Machine Learning Course
basic track

Introduction to Deep Learning

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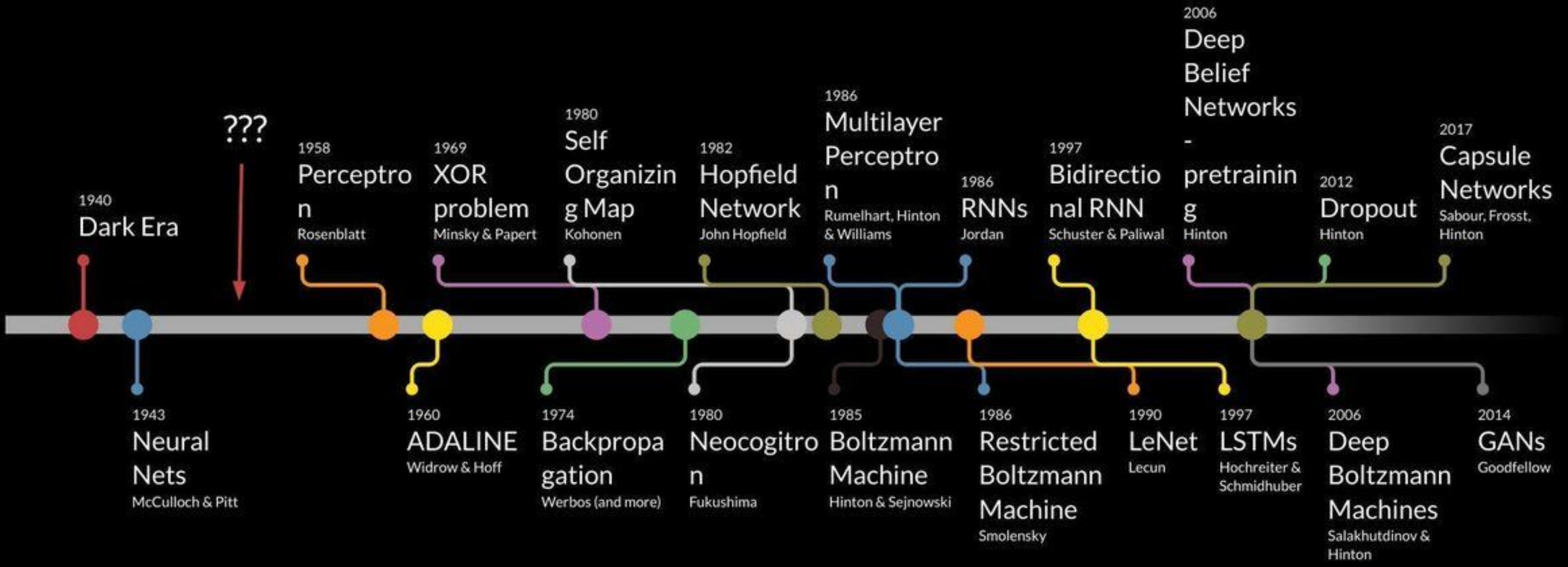
Moscow, Russia

Outline

1. Neural Networks in different areas. Historical overview.
2. Backpropagation.
3. Playground.
4. More on backpropagation.
5. Activation functions.
6. PyTorch practice

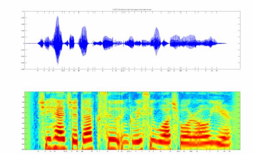
Deep Learning Timeline



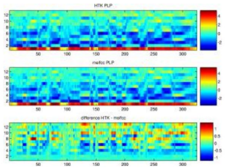
Made by Favio Vázquez

Real world problems

Audio Features

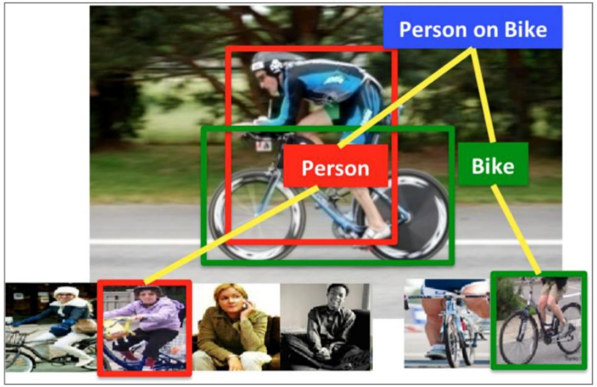


Spectrogram



MFCC

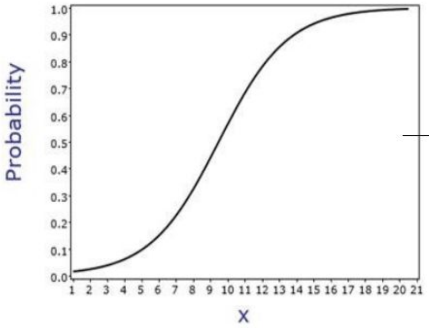
- Object detection
- Action classification
- Image captioning
- …



"man in black shirt is playing guitar."

Logistic regression

X $\longrightarrow$ Wx +b $\longrightarrow$

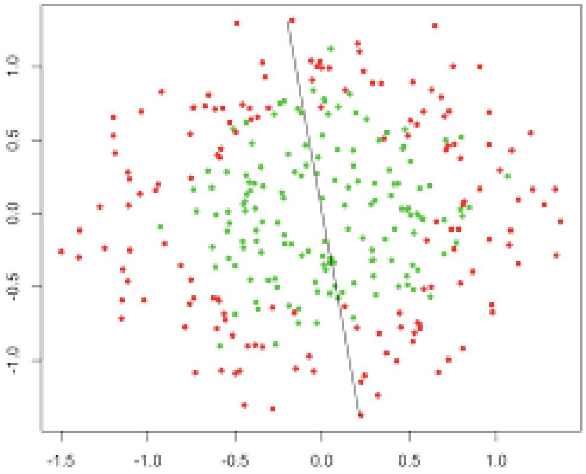


$\longrightarrow$ P(y)

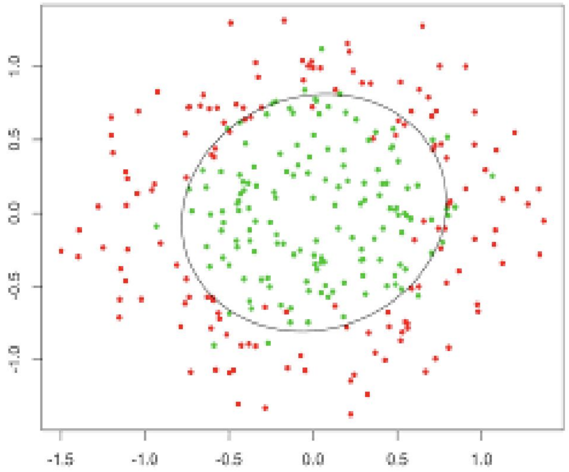
$$P(y|x) = \sigma(w \cdot x + b)$$

$$L = -\sum_i y_i \log P(y|x_i) + (1 - y_i) \log(1 - P(y|x_i))$$

Problem: nonlinear dependencies



What we have

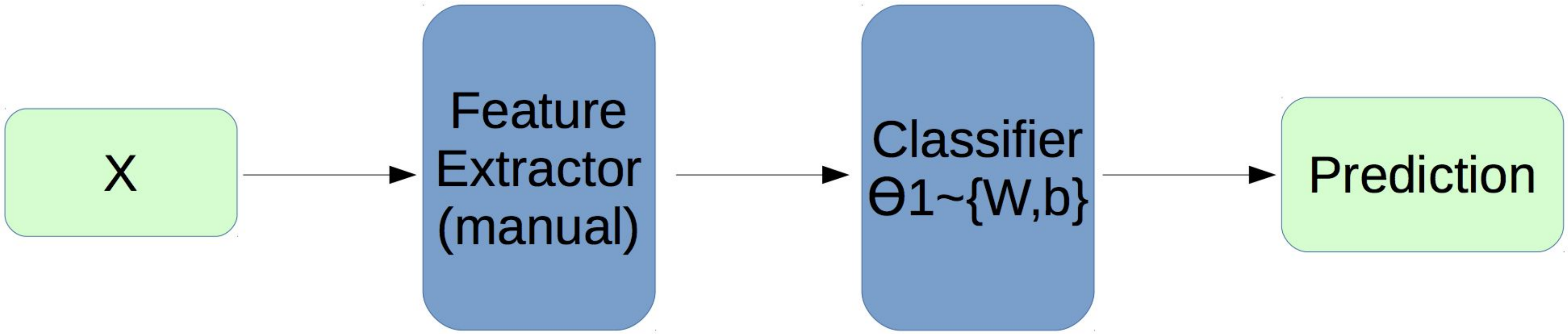


What we want

Logistic regression (generally, linear model) need feature engineering to show good results.

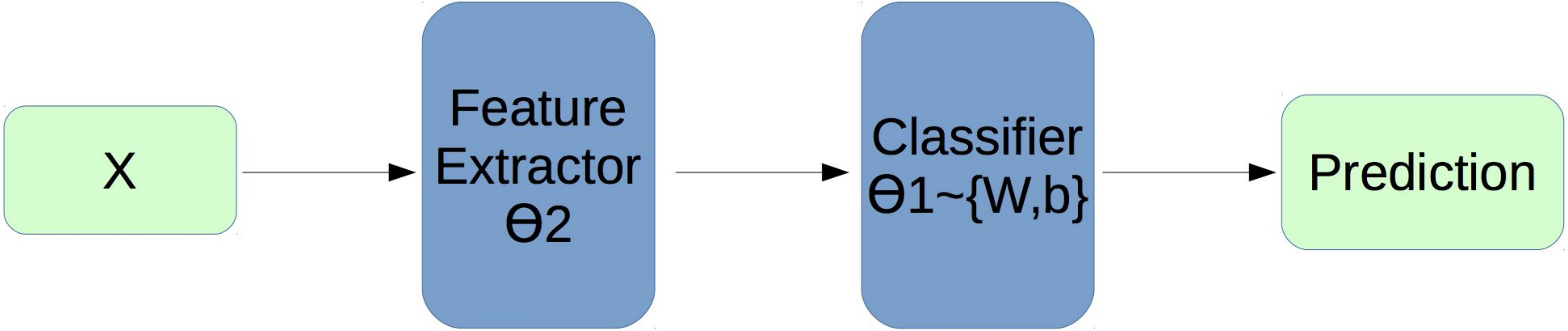
And feature engineering is an *art*.

Classic pipeline



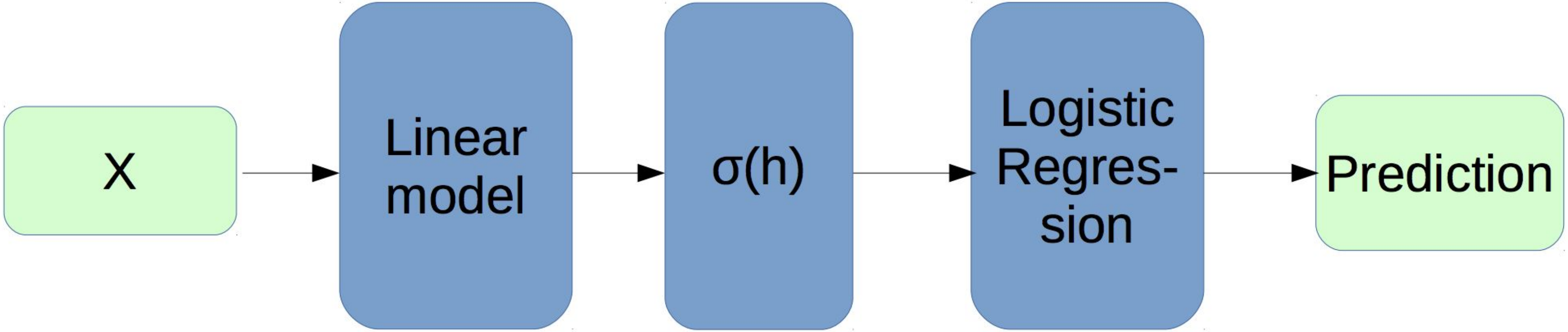
Handcrafted features, generated by experts.

NN pipeline



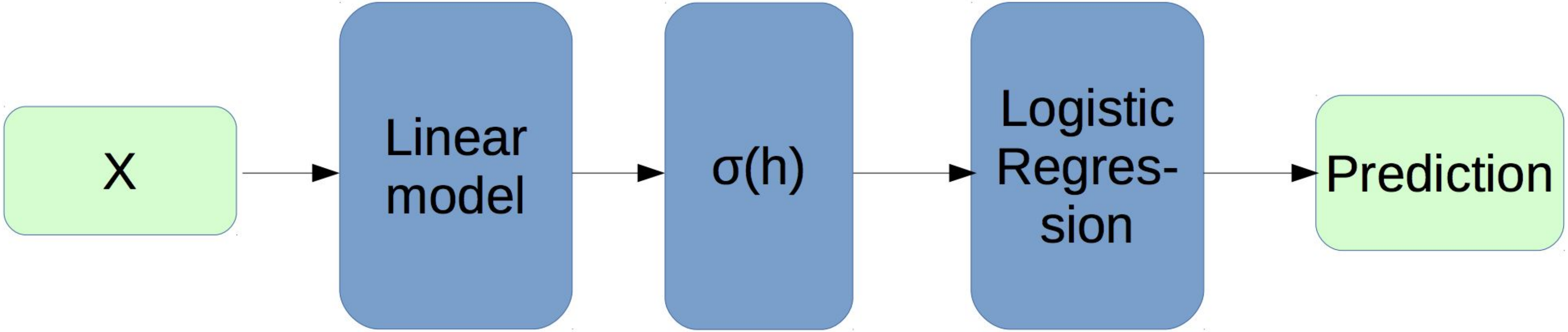
Automatically extracted features.

NN pipeline: example



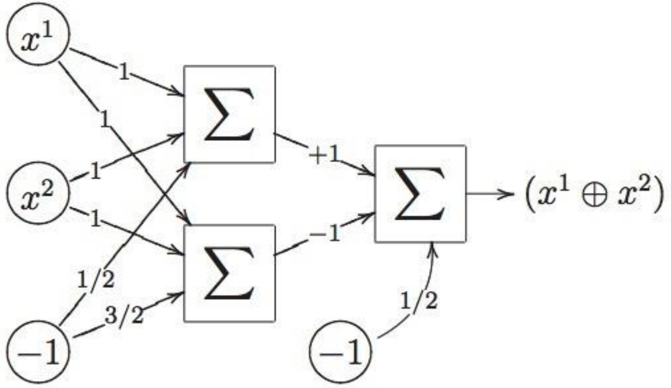
E.g. two logistic regressions one after another.

NN pipeline: example



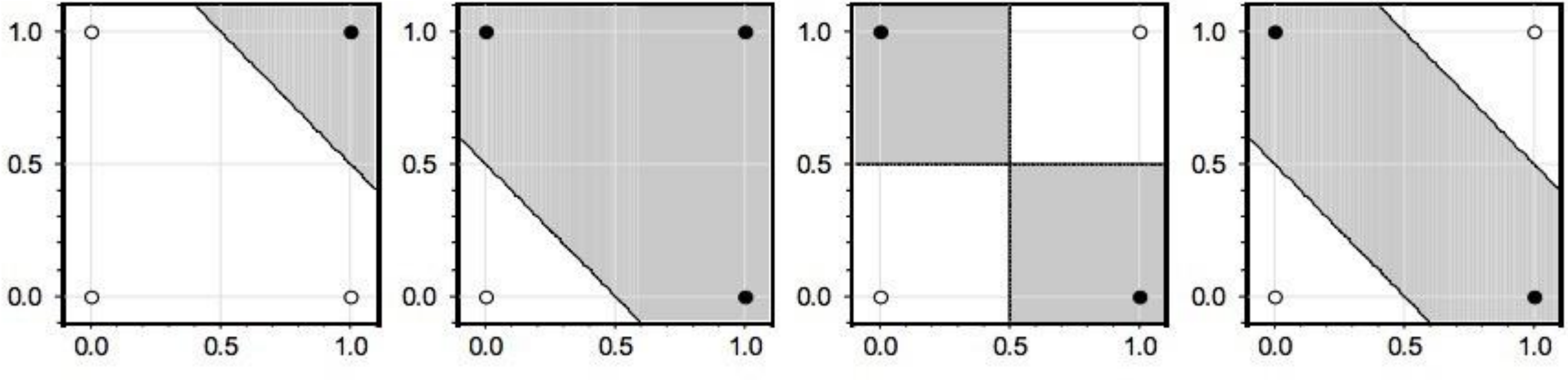
Actually, it’s a neural network.

XOR problem



This 2-layer NN (on the left) implements XOR with only x1 and x2 features.

1-layer NN also can succeed, but only with extra feature x1*x2.



AND OR XOR(with x1*x2) XOR

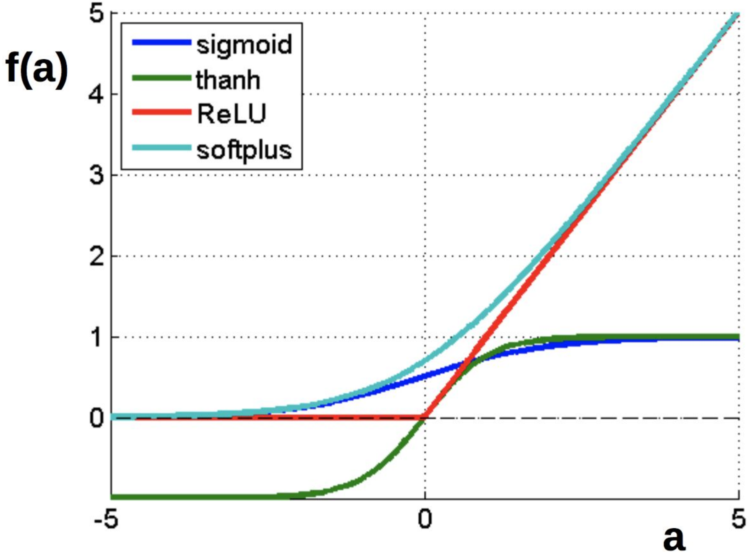
Activation functions: nonlinearities

$$f(a) = \frac{1}{1+e^{a}}$$

$$f(a) = \tanh(a)$$

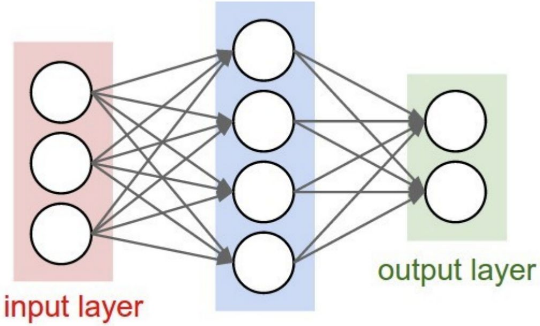
$$f(a) = \max(0, a)$$

$$f(a) = \log(1+e^{a})$$



Some generally accepted terms

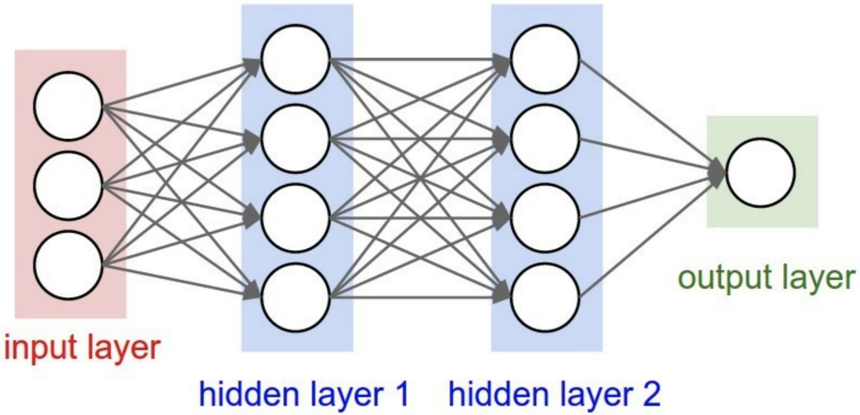
- Layer – a building block for NNs :
  - Dense layer: f(x) = Wx+b
  - Nonlinearity layer: f(x) = σ(x)
  - Input layer, output layer
  - A few more we will cover later
- Activation function – function applied to layer output
  - Sigmoid
  - tanh
  - ReLU
  - Any other function to get nonlinear intermediate signal in NN
- Backpropagation – a fancy word for “chain rule”



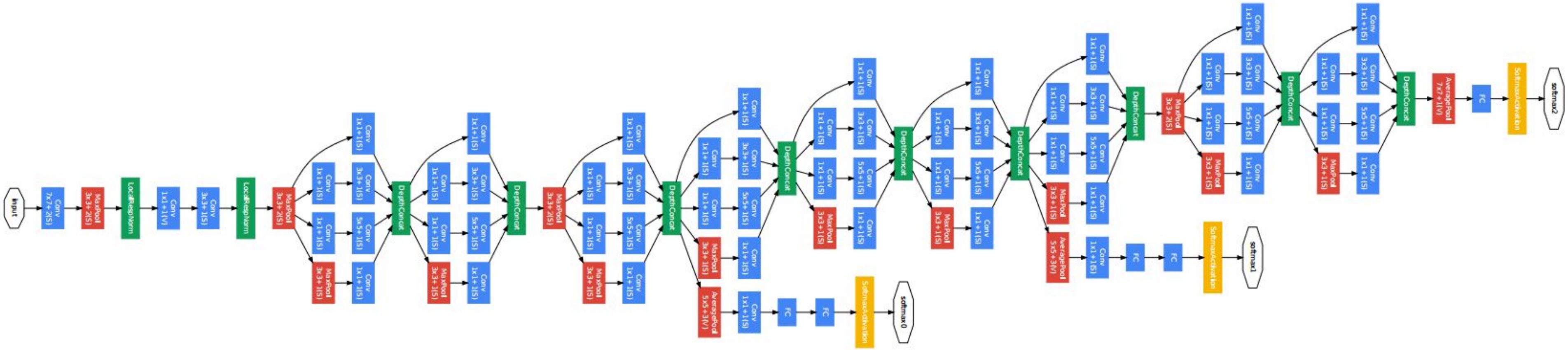
Dense layer
with a nonlinearity

“Train it via backprop!”

Actually, it can be deeper



Much deeper...



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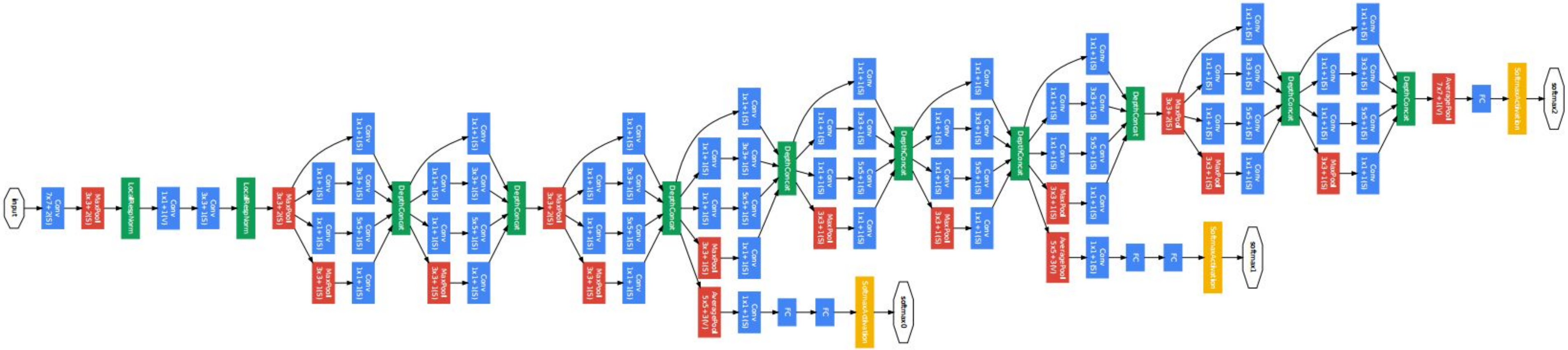
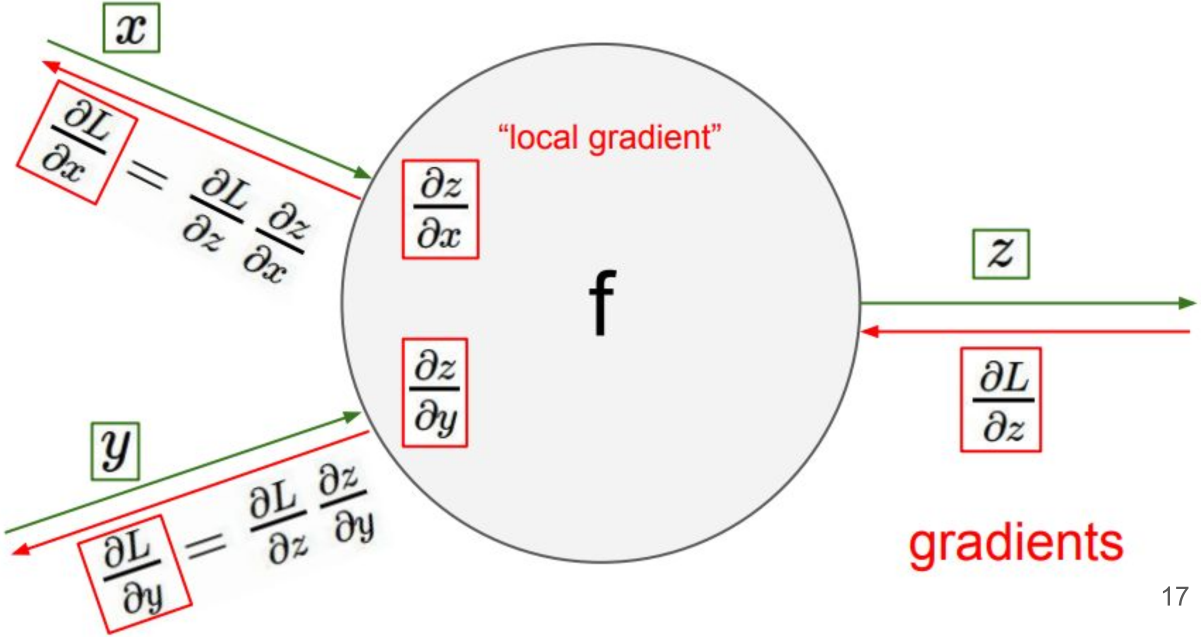


How to train it?

Backpropagation and chain rule

Chain rule is just simple math: $$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$$

Backprop is just way to use it in NN training.



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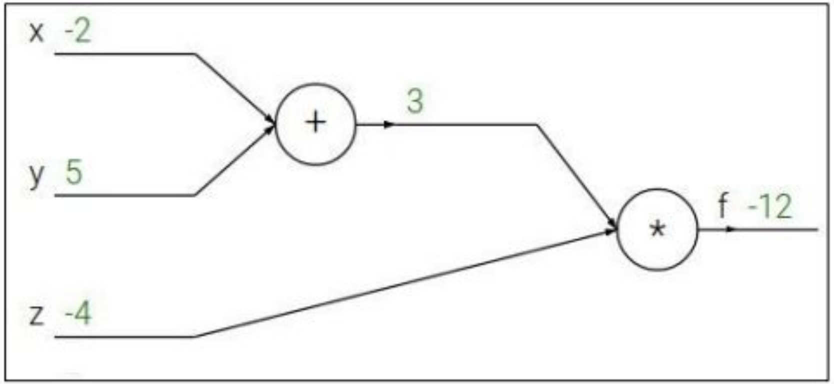
Backpropagation example

$$f(x, y, z) = (x + y)z$$

e.g. x = -2, y = 5, z = -4



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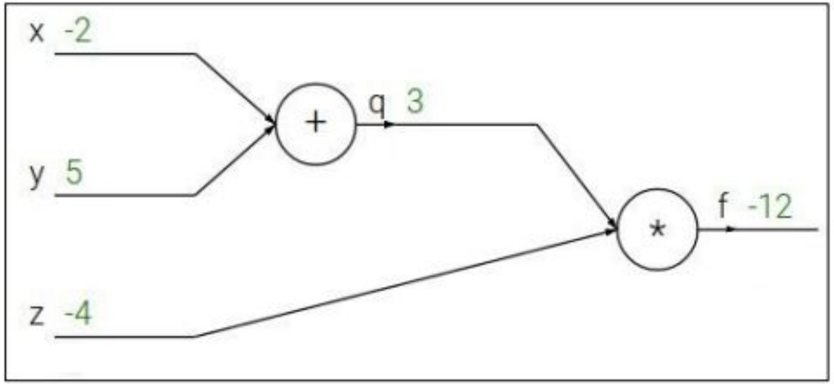

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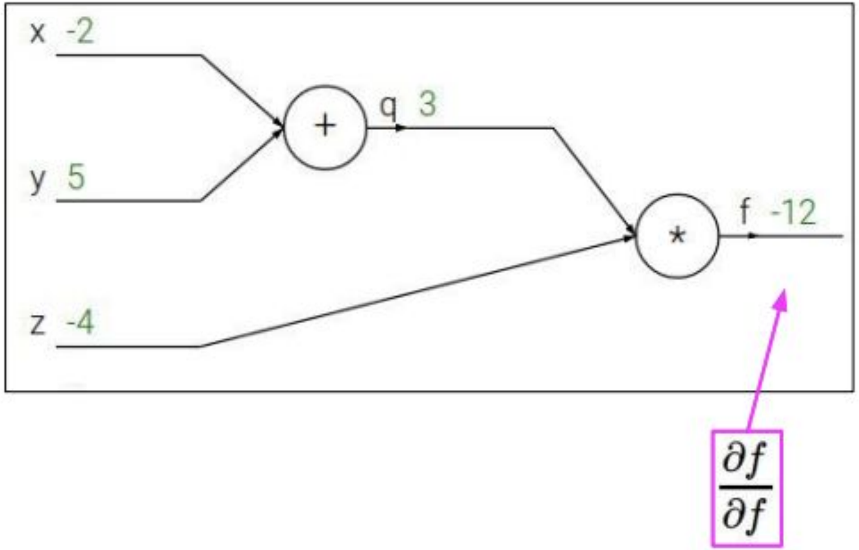

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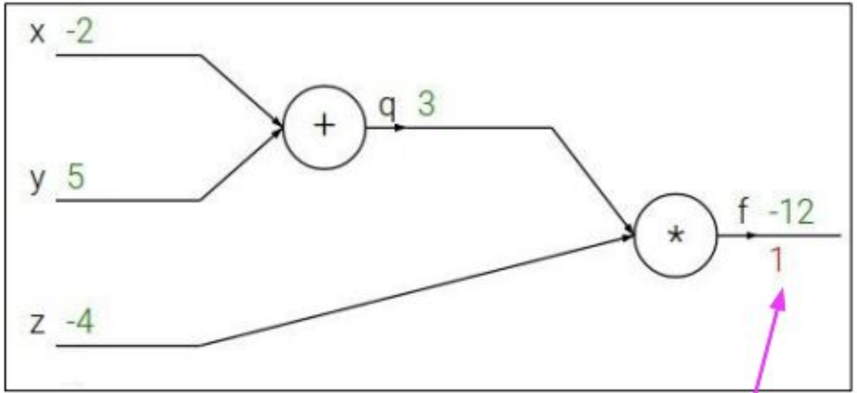

$$\frac{\partial f}{\partial f}$$

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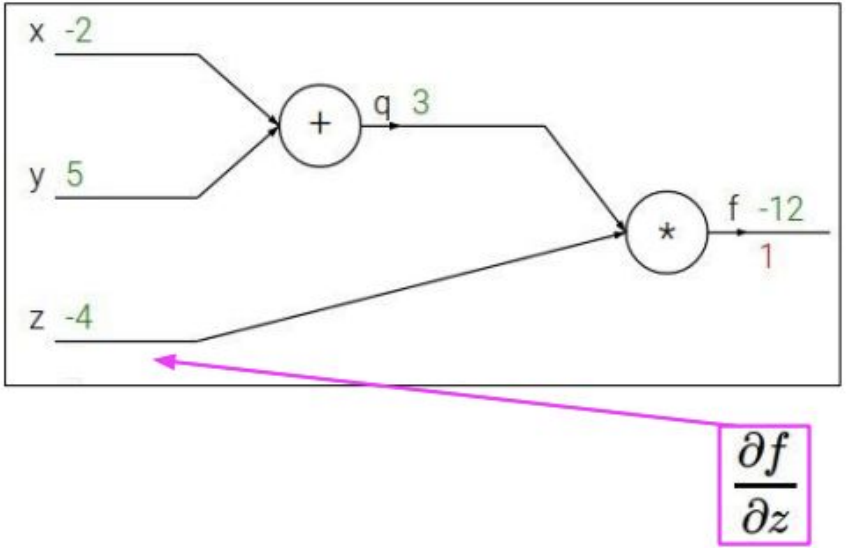

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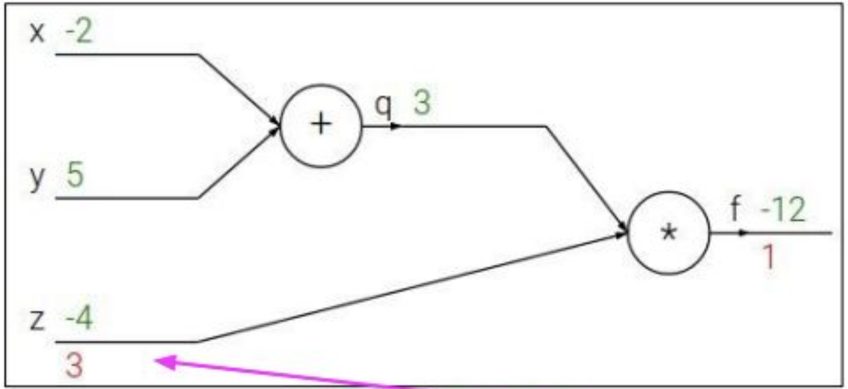

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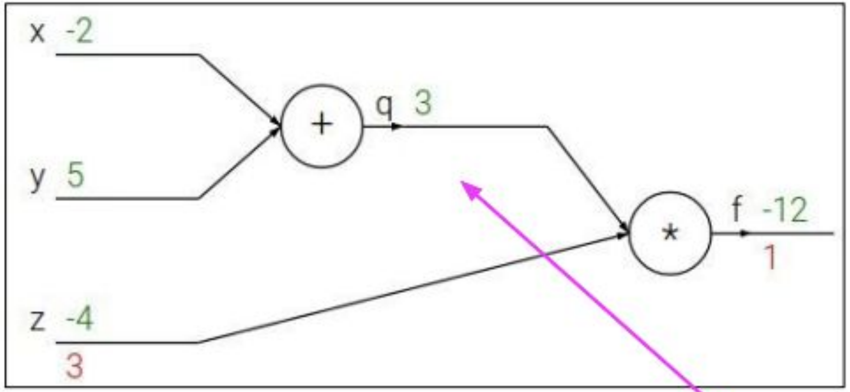

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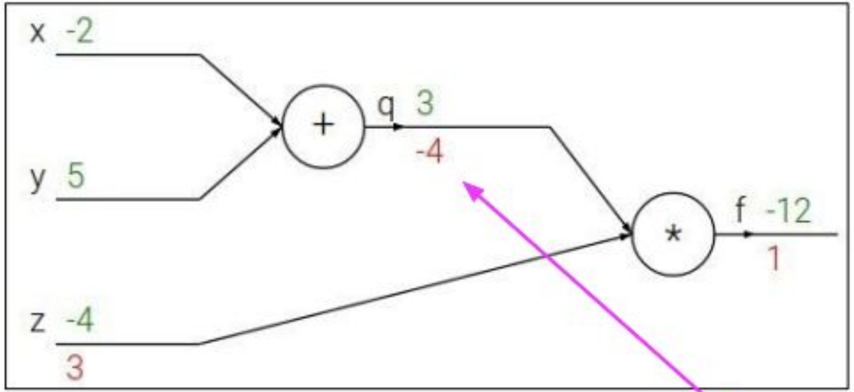

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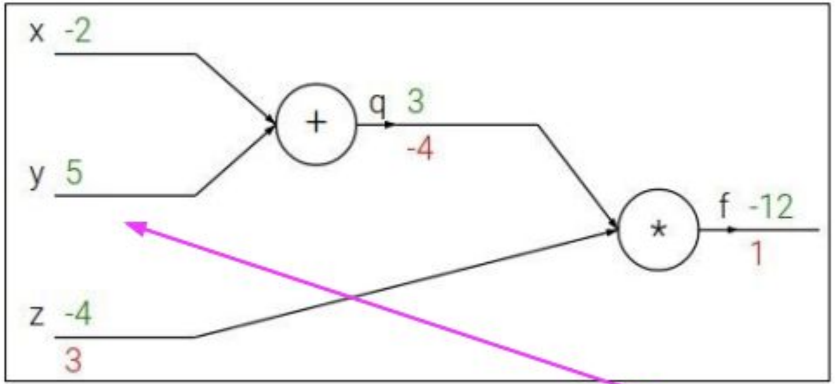

$$\frac{\partial f}{\partial y}$$

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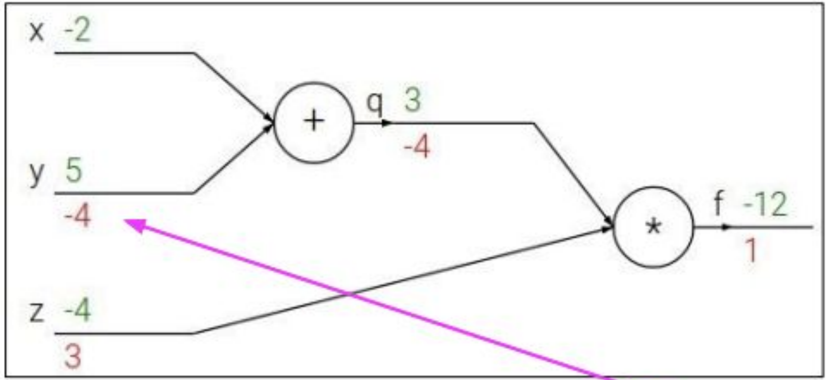

$\frac{\partial f}{\partial y}$

Chain rule:

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial y}$$

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Backpropagation example

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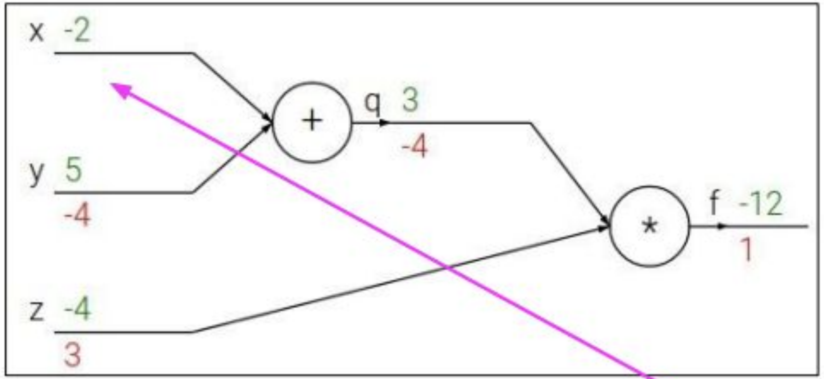

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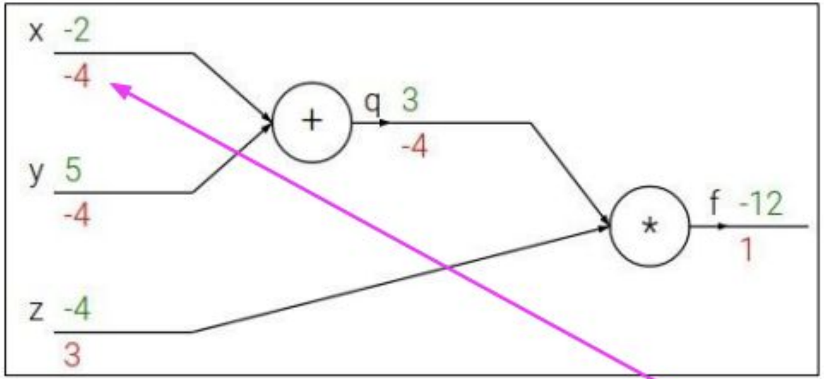

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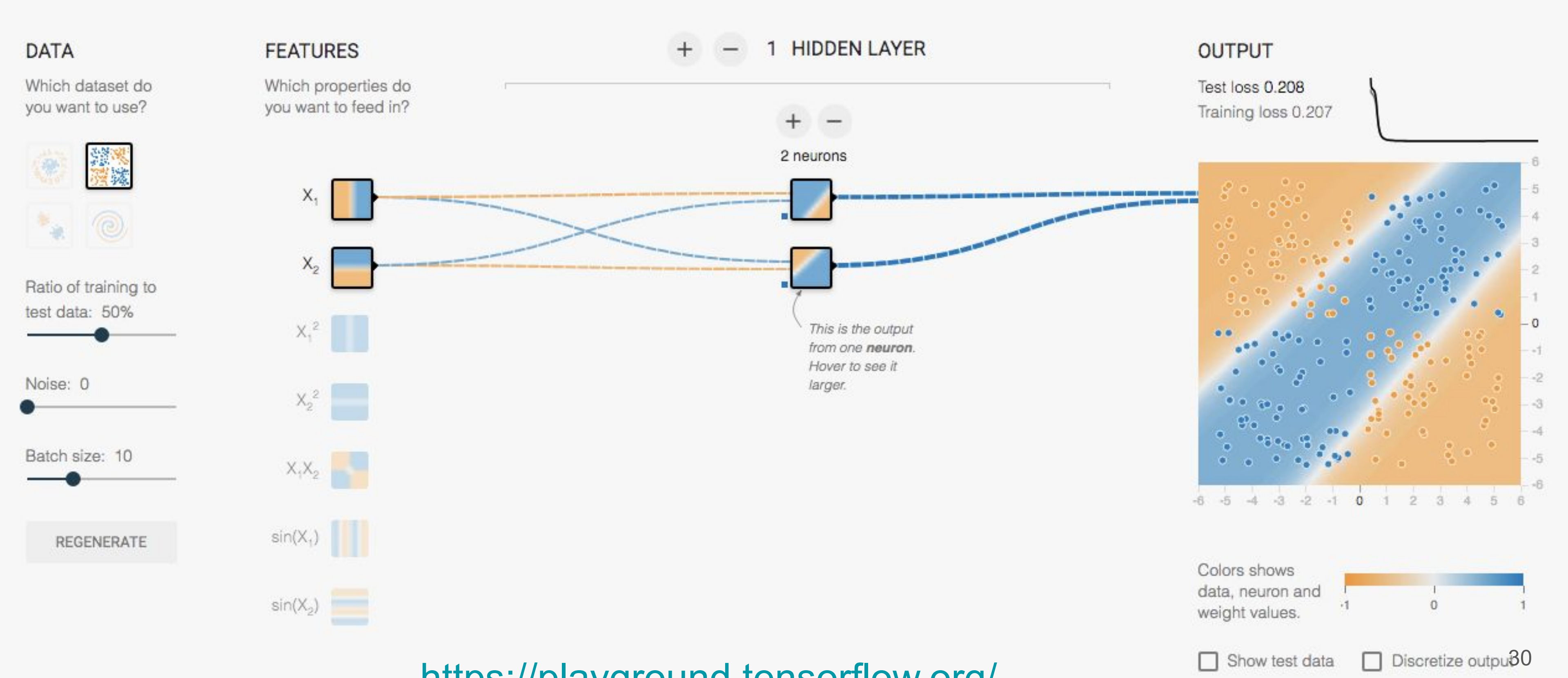
Practice time: interactive playground



https://playground.tensorflow.org/

Backpropagation and chain rule

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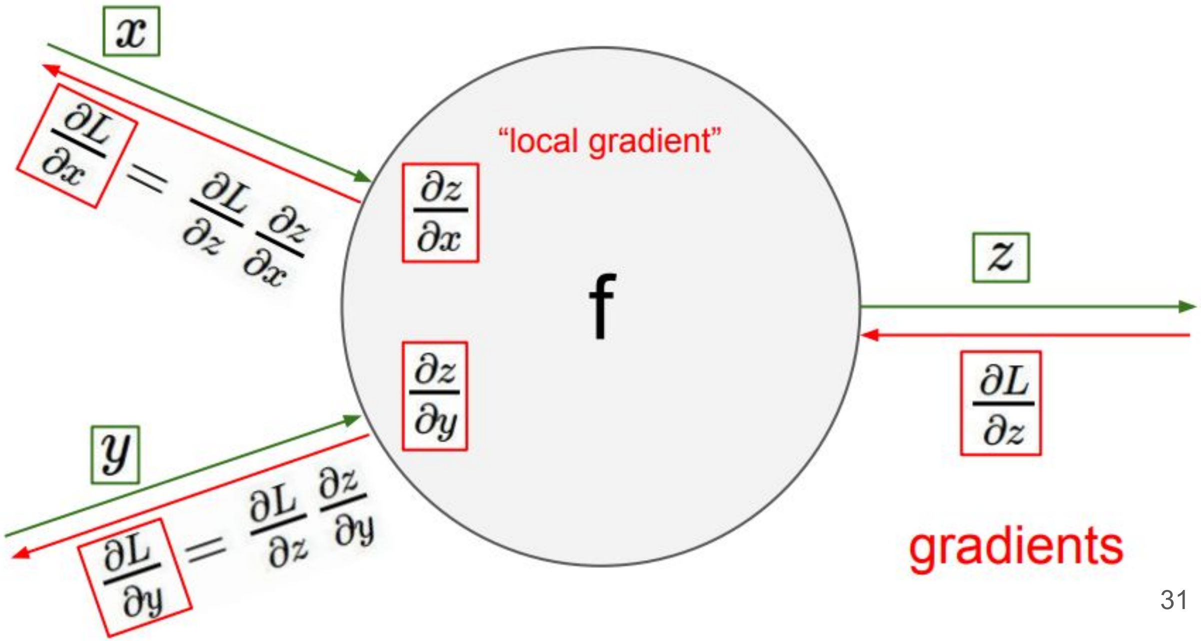
Backprop is just way to use it in NN training.



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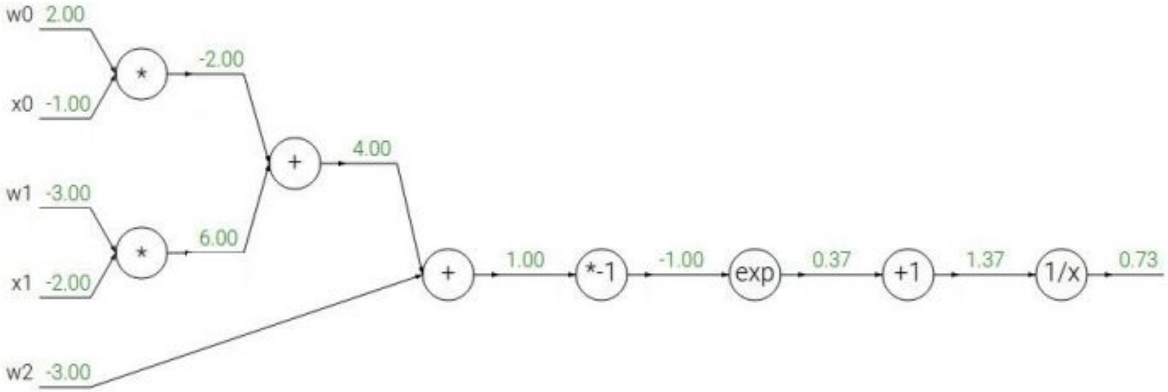
Backpropagation example

Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



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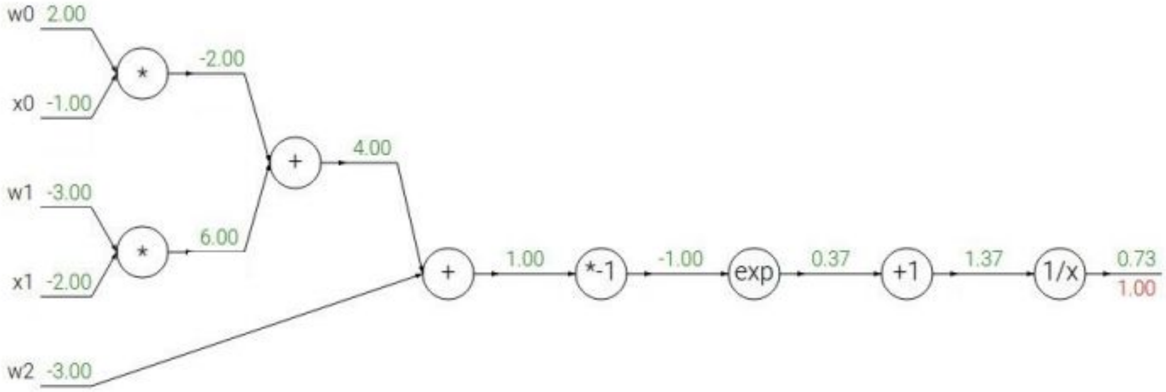

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$f_a(x) = ax \quad \rightarrow \quad \dfrac{df}{dx} = a$

$f(x) = \dfrac{1}{x} \quad \rightarrow \quad \dfrac{df}{dx} = -1/x^2$

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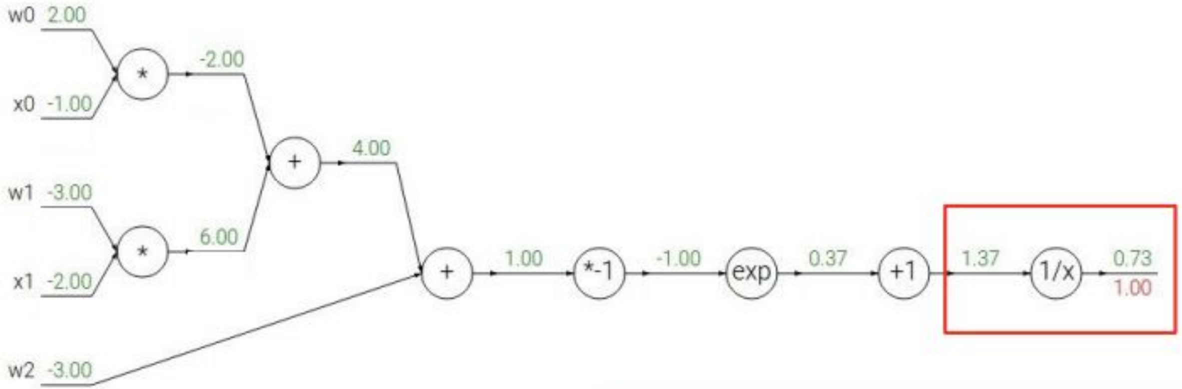

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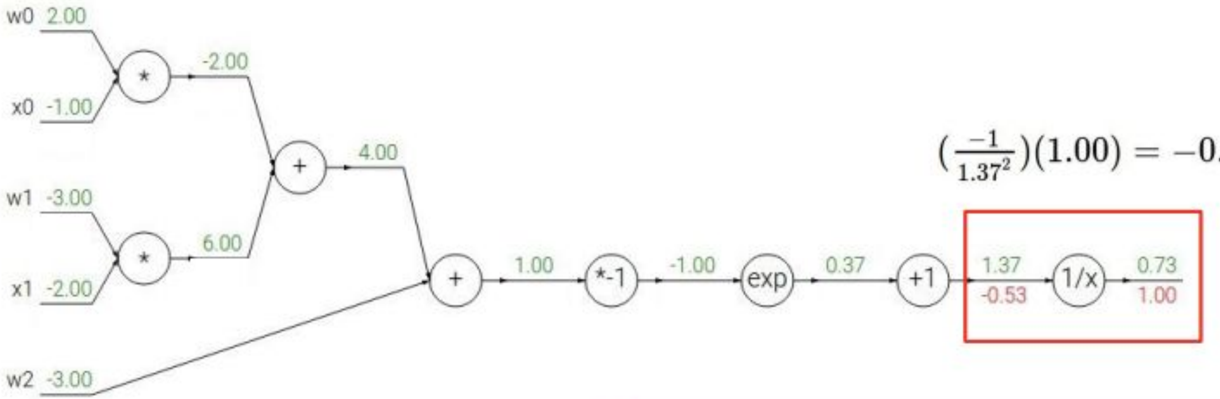

$$\left(\frac{-1}{1.37^2}\right)(1.00) = -0.53$$

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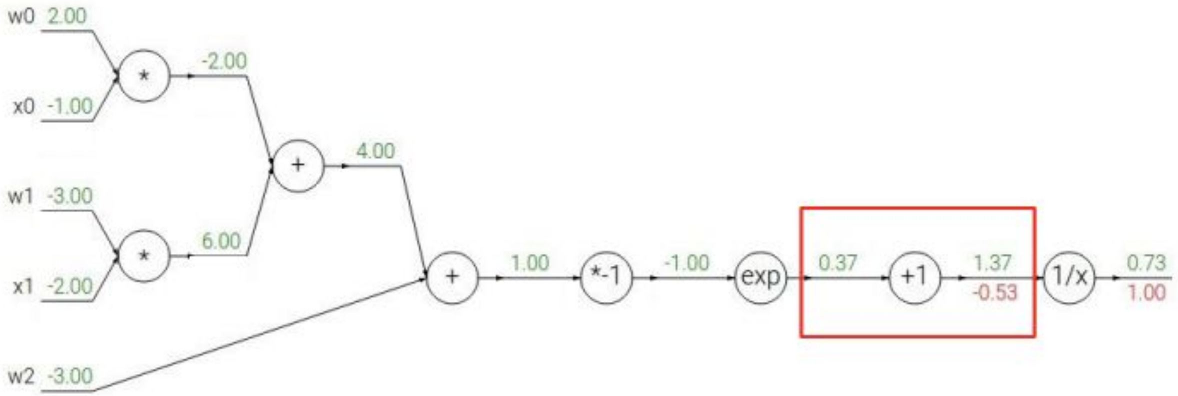

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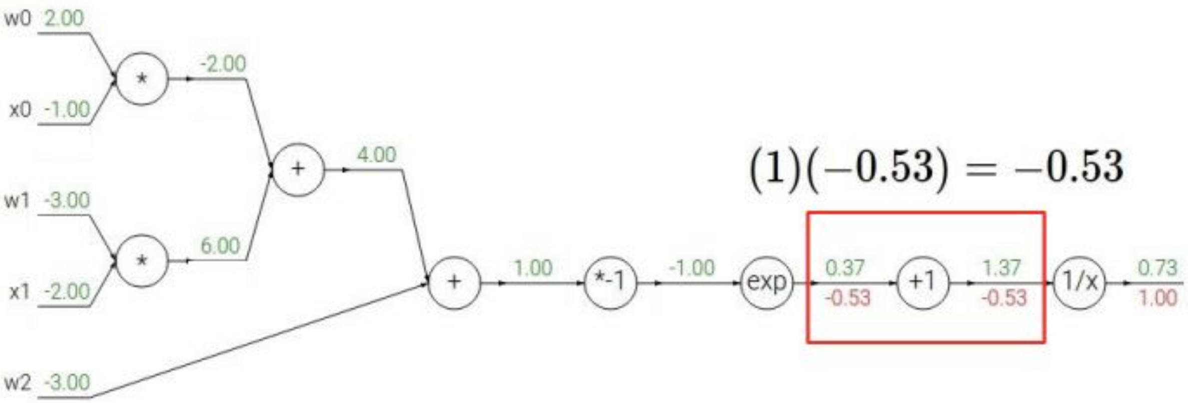

$$(1)(-0.53) = -0.53$$

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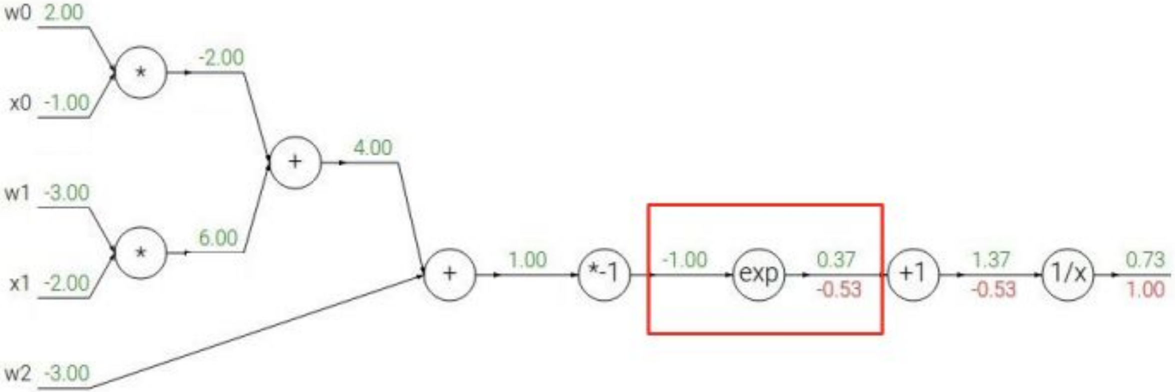

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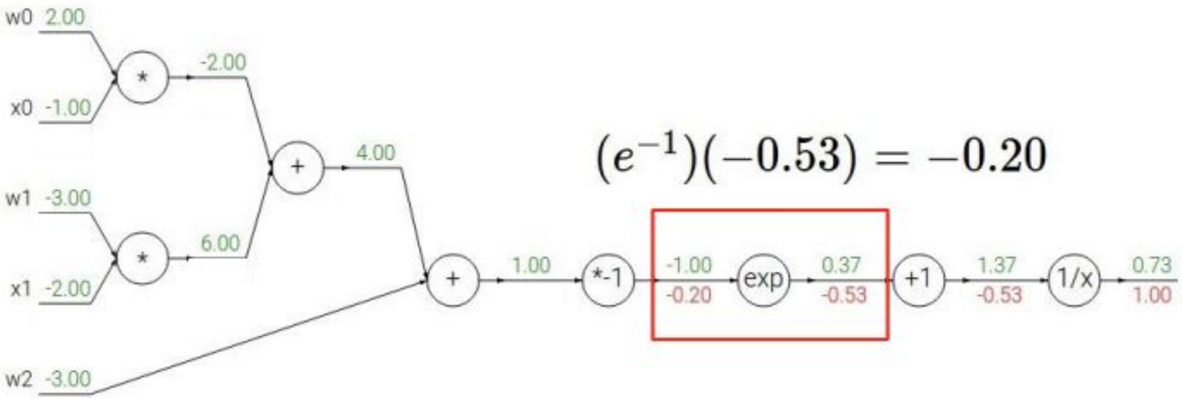
source: http://cs231n.github.io

Backpropagation example

Another example: $f(w,x) = \dfrac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$

$$(e^{-1})(-0.53) = -0.20$$



$$\boxed{f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x}$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

$$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

$$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$$

source: http://cs231n.github.io

Backpropagation example

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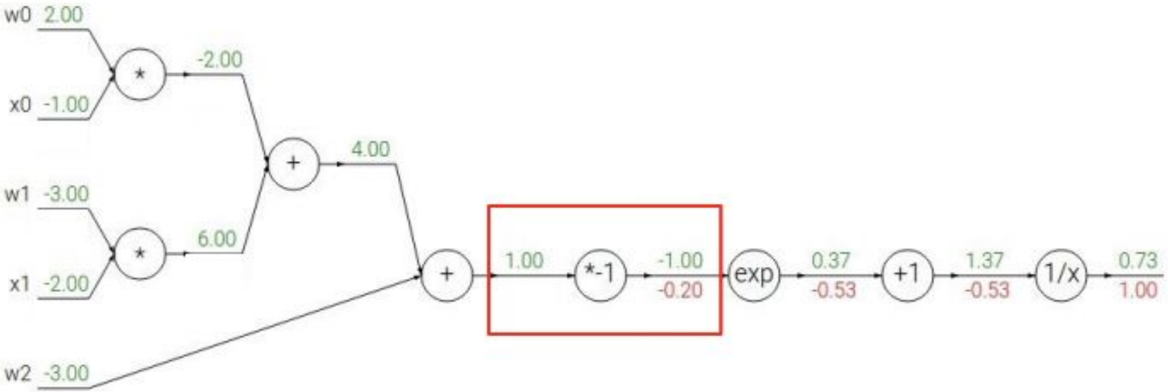

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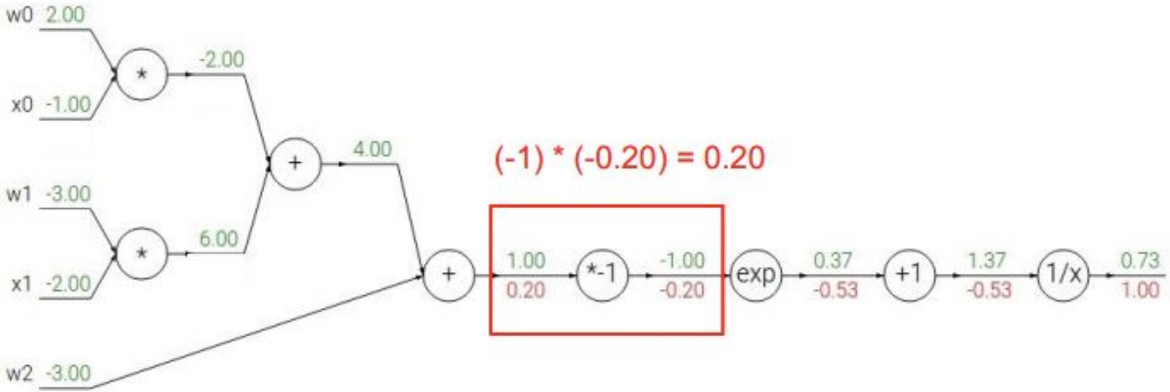

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Backpropagation example

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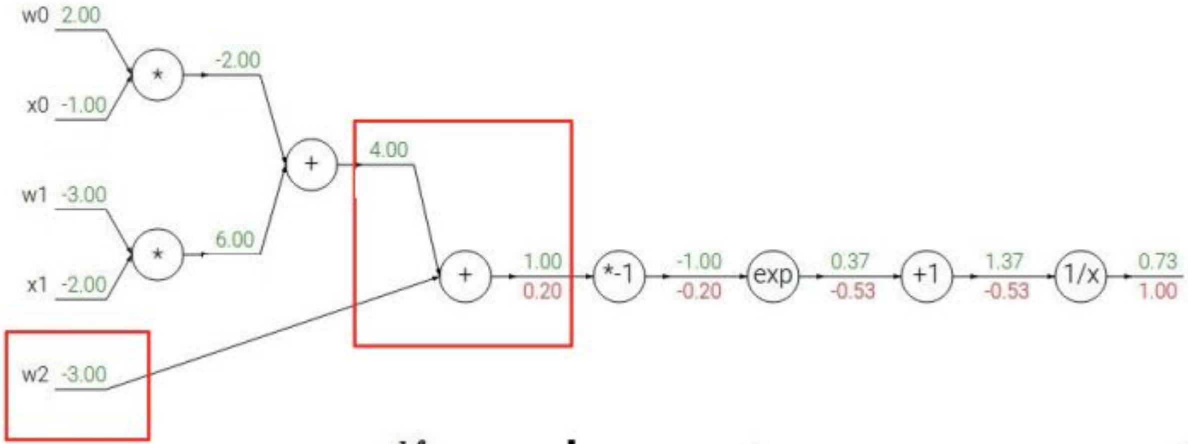
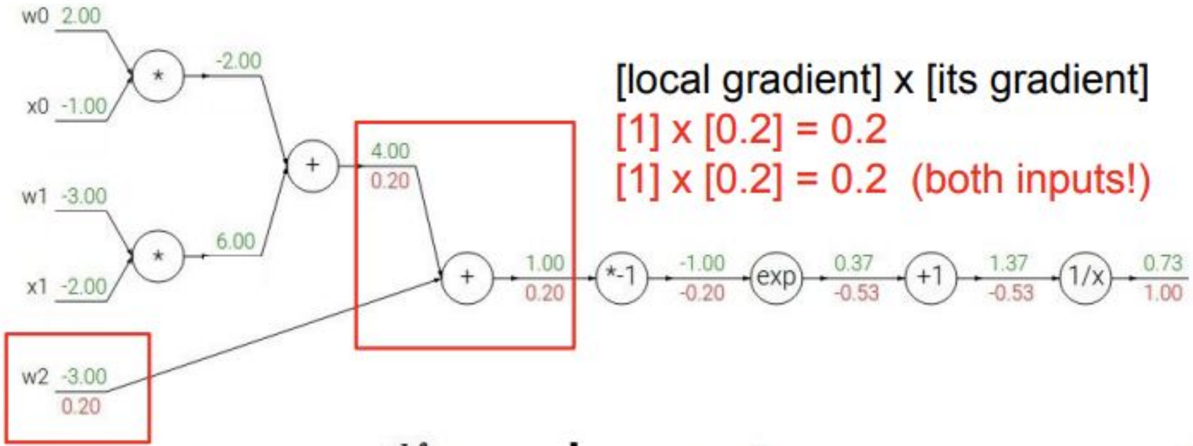


$f(x) = e^x \rightarrow \frac{df}{dx} = e^x$		$f(x) = \frac{1}{x} \rightarrow \frac{df}{dx} = -1/x^2$
$f_a(x) = ax \rightarrow \frac{df}{dx} = a$		$f_c(x) = c + x \rightarrow \frac{df}{dx} = 1$

source: http://cs231n.github.io

Backpropagation example

Another example: $$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$



[local gradient] x [its gradient]
[1] x [0.2] = 0.2
[1] x [0.2] = 0.2 (both inputs!)

$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$

$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$

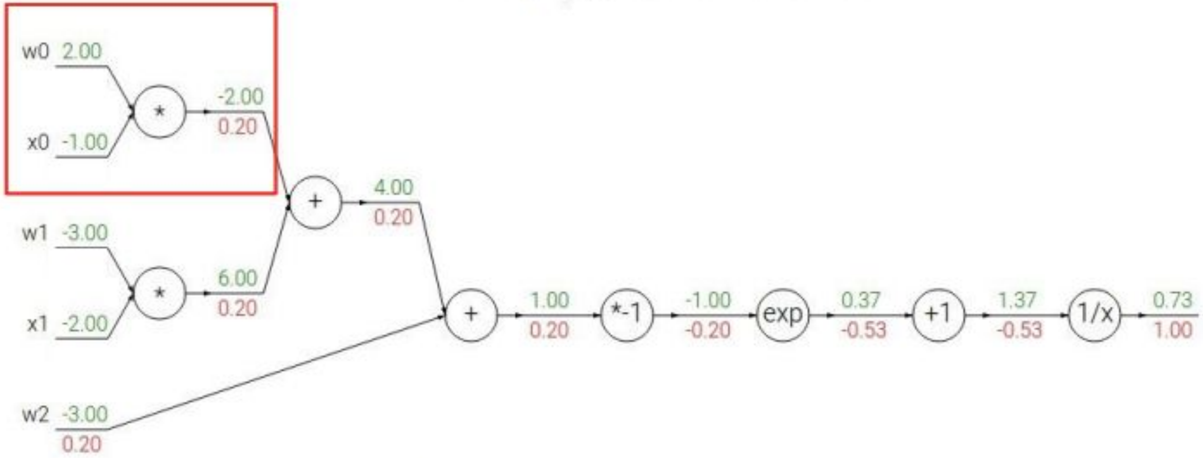
$f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$

$f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$

source: http://cs231n.github.io

Backpropagation example

Another example: $f(w,x) = \frac{1}{1+e^{-(w_0 x_0 + w_1 x_1 + w_2)}}$



$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

$$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$$

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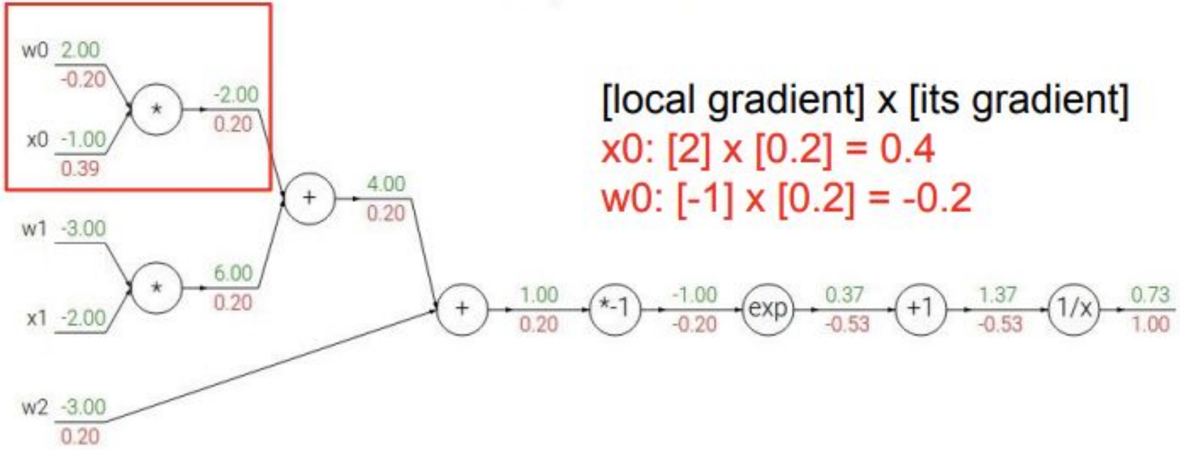


[local gradient] x [its gradient]

x0: [2] x [0.2] = 0.4

w0: [-1] x [0.2] = -0.2

$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$ | $f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$

$f_a(x) = ax \quad \rightarrow \quad \frac{df}{dx} = a$ | $f_c(x) = c + x \quad \rightarrow \quad \frac{df}{dx} = 1$

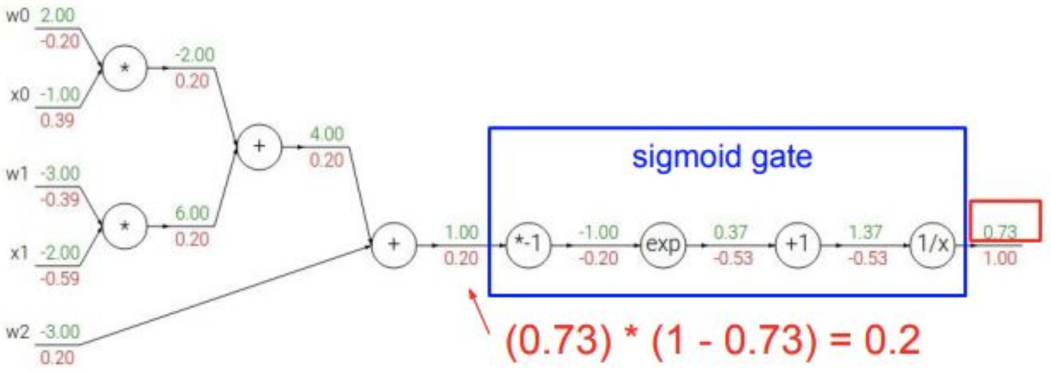
source: http://cs231n.github.io

Backpropagation example

$$f(w,x) = \frac{1}{1+e^{-(w_0x_0+w_1x_1+w_2)}}$$

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

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

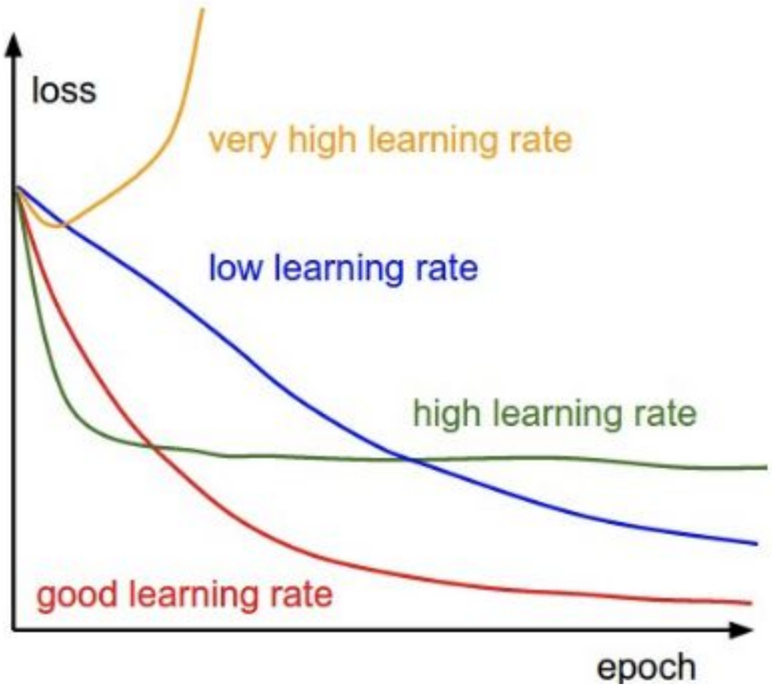


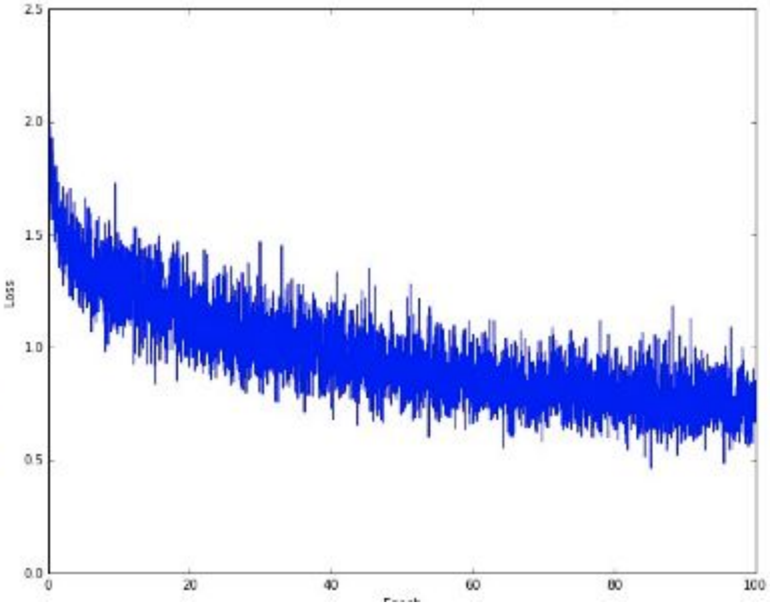
source: http://cs231n.github.io

Gradient optimization

Stochastic gradient descent (and variations) is used to optimize NN parameters.

$$x_{t+1} = x_t - \text{learning rate} \cdot dx$$





source: http://cs231n.github.io/neural-networks-3/

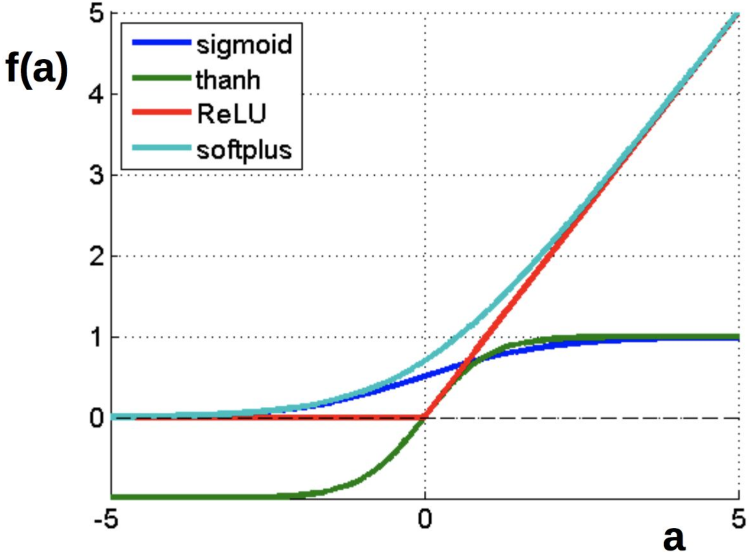
Once more: nonlinearities

$$f(a) = \frac{1}{1+e^a}$$

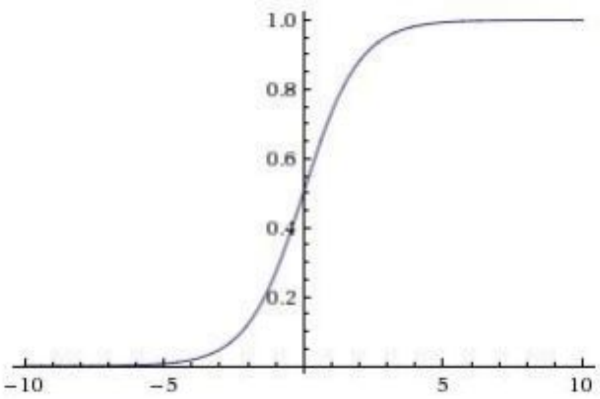
$$f(a) = \tanh(a)$$

$$f(a) = \max(0, a)$$

$$f(a) = \log(1 + e^a)$$



Activation functions



Sigmoid

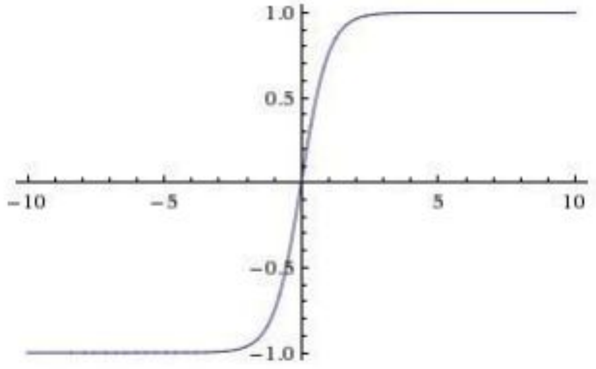
$$f(a) = \frac{1}{1 + e^{a}}$$

- Squashes numbers to range [0,1]
- Historically popular since they have nice interpretation as a saturating "firing rate" of a neuron

3 problems:

1. Saturated neurons "kill" the gradients
2. Sigmoid outputs are not zero-centered
3. exp() is a bit compute expensive

Activation functions

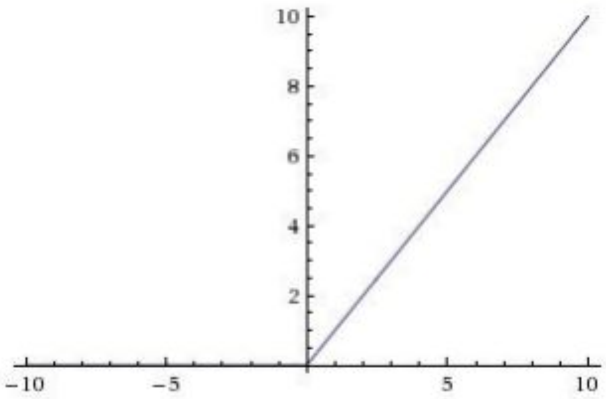


tanh(x)

- Squashes numbers to range [-1,1]
- zero centered (nice)
- still kills gradients when saturated :(

$$f(a) = \tanh(a)$$

Activation functions



ReLU
(Rectified Linear Unit)

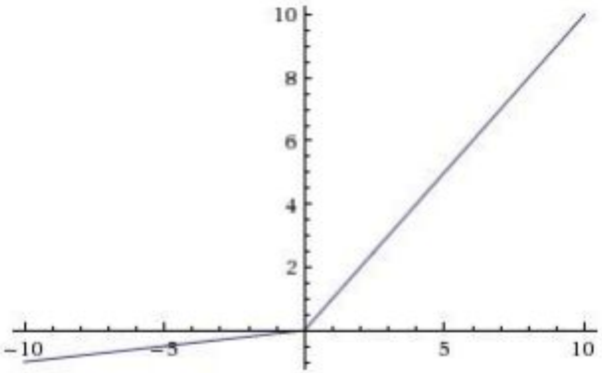
$$f(a) = \max(0, a)$$

- Does not saturate (in +region)
- Very computationally efficient
- Converges much faster than sigmoid/tanh in practice (e.g. 6x)

- Not zero-centered output
- An annoyance:

hint: what is the gradient when x < 0?

Activation functions

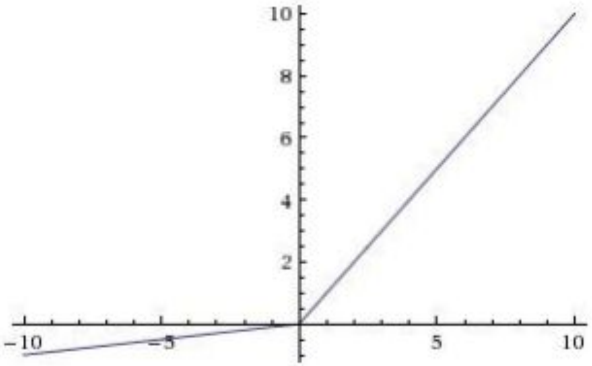


- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not “die”.**

Leaky ReLU

$$f(x) = \max(0.01x, x)$$

Activation functions



- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not "die".**

Leaky ReLU

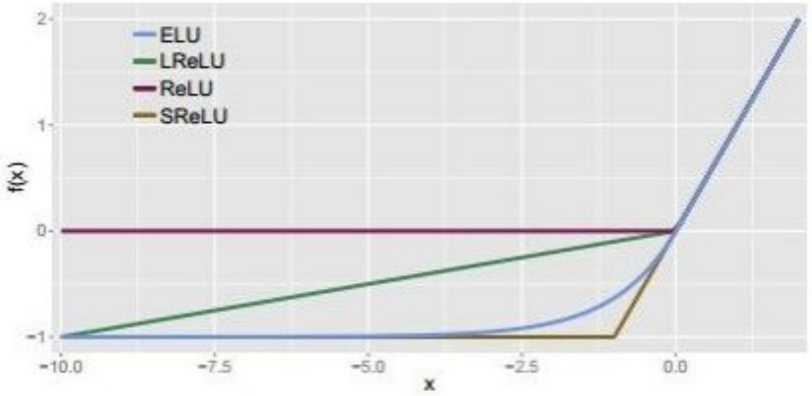
$$f(x) = \max(0.01x, x)$$

Parametric Rectifier (PReLU)

$$f(x) = \max(\alpha x, x)$$

backprop into \alpha
(parameter)

Exponential Linear Units (ELU)



$$f(x) = \begin{cases} x & \text{if } x > 0 \\ \alpha\,(\exp(x) - 1) & \text{if } x \leq 0 \end{cases}$$

- All benefits of ReLU
- Does not die
- Closer to zero mean outputs

- Computation requires exp()

Activation functions: sum up

- Use ReLU as baseline approach
- Be careful with the learning rates
- Try out Leaky ReLU or ELU
- Try out tanh but do not expect much from it
- Do not use Sigmoid

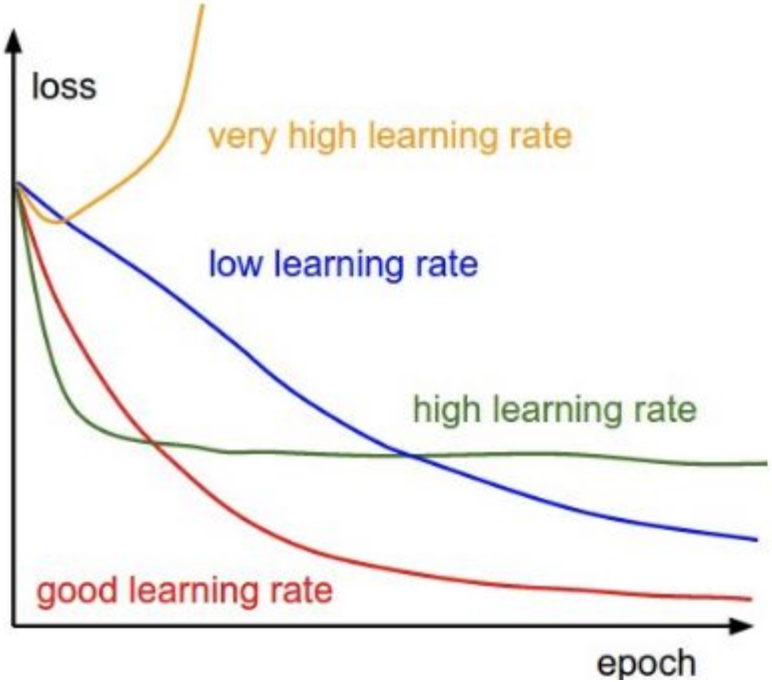
That’s all. Time to build some NN.

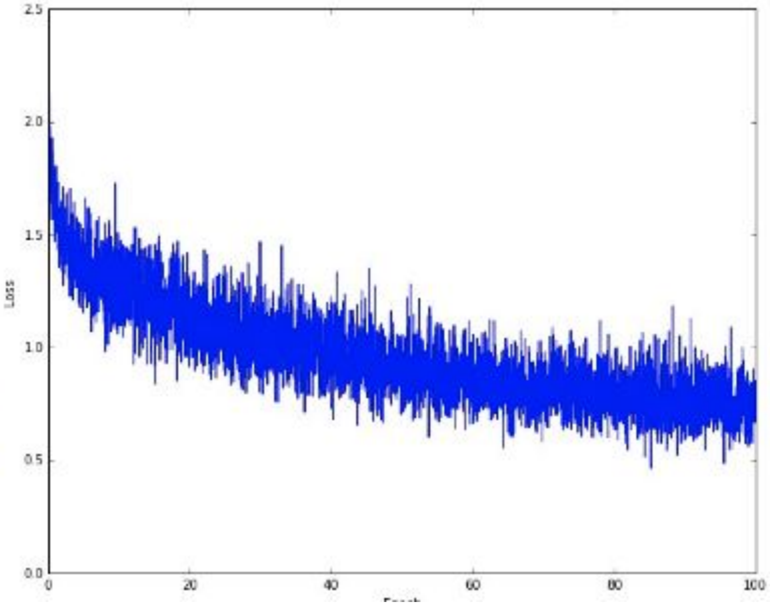
Backup

Optimizers

Stochastic gradient descent is used to optimize NN parameters.

$$x_{t+1} = x_t - \text{learning rate} \cdot dx$$



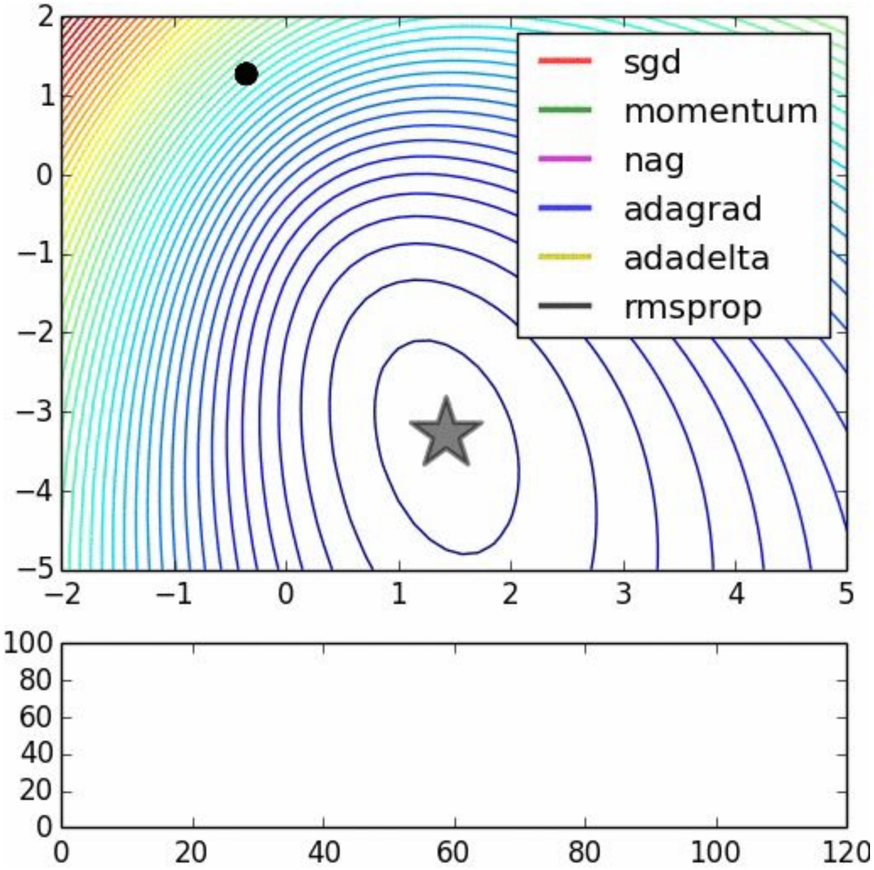


source: http://cs231n.github.io/neural-networks-3/

Optimizers

There are much more optimizers:

- Momentum
- Adagrad
- Adadelta
- RMSprop
- Adam
- …
- even other NNs

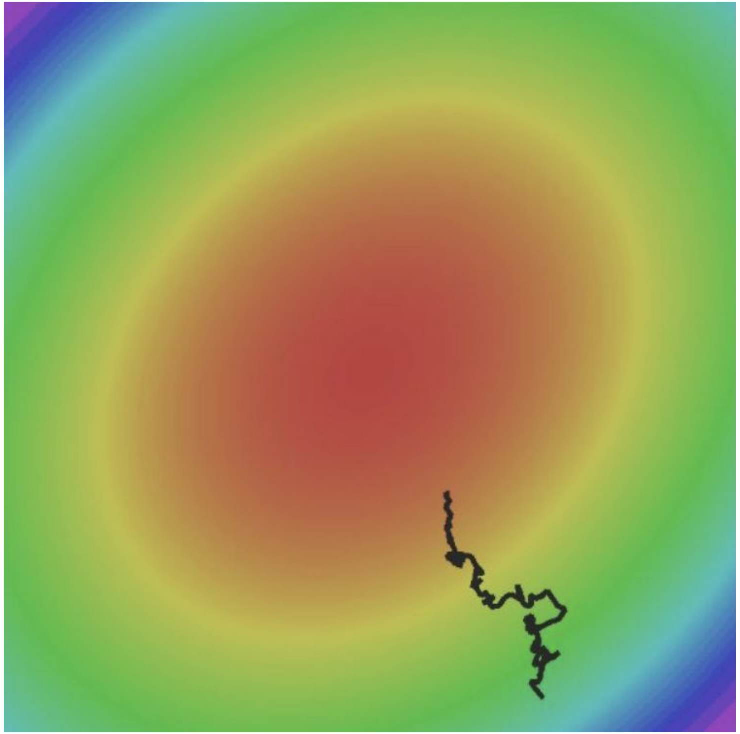


Optimization: SGD

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(x_i, y_i, W)$$

$$\nabla_W L(W) = \frac{1}{N} \sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W)$$

Averaging over minibatches ---> noisy gradient



source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

First idea: momentum

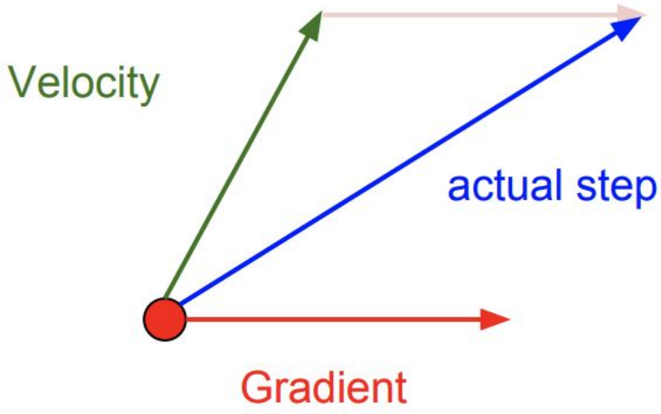
Simple SGD

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

SGD with momentum

$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

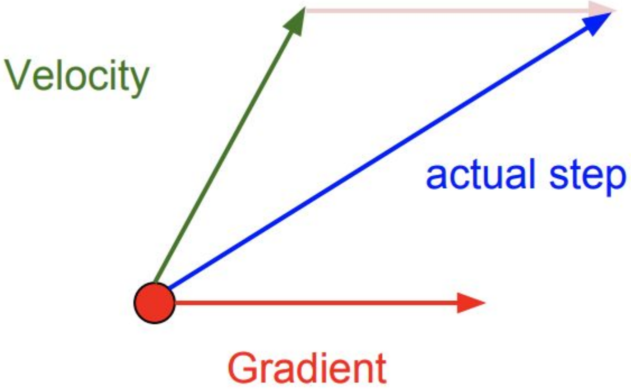
Momentum update:



source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

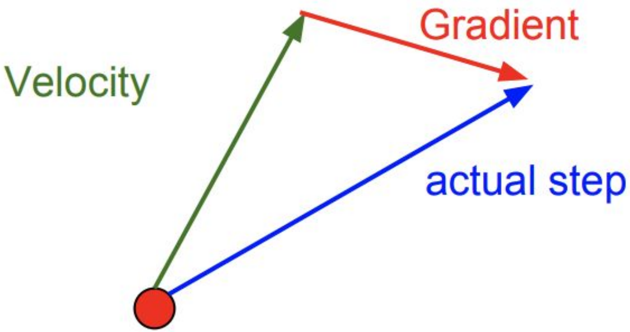
Nesterov momentum

Momentum update:



$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

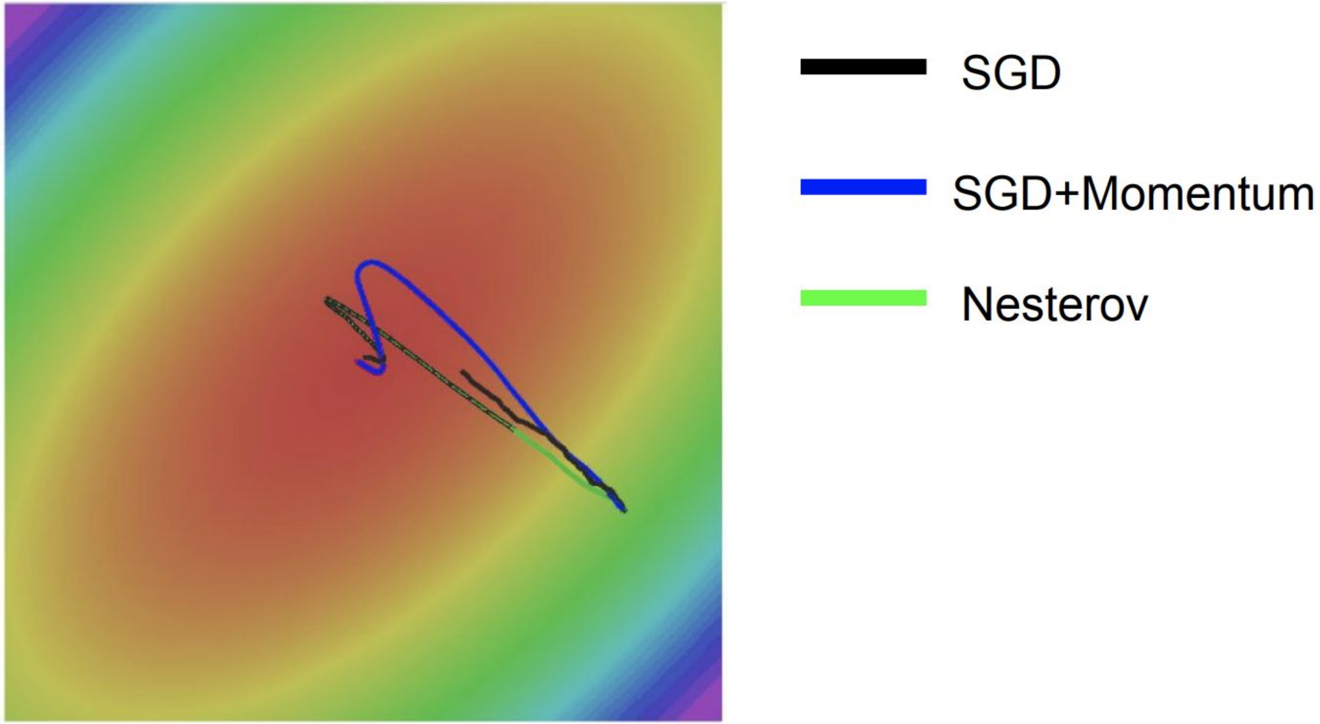
Nesterov Momentum



$$v_{t+1} = \rho v_t - \alpha \nabla f(\boxed{x_t + \rho v_t})$$
$$x_{t+1} = x_t + v_{t+1}$$

source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

Comparing momentums



source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

Second idea: different dimensions are different

Adagrad: SGD with cache

$$\text{cache}_{t+1} = \text{cache}_t + (\nabla f(x_t))^2$$
$$x_{t+1} = x_t - \alpha \frac{\nabla f(x_t)}{\text{cache}_{t+1} + \varepsilon}$$

Second idea: different dimensions are different

Adagrad: SGD with cache

$$\mathrm{cache}_{t+1} = \mathrm{cache}_t + (\nabla f(x_t))^2$$

$$x_{t+1} = x_t - \alpha \frac{\nabla f(x_t)}{\mathrm{cache}_{t+1} + \varepsilon}$$

Problem: gradient fades with time

Second idea: different dimensions are different

Adagrad: SGD with cache

$$\text{cache}_{t+1} = \text{cache}_t + (\nabla f(x_t))^2$$

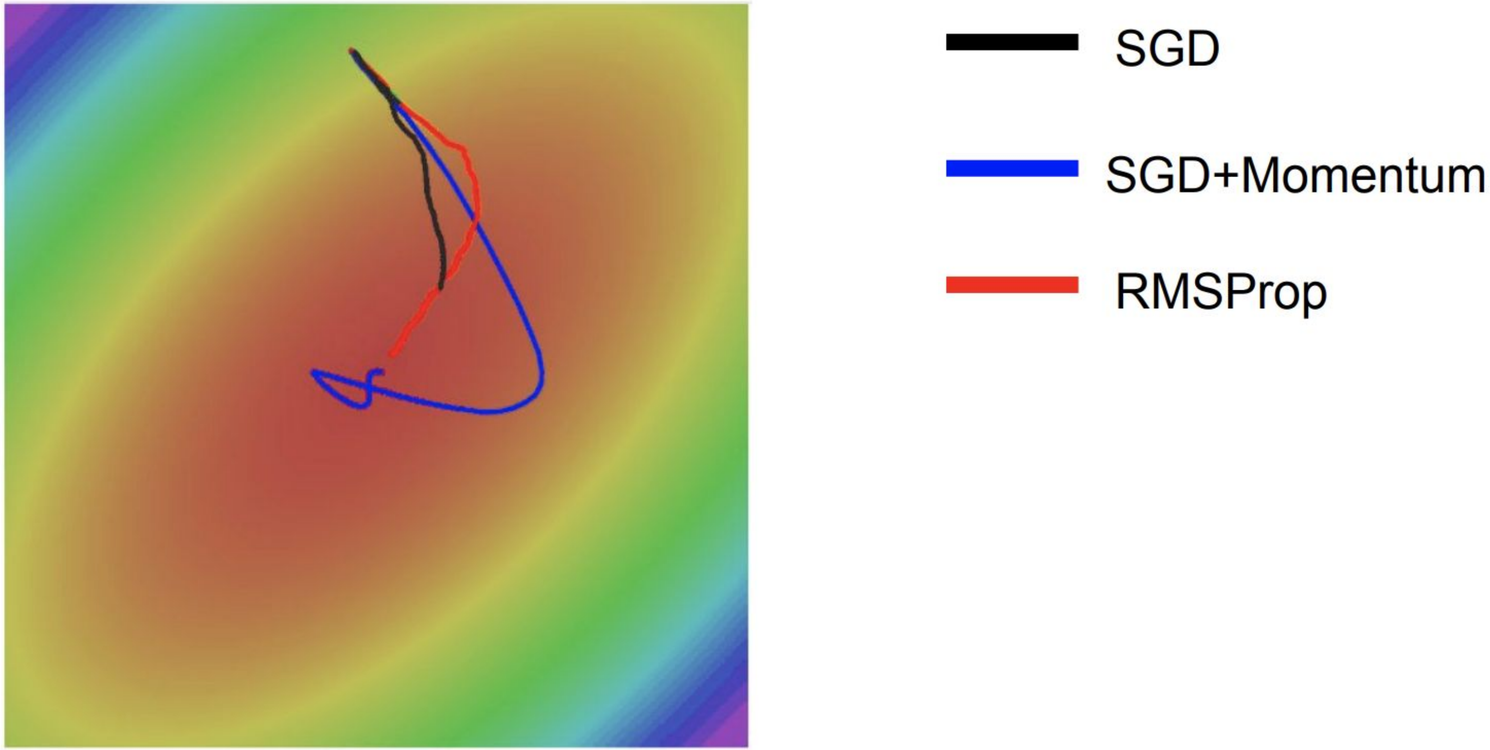
$$x_{t+1} = x_t - \alpha \frac{\nabla f(x_t)}{\text{cache}_{t+1} + \varepsilon}$$

RMSProp: SGD with cache with exp. Smoothing

$$\text{cache}_{t+1} = \beta \text{cache}_t + (1-\beta)(\nabla f(x_t))^2$$

$$x_{t+1} = x_t - \alpha \frac{\nabla f(x_t)}{\text{cache}_{t+1} + \varepsilon}$$

Slide 29 Lecture 6 of Geoff Hinton's Coursera class
http://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_lec6.pdf



source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

Adam

Let's combine the momentum idea and RMSProp normalization:

$$v_{t+1} = \gamma v_t + (1-\gamma)\nabla f(x_t)$$

$$\text{cache}_{t+1} = \beta \text{cache}_t + (1-\beta)(\nabla f(x_t))^2$$

$$x_{t+1} = x_t - \alpha \frac{v_{t+1}}{\text{cache}_{t+1} + \varepsilon}$$

Adam full form involves bias correction term. See http://cs231n.github.io/neural-networks-3/ for more info.

Adam

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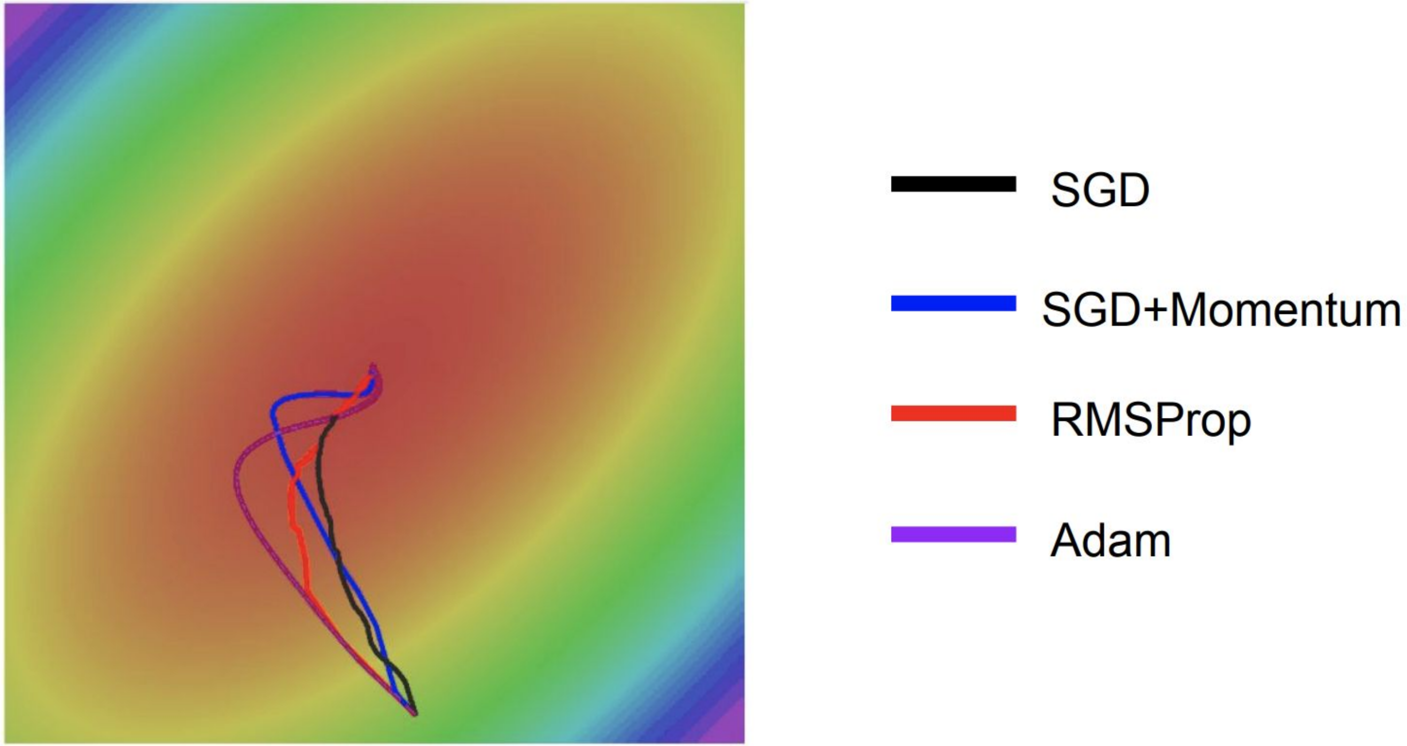
$$x_{t+1} = x_t - \alpha \frac{v_{t+1}}{\text{cache}_{t+1} + \varepsilon}$$

Actually, that’s not quite Adam.

Adam full form involves bias correction term. See http://cs231n.github.io/neural-networks-3/ for more info.

Comparing optimizers



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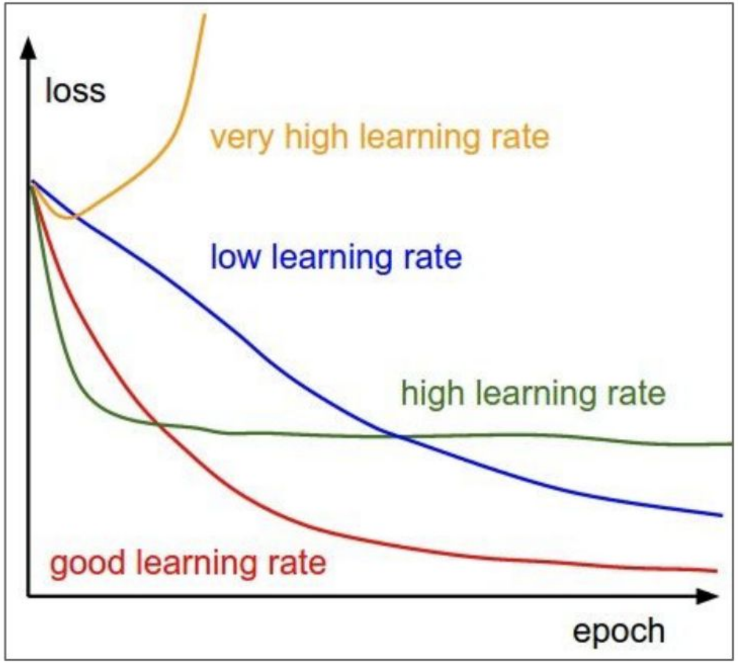
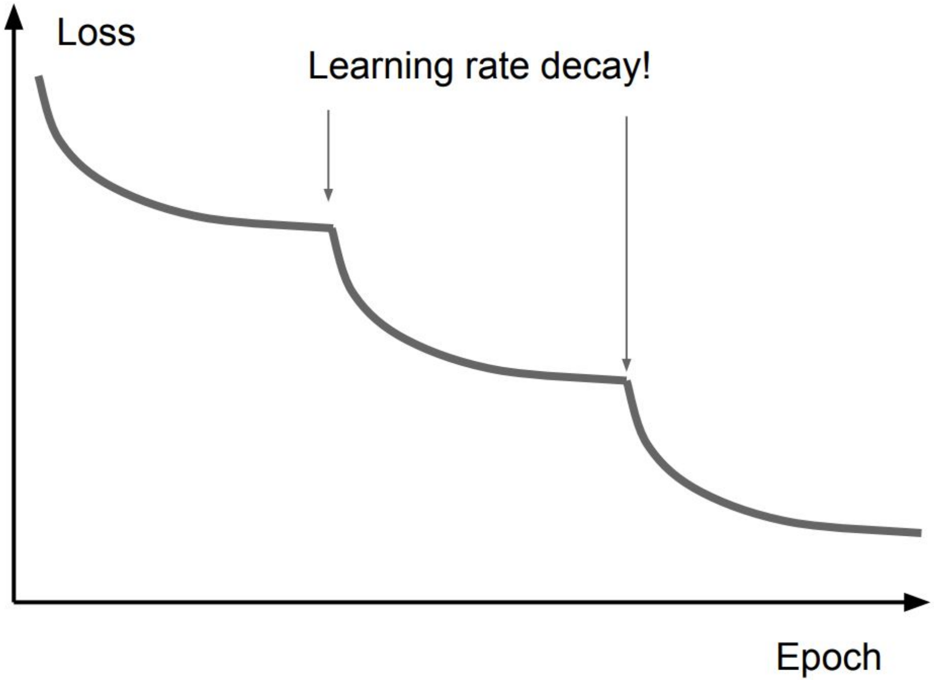
Once more: learning rate





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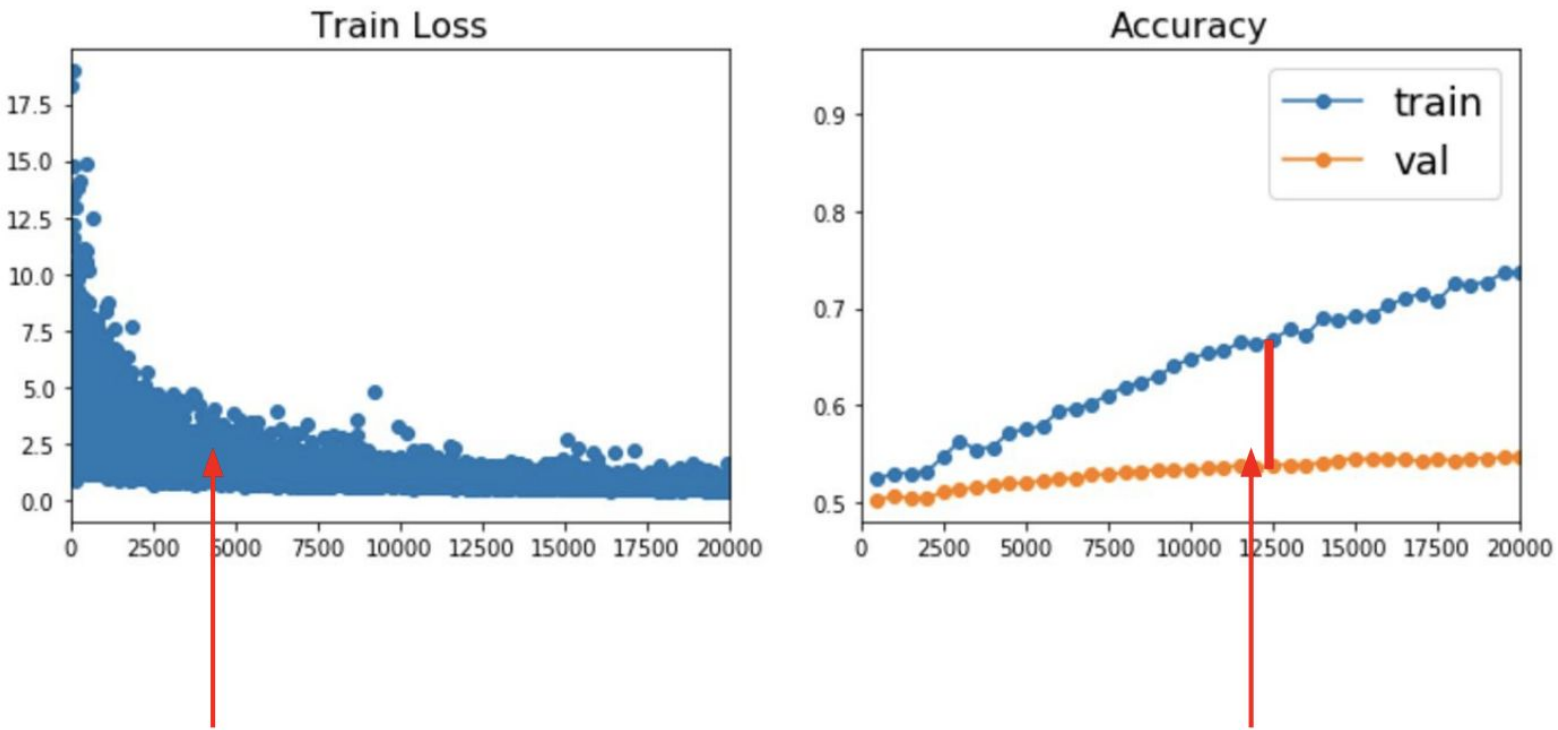
Sum up: optimization

- Adam is great basic choice
- Even for Adam/RMSProp learning rate matters
- Use learning rate decay
- Monitor your model quality



Better optimization algorithms help reduce training loss

But we really care about error on new data - how to reduce the gap?

source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf