Advanced ML course

Lecture 3: Introduction to Deep Learning

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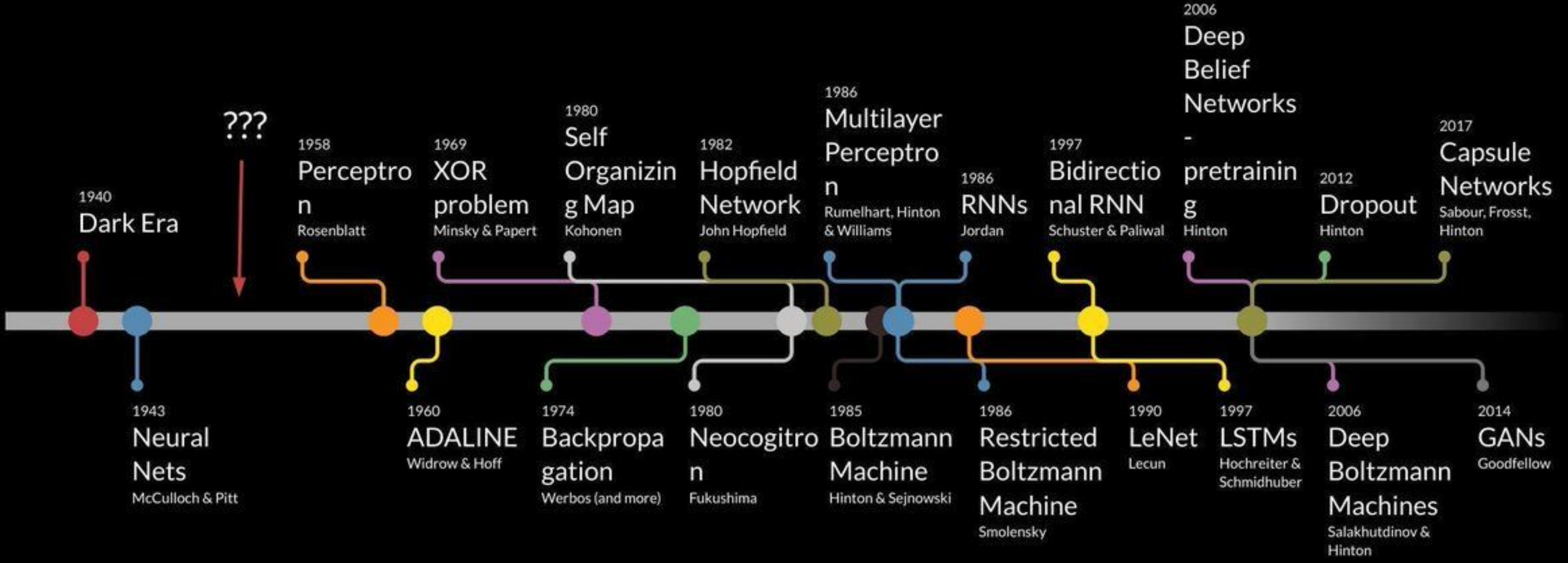
Outline

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



1940
Dark Era

1943
Neural Nets
McCulloch & Pitt

???

1958
Perceptron
Rosenblatt

1960
ADALINE
Widrow & Hoff

1969
XOR problem
Minsky & Papert

1974
Backpropagation
Werbos (and more)

1980
Self Organizing Map
Kohonen

1980
Neocogitron
Fukushima

1982
Hopfield Network
John Hopfield

1985
Boltzmann Machine
Hinton & Sejnowski

1986
Multilayer Perceptron
Rumelhart, Hinton & Williams

1986
Restricted Boltzmann Machine
Smolensky

1986
RNNs
Jordan

1990
LeNet
Lecun

1997
Bidirectional RNN
Schuster & Paliwal

1997
LSTMs
Hochreiter & Schmidhuber

2006
Deep Belief Networks - pretraining
Hinton

2006
Deep Boltzmann Machines
Salakhutdinov & Hinton

2012
Dropout
Hinton

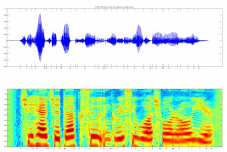
2014
GANs
Goodfellow

2017
Capsule Networks
Sabour, Frosst, Hinton

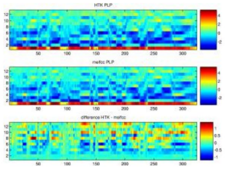
Made by Favio Vázquez

Real world problems

Audio Features

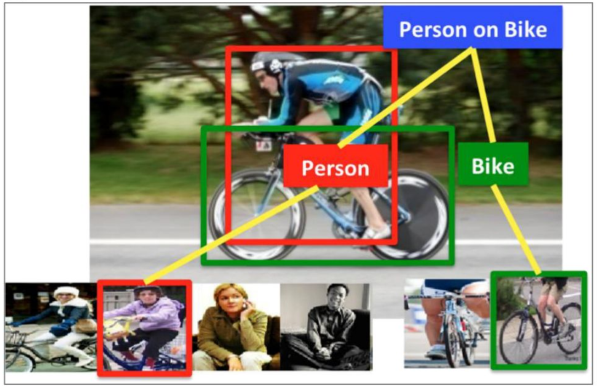


Spectrogram



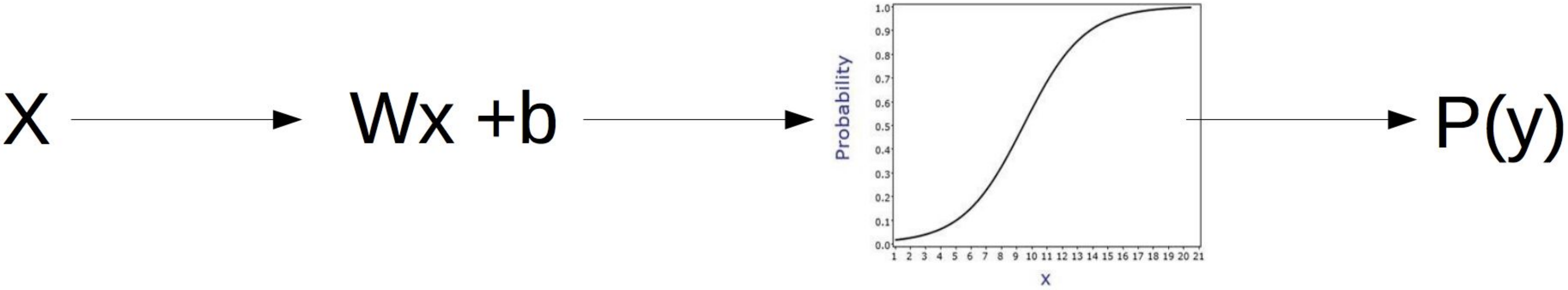
MFCC

- Object detection
- Action classification
- Image captioning
- …



"man in black shirt is playing guitar."

Logistic regression

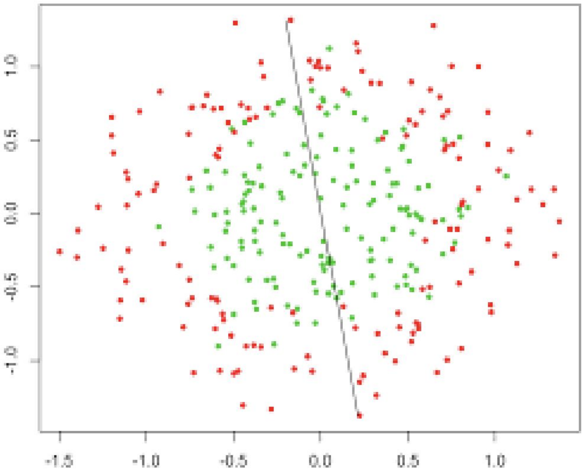


X → Wx +b → → P(y)

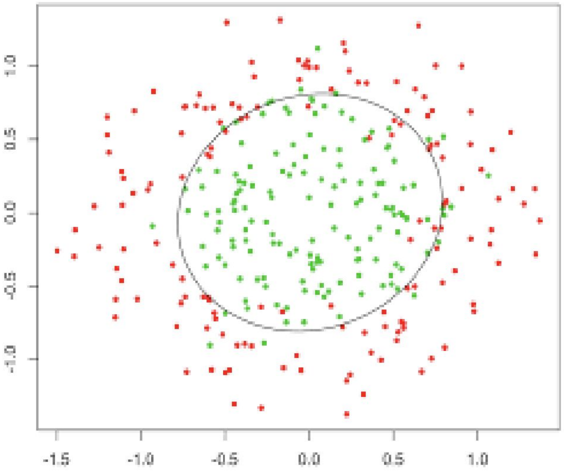
$$P(y|x)=\sigma(w\cdot x+b)$$

$$L=-\sum_{i} y_i \log P(y|x_i)+(1-y_i)\log(1-P(y|x_i))$$

Problem: nonlinear dependencies



What we have

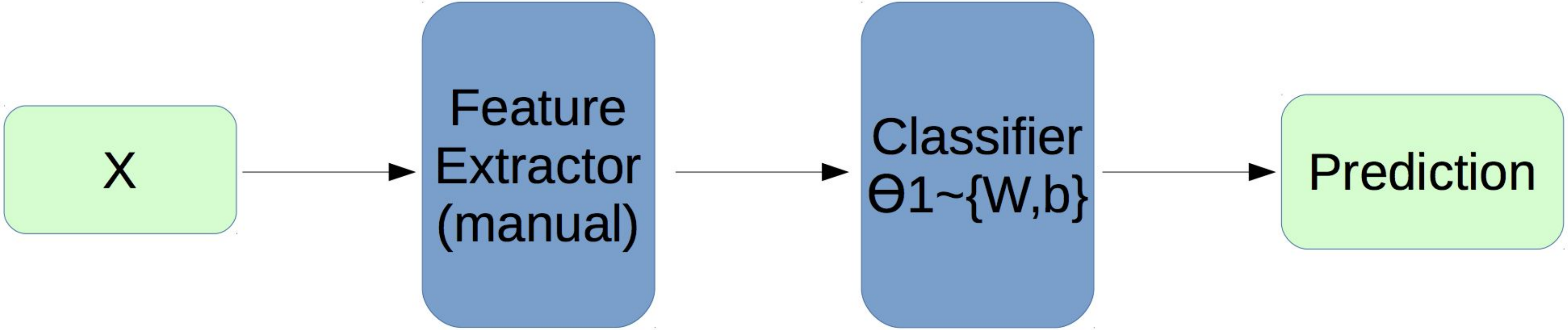


What we want

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

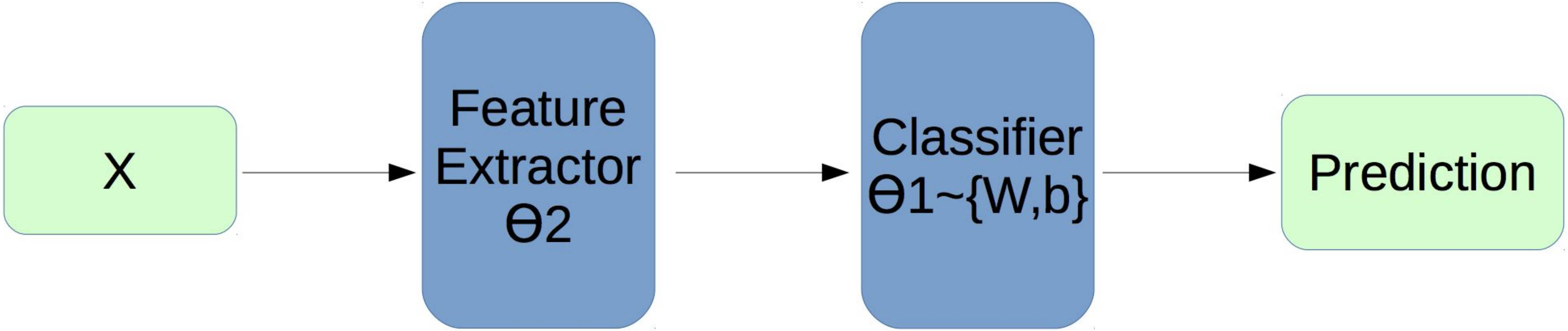
And feature engineering is an *art*.

Classic pipeline



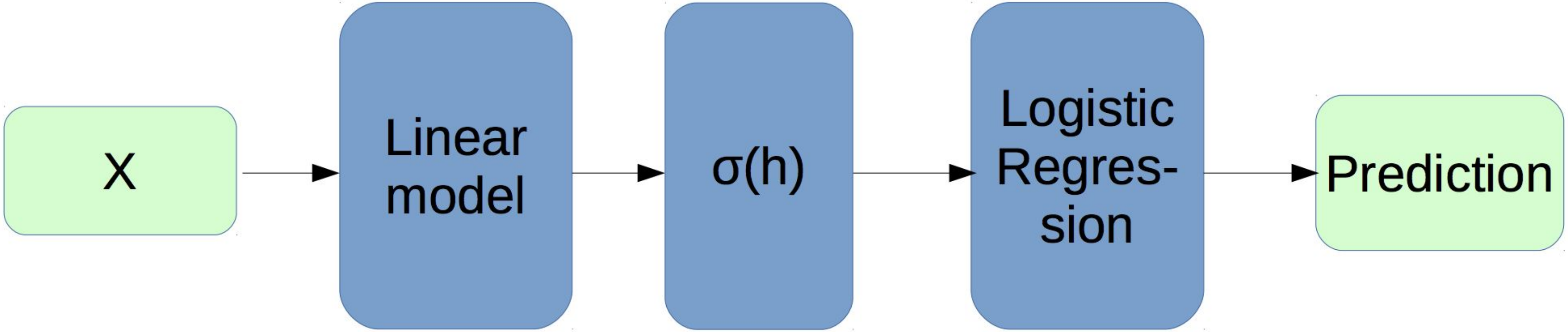
Handcrafted features, generated by experts.

NN pipeline



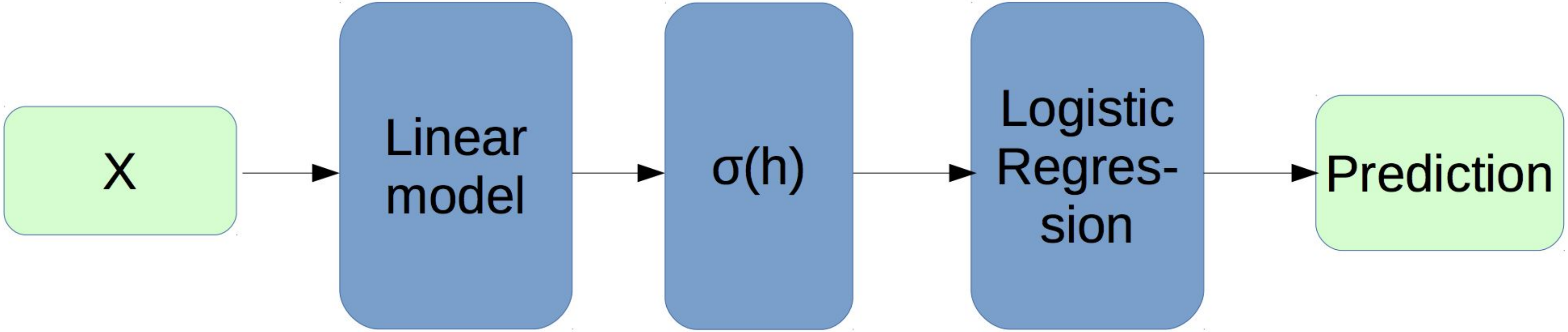
Automatically extracted features.

NN pipeline: example



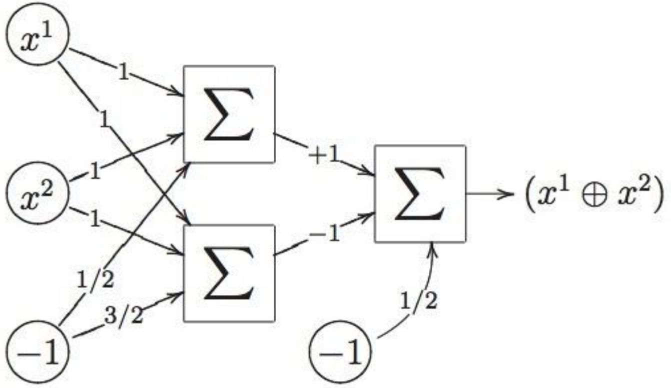
E.g. two logistic regressions one after another.

NN pipeline: example



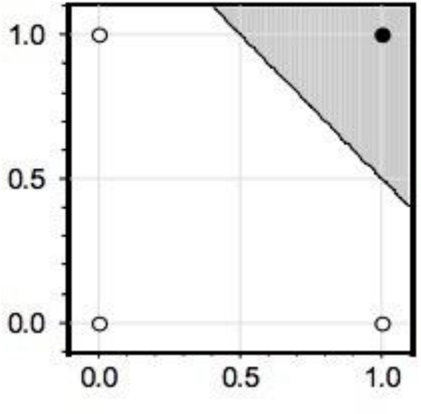
Actually, it’s a neural network.

XOR problem

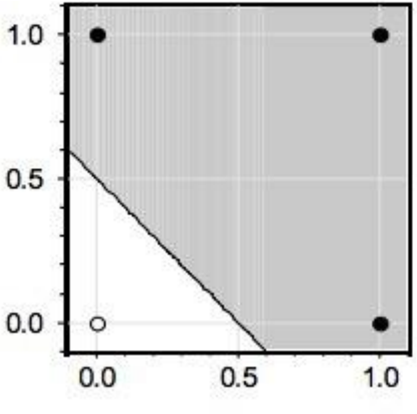


This 2-layer NN (on the left) implements XOR with only x1 and x2 features.

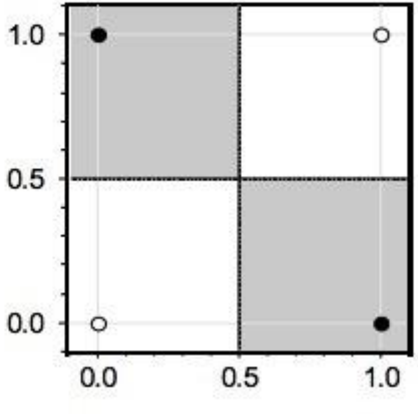
1-layer NN also can succeed, but only with extra feature x1*x2.



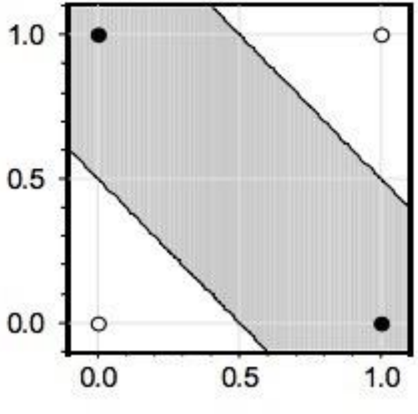
AND



OR



XOR(with x1*x2)



XOR

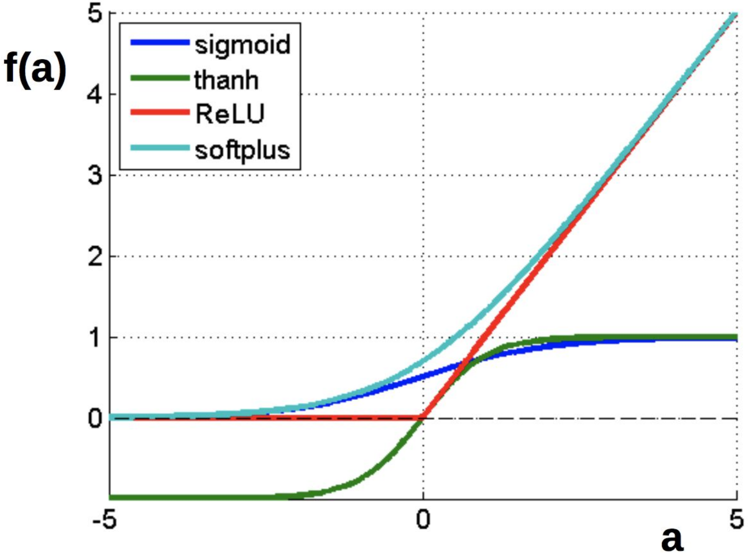
Activation functions: nonlinearities

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

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

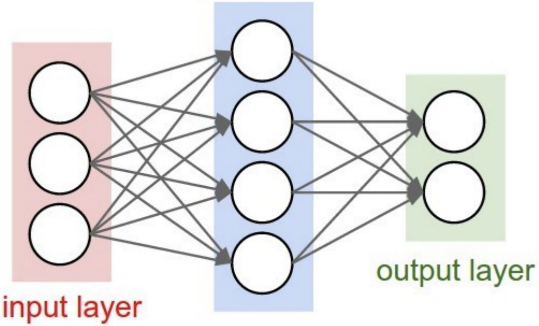
$$f(a) = \max(0, a)$$

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



Some generally accepted terms

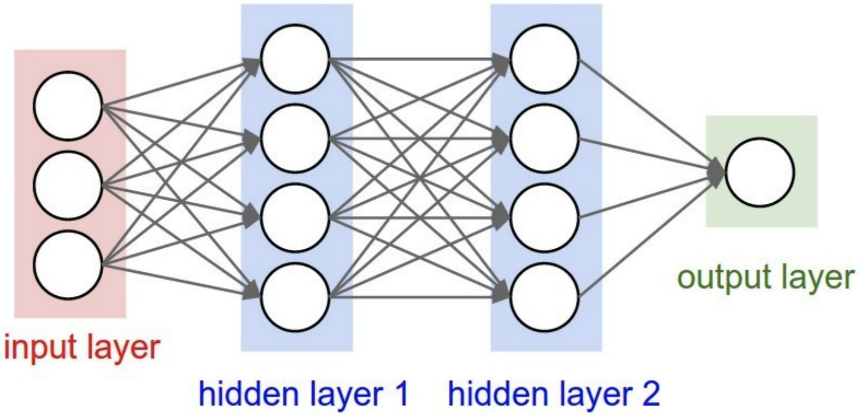
- Layer – a building block for NNs :
    - Dense layer: f(x) = Wx+b
    - Nonlinearity layer: f(x) = σ(x)
    - Input layer, output layer
    - A few more we will cover later
- Activation function – function applied to layer output
    - Sigmoid
    - tanh
    - ReLU
    - Any other function to get nonlinear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



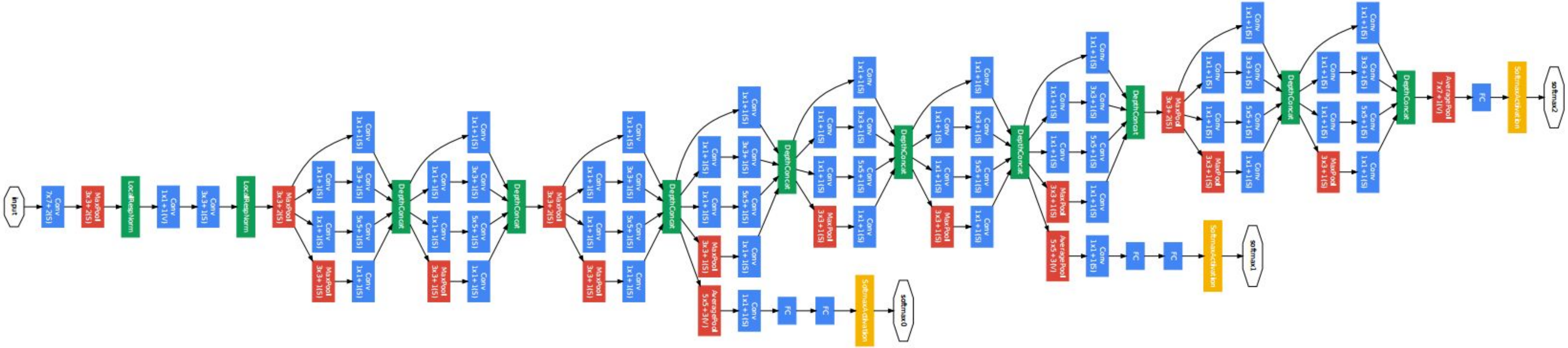
Dense layer
with a nonlinearity

“Train it via backprop!”

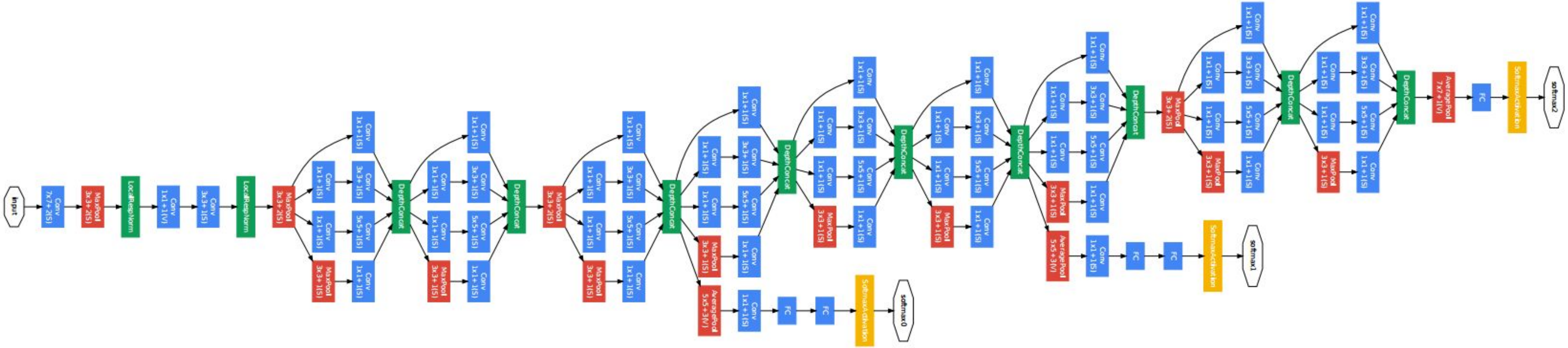
Actually, it can be deeper



Much deeper...


input
Conv 7x7+2(S)
MaxPool 3x3+2(S)
LocalRespNorm
Conv 1x1+1(V)
Conv 3x3+1(S)
LocalRespNorm
MaxPool 3x3+2(S)
Conv 1x1+1(S)
Conv 1x1+1(S)
Conv 1x1+1(S)
MaxPool 3x3+1(S)
Conv 1x1+1(S)
Conv 3x3+1(S)
Conv 5x5+1(S)
Conv 1x1+1(S)
DepthConcat
Conv 1x1+1(S)
Conv 1x1+1(S)
MaxPool 3x3+1(S)
Conv 1x1+1(S)
Conv 3x3+1(S)
Conv 5x5+1(S)
Conv 1x1+1(S)
DepthConcat
MaxPool 3x3+2(S)
Conv 1x1+1(S)
Conv 1x1+1(S)
MaxPool 3x3+1(S)
Conv 1x1+1(S)
Conv 3x3+1(S)
Conv 5x5+1(S)
Conv 1x1+1(S)
DepthConcat
Conv 1x1+1(S)
Conv 1x1+1(S)
MaxPool 3x3+1(S)
AveragePool 5x5+3(V)
Conv 1x1+1(S)
Conv 3x3+1(S)
Conv 5x5+1(S)
Conv 1x1+1(S)
Conv 1x1+1(S)
FC
FC
SoftmaxActivation
softmax0
DepthConcat
Conv 1x1+1(S)
Conv 1x1+1(S)
MaxPool 3x3+1(S)
Conv 1x1+1(S)
Conv 3x3+1(S)
Conv 5x5+1(S)
Conv 1x1+1(S)
DepthConcat
Conv 1x1+1(S)
Conv 1x1+1(S)
MaxPool 3x3+1(S)
Conv 1x1+1(S)
Conv 3x3+1(S)
Conv 5x5+1(S)
Conv 1x1+1(S)
DepthConcat
Conv 1x1+1(S)
Conv 1x1+1(S)
MaxPool 3x3+1(S)
AveragePool 5x5+3(V)
Conv 1x1+1(S)
Conv 3x3+1(S)
Conv 5x5+1(S)
Conv 1x1+1(S)
Conv 1x1+1(S)
FC
FC
SoftmaxActivation
softmax1
DepthConcat
MaxPool 3x3+2(S)
Conv 1x1+1(S)
Conv 1x1+1(S)
MaxPool 3x3+1(S)
Conv 1x1+1(S)
Conv 3x3+1(S)
Conv 5x5+1(S)
Conv 1x1+1(S)
DepthConcat
Conv 1x1+1(S)
Conv 1x1+1(S)
MaxPool 3x3+1(S)
Conv 1x1+1(S)
Conv 3x3+1(S)
Conv 5x5+1(S)
Conv 1x1+1(S)
DepthConcat
AveragePool 7x7+1(V)
FC
SoftmaxActivation
softmax2

Much deeper...

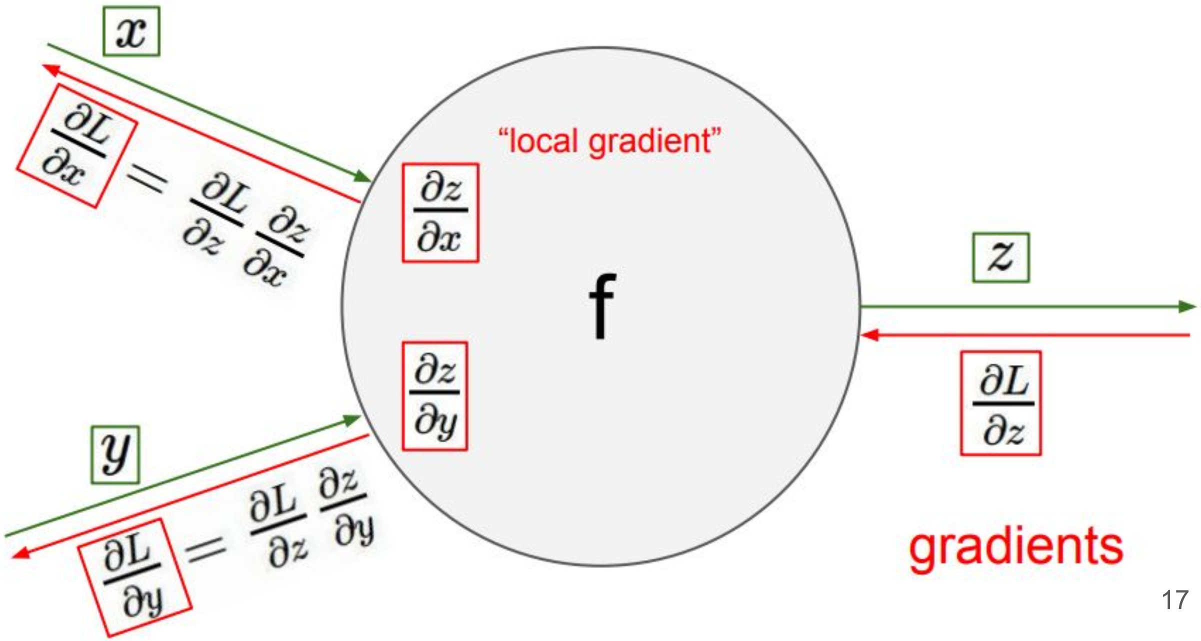


How to train it?

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.



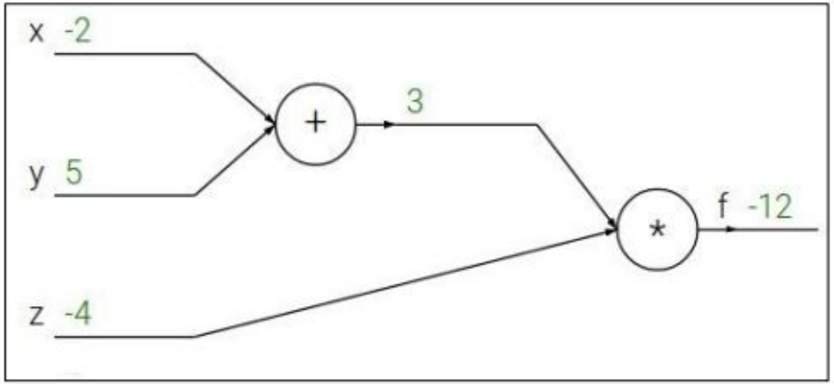
x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"local gradient"
$\frac{\partial z}{\partial x}$
f
$\frac{\partial z}{\partial y}$
z
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
gradients

source: http://cs231n.github.io

Backpropagation example

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

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



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Backpropagation example

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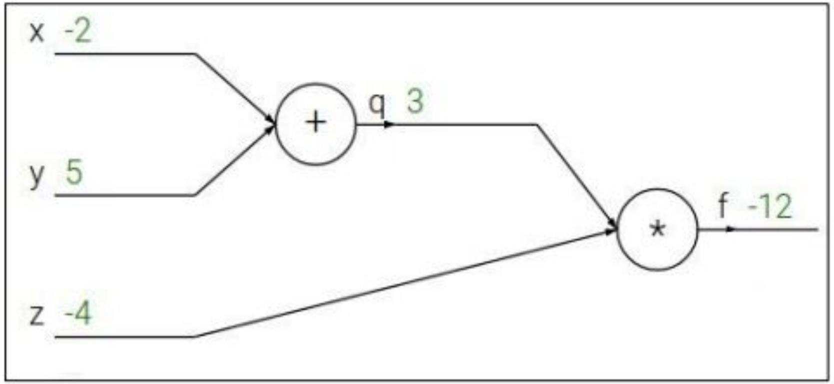
Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



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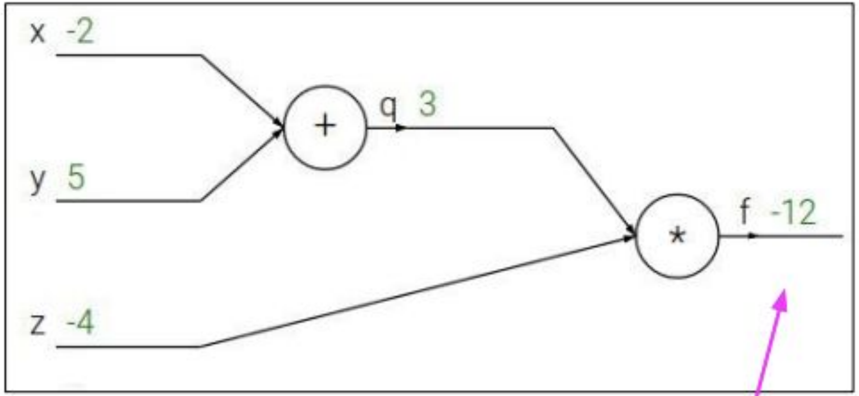

$\frac{\partial f}{\partial f}$

source: http://cs231n.github.io

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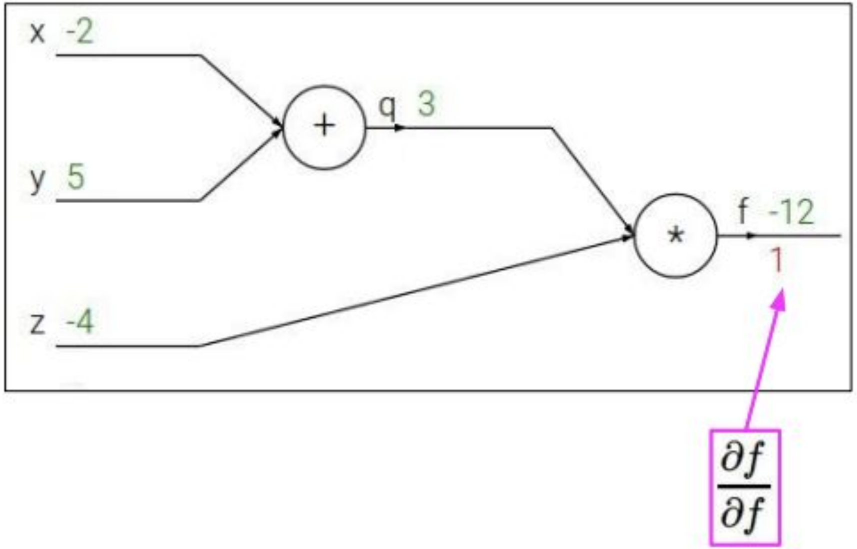

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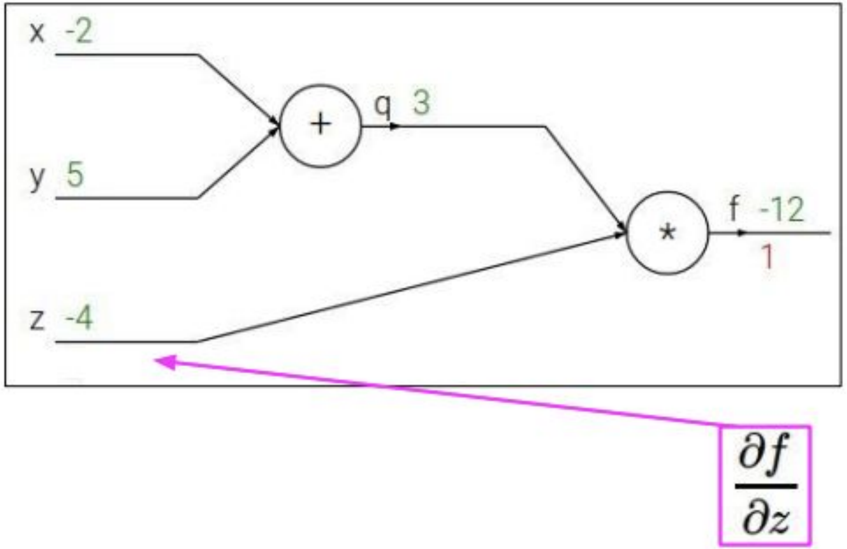

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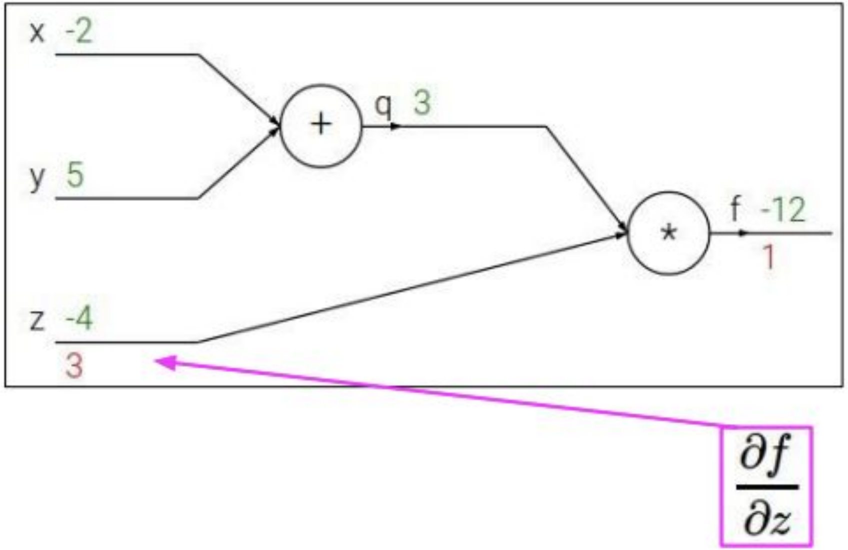

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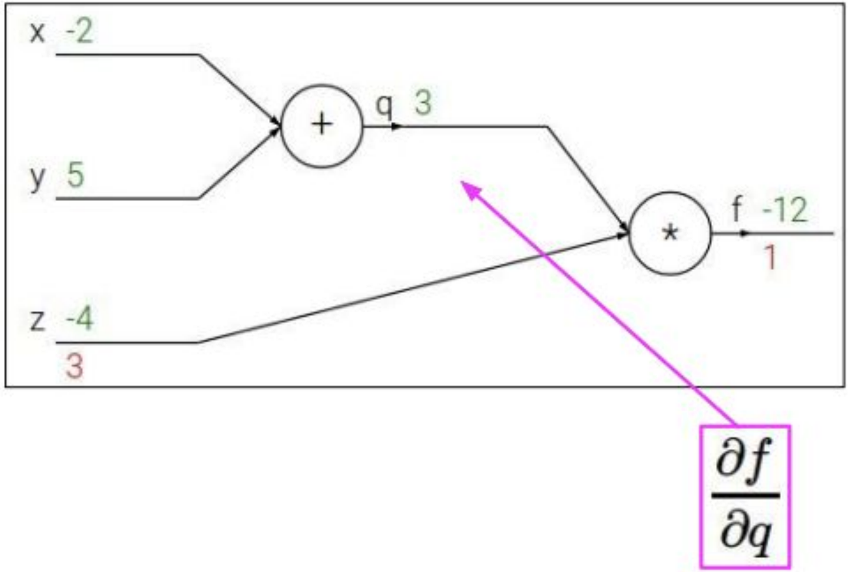

$$\frac{\partial f}{\partial q}$$

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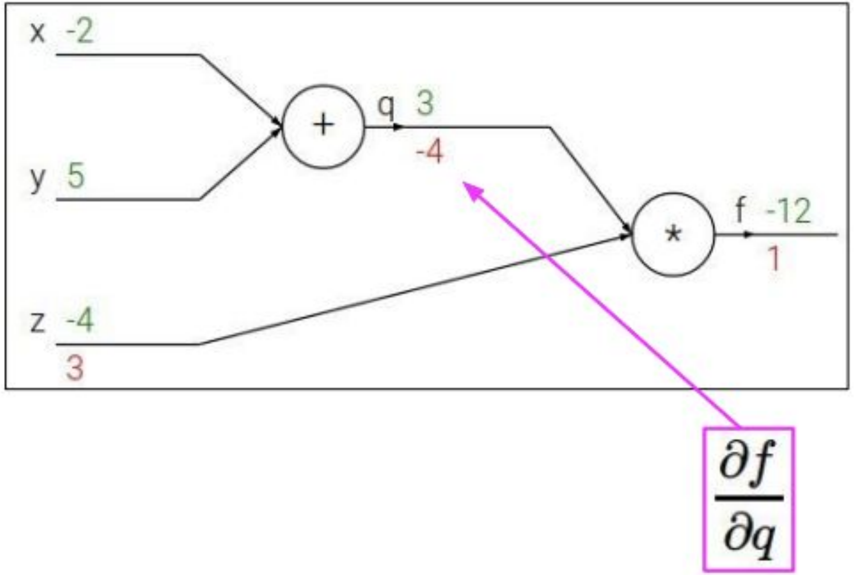

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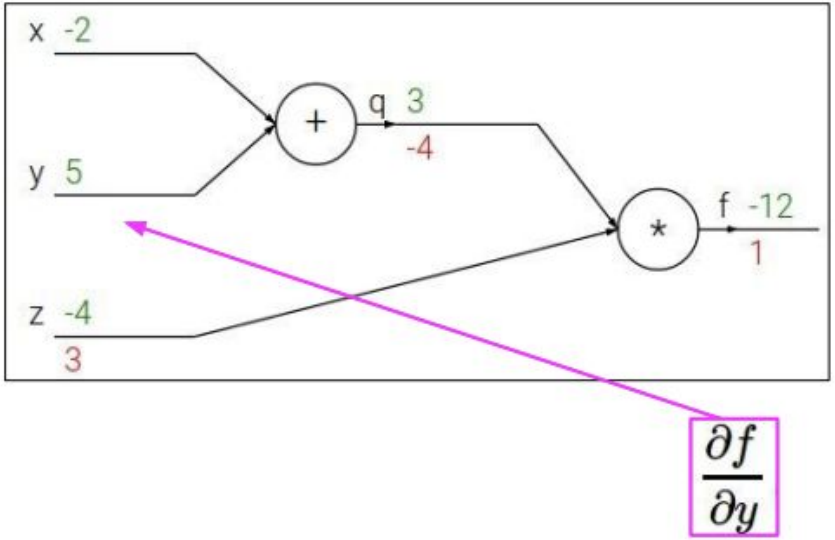

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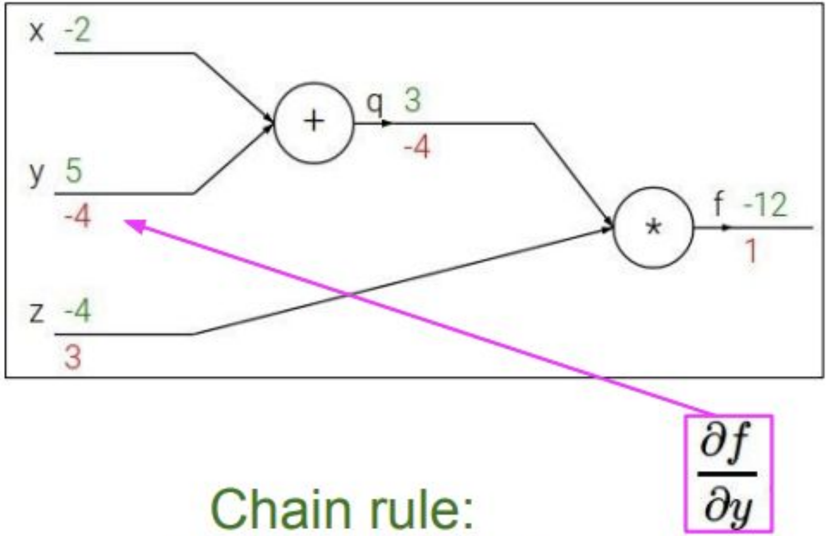

Chain rule:

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

source: http://cs231n.github.io

Backpropagation example

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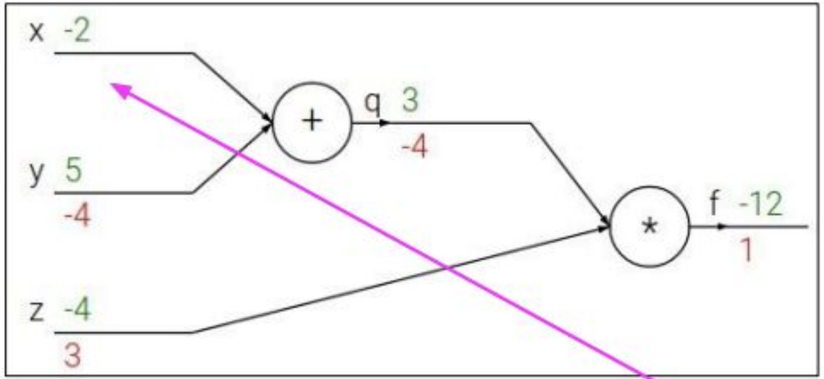

$$\frac{\partial f}{\partial x}$$

source: http://cs231n.github.io

Backpropagation example

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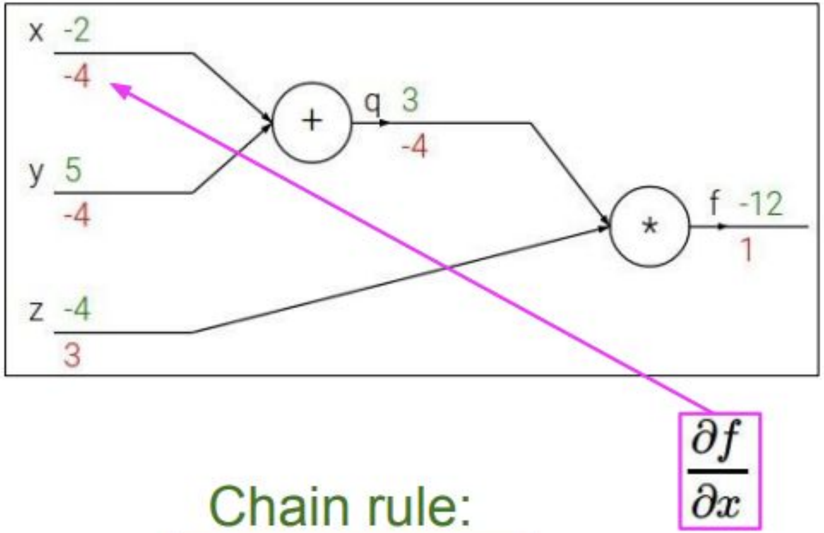


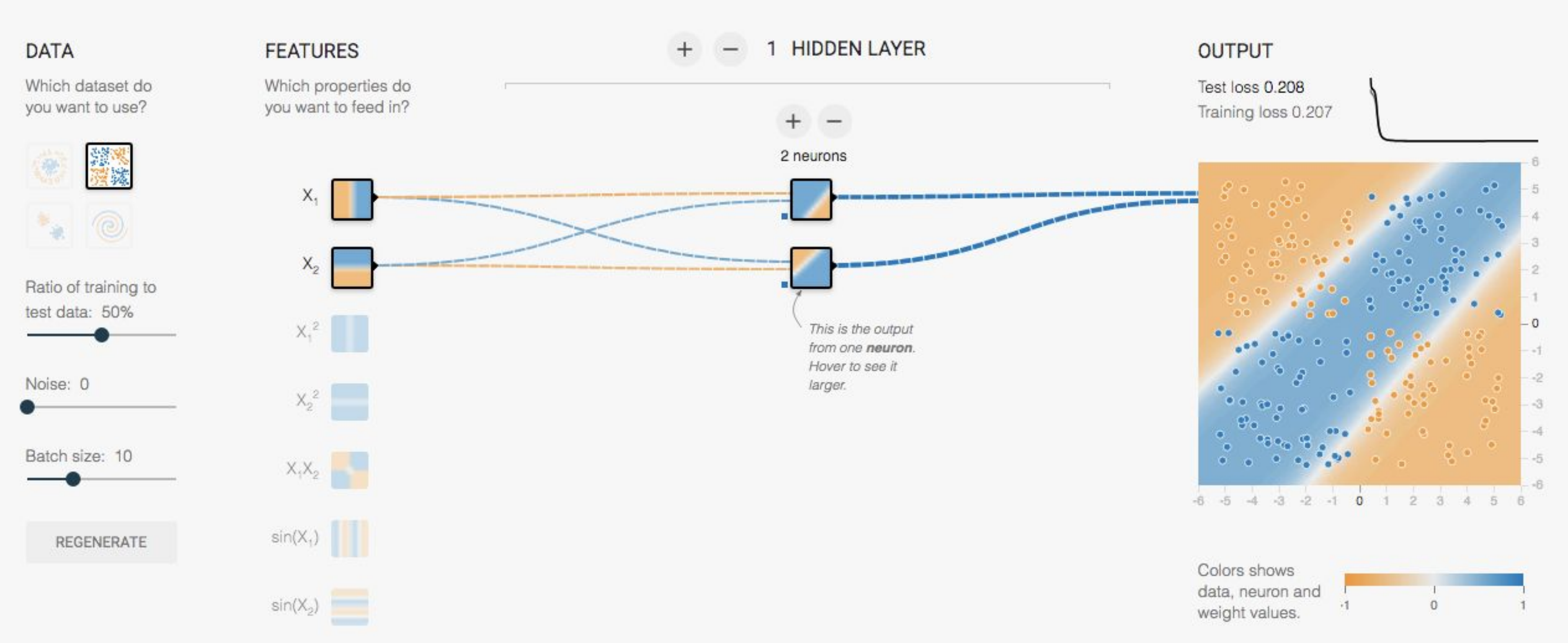
$\frac{\partial f}{\partial x}$

Chain rule:

$$\boxed{\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q}\frac{\partial q}{\partial x}}$$

source: http://cs231n.github.io

Practice time: interactive playground



DATA

Which dataset do you want to use?

Ratio of training to test data: 50%

Noise: 0

Batch size: 10

REGENERATE

FEATURES

Which properties do you want to feed in?

1 HIDDEN LAYER

2 neurons

*This is the output from one **neuron**. Hover to see it larger.*

OUTPUT

Test loss 0.208

Training loss 0.207

Colors shows data, neuron and weight values.

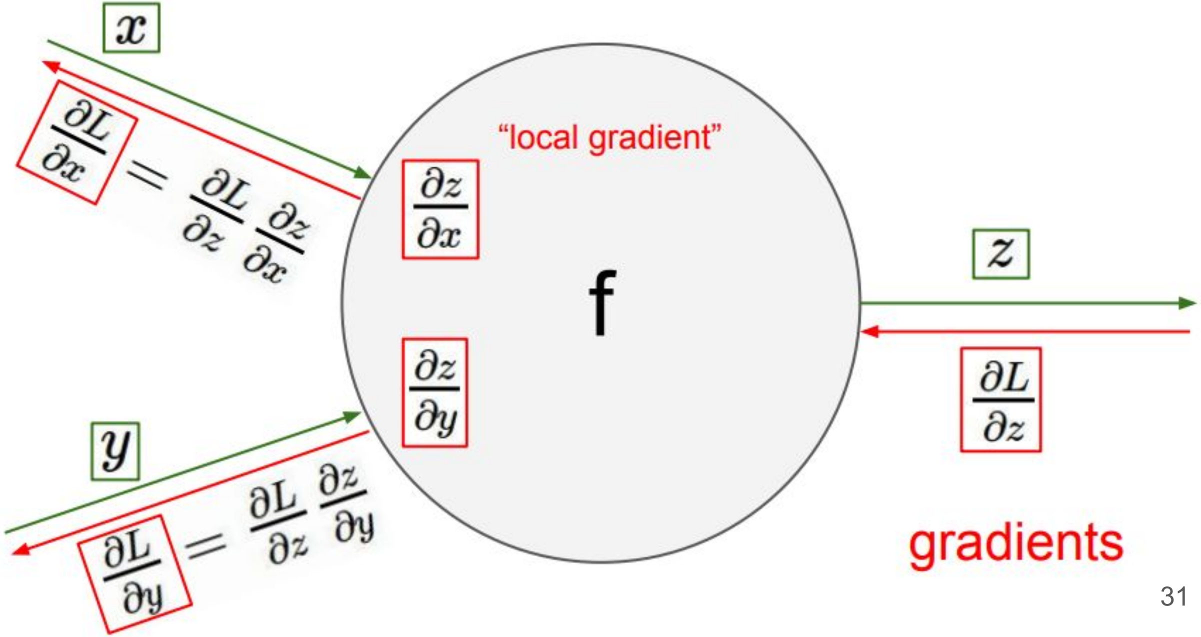
□ Show test data □ Discretize output

https://playground.tensorflow.org/

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.



x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
"local gradient"
$\frac{\partial z}{\partial x}$
f
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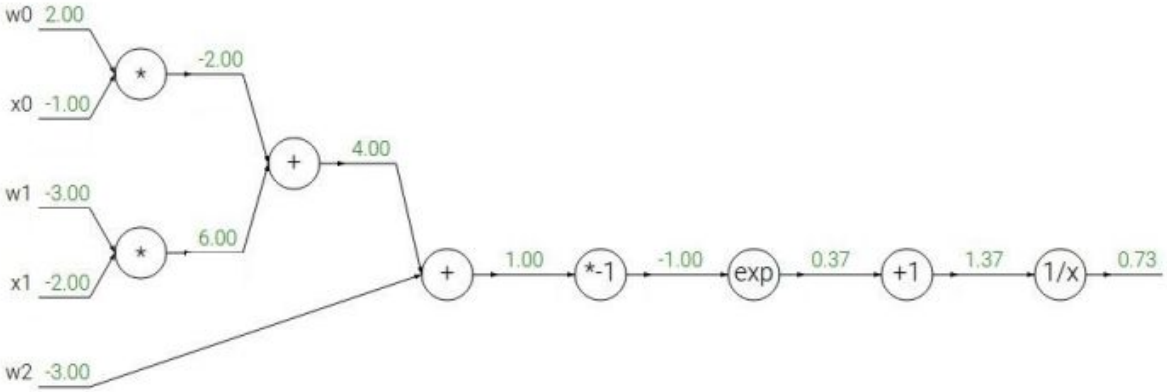
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
gradients

source: http://cs231n.github.io

Backpropagation example

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



source: http://cs231n.github.io

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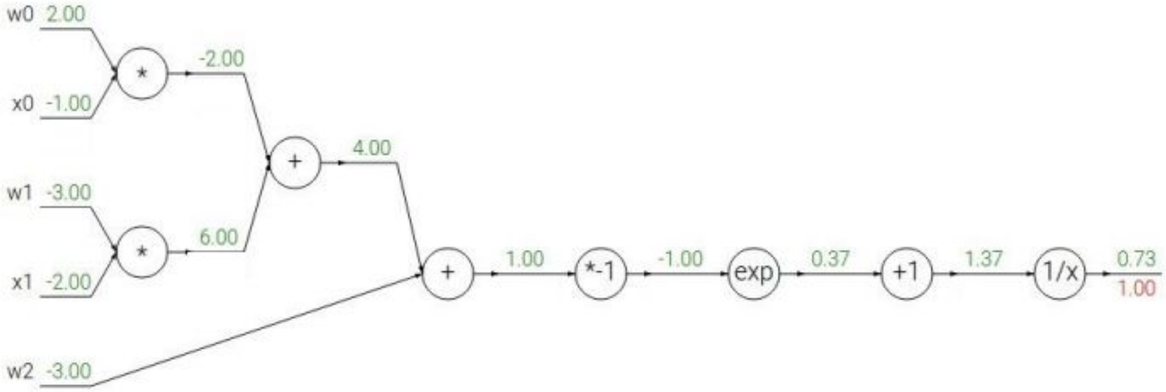

$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$

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

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

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

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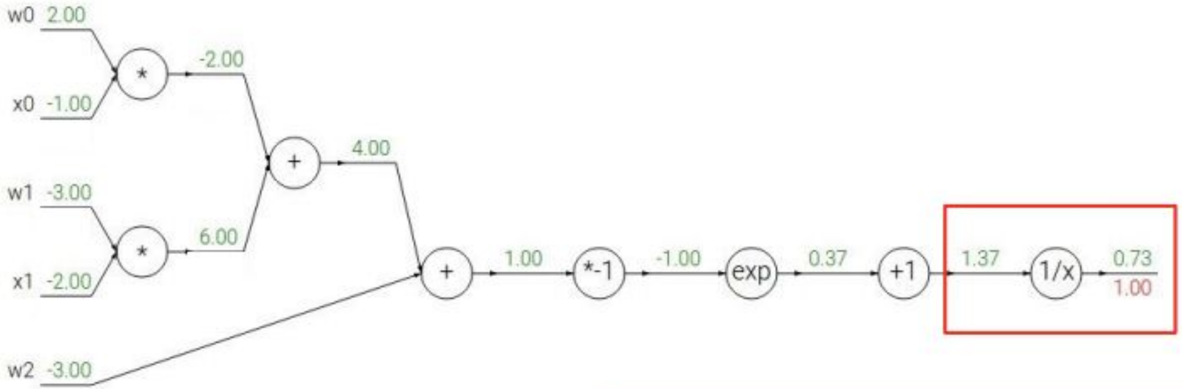

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$$\boxed{f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2}$$

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

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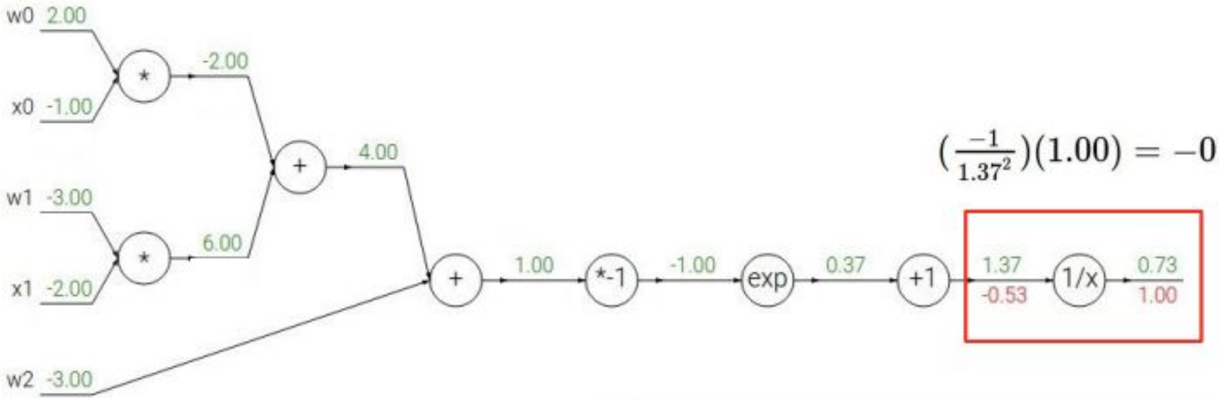

$(\frac{-1}{1.37^2})(1.00) = -0.53$

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

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

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

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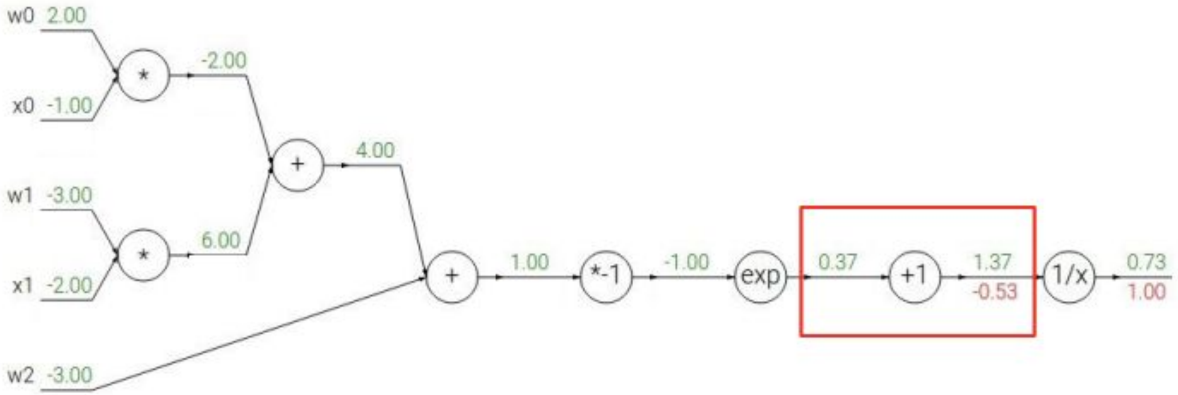


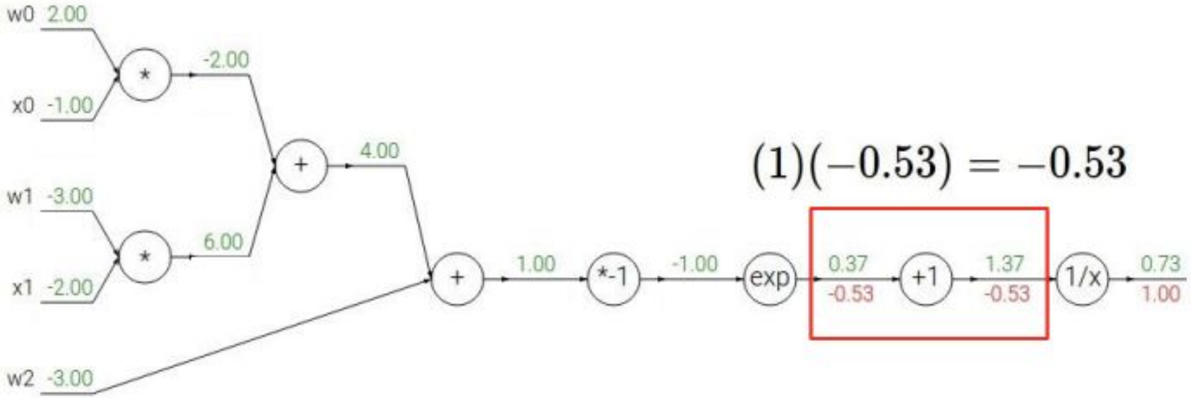
$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x \qquad\qquad f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$$

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

source: http://cs231n.github.io

Backpropagation example

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



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

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

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

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

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Backpropagation example

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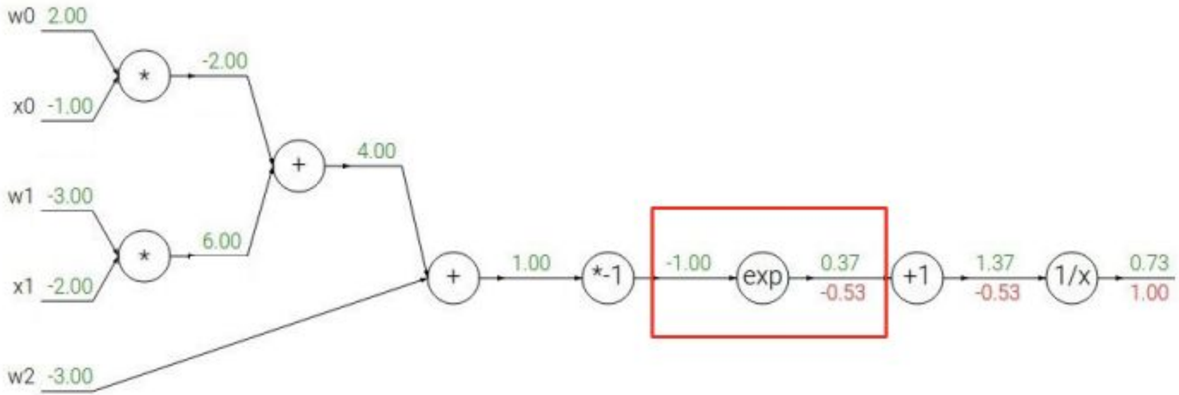

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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

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Backpropagation example

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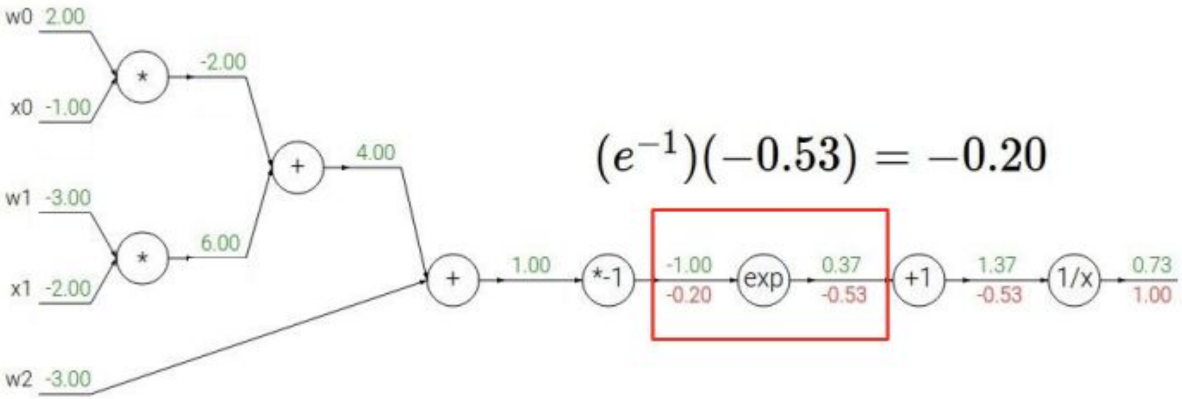

$$(e^{-1})(-0.53) = -0.20$$

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

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

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

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Backpropagation example

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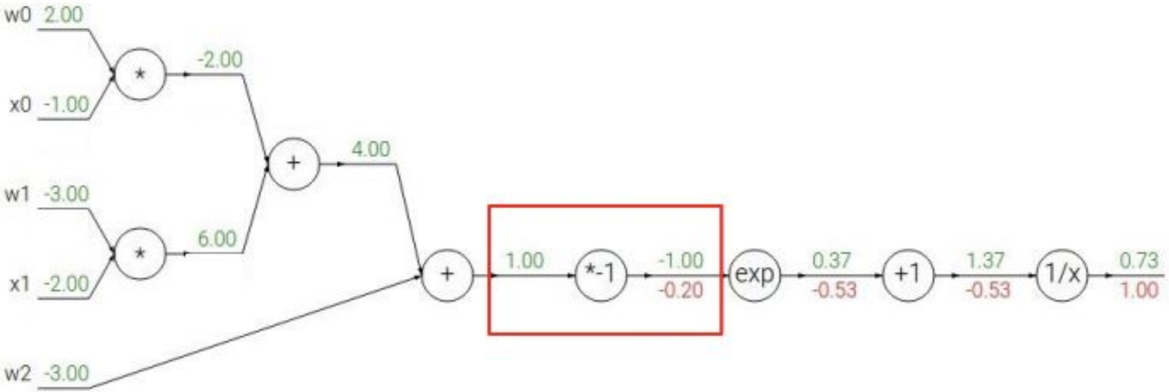

$$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$$

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

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Backpropagation example

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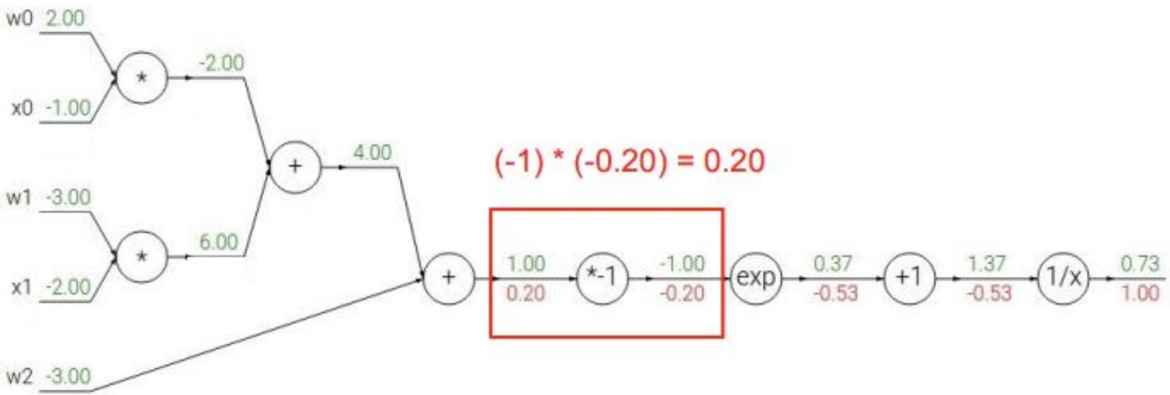

(-1) * (-0.20) = 0.20

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

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

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Backpropagation example

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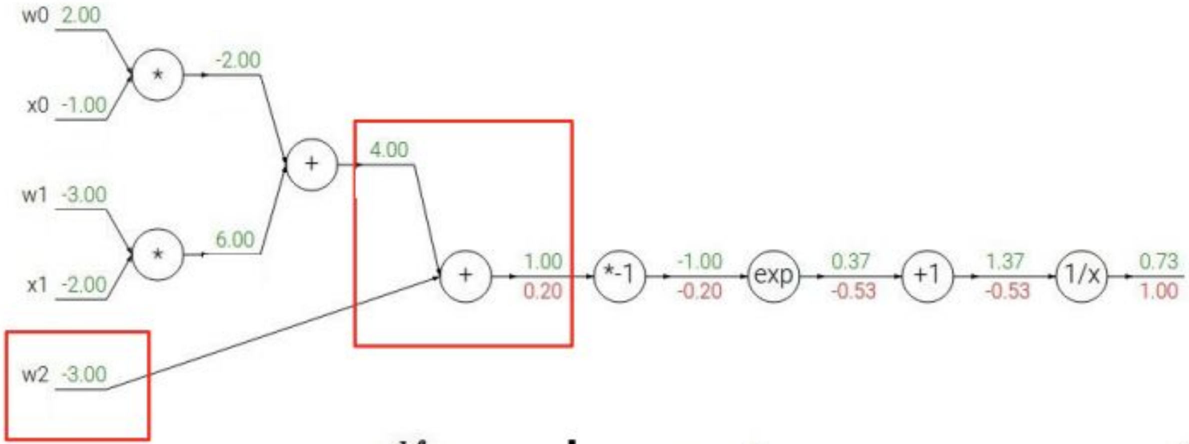

$f(x) = e^x \quad \rightarrow \quad \frac{df}{dx} = e^x$ | $f(x) = \frac{1}{x} \quad \rightarrow \quad \frac{df}{dx} = -1/x^2$

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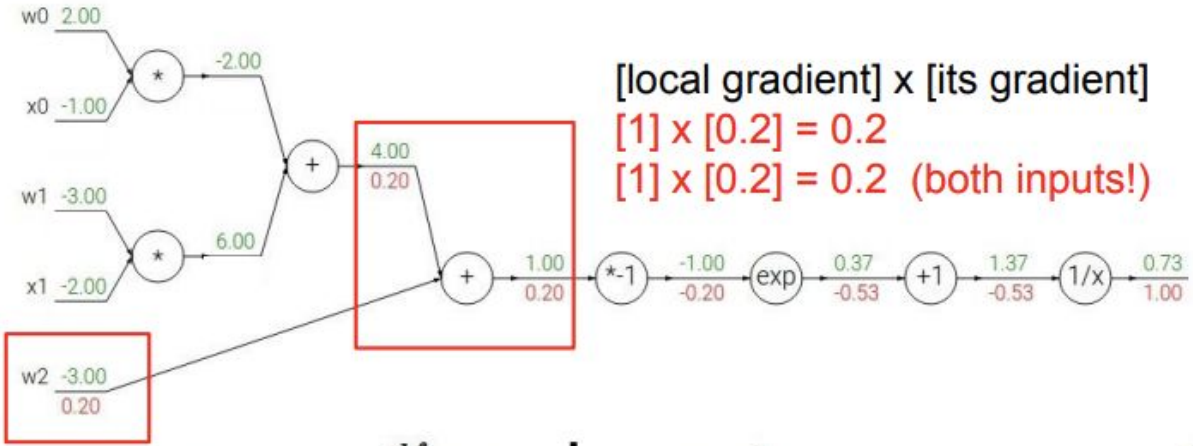


[local gradient] x [its gradient]

[1] x [0.2] = 0.2

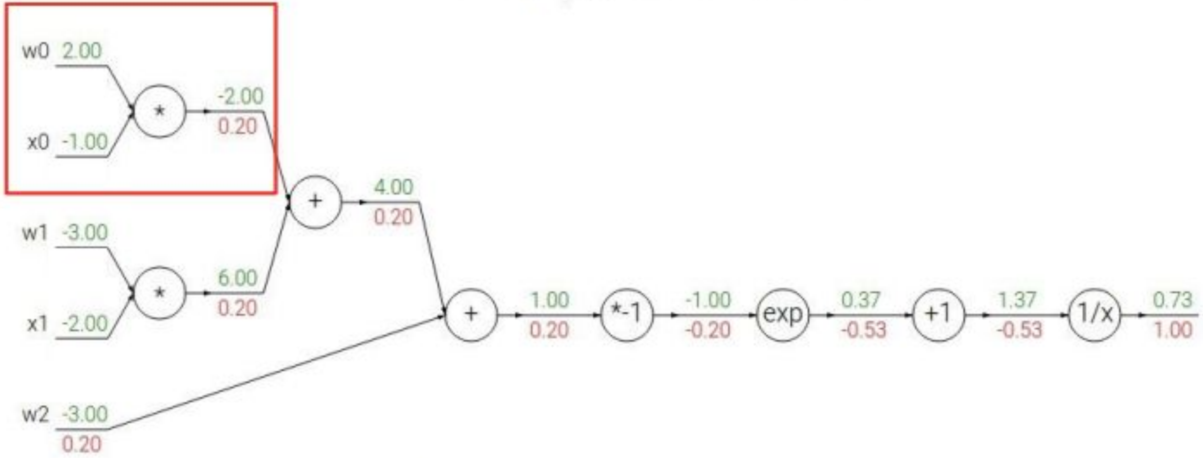
[1] x [0.2] = 0.2 (both inputs!)

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

source: http://cs231n.github.io

Backpropagation example

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



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

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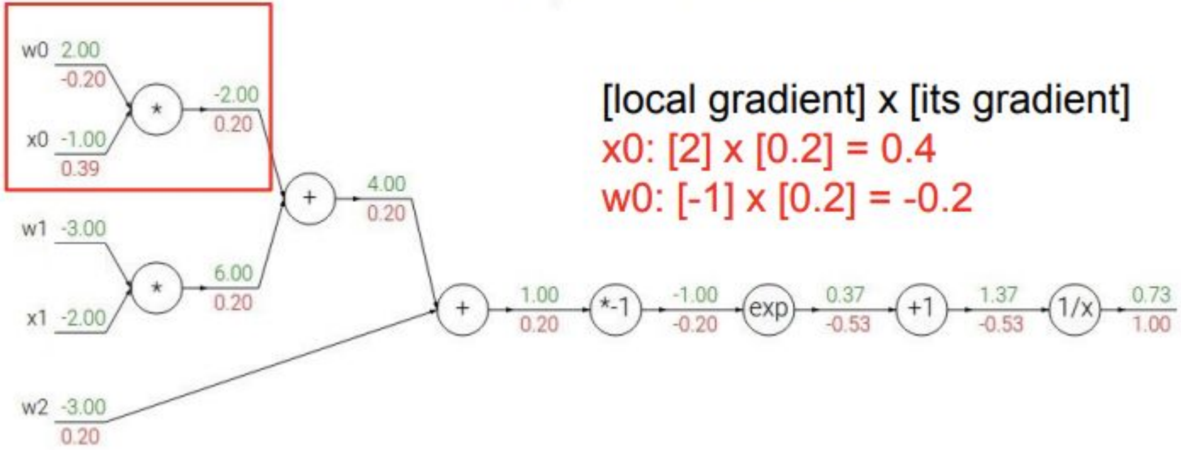
Backpropagation example

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



[local gradient] x [its gradient]

x0: [2] x [0.2] = 0.4

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

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

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

source: http://cs231n.github.io

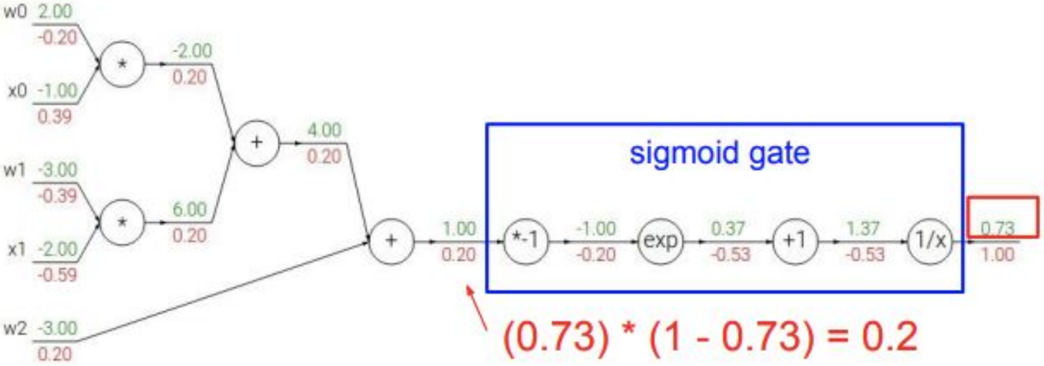
Backpropagation example

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

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

sigmoid function

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



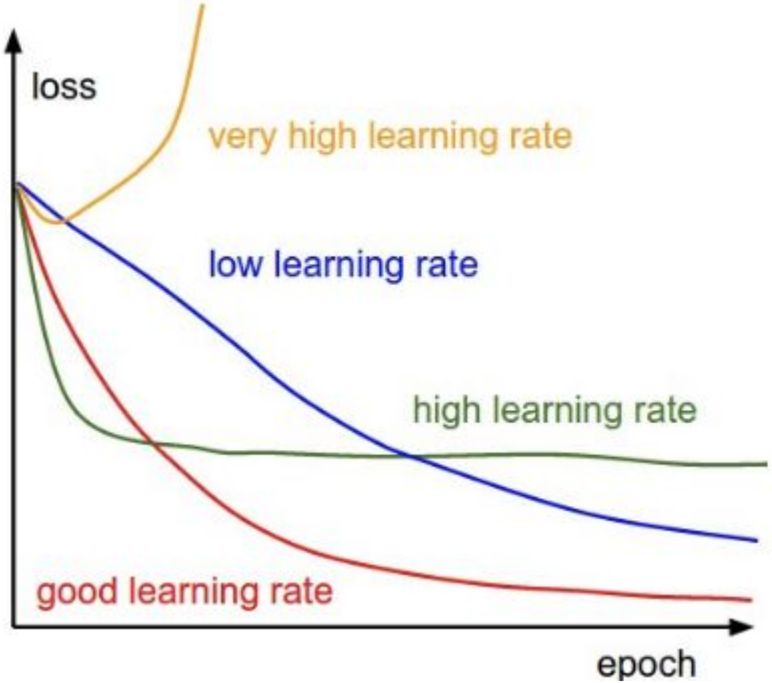
(0.73) * (1 - 0.73) = 0.2

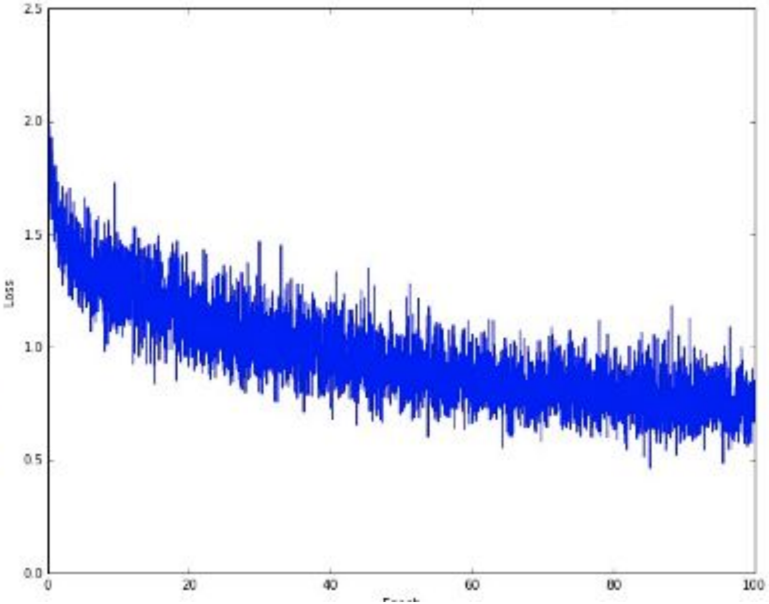
source: http://cs231n.github.io

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/

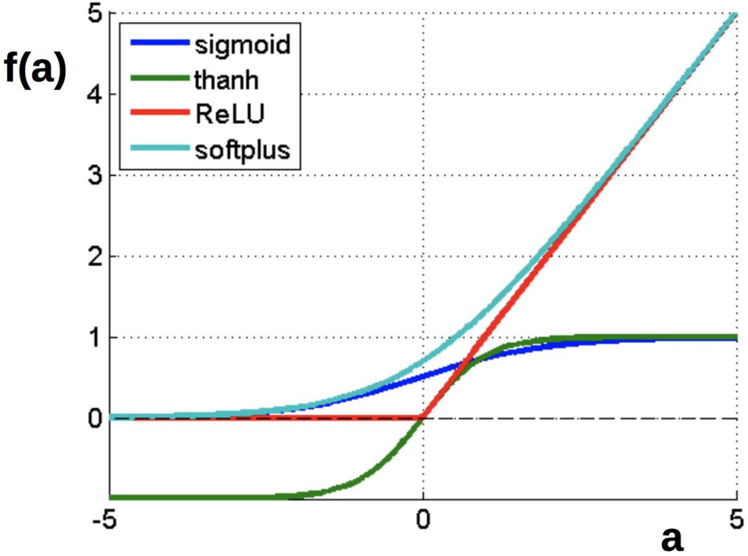
Once more: nonlinearities

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

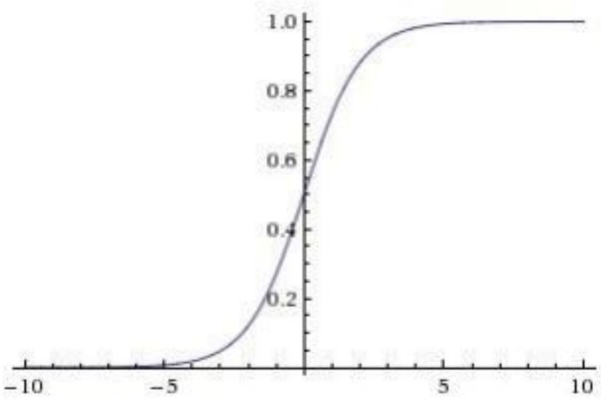
$$f(a) = \tanh(a)$$

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

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



Activation functions



Sigmoid

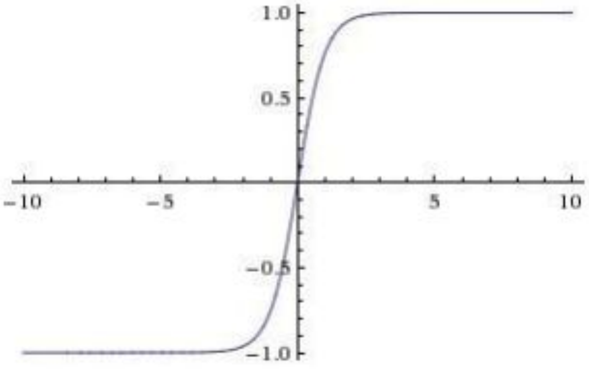
$$f(a) = \frac{1}{1 + e^{a}}$$

- 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

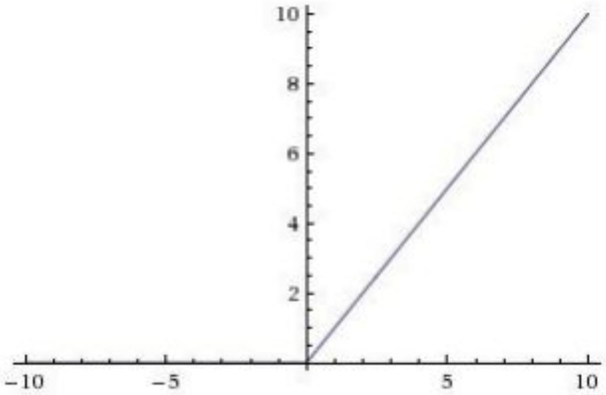


tanh(x)

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

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

Activation functions



ReLU
(Rectified Linear Unit)

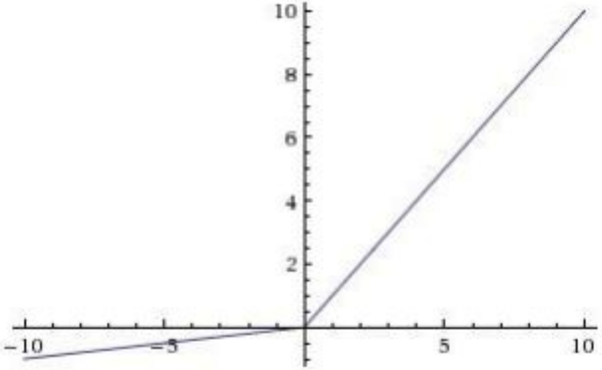
$$f(a) = \max(0, a)$$

- 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

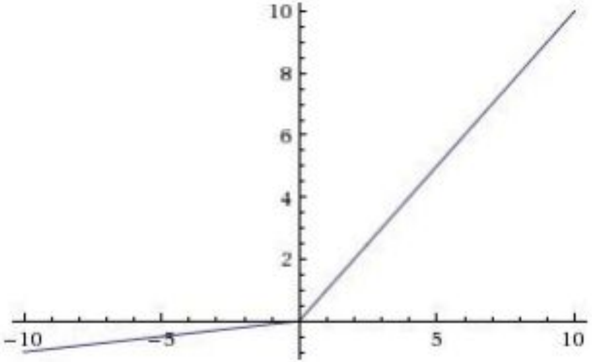


Leaky ReLU

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

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

Activation functions



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

Leaky ReLU

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

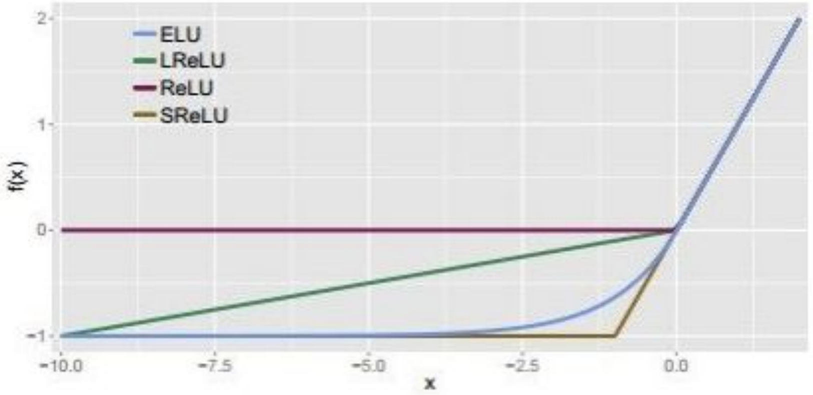
Parametric Rectifier (PReLU)

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

backprop into \alpha (parameter)

Activation functions

Exponential Linear Units (ELU)



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

- 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

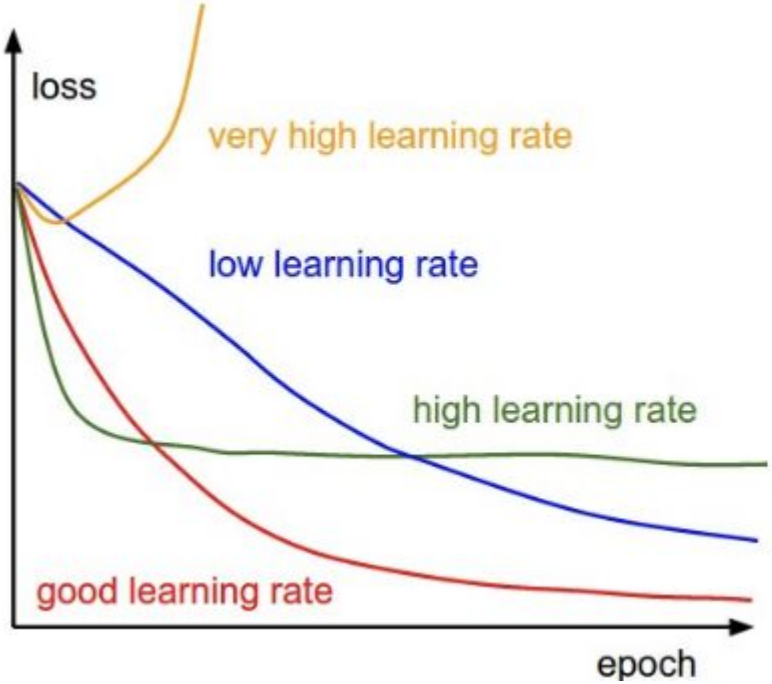
That’s all. Time to build some NN.

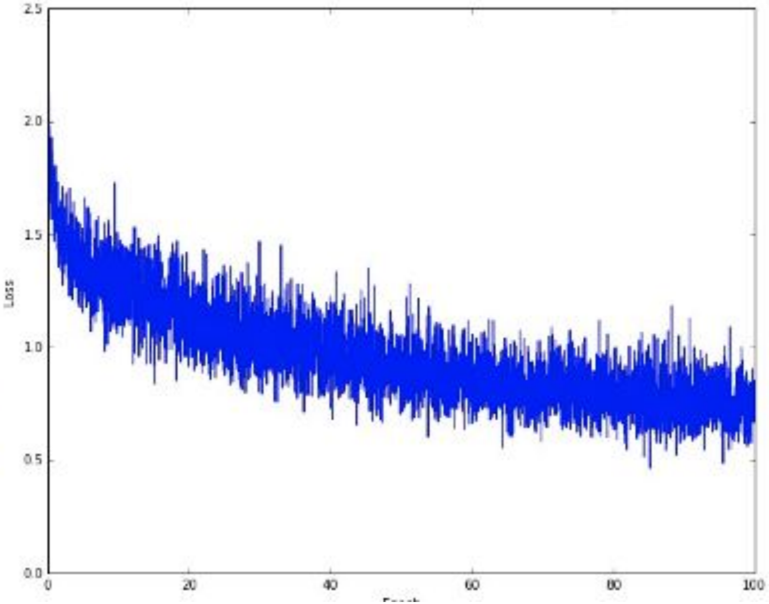
Backup

Optimizers

Stochastic gradient descent is used to optimize NN parameters.

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



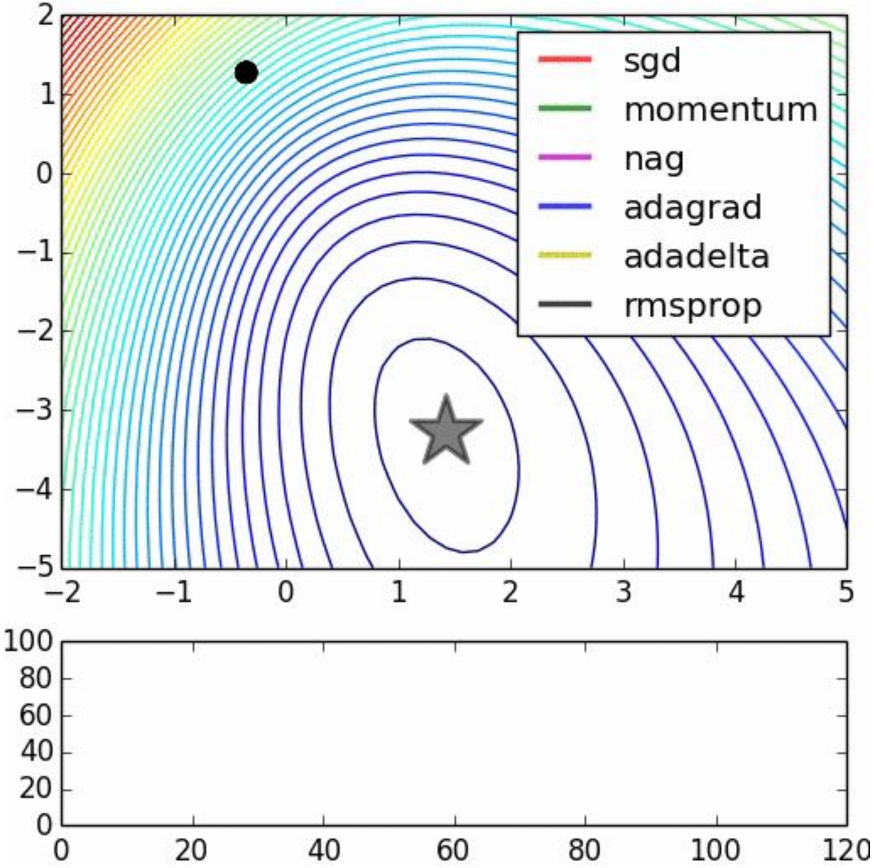


source: http://cs231n.github.io/neural-networks-3/

Optimizers

There are much more optimizers:

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

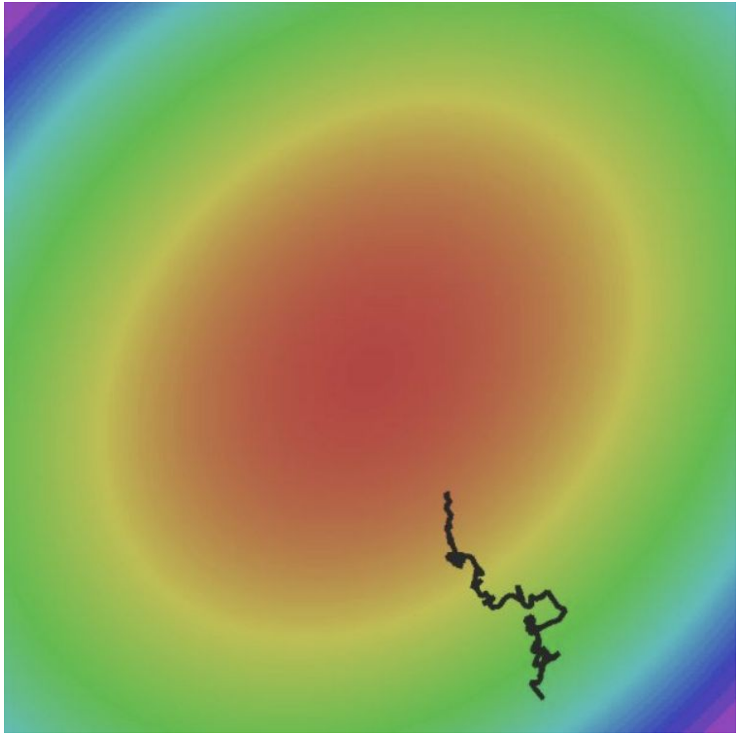


Optimization: SGD

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

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

Averaging over minibatches ---> noisy gradient



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

First idea: momentum

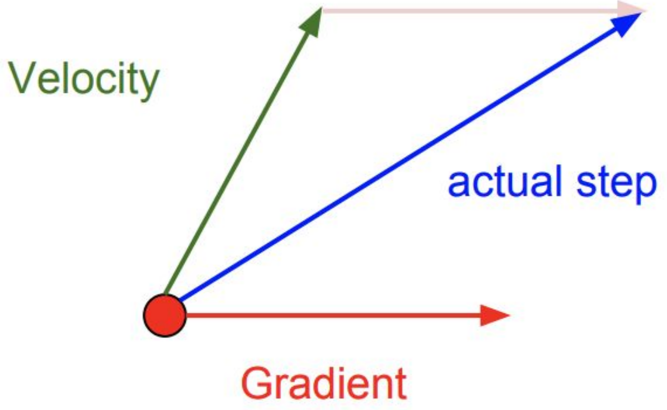
Simple SGD

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

SGD with momentum

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

Momentum update:



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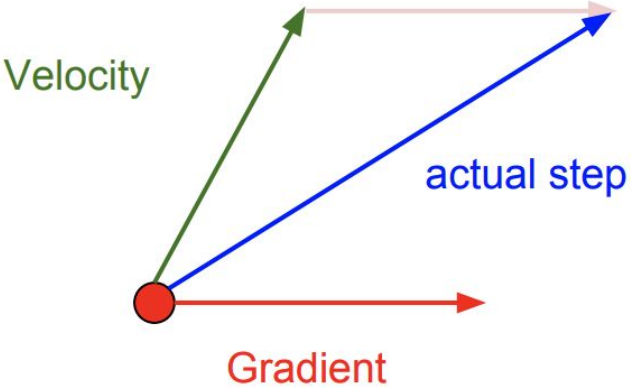
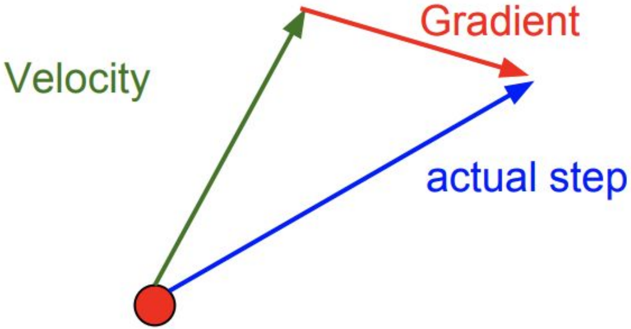
Nesterov momentum

Momentum update:



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

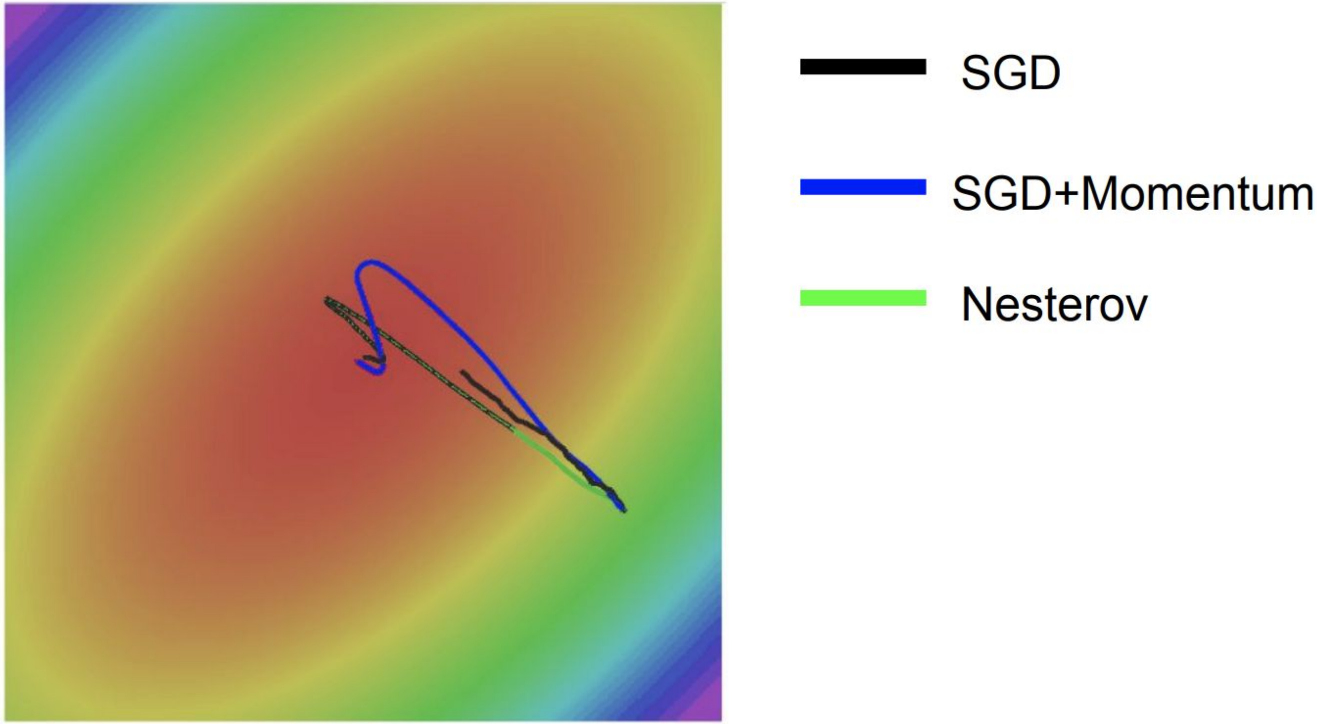
Nesterov Momentum



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

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

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

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

Problem: gradient fades with time

Second idea: different dimensions are different

Adagrad: SGD with cache

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

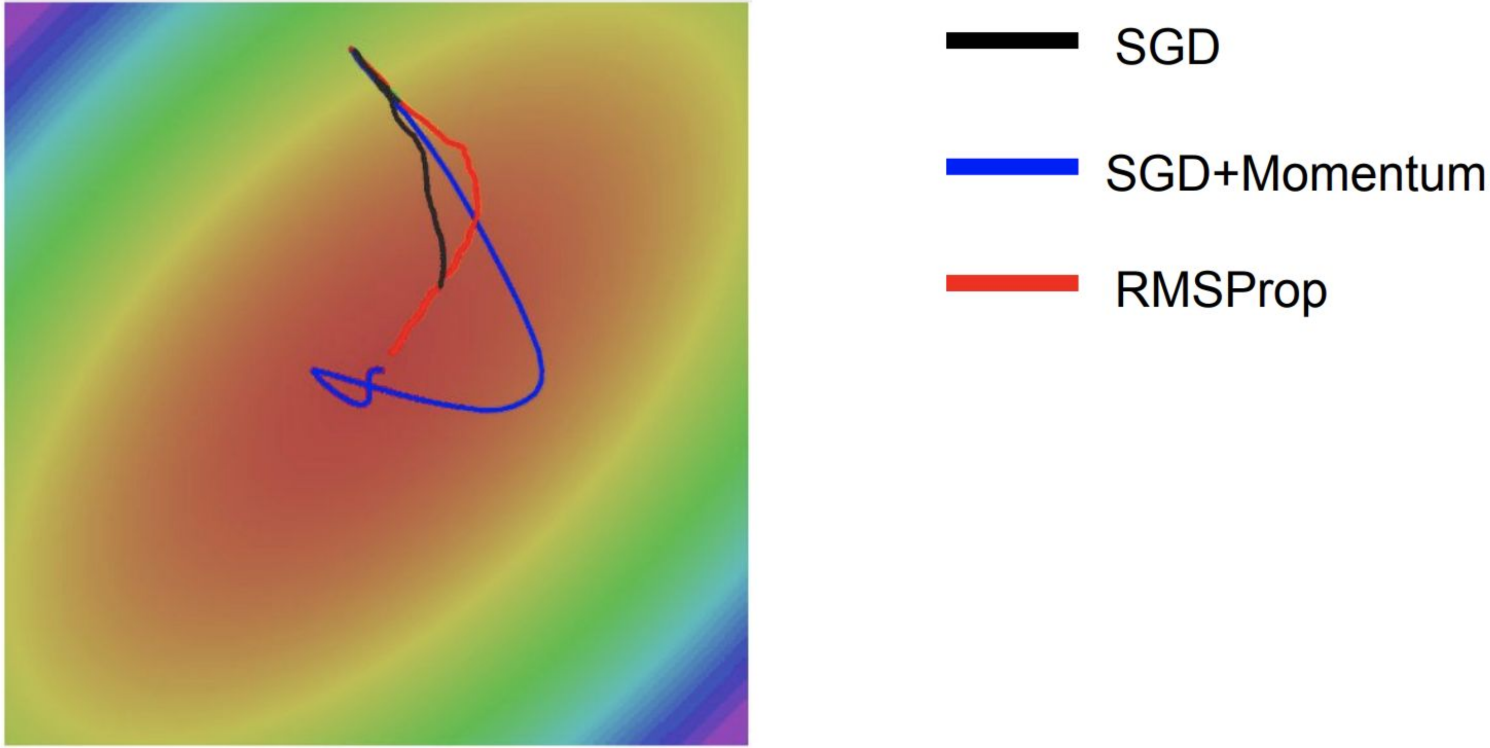
$$x_{t+1} = x_t - \alpha \frac{\nabla f(x_t)}{\text{cache}_{t+1} + \varepsilon}$$

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

Let’s combine the momentum idea and RMSProp normalization:

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

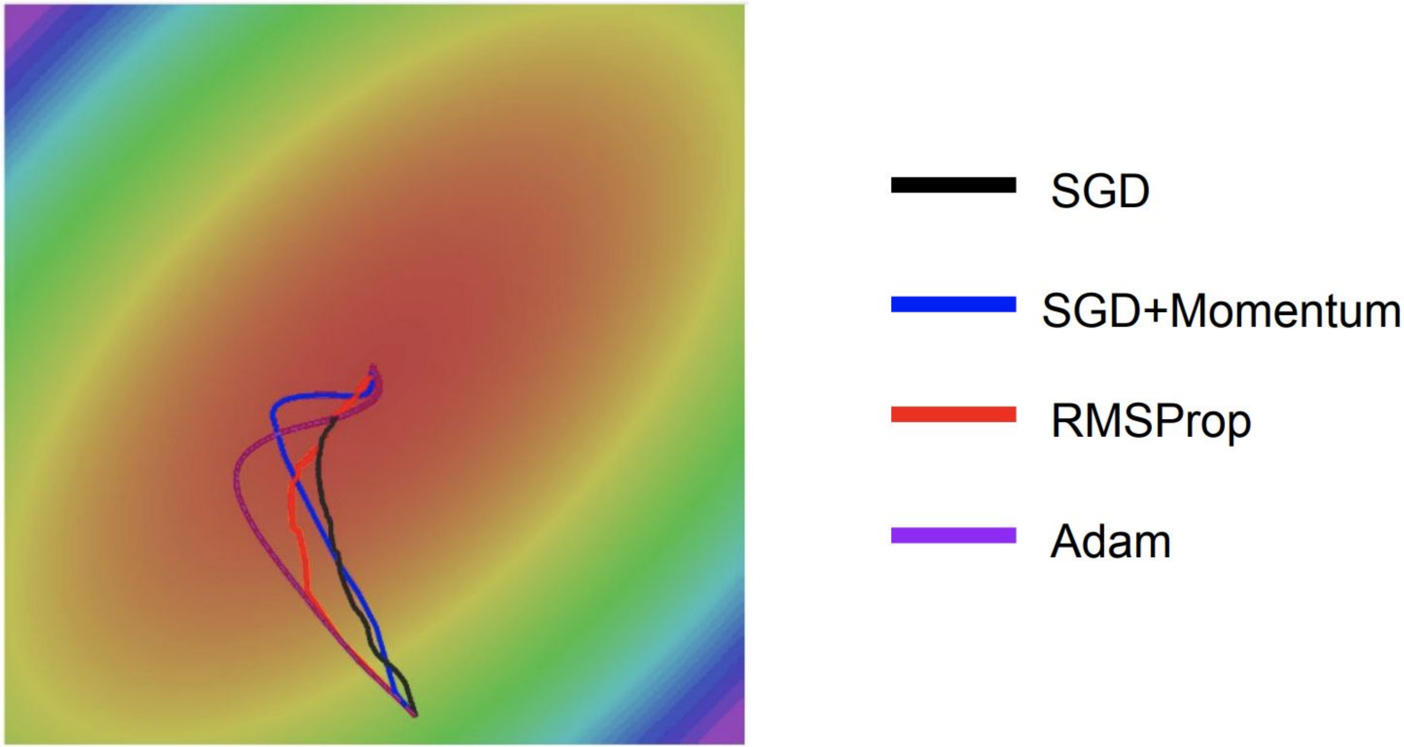
$$\text{cache}_{t+1} = \beta \text{cache}_t + (1-\beta)(\nabla f(x_t))^2$$

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

Actually, that’s not quite Adam.

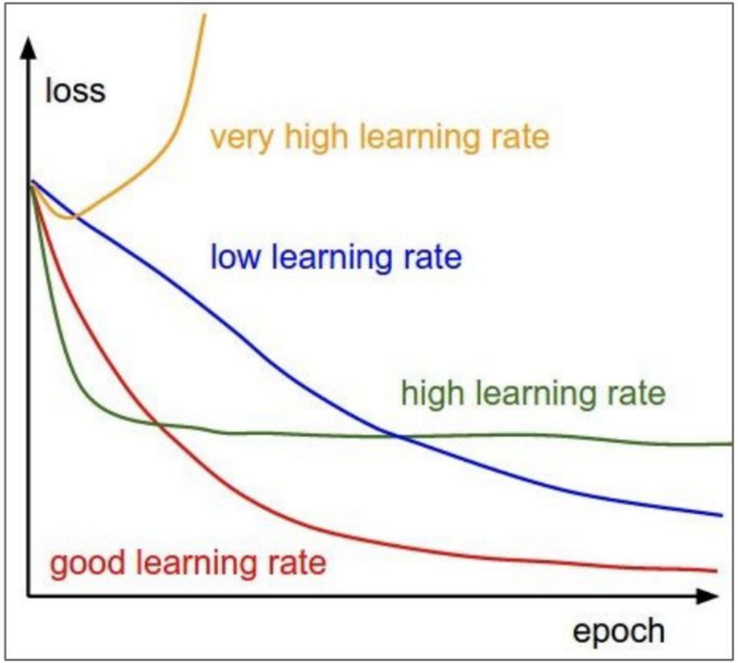
Adam full form involves bias correction term. See http://cs231n.github.io/neural-networks-3/ for more info.

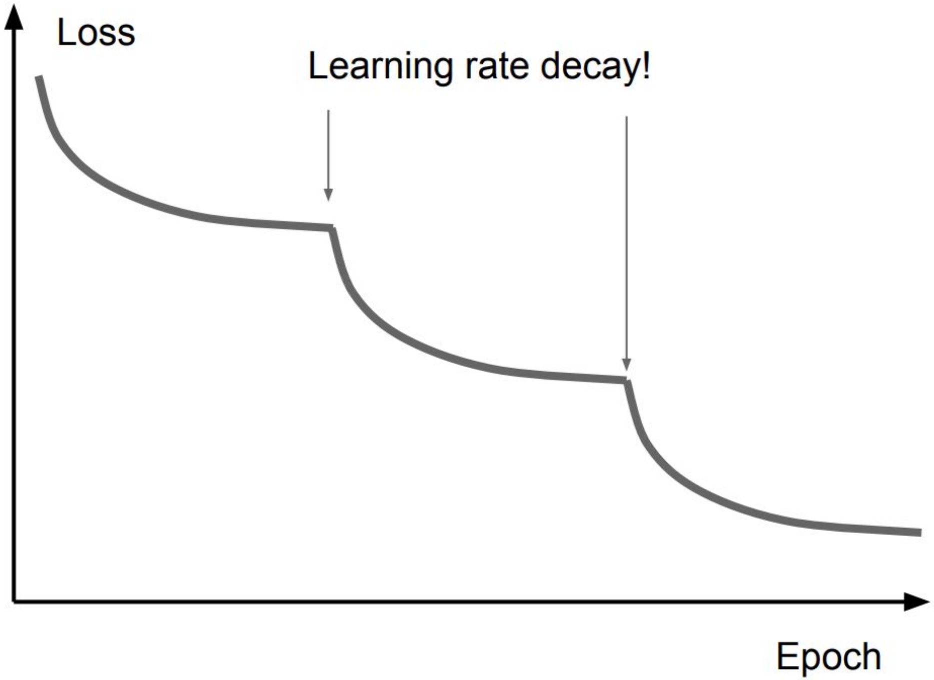
Comparing optimizers



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

Once more: learning rate

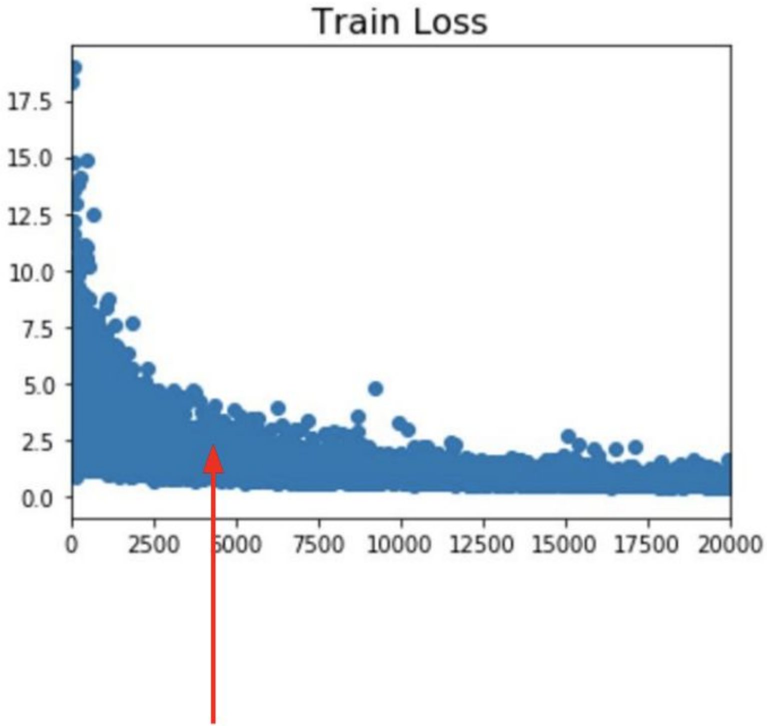




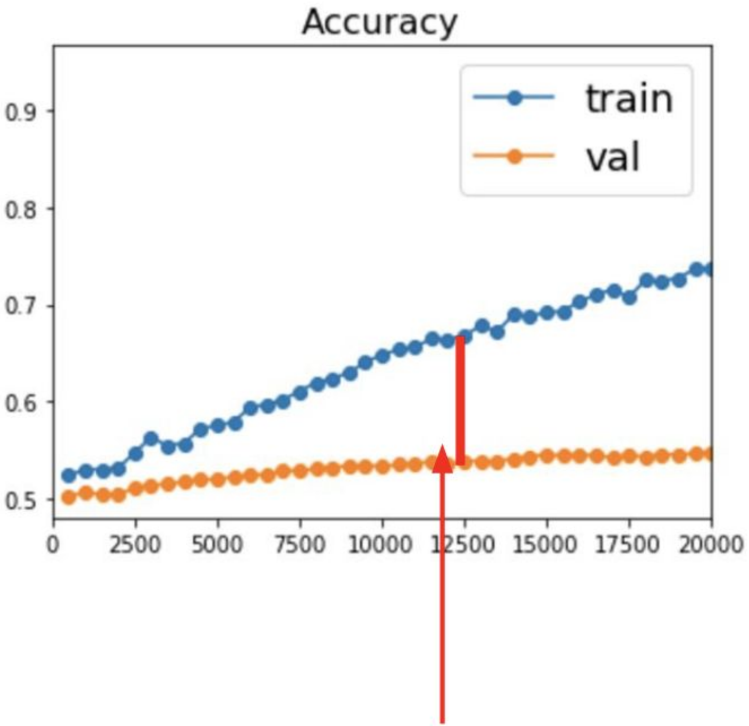
source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

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