

Machine Learning: short introduction (trees and ANN), part 3

Sergey Korpachev on behalf of Dépôt

Outline

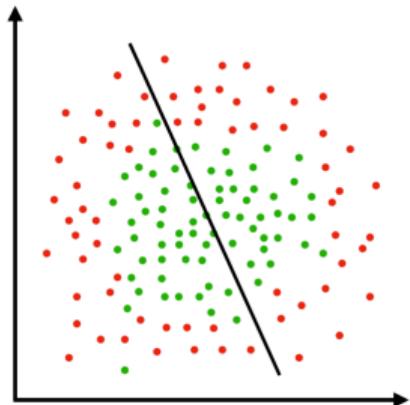
- Machine learning (ML)
 - Data
 - Features in ML
 - ML pipeline
 - Linear model
 - Decision tree
 - Neural network
 - Summary

Modelling nonlinearities

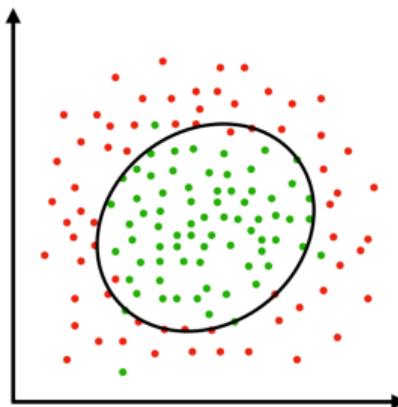
Modelling nonlinearities

linear models

What we have



What we want

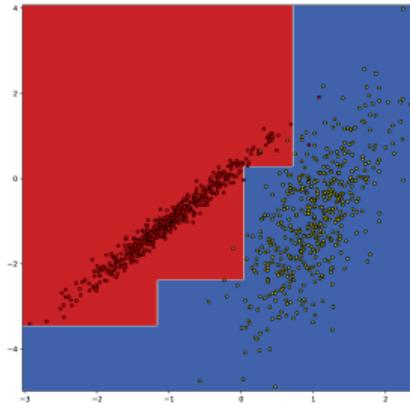
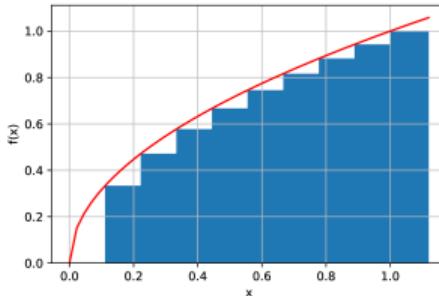


Linear models can't simply describe complex nonlinear data

Modelling nonlinearities

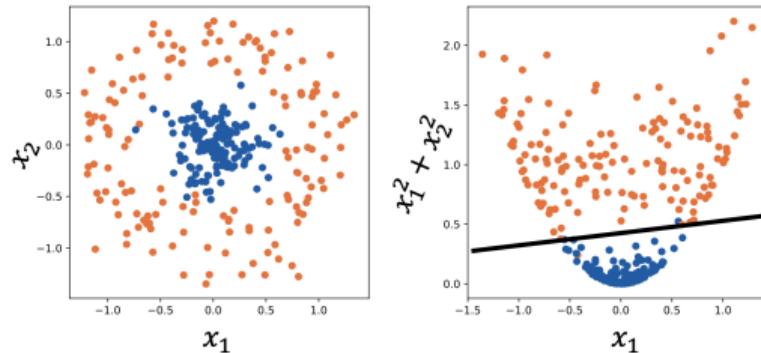
—○ trees

- (Ensembles of) Trees were designed to approximate nonlinearities and are **pretty good** in it + they are **fast and interpretable**
- But they are just “brute-force” algorithms – **don’t infer symmetries** in data by design
- **Ad-hoc, cut-based and piecewise approximations** of data at hand + not differentiable and smooth



Modelling nonlinearities

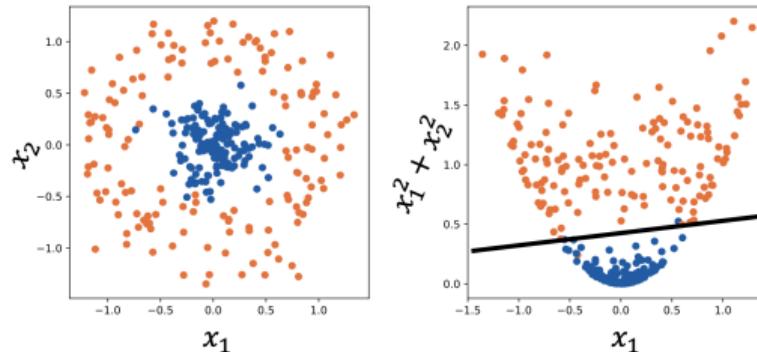
—○ feature engineering



- But sometimes we know *a priori* that there are transformations simplifying the problem → even linear model can do the job
- However, this **feature engineering** is non-trivial, requires domain knowledge and is time-consuming

Modelling nonlinearities

—○ feature engineering



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- However, this **feature engineering** is non-trivial, requires domain knowledge and is time-consuming

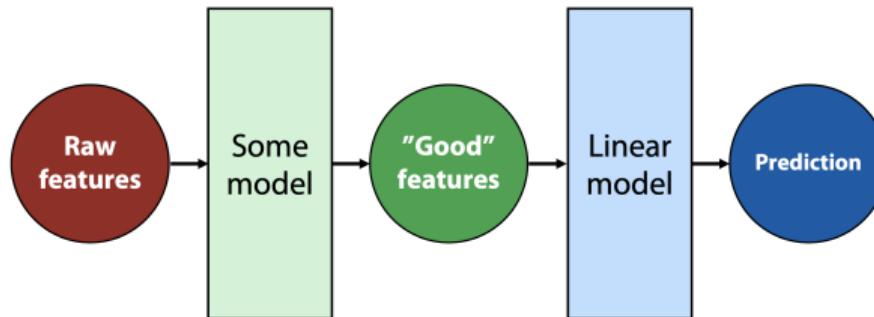
What if we design a model which could **automatically** feature-engineer itself?

Neural Network

Neural Network

—○ automating FE

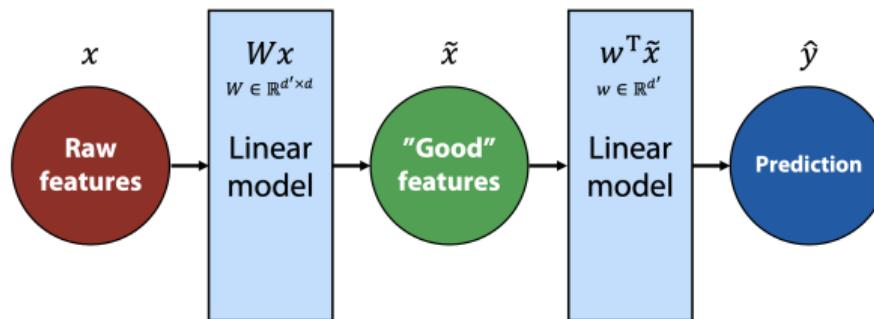
NN illustrations from
ML in HEP 2020



- Let's use a **simple linear model** to solve our supervised problem
- Add a block to a linear model which will automatically **generate new features** for it
- Two blocks would work together as a **single model** ⇒ their parameters are updated simultaneously
- And **automatically**, by e.g. gradient descent (given their differentiability)

Neural Network

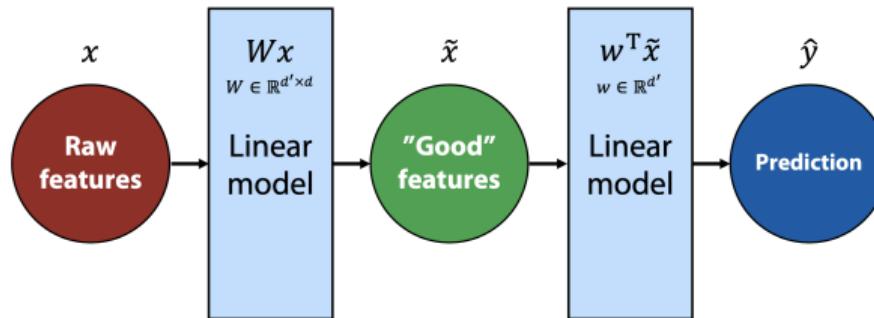
—○ automating FE



- Would a linear model work as a feature generating model?

Neural Network

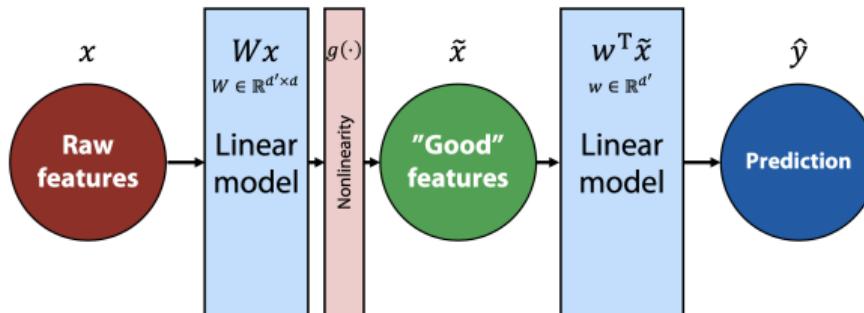
—○ automating FE



- Would a linear model work as a feature generating model? **No**
- $\hat{y} = w^T \tilde{x} = w^T (Wx) = (w^T W)x = w'^T x \Rightarrow$ it is still a linear model
- Input feature space has not changed, only the model weights

Neural Network

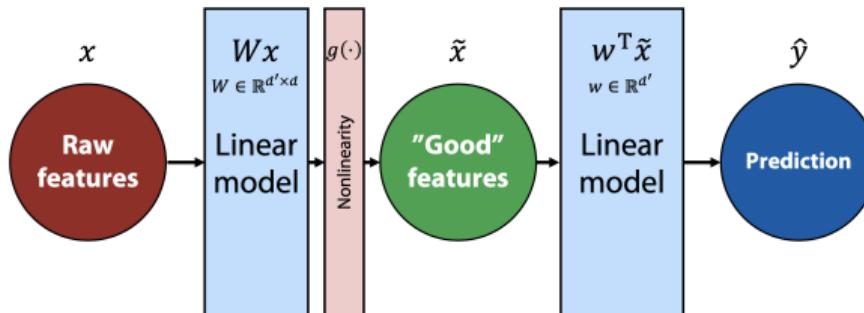
—○ automating FE



- Let's then introduce **nonlinearity** to our model
→ $\hat{y} = w^T \tilde{x} = w^T g(Wx)$,
where $g(\cdot)$ – some nonlinear scalar function (applied elementwise)

Neural Network

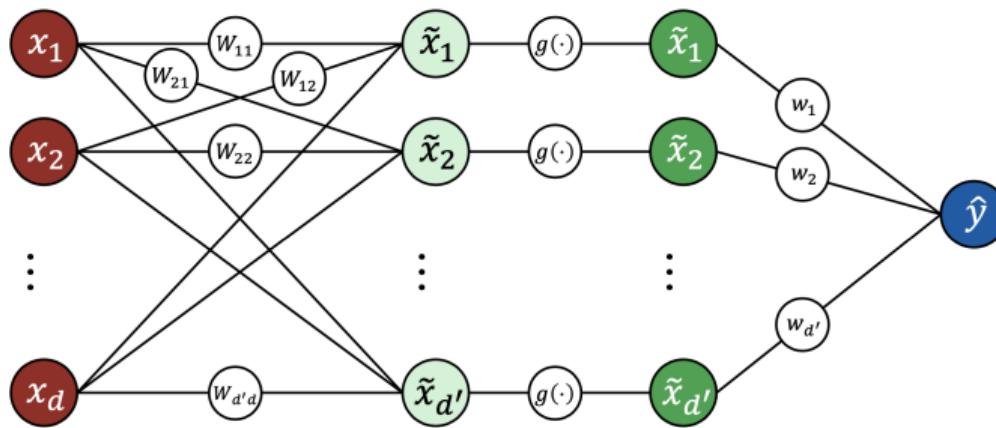
—○ automating FE



- Let's then introduce **nonlinearity** to our model
 - $\hat{y} = w^T \tilde{x} = w^T g(Wx)$,
where $g(\cdot)$ – some nonlinear scalar function (applied elementwise)
 - This is the simplest example of a **neural network**

Neural Network

—○ architecture



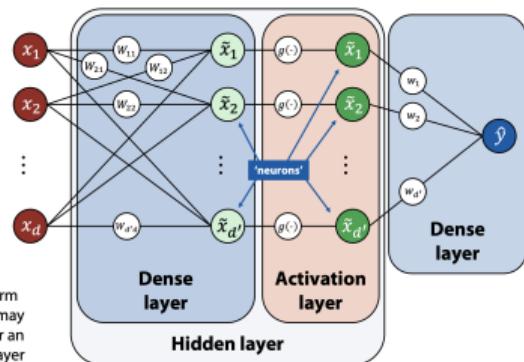
Essentially, NN is just a **composite function** that maps a set of X to a set of Y

$$\hat{y} = w^T \tilde{x} = w^T g(Wx)$$

Neural Network

 ——○ terminology

Feed-forward network:



Note: the term "activation" may also stand for an output of a layer

- Brown nodes x_1, x_2, \dots, x_d – features from an **input layer**
- Green nodes $\tilde{x}_1, \tilde{x}_2, \dots, \tilde{x}_{d'}$ – **neurons** from a **hidden layer**
- Blue node \hat{y} – neuron from an **output layer**
- Straight lines (edges) between neurons – **weights** w_{ij}
- $g(\cdot)$ – nonlinear **activation** function, e.g. sigmoid $\sigma(\cdot)$
- **Important:** each neuron has additional **bias** b associated to it and added to other inputs (not illustrated)

Training

Training —— o how to train?

- Since NN fundamentally is a parametrized differentiable model we can optimise the loss function and use **gradient descent** to train it:

$$\omega_{k+1} \leftarrow \omega_k - \eta \cdot \nabla Q(\omega_k)$$

- But **gradients** are hard to derive analytically – writing down all the derivatives is tough and tedious (especially for large NN)
- Note that NN is just a **composite model** \Rightarrow can use **chain rule** for differentiating it

Training —— o chain rule

- Computing derivative of a "base" function is simple \Rightarrow decompose composite function into a set of base ones and differentiate them one by one
- Let's recall the rule:

$$\frac{\partial f(t(x))}{\partial x} = \frac{\partial f(t)}{\partial t} \cdot \frac{\partial t(x)}{\partial x}$$

Exercise: can you compute derivative of sigmoid function by decomposing it into base functions?

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

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$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

$$\sigma(x) = f(g(h(p(x)))), \quad f(z) = \frac{1}{z}, \quad g(z) = 1 + z, \quad h(z) = e^z, \quad p(z) = -z$$

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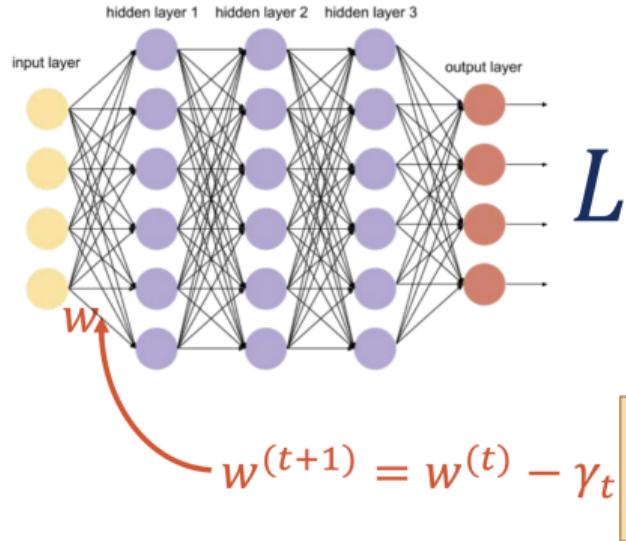
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$$\sigma'(x) = \frac{\partial f}{\partial g} \cdot \frac{\partial g}{\partial h} \cdot \frac{\partial h}{\partial p} \cdot \frac{\partial p}{\partial x} = -\frac{1}{g^2} \cdot 1 \cdot e^p \cdot (-1) = \dots = \sigma(x) \cdot (1 - \sigma(x))$$

Training — o backpropagation

backprop illustrations from [DMIA](#)

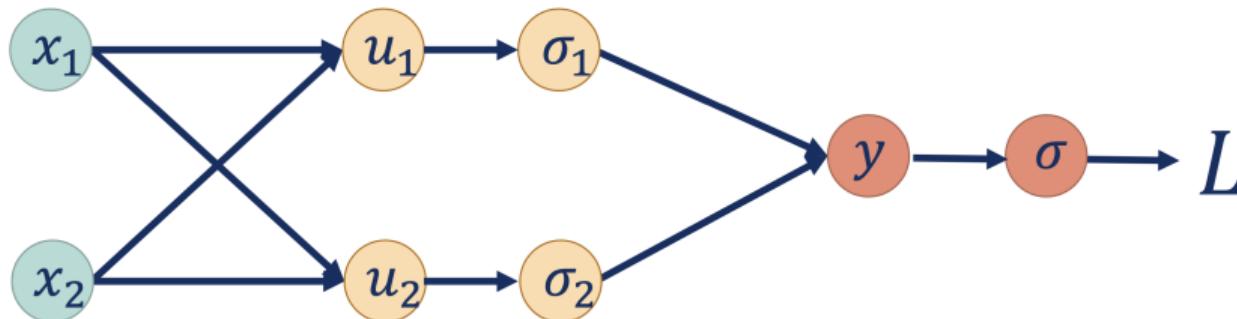


- So how to find partial derivatives of loss function with respect to some weight?

Training

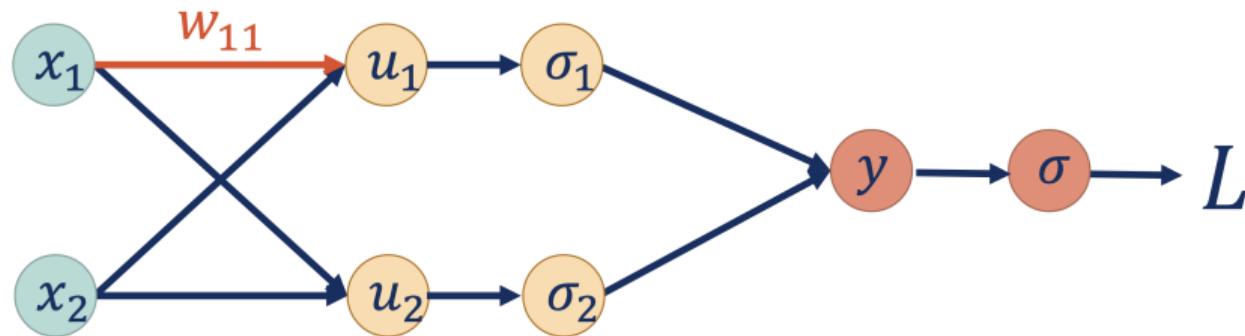
—○ backpropagation

backprop illustrations from [DMIA](#)



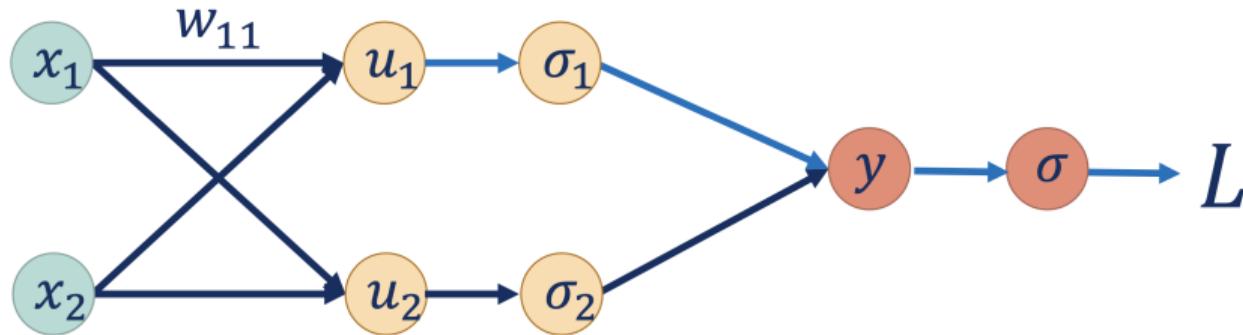
- Let's consider a simplified neural network
- Represent it in the form of a **computational graph**

Training —○ backpropagation



$$w_{11}^{(t+1)} = w_{11}^{(t)} - \gamma_t \frac{\partial L}{\partial w_{11}}$$

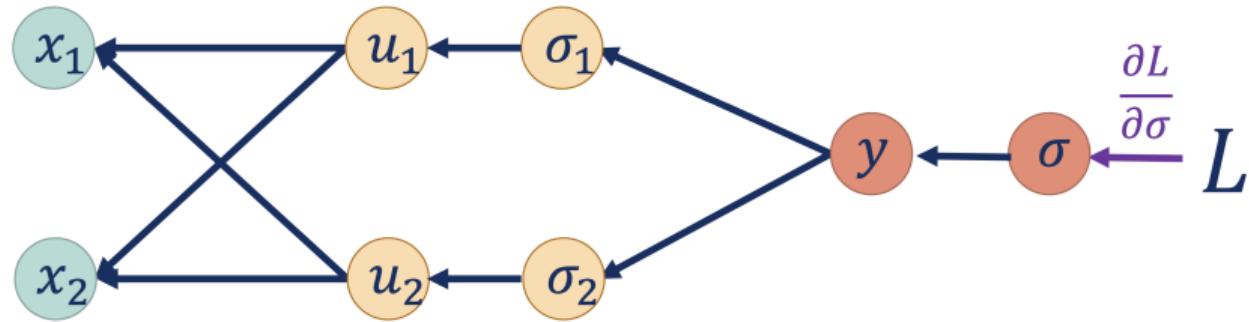
Training —○ backpropagation



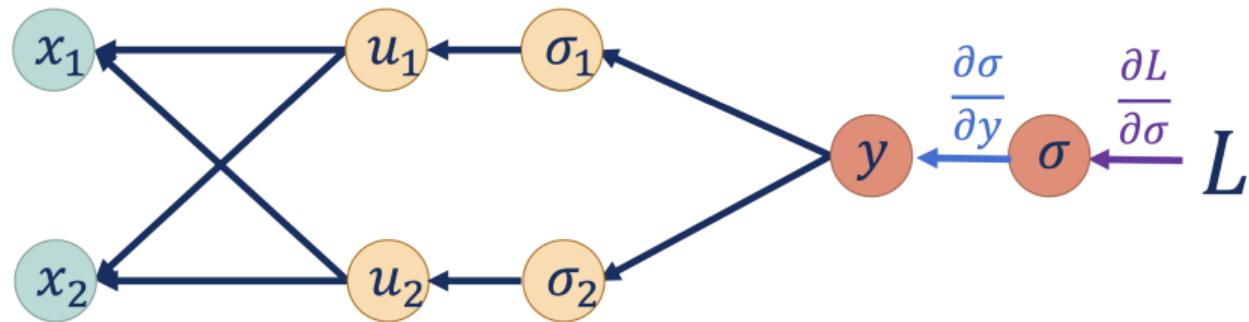
$$w_{11}^{(t+1)} = w_{11}^{(t)} - \gamma_t \frac{\partial L}{\partial w_{11}}$$

$$\frac{\partial L}{\partial w_{11}} = \frac{\partial L}{\partial u_1} \frac{\partial u_1}{\partial w_{11}} = \frac{\partial L}{\partial u_1} x_1$$

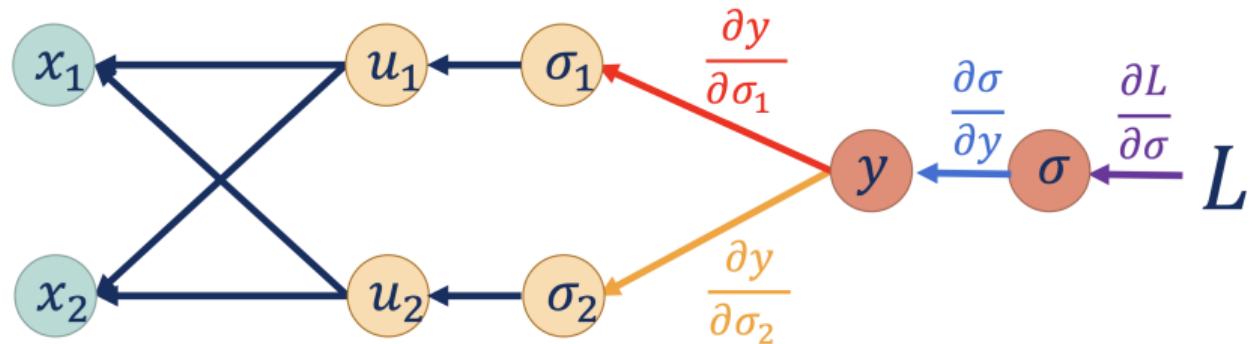
Training —○ backpropagation



Training —○ backpropagation

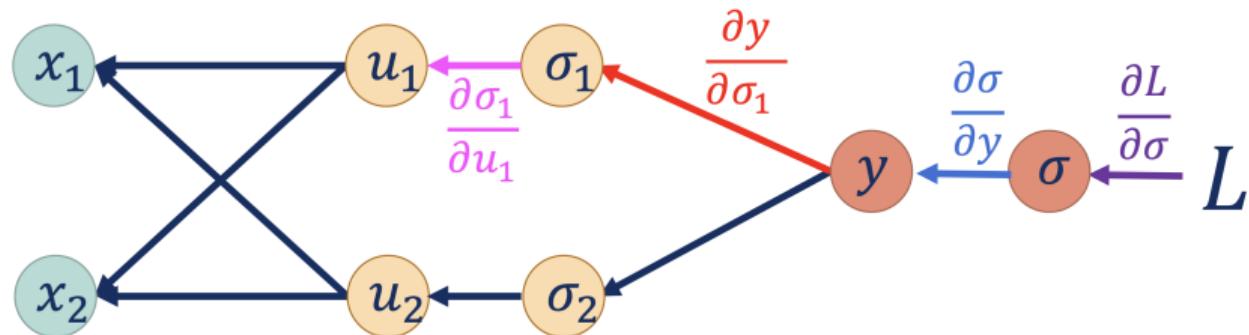


Training —○ backpropagation



Training

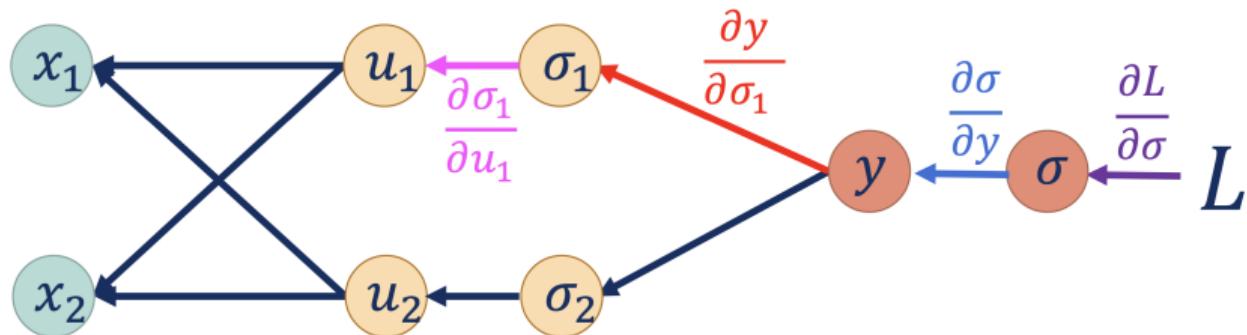
—○ backpropagation



$$\frac{\partial L}{\partial u_1} = \frac{\partial L}{\partial \sigma} \frac{\partial \sigma}{\partial y} \frac{\partial y}{\partial \sigma_1} \frac{\partial \sigma_1}{\partial u_1}$$

Training

—○ backpropagation



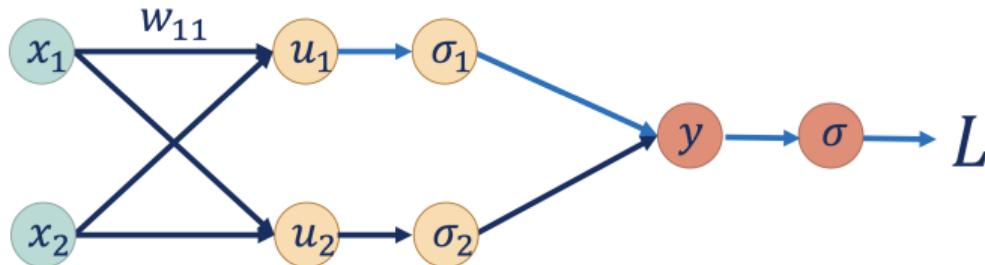
$$\frac{\partial L}{\partial u_1} = \frac{\partial L}{\partial \sigma} \frac{\partial \sigma}{\partial y} \frac{\partial y}{\partial \sigma_1} \frac{\partial \sigma_1}{\partial u_1}$$

- this procedure is called **backpropagation**
- its idea is to **collect derivatives** at each step in the computational graph w/o recalculating them every single time for every weight

Training

—○ wrap it up

train NN in your browser!

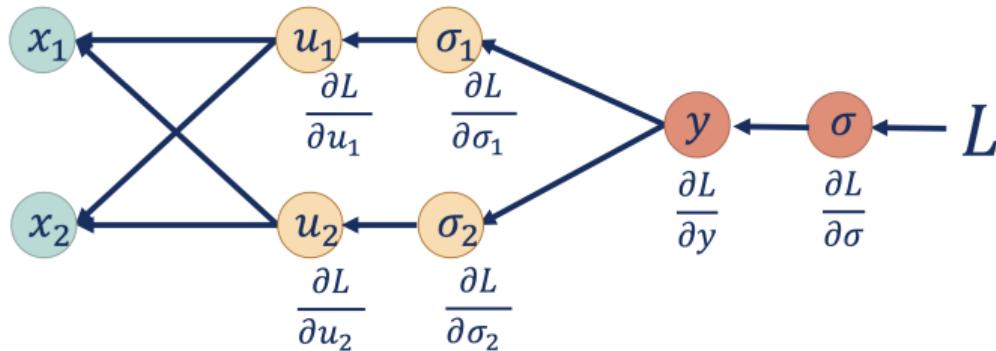


- 1 make **forward pass** through NN to calculate the output of each neuron and value of loss function

Training

—○ wrap it up

[train NN in your browser!](#)

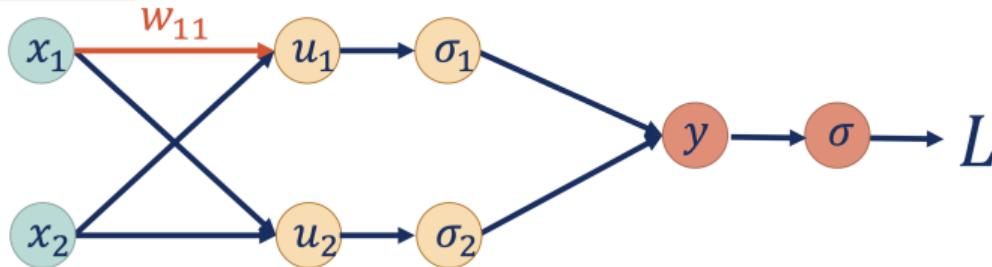


- 1 make **forward pass** through NN to calculate the output of each neuron and value of loss function
- 2 with **backward pass** go back through NN to calculate gradients for all weights

Training

—○ wrap it up

train NN in your browser!



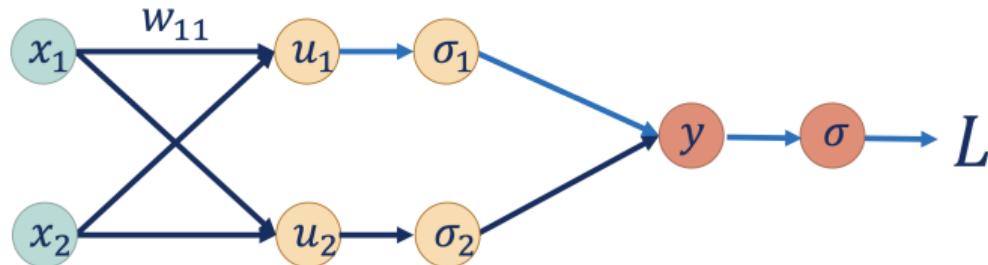
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- 1 make **forward pass** through NN to calculate the output of each neuron and value of loss function
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- 3 update weights with their gradients

Training

—○ wrap it up

train NN in your browser!



- 1 make **forward pass** through NN to calculate the output of each neuron and value of loss function
- 2 with **backward pass** go back through NN to calculate gradients for all weights
- 3 update weights with their gradients
- 4 repeat until convergence

*one iteration (**epoch**) = forward and backward pass

Summary

Summary — o Socratic method

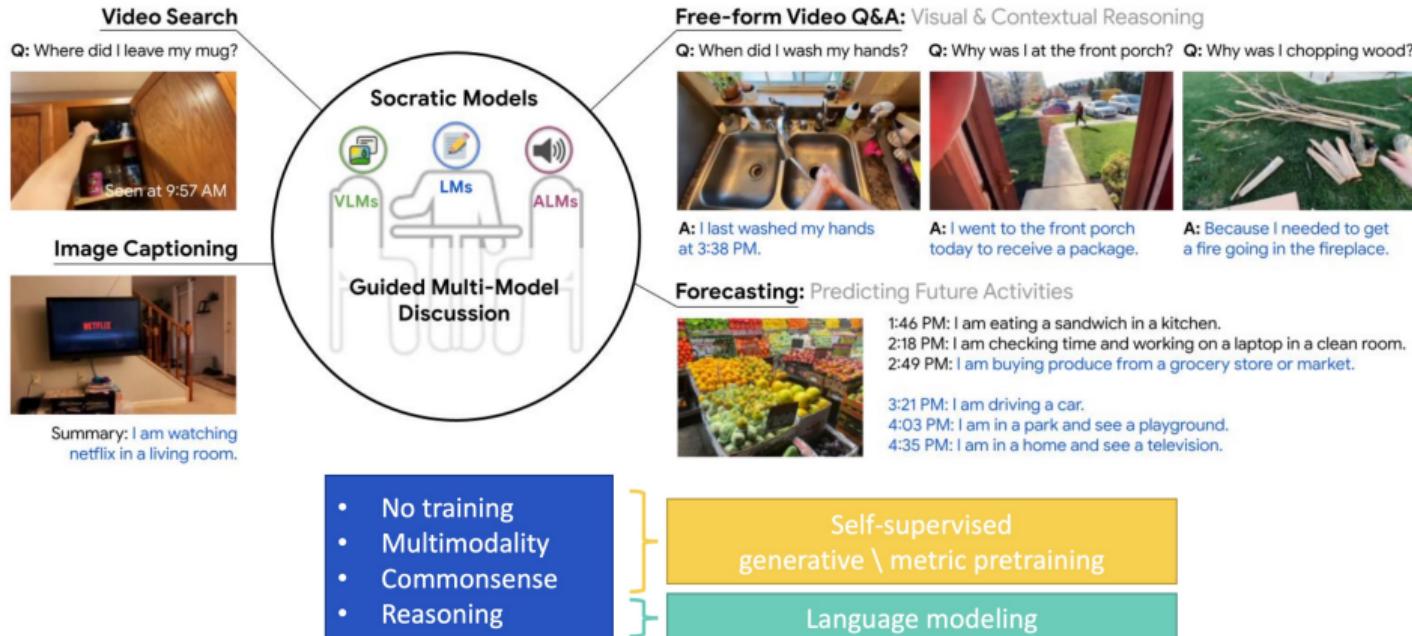
From Wikipedia, the free encyclopedia

The **Socratic method** (also known as **method of Elenchus** or **Socratic debate**) is a form of [argumentative dialogue](#) between individuals, based on asking and answering questions.

In [Plato's](#) dialogue "[Theaetetus](#)", [Socrates](#) describes his method as a form of "midwifery" because it is employed to help his interlocutors develop their understanding in a way analogous to a child developing in the womb. The Socratic method begins with commonly held beliefs and scrutinizes them by way of questioning to determine their internal consistency and their coherence with other beliefs and so to bring everyone closer to the truth.

In modified forms, it is employed today in a variety of pedagogical contexts.

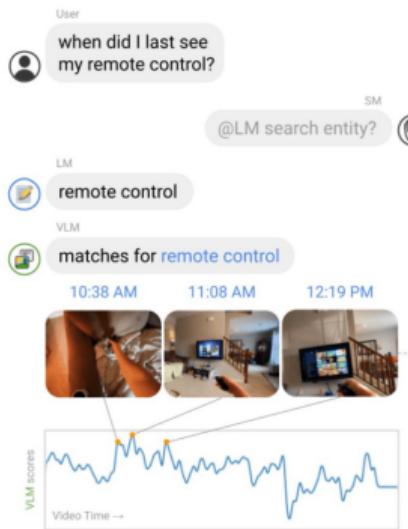
Summary —○ ML today



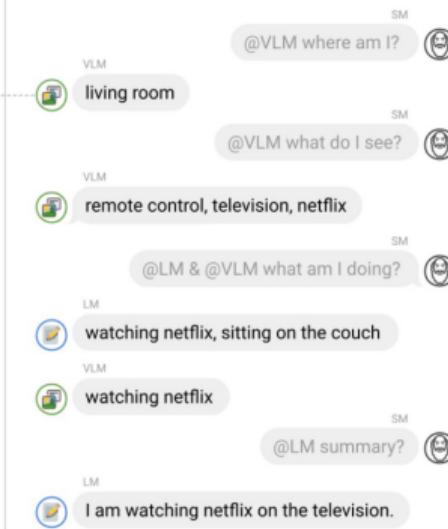
Zeng, Andy, et al. "Socratic models: Composing zero-shot multimodal reasoning with language." *arXiv preprint arXiv:2204.00598* (2022).

Summary ——○ ML today

Socratic Question to Video Search



Socratic Egocentric Image Summaries



Socratic Video Q&A with Linguistic World-State History

Generated Linguistic World-State History from Video

10:38 AM: Places: living room. Objects: sofa bed, loveseat, coffee table.
Activities: watching TV. I was watching TV in a living room.
11:08 AM: Places: living room. Objects: remote control, television, netflix.
Activities: watching netflix. I was watching netflix on the television.
12:19 PM: Places: television room. Objects: television, remote control, netflix. Activities: watching netflix. I was watching netflix on a television.

User
where did I leave my remote control?

LM
I left my remote control in the living room.

SM
@LM explain? (User)

LM
I was watching TV in the living room and I needed it to change the channel.

Zeng, Andy, et al. "Socratic models: Composing zero-shot multimodal reasoning with language." *arXiv preprint arXiv:2204.00598* (2022).

Summary —○ ChatGPT3 problems

ChatGPT3 on fractions :

Me: what is larger, two fourths or one half?

ChatGPT :

One half is larger than two fourths.

Two fourths can be written as $2/4$, which is equal to $1/2$.
Therefore, one half is equal to two fourths.

Me: didn't you just contradict yourself?

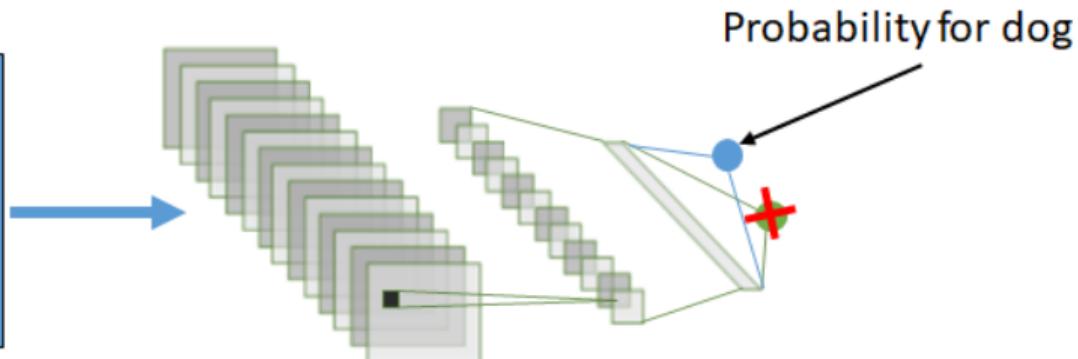
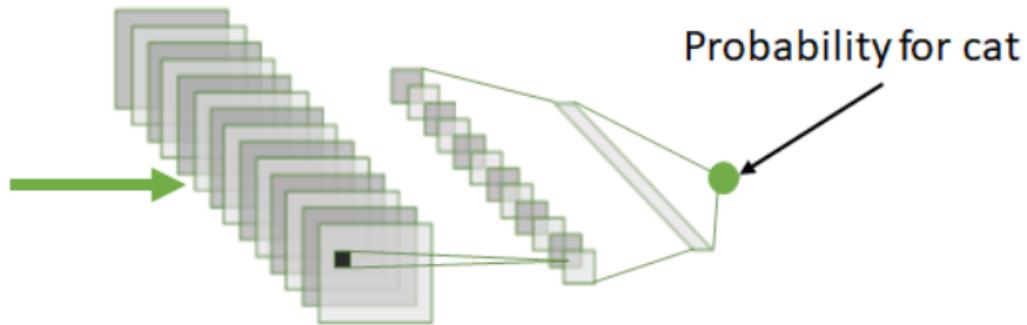
ChatGPT: I apologize, I made a mistake in my previous answer.
Two fourths ($2/4$) is smaller than one half ($1/2$).

Me : Are you sure?

ChatGPT: Yes, I am sure. Two fourths ($2/4$) is equal to $1/2$. Since $1/2$ is larger than $2/4$, it follows that one half is larger than two fourths.



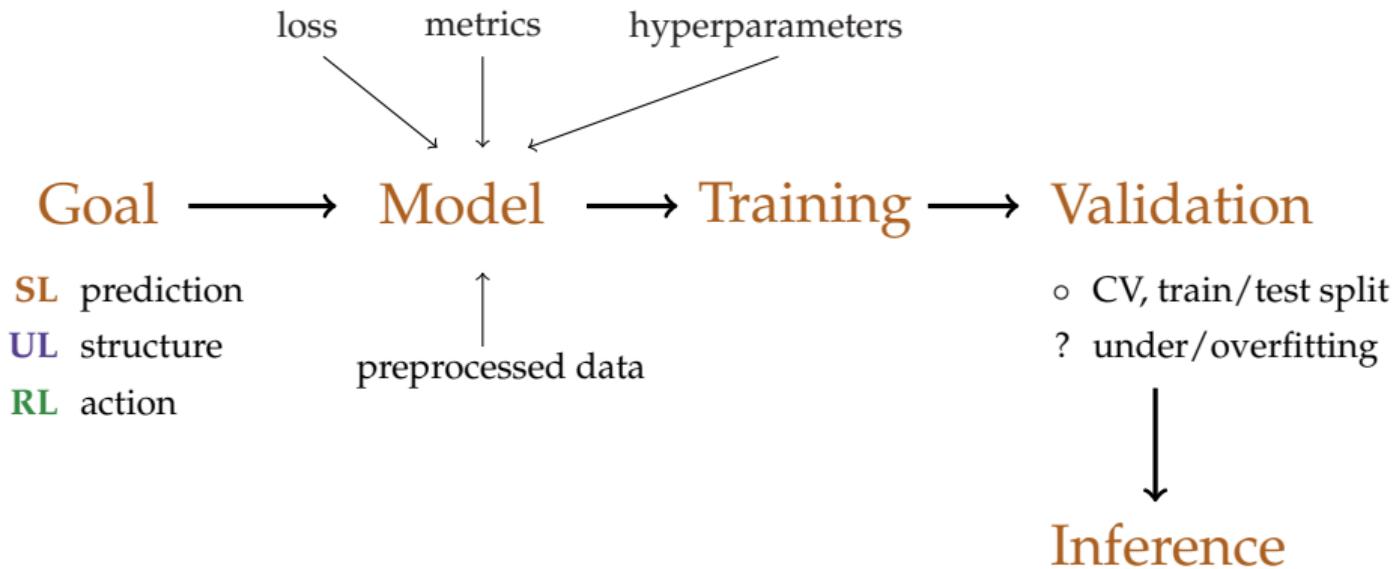
Summary —○ Transfer learning



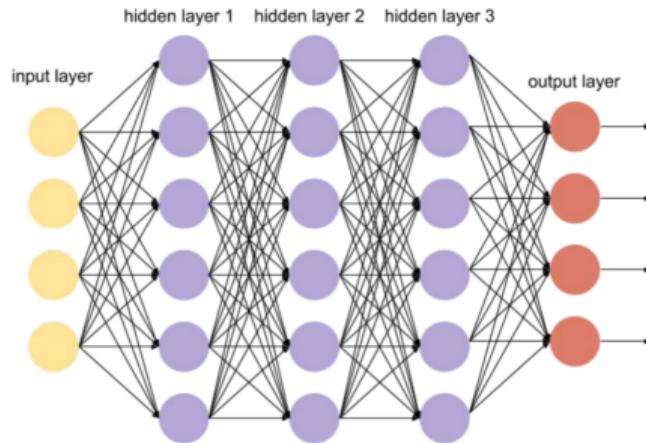
Backup slides

Backup slides

—○ what is ML pipeline?



Backup slides —○ NN formula



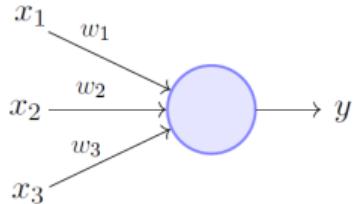
$$h_t = f(W h_{t-1} + b)$$

$$a(x) = f_3(W_3 f_2(W_2 f_1(W_1 f_0(W_0 x + b_0) + b_1) + b_2) + b_3)$$



Backup slides

—○ calculating weights: slide 1



Perceptron Model (Minsky-Papert in 1969)

Source

$$Q(y_{model}, y_{target}) = Q(y(x, w, b), y_{target})$$

$$out = y = \sigma(sum) = \sigma\left(\sum_{i=1}^3 (x_i \cdot w_i) + b\right)$$

$$\frac{\partial Q}{\partial w_i} = \frac{\partial Q}{\partial y} \cdot \frac{\partial y}{\partial \sigma} \cdot \frac{\partial \sigma}{\partial sum} \cdot \frac{\partial sum}{\partial w_i} = \frac{\partial Q}{\partial y} \cdot \mathbf{1} \cdot \frac{\partial \sigma}{\partial sum} \cdot \frac{\partial sum}{\partial w_i}$$

$$\frac{\partial \sigma}{\partial sum} = \sigma(sum) \cdot (1 - \sigma(sum))$$

Backup slides —○ calculating weights: slide 2

$$Q(y(x, w, b), y_{target})$$

$$Q = (y_{target} - y(x_1, w_1, b))^2$$

$$out = y = (x \cdot w) + b$$

$$\frac{\partial Q}{\partial w_i} = \frac{\partial Q}{\partial y} \cdot \frac{\partial y}{\partial w_i}$$

Input: $x = 1$, $w = 0.1$ and $b = 1$

$y_{target} = 2$ and learning rate: $\eta = 0.1$

Backup slides —○ calculating weights: slide 2

$$\begin{aligned}Q &= Q(y(x, w, b), y_{target}) \\Q &= (y_{target} - y(x_1, w_1, b))^2 \\out &= y = (x \cdot w) + b \\ \frac{\partial Q}{\partial w_i} &= \frac{\partial Q}{\partial y} \cdot \frac{\partial y}{\partial w_i}\end{aligned}$$

Input: $x = 1$, $w = 0.1$ and $b = 1$

$y_{target} = 2$ and learning rate: $\eta = 0.1$

How to find w_{new} and b_{new} ?

$$\begin{aligned}\frac{\partial Q}{\partial y} &= -2 \cdot (y_{target} - y) \\\frac{\partial Q}{\partial w} &= \frac{\partial Q}{\partial y} \cdot \frac{\partial y}{\partial w} = -2 \cdot x \cdot (y_{target} - y) \\\frac{\partial Q}{\partial b} &= \frac{\partial Q}{\partial y} \cdot \frac{\partial y}{\partial b} = -2 \cdot (y_{target} - y) \\[w_{new}, b_{new}] &\Rightarrow \theta_{i+1} = \theta_i - \eta \cdot \frac{\partial Q(\theta_i)}{\partial \theta_i}\end{aligned}$$

Backup slides

—○ calculating weights: slide 2

$$Q(y(x, w, b), y_{target})$$

$$Q = (y_{target} - y(x_1, w_1, b))^2$$

$$out = y = (x \cdot w) + b$$

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$$\frac{\partial Q}{\partial b} = \frac{\partial Q}{\partial y} \cdot \frac{\partial y}{\partial b} = -2 \cdot (y_{target} - y)$$

$$[w_{new}, b_{new}] \Rightarrow \theta_{i+1} = \theta_i - \eta \cdot \frac{\partial Q(\theta_i)}{\partial \theta_i}$$

y	Q	$\frac{\partial Q}{\partial y}$	$\frac{\partial Q}{\partial w}$	$\frac{\partial Q}{\partial b}$	w_{new}	b_{new}
1.1	0.81	-1.8	-1.8	-1.8	0.28	1.18

Backup slides

—○ human brain

