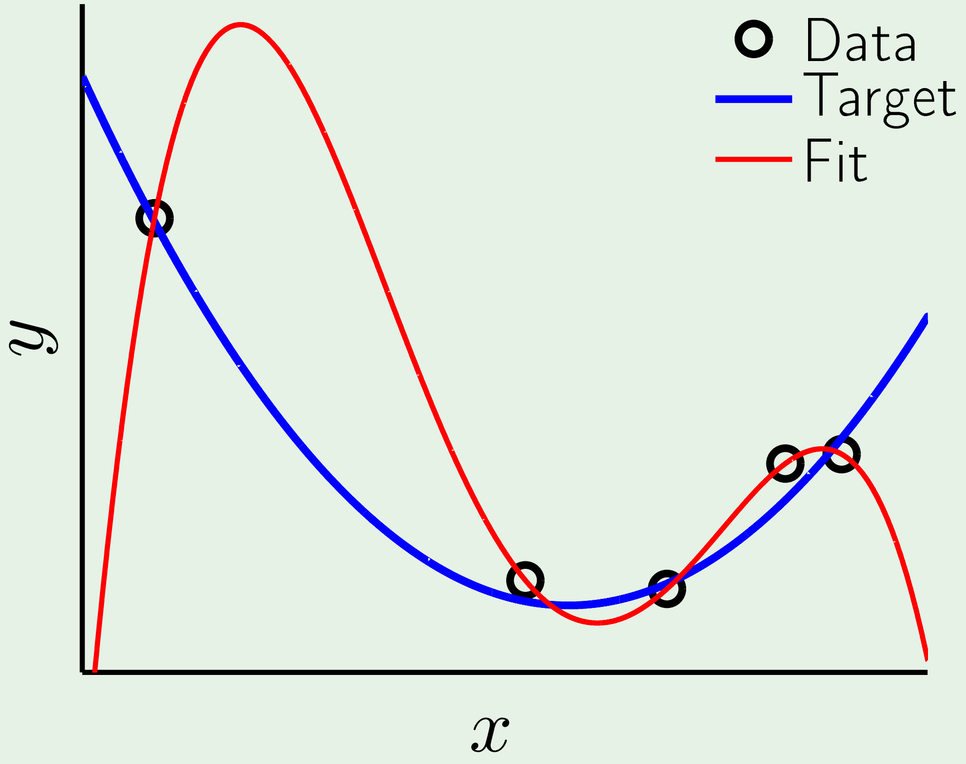


restrained fit

Review of Lecture 11

- **Overfitting**

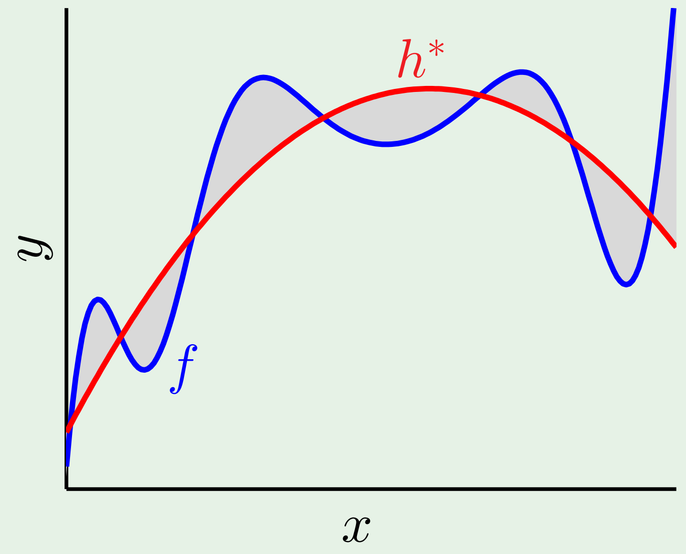
Fitting the data more than is warranted

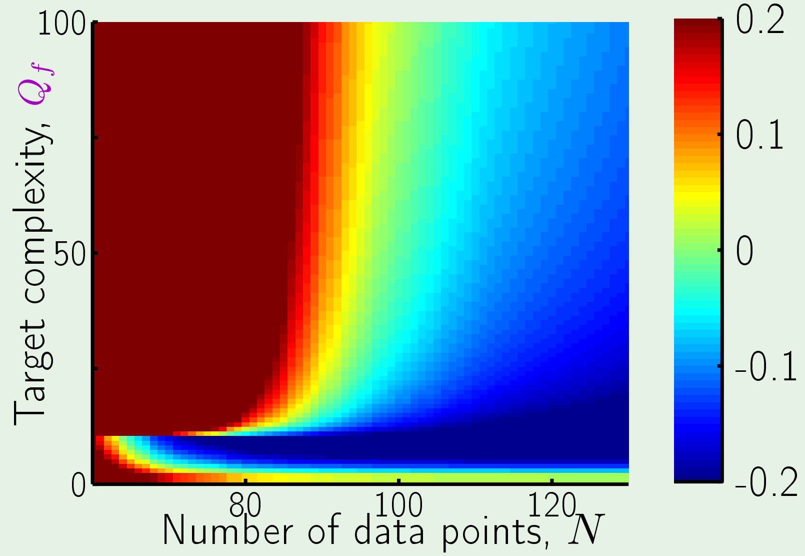


VC allows it; doesn't predict it

Fitting the noise, stochastic/deterministic

- **Deterministic noise**





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Lecture 12: Regularization

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Outline

- Regularization - informal
- Regularization - formal
- Weight decay
- Choosing a regularizer

Two approaches to regularization

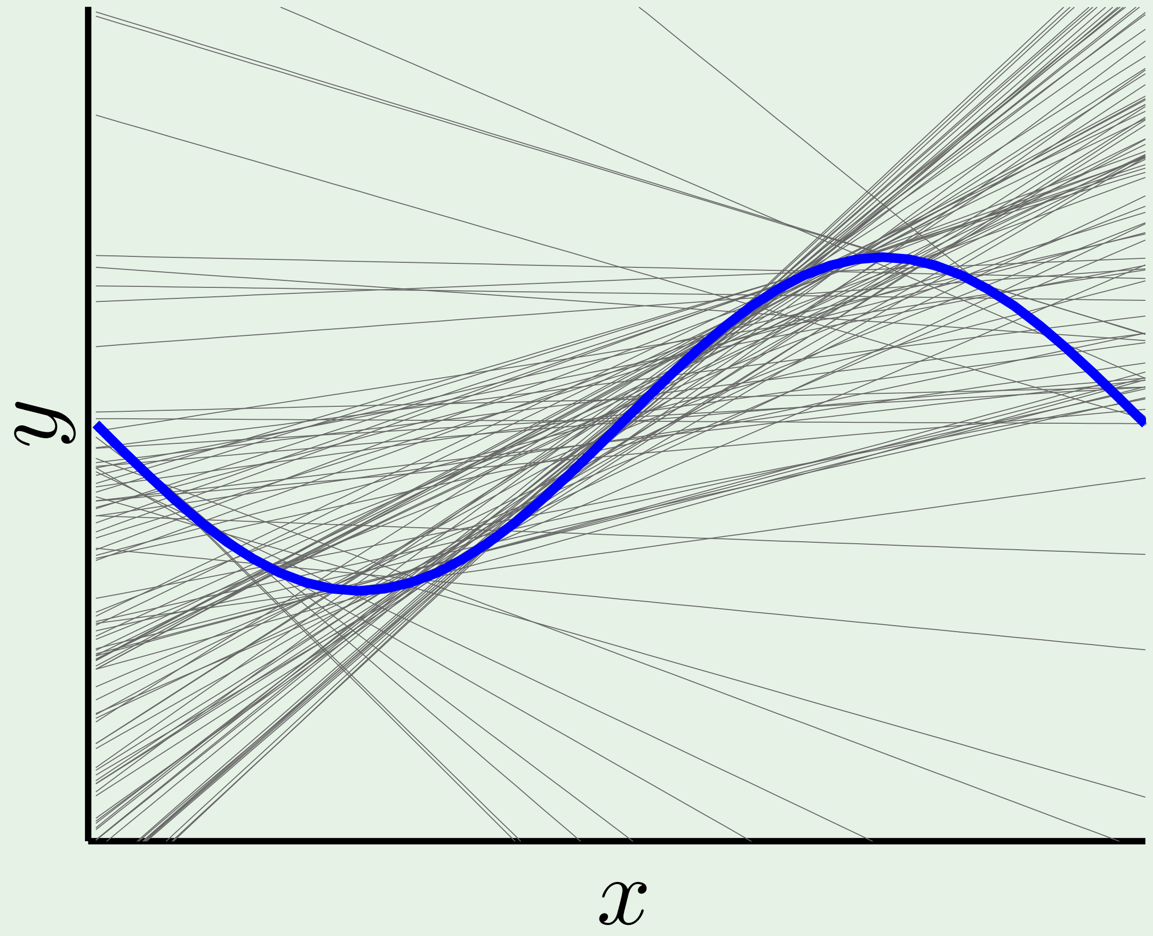
Mathematical:

Ill-posed problems in function approximation

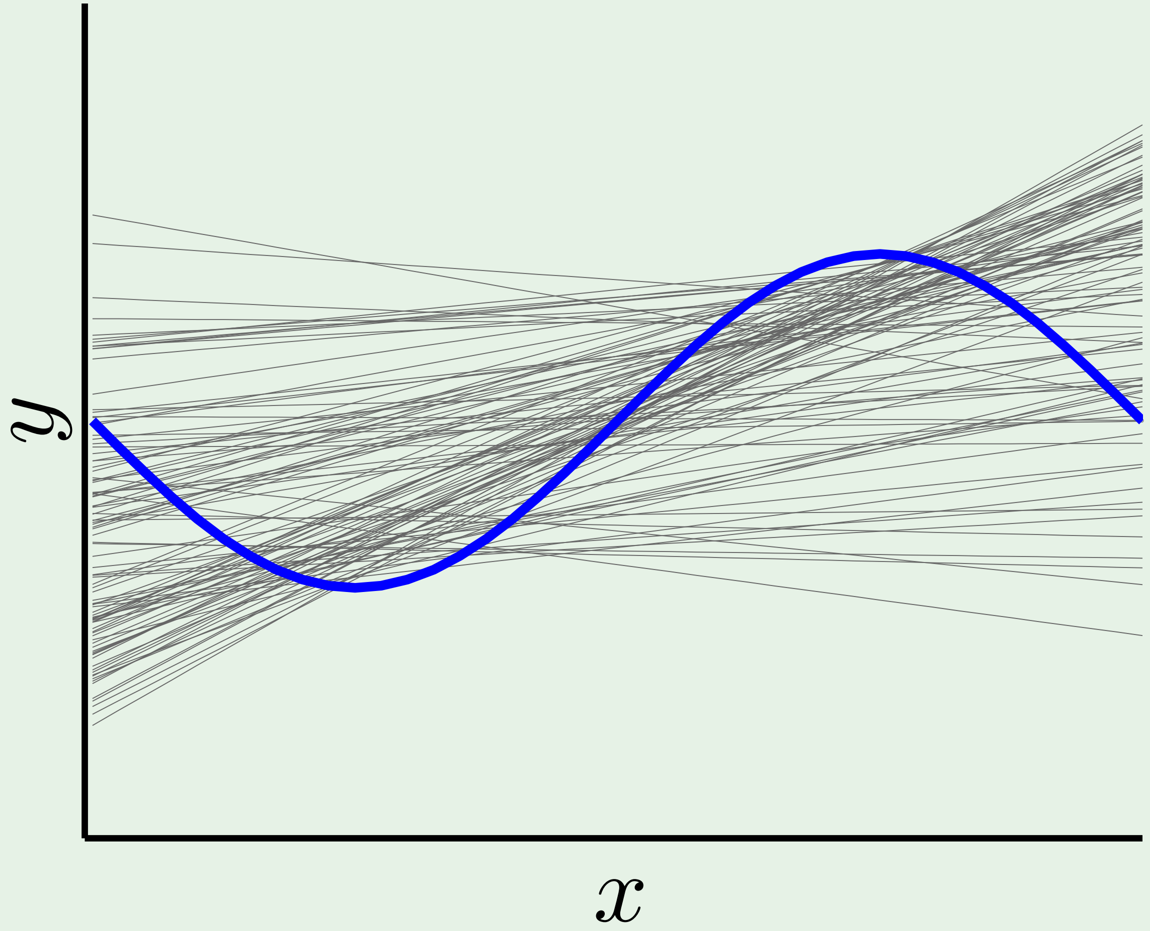
Heuristic:

Handicapping the minimization of E_{in}

A familiar example



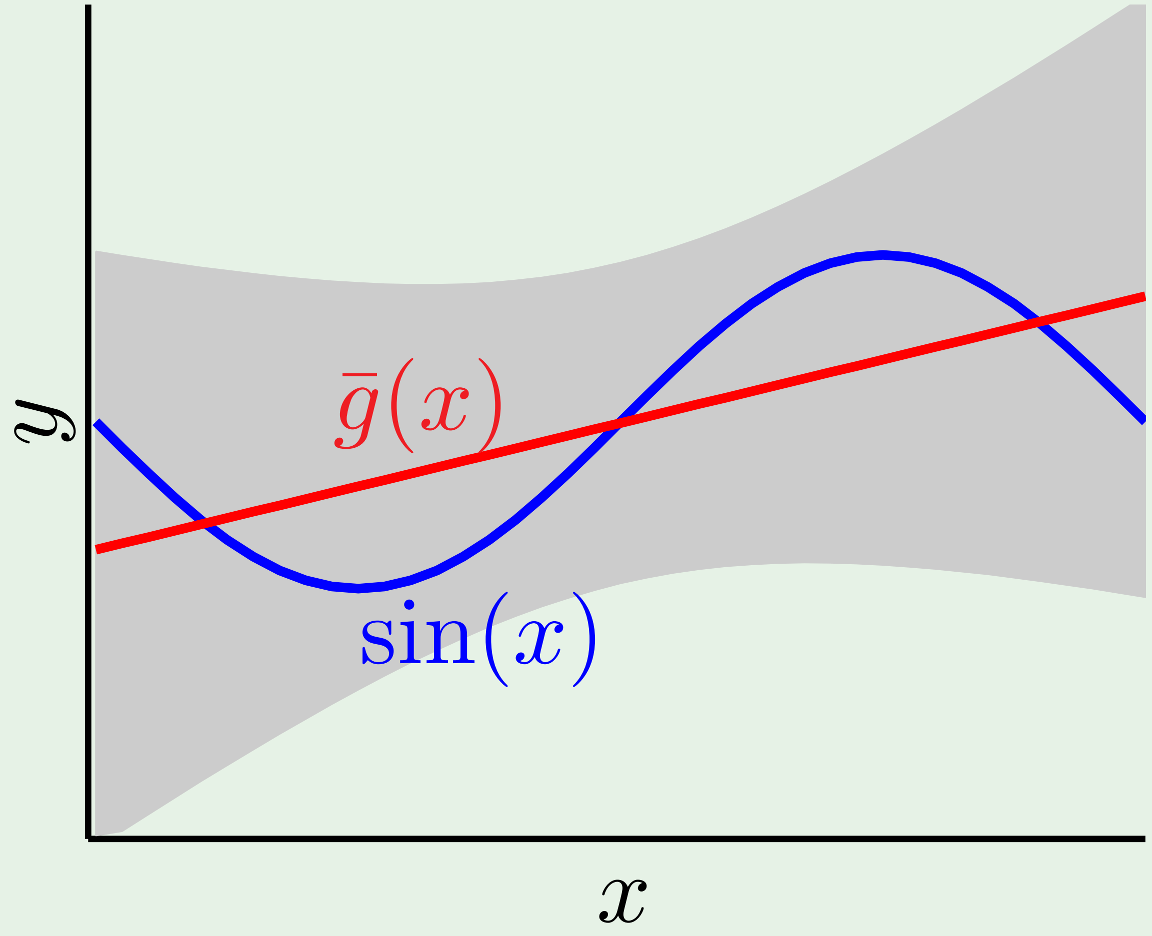
without regularization



with regularization

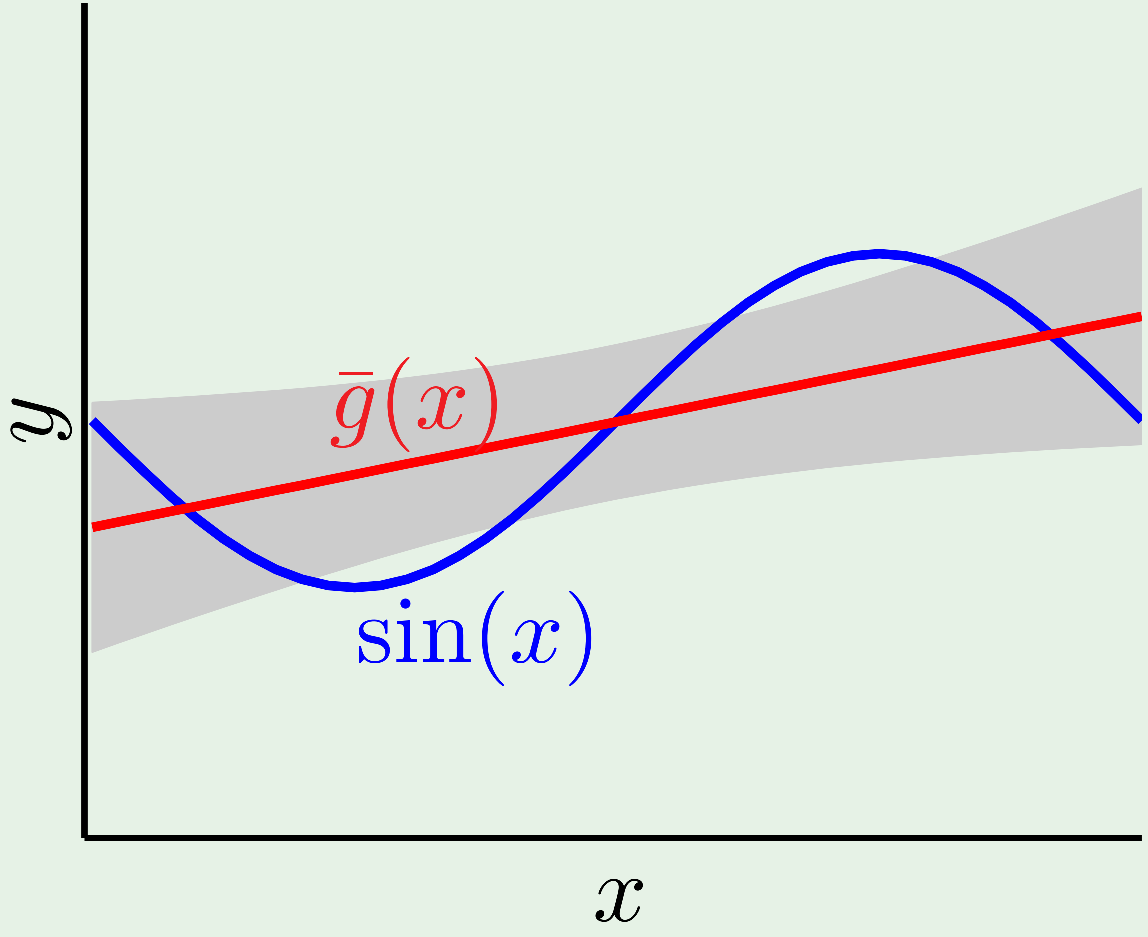
and the winner is ...

without regularization



bias $= \mathbf{0.21}$ var $= \mathbf{1.69}$

with regularization



bias $= \mathbf{0.23}$ var $= \mathbf{0.33}$

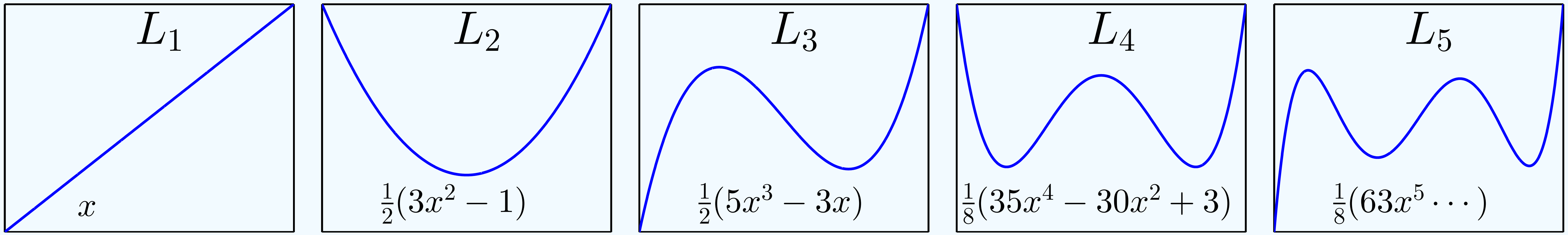
The polynomial model

$\mathcal{H}_Q$: polynomials of order Q

linear regression in $\mathcal{Z}$ space

$$\mathbf{z} = \begin{bmatrix} 1 \\ L_1(x) \\ \vdots \\ L_Q(x) \end{bmatrix} \qquad \mathcal{H}_Q = \left\{ \sum_{q=0}^{Q} w_q \, L_q(x) \right\}$$

Legendre polynomials:



Unconstrained solution

Given $(x_1, y_1), \cdots, (x_N, y_n) \quad \longrightarrow \quad (\mathbf{z}_1, y_1), \cdots, (\mathbf{z}_N, y_n)$

Minimize $E_{\text{in}}(\mathbf{w}) = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{w}^{\intercal}\mathbf{z}_n - y_n)^2$

Minimize $\frac{1}{N} (\mathrm{Z}\mathbf{w} - \mathbf{y})^{\intercal}(\mathrm{Z}\mathbf{w} - \mathbf{y})$

$$\mathbf{w}_{\text{lin}} = (\mathrm{Z}^{\intercal}\mathrm{Z})^{-1}\mathrm{Z}^{\intercal}\mathbf{y}$$

Constraining the weights

Hard constraint: $\mathcal{H}_2$ is constrained version of $\mathcal{H}_{10}$ with $w_q = 0$ for $q > 2$

Softer version: $\sum_{q=0}^{Q} w_q^2 \leq C$ "**soft-order**" constraint

Minimize $\frac{1}{N}(\mathrm{Z}\mathbf{w} - \mathbf{y})^{\intercal}(\mathrm{Z}\mathbf{w} - \mathbf{y})$

subject to: $\mathbf{w}^{\intercal}\mathbf{w} \leq C$

Solution: $\mathbf{w}_{\text{reg}}$ instead of $\mathbf{w}_{\text{lin}}$

Solving for $\mathbf{w}_{\text{reg}}$

Minimize $\quad E_{\text{in}}(\mathbf{w}) \;=\; \frac{1}{N}\,(\mathrm{Z}\mathbf{w}-\mathbf{y})^{\mathsf{T}}(\mathrm{Z}\mathbf{w}-\mathbf{y})$

subject to: $\quad \mathbf{w}^{\mathsf{T}}\mathbf{w} \le C$

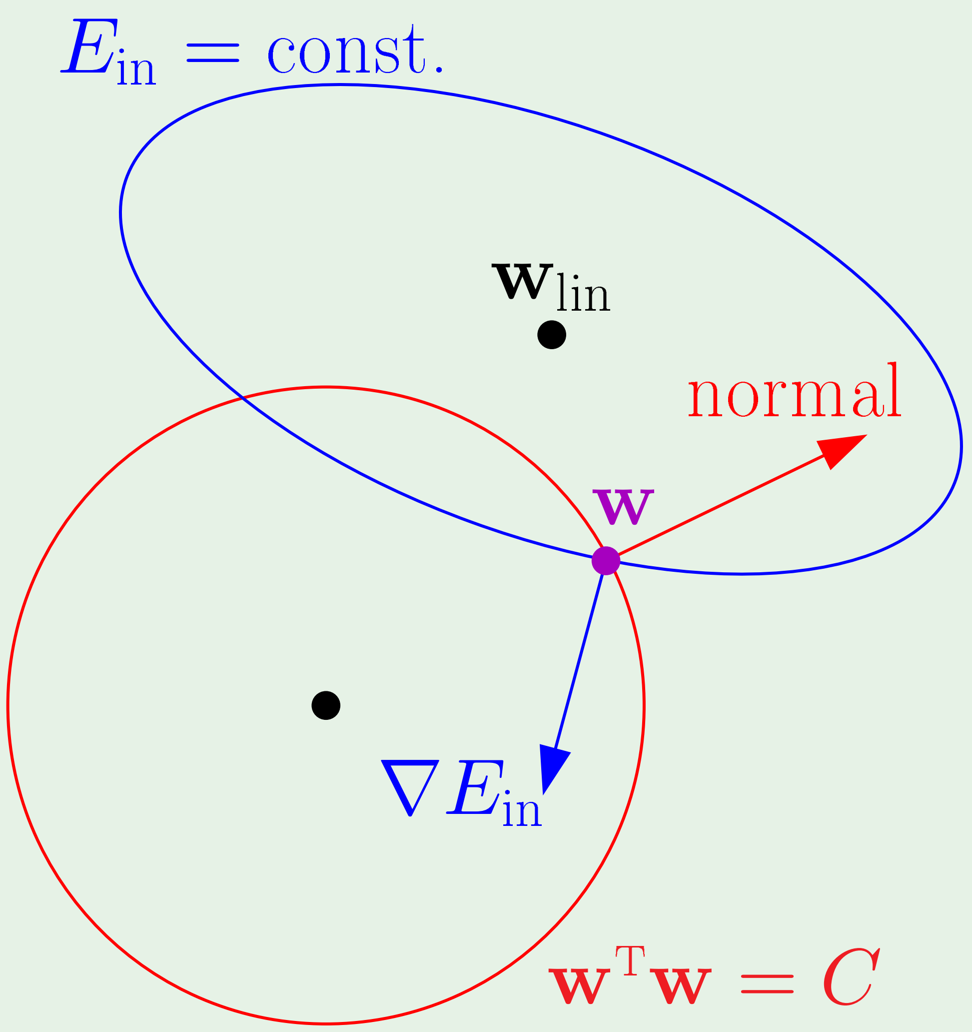
$$\nabla E_{\text{in}}(\mathbf{w}_{\text{reg}}) \propto \; -\mathbf{w}_{\text{reg}}$$

$$= \; -2\frac{\lambda}{N}\mathbf{w}_{\text{reg}}$$

$$\nabla E_{\text{in}}(\mathbf{w}_{\text{reg}}) + 2\frac{\lambda}{N}\mathbf{w}_{\text{reg}} \;=\; \mathbf{0}$$

Minimize $\quad E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\mathbf{w}^{\mathsf{T}}\mathbf{w}$

$C\uparrow \quad \lambda\downarrow$



Augmented error

Minimizing $$E_{\text{aug}}(\mathbf{w}) = E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\mathbf{w}^{\mathsf{T}}\mathbf{w}$$

$$= \frac{1}{N}(\mathrm{Z}\mathbf{w} - \mathbf{y})^{\mathsf{T}}(\mathrm{Z}\mathbf{w} - \mathbf{y}) + \frac{\lambda}{N}\mathbf{w}^{\mathsf{T}}\mathbf{w}$$ unconditionally

– solves –

Minimizing $$E_{\text{in}}(\mathbf{w}) = \frac{1}{N}(\mathrm{Z}\mathbf{w} - \mathbf{y})^{\mathsf{T}}(\mathrm{Z}\mathbf{w} - \mathbf{y})$$

subject to: $\mathbf{w}^{\mathsf{T}}\mathbf{w} \leq C$ $\longleftarrow$ VC formulation

The solution

Minimize $\quad E_{\text{aug}}(\mathbf{w}) \;=\; E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\mathbf{w}^{\mathsf{T}}\mathbf{w}$

$$= \frac{1}{N}\left((\mathrm{Z}\mathbf{w}-\mathbf{y})^{\mathsf{T}}(\mathrm{Z}\mathbf{w}-\mathbf{y}) \;+\; \lambda\,\mathbf{w}^{\mathsf{T}}\mathbf{w}\right)$$

$\nabla E_{\text{aug}}(\mathbf{w}) \;=\; \mathbf{0} \qquad \Longrightarrow \qquad \mathrm{Z}^{\mathsf{T}}(\mathrm{Z}\mathbf{w}-\mathbf{y}) + \lambda\mathbf{w} = \mathbf{0}$

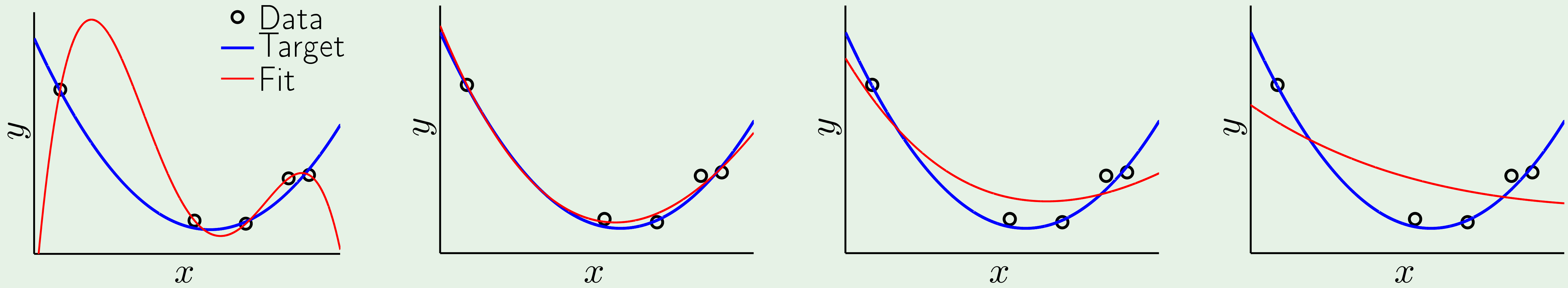
$$\boxed{\mathbf{w}_{\text{reg}} \;=\; (\mathrm{Z}^{\mathsf{T}}\mathrm{Z} + \lambda\mathrm{I})^{-1}\,\mathrm{Z}^{\mathsf{T}}\mathbf{y}}$$ (with regularization)

as opposed to $\quad \mathbf{w}_{\text{lin}} \;=\; (\mathrm{Z}^{\mathsf{T}}\mathrm{Z})^{-1}\mathrm{Z}^{\mathsf{T}}\mathbf{y}$ (without regularization)

The result

Minimizing $\quad E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\,\mathbf{w}^{\intercal}\mathbf{w} \quad$ for different λ's:

$\lambda = 0$ $\qquad$ $\lambda = 0.0001$ $\qquad$ $\lambda = 0.01$ $\qquad$ $\lambda = 1$



overfitting $\longrightarrow$ $\longrightarrow$ $\longrightarrow$ $\longrightarrow$ **underfitting**

Weight 'decay'

Minimizing $E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\,\mathbf{w}^{\mathsf{T}}\mathbf{w}$ is called weight *decay*. Why?

Gradient descent:

$$\mathbf{w}(t+1) = \mathbf{w}(t) \;-\; \eta\,\nabla E_{\text{in}}\left(\mathbf{w}(t)\right) \;-\; 2\,\eta\,\frac{\lambda}{N}\,\mathbf{w}(t)$$

$$= \mathbf{w}(t)\;(1 - 2\eta\frac{\lambda}{N}) \;-\; \eta\,\nabla E_{\text{in}}\left(\mathbf{w}(t)\right)$$

Applies in neural networks:

$$\mathbf{w}^{\mathsf{T}}\mathbf{w} = \sum_{l=1}^{L}\sum_{i=0}^{d^{(l-1)}}\sum_{j=1}^{d^{(l)}}\left(w_{ij}^{(l)}\right)^2$$

Variations of weight decay

Emphasis of certain weights: $\sum_{q=0}^{Q} \gamma_q \, w_q^2$

Examples:

$\gamma_q = 2^q \implies$ low-order fit

$\gamma_q = 2^{-q} \implies$ high-order fit

Neural networks: different layers get different γ's

Tikhonov regularizer: $\mathbf{w}^{\mathsf{T}}\Gamma^{\mathsf{T}}\Gamma\mathbf{w}$

Even weight growth!

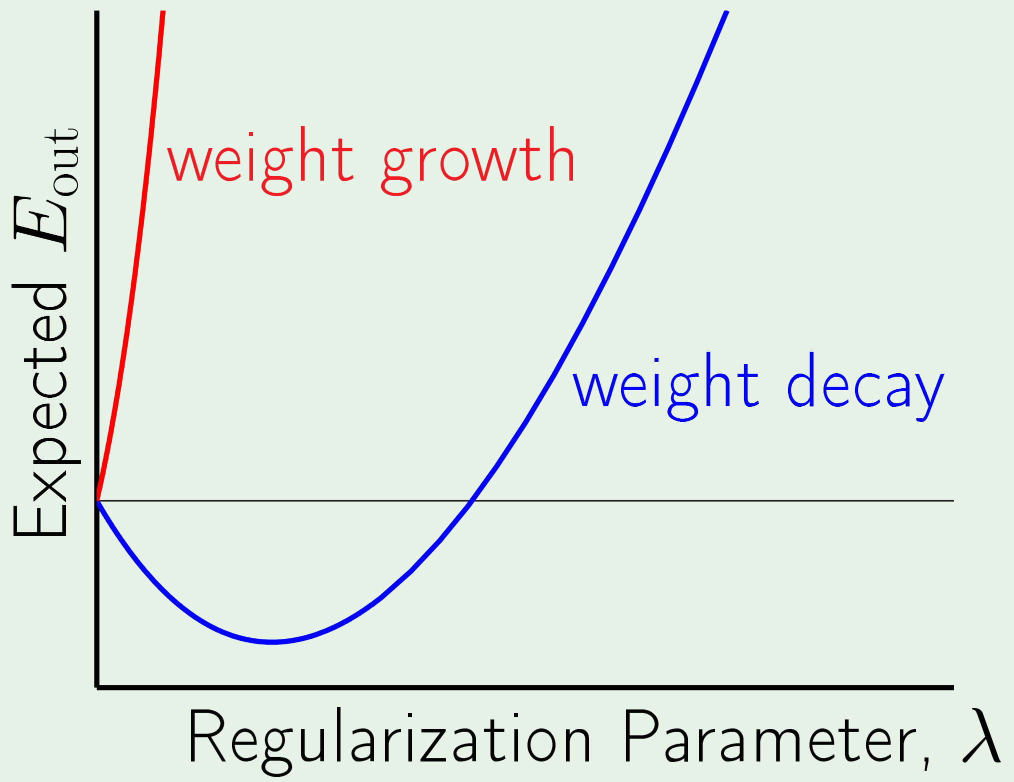
We 'constrain' the weights to be large - bad!

Practical rule:

stochastic noise is 'high-frequency'

deterministic noise is also non-smooth

$\Longrightarrow$ constrain learning towards smoother hypotheses



General form of augmented error

Calling the regularizer $\Omega = \Omega(h)$, we minimize

$$E_{\text{aug}}(h) = E_{\text{in}}(h) + \frac{\lambda}{N}\Omega(h)$$

Rings a bell? $\downarrow \downarrow$

$$E_{\text{out}}(h) \leq E_{\text{in}}(h) + \Omega(\mathcal{H})$$

E_{aug} is better than E_{in} as a proxy for E_{out}

Outline

- Regularization - informal
- Regularization - formal
- Weight decay
- Choosing a regularizer

The perfect regularizer Ω

Constraint in the 'direction' of the target function (going in circles ☺)

Guiding principle:

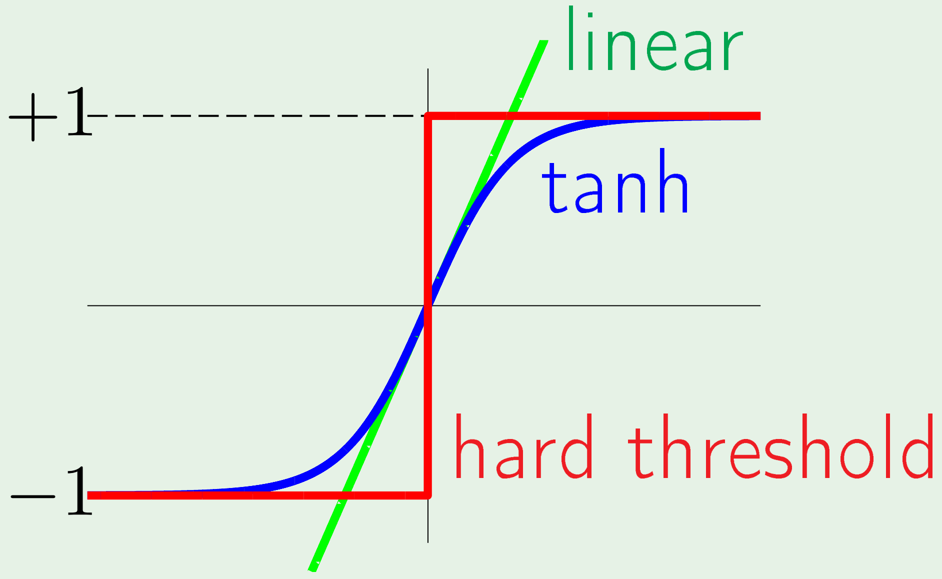
Direction of **smoother** or "simpler"

Chose a bad Ω?

We still have λ!

Neural-network regularizers

Weight decay: From linear to logical



Weight elimination:

Fewer weights $\Longrightarrow$ smaller VC dimension

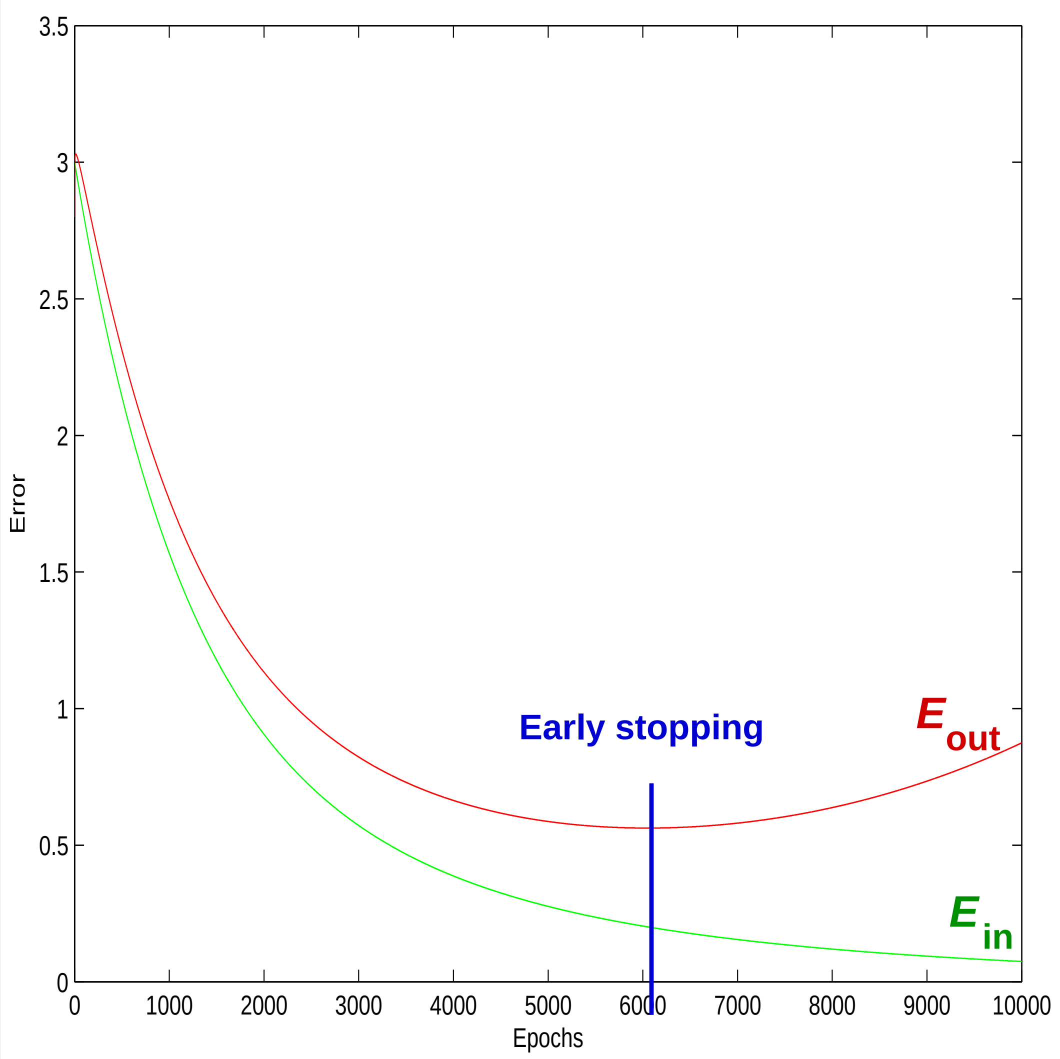
Soft weight elimination:

$$\Omega(\mathbf{w}) = \sum_{i,j,l} \frac{\left(w_{ij}^{(l)}\right)^2}{\beta^2 + \left(w_{ij}^{(l)}\right)^2}$$

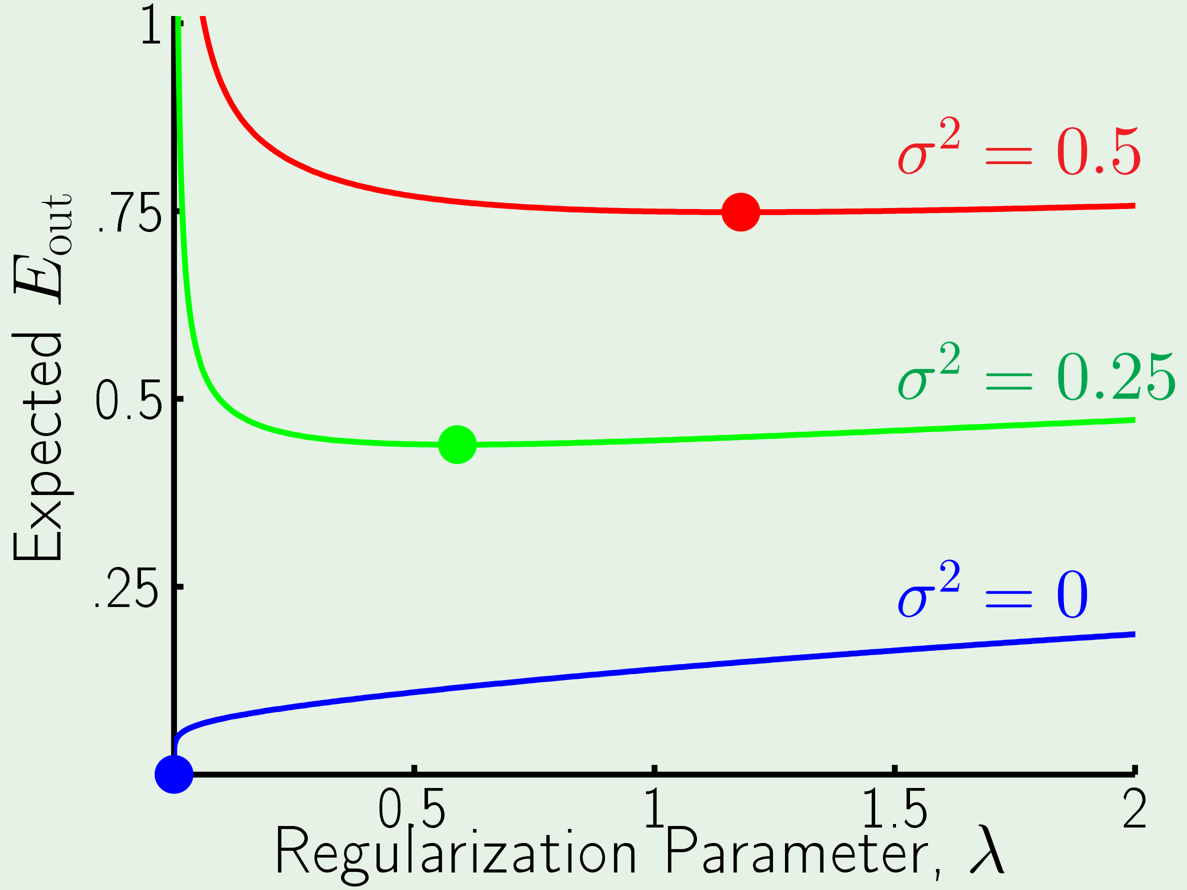
Early stopping as a regularizer

Regularization through the optimizer!

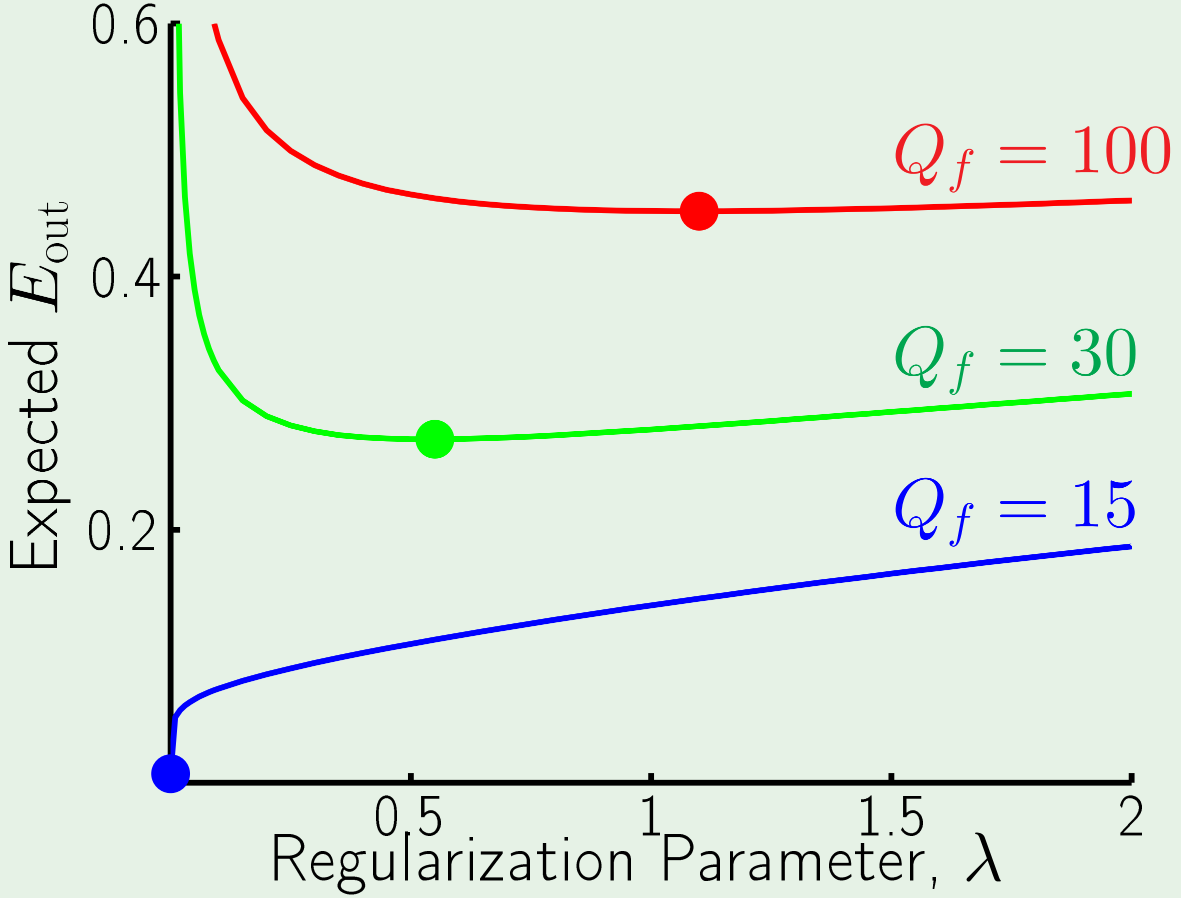
When to stop? **validation**



The optimal λ



Stochastic noise

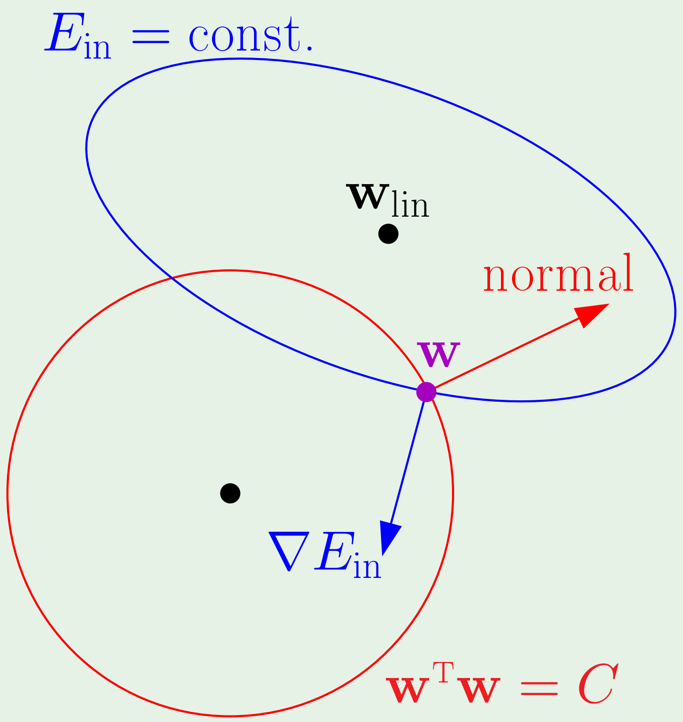


Deterministic noise

Review of Lecture 12

- Regularization

constrained $\longrightarrow$ unconstrained



Minimize $E_{\text{aug}}(\mathbf{w}) = E_{\text{in}}(\mathbf{w}) + \frac{\lambda}{N}\mathbf{w}^{\mathsf{T}}\mathbf{w}$

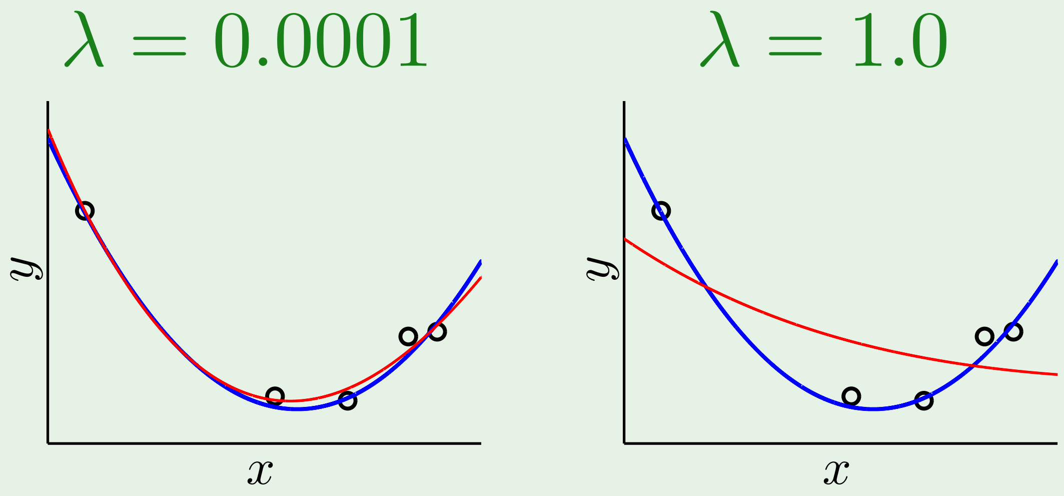
- Choosing a regularizer

$$E_{\text{aug}}(h) = E_{\text{in}}(h) + \frac{\lambda}{N}\Omega(h)$$

$\Omega(h)$: heuristic $\rightarrow$ smooth, simple h

most used: **weight decay**

λ: principled; validation



Learning From Data

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Lecture 13: **Validation**

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Tuesday, May 15, 2012

Outline

- The validation set
- Model selection
- Cross validation

Validation versus regularization

In one form or another, $E_{\text{out}}(h) \;=\; E_{\text{in}}(h) \;+\;$ overfit penalty

Regularization:

$$E_{\text{out}}(h) \;=\; E_{\text{in}}(h) + \underbrace{\text{overfit penalty}}_{\text{regularization estimates this quantity}}$$

Validation:

$$\underbrace{E_{\text{out}}(h)}_{\text{validation estimates this quantity}} = \; E_{\text{in}}(h) \;+\; \text{overfit penalty}$$

Analyzing the estimate

On out-of-sample point $(\mathbf{x}, y)$, the error is $\mathbf{e}(h(\mathbf{x}), y)$

Squared error: $\left(h(\mathbf{x}) - y\right)^2$

Binary error: $[\![h(\mathbf{x}) \neq y]\!]$

$$\mathbb{E}\left[\mathbf{e}(h(\mathbf{x}), y)\right] = E_{\text{out}}(h)$$

$$\text{var}\left[\mathbf{e}(h(\mathbf{x}), y)\right] = \sigma^2$$

From a point to a set

On a validation set $(\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_K, y_K)$, the error is $E_{\text{val}}(h) = \frac{1}{K} \sum_{k=1}^{K} \mathrm{e}(h(\mathbf{x}_k), y_k)$

$$\mathbb{E}\left[E_{\text{val}}(h)\right] = \frac{1}{K} \sum_{k=1}^{K} \mathbb{E}\left[\mathrm{e}(h(\mathbf{x}_k), y_k)\right] = E_{\text{out}}(h)$$

$$\text{var}\left[E_{\text{val}}(h)\right] = \frac{1}{K^2} \sum_{k=1}^{K} \text{var}\left[\mathrm{e}(h(\mathbf{x}_k), y_k)\right] = \frac{\sigma^2}{K}$$

$$E_{\text{val}}(h) = E_{\text{out}}(h) \pm O\left(\frac{1}{\sqrt{K}}\right)$$

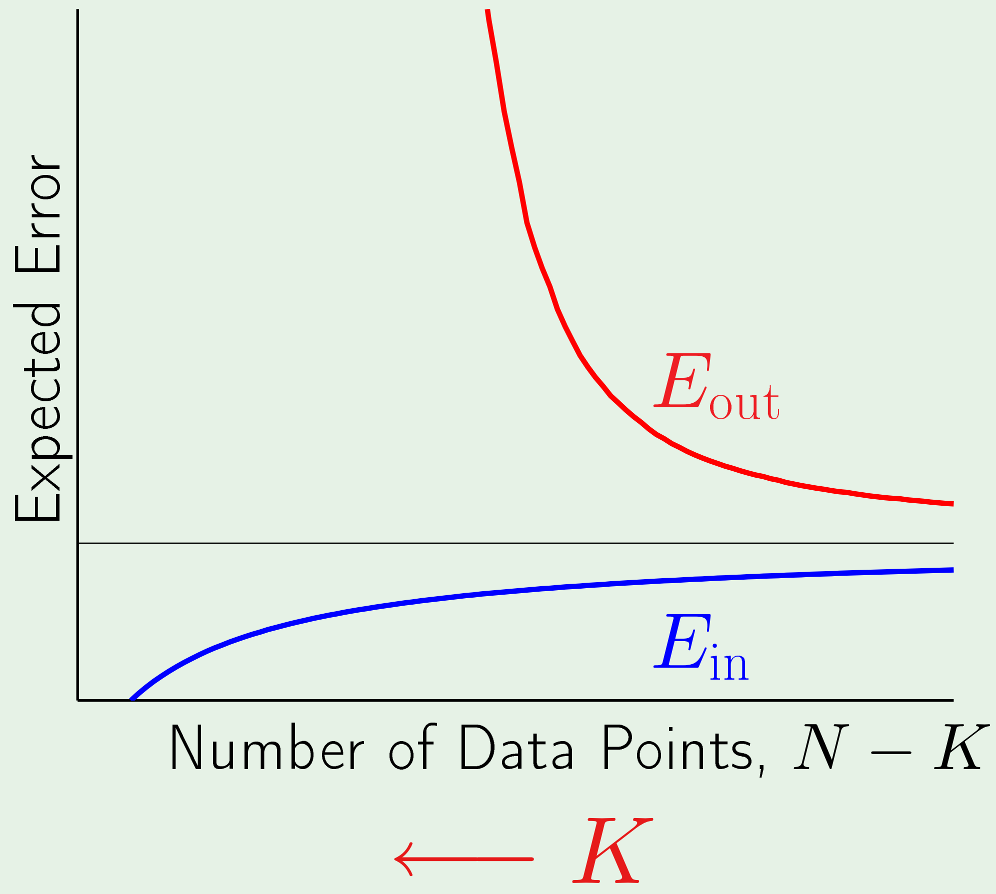
K is taken out of N

Given the data set $\mathcal{D} = (\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$

$\underbrace{K \text{ points}}_{\mathcal{D}_{\text{val}}} \rightarrow$ validation $\quad \underbrace{N-K \text{ points}}_{\mathcal{D}_{\text{train}}} \rightarrow$ training

$O\left(\frac{1}{\sqrt{K}}\right)$: Small $K \implies$ bad estimate

Large $K \implies$?



K is put back into N

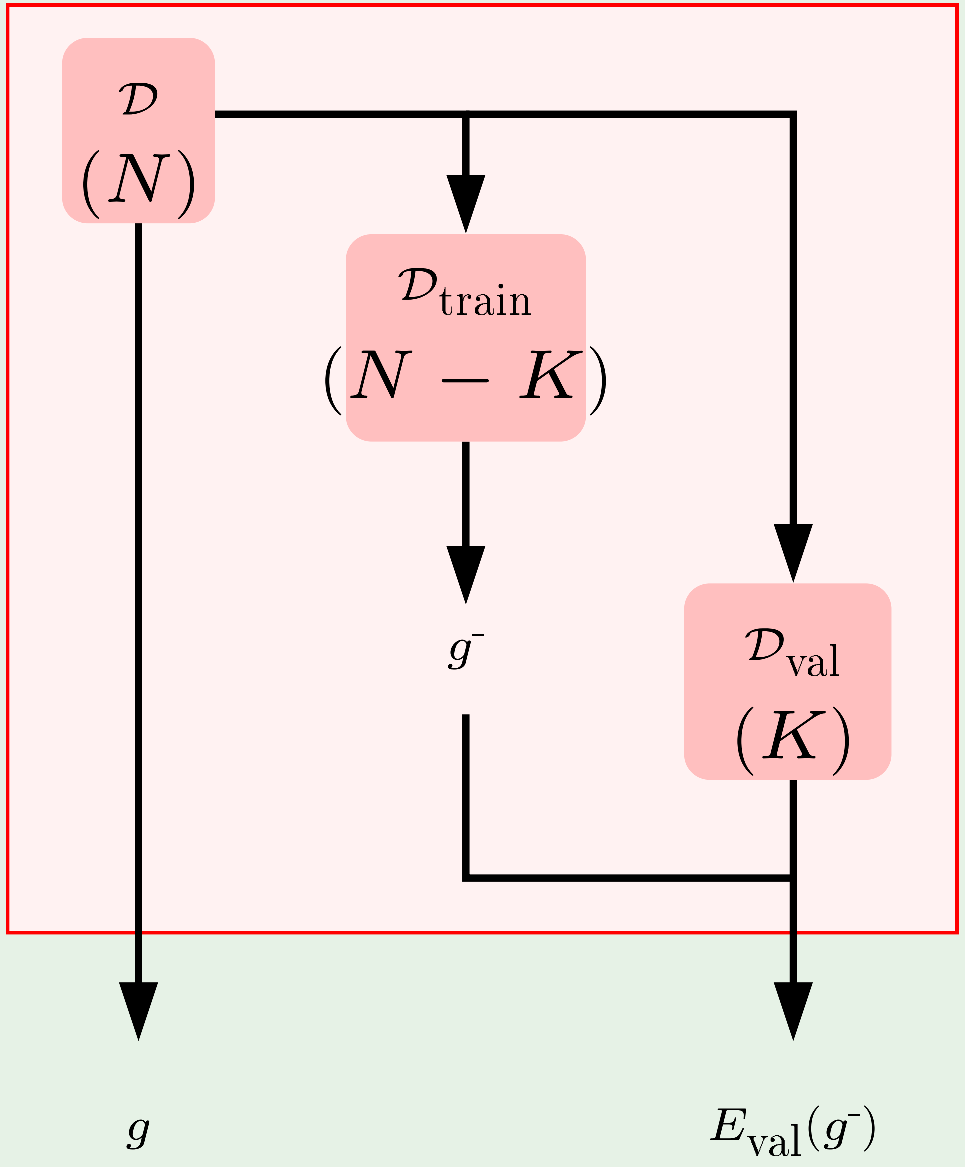
$$\begin{array}{ccc} \mathcal{D} & \longrightarrow & \mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{val}} \\ \downarrow & & \downarrow \qquad \downarrow \\ N & & N-K \qquad K \end{array}$$

$\mathcal{D} \Longrightarrow g \qquad \mathcal{D}_{\text{train}} \Longrightarrow g^-$

$E_{\text{val}} = E_{\text{val}}(g^-)$ Large $K \Longrightarrow$ bad estimate!

Rule of Thumb:

$$K = \frac{N}{5}$$



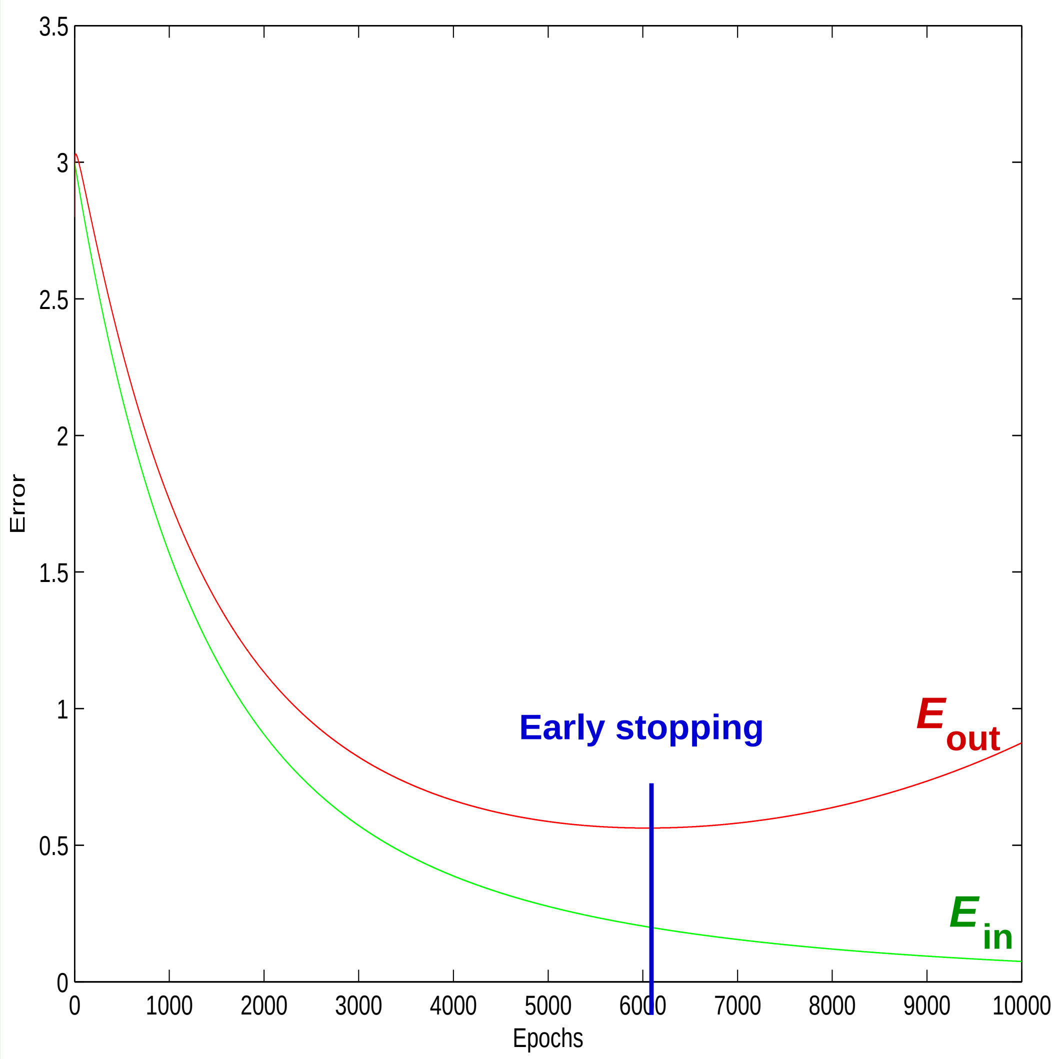
Why 'validation'

$\mathcal{D}_{\rm val}$ is used to make learning choices

If an estimate of $E_{\rm out}$ affects learning:

the set is no longer a **test** set!

It becomes a validation set



What's the difference?

Test set is unbiased; validation set has optimistic bias

Two hypotheses h_1 and h_2 with $E_{\text{out}}(h_1) = E_{\text{out}}(h_2) = 0.5$

Error estimates $\mathbf{e}_1$ and $\mathbf{e}_2$ uniform on $[0, 1]$

Pick $h \in \{h_1, h_2\}$ with $\mathbf{e} = \min(\mathbf{e}_1, \mathbf{e}_2)$

$\mathbb{E}(\mathbf{e}) < 0.5$ optimistic bias

Outline

- The validation set
- Model selection
- Cross validation

Using $\mathcal{D}_{\text{val}}$ more than once

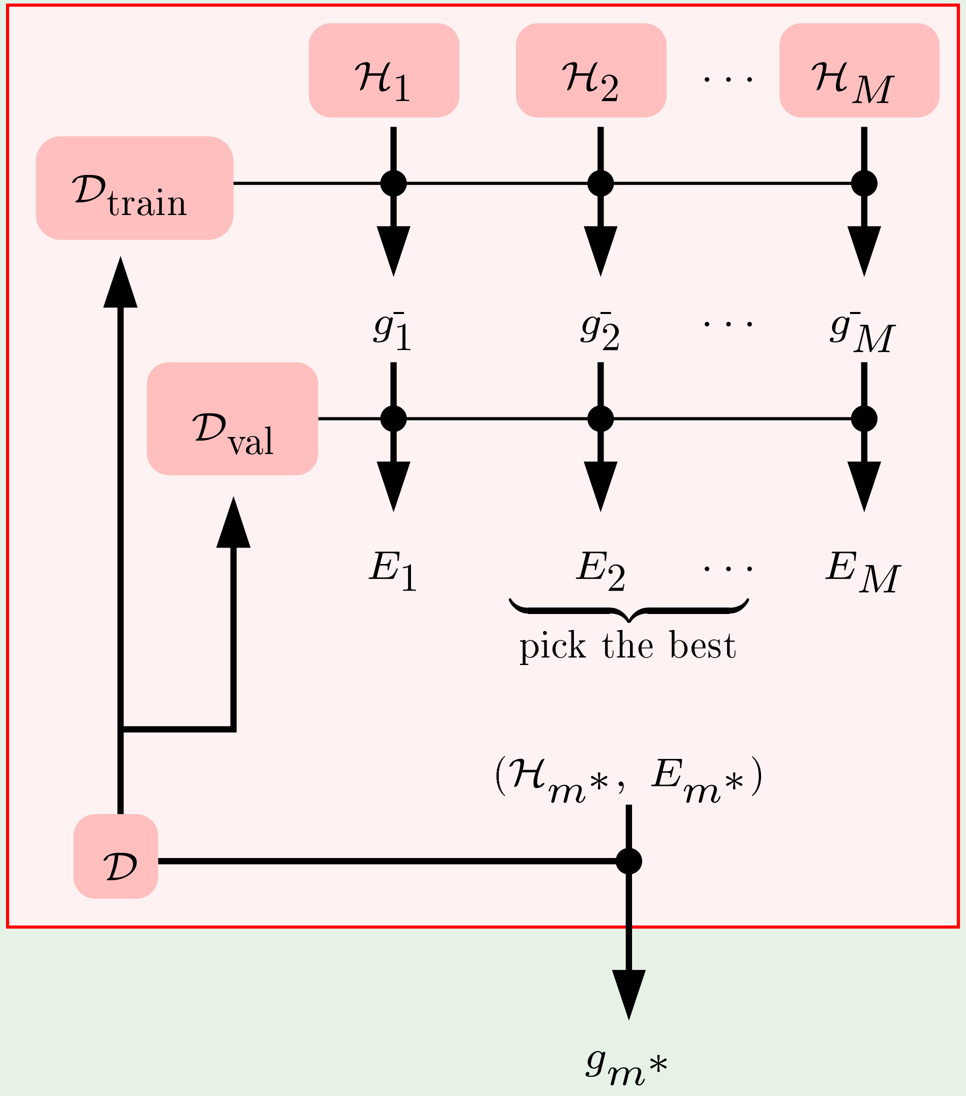
M models $\mathcal{H}_1, \ldots, \mathcal{H}_M$

Use $\mathcal{D}_{\text{train}}$ to learn g_m^- for each model

Evaluate g_m^- using $\mathcal{D}_{\text{val}}$:

$$E_m = E_{\text{val}}(g_m^-); \quad m = 1, \ldots, M$$

Pick model $m = m^*$ with smallest E_m

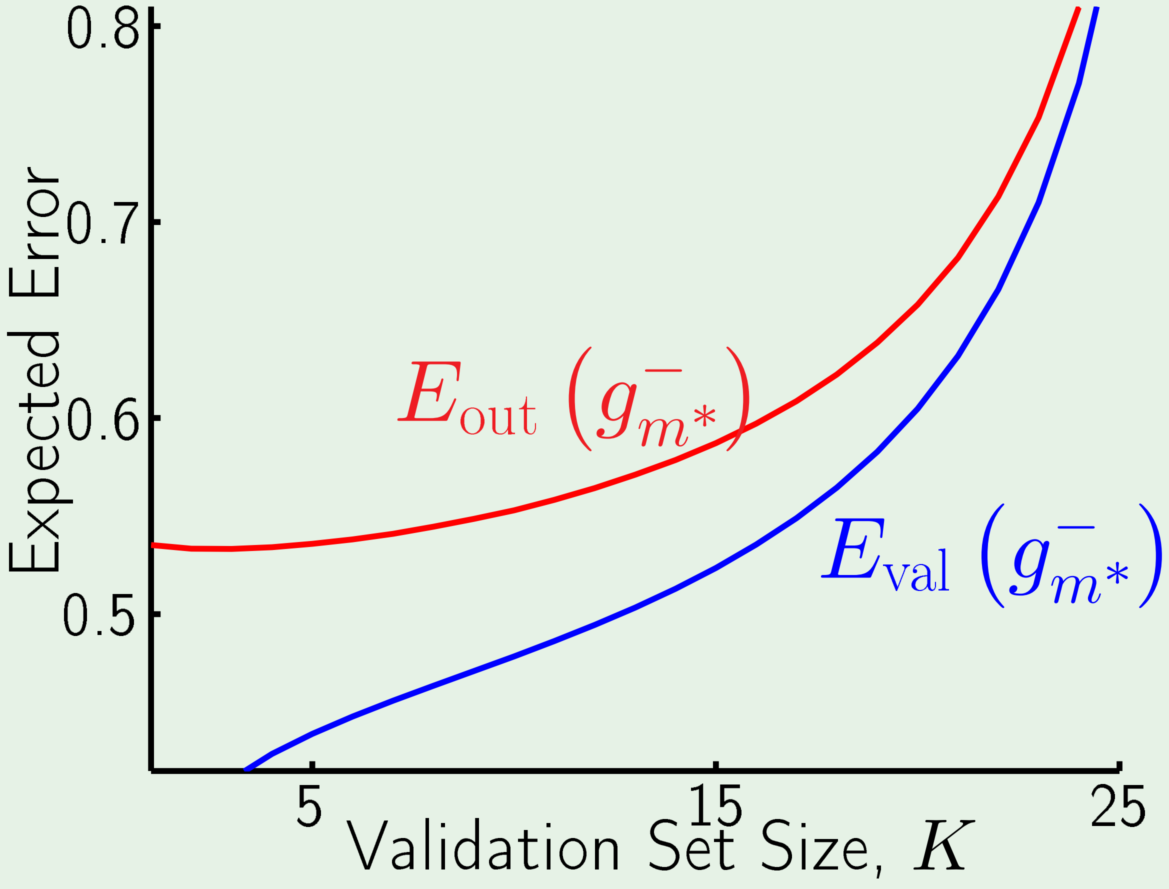


The bias

We selected the model $\mathcal{H}_{m^*}$ using $\mathcal{D}_{\text{val}}$

$E_{\text{val}}(g^-_{m^*})$ is a biased estimate of $E_{\text{out}}(g^-_{m^*})$

Illustration: selecting between 2 models



How much bias

For M models: $\mathcal{H}_1, \ldots, \mathcal{H}_M$

$\mathcal{D}_{\text{val}}$ is used for "training" on the **finalists model**:

$$\mathcal{H}_{\text{val}} = \{g_1^-, g_2^-, \ldots, g_M^-\}$$

Back to Hoeffding and VC!

$$E_{\text{out}}(g_{m^*}^-) \leq E_{\text{val}}(g_{m^*}^-) + O\left(\sqrt{\frac{\ln M}{K}}\right)$$

regularization λ early-stopping T

Data contamination

Error estimates: E_{in}, E_{test}, E_{val}

Contamination: Optimistic (deceptive) bias in estimating E_{out}

Training set: totally contaminated

Validation set: slightly contaminated

Test set: totally ‘clean’

Outline

- The validation set

- Model selection

- Cross validation

The dilemma about K

The following chain of reasoning:

$$E_{\text{out}}(g) \underset{\text{(small } K)}{\approx} E_{\text{out}}(g^-) \underset{\text{(large } K)}{\approx} E_{\text{val}}(g^-)$$

highlights the dilemma in selecting K:

Can we have K both small and large? ☺

Leave one out

$N - 1$ points for training, and 1 point for validation!

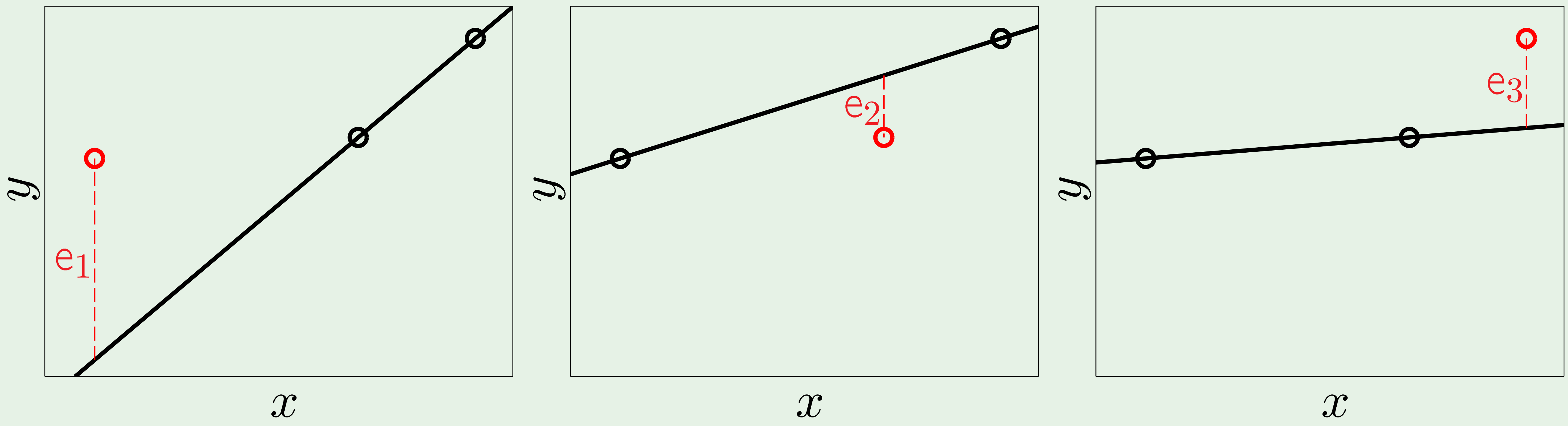
$$\mathcal{D}_n = (\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_{n-1}, y_{n-1}), \cancel{(\mathbf{x}_n, y_n)}, (\mathbf{x}_{n+1}, y_{n+1}), \ldots, (\mathbf{x}_N, y_N)$$

Final hypothesis learned from $\mathcal{D}_n$ is g_n^-

$$\mathbf{e}_n = E_{\text{val}}(g_n^-) = \mathbf{e}\left(g_n^-(\mathbf{x}_n), y_n\right)$$

cross validation error: $E_{\text{cv}} = \dfrac{1}{N} \displaystyle\sum_{n=1}^{N} \mathbf{e}_n$

Illustration of cross validation

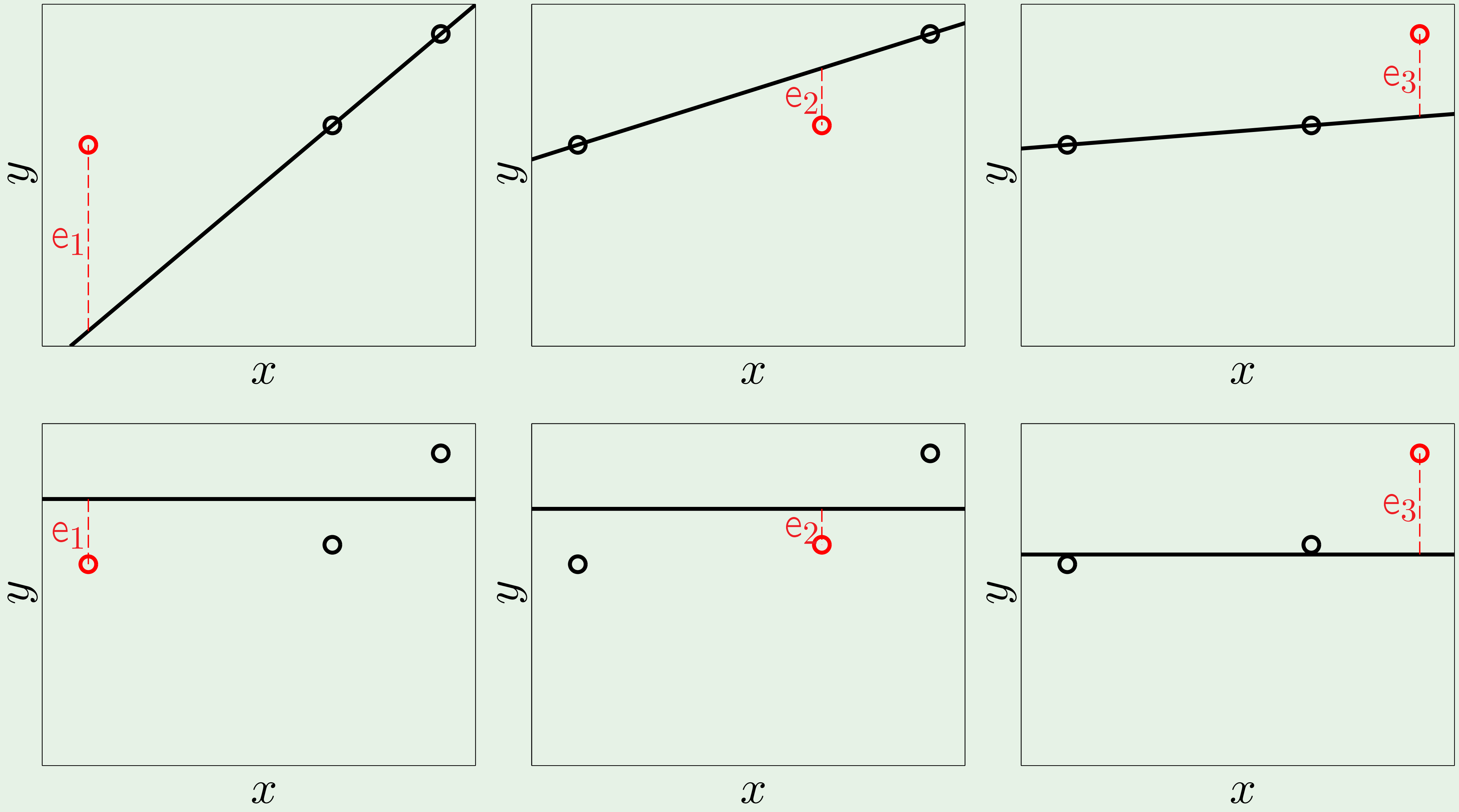


$$E_{\text{cv}} = \frac{1}{3}\left(\mathrm{e}_1 + \mathrm{e}_2 + \mathrm{e}_3 \right)$$

Model selection using CV

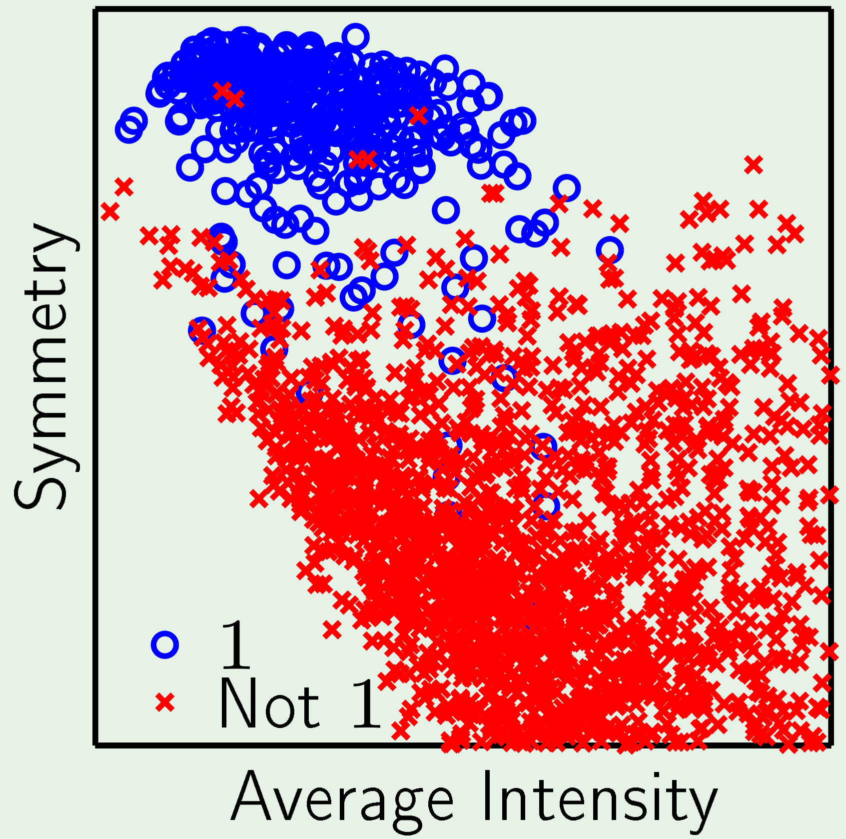
Linear:

Constant:

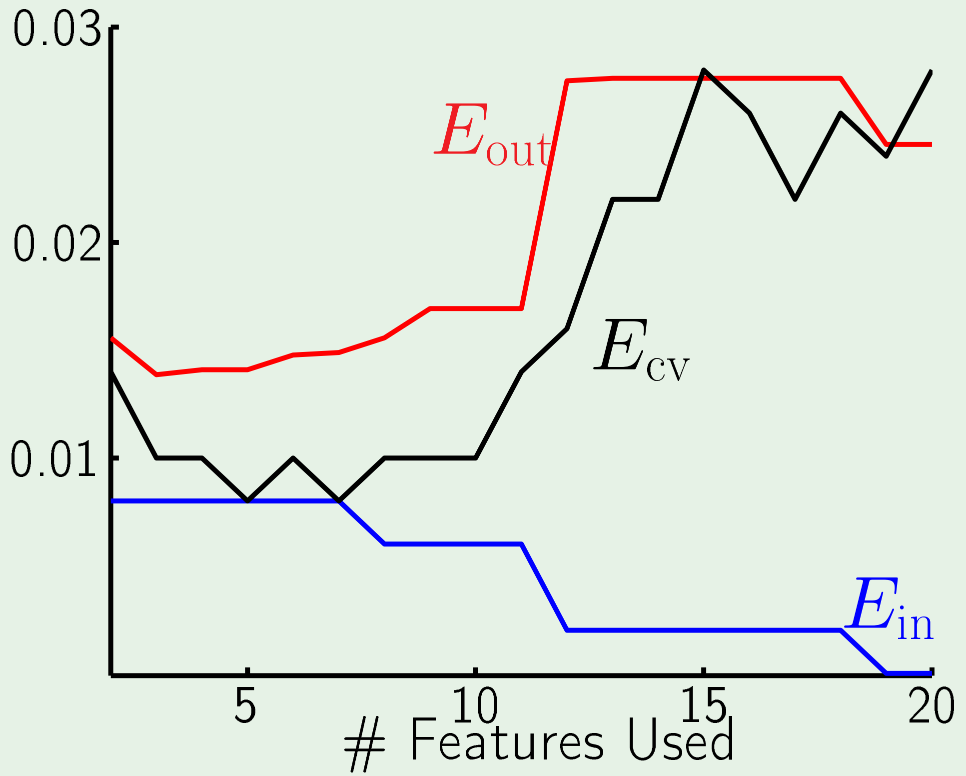


Cross validation in action

Digits classification task



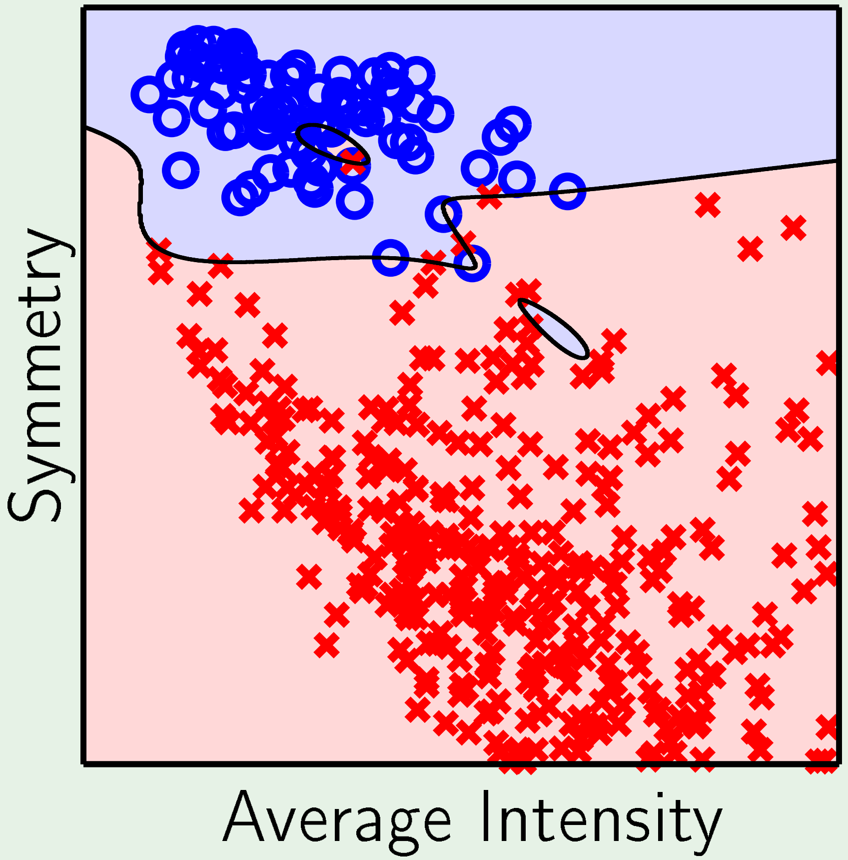
Different errors



$$(1, x_1, x_2) \to (1, x_1, x_2, x_1^2, x_1x_2, x_2^2, x_1^3, x_1^2x_2, \ldots, x_1^5, x_1^4x_2, x_1^3x_2^2, x_1^2x_2^3, x_1x_2^4, x_2^5)$$

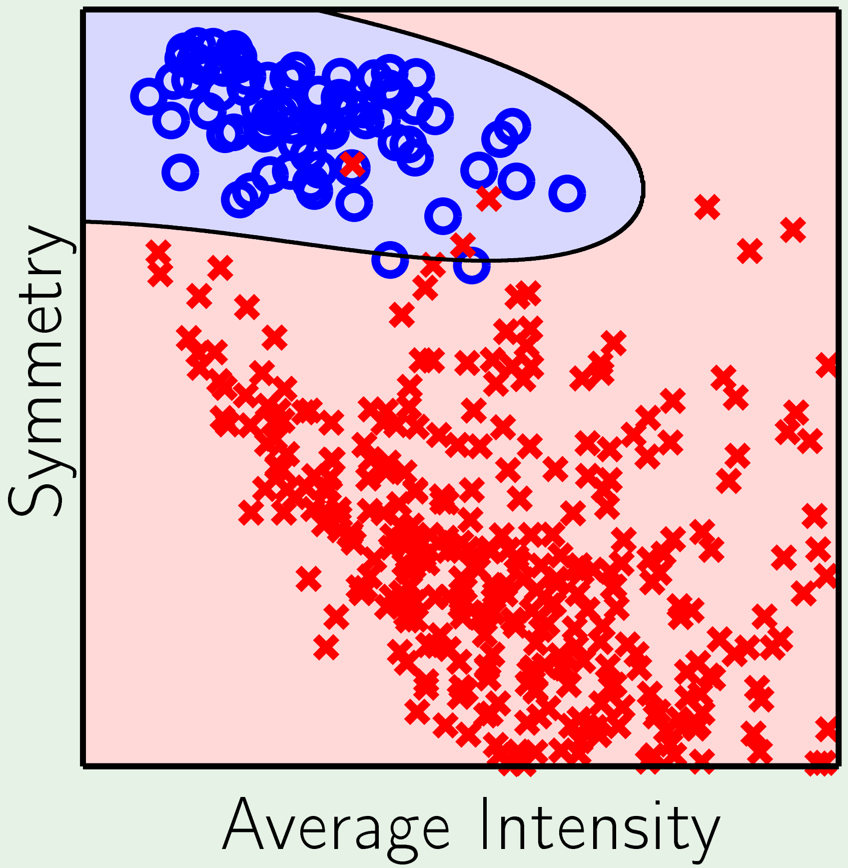
The result

without validation



$E_{\text{in}} = 0\%$ $E_{\text{out}} = 2.5\%$

with validation

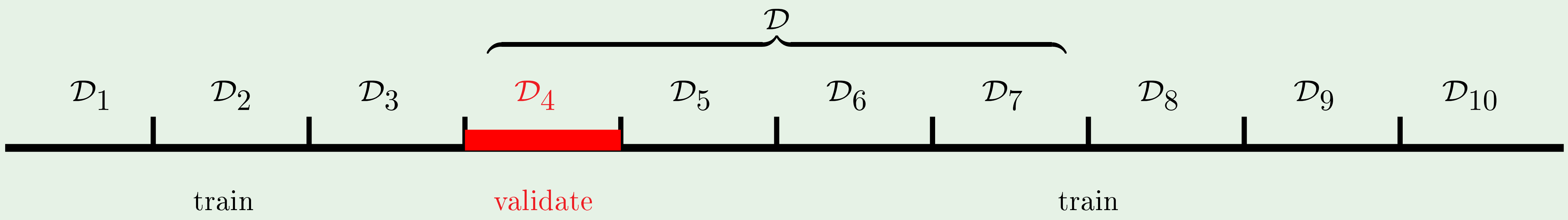


$E_{\text{in}} = 0.8\%$ $E_{\text{out}} = 1.5\%$

Leave more than one out

Leave one out: N training sessions on $N-1$ points each

More points for validation?

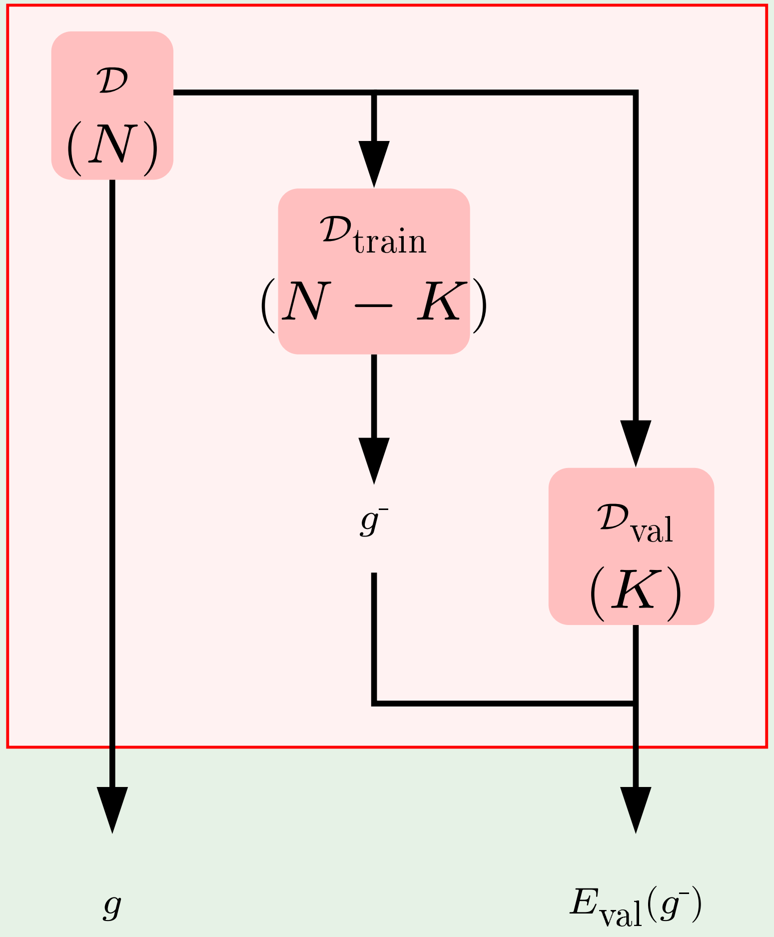


$\frac{N}{K}$ training sessions on $N-K$ points each

10-fold cross validation: $K = \frac{N}{10}$

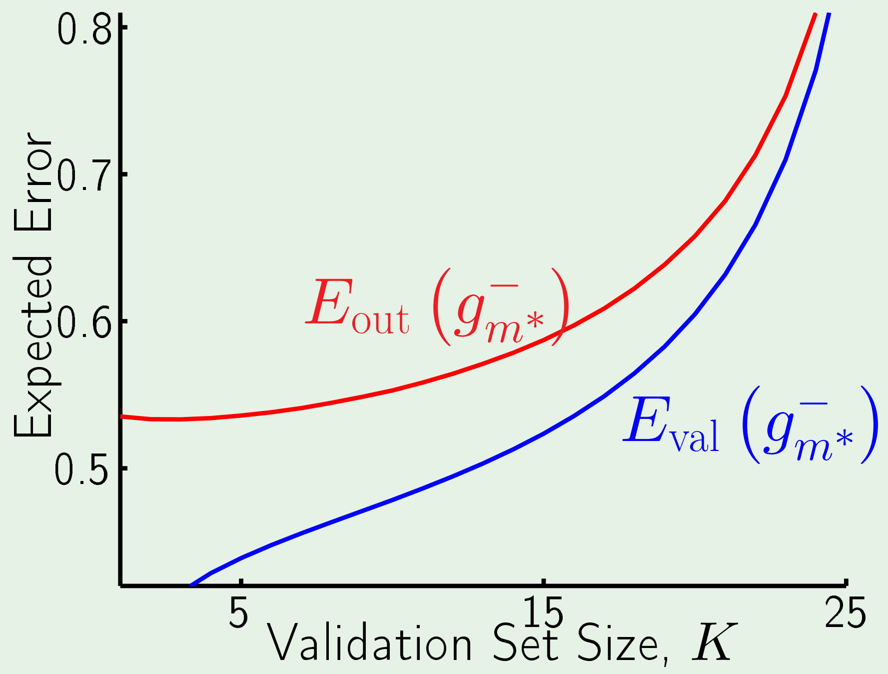
Review of Lecture 13

- Validation



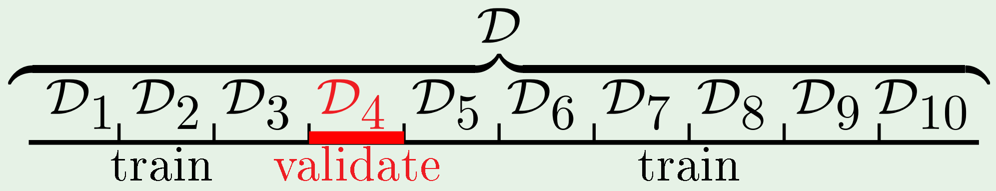
$E_{\text{val}}(g^-)$ estimates $E_{\text{out}}(g)$

- Data contamination



$\mathcal{D}_{\text{val}}$ slightly contaminated

- Cross validation



10-fold cross validation

Learning From Data

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Lecture 14: Support Vector Machines

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Thursday, May 17, 2012

Outline

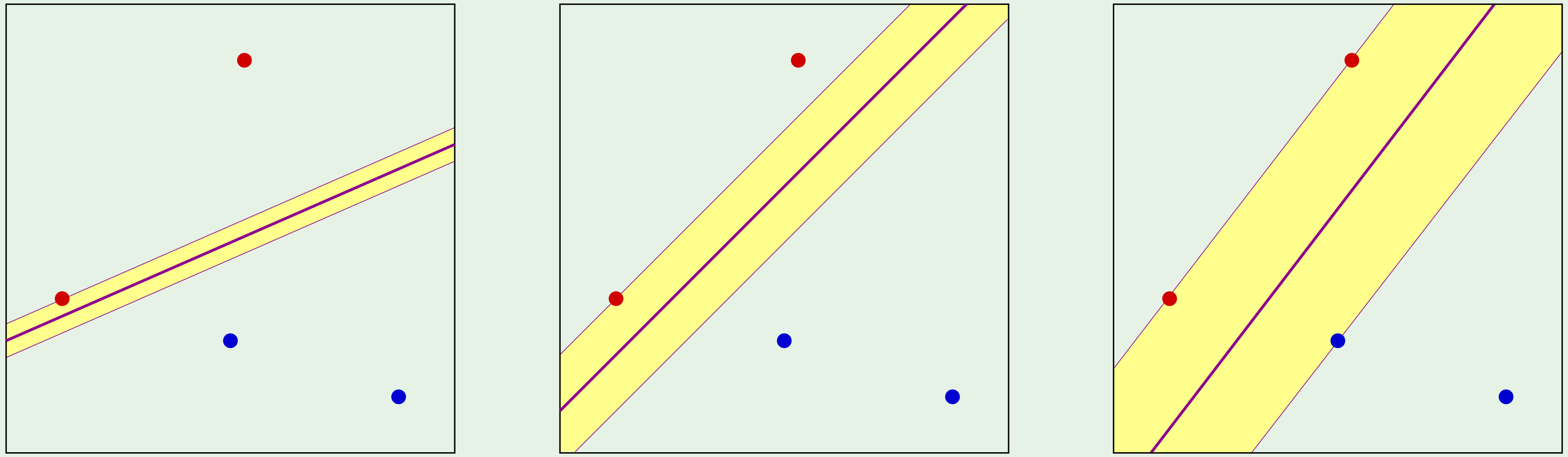
- Maximizing the margin
- The solution
- Nonlinear transforms

Better linear separation

Linearly separable data

Different separating lines

Which is best?

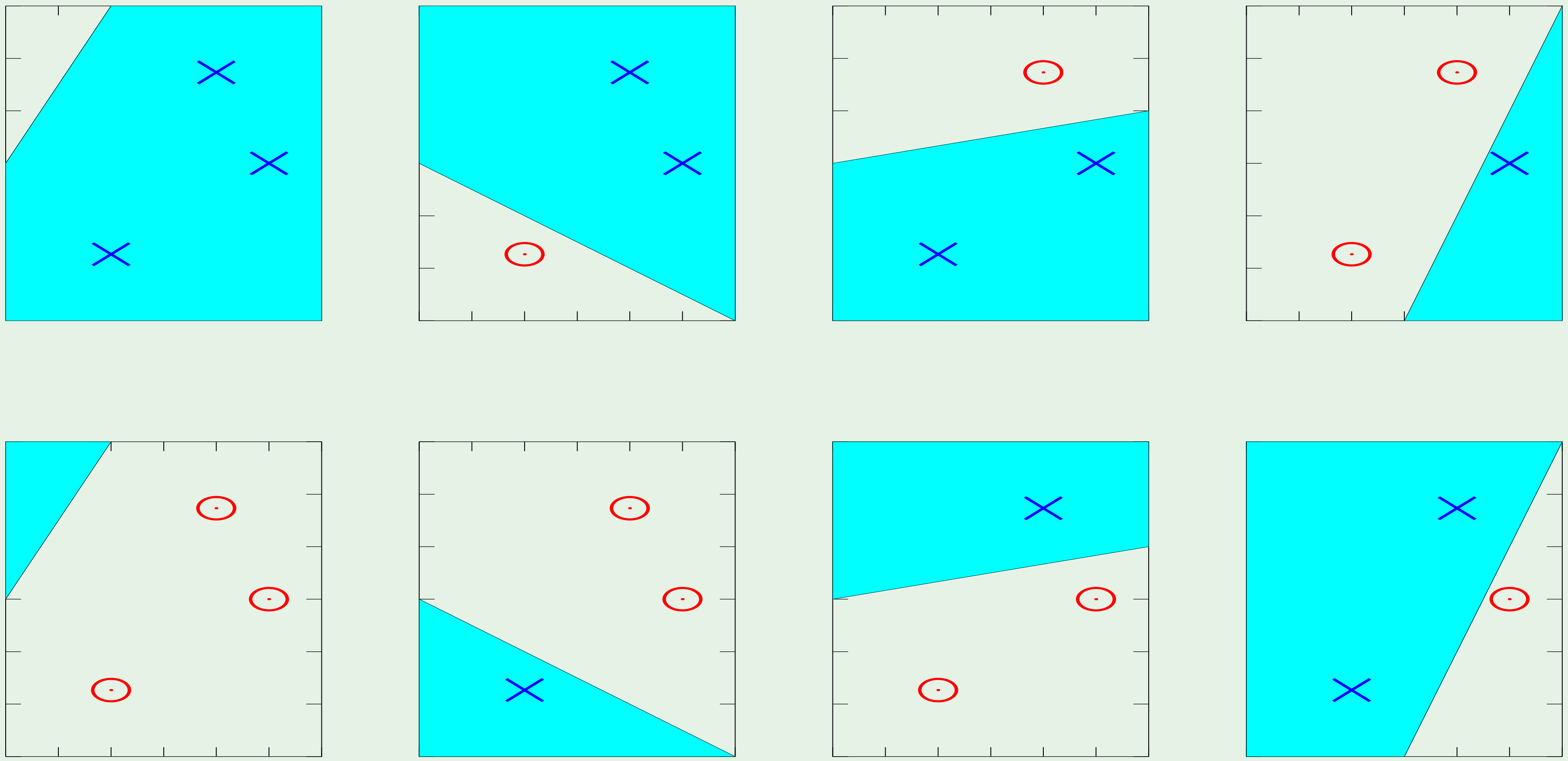


Two questions:

1. Why is bigger margin better?
2. Which $\mathbf{w}$ maximizes the margin?

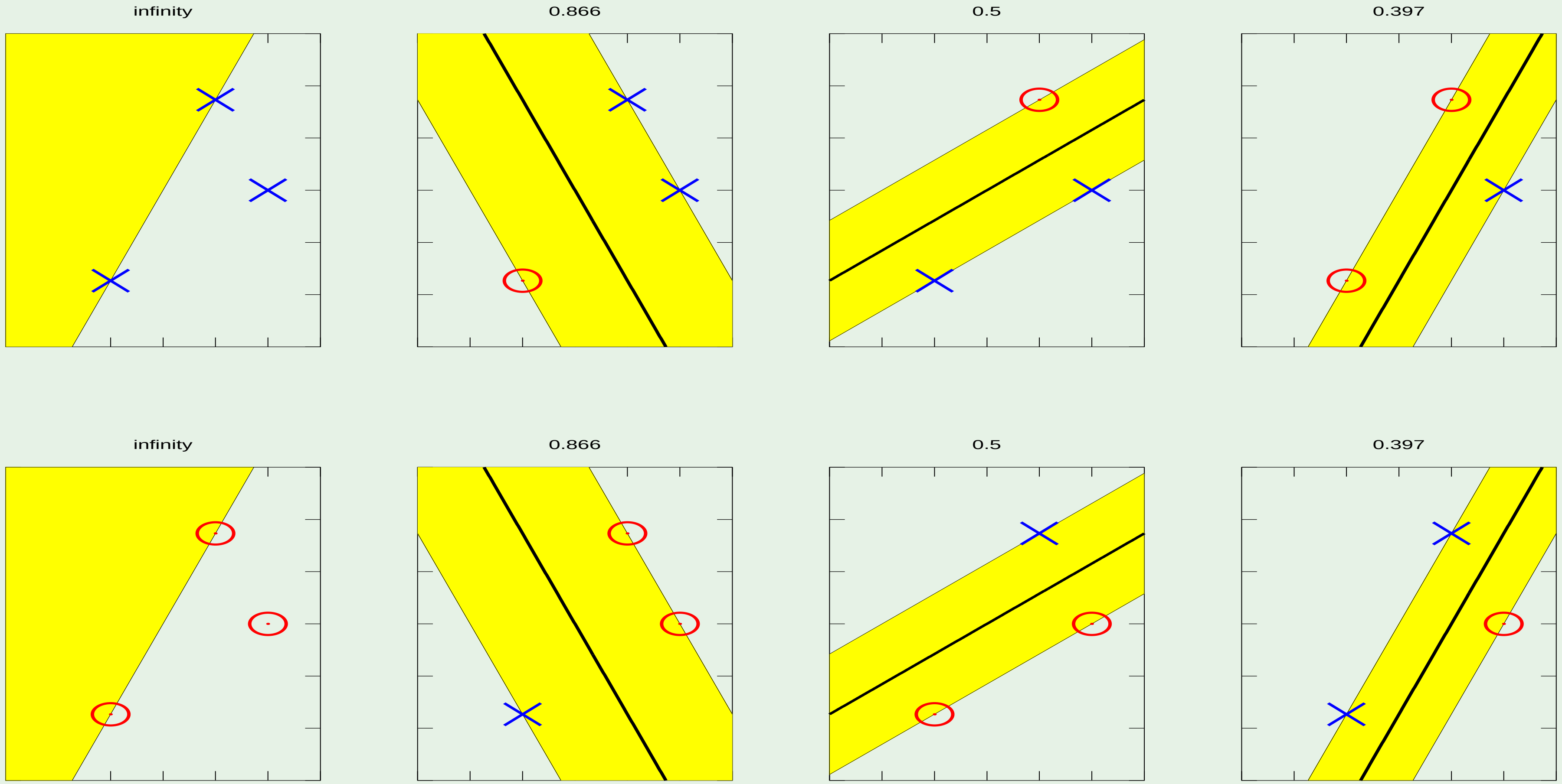
Remember the growth function?

All dichotomies with any line:



Dichotomies with fat margin

Fat margins imply fewer dichotomies



Finding $\mathbf{w}$ with large margin

Let $\mathbf{x}_n$ be the nearest data point to the plane $\mathbf{w}^{\intercal}\mathbf{x} = 0$. How far is it?

2 preliminary technicalities:

1. **Normalize $\mathbf{w}$:**

   $|\mathbf{w}^{\intercal}\mathbf{x}_n| = 1$

2. **Pull out w_0:**

   $\mathbf{w} = (w_1, \cdots, w_d)$ apart from b

   The plane is now $\boxed{\mathbf{w}^{\intercal}\mathbf{x} + b = 0}$ (no x_0)

Computing the distance

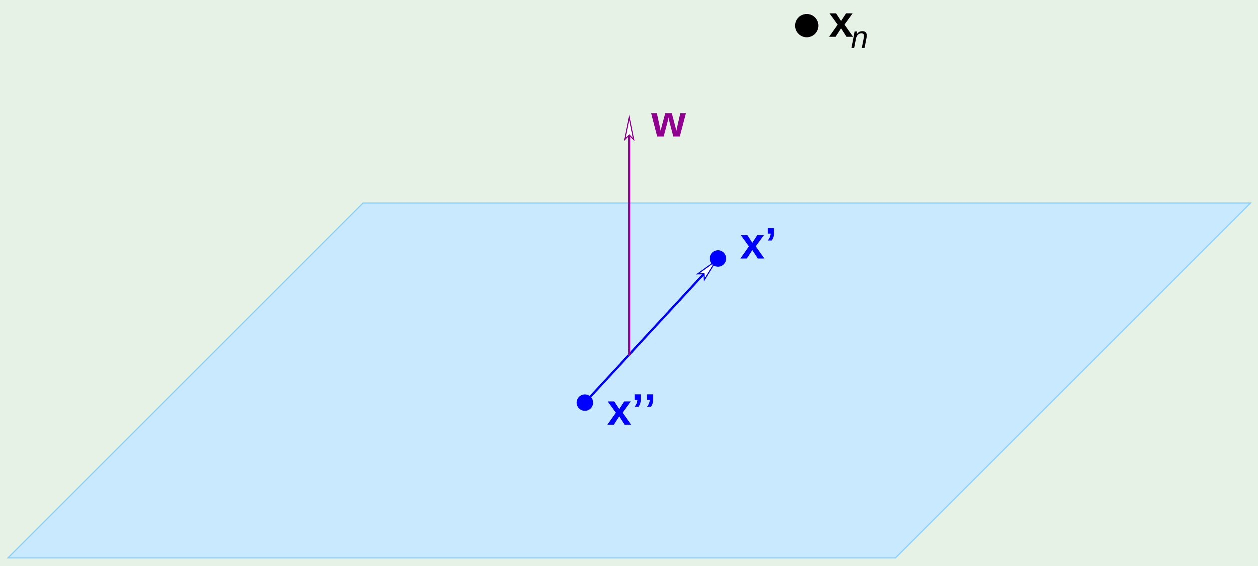
The distance between $\mathbf{x}_n$ and the plane $\mathbf{w}^\intercal\mathbf{x} + b = 0$ where $|\mathbf{w}^\intercal\mathbf{x}_n + b| = 1$

The vector $\mathbf{w}$ is $\perp$ to the plane in the $\mathcal{X}$ space:

Take $\mathbf{x}'$ and $\mathbf{x}''$ on the plane

$$\mathbf{w}^\intercal\mathbf{x}' + b = 0 \quad \text{and} \quad \mathbf{w}^\intercal\mathbf{x}'' + b = 0$$

$$\Longrightarrow \quad \mathbf{w}^\intercal(\mathbf{x}' - \mathbf{x}'') = 0$$



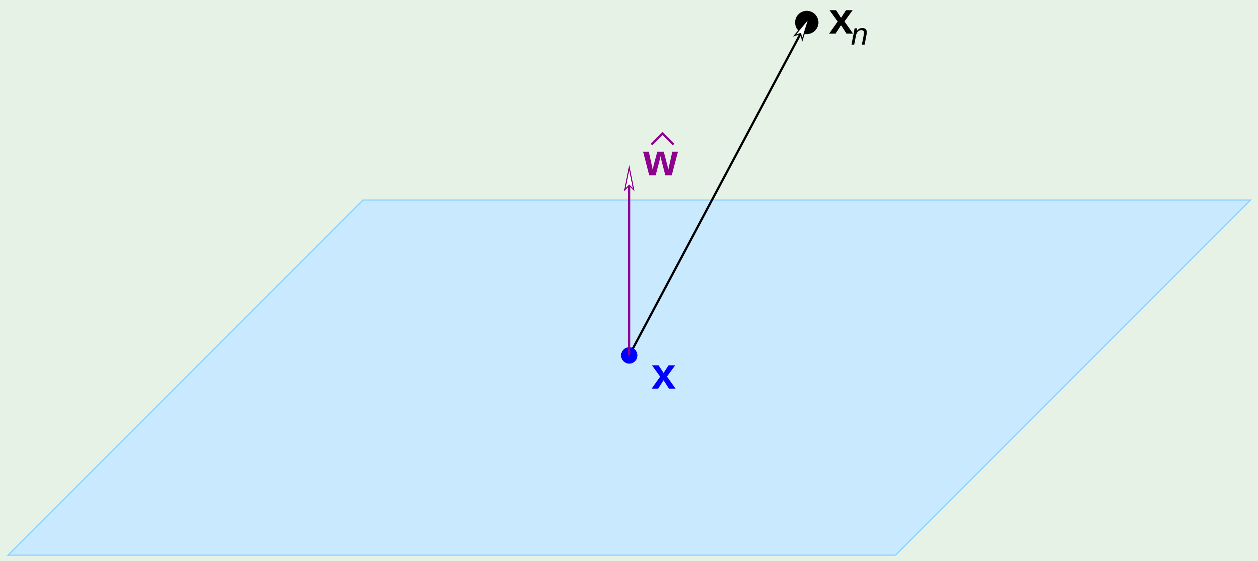
and the distance is ...

Distance between $\mathbf{x}_n$ and the plane:

Take any point $\mathbf{x}$ on the plane

Projection of $\mathbf{x}_n - \mathbf{x}$ on $\mathbf{w}$

$$\hat{\mathbf{w}} = \frac{\mathbf{w}}{\|\mathbf{w}\|} \implies \text{distance} = \left|\hat{\mathbf{w}}^{\mathsf{T}}(\mathbf{x}_n - \mathbf{x})\right|$$



$$\text{distance} = \frac{1}{\|\mathbf{w}\|}\left|\mathbf{w}^{\mathsf{T}}\mathbf{x}_n - \mathbf{w}^{\mathsf{T}}\mathbf{x}\right| = \frac{1}{\|\mathbf{w}\|}\left|\mathbf{w}^{\mathsf{T}}\mathbf{x}_n + b - \mathbf{w}^{\mathsf{T}}\mathbf{x} - b\right| = \frac{1}{\|\mathbf{w}\|}$$

The optimization problem

Maximize $\frac{1}{\|\mathbf{w}\|}$

subject to $\min_{n=1,2,\ldots,N} |\mathbf{w}^\intercal \mathbf{x}_n + b| = 1$

Notice: $|\mathbf{w}^\intercal \mathbf{x}_n + b| = y_n \left(\mathbf{w}^\intercal \mathbf{x}_n + b\right)$

Minimize $\frac{1}{2} \mathbf{w}^\intercal \mathbf{w}$

subject to $y_n \left(\mathbf{w}^\intercal \mathbf{x}_n + b\right) \geq 1$ for $n = 1, 2, \ldots, N$

Outline

- Maximizing the margin
- The solution
- Nonlinear transforms

Constrained optimization

Minimize $\frac{1}{2}\,\mathbf{w}^{\intercal}\mathbf{w}$

subject to $y_n\left(\mathbf{w}^{\intercal}\mathbf{x}_n + b\right) \geq 1$ for $n = 1, 2, \ldots, N$

$\mathbf{w} \in \mathbb{R}^d,\ b \in \mathbb{R}$

Lagrange? inequality constraints $\Longrightarrow$ KKT

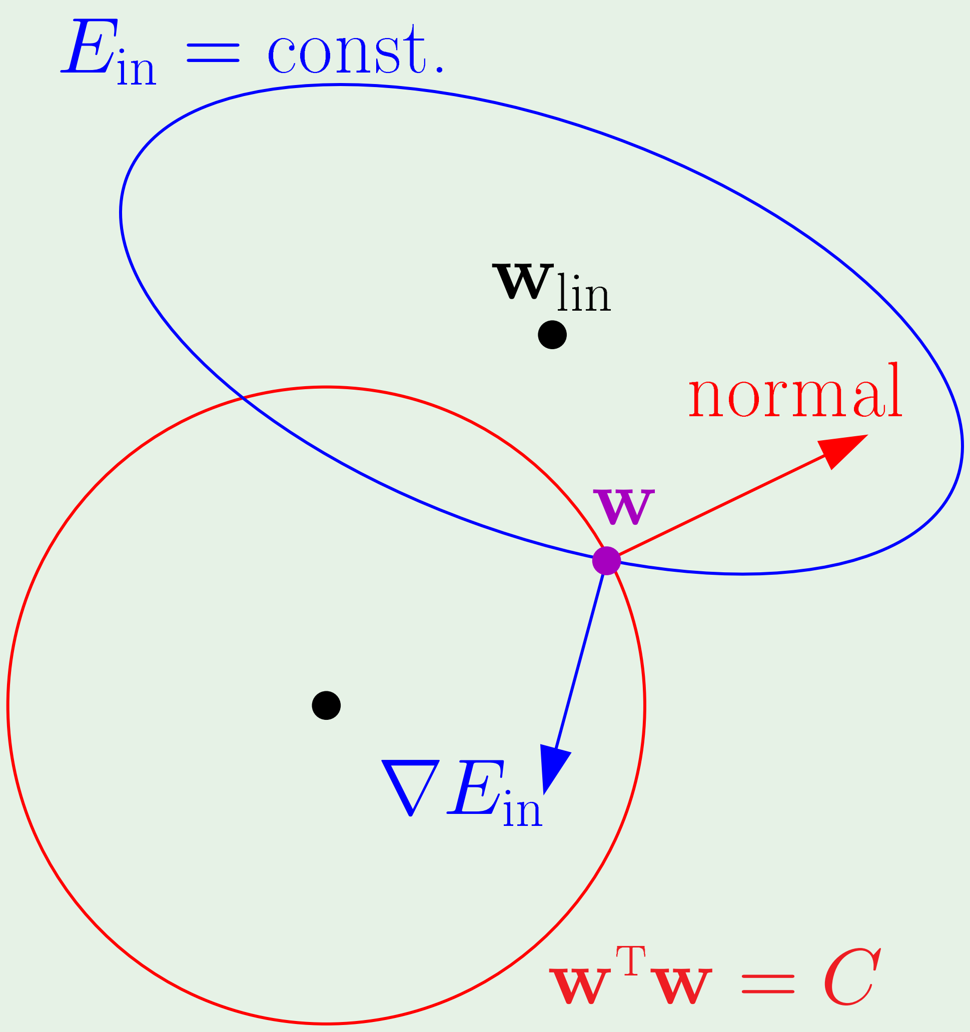
We saw this before

Remember regularization?

Minimize $E_{\text{in}}(\mathbf{w}) \;=\; \frac{1}{N}\,(\mathrm{Z}\mathbf{w}-\mathbf{y})^{\mathsf{T}}(\mathrm{Z}\mathbf{w}-\mathbf{y})$

subject to: $\mathbf{w}^{\mathsf{T}}\mathbf{w} \leq C$

∇E_{in} normal to constraint



	optimize	constrain
Regularization:	E_{in}	$\mathbf{w}^{\mathsf{T}}\mathbf{w}$
SVM:	$\mathbf{w}^{\mathsf{T}}\mathbf{w}$	E_{in}

Lagrange formulation

Minimize $\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\,\mathbf{w}^{\intercal}\mathbf{w} - \sum_{n=1}^{N} \alpha_n (y_n\,(\mathbf{w}^{\intercal}\mathbf{x}_n + b) - 1)$

w.r.t. $\mathbf{w}$ and b and maximize w.r.t. each $\alpha_n \geq 0$

$$\nabla_{\mathbf{w}}\mathcal{L} = \mathbf{w} - \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n = \mathbf{0}$$

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{n=1}^{N} \alpha_n y_n = 0$$

Substituting ...

$$\mathbf{w} \;=\; \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n \qquad \text{and} \qquad \sum_{n=1}^{N} \alpha_n y_n \;=\; 0$$

in the Lagrangian

$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\,\mathbf{w}^{\intercal}\mathbf{w} \;-\; \sum_{n=1}^{N} \alpha_n \left(y_n \left(\mathbf{w}^{\intercal}\mathbf{x}_n + b\right) - 1\right)$$

we get

$$\mathcal{L}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \,\alpha_n \alpha_m\, \mathbf{x}_n^{\intercal}\mathbf{x}_m$$

Maximize w.r.t. to $\boldsymbol{\alpha}$ subject to $\alpha_n \geq 0$ for $n = 1, \cdots, N$ **and** $\sum_{n=1}^{N} \alpha_n y_n = 0$

The solution - quadratic programming

$$\min_{\boldsymbol{\alpha}} \quad \frac{1}{2}\,\boldsymbol{\alpha}^{\intercal} \underbrace{\begin{bmatrix} y_1y_1\ \mathbf{x}_1^{\intercal}\mathbf{x}_1 & y_1y_2\ \mathbf{x}_1^{\intercal}\mathbf{x}_2 & \ldots & y_1y_N\ \mathbf{x}_1^{\intercal}\mathbf{x}_N \\ y_2y_1\ \mathbf{x}_2^{\intercal}\mathbf{x}_1 & y_2y_2\ \mathbf{x}_2^{\intercal}\mathbf{x}_2 & \ldots & y_2y_N\ \mathbf{x}_2^{\intercal}\mathbf{x}_N \\ \ldots & \ldots & \ldots & \ldots \\ y_Ny_1\ \mathbf{x}_N^{\intercal}\mathbf{x}_1 & y_Ny_2\ \mathbf{x}_N^{\intercal}\mathbf{x}_2 & \ldots & y_Ny_N\ \mathbf{x}_N^{\intercal}\mathbf{x}_N \end{bmatrix}}_{\text{quadratic coefficients}} \boldsymbol{\alpha} + \underbrace{\left(-\mathbf{1}^{\intercal}\right)}_{\text{linear}} \boldsymbol{\alpha}$$

subject to $\underbrace{\mathbf{y}^{\intercal}\boldsymbol{\alpha} = 0}_{\text{linear constraint}}$

$$\underbrace{\mathbf{0}}_{\text{lower bounds}} \leq \boldsymbol{\alpha} \leq \underbrace{\infty}_{\text{upper bounds}}$$

QP hands us $\boldsymbol{\alpha}$

Solution: $\boldsymbol{\alpha} = \alpha_1, \cdots, \alpha_N$

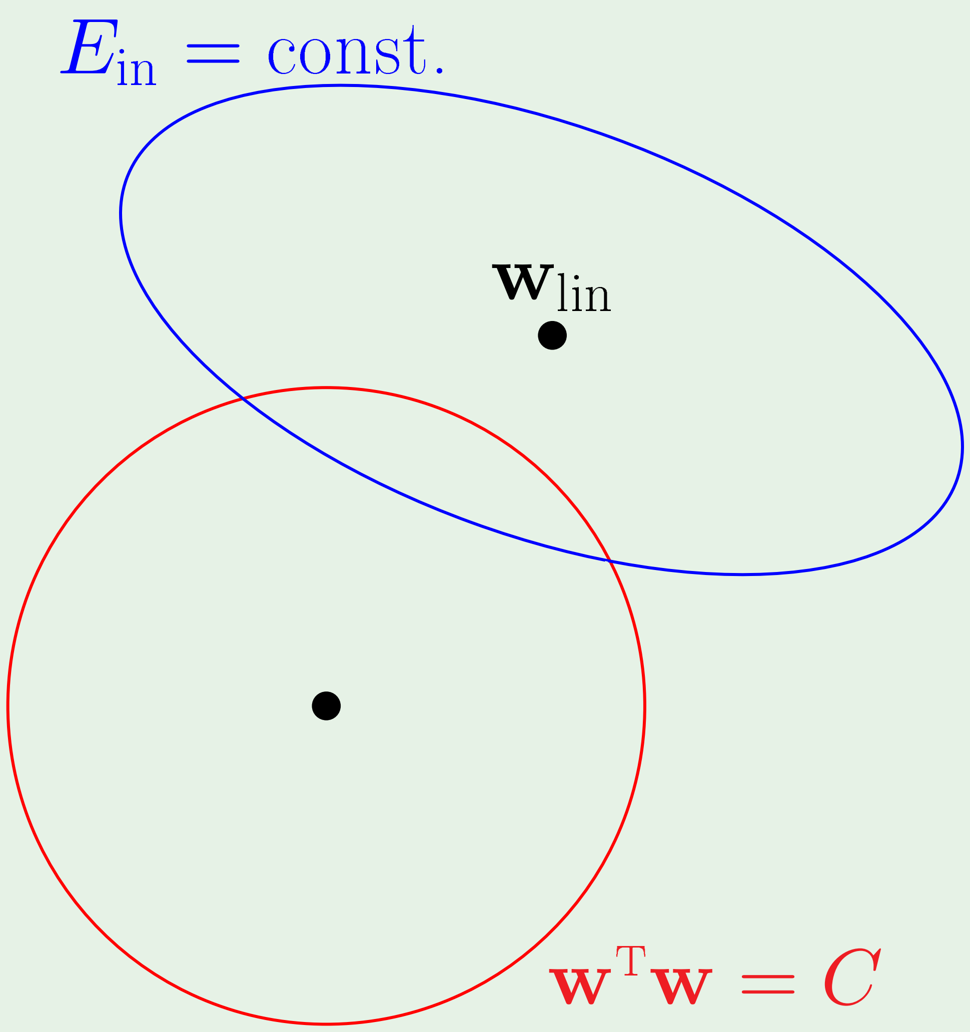
$$\Longrightarrow \quad \mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n$$

KKT condition: For $n = 1, \cdots, N$

$$\alpha_n \left(y_n \left(\mathbf{w}^{\intercal} \mathbf{x}_n + b \right) - 1 \right) = 0$$

We saw this before!

$\alpha_n > 0 \implies \mathbf{x}_n$ is a **support vector**



Support vectors

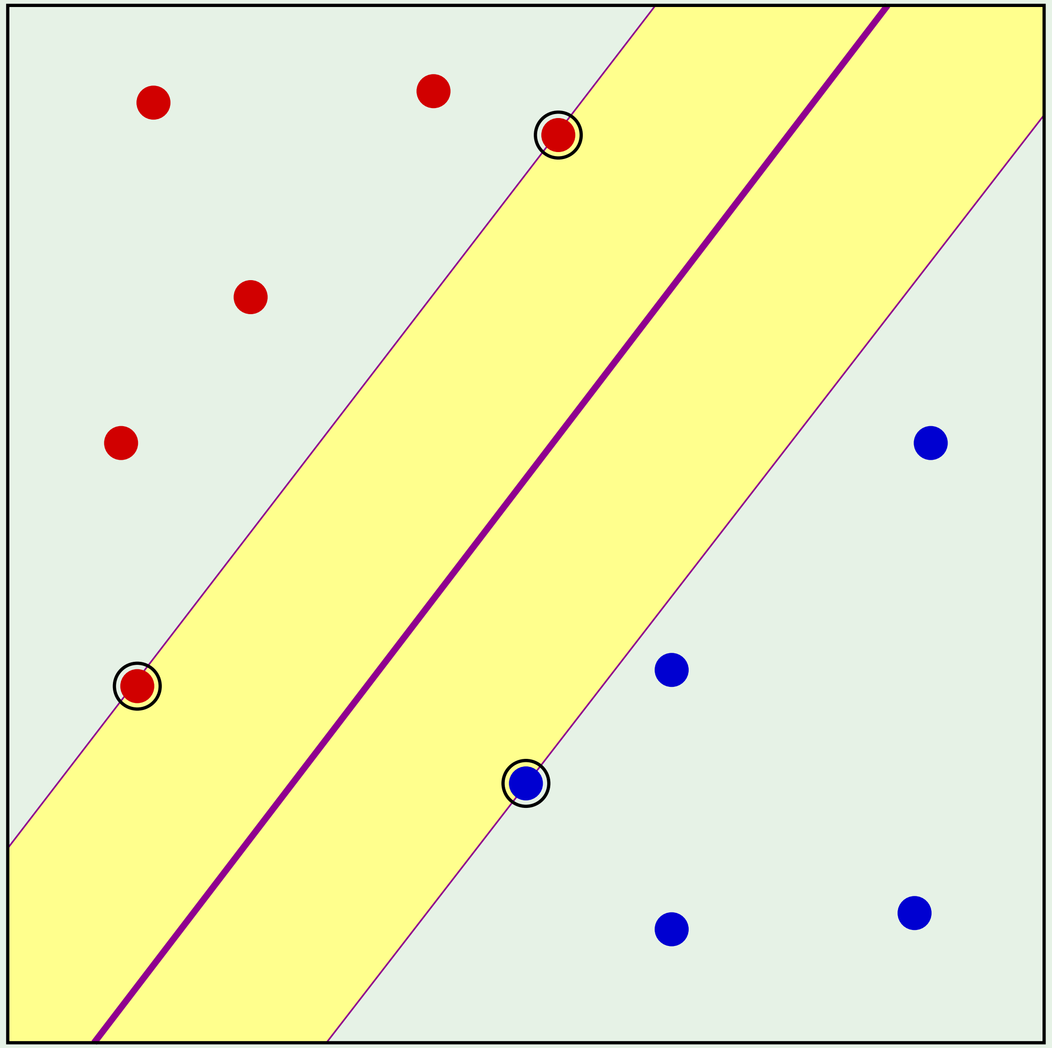
Closest $\mathbf{x}_n$'s to the plane: achieve the margin

$$\Longrightarrow \quad y_n\left(\mathbf{w}^\intercal \mathbf{x}_n + b\right) = 1$$

$$\mathbf{w} = \sum_{\mathbf{x}_n \text{ is SV}} \alpha_n y_n \mathbf{x}_n$$

Solve for b using any SV:

$$y_n\left(\mathbf{w}^\intercal \mathbf{x}_n + b\right) = 1$$

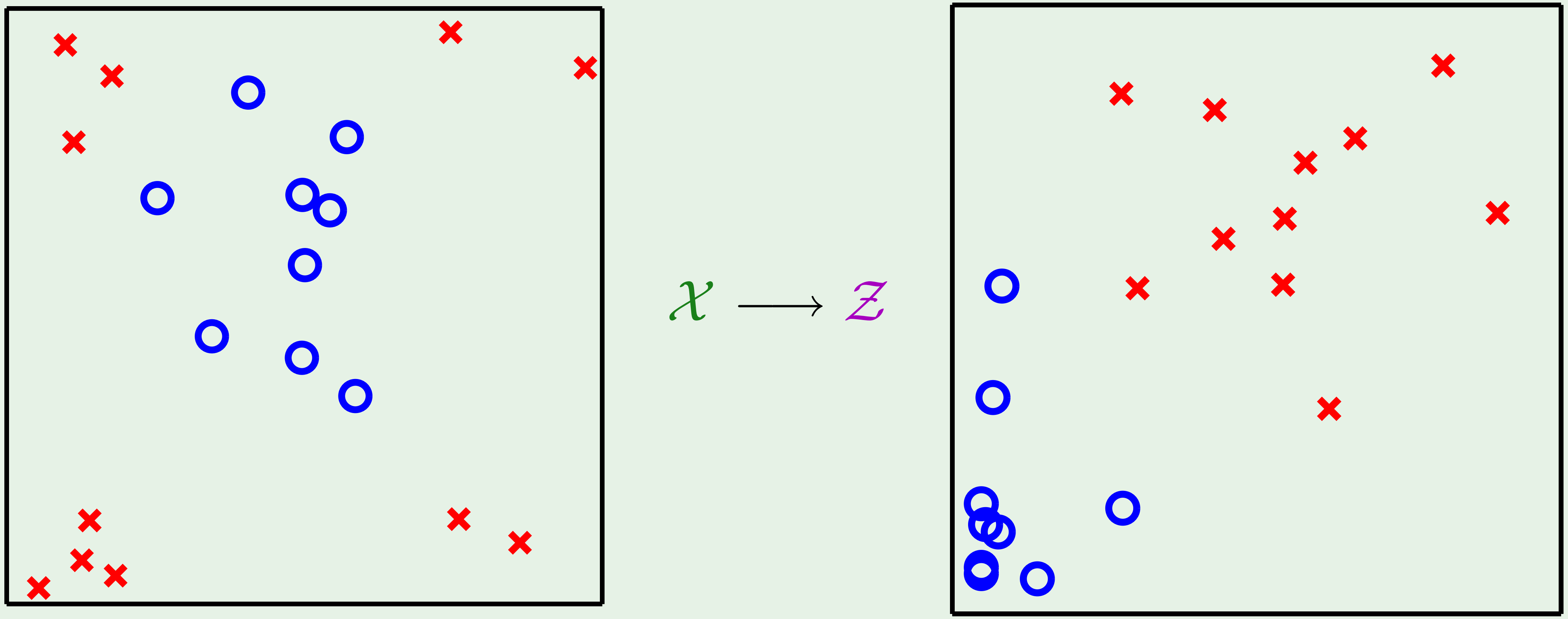


Outline

- Maximizing the margin
- The solution
- Nonlinear transforms

z instead of x

$$\mathcal{L}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \, \alpha_n \alpha_m \, \mathbf{z}_n^{\mathsf{T}} \mathbf{z}_m$$



"Support vectors" in $\mathcal{X}$ space

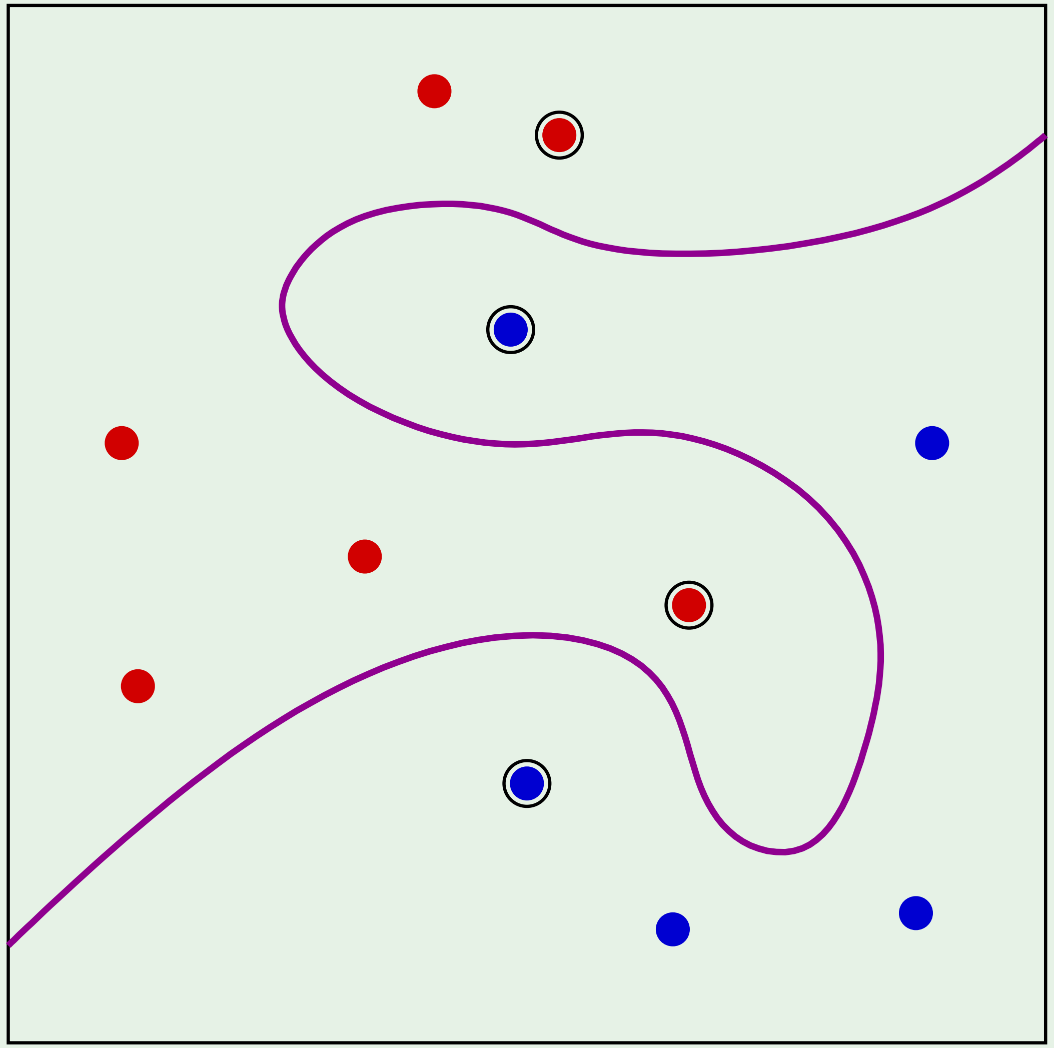
Support vectors live in $\mathcal{Z}$ space

In $\mathcal{X}$ space, "pre-images" of support vectors

The margin is maintained in $\mathcal{Z}$ space

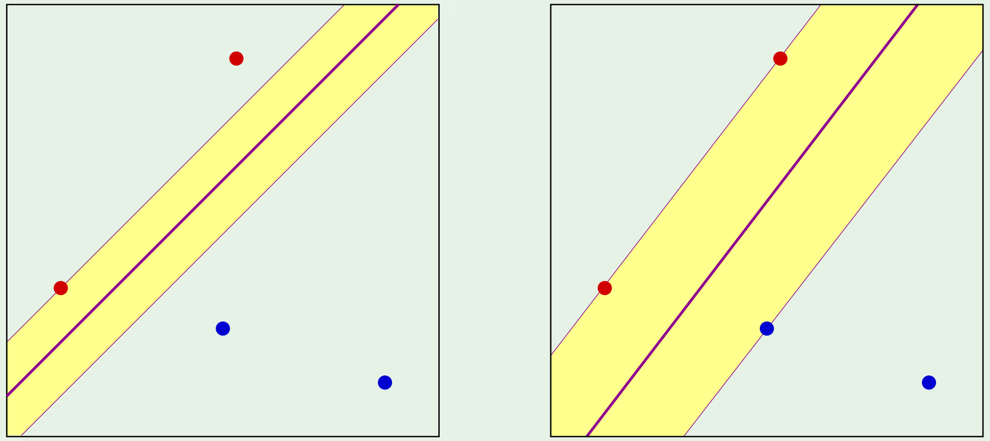
Generalization result

$$\mathbb{E}[E_{\text{out}}] \leq \frac{\mathbb{E}[\text{\# of SV's}]}{N-1}$$



Review of Lecture 14

- The margin

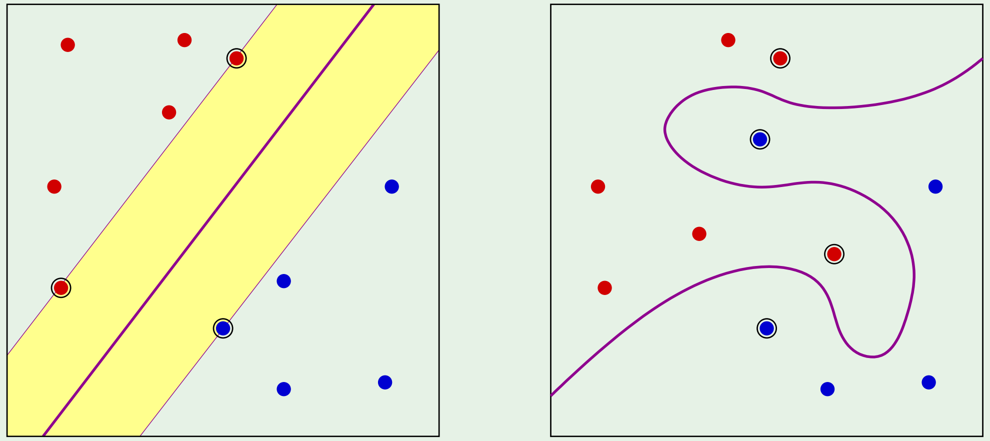


Maximizing the margin $\Longrightarrow$ dual problem:

$$\mathcal{L}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \, \alpha_n \alpha_m \, \mathbf{x}_n^{\mathsf{T}} \mathbf{x}_m$$

quadratic programming

- Support vectors



$\mathbf{x}_n$ (or $\mathbf{z}_n$) with Lagrange $\alpha_n > 0$

$$\mathbb{E}[E_{\text{out}}] \le \frac{\mathbb{E}[\text{\# of SV's}]}{N-1}$$

(in-sample check of out-of-sample error)

- Nonlinear transform

Complex h, but simple $\mathcal{H}$ ☺

Learning From Data

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Lecture 15: Kernel Methods

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Tuesday, May 22, 2012

Outline

- The kernel trick

- Soft-margin SVM

What do we need from the $\mathcal{Z}$ space?

$$\mathcal{L}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \, \alpha_n \alpha_m \, \mathbf{z}_n^{\mathsf{T}} \mathbf{z}_m$$

Constraints: $\alpha_n \geq 0$ for $n = 1, \cdots, N$ and $\sum_{n=1}^{N} \alpha_n y_n = 0$

$$\boxed{g(\mathbf{x}) = \operatorname{sign}\left(\mathbf{w}^{\mathsf{T}} \mathbf{z} + b\right)}$$ need $\mathbf{z}_n^{\mathsf{T}} \mathbf{z}$

where $\mathbf{w} = \sum_{\mathbf{z}_n \text{ is SV}} \alpha_n y_n \mathbf{z}_n$

and b: $y_m \left(\mathbf{w}^{\mathsf{T}} \mathbf{z}_m + b\right) = 1$ need $\mathbf{z}_n^{\mathsf{T}} \mathbf{z}_m$

Generalized inner product

Given two points $\mathbf{x}$ and $\mathbf{x}' \in \mathcal{X}$, we need $\mathbf{z}^\intercal\mathbf{z}'$

Let $\mathbf{z}^\intercal\mathbf{z}' = K(\mathbf{x}, \mathbf{x}')$ (the kernel) "inner product" of $\mathbf{x}$ and $\mathbf{x}'$

Example: $\mathbf{x} = (x_1, x_2) \longrightarrow$ 2nd-order Φ

$$\mathbf{z} = \Phi(\mathbf{x}) = (1, x_1, x_2, x_1^2, x_2^2, x_1 x_2)$$

$$K(\mathbf{x}, \mathbf{x}') = \mathbf{z}^\intercal\mathbf{z}' = 1 + x_1 {x'}_1 + x_2 {x'}_2 + x_1^2 {x'}_1^2 + x_2^2 {x'}_2^2 + x_1 {x'}_1 x_2 {x'}_2$$

The trick

Can we compute $K(\mathbf{x}, \mathbf{x}')$ **without** transforming $\mathbf{x}$ and $\mathbf{x}'$?

Example: Consider $K(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^\intercal \mathbf{x}')^2 = (1 + x_1 x'_1 + x_2 x'_2)^2$

$$= 1 + x_1^2 x'^2_1 + x_2^2 x'^2_2 + 2 x_1 x'_1 + 2 x_2 x'_2 + 2 x_1 x'_1 x_2 x'_2$$

This is an inner product!

$$(1 , x_1^2 , x_2^2 , \sqrt{2}\, x_1 , \sqrt{2}\, x_2 , \sqrt{2}\, x_1 x_2)$$

$$(1 , x'^2_1 , x'^2_2 , \sqrt{2} x'_1 , \sqrt{2} x'_2 , \sqrt{2} x'_1 x'_2)$$

The polynomial kernel

$\mathcal{X} = \mathbb{R}^d$ and $\Phi : \mathcal{X} \to \mathcal{Z}$ is polynomial of order Q

The "equivalent" kernel $K(\mathbf{x}, \mathbf{x}') = (1 + \mathbf{x}^\intercal \mathbf{x}')^Q$

$$= (1 + x_1 x'_1 + x_2 x'_2 + \cdots + x_d x'_d)^Q$$

Compare for $d = 10$ and $Q = 100$

Can adjust scale: $K(\mathbf{x}, \mathbf{x}') = (a\mathbf{x}^\intercal \mathbf{x}' + b)^Q$

We only need $\mathcal{Z}$ to exist!

If $K(\mathbf{x}, \mathbf{x}')$ is an inner product in some space $\mathcal{Z}$, we are good.

Example: $$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\gamma \left\|\mathbf{x} - \mathbf{x}'\right\|^2\right)$$

Infinite-dimensional $\mathcal{Z}$: take simple case

$$K(x, x') = \exp\left(-(x - x')^2\right)$$

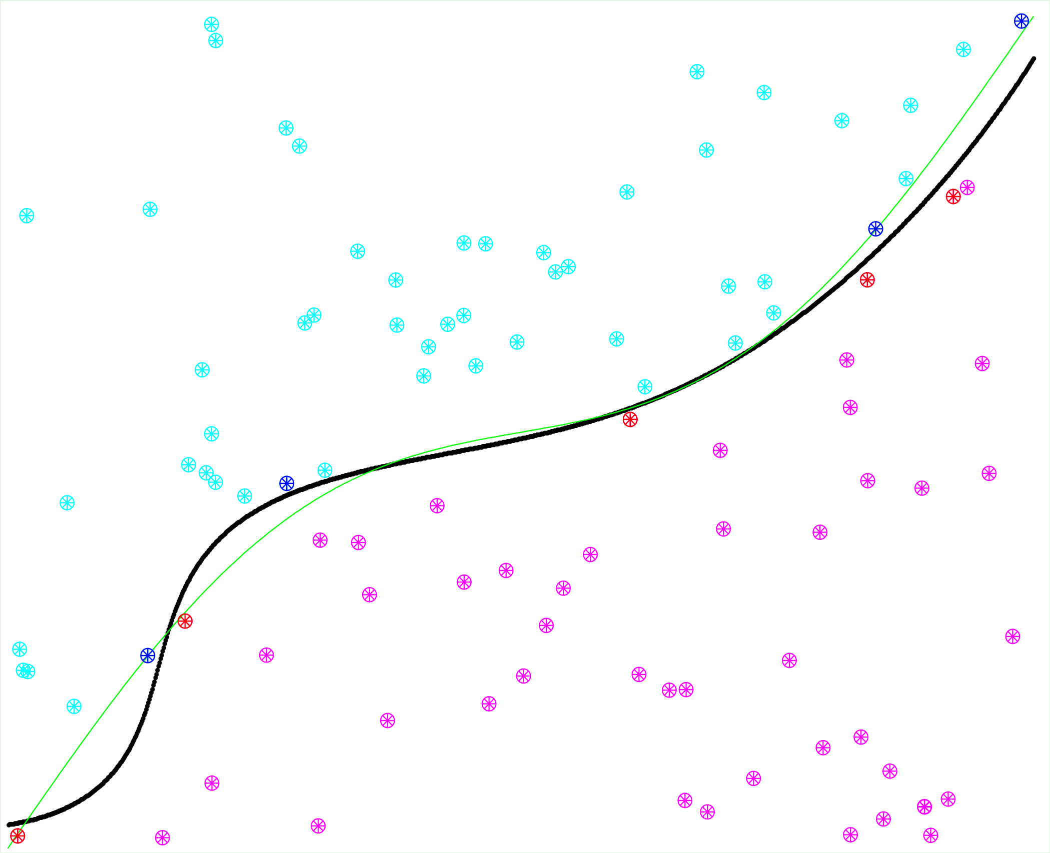
$$= \exp\left(-x^2\right) \exp\left(-x'^2\right) \underbrace{\sum_{k=0}^{\infty} \frac{2^k (x)^k (x')^k}{k!}}_{\exp(2xx')}$$

This kernel in action

Slightly non-separable case:

Transforming $\mathcal{X}$ into ∞-dimensional $\mathcal{Z}$

Overkill? Count the support vectors



Kernel formulation of SVM

Remember quadratic programming? The only difference now is:

$$\underbrace{\begin{bmatrix} y_1y_1\,K(\mathbf{x}_1,\mathbf{x}_1) & y_1y_2\,K(\mathbf{x}_1,\mathbf{x}_2) & \ldots & y_1y_N K(\mathbf{x}_1,\mathbf{x}_N) \\ y_2y_1\,K(\mathbf{x}_2,\mathbf{x}_1) & y_2y_2\,K(\mathbf{x}_2,\mathbf{x}_2) & \ldots & y_2y_N K(\mathbf{x}_2,\mathbf{x}_N) \\ \ldots & \ldots & \ldots & \ldots \\ y_Ny_1 K(\mathbf{x}_N,\mathbf{x}_1) & y_Ny_2 K(\mathbf{x}_N,\mathbf{x}_2) & \ldots & y_Ny_N K(\mathbf{x}_N,\mathbf{x}_N) \end{bmatrix}}_{\text{quadratic coefficients}}$$

Everything else is the same.

The final hypothesis

Express $g(\mathbf{x}) = \text{sign}\left(\mathbf{w}^\intercal \mathbf{z} + b\right)$ in terms of $K(-,-)$

$$\mathbf{w} = \sum_{\mathbf{z}_n \text{ is SV}} \alpha_n y_n \mathbf{z}_n \quad \Longrightarrow \quad g(\mathbf{x}) = \text{sign}\left(\sum_{\alpha_n > 0} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}) + b\right)$$

where $$b = y_m - \sum_{\alpha_n > 0} \alpha_n y_n K(\mathbf{x}_n, \mathbf{x}_m)$$

for any support vector $(\alpha_m > 0)$

How do we know that $\mathcal{Z}$ exists ...

... for a given $K(\mathbf{x}, \mathbf{x}')$? valid kernel

Three approaches:

1. By construction
2. Math properties (*Mercer's condition*)
3. Who cares? ☺

Design your own kernel

$K(\mathbf{x}, \mathbf{x}')$ is a valid kernel iff

1. It is symmetric and **2.** The matrix:

$$\begin{bmatrix} K(\mathbf{x}_1, \mathbf{x}_1) & K(\mathbf{x}_1, \mathbf{x}_2) & \dots & K(\mathbf{x}_1, \mathbf{x}_N) \\ K(\mathbf{x}_2, \mathbf{x}_1) & K(\mathbf{x}_2, \mathbf{x}_2) & \dots & K(\mathbf{x}_2, \mathbf{x}_N) \\ \dots & \dots & \dots & \dots \\ K(\mathbf{x}_N, \mathbf{x}_1) & K(\mathbf{x}_N, \mathbf{x}_2) & \dots & K(\mathbf{x}_N, \mathbf{x}_N) \end{bmatrix}$$

is **positive semi-definite**

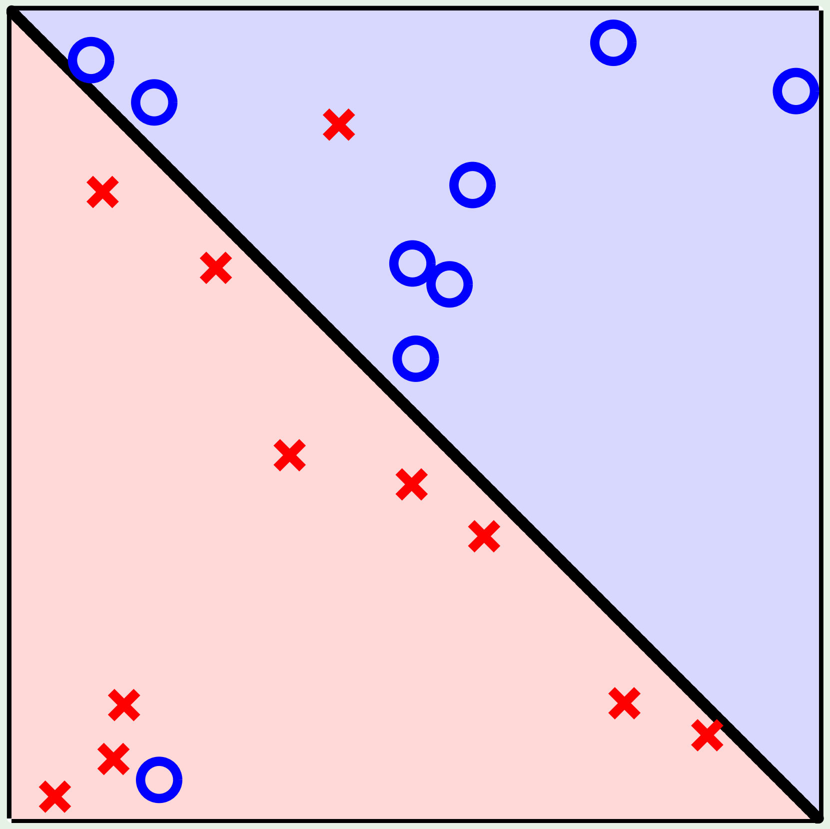
for any $\mathbf{x}_1, \cdots, \mathbf{x}_N$ (Mercer's condition)

Outline

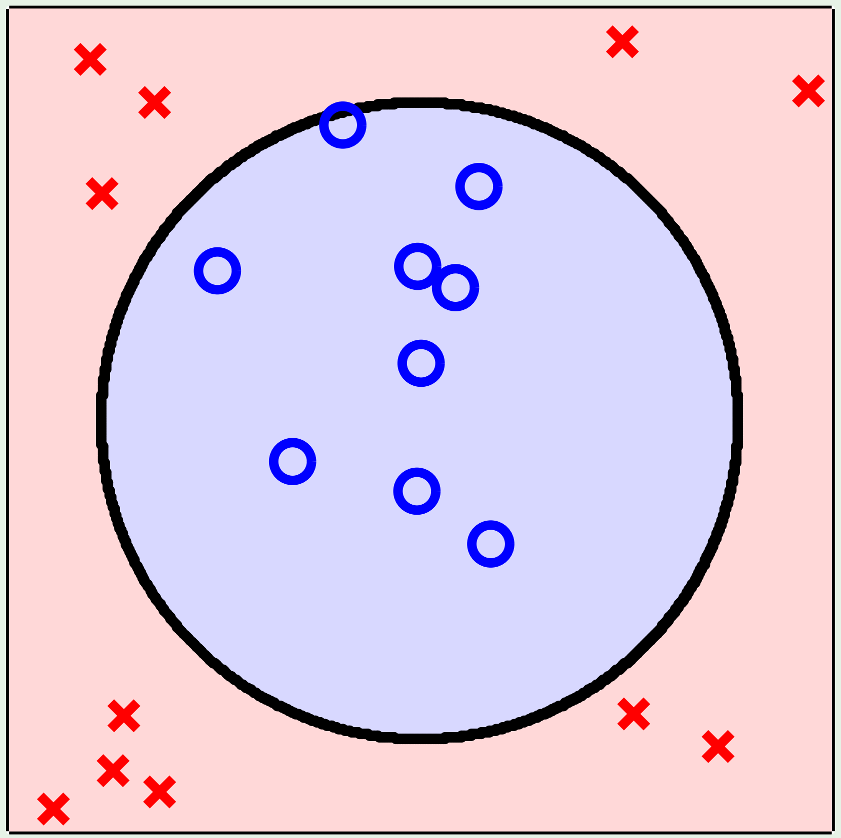
- The kernel trick
- Soft-margin SVM

Two types of non-separable

slightly:



seriously:

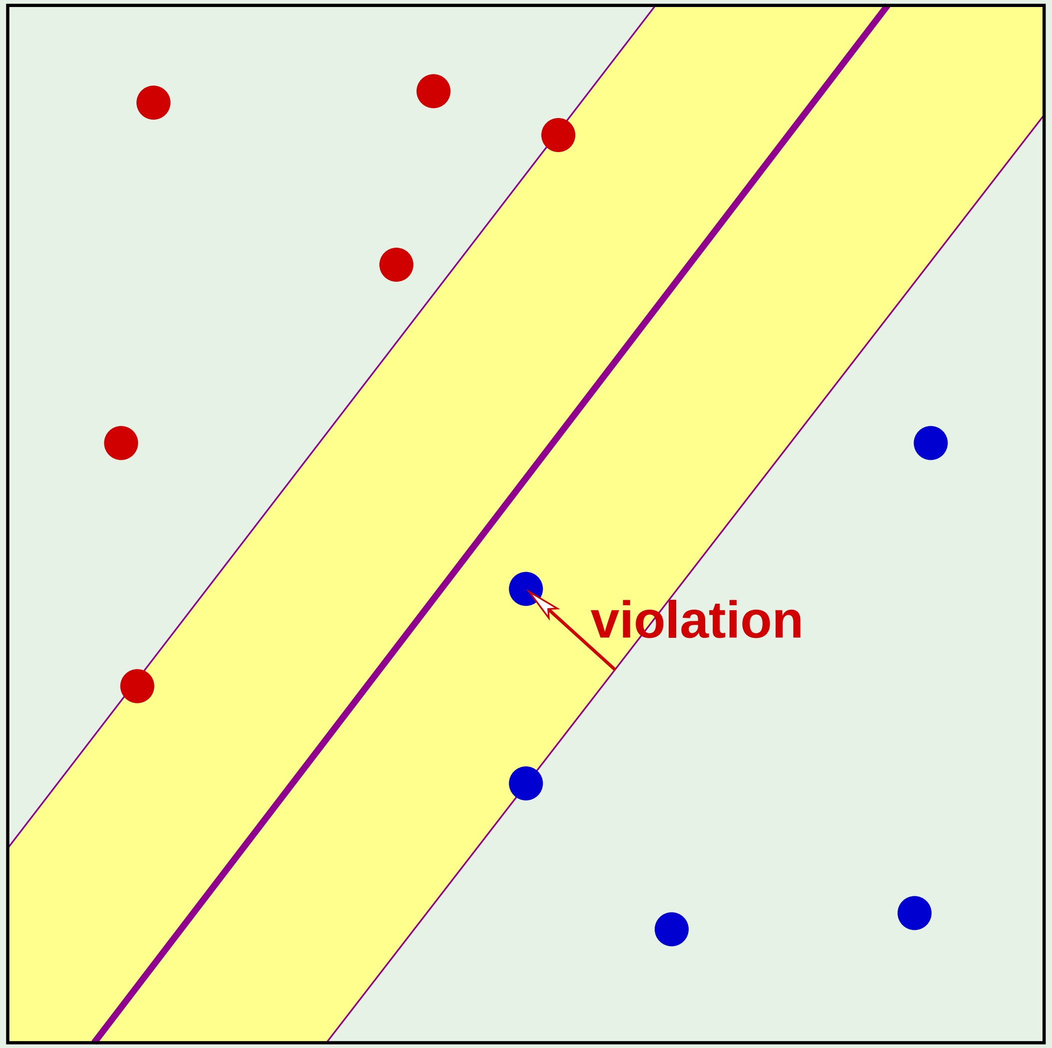


Error measure

Margin violation: $y_n \left(\mathbf{w}^\intercal \mathbf{x}_n + b \right) \geq 1$ fails

Quantify: $y_n \left(\mathbf{w}^\intercal \mathbf{x}_n + b \right) \geq 1 - \xi_n \qquad \xi_n \geq 0$

$$\text{Total violation} = \sum_{n=1}^{N} \xi_n$$



The new optimization

Minimize $\quad \frac{1}{2}\,\mathbf{w}^{\intercal}\mathbf{w} + C\sum_{n=1}^{N}\xi_n$

subject to $\quad y_n\left(\mathbf{w}^{\intercal}\mathbf{x}_n + b\right) \geq 1 - \xi_n \quad$ for $\quad n = 1, \ldots, N$

and $\quad \xi_n \geq 0 \quad$ for $\quad n = 1, \ldots, N$

$\mathbf{w} \in \mathbb{R}^d \;,\quad b \in \mathbb{R} \;,\quad \boldsymbol{\xi} \in \mathbb{R}^N$

Lagrange formulation

$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta}) = \frac{1}{2}\,\mathbf{w}^{\mathsf{T}}\mathbf{w} + C\sum_{n=1}^{N} \xi_n - \sum_{n=1}^{N} \alpha_n(y_n\,(\mathbf{w}^{\mathsf{T}}\mathbf{x}_n + b) - 1 + \xi_n) - \sum_{n=1}^{N} \beta_n\,\xi_n$$

Minimize w.r.t. $\mathbf{w}$, b, and $\boldsymbol{\xi}$ and maximize w.r.t. each $\alpha_n \geq 0$ and $\beta_n \geq 0$

$$\nabla_{\mathbf{w}}\mathcal{L} = \mathbf{w} - \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n = \mathbf{0}$$

$$\frac{\partial \mathcal{L}}{\partial b} = -\sum_{n=1}^{N} \alpha_n y_n = 0$$

$$\frac{\partial \mathcal{L}}{\partial \xi_n} = C - \alpha_n - \beta_n = 0$$

and the solution is . . .

Maximize $\mathcal{L}(\boldsymbol{\alpha}) = \sum_{n=1}^{N} \alpha_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} y_n y_m \, \alpha_n \alpha_m \, \mathbf{x}_n^{\mathsf{T}} \mathbf{x}_m$ w.r.t. to $\boldsymbol{\alpha}$

subject to $0 \leq \alpha_n \leq C$ for $n = 1, \cdots, N$ and $\sum_{n=1}^{N} \alpha_n y_n = 0$

$$\Longrightarrow \quad \mathbf{w} = \sum_{n=1}^{N} \alpha_n y_n \mathbf{x}_n$$

minimizes $\frac{1}{2} \mathbf{w}^{\mathsf{T}} \mathbf{w} + C \sum_{n=1}^{N} \xi_n$

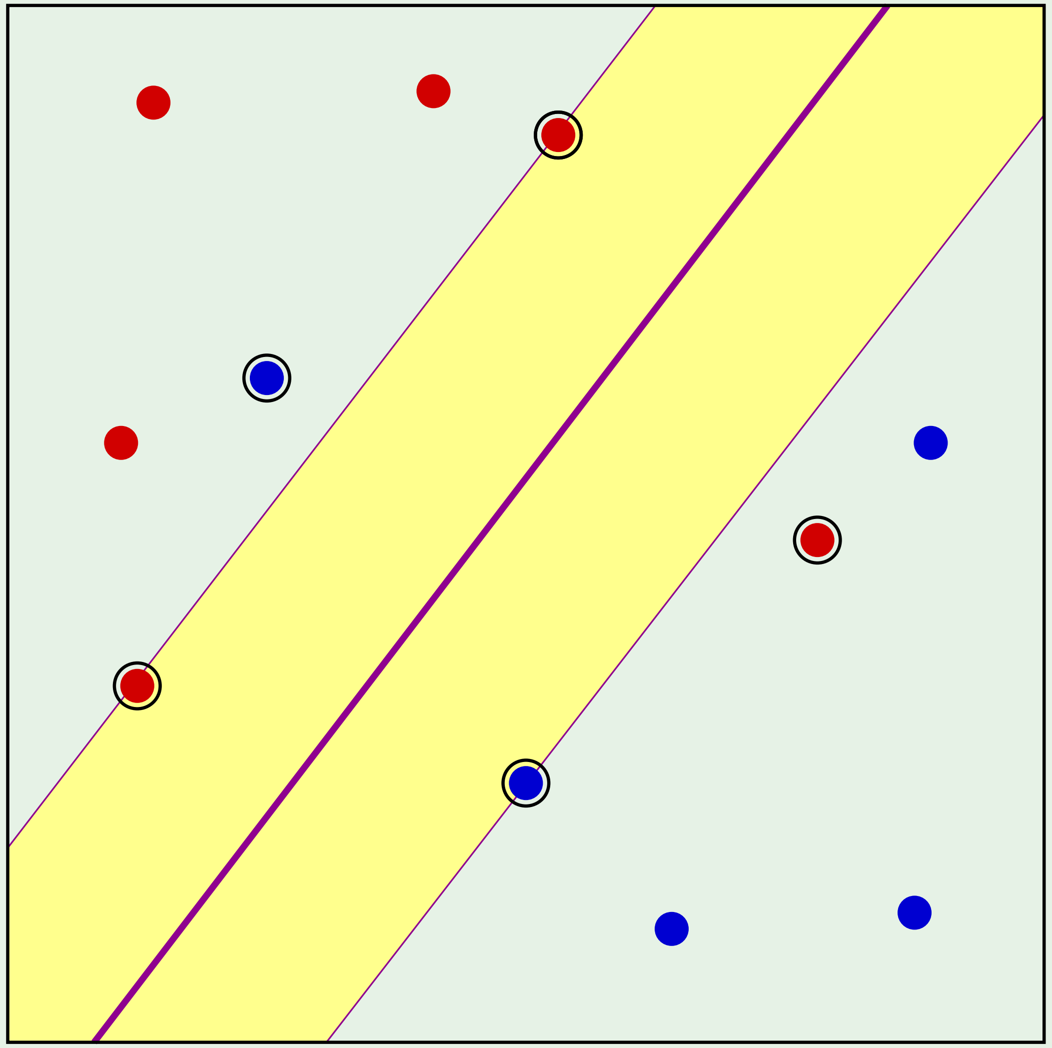
Types of support vectors

margin support vectors $(0 < \alpha_n < C)$

$$y_n\left(\mathbf{w}^{\intercal}\mathbf{x}_n + b\right) = 1 \qquad (\xi_n = 0)$$

non-margin support vectors $(\alpha_n = C)$

$$y_n\left(\mathbf{w}^{\intercal}\mathbf{x}_n + b\right) < 1 \qquad (\xi_n > 0)$$



Two technical observations

1. Hard margin: What if data is not linearly separable?

"primal $\longrightarrow$ dual" breaks down

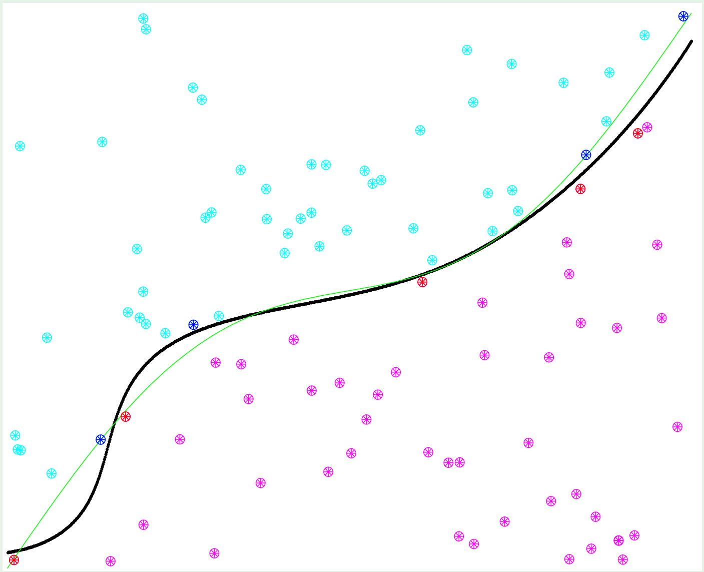
2. $\mathcal{Z}$: What if there is w_0?

All goes to b and $w_0 \to 0$

Review of Lecture 15

- Kernel methods

$$K(\mathbf{x}, \mathbf{x}') = \mathbf{z}^\intercal \mathbf{z}' \text{ for some } \mathcal{Z} \text{ space}$$

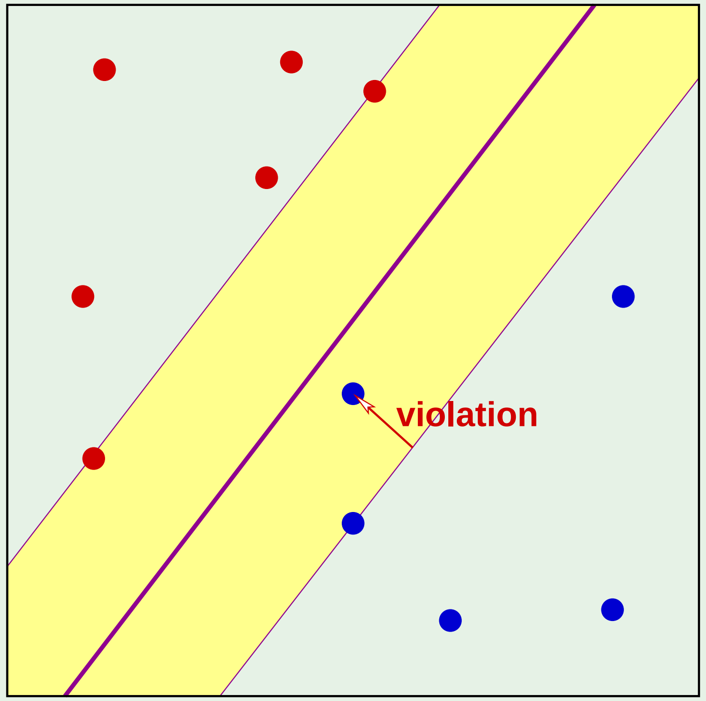


$\uparrow$

$$K(\mathbf{x}, \mathbf{x}') = \exp\left(-\gamma \, \|\mathbf{x} - \mathbf{x}'\|^2\right)$$

- Soft-margin SVM

$$\text{Minimize} \quad \frac{1}{2}\mathbf{w}^\intercal \mathbf{w} + C \sum_{n=1}^{N} \xi_n$$



Same as hard margin, but $0 \le \alpha_n \le C$

Learning From Data

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Lecture 16: Radial Basis Functions

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Thursday, May 24, 2012

Outline

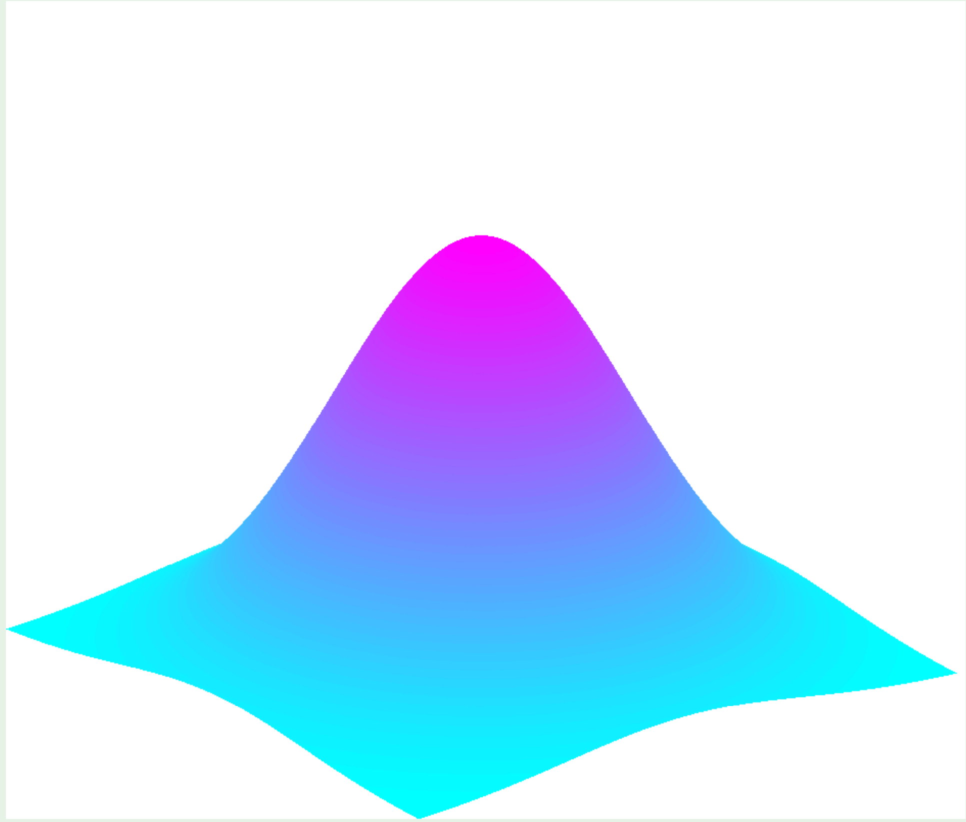
- RBF and nearest neighbors
- RBF and neural networks
- RBF and kernel methods
- RBF and regularization

Basic RBF model

Each $(\mathbf{x}_n, y_n) \in \mathcal{D}$ influences $h(\mathbf{x})$ based on $\underbrace{\|\mathbf{x} - \mathbf{x}_n\|}_{\text{radial}}$

Standard form:

$$h(\mathbf{x}) = \sum_{n=1}^{N} w_n \underbrace{\exp\left(-\gamma \|\mathbf{x} - \mathbf{x}_n\|^2\right)}_{\text{basis function}}$$



The learning algorithm

Finding $w_1, \cdots, w_N$:
$$h(\mathbf{x}) = \sum_{n=1}^{N} w_n \exp\left(-\gamma \left\|\mathbf{x} - \mathbf{x}_n\right\|^2\right)$$

based on $\mathcal{D} = (\mathbf{x}_1, y_1), \cdots, (\mathbf{x}_N, y_N)$

$E_{\text{in}} = 0$: $\quad h(\mathbf{x}_n) = y_n$ for $n = 1, \cdots, N$:

$$\sum_{m=1}^{N} w_m \exp\left(-\gamma \left\|\mathbf{x}_n - \mathbf{x}_m\right\|^2\right) = y_n$$

The solution

$$\sum_{m=1}^{N} w_m \exp\left(-\gamma \left\|\mathbf{x}_n - \mathbf{x}_m\right\|^2\right) = y_n$$

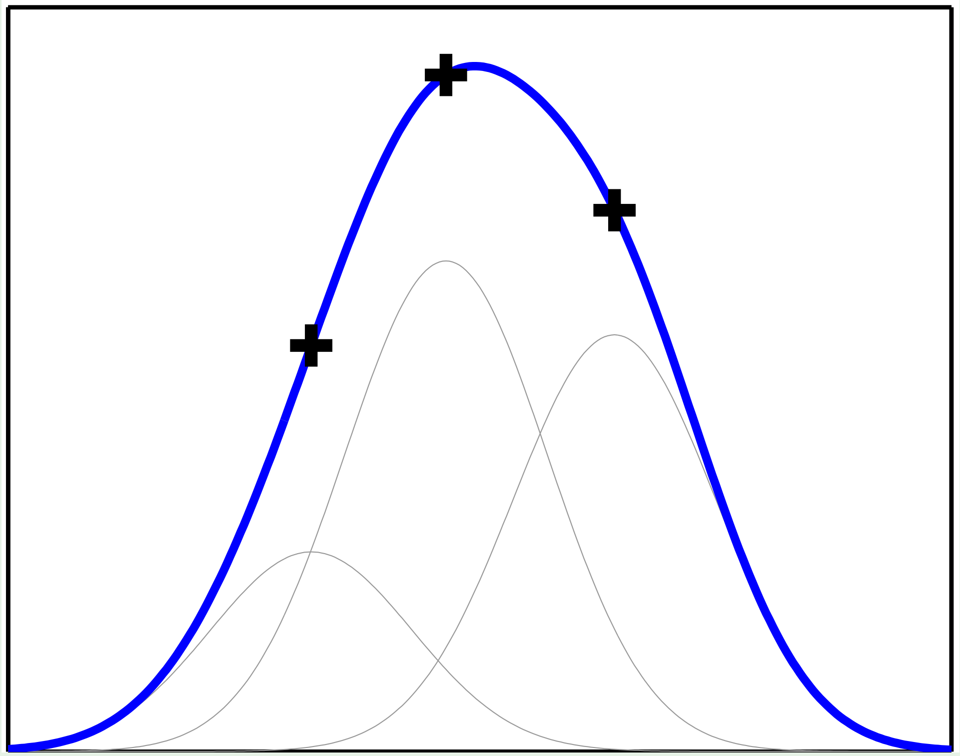
N equations in N unknowns

$$\underbrace{\begin{bmatrix} \exp(-\gamma \left\|\mathbf{x}_1 - \mathbf{x}_1\right\|^2) & \ldots & \exp(-\gamma \left\|\mathbf{x}_1 - \mathbf{x}_N\right\|^2) \\ \exp(-\gamma \left\|\mathbf{x}_2 - \mathbf{x}_1\right\|^2) & \ldots & \exp(-\gamma \left\|\mathbf{x}_2 - \mathbf{x}_N\right\|^2) \\ \vdots & \vdots & \vdots \\ \exp(-\gamma \left\|\mathbf{x}_N - \mathbf{x}_1\right\|^2) & \ldots & \exp(-\gamma \left\|\mathbf{x}_N - \mathbf{x}_N\right\|^2) \end{bmatrix}}_{\Phi} \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_N \end{bmatrix}}_{\mathbf{w}} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\mathbf{y}}$$

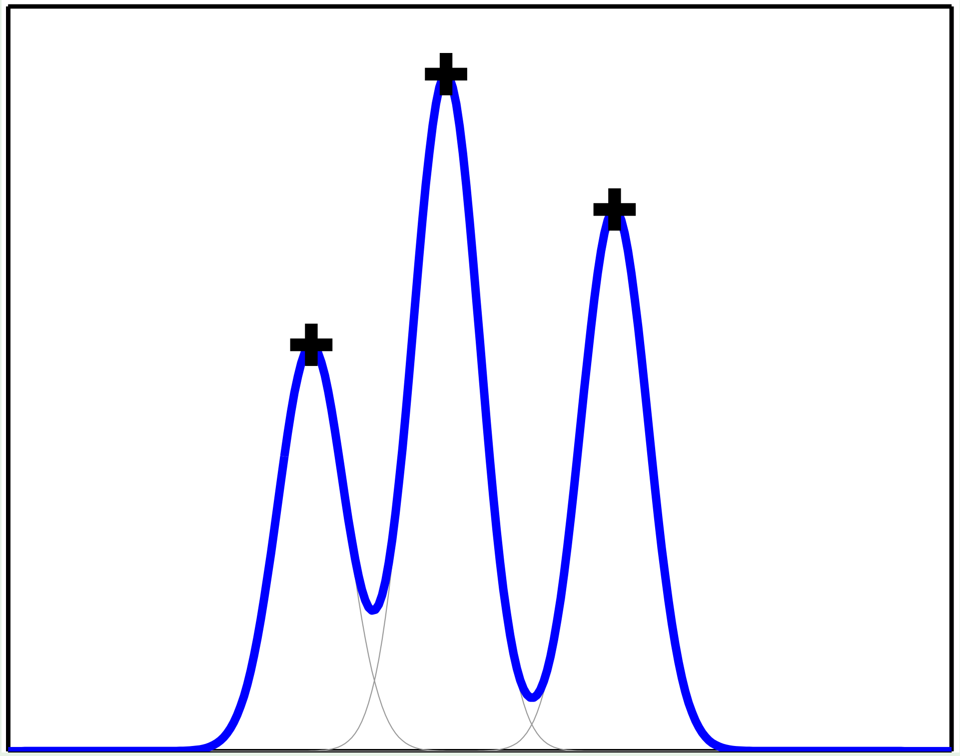
If Φ is invertible, $\boxed{\mathbf{w} = \Phi^{-1}\mathbf{y}}$ "exact interpolation"

The effect of γ

$$h(\mathbf{x}) = \sum_{n=1}^{N} w_n \exp\left(-\gamma \left\|\mathbf{x} - \mathbf{x}_n\right\|^2\right)$$



small γ



large γ

RBF for classification

$$h(\mathbf{x}) \; = \mathrm{sign}\left(\sum_{n=1}^{N} w_n \; \exp\left(-\gamma \; \|\mathbf{x} - \mathbf{x}_n\|^2\right)\right)$$

Learning: $\sim$ linear regression for classification

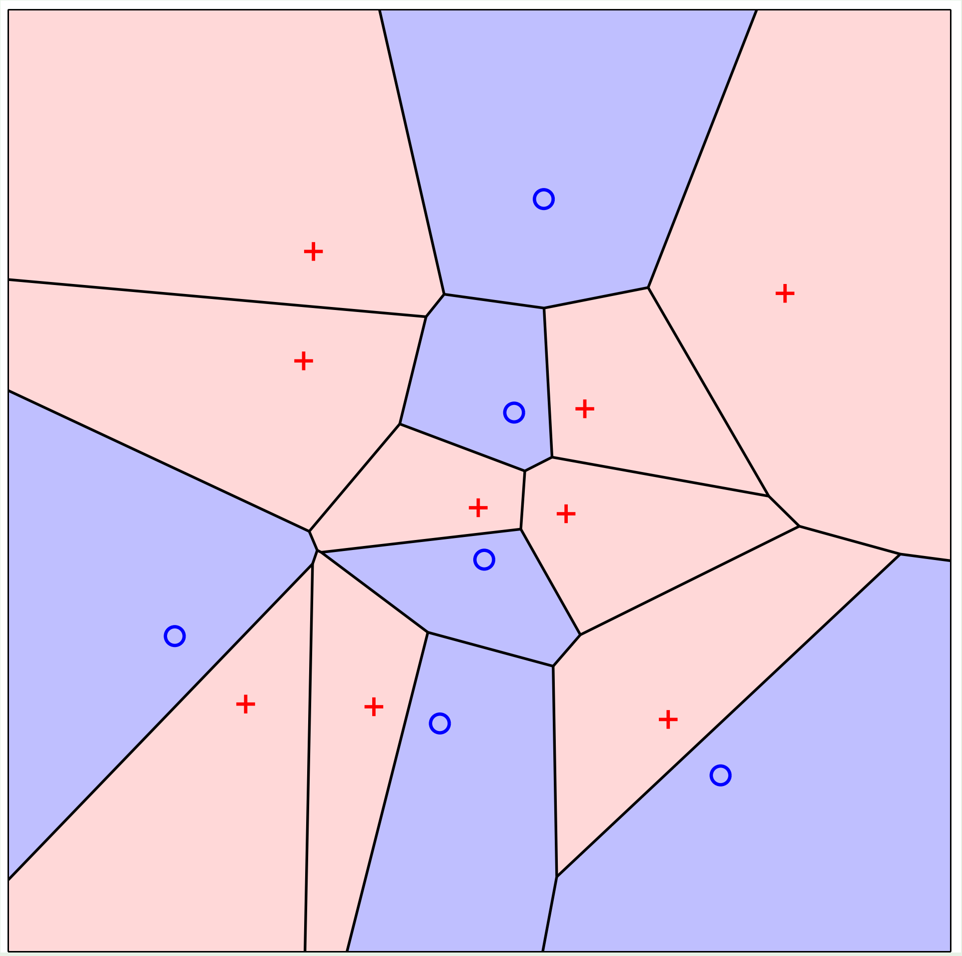
$$s \; = \sum_{n=1}^{N} w_n \; \exp\left(-\gamma \; \|\mathbf{x} - \mathbf{x}_n\|^2\right)$$

Minimize $(s - y)^2$ on $\mathcal{D}$ $\qquad y = \pm 1$

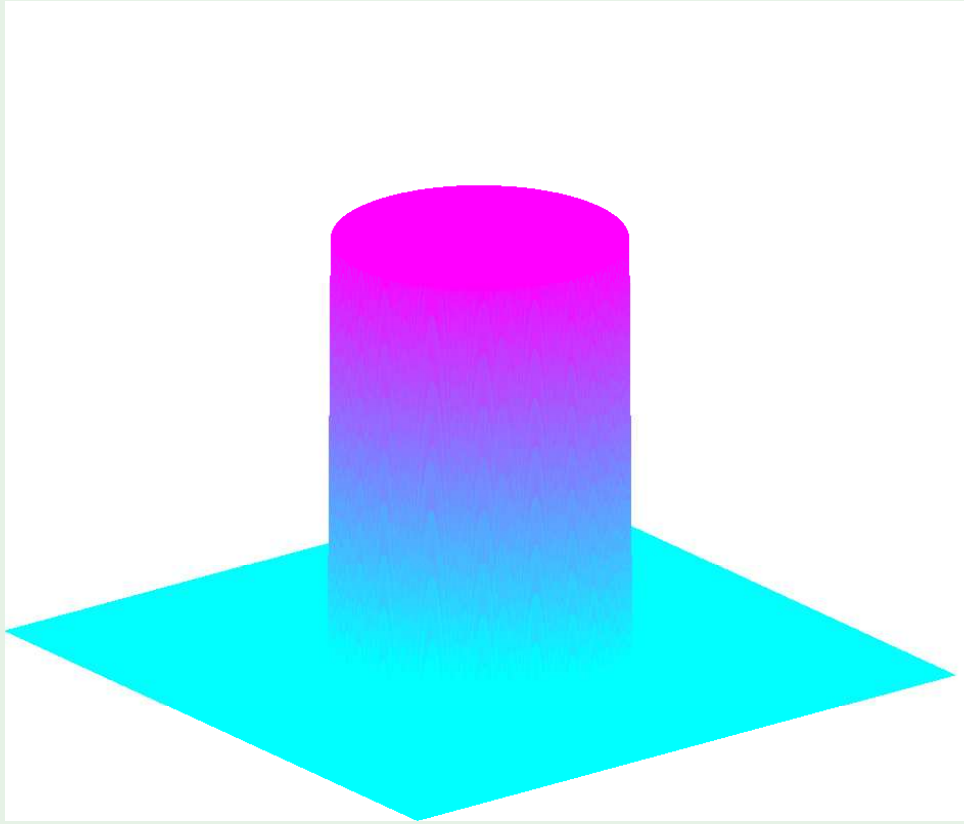
$h(\mathbf{x}) = \mathrm{sign}(s)$

Relationship to nearest-neighbor method

Adopt the y value of a nearby point:



similar effect by a basis function:



RBF with K centers

N parameters $w_1, \cdots, w_N$ based on N data points

Use $K \ll N$ centers: $\boldsymbol{\mu}_1, \cdots, \boldsymbol{\mu}_K$ instead of $\mathbf{x}_1, \cdots, \mathbf{x}_N$

$$h(\mathbf{x}) = \sum_{k=1}^{K} w_k \exp\left(-\gamma \left\|\mathbf{x} - \boldsymbol{\mu}_k\right\|^2\right)$$

1. How to choose the centers $\boldsymbol{\mu}_k$

2. How to choose the weights w_k

Choosing the centers

Minimize the distance between $\mathbf{x}_n$ and the **closest** center $\boldsymbol{\mu}_k$: K-means clustering

Split $\mathbf{x}_1, \cdots, \mathbf{x}_N$ into clusters $S_1, \cdots, S_K$

Minimize $\displaystyle\sum_{k=1}^{K} \sum_{\mathbf{x}_n \in S_k} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$

Unsupervised learning ☺

NP-hard ☹

An iterative algorithm

Lloyd's algorithm: Iteratively minimize $\sum_{k=1}^{K} \sum_{\mathbf{x}_n \in S_k} \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2$ w.r.t. $\boldsymbol{\mu}_k, S_k$

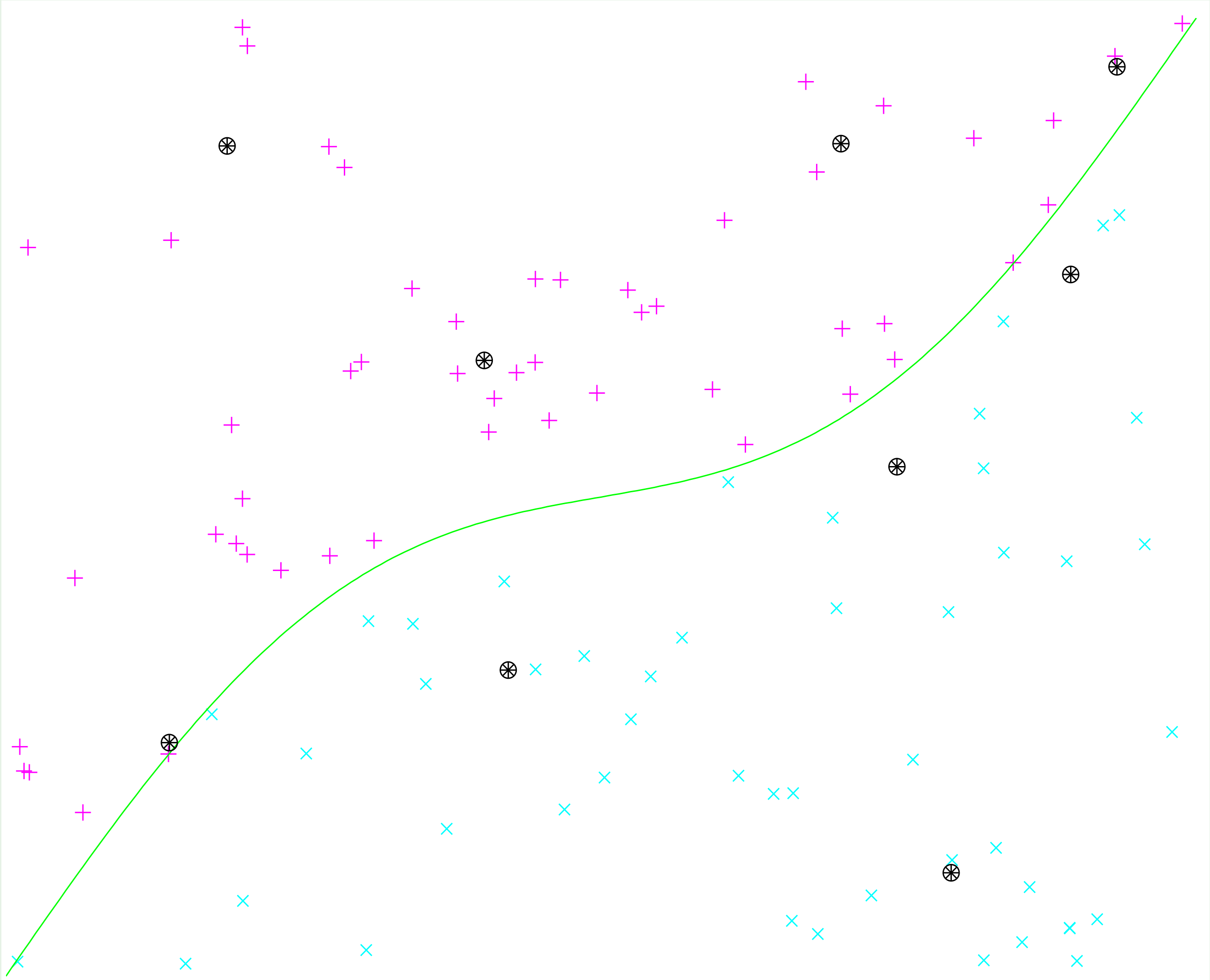
$$\boldsymbol{\mu}_k \leftarrow \frac{1}{|S_k|} \sum_{\mathbf{x}_n \in S_k} \mathbf{x}_n$$

$$S_k \leftarrow \{\mathbf{x}_n : \|\mathbf{x}_n - \boldsymbol{\mu}_k\| \leq \text{all } \|\mathbf{x}_n - \boldsymbol{\mu}_\ell\|\}$$

Convergence $\longrightarrow$ **local minimum**

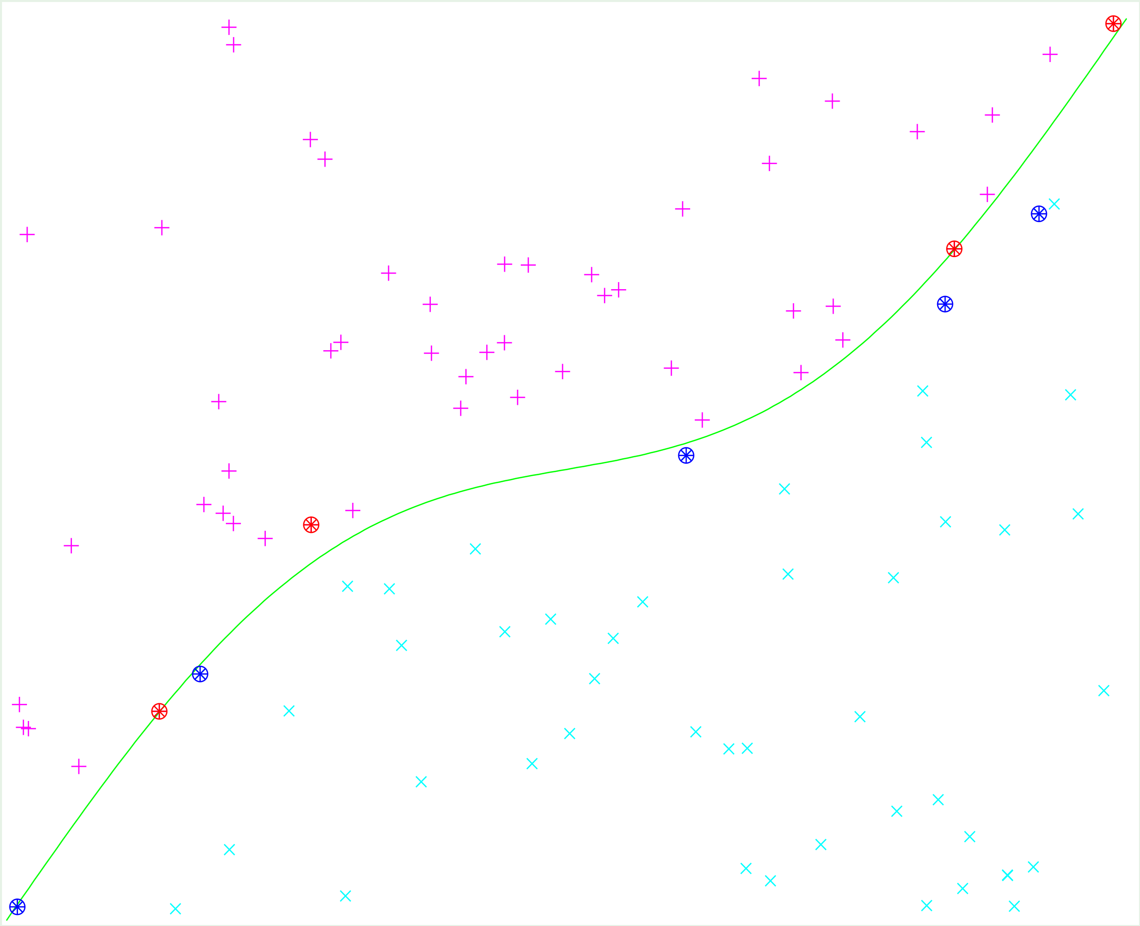
Lloyd's algorithm in action

1. Get the data points
2. Only the inputs!
3. Initialize the centers
4. Iterate
5. These are your $\boldsymbol{\mu}_k$'s

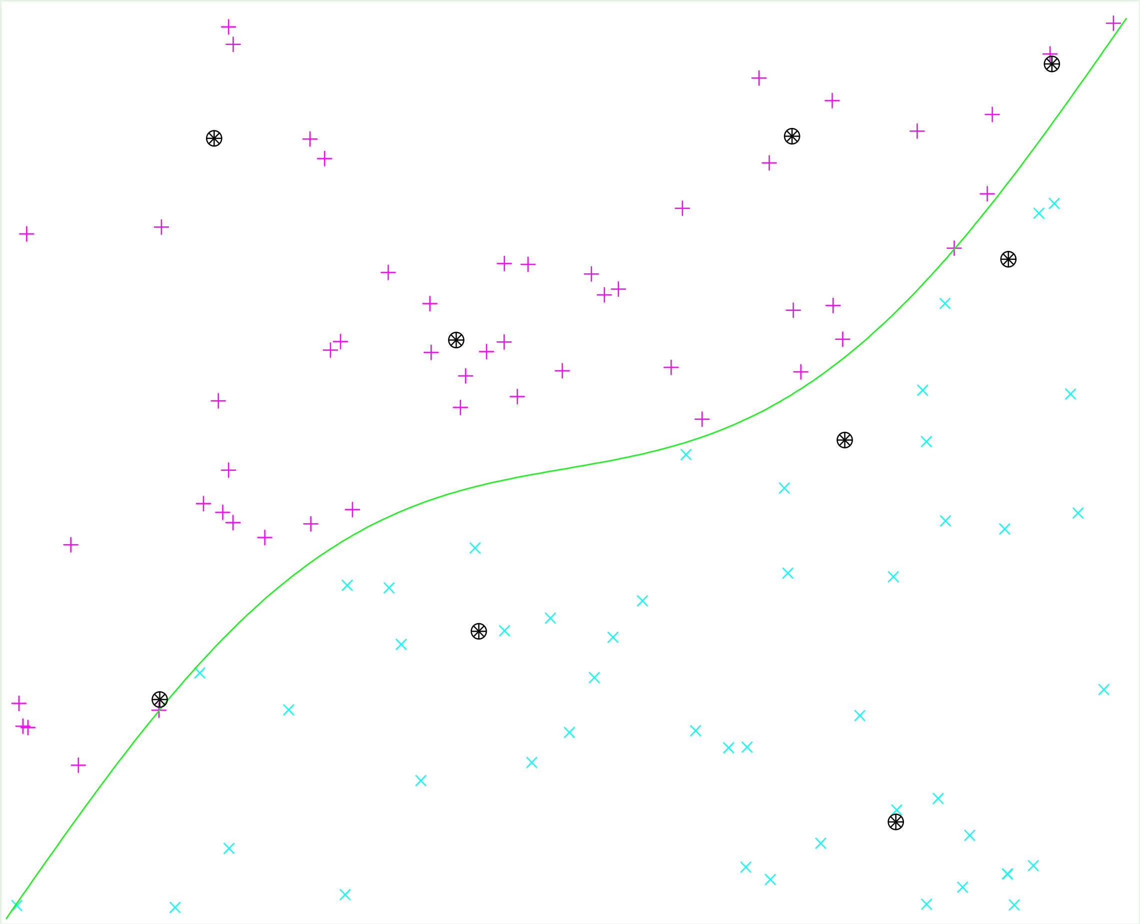


Centers versus support vectors

support vectors



RBF centers



Choosing the weights

$$\sum_{k=1}^{K} w_k \, \exp\left(-\gamma \, \|\mathbf{x}_n - \boldsymbol{\mu}_k\|^2\right) \approx \, y_n$$

N equations in $K < N$ unknowns

$$\underbrace{\begin{bmatrix} \exp(-\gamma \, \|\mathbf{x}_1 - \boldsymbol{\mu}_1\|^2) & \dots & \exp(-\gamma \, \|\mathbf{x}_1 - \boldsymbol{\mu}_K\|^2) \\ \exp(-\gamma \, \|\mathbf{x}_2 - \boldsymbol{\mu}_1\|^2) & \dots & \exp(-\gamma \, \|\mathbf{x}_2 - \boldsymbol{\mu}_K\|^2) \\ \vdots & \vdots & \vdots \\ \exp(-\gamma \, \|\mathbf{x}_N - \boldsymbol{\mu}_1\|^2) & \dots & \exp(-\gamma \, \|\mathbf{x}_N - \boldsymbol{\mu}_K\|^2) \end{bmatrix}}_{\Phi} \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_K \end{bmatrix}}_{\mathbf{w}} \approx \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\mathbf{y}}$$

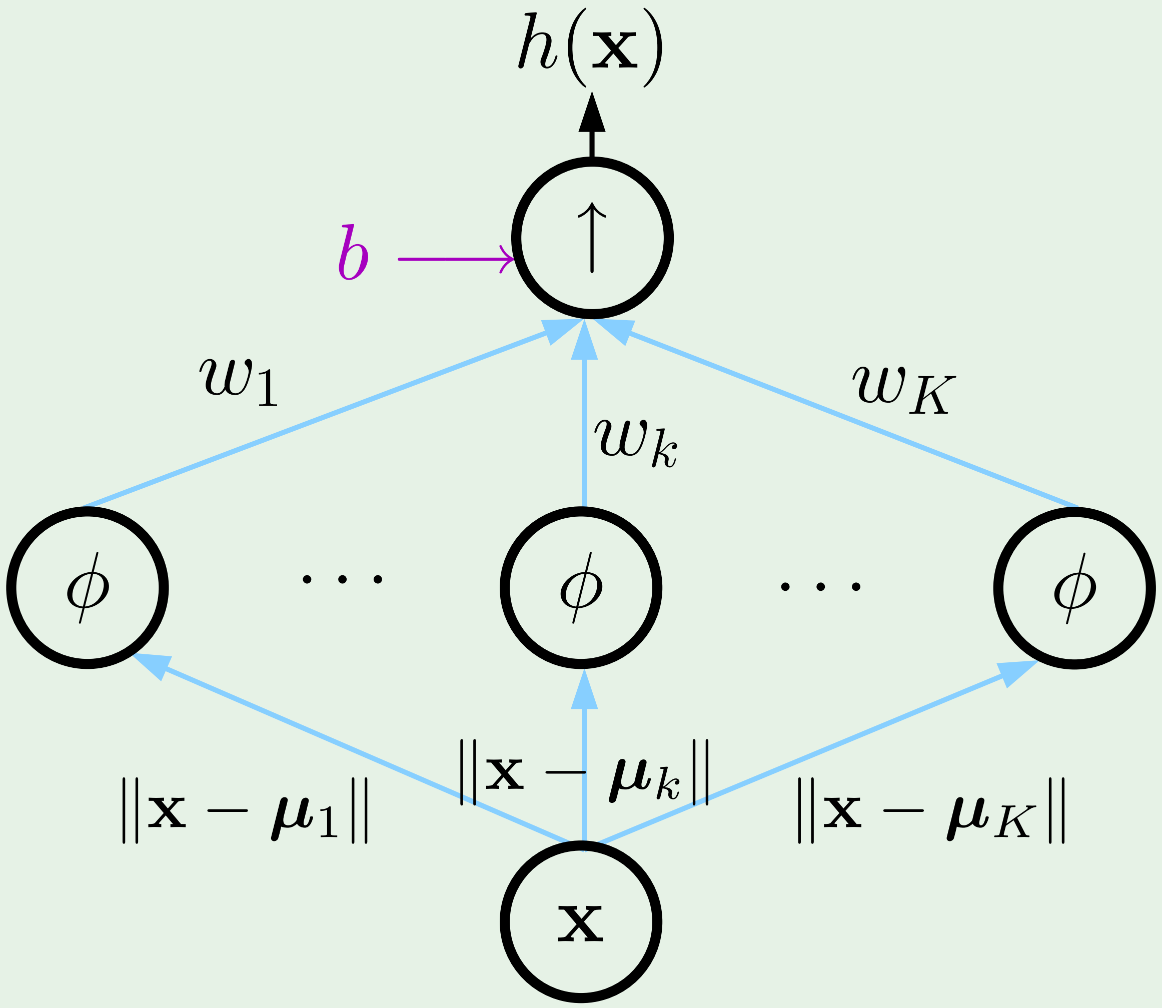
If $\Phi^\top \Phi$ is invertible, $\boxed{\mathbf{w} = (\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{y}}$ **pseudo-inverse**

RBF network

The "features" are $\exp\left(-\gamma \left\|\mathbf{x} - \boldsymbol{\mu}_k\right\|^2\right)$

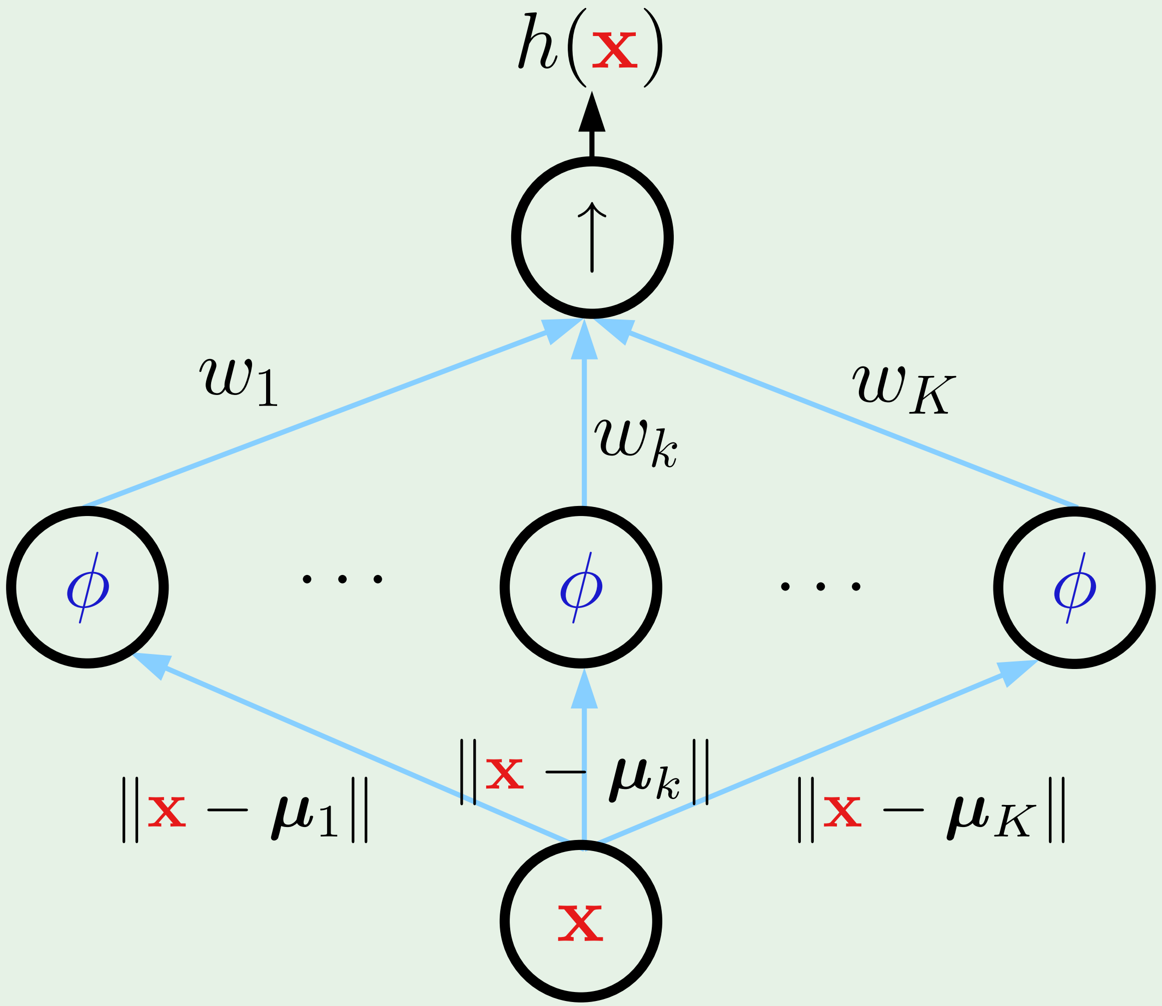
Nonlinear transform depends on $\mathcal{D}$

$\Longrightarrow$ No longer a linear model

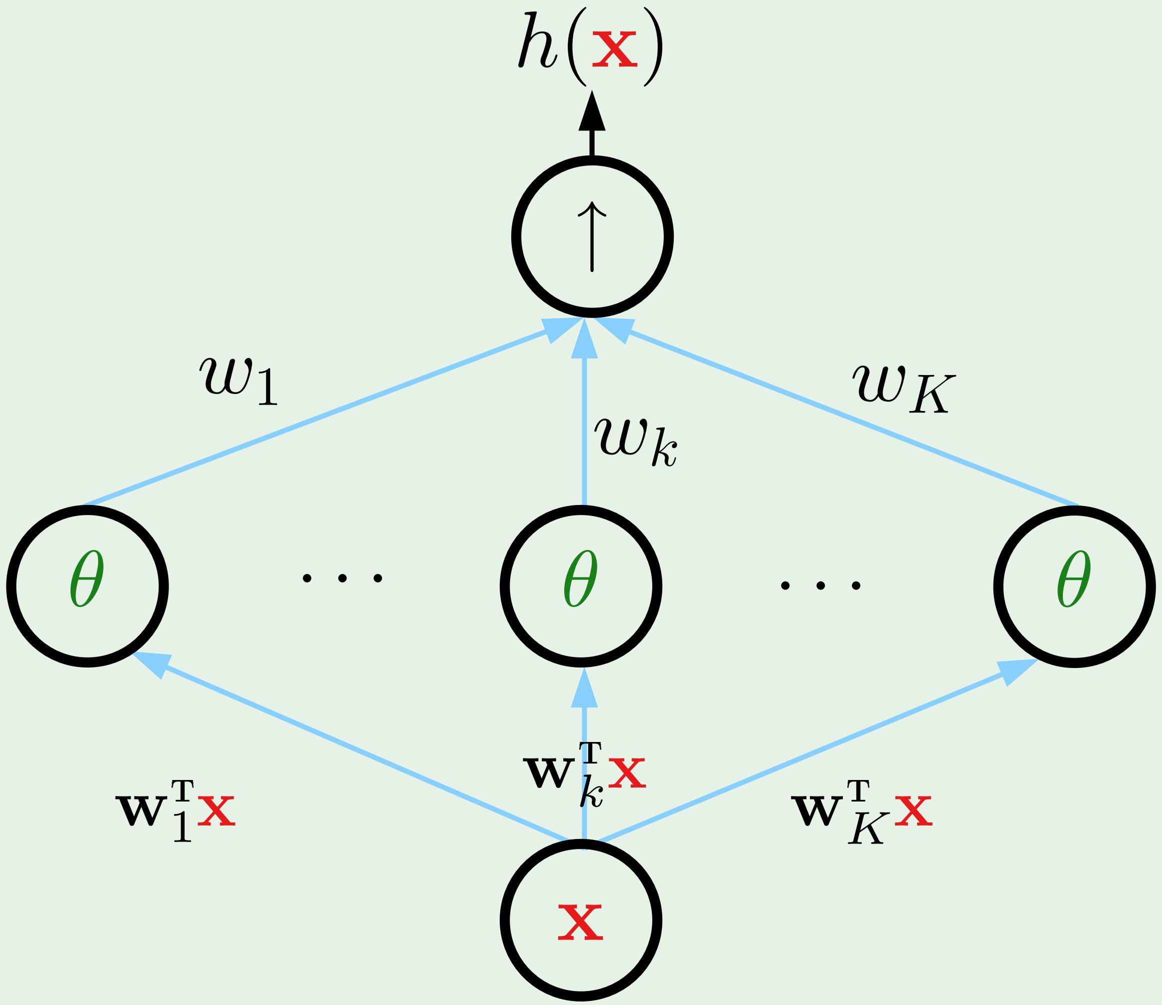


A bias term (b or w_0) is often added

Compare to neural networks



RBF network



neural network

Choosing γ

Treating γ as a parameter to be learned $\qquad h(\mathbf{x}) = \sum_{k=1}^{K} w_k \exp\left(-\gamma \left\|\mathbf{x} - \boldsymbol{\mu}_k\right\|^2\right)$

Iterative approach ($\sim$ **EM algorithm** in mixture of Gaussians):

1. Fix γ, solve for $w_1, \cdots, w_K$
2. Fix $w_1, \cdots, w_K$, minimize error w.r.t. γ

We can have a different γ_k for each center $\boldsymbol{\mu}_k$

Outline

- RBF and nearest neighbors
- RBF and neural networks
- RBF and kernel methods
- RBF and regularization

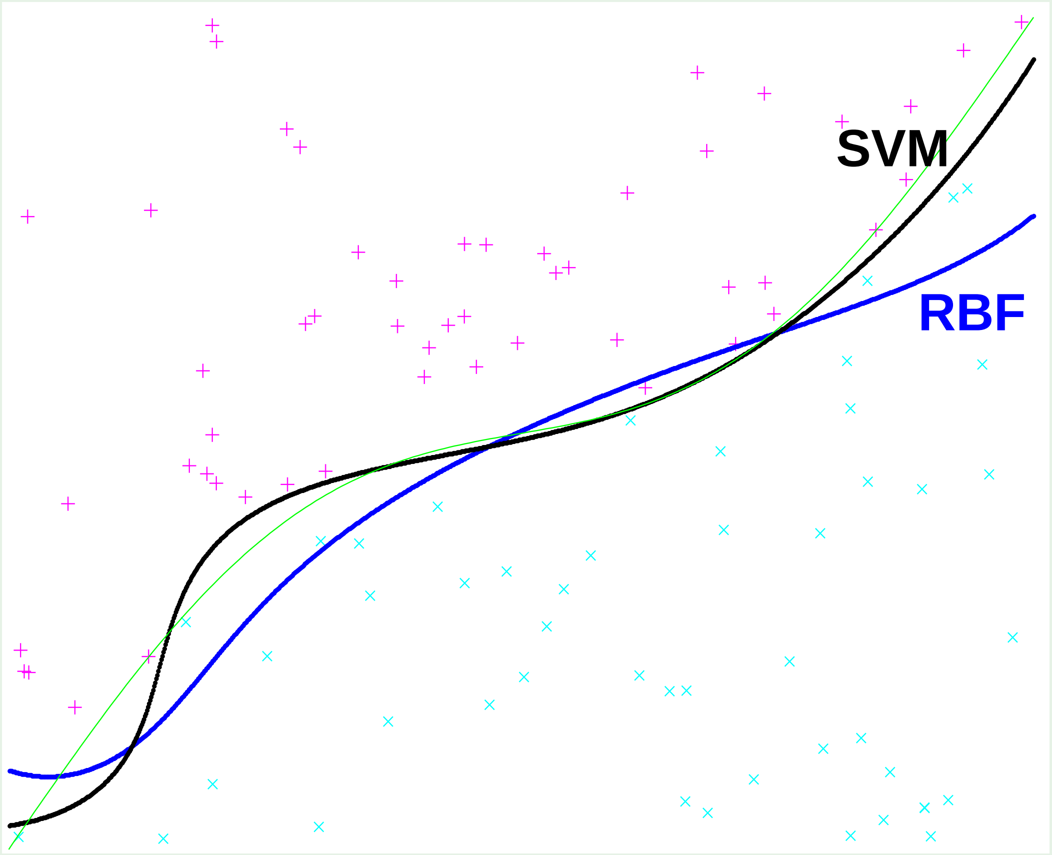
RBF versus its SVM kernel

SVM kernel implements:

$$\text{sign}\left(\sum_{\alpha_n>0} \alpha_n y_n \exp\left(-\gamma\left\|\mathbf{x}-\mathbf{x}_n\right\|^2\right)+b\right)$$

Straight RBF implements:

$$\text{sign}\left(\sum_{k=1}^{K} w_k \exp\left(-\gamma\left\|\mathbf{x}-\boldsymbol{\mu}_k\right\|^2\right)+b\right)$$



RBF and regularization

RBF can be derived based purely on regularization:

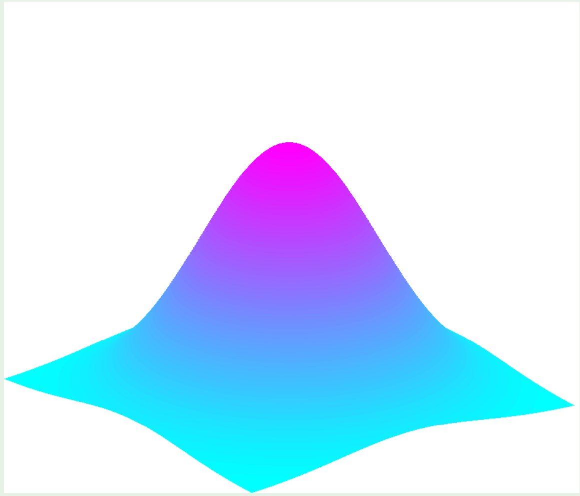
$$\sum_{n=1}^{N} \left(h(x_n) - y_n\right)^2 + \lambda \sum_{k=0}^{\infty} a_k \int_{-\infty}^{\infty} \left(\frac{d^k h}{dx^k}\right)^2 dx$$

"smoothest interpolation"

Review of Lecture 16

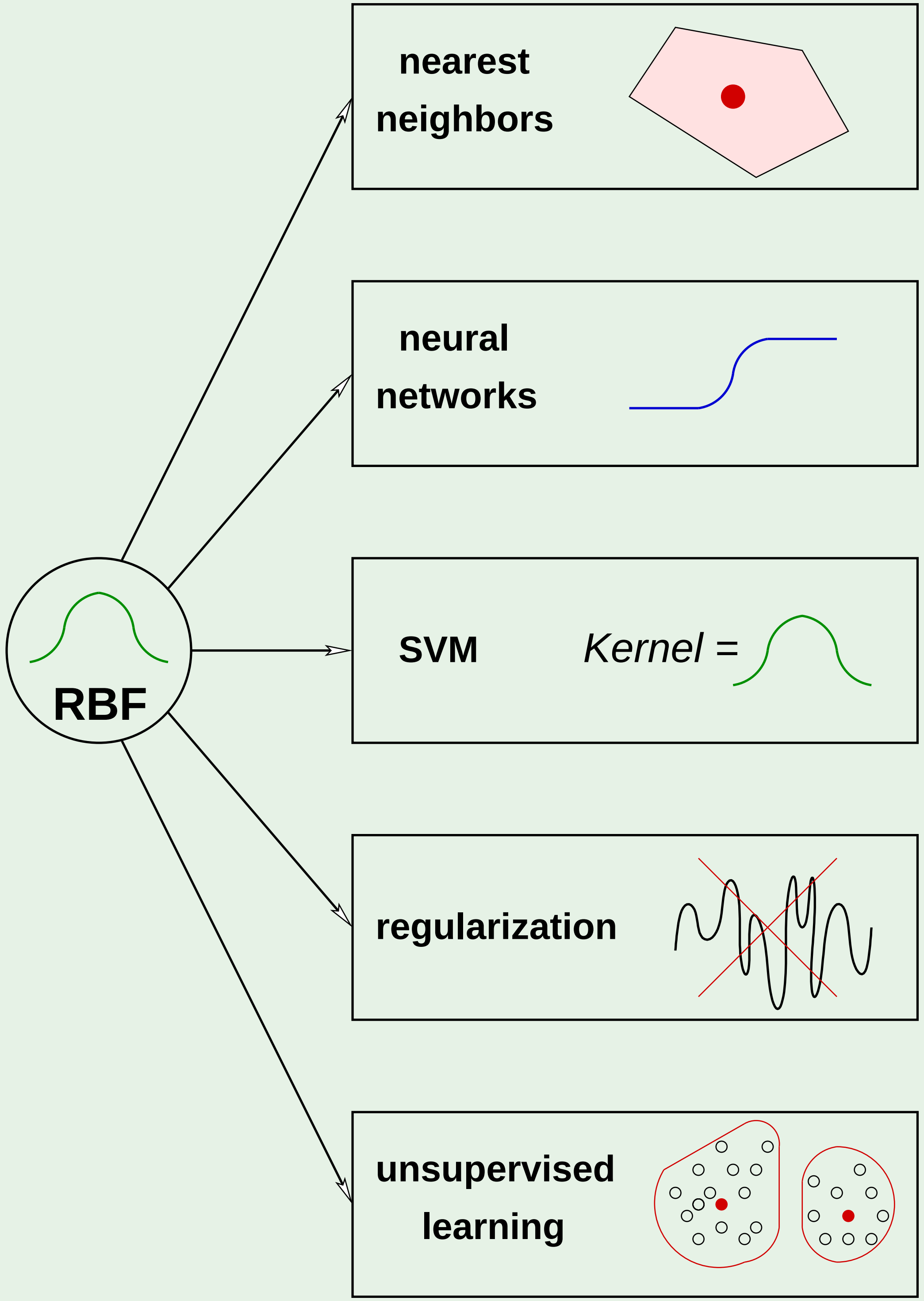
- Radial Basis Functions

$$h(\mathbf{x}) = \sum_{k=1}^{K} w_k \exp\left(-\gamma \left\|\mathbf{x} - \boldsymbol{\mu}_k\right\|^2\right)$$



Choose $\boldsymbol{\mu}_k$'s: Lloyd's algorithm

Choose w_k's: Pseudo-inverse



Learning From Data

Yaser S. Abu-Mostafa
California Institute of Technology

Lecture 17: Three Learning Principles

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Tuesday, May 29, 2012

Outline

- Occam's Razor
- Sampling Bias
- Data Snooping

Recurring theme - simple hypotheses

A "quote" by Einstein:

> An explanation of the data should be made *as simple as possible, but no simpler*

The razor: symbolic of a principle set by William of Occam

Occam's Razor

The simplest model that fits the data is also the most plausible.

Two questions:

1. What does it mean for a model to be simple?

2. How do we know that simpler is better?

First question: ‘simple’ means?

Measures of complexity - two types: **complexity of h** and **complexity of $\mathcal{H}$**

Complexity of h: MDL, order of a polynomial

Complexity of $\mathcal{H}$: Entropy, VC dimension

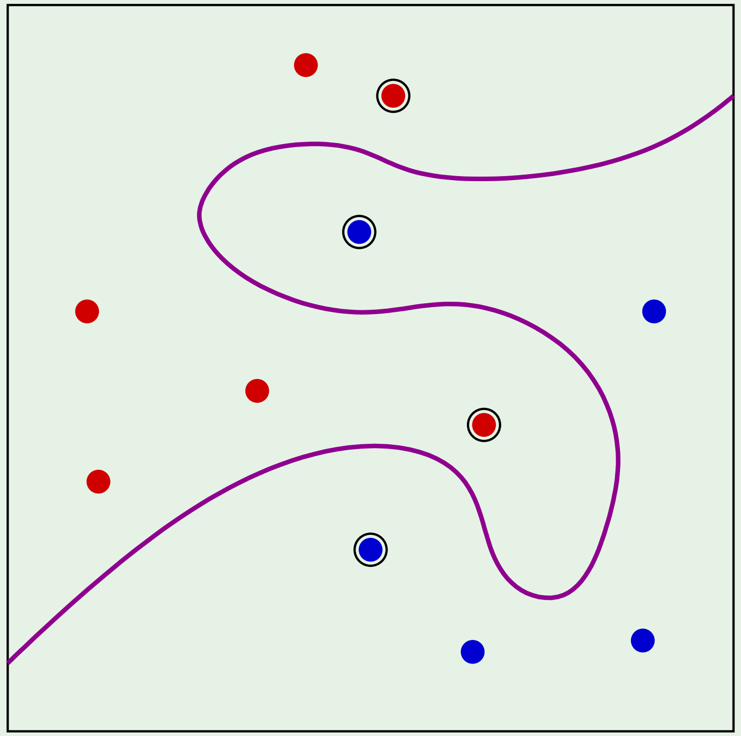
- When we think of simple, it's in terms of h
- Proofs use simple in terms of $\mathcal{H}$

and the link is ...

counting: ℓ bits specify h $\Longrightarrow$ h is one of 2^ℓ elements of a set $\mathcal{H}$

Real-valued parameters? **Example:** 17th order polynomial - complex and one of "many"

Exceptions? Looks complex but is one of few - **SVM**



Puzzle 1: Football oracle

00000000000000001111111111111111	0
00000000111111110000000011111111	1
00001111000011110000111100001111	0
00110011001100110011001100110011	1
01010101010101010101010101010101	1

$\uparrow$

- Letter predicting game outcome
- Good call!
- More letters - for 5 weeks
- Perfect record!
- Want more? $50 charge ☺
- **Should you pay?**

Second question: Why is simpler better?

Better doesn't mean more elegant! It means better out-of-sample performance

The basic argument: (formal proof under different idealized conditions)

Fewer simple hypotheses than complex ones

$$m_{\mathcal{H}}(N)$$

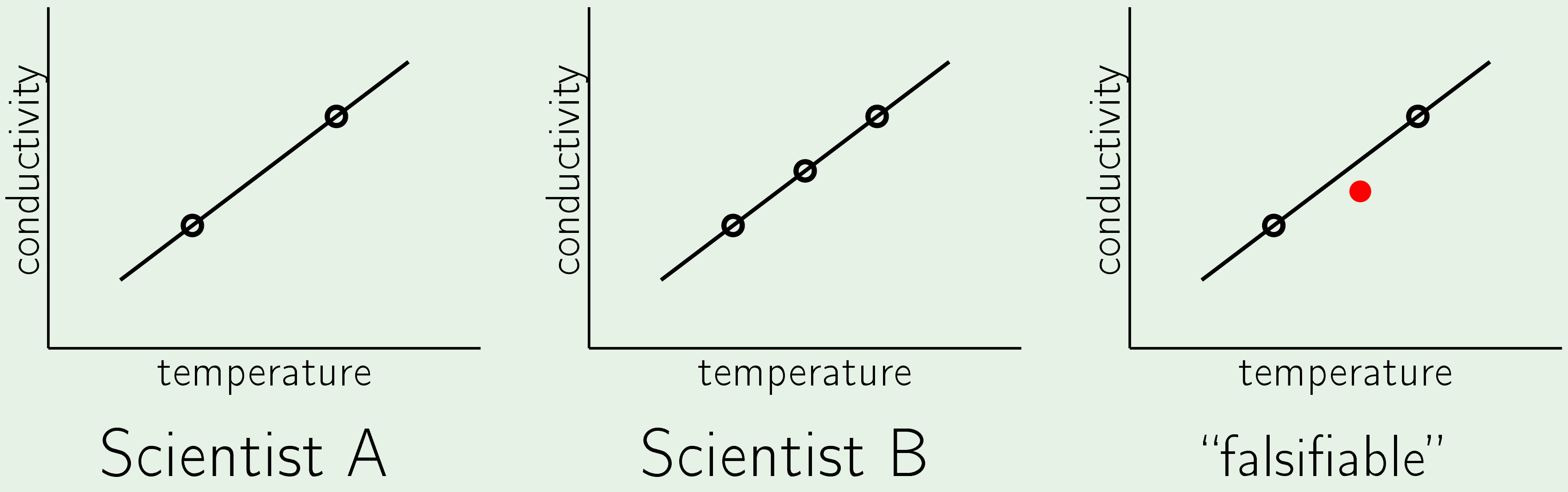
$\Rightarrow$ less likely to fit a given data set

$$m_{\mathcal{H}}(N)/2^N$$

$\Rightarrow$ more significant when it happens

The postal scam: $m_{\mathcal{H}}(N) = 1$ versus 2^N

A fit that means nothing



Conductivity linear in temperature?

Two scientists conduct experiments

What evidence do A and B provide?

Outline

- Occam's Razor
- Sampling Bias
- Data Snooping

Puzzle 2: Presidential election

In 1948, **Truman** ran against **Dewey** in close elections

A newspaper ran a phone poll of how people voted

Dewey won the poll decisively - newspaper declared:

On to the victory rally . . .

. . . of Truman ☺

It's not δ's fault:

$$\mathbb{P}\left[\,|E_{\rm in} - E_{\rm out}| > \epsilon\,\right] \;\leq\; \delta$$

The bias

In 1948, phones were expensive.

> **If the data is sampled in a biased way, learning will produce a similarly biased outcome.**

Example: normal period in the market

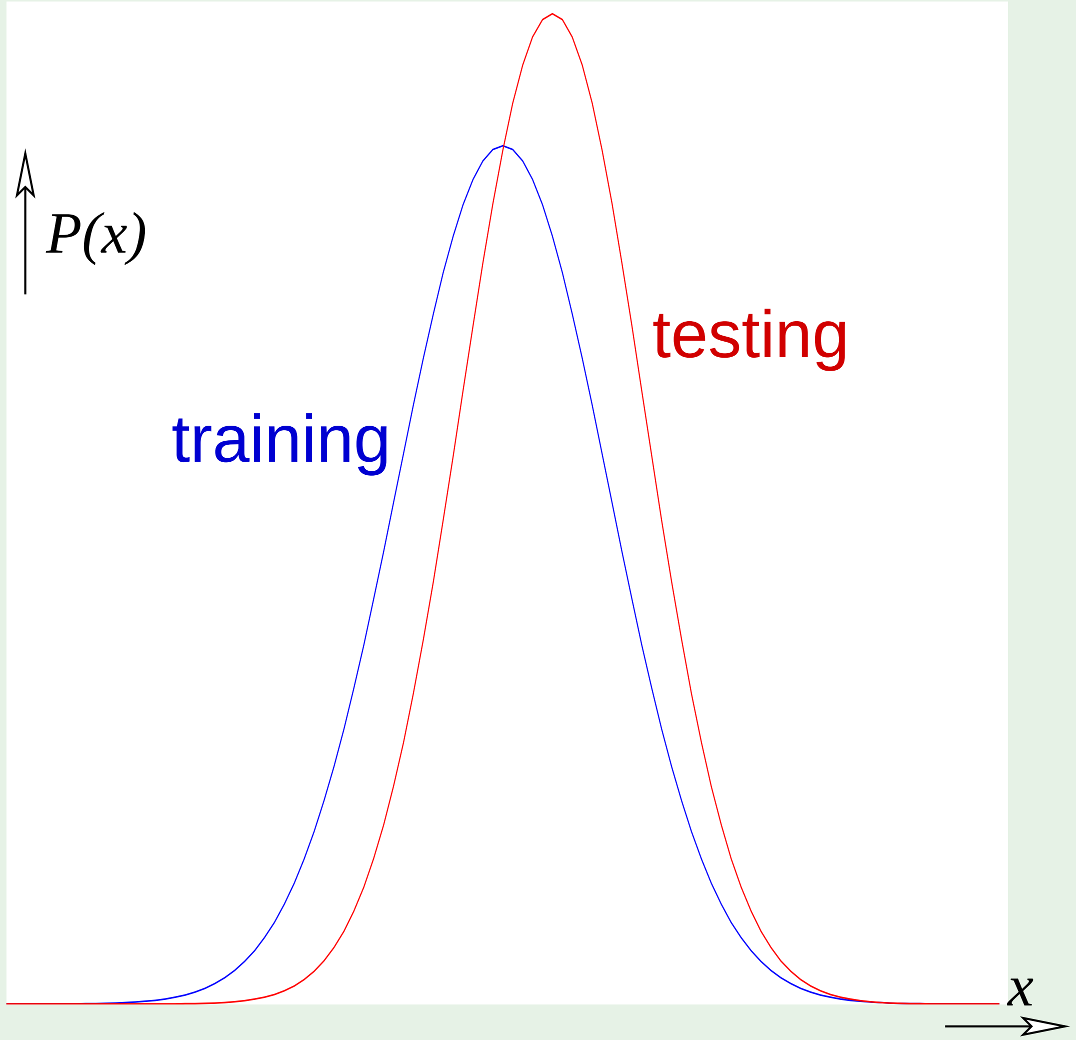
Testing: live trading in real market

Matching the distributions

Methods to match training and testing distributions

Doesn't work if:

Region has $P = 0$ in training, but $P > 0$ in testing



Puzzle 3: Credit approval

Historical records of customers

Input: information on credit application:

Target: profitable for the bank

age	23 years
gender	male
annual salary	$30,000
years in residence	1 year
years in job	1 year
current debt	$15,000
...	...

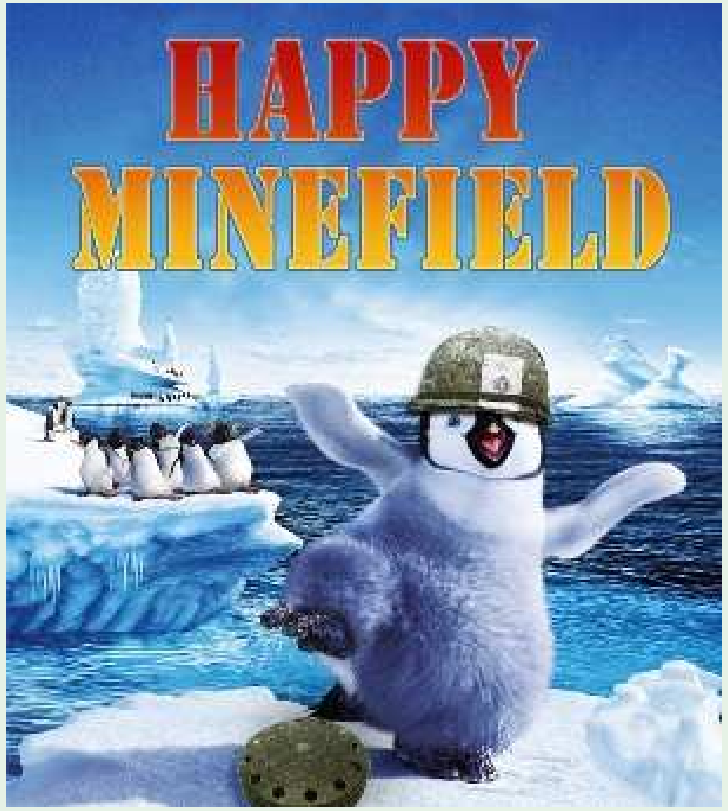
Outline

- Occam's Razor
- Sampling Bias
- Data Snooping

The principle

If a data set has affected any step in the learning process, its ability to assess the outcome has been compromised.

Most common trap for practitioners - many ways to slip ☹



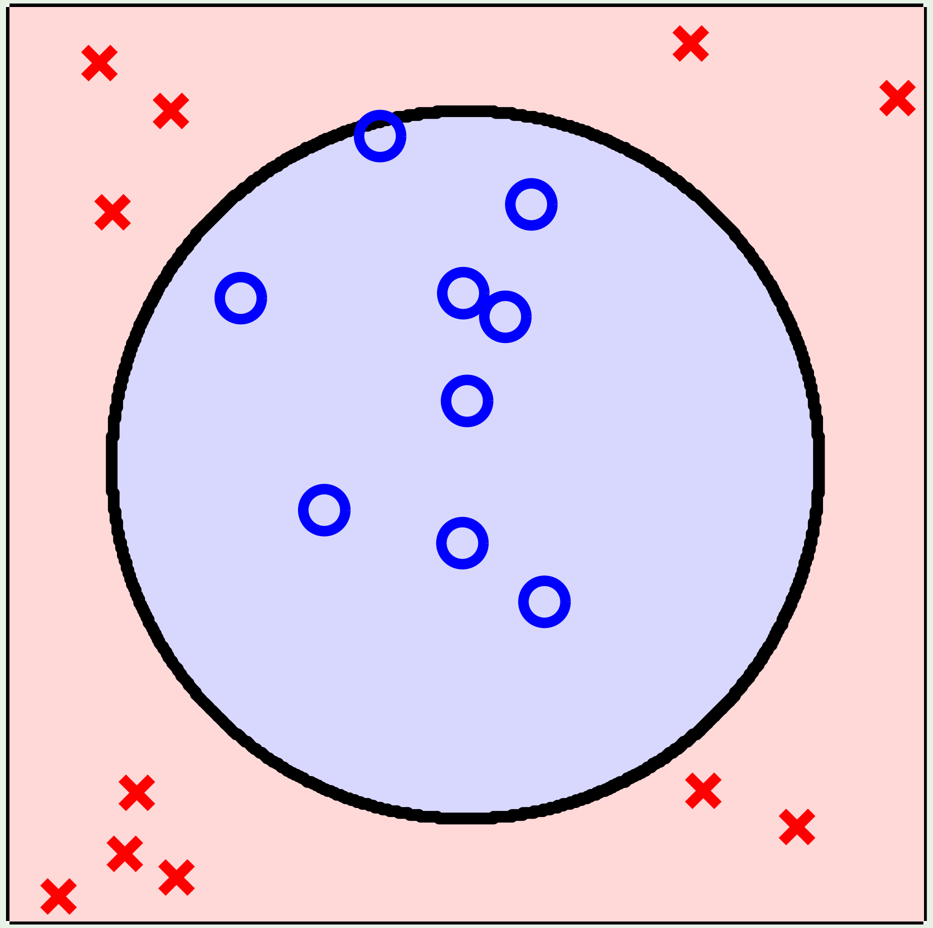
Looking at the data

Remember nonlinear transforms?

$\mathbf{z} = (1, x_1, x_2, x_1x_2, x_1^2, x_2^2)$

or $\mathbf{z} = (1, x_1^2, x_2^2)$ or $\mathbf{z} = (1, x_1^2 + x_2^2)$

Snooping involves $\mathcal{D}$, not other information

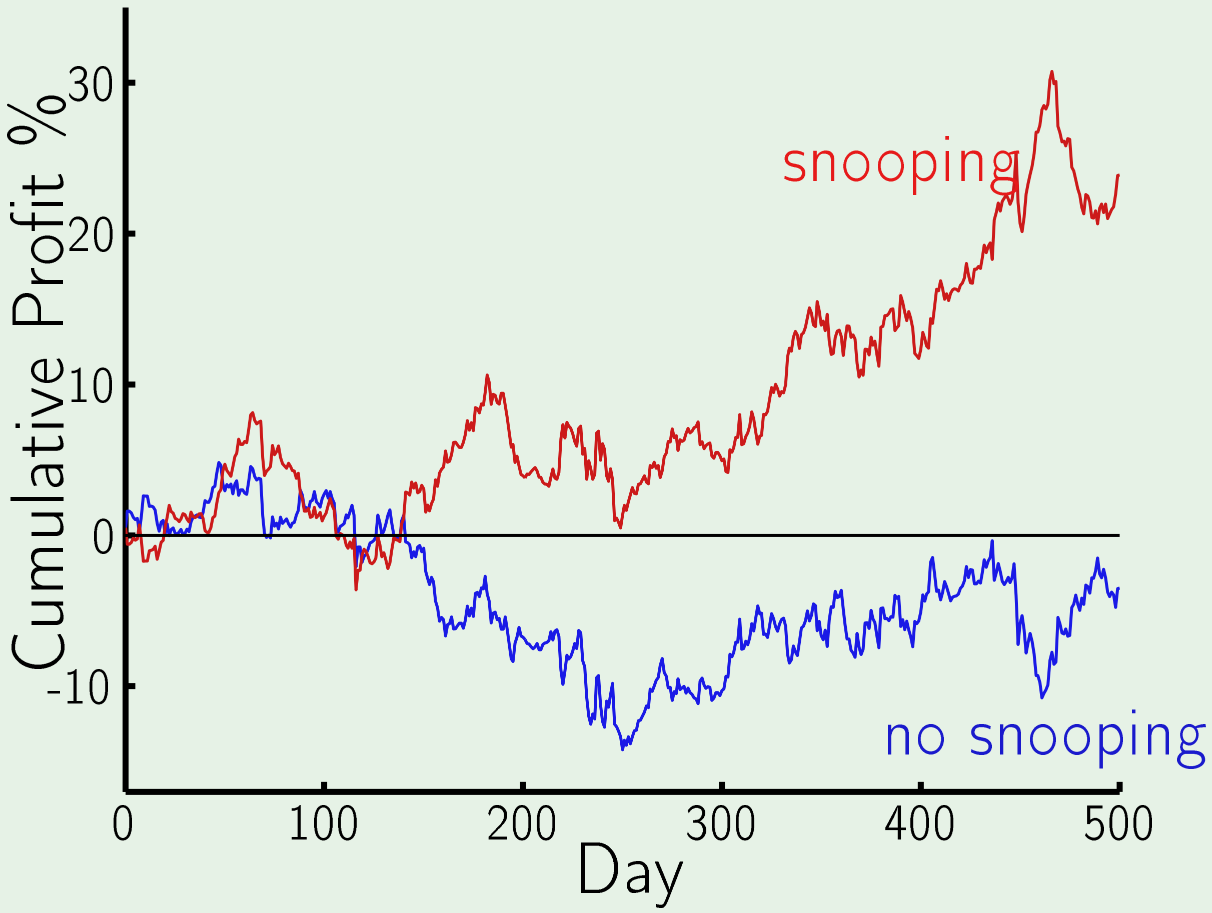


Puzzle 4: Financial forecasting

Predict US Dollar versus British Pound

Normalize data, split randomly: $\mathcal{D}_{\text{train}}$, $\mathcal{D}_{\text{test}}$

Train on $\mathcal{D}_{\text{train}}$ only, test g on $\mathcal{D}_{\text{test}}$



$$\Delta r_{-20}, \Delta r_{-19}, \cdots, \Delta r_{-1} \rightarrow \Delta r_0$$

Reuse of a data set

Trying one model after the other **on the same data set**, you will eventually 'succeed'

If you torture the data long enough, it will confess

VC dimension of the **total** learning model

May include what **others** tried!

Key problem: matching a *particular* data set

Two remedies

1. **Avoid** data snooping

   strict discipline

2. **Account for** data snooping

   how much data contamination

Puzzle 5: Bias via snooping

Testing long-term performance of "buy and hold" in stocks. Use **50 years** worth of data

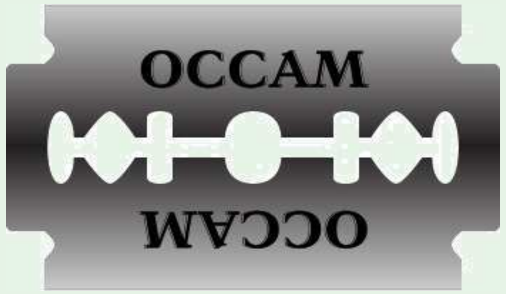
- All currently traded companies in S&P500
- Assume you strictly followed buy and hold
- Would have made great profit!

Sampling bias caused by 'snooping'

Review of Lecture 17

- Occam's Razor

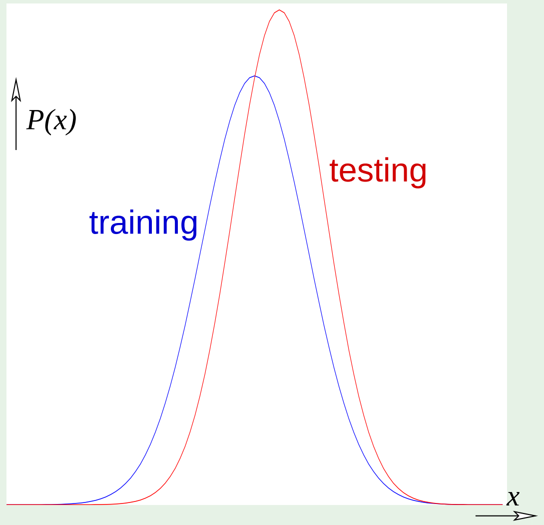
> The simplest model that fits the data is also the most plausible.



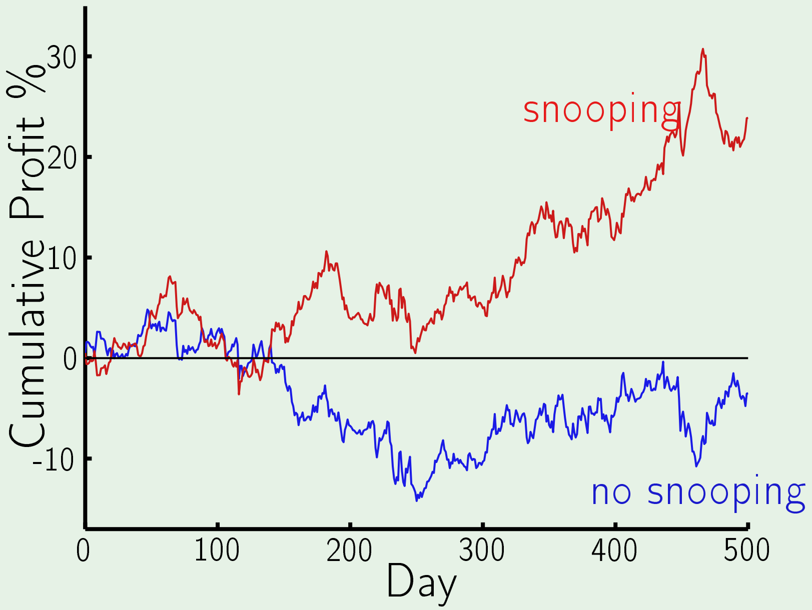
complexity of h $\longleftrightarrow$ complexity of $\mathcal{H}$

unlikely event $\longleftrightarrow$ significant if it happens

- Sampling bias



- Data snooping



Learning From Data

Yaser S. Abu-Mostafa
California Institute of Technology

Lecture 18: Epilogue

Sponsored by Caltech's Provost Office, E&AS Division, and IST • Thursday, May 31, 2012

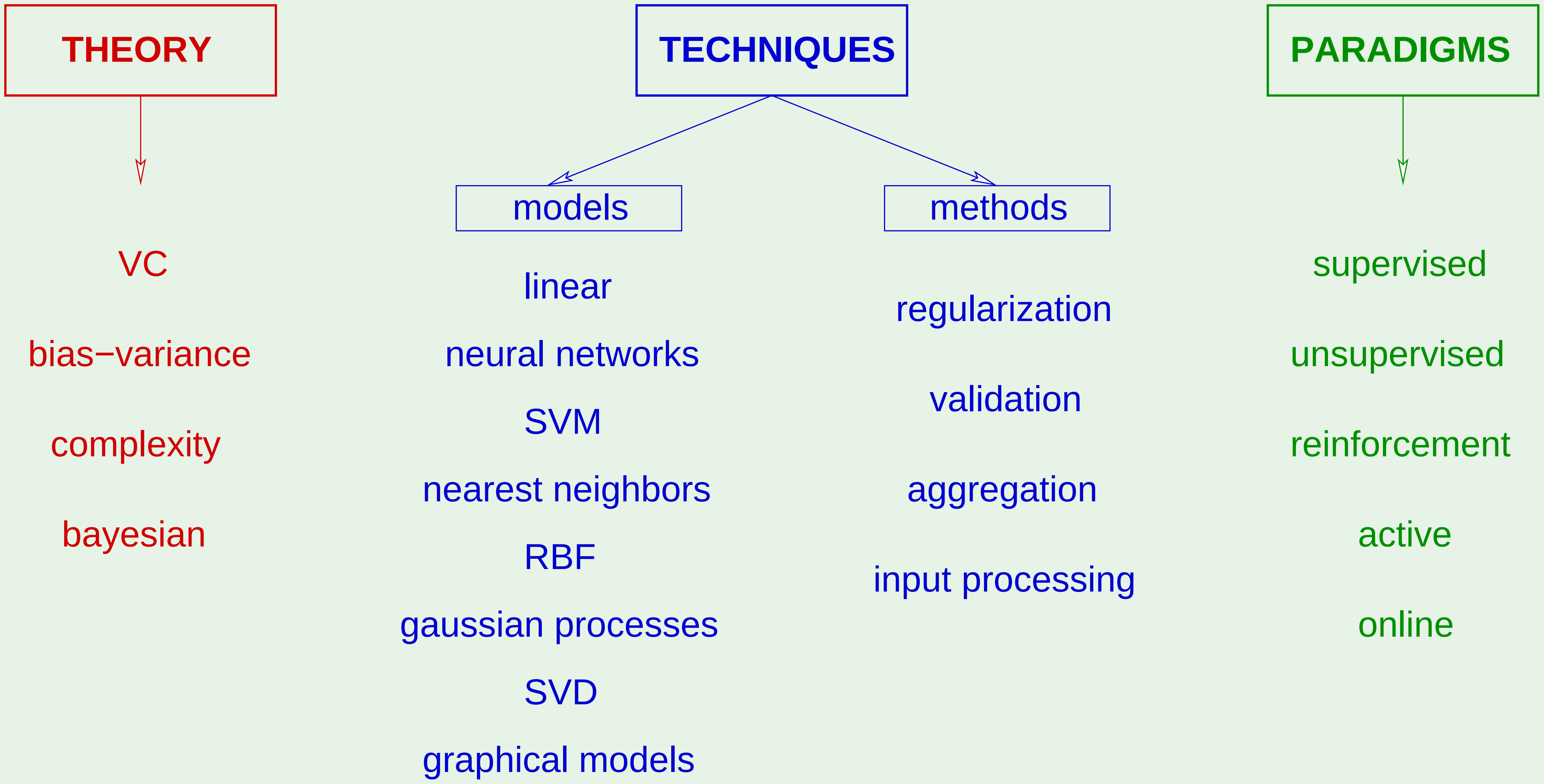
Outline

- The map of machine learning
- Bayesian learning
- Aggregation methods
- Acknowledgments

It's a jungle out there

semi−supervised learning
overfitting
stochastic gradient descent
SVM
Q learning
Gaussian processes
deterministic noise
data snooping
distribution−free
linear regression
learning curves
VC dimension
collaborative filtering
mixture of expe
decision trees
nonlinear transformation
sampling bias
neural networks
no free
RBF
training versus testing
noisy targets
Bayesian prior
active learning
linear models
bias−variance tradeoff
weak learners
ordinal regression
logistic regression
data contamination
cross validation
ensemble learning
types of learning
perceptrons
hidden Markov mo
error measures
kernel methods
xploration versus exploitation
graphical models
is learning feasible?
soft−order constraint
clustering
weight decay
Boltzmann mach
regularization
Occam's razor

The map


THEORY
VC
bias−variance
complexity
bayesian
TECHNIQUES
models
linear
neural networks
SVM
nearest neighbors
RBF
gaussian processes
SVD
graphical models
methods
regularization
validation
aggregation
input processing
PARADIGMS
supervised
unsupervised
reinforcement
active
online

Outline

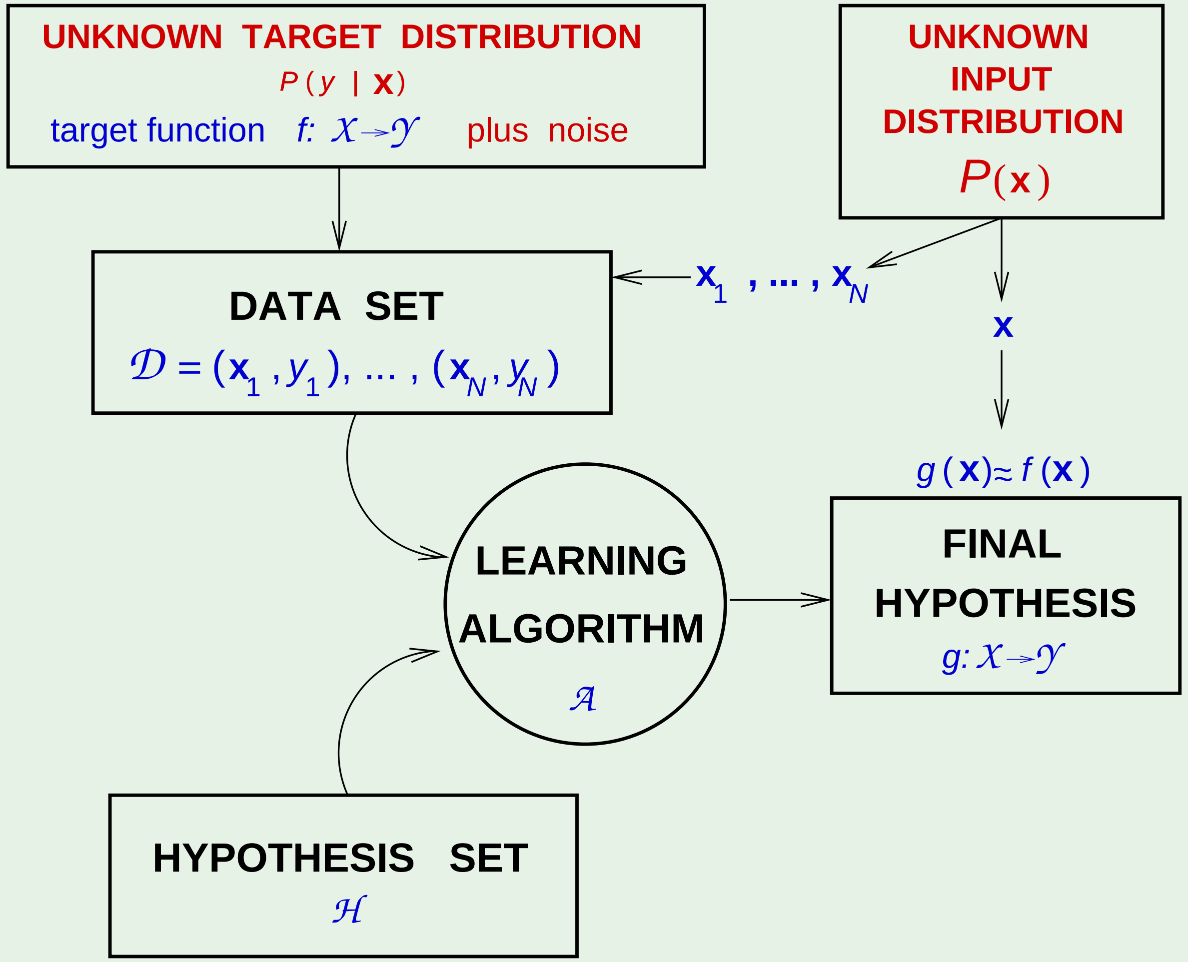
- The map of machine learning
- Bayesian learning
- Aggregation methods
- Acknowledgments

Probabilistic approach

Extend probabilistic role to all components

$P(\mathcal{D} \mid h = f)$ decides which h (likelihood)

How about $P(h = f \mid \mathcal{D})$?



The prior

$P(h = f \mid \mathcal{D})$ requires an additional probability distribution:

$$P(h = f \mid \mathcal{D}) = \frac{P(\mathcal{D} \mid h = f)\ P(h = f)}{P(\mathcal{D})} \propto P(\mathcal{D} \mid h = f)\ P(h = f)$$

$P(h = f)$ is the **prior**

$P(h = f \mid \mathcal{D})$ is the **posterior**

Given the prior, we have the full distribution

Example of a prior

Consider a perceptron: h is determined by $\mathbf{w} = w_0, w_1, \cdots, w_d$

A possible prior on $\mathbf{w}$: Each w_i is independent, uniform over $[-1, 1]$

This determines the prior over h - $P(h = f)$

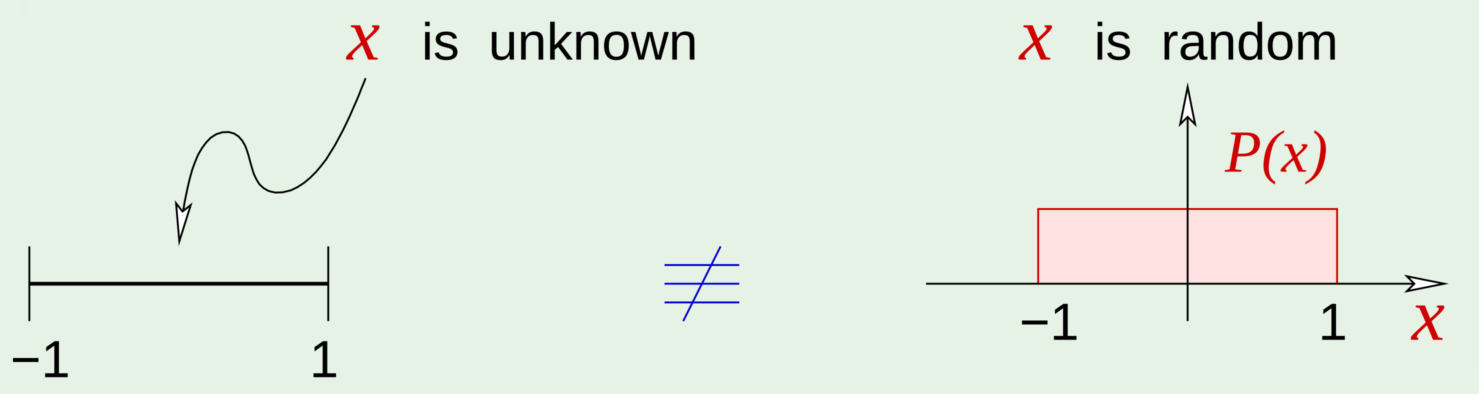
Given $\mathcal{D}$, we can compute $P(\mathcal{D} \mid h = f)$

Putting them together, we get $P(h = f \mid \mathcal{D})$

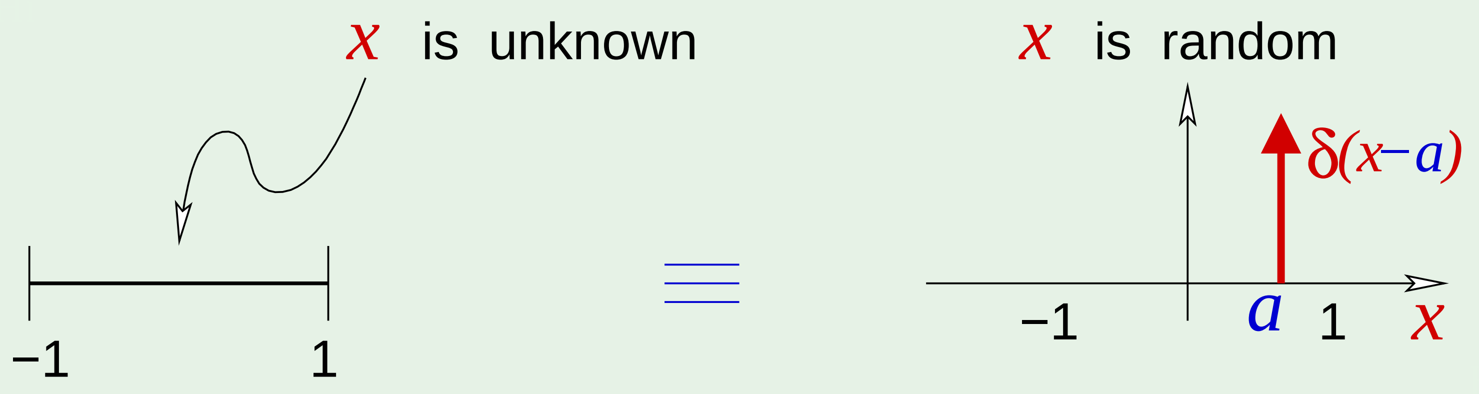
$$\propto \quad P(h = f)P(\mathcal{D} \mid h = f)$$

A prior is an assumption

Even the most "neutral" prior:



The true equivalent would be:



If we knew the prior

... we could compute $P(h = f \mid \mathcal{D})$ for every $h \in \mathcal{H}$

$\Longrightarrow$ we can find the most probable h given the data

we can derive $\mathbb{E}(h(\mathbf{x}))$ for every $\mathbf{x}$

we can derive the **error bar** for every $\mathbf{x}$

we can derive everything in a principled way

When is Bayesian learning justified?

1. The prior is **valid**

   trumps all other methods

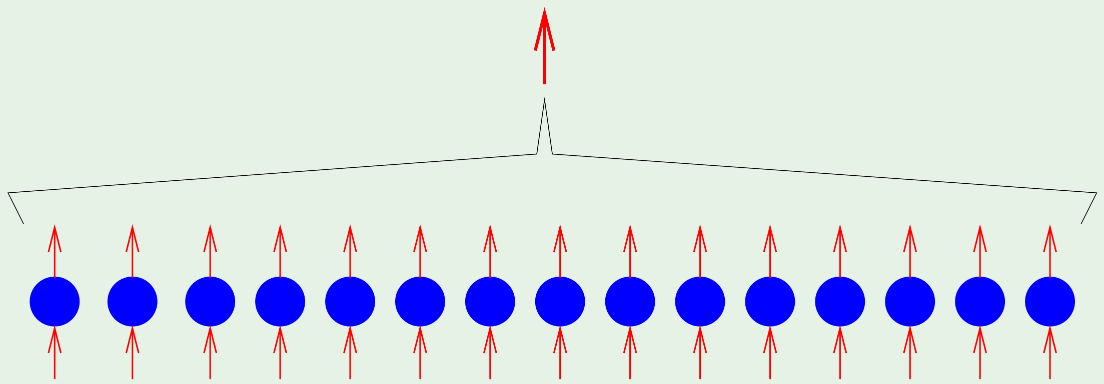
2. The prior is **irrelevant**

   just a computational catalyst

Outline

What is aggregation?

Combining different solutions $h_1, h_2, \cdots, h_T$ that were trained on $\mathcal{D}$:



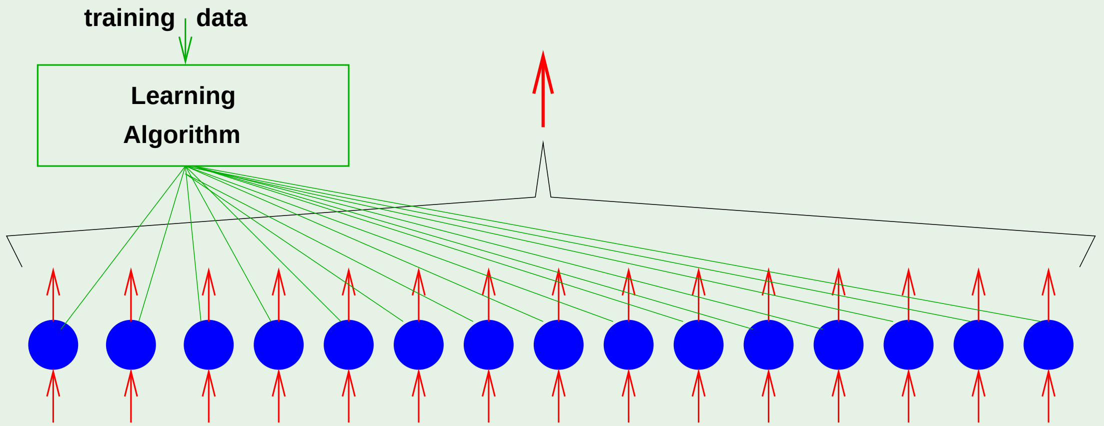
Regression: take an average

Classification: take a vote

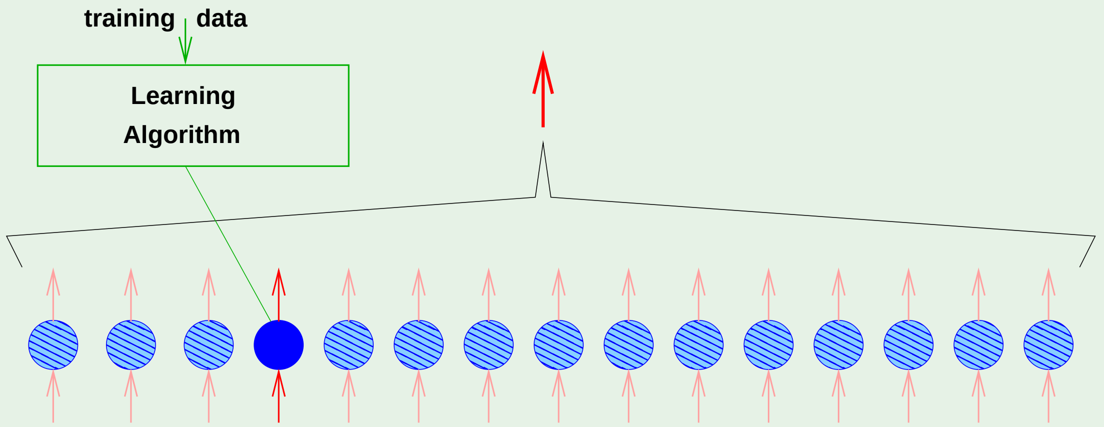
a.k.a. *ensemble learning* and *boosting*

Different from 2-layer learning

In a 2-layer model, all units learn **jointly**:



In aggregation, they learn **independently** then get combined:



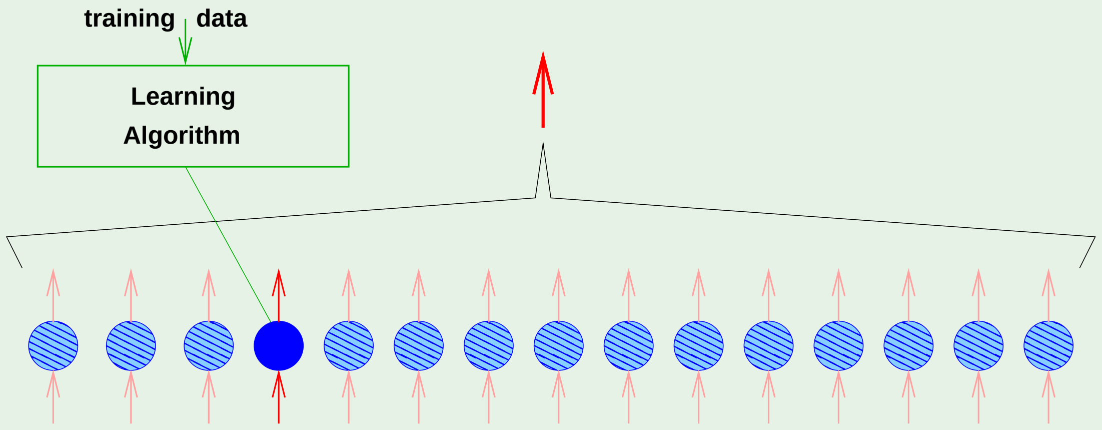
Two types of aggregation

1. **After the fact:** combines existing solutions

Example. Netflix teams merging "blending"

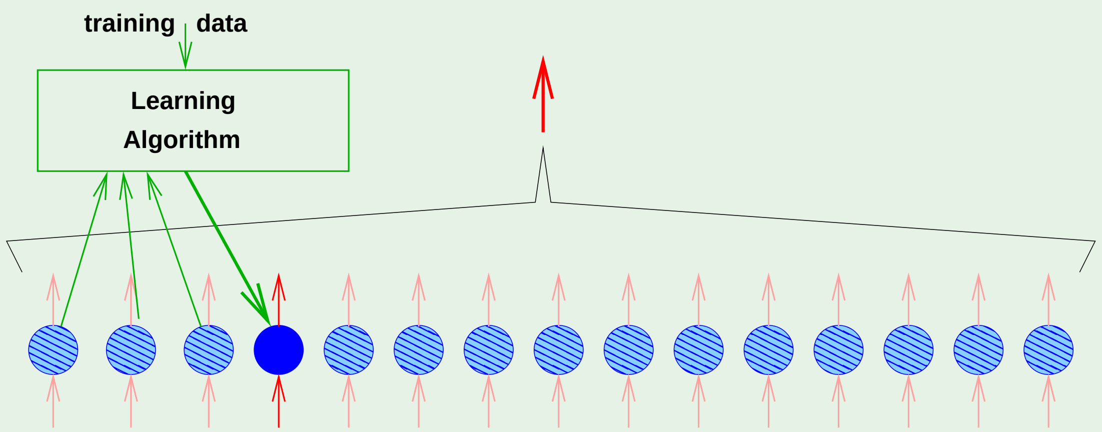
2. **Before the fact:** creates solutions to be combined

Example. Bagging - resampling $\mathcal{D}$



Decorrelation - boosting

Create $h_1, \cdots, h_t, \cdots$ sequentially: Make h_t decorrelated with previous h's:



Emphasize points in $\mathcal{D}$ that were misclassified

Choose weight of h_t based on $E_{\text{in}}(h_t)$

Blending - after the fact

For regression, $h_1, h_2, \cdots, h_T \longrightarrow g(\mathbf{x}) = \sum_{t=1}^{T} \alpha_t \, h_t(\mathbf{x})$

Principled choice of α_t's: minimize the error on an "aggregation data set" pseudo-inverse

Some α_t's can come out negative

Most valuable h_t in the blend?

Outline

- The map of machine learning
- Bayesian learning
- Aggregation methods
- Acknowledgments

Course content

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IST - Mathieu Desbrun

E&AS Division - Ares Rosakis and Mani Chandy

Provost's Office - Ed Stolper and Melany Hunt

Many others

Caltech TA's and staff members

Caltech alumni and Alumni Association

Colleagues all over the world

To the fond memory of

Faiza A. Ibrahim