

MRL 2020 - Day 9 - Part 1

How to train your neural network

Organizers











+ info: http://bit.ly/upcrl-2020

https://telecombcn-dl.github.io/mrl-2020/



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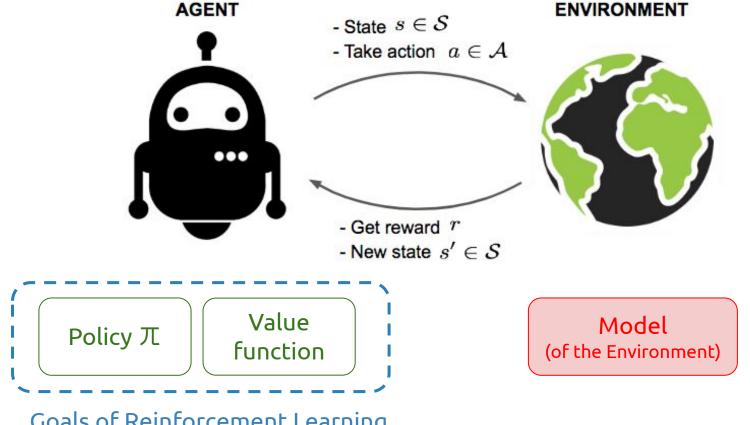
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Outline

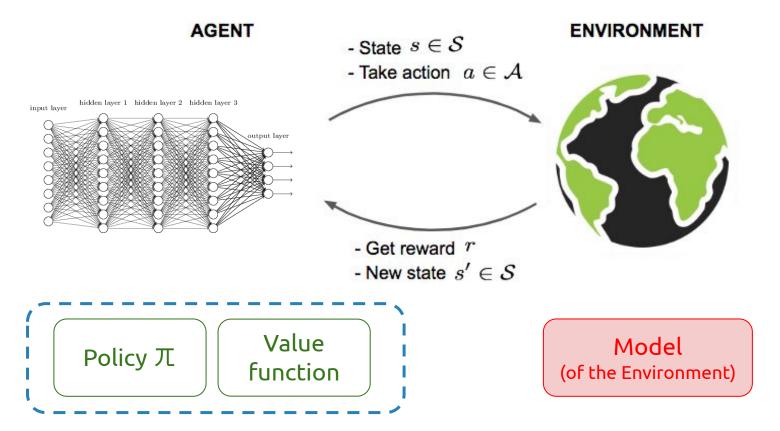
- 1. RL with Neural Networks
- 2. Loss functions
- 3. Backpropagation
- 4. Optimizers

Reinforcement Learning (with extrinsic reward)



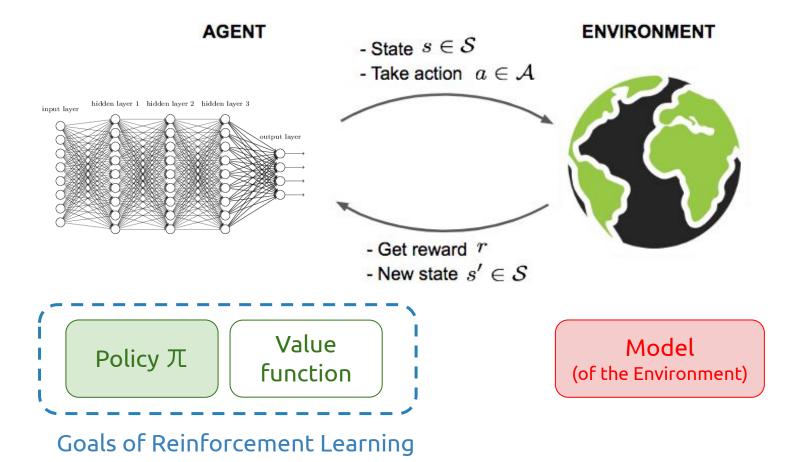
Goals of Reinforcement Learning

Reinforcement Learning with Neural Networks (NN)



Goals of Reinforcement Learning

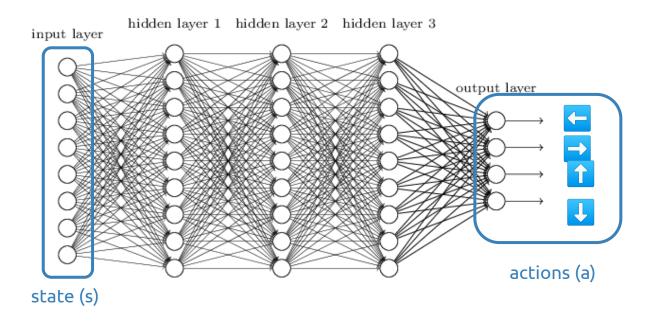
Policy-based RL with Neural Networks (NN)



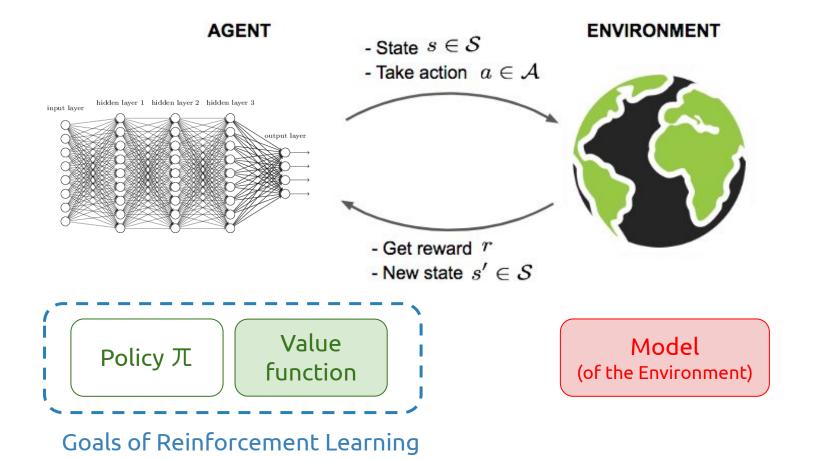
Policy-based RL with Neural Networks (NN)

The <u>Policy</u> π is a function S \rightarrow A that specifies which action to take in each state:

A Multi-Layer Perceptron (MLP) can implement a <u>classifier</u> to predict the distribution of actions given a state.



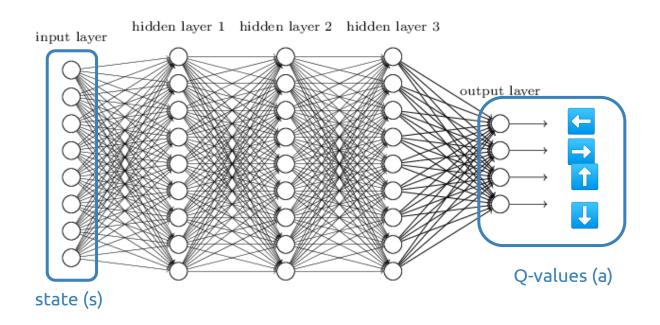
Value-based RL with Neural Networks (NN)



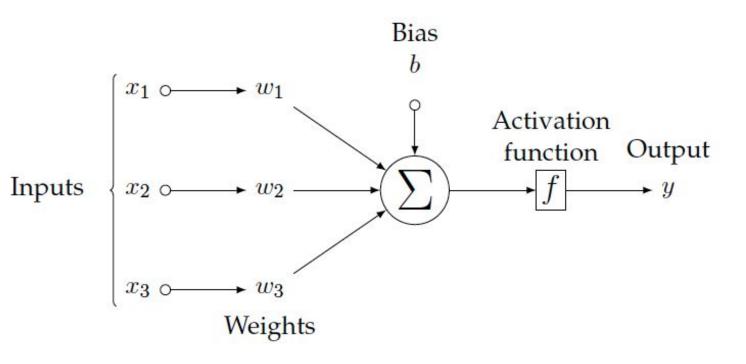
Value-based RL with Neural Networks (NN)

The <u>action-value Q_{π} (s,a)</u> function is the expected return for taking action a when being in state s.

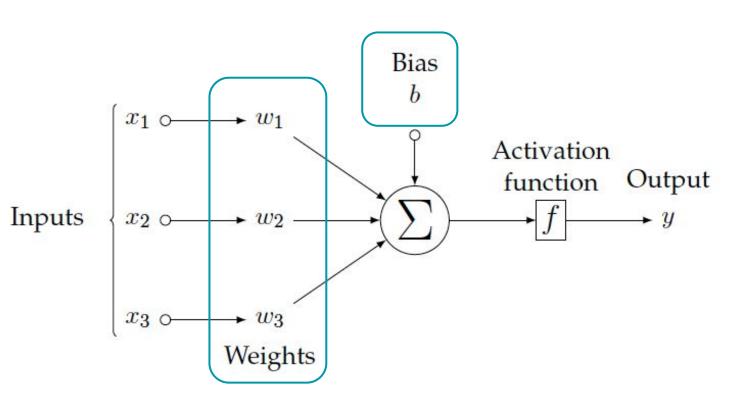
A Multi-Layer Perceptron (MLP) can implement a <u>regressor</u> to predict $Q_{\pi}(s,a)$.



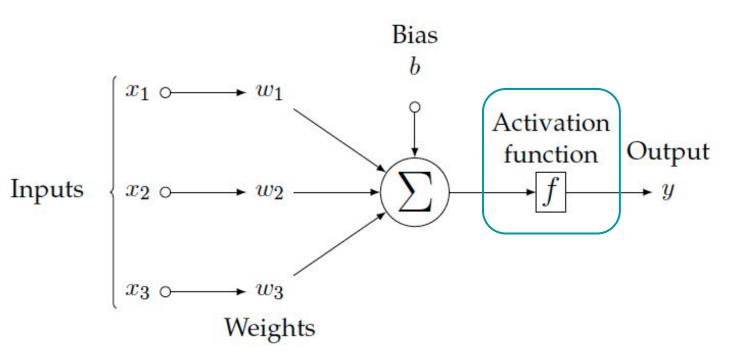
Which components of the neurons must be estimated during training?



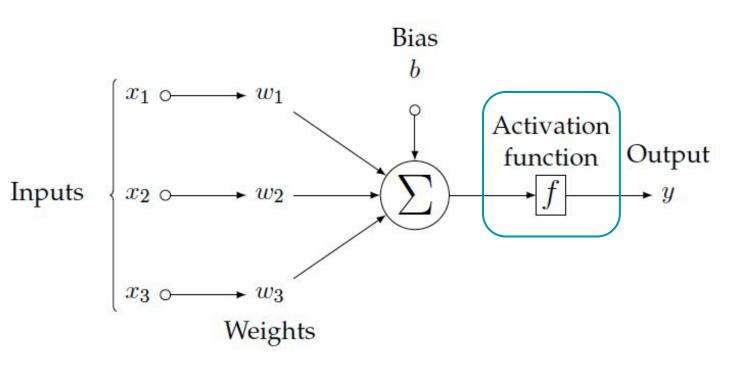
The weights (w_i) and bias (b) must be estimated during training.



The **activation function (f)** is a design choice.



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Activation functions:

• They act as a threshold

Desirable properties

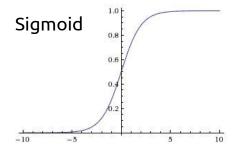
- Mostly smooth, continuous, differentiable
- Fairly linear

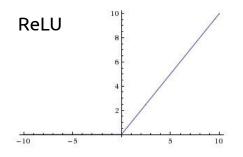
Common nonlinearities

- Sigmoid
- Tanh
- ReLU = max(0, x)

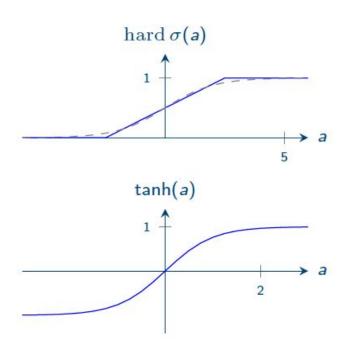
Why do we need them?

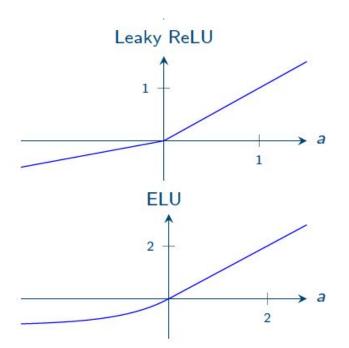
If we only use linear layers we are only able to learn linear transformations of our input.





Other popular activation functions:





When each node in each layer is a linear combination of all inputs from the previous layer then the network is called a multilayer perceptron (MLP)

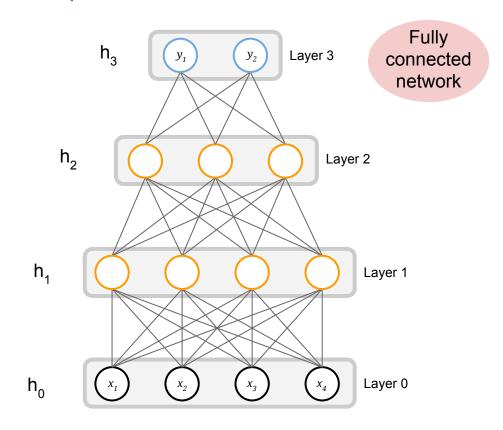
Weights can be organized into matrices.

Forward pass computes

$$\mathbf{h}_0 = \mathbf{x}$$

$$\mathbf{h}^{(t)} = g(W^{(t)}\mathbf{h}^{(t-1)} + \mathbf{b}^{(t)})$$

$$f(\mathbf{x}) = \mathbf{h}^{(L)}$$



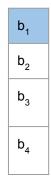
Slide: Kevin McGuinness (DCU)

 W_1

W ₁₁	W ₁₂	w ₁₃	W ₁₄
W ₂₁	W ₂₂	W ₂₃	W ₂₄
W ₃₁	W ₃₂	W ₃₃	W ₃₄
W ₄₁	W ₄₂	W ₄₃	W ₄₄

 h_0

 b_1

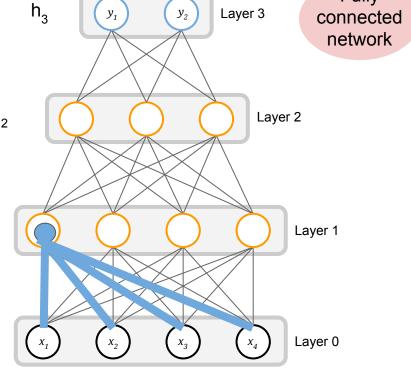


 $h_{11} = g(wx + b)$

 h_2

h₁

 h_0



Forward pass computes

$$\mathbf{h}_0 = \mathbf{x}$$

$$\mathbf{h}^{(t)} = g(W^{(t)}\mathbf{h}^{(t-1)} + \mathbf{b}^{(t)})$$

$$f(\mathbf{x}) = \mathbf{h}^{(L)}$$

Slide: Kevin McGuinness (DCU)

Fully

 W_1

W ₁₁	W ₁₂	w ₁₃	W ₁₄
W ₂₁	W ₂₂	W ₂₃	W ₂₄
W ₃₁	W ₃₂	W ₃₃	w ₃₄
W ₄₁	W ₄₂	W ₄₃	W ₄₄

 h_0

 b_1

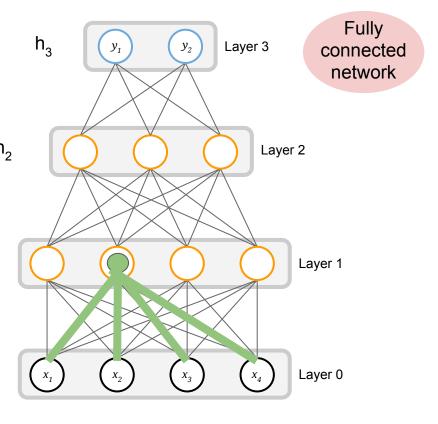
b₁
b₂
b₃
b₄

 $h_{11} = g(wx + b)$

 $h_{12} = g(wx + b)h_2$

 h_1

 h_0



Forward pass computes

$$\mathbf{h}_0 = \mathbf{x}$$

$$\mathbf{h}^{(t)} = g(W^{(t)}\mathbf{h}^{(t-1)} + \mathbf{b}^{(t)})$$

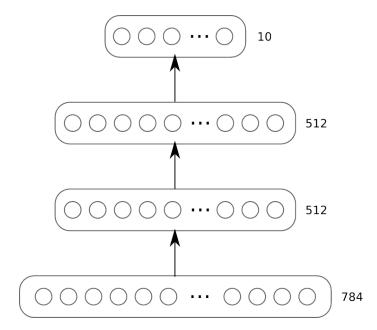
$$f(\mathbf{x}) = \mathbf{h}^{(L)}$$

Slide: Kevin McGuinness (DCU)

How many parameters contains the following MLP?

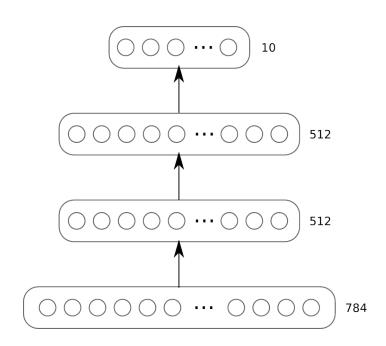
Model

- 3 layer neural network (2 hidden layers)
- Tanh units (activation function)
- 512-512-10



How many parameters contains the following MLP?

Layer	#Weights	#Biases	Total
1	784 x 512	512	401,920
2	512 x 512	512	262,656
3	512 x 10	10	5,130
			669,706

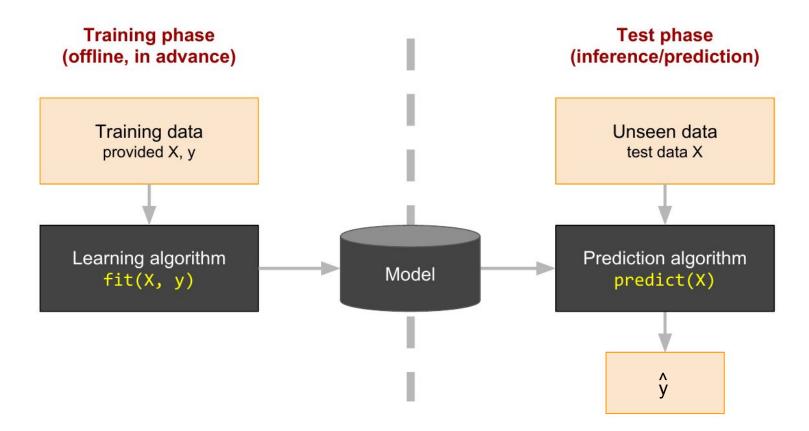




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Black box abstraction of supervised learning



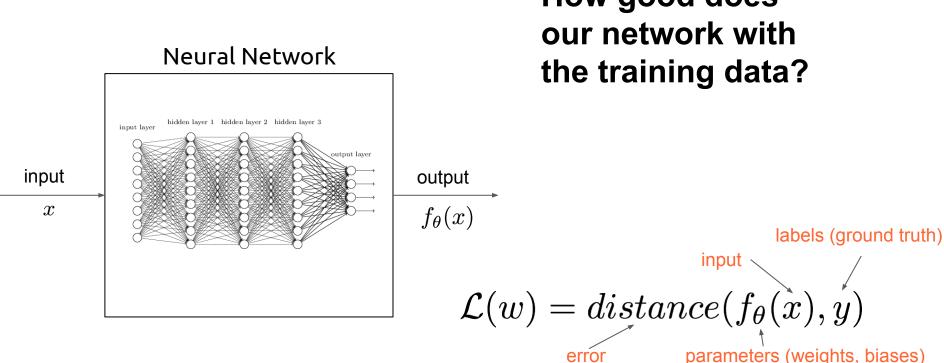
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loss function

= cost function

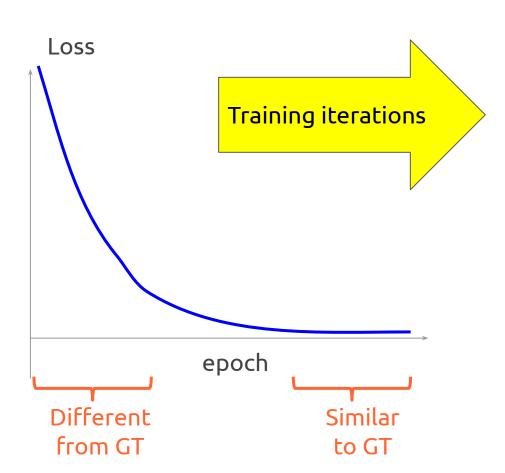
= objective function

= error function



How good does

The Loss value should decrease when the more the NN output matches the ground truth (GT).



Regression: the network predicts continuous, numeric variables

• Example: Price of a house

$$y = \mathbf{w}^{T} \cdot \mathbf{x} + b = w1 \cdot x1 + w2 \cdot x2 + w3 \cdot x3 + ... + wM \cdot xM + b$$

Which loss function would you choose for this problem?

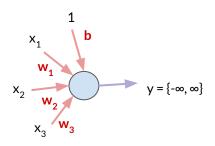


The **loss function** assesses the performance of our model by comparing its predictions (\hat{y}) to an expected value (y), typically coming from annotations.

Example: the predicted price (ŷ) and one actually paid (y) could be compared with the Euclidean distance (also referred as L2 distance or Mean Square Error - MSE):

$$y = w_1 \cdot x_1 + w_2 \cdot x_2 + w_3 \cdot x_3 + b = \mathbf{w}^T \cdot \mathbf{x} + b$$



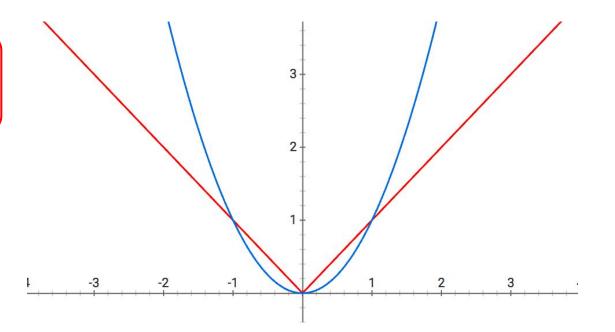


L1 Loss

$$\mathcal{L} = \frac{1}{n} \sum_{i=1}^{n} |y_i - f_{\theta}(x_i)|$$

L2 Loss

$$\mathcal{L} = \frac{1}{n} \sum_{i=1}^{n} (y_i - f_{\theta}(x_i))^2$$



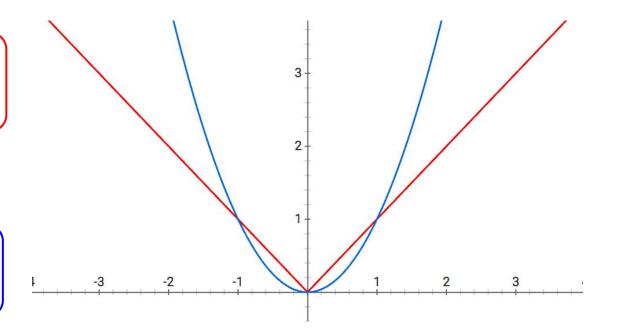
Which of these two losses is lighter to compute?

L1 Loss

$$\mathcal{L} = \frac{1}{n} \sum_{i=1}^{n} |y_i - f_{\theta}(x_i)|$$

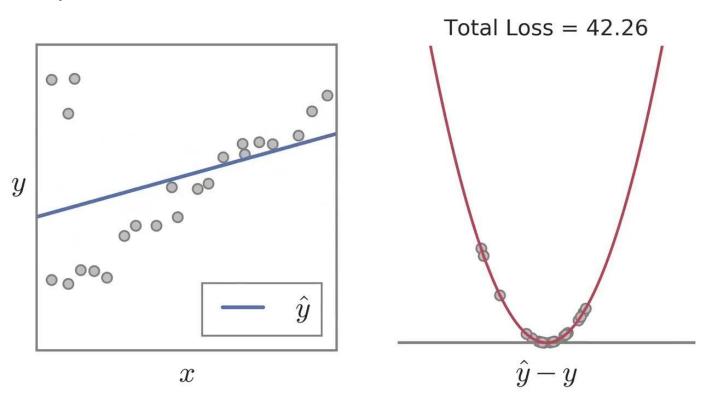
L2 Loss

$$\mathcal{L} = \frac{1}{n} \sum_{i=1}^{n} (y_i - f_{\theta}(x_i))^2$$

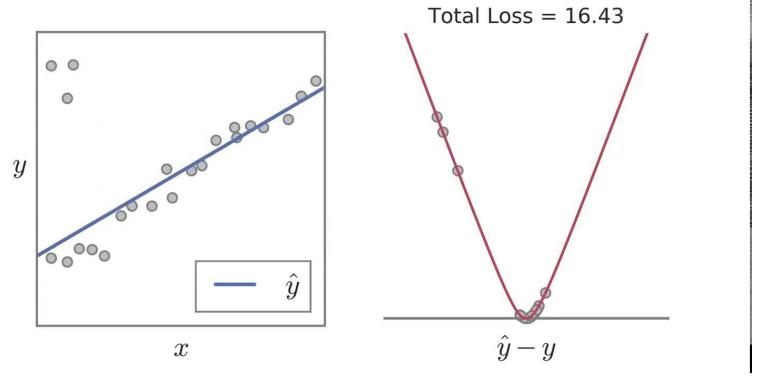


Which of these two losses is more sensitive to outliers ($|y_i-f_\theta(x_i)|>>1$)?

<u>L2 loss</u> has problems when there are outliers in the data



Pseudo-Huber loss (Charbonnier, Smooth L $_1$) is generally more resilient to outliers than L2.



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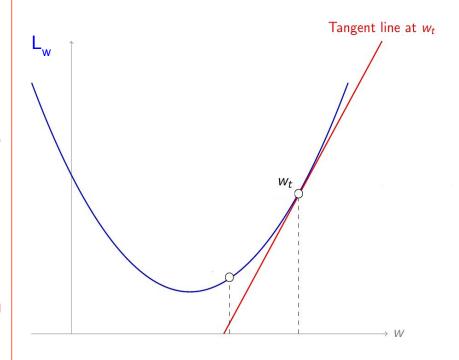
Backpropagation

<u>Discussion</u>: Consider the single parameter model...

$$\hat{y} = x \cdot w$$

...and that, given a pair (y, \hat{y}) , we would like to update the current w_t value to a new w_{t+1} based on the loss function L_w .

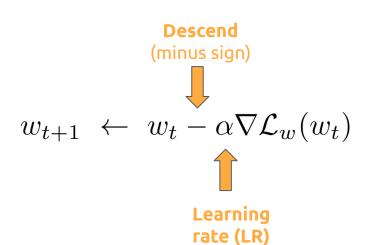
- (a) Would you increase or decrease w₊?
- (b) What operation could indicate which way to go?
- (c) How much would you increase or decrease w₊?

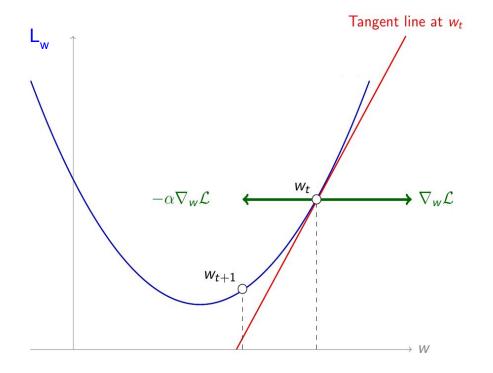


Gradient Descent (GD)

Motivation for this lecture:

if we had a way to estimate the gradient of the loss (∇ L) with respect to the parameter(s), we could use gradient descent to optimize them.



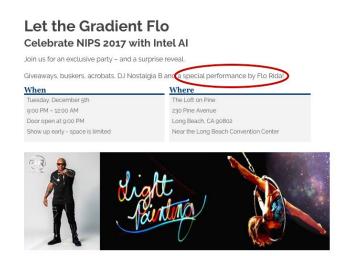


Gradient Descent (GD)

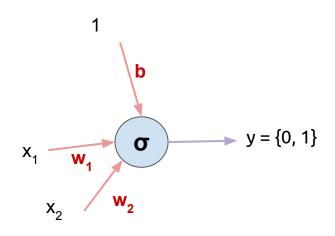
Backpropagation will allow us to compute the <u>gradients of the loss function</u> with respect to:

- all model parameters (w & b) final goal during training
- input/intermediate data visualization & interpretability purposes.

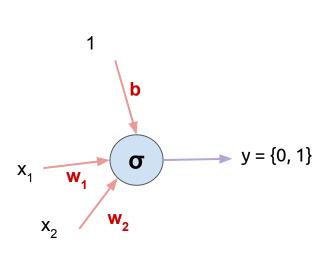
Gradients will "flow" from the output of the model towards the input ("back").

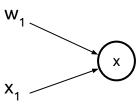


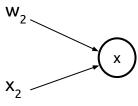


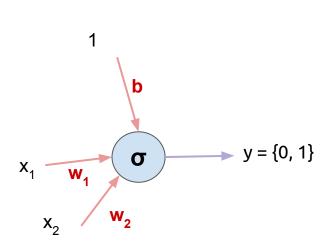


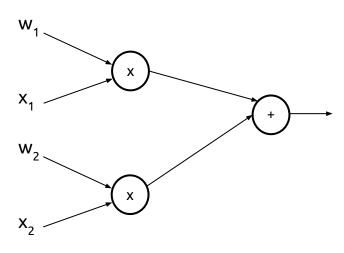
<u>Question</u>: What is the order of operations of this perceptron with a sigmoid activation?

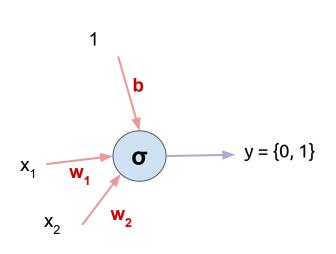


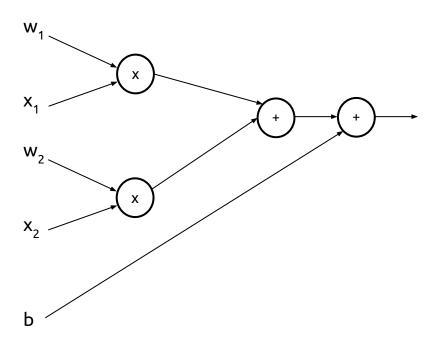


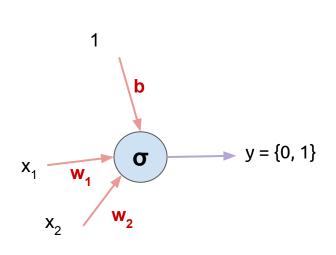


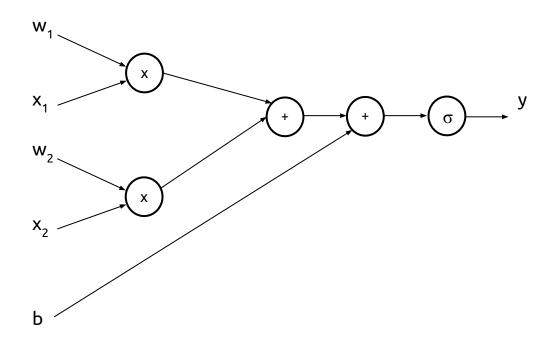


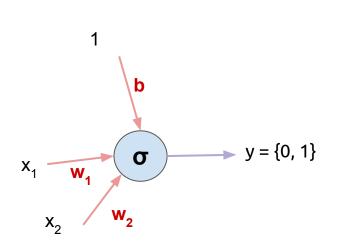


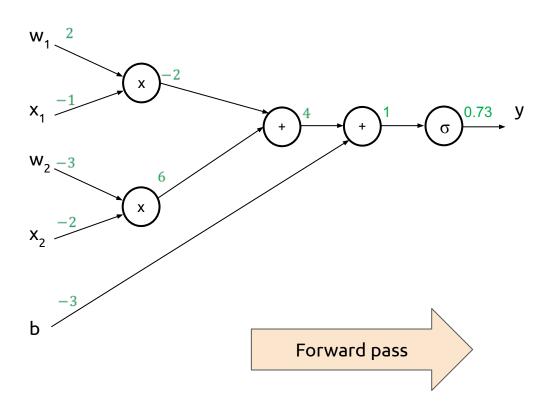










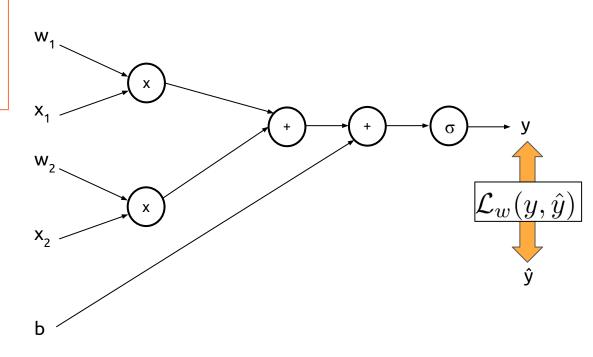


<u>Challenge</u>: How to compute the gradient of the loss function with respect to w_1 , w_2 or b?

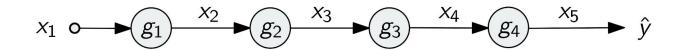
$$\frac{\partial \mathcal{L}(y, \hat{y})}{\partial w_1} = ?$$

$$\frac{\partial \mathcal{L}(y, \hat{y})}{\partial w_2} = ?$$

$$\frac{\partial \mathcal{L}(y, \hat{y})}{\partial b} = ?$$



$$\hat{y} = g_4(g_3(g_2(g_1(x_1))))$$

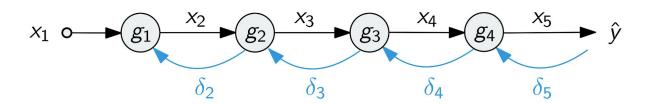


Decompose into steps (**forward propagation**):

$$x_2 = g_1(x_1)$$
 $x_3 = g_2(x_2)$
 $x_4 = g_3(x_3)$
 $\hat{y} = x_5 = g_4(x_4)$

Forward pass

$$\hat{y} = g_4(g_3(g_2(g_1(x_1))))$$

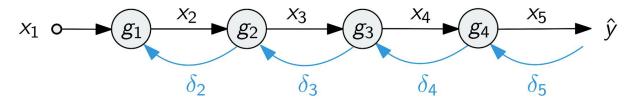


Want to find $\frac{\partial \hat{y}}{\partial x_1}$. Chain rule:

How does a variation ("difference") on the input affect the prediction?

$$\frac{\partial \hat{y}}{\partial x_1} = \frac{\partial \hat{y}}{\partial x_4} \frac{\partial x_4}{\partial x_3} \frac{\partial x_3}{\partial x_2} \frac{\partial x_2}{\partial x_1}$$

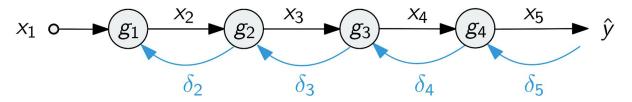
Backward pass



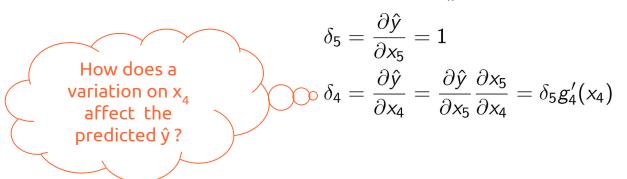
Decompose into steps again. Let $\delta_k = \frac{\partial \hat{y}}{\partial x_k}$. Backpropagation:

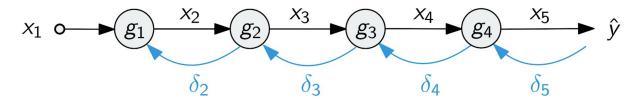
$$\delta_5 = \frac{\partial \hat{y}}{\partial x_5} = 1$$



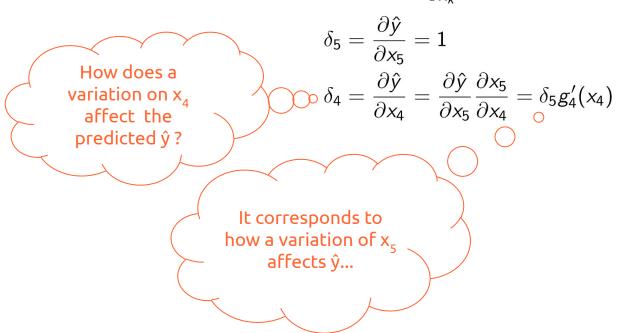


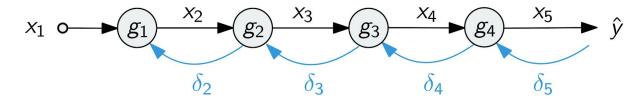
Decompose into steps again. Let $\delta_k = \frac{\partial \hat{y}}{\partial x_k}$. Backpropagation:



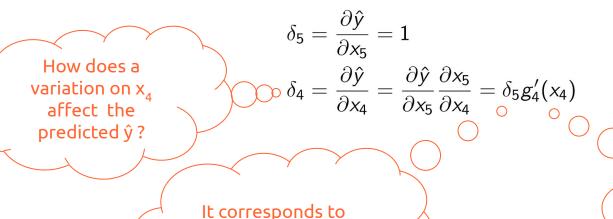


Decompose into steps again. Let $\delta_k = \frac{\partial \hat{y}}{\partial x_k}$. Backpropagation:





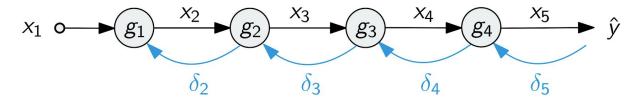
Decompose into steps again. Let $\delta_k = \frac{\partial \hat{y}}{\partial x_k}$. Backpropagation:



how a variation of x_{ϵ}

affects ŷ ...

...multiplied by how a variation near the input x_4 affects the output $g_4(x_4)$.



The same reasoning can be iteratively applied until reaching $\frac{\partial \hat{y}}{\partial x_1}$:

$$\delta_{5} = \frac{\partial \hat{y}}{\partial x_{5}} = 1$$

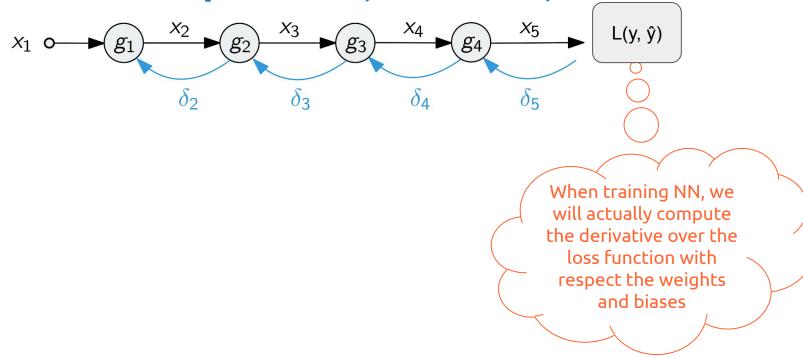
$$\delta_{4} = \frac{\partial \hat{y}}{\partial x_{4}} = \frac{\partial \hat{y}}{\partial x_{5}} \frac{\partial x_{5}}{\partial x_{4}} = \delta_{5} g_{4}'(x_{4})$$

$$\delta_{3} = \frac{\partial \hat{y}}{\partial x_{3}} = \frac{\partial \hat{y}}{\partial x_{4}} \frac{\partial x_{4}}{\partial x_{3}} = \delta_{4} g_{3}'(x_{3})$$

$$\delta_{2} = \frac{\partial \hat{y}}{\partial x_{2}} = \frac{\partial \hat{y}}{\partial x_{3}} \frac{\partial x_{3}}{\partial x_{2}} = \delta_{3} g_{2}'(x_{2})$$

$$\delta_{1} = \frac{\partial \hat{y}}{\partial x_{1}} = \frac{\partial \hat{y}}{\partial x_{2}} \frac{\partial x_{2}}{\partial x_{1}} = \delta_{2} g_{1}'(x_{1})$$

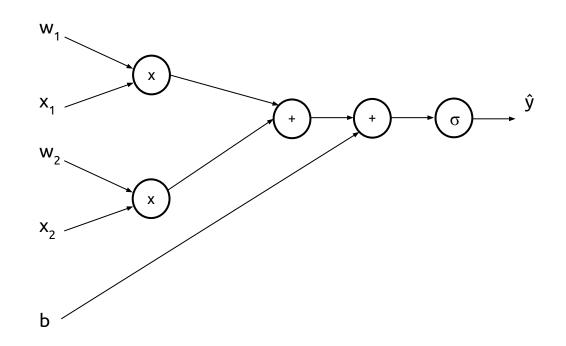
Backward pass



Backward pass

Question: What are the derivatives of the function involved in the computational graph of a perceptron?

- SUM (+) $\frac{\partial (a+b)}{\partial a}$
- PRODUCT (x) $\frac{\partial (a \cdot b)}{\partial a}$
- SIGMOID (σ) $\frac{\partial \sigma(x)}{\partial x}$



Gradient weights for sigmoid σ

$$\frac{\partial \sigma(x)}{\partial x} = \frac{\partial}{\partial x} \left(\frac{1}{1 + e^{-x}} \right) = \frac{-1}{(1 + e^{-x})^2} \frac{\partial (1 + e^{-x})}{\partial x} = \frac{-1}{(1 + e^{-x})^2} \frac{\partial (e^{-x})}{\partial x}$$

(*)
$$f(x) = \frac{g(x)}{h(x)}$$
 $f'(x) = \frac{g'(x)h(x) - g(x)h'(x)}{h^2}$

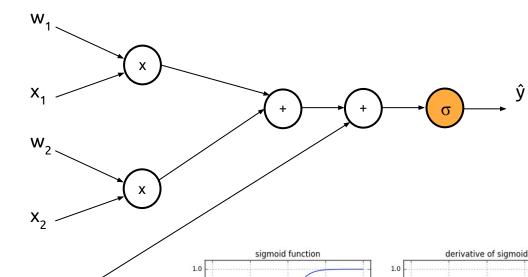
$$\frac{\partial \sigma(x)}{\partial x} = \frac{-1}{(1+e^{-x})^2}(-e^{-x}) = \frac{e^{-x}}{(1+e^{-x})^2}$$

...which can be re-arranged as...

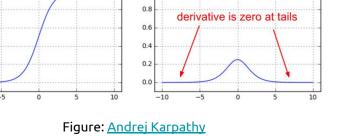
$$\frac{\partial \sigma(x)}{\partial x} = \frac{e^{-x}}{(1+e^{-x})^2} = \frac{e^{-x}}{(1+e^{-x})} \frac{1}{(1+e^{-x})}$$

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

$$\frac{\partial \sigma(x)}{\partial x} = (1 - \sigma(x)) \, \sigma(x) \quad {}^{\mathrm{b}}$$

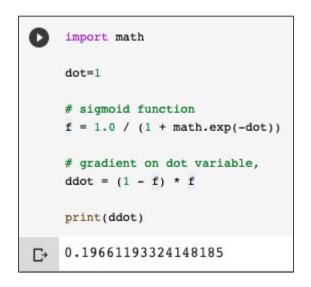


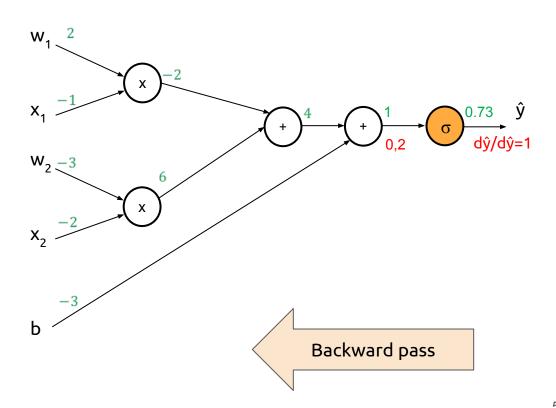
0.6



Even more details: Arunava, "Derivative of the Sigmoid function" (2018)

$$\frac{\partial \sigma(x)}{\partial x} = (1 - \sigma(x)) \, \sigma(x)$$

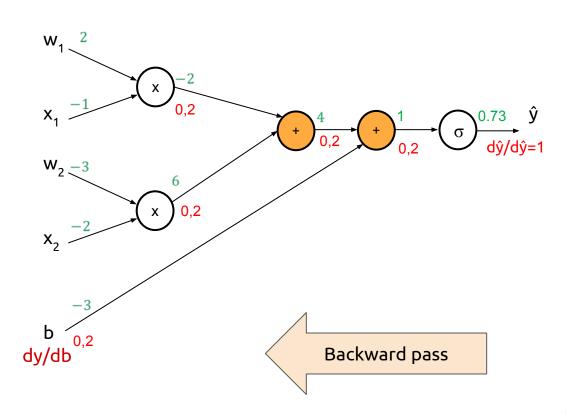




SUM

$$\frac{\partial(a+b)}{\partial a} = 1$$

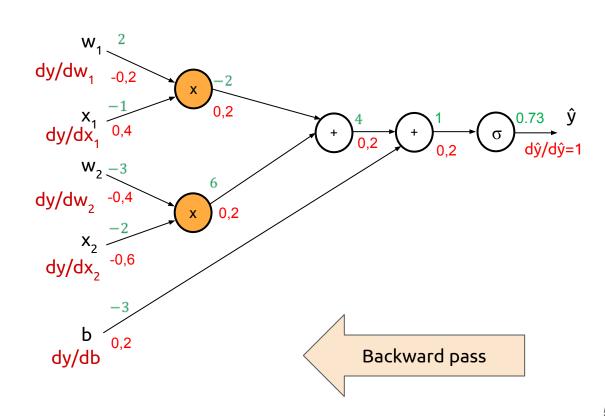
$$\frac{\partial(a+b)}{\partial b} = 1$$



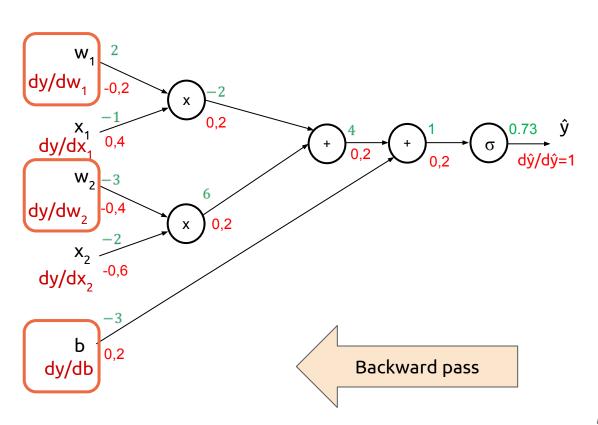
Product

$$\frac{\partial(a\cdot b)}{\partial a} = b$$

$$\frac{\partial(a\cdot b)}{\partial b} = a$$

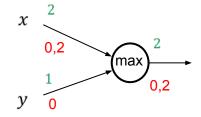


Normally, we will be interested only on the weights (w_i) and biases (b), not the inputs (x_i). The weights are the parameters to learn in our models.

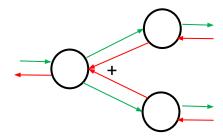


(bonus) Gradients weights for MAX & SPLIT

Max: Routes the gradient only to the higher input branch (not sensitive to the lower branches).



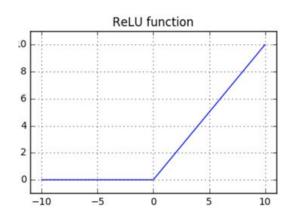
Split: Branches that split in the forward pass and merge in the backward pass, add gradients

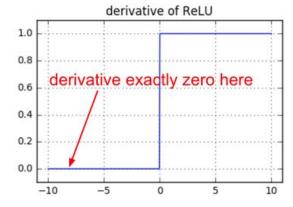


(bonus) Gradient weights for ReLU

$$ReLU(x) = \left\{ \begin{array}{ll} x & \text{if } x \ge 0 \\ 0 & \text{if } x < 0 \end{array} \right\}$$

$$\frac{\partial ReLU(x)}{\partial x} = u(x) = \left\{ \begin{array}{ll} 1 & \text{if } x > 0 \\ 0 & \text{if } x < 0 \end{array} \right\}$$

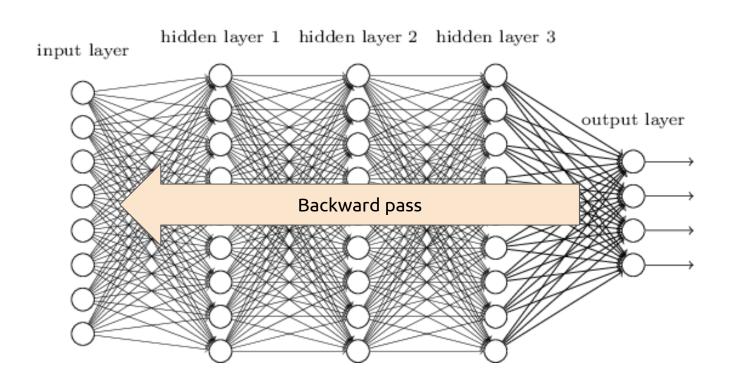




Figures: Andrei Karpathy

Backpropagation across layers

Gradients can flow across stacked layers of neurons to estimate their parameters.



Backpropagation & RL





For differentiable problems, there's backpropagation. For everything else, there's RL.

Tradueix el tuit

18:11 - 31 de gen. de 2019





En resposta a @gdb

Not quite right.

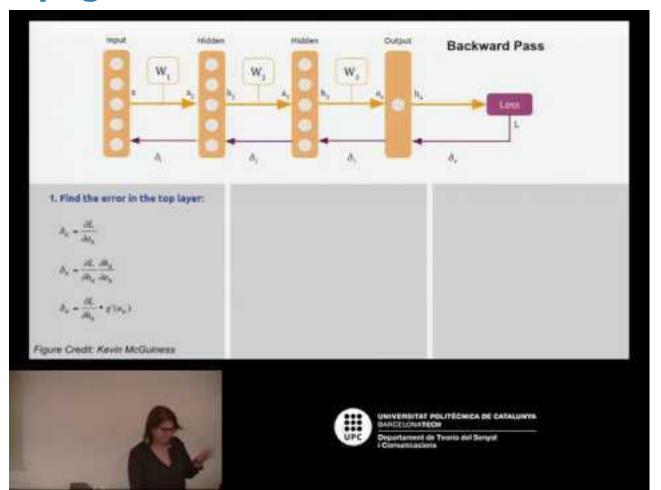
A more accurate statement would be "for everything else, there is gradient-free (zerothorder) optimization."

RL is when there is a sequential decision process and what you see depends on previous actions you took.

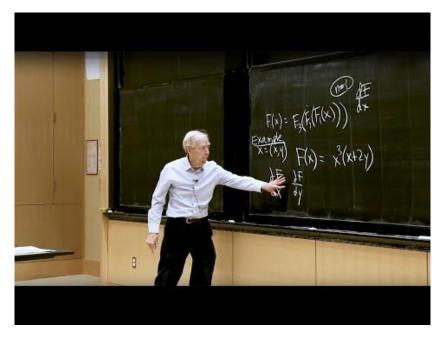
Tradueix el tuit

2:38 - 1 de febr. de 2019

Backpropagation: Learn more



Backpropagation: Learn more



Gilbert Strang, <u>"27. Backpropagation: Find Partial Derivatives"</u>. MIT 18.065 (2018)



Creative Commons, <u>"Yoshua Bengio Extra</u> <u>Footage 1: Brainstorm with students"</u> (2018)

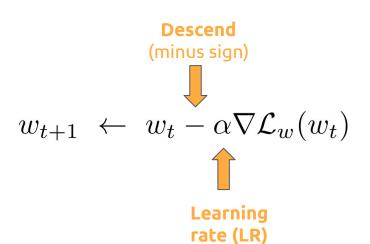
Outline

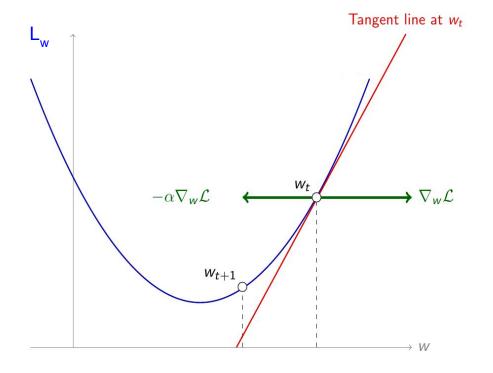
- 1. RL with Neural Networks
- 2. Loss functions
- 3. Backpropagation
- 4. Optimizers

Gradient Descent (GD)

Motivation for this lecture:

if we had a way to estimate the gradient of the loss (∇ L) with respect to the parameter(s), we could use gradient descent to optimize them.





Gradient descent (GD)

Computing the gradient for the full dataset at each step is slow

Especially if the dataset is large!

For most losses we care about, the total loss can be expressed as a sum (or average) of losses on the individual examples

$$\mathcal{L} = \frac{1}{N} \sum_{i=1}^{N} L(\mathbf{y}_i, \hat{\mathbf{y}}_i)$$

The gradient is the average of the gradients on individual examples

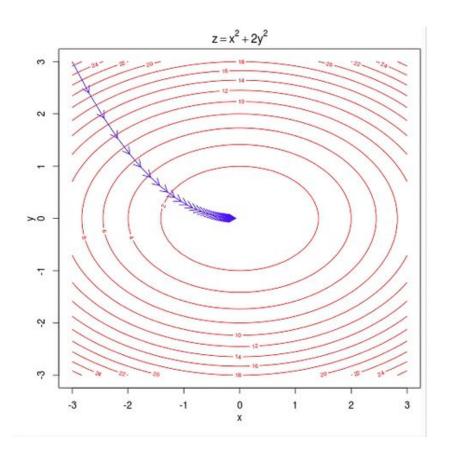
$$abla \mathcal{L} = rac{1}{N} \sum_{i=1}^{N}
abla L(\mathbf{y}_i, \hat{\mathbf{y}}_i)$$

Stochastic gradient descent (SGD)

SGD: estimate the gradient using a subset of the examples

- Pick a single random training example
- **Estimate** a (noisy) loss on this single training example (the *stochastic* gradient)
- Compute gradient wrt. this loss
- Take a step of gradient descent using the estimated loss

Stochastic gradient descent



Stochastic Gradient Descent (SGD)

SGD Advantages

- Very fast (only need to compute gradient on single example)
- Memory efficient (does not need the full dataset to compute gradient)
- Online (don't need full dataset at each step)

SGD Disadvantages

- Gradient is very noisy, may not always point in correct direction
- Convergence can be slower

In practice: Mini-batch SGD

- Estimate gradient on small batch of training examples (say 50)
- Known as mini-batch stochastic gradient descent

Vanilla mini-batch SGD

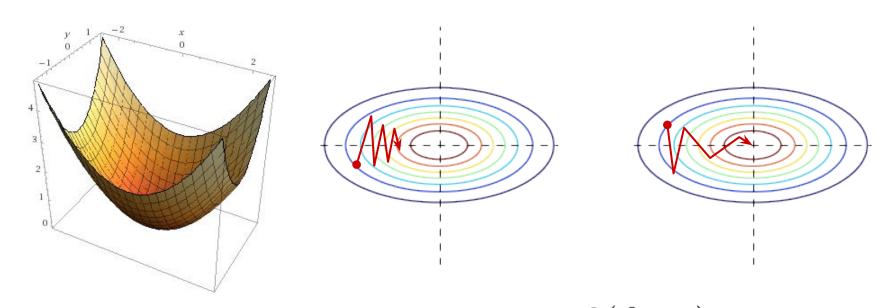
$$\theta_t = \theta_{t-1} - \alpha \nabla_{\theta} \mathcal{L}(\theta_{t-1})$$
Evaluated on a mini-batch

Momentum

Velocity
$$\longrightarrow v_t = \gamma v_{t-1} + \alpha \nabla_{\theta} \mathcal{L}(\theta_{t-1})$$

$$\theta_t = \theta_{t-1} - v_t \qquad \text{2x memory for parameters!}$$

Momentum



$$v_t = \gamma v_{t-1} + \alpha \nabla_{\theta} \mathcal{L}(\theta_{t-1})$$

$$\theta_t = \theta_{t-1} - v_t$$

2x memory for parameters!

Adagrad

<u>Adapts the learning rate</u> for each of the parameters based on sizes of previous updates.

- Scales updates to be larger for parameters that are updated less
- Scales updates to be smaller for parameters that are updated more

Store $\underline{\text{sum of squares}}$ of gradients so far in diagonal of matrix G_t

$$G_t = \sum_{i=0}^t \mathrm{diag}(
abla \mathcal{L}(heta)_i)^2$$
 Gradient of loss at timestep i

Update rule:
$$\theta_t = \theta_{t-1} - \alpha G_t^{-\frac{1}{2}} \nabla \mathcal{L}(\theta_{t-1})$$

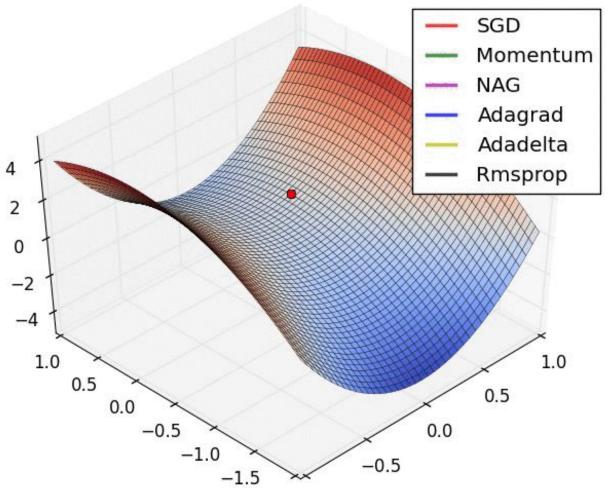
RMSProp

Modification of Adagrad to address aggressively decaying learning rate.

Instead of storing sum of squares of gradient over all time steps so far, use a **decayed moving average** of sum of squares of gradients

$$G_t = \gamma G_{t-1} + (1 - \gamma) \operatorname{diag}(\nabla \mathcal{L}(\theta))^2$$

Update rule:
$$\theta_t = \theta_{t-1} - \alpha G_t^{-\frac{1}{2}} \nabla \mathcal{L}(\theta_{t-1})$$



Adam

Combines momentum and RMSProp

Keep decaying average of both first-order moment of gradient (momentum) and second-order moment (like RMSProp)

First-order:
$$v_t = \gamma_1 v_{t-1} + (1 - \gamma_1) \nabla \mathcal{L}(\theta_{t-1})$$

Second-order:
$$G_t = \gamma_2 G_{t-1} + (1 - \gamma_2) \operatorname{diag}(\nabla \mathcal{L}(\theta))^2$$

Update rule:
$$\theta_t = \theta_{t-1} - \alpha G_t^{-\frac{1}{2}} v_t$$
 3x memory!

Summary

We need an algorithm to find **good weight configurations**.

This is an unconstrained continuous optimization problem.

We can use standard iterative optimization methods like gradient descent.

To use gradient descent, we need a way to find the **gradient of the loss with** respect to the parameters (weights and biases) of the network.

Error **backpropagation** is an efficient algorithm for finding these gradients.

Basically an application of the multivariate **chain rule** and **dynamic programming**.

In practice, computing the full gradient is expensive. Backpropagation is typically used with **stochastic gradient descent**.

Slide: Kevin McGuinness (DCU)

Outline

- 1. RL with Neural Networks
- 2. Loss functions
- 3. Backpropagation
- 4. Optimizers

Undergradese

What undergrads ask vs. what they're REALLY asking

"Is it going to be an open book exam?"

Translation: "I don't have to actually memorize anything, do I?"

"Hmm, what do you mean by that?"

> Translation: "What's the answer so we can all go home."

"Are you going to have office hours today?"

> Translation: "Can I do my homework in your office?"

"Can i get an extension?"

> Translation: "Can you re-arrange your life around mine?"

> > "Is grading going to be curved?"

W. PHDCOMICS. COM

Translation: "Can I do a mediocre job and still get an A?"

