Machine Learning is a Search Problem

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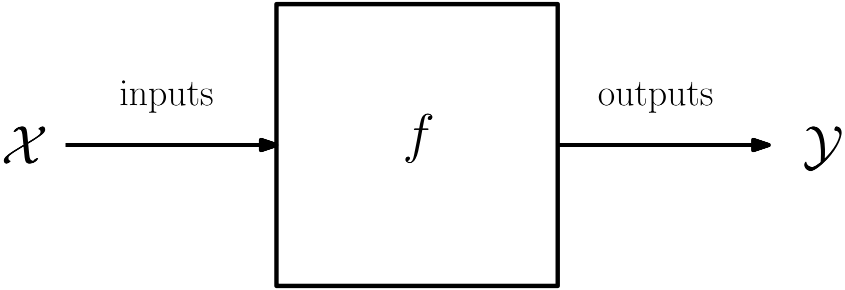
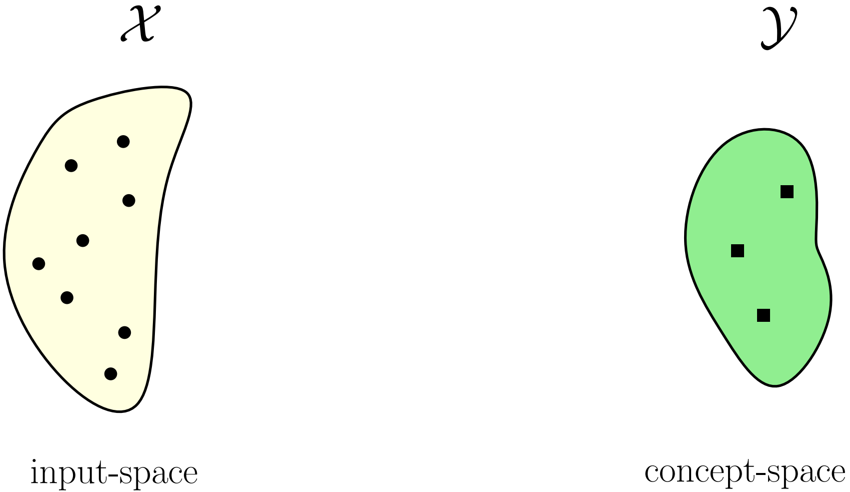

$\mathcal{X}$
inputs
f
outputs
$\mathcal{Y}$

"No learner can ever beat random guessing over all possible functions to be learned"

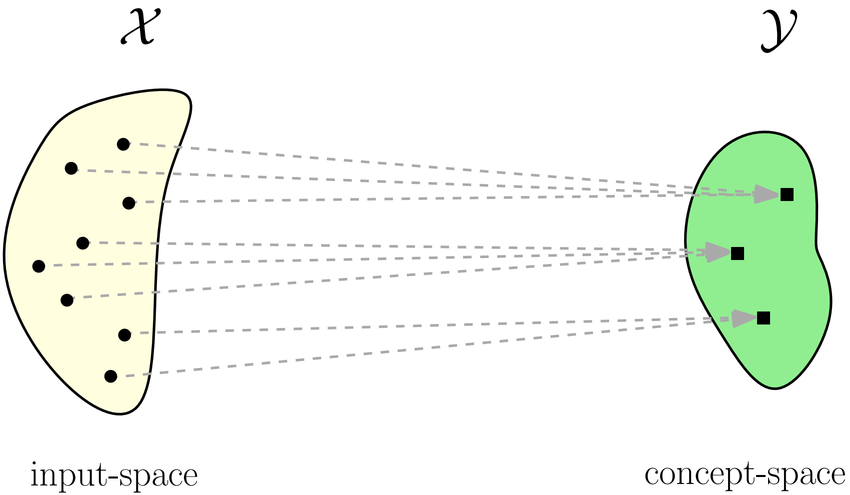
– *No free lunch theorem*, D. Wolpert.

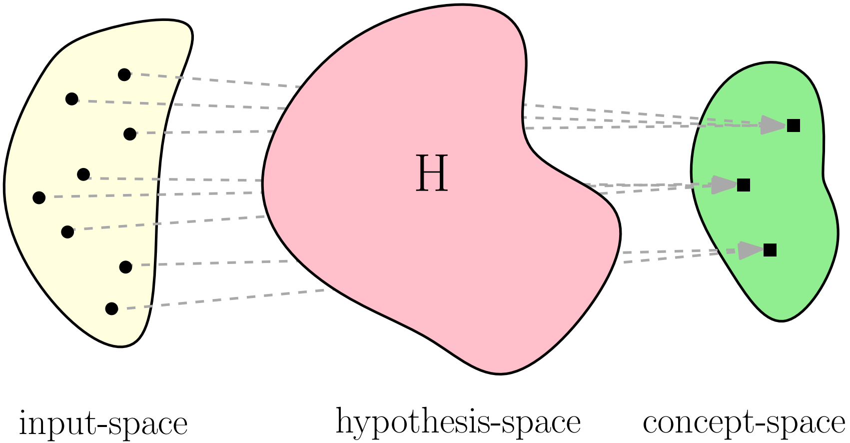
$\mathcal{X}$ $\mathcal{Y}$

inputs outputs

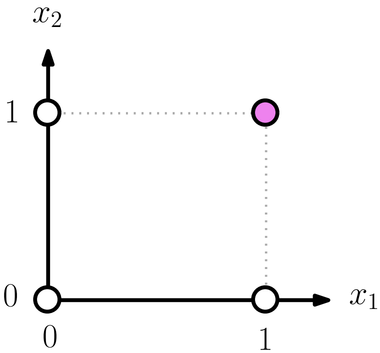

$\mathcal{X}$
$\mathcal{Y}$
input-space
concept-space

Search the unknown target function $f : \mathcal{X} \to \mathcal{Y}$




H
input-space
hypothesis-space
concept-space

	x_1	x_2	y
1:	0	0	0
2:	0	1	0
3:	1	0	0
4:	1	1	1



	x_1	x_2	y
1:	0	0	0
2:	0	1	0
3:	1	0	0
4:	1	1	1

$y = f(\mathbf{x})$, where $\mathbf{x} = \langle x_1, \ldots, x_d \rangle$

number of inputs $d = 2$
each x_i takes 2 options 0 or 1
input-space $\mathcal{X} = 2^d = 2^2 = 4$

number of outputs 1
output y takes 2 options in $\{0, 1\}$
concept-space $\mathcal{C} = 2^I = 2^{2^2} = 16$

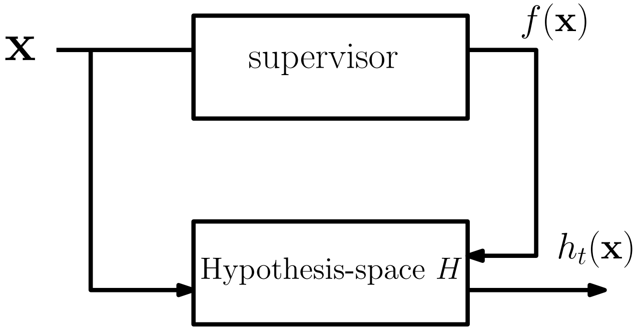
	x_1	x_2	y
1:	0	0	0
2:	0	1	0
3:	1	0	0
4:	1	1	1

input-space: $\mathcal{X} = 4$

concept-space: $\mathcal{C} = 16$

hypothesis-space : H is a set of all possible functions such that $h_t \in H$ produces a function $g : \mathcal{X} \to \mathcal{Y}$ that approximates f i.e. $g \approx f$.

data-space (training data):
$\mathcal{D} = \{(\mathbf{x}_1, f(\mathbf{x}_1)), \ldots, (\mathbf{x}_N, f(\mathbf{x}_N))\}$, where $\mathcal{D} \in C$ are N training examples.


$\mathbf{x}$
supervisor
$f(\mathbf{x})$
Hypothesis-space H
$h_t(\mathbf{x})$

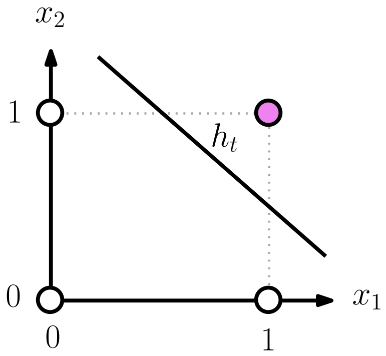
What learning needs?

Learning needs the method(s) to

- Represent
- Evaluate
- Optimize

a hypothesis h_t:

	x_1	x_2	y
1:	0	0	0
2:	0	1	0
3:	1	0	0
4:	1	1	1



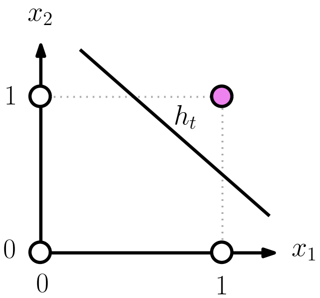
How to represent a hypothesis $h_t \in H$

A hypothesis h_t as a perceptron. A simple linear combination of inputs.

$$h_t = g(\mathbf{x}) = \sum_{i=1}^{d} w_i x_i \geq w_0$$

where w_0 is a threshold.

The hypothesis h_t has the parameters inputs weights w_i and the threshold w_0.



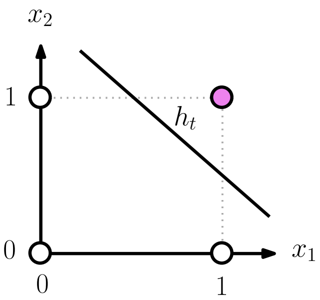
A hypothesis h_t as a perceptron.

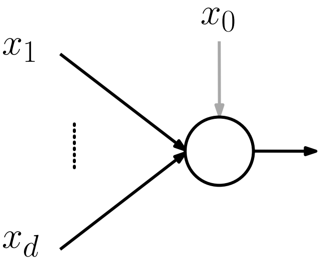
$$\sum_{i=1}^{d} w_i x_i \geq w_0$$

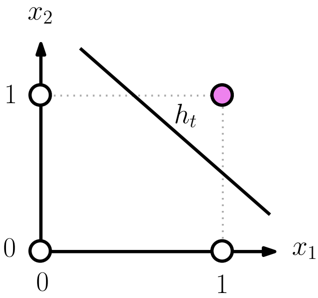
$$\sum_{i=1}^{d} w_i x_i - w_0 = 0$$

For an artificial input $x_0 = 1$

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




x_0
x_1
x_d

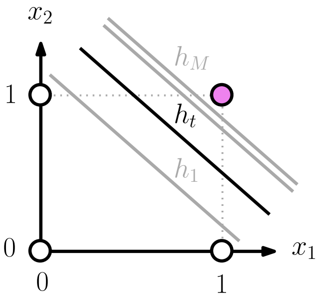

x_2
1
h_t
0
0
1
x_1

Which hypothesis to pick?

	x_1	x_2	y
1:	0	0	0
2:	0	1	0
3:	1	0	0
4:	1	1	1

Cost function such as the error rate:

$$E(h_t(\mathcal{D})) = \frac{1}{N}\sum_{j=1}^{N}\left(g(\mathbf{x}_j) \neq f(\mathbf{x}_j)\right)$$



How to search optimum hypothesis?

Function g of the hypothesis has parameter $\mathbf{w}$:

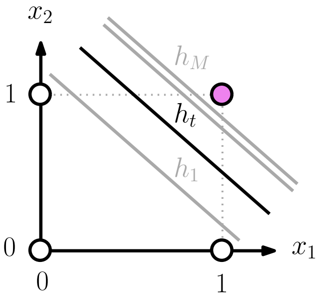
$$g_{\mathbf{w}}(\mathbf{x}) = \sum_{i=0}^{d} w_i x_i = 0$$

Simple algorithm:

Repeat parameter $\mathbf{w}$ update for $t = 2, 3, \ldots, M$

$$\mathbf{w}_t = \mathbf{w}_{t-1} + y\mathbf{x}$$

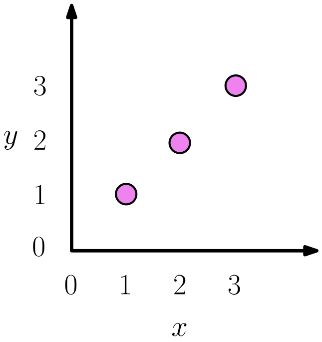
Until error rate $E(h_t(\mathcal{D}))$ is acceptable.



Does error $E(h_t(\mathcal{D}))$ minimization work?

Let's see an example (house price):

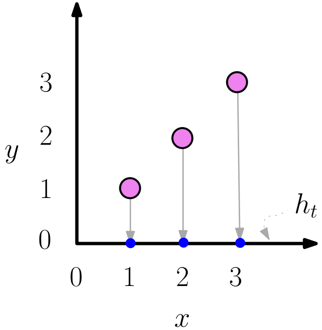
	$x = area(m^2)$	$y = price(in\ £)$
1:	1000	100K
2:	2000	200K
3:	3000	300K

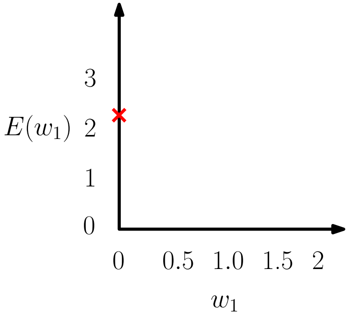


Now, cost function is a squared error:

$$E(h_t(\mathbf{x})) = \frac{1}{2N}\sum_{j=1}^{N}\left(g(\mathbf{x}_j) - f(\mathbf{x}_j)\right)^2$$

Does error $E(h_t(\mathcal{D}))$ minimization work?





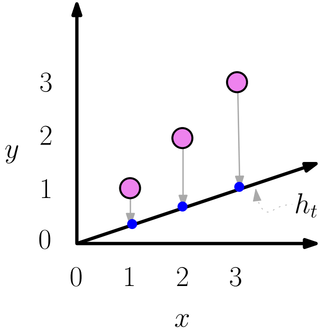
Hypothesis h_t for $w_0 = 0$ and $w_1 = 0.0$:

$$g(\mathbf{x}) = w_0 + w_1 x$$

Error $E(w_1)$ for $w_0 = 0$ and $w_1 = 0$:

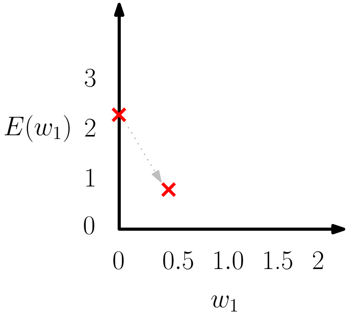
$$E(g_{\mathbf{w}}(\mathbf{x})) = 2.33$$

Does error $E(h_t(\mathcal{D}))$ minimization work?



Hypothesis h_t for $w_0 = 0$ and $w_1 = 0.5$:

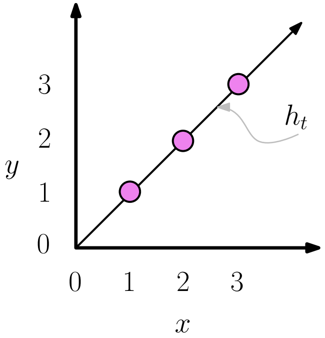
$$g(\mathbf{x}) = w_0 + w_1 x$$

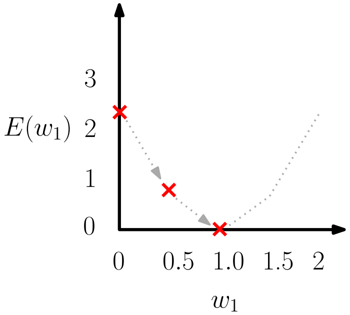


Error $E(w_1)$ for $w_0 = 0$ and $w_1 = 0.5$:

$$E(g_{\mathbf{w}}(\mathbf{x})) = 0.625$$

Does error $E(h_t(\mathcal{D}))$ minimization work?





Hypothesis h_t for $w_0 = 0$ and $w_1 = 1$:

$$g(\mathbf{x}) = w_0 + w_1 x$$

Error $E(w_1)$ for $w_0 = 0$ and $w_1 = 1$:

$$E(g_{\mathbf{w}}(\mathbf{x})) = 0.0$$

Gradient Descent

Function g of the hypothesis has parameter $\mathbf{w}$:

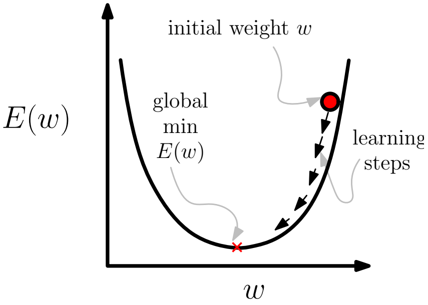
$$g_{\mathbf{w}}(\mathbf{x}) = \sum_{i=0}^{d} w_i x_i = 0$$

Repeat parameter $\mathbf{w}$ update for $t = 2, 3, \ldots, M$

$$\mathbf{w}_t = \mathbf{w}_{t-1} + \alpha \frac{\partial}{\partial \mathbf{w}} E(\mathbf{x})$$

for a learning-rate α.

Until error rate $E(h_t(\mathcal{D}))$ is acceptable.



Gradient Descent

Function g of the hypothesis has parameter $\mathbf{w}$:

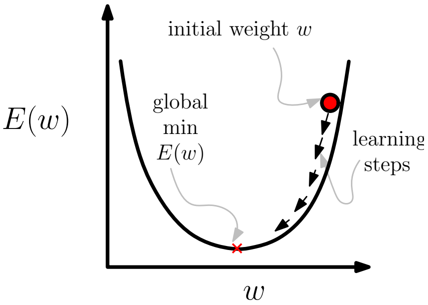
$$g_{\mathbf{w}}(\mathbf{x}) = \sum_{i=0}^{d} w_i x_i = 0$$

Repeat parameter $\mathbf{w}$ update for $t = 2, 3, \ldots, M$

$$\mathbf{w}_t = \mathbf{w}_{t-1} + \alpha \Delta \mathbf{w}$$

where $\Delta \mathbf{w}$ is gradient and α learning-rate.

Until error rate $E(h_t(\mathcal{D}))$ is acceptable.



Gradient Descent: Versions

Stochastic Gradient Descent

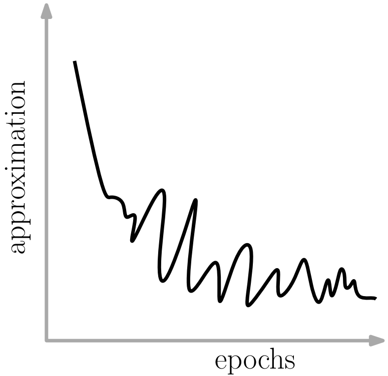
$t = 0$
$\mathbf{w}$ initial weights
for t in epochs **do**
  $\mathcal{D} \leftarrow \mathit{shuffle}(\mathcal{D})$
  for $\mathbf{x}_j$ in $\mathcal{D}$ **do**
    $\Delta\mathbf{w} = g_{\mathbf{w}}(\mathbf{x}_j)$
    $\mathbf{w}_j = \mathbf{w}_{j-1} + \alpha\Delta\mathbf{w}$

Batch Gradient Descent

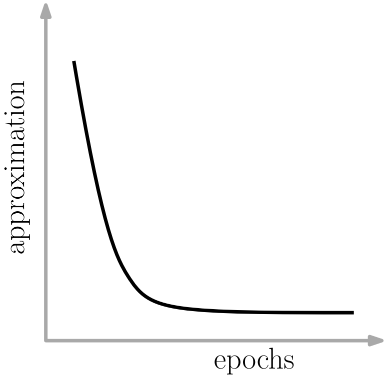
$t = 0$
$\mathbf{w}$ initial weights
for t in epochs **do**
  for $\mathbf{x}_j$ in $\mathcal{D}$ **do**
    $\Delta\mathbf{w} = \Delta\mathbf{w} + g_{\mathbf{w}}(\mathbf{x}_j)$
  $\Delta\mathbf{w} = \frac{\Delta\mathbf{w}}{|\mathcal{D}|}$
  $\mathbf{w}_t = \mathbf{w}_{t-1} + \alpha\Delta\mathbf{w}$

Gradient Descent: Versions

Stochastic Gradient Descent

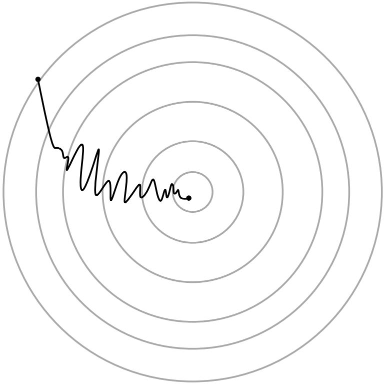


Batch Gradient Descent

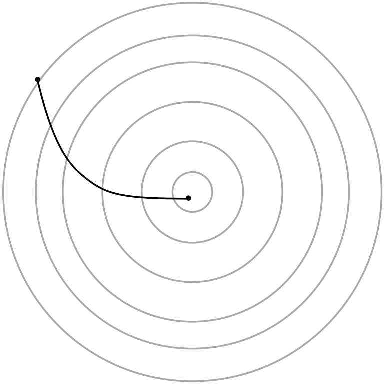


Gradient Descent: Versions

Stochastic Gradient Descent



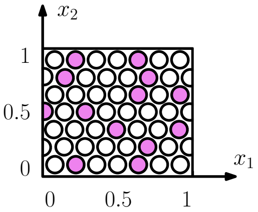
Batch Gradient Descent



What is learning?

Is learning possible?

What is learning?



Box $\mathcal{X}$ full of red and white marbles:

i.e., all possible data points $\mathbf{x} \in \mathbb{R}^2$ space.

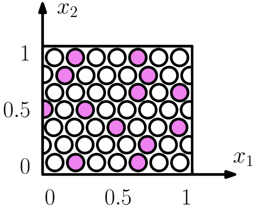
Random sample $\mathcal{D}$

Learning answers, the question:

What is the probability of picking a red marble from box $\mathcal{X}$ by just seeing sample $\mathcal{D}$.

Q: Is learning possible?

What is learning?



Box $\mathcal{X}$ full of red and white marbles:

i.e. all possible data points $\mathbf{x} \in \mathbb{R}^2$ space.

Random sample $\mathcal{D}$

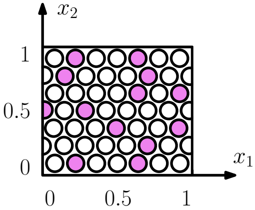
Learning answers the question:

What is the probability of picking a red marble from box $\mathcal{X}$ by just seeing sample $\mathcal{D}$.

Q: Is learning possible?

A: If we can tell the probability of picking red marble from the box $\mathcal{X}$ then yes!

Probability of picking a marble



The probability of picking red marble from the box $\mathcal{X}$ is μ.

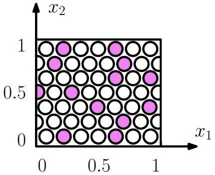
The probability of picking red marble from the sample $\mathcal{D}$ is ν.

We can confirm the probability μ iff the following holds:

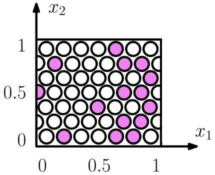
$$P[|\nu - \mu| > \epsilon] \leq 2e^{-2\epsilon^2 N}$$

This inequality is Hoeffding's Inequality. Or Probability approximate correct learning.

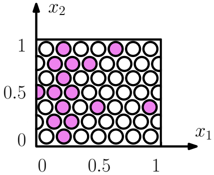
Probably approximately correct learning



$E(h_1(\mathcal{X}))$



$E(h_2(\mathcal{X}))$



$E(h_M(\mathcal{X}))$

$E(h_1(\mathcal{D}))$

$E(h_2(\mathcal{D}))$

$\cdots$

$E(h_M(\mathcal{D}))$

Union bound:

$$P[|E(h_{\mathcal{D}}) - E(h_{\mathcal{X}})| > \epsilon] \leq \sum_{t=1}^{M} P[|E(h_{\mathcal{D}}) - E(h_{\mathcal{X}})| > \epsilon] \leq 2Me^{-2\epsilon^2 N}$$

How many training example required to learn?

Lets δ be the probability of error rate greater than ϵ, i.e. $P[|E(h_{\mathcal{D}}) - E(h_{\mathcal{X}})| > \epsilon] \leq \delta$.

$$\delta \leq 2Me^{-2\epsilon^2 N}$$

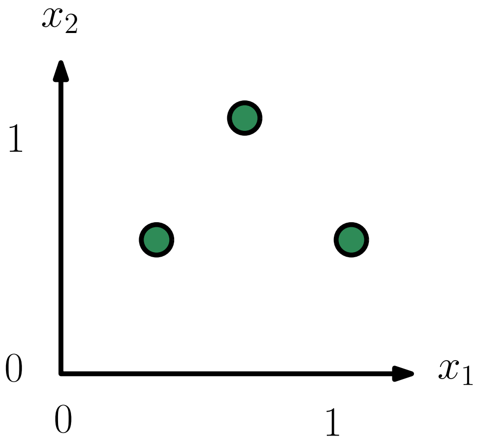
For $M \leq \mathcal{C}$, and $\mathcal{C} = 2^{2^d}$, and d is input-space dimension.
We can also summaries it for bound on N as:

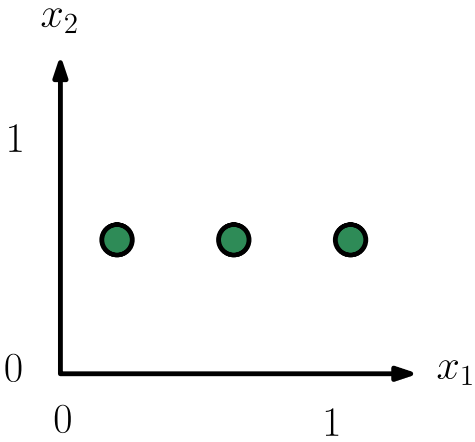
$$N > \frac{1}{\epsilon}\left(\ln M + \ln \frac{1}{\delta}\right)$$

N grows exponentially in # input attributes d.

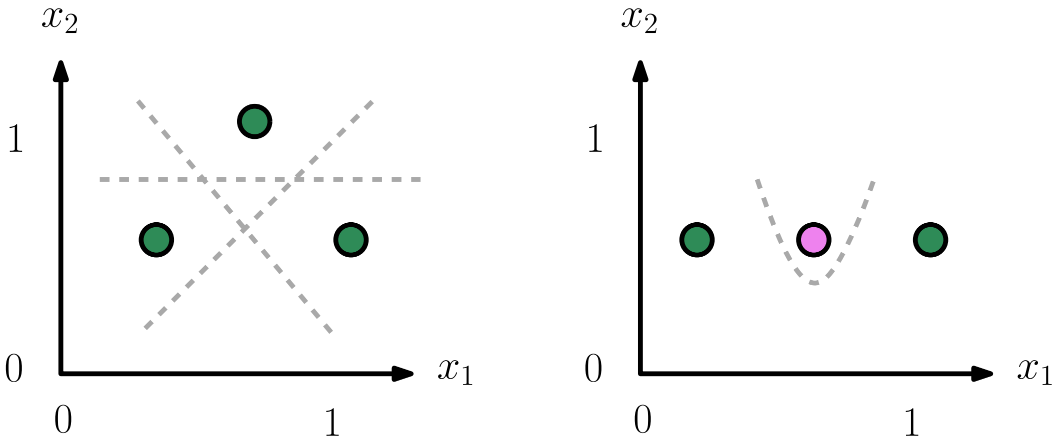
Conclusion: Larger N require for higher accuracy and for improving probability of finding correct hypothesis.

How do we choose a hypothesis class?

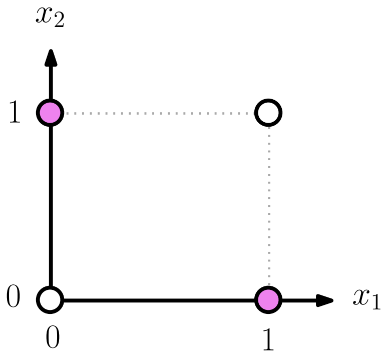


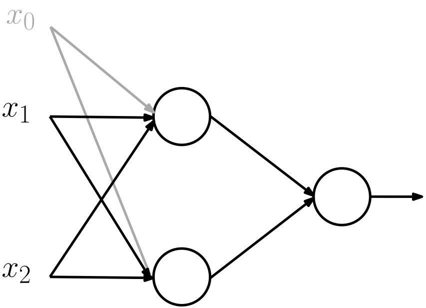


How do we choose a hypothesis class?

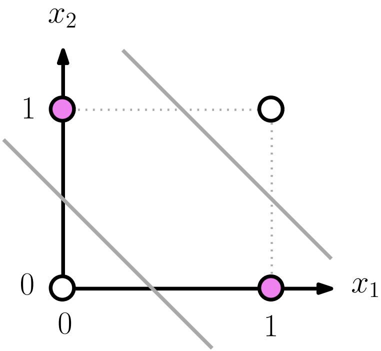


	x_1	x_2	y
1:	0	0	0
2:	0	1	1
3:	1	0	1
4:	1	1	0



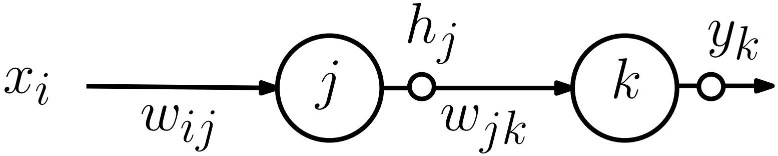


x_0
x_1
x_2

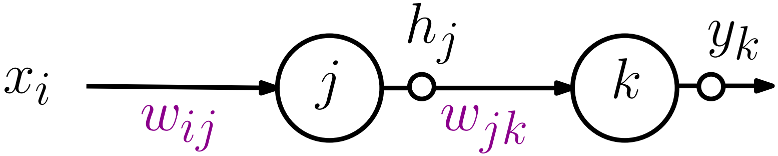


x_2
1
0
0
1
x_1

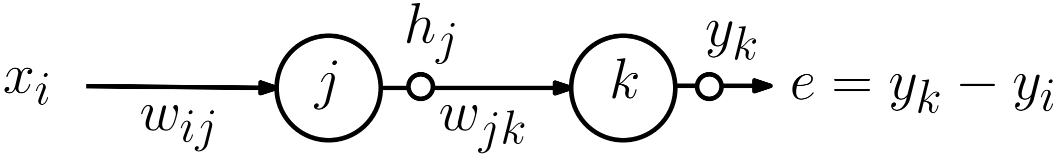
Backpropagation: Forward pass



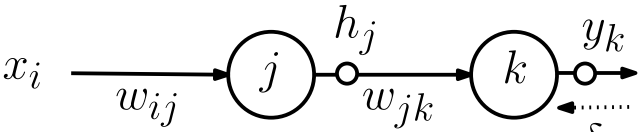
Backpropagation: Forward pass



Backpropagation: Error at the output layer



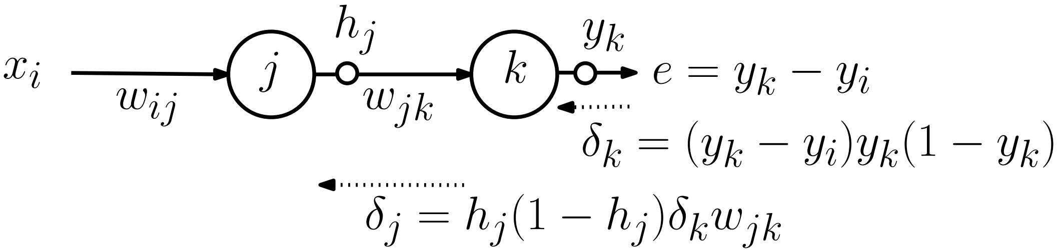
Backpropagation: Backward pass (output layer δ)



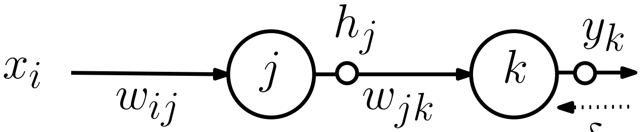
$$e = y_k - y_i$$

$$\delta_k = (y_k - y_i)y_k(1 - y_k)$$

Backpropagation: Backward pass (hidden layer δ)



Backpropagation: Backward pass (input layer δ)



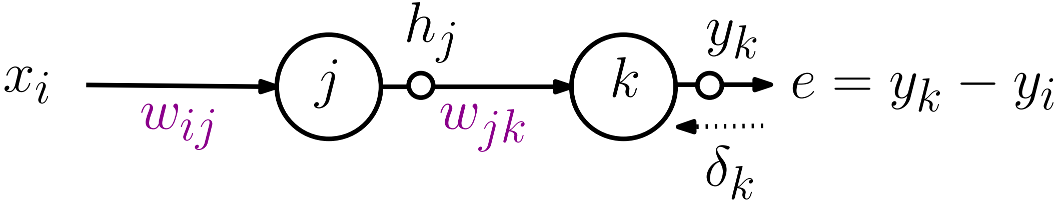
$$e = y_k - y_i$$

$$\delta_k = (y_k - y_i)y_k(1 - y_k)$$

$$\delta_j = h_j(1 - h_j)\delta_k w_{jk}$$

$$\delta_i = \delta_j w_{ik}$$

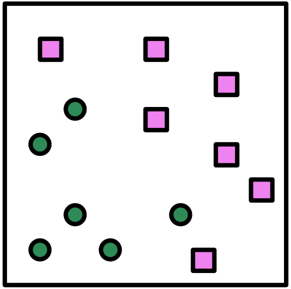
Backpropagation: Backward pass (input layer δ)



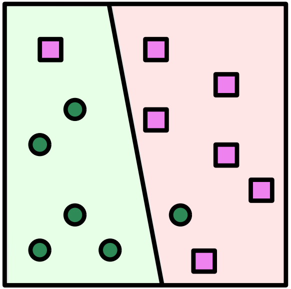
$$\Delta w_{jk} = \delta_j h_j$$

$$\Delta w_{ij} = \delta_i x_i$$

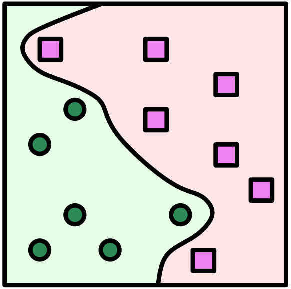
Is the chosen hypothesis good?



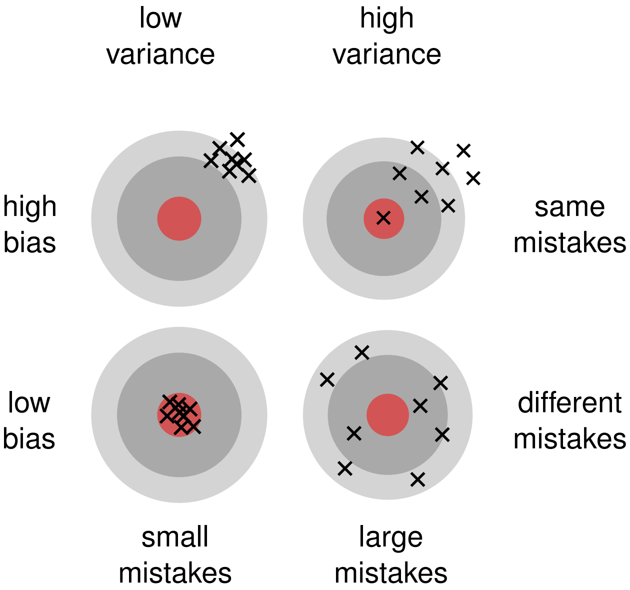
Training data



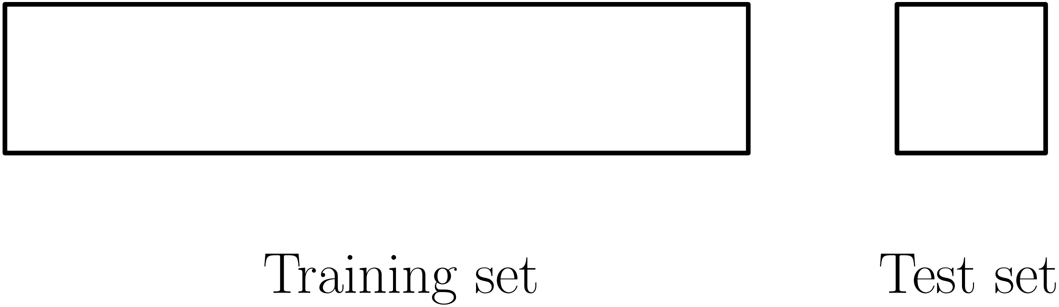
Underfit



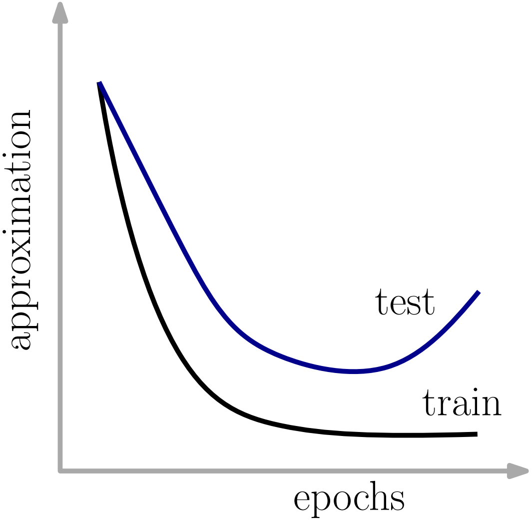
Overfit


low
variance
high
variance
high
bias
same
mistakes
low
bias
different
mistakes
small
mistakes
large
mistakes

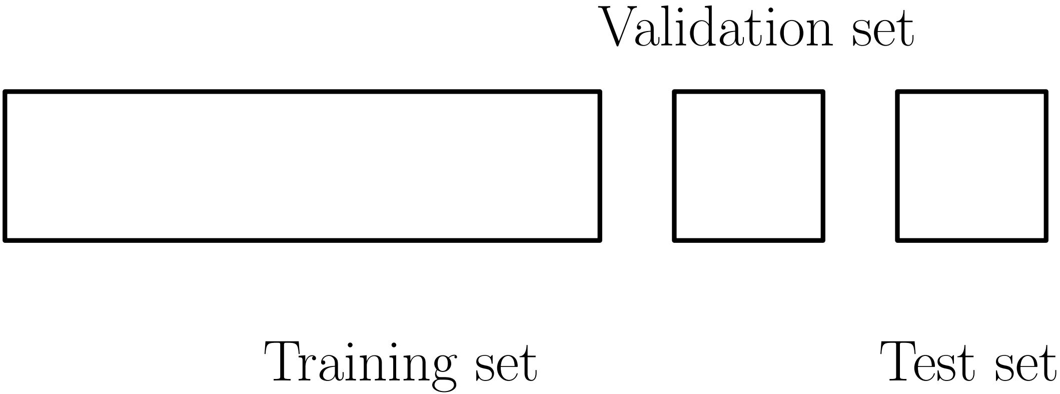
Training: Cross Validation



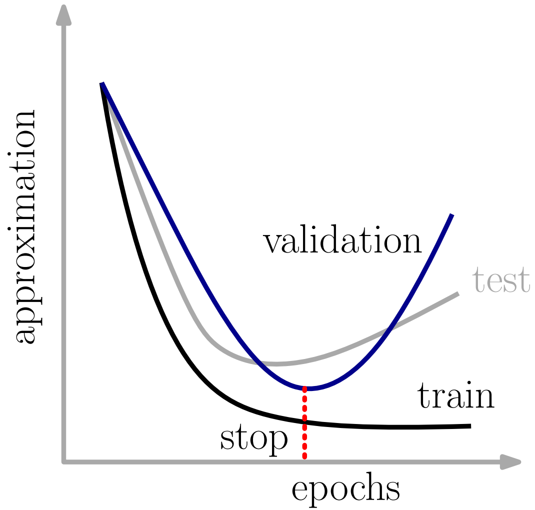
Training



Training: Take another set



Training: Early Stopping



Among all generated hypothesis from H, chose the simplest one.

– *Occam's Razor*, William of Ockham.