

Lecture 01: Introduction and DL recap

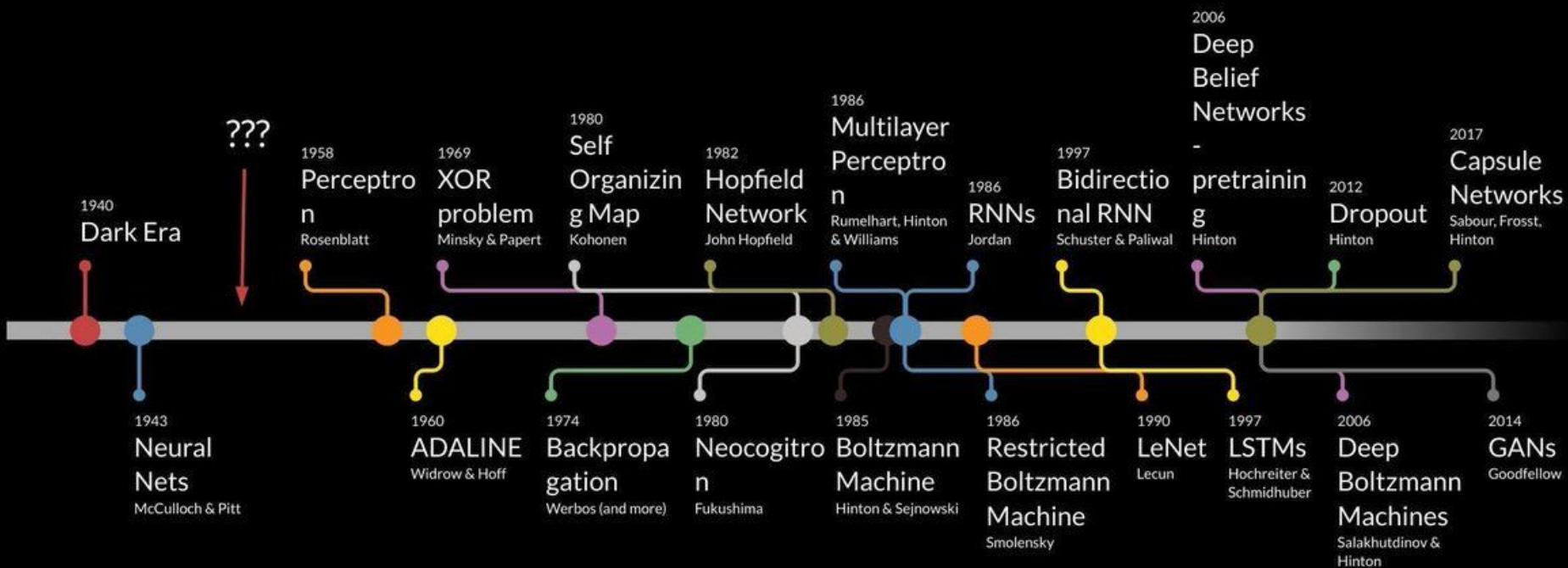
MADE, Moscow
25.03.2020

Radoslav Neychev

Outline

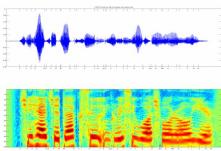
1. Neural Networks in different areas. Historical overview.
2. Backpropagation recap.
3. Activation functions
4. Optimization.
5. Regularization.

Deep Learning Timeline

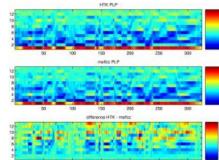


Audio Features

Real world problems

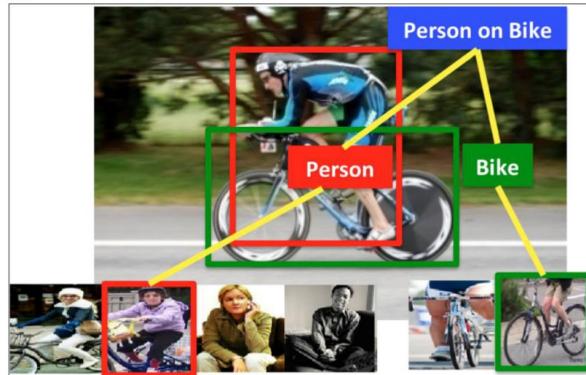


Spectrogram

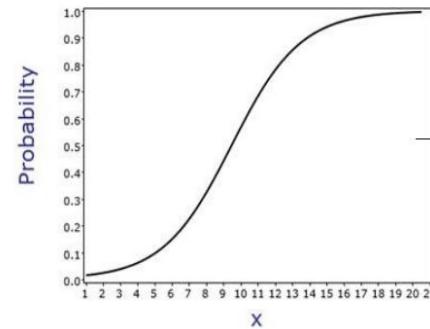
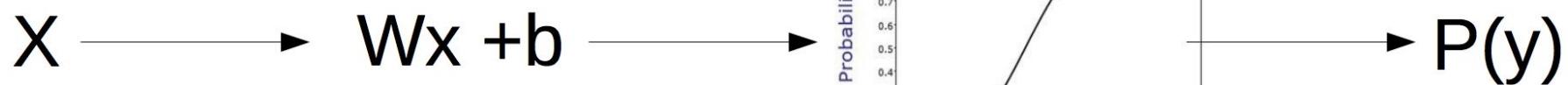


MFCC

- Object detection
- Action classification
- Image captioning
- ...



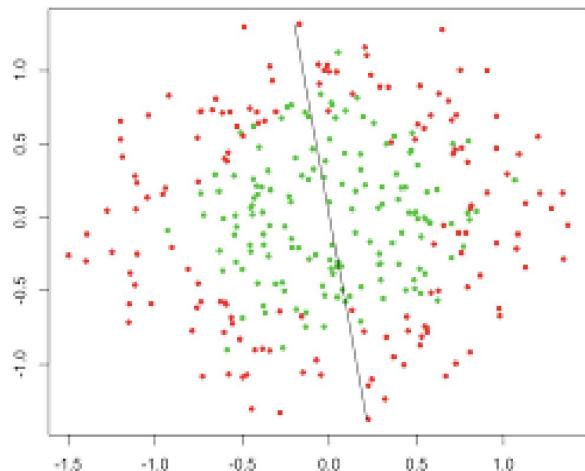
Logistic regression



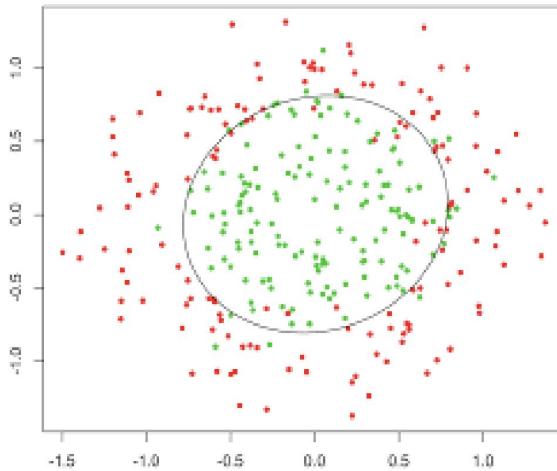
$$P(y|x) = \sigma(w \cdot x + b)$$

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

Problem: nonlinear dependencies



What we have

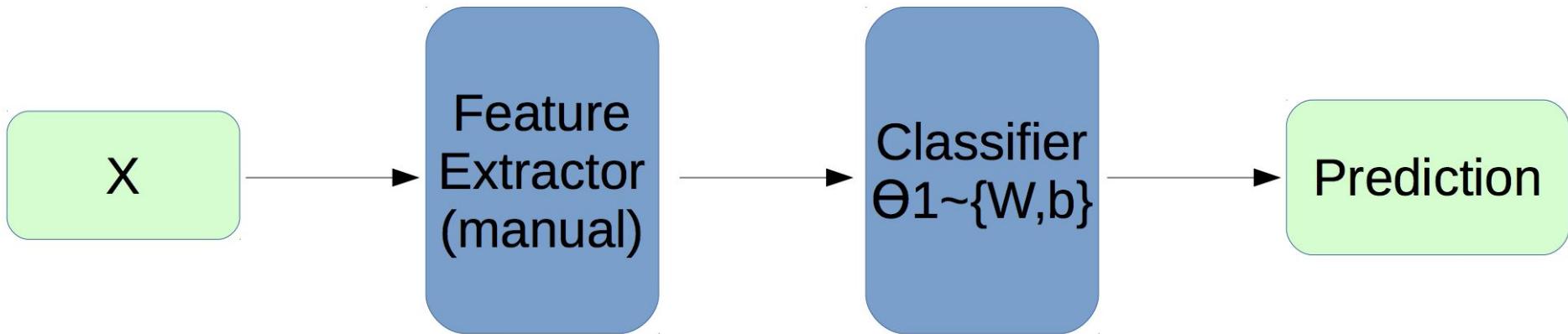


What we want

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

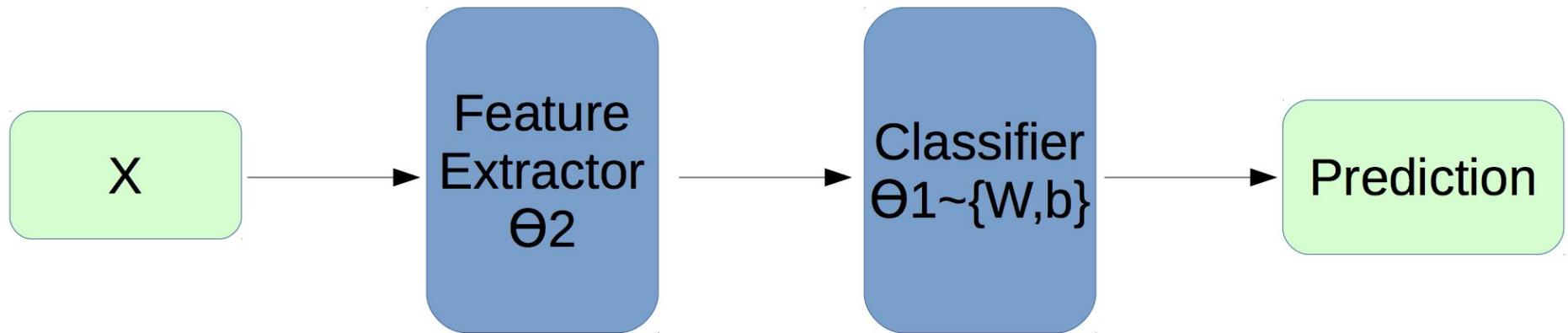
And feature engineering is
an *art*.

Classic pipeline



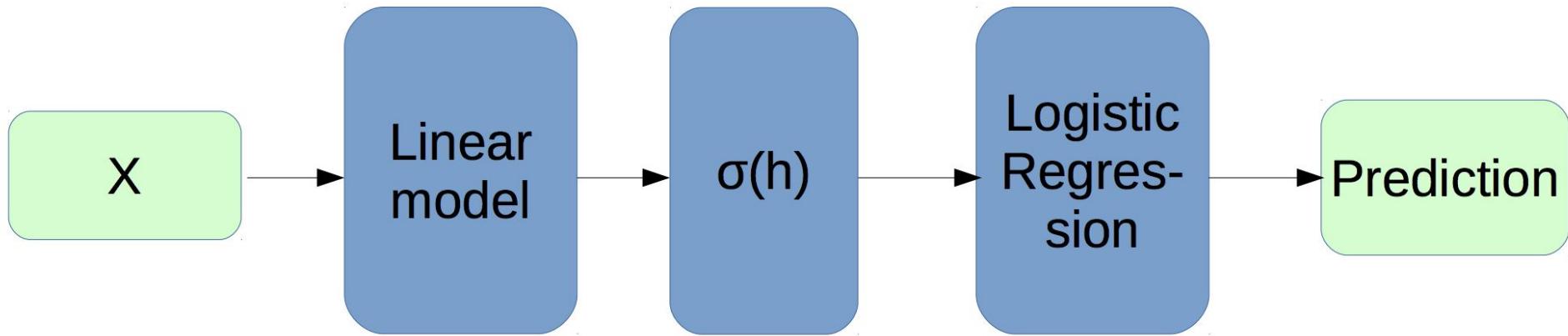
Handcrafted features, generated by experts.

NN pipeline



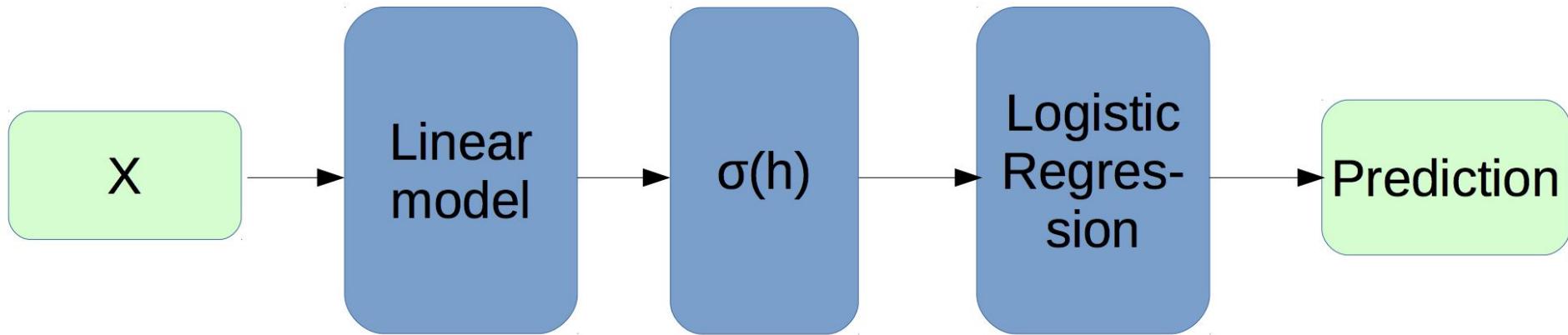
Automatically extracted features.

NN pipeline: example



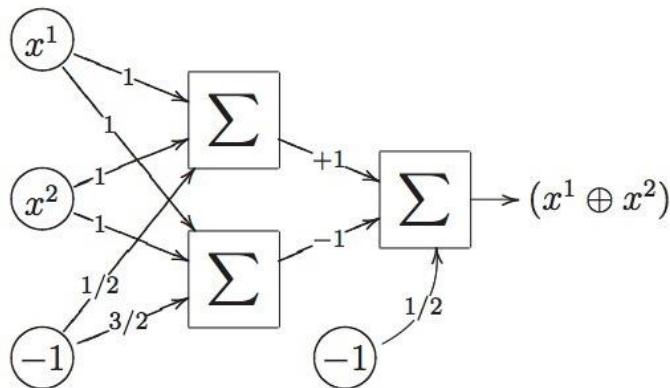
E.g. two logistic regressions one after another.

NN pipeline: example



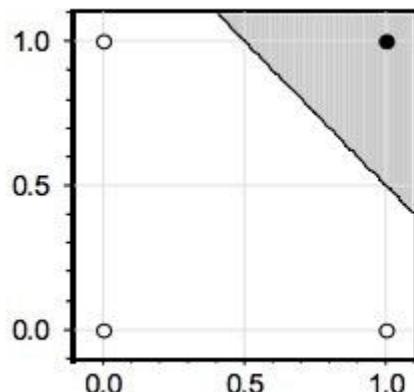
Actually, it's a neural network.

XOR problem

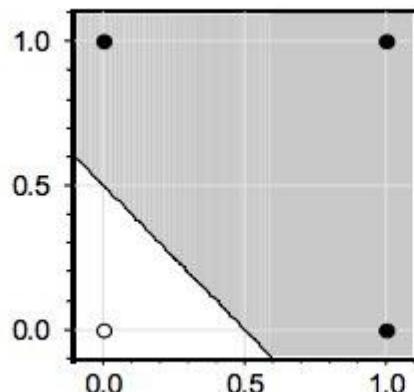


This 2-layer NN (on the left) implements XOR with only x_1 and x_2 features.

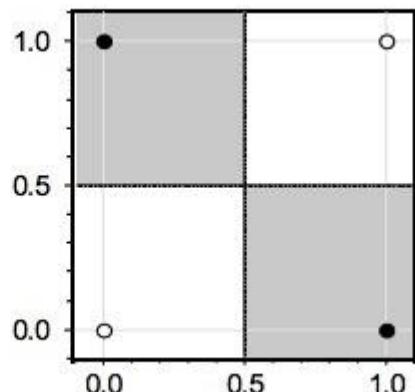
1-layer NN also can succeed, but only with extra feature $x_1 \cdot x_2$.



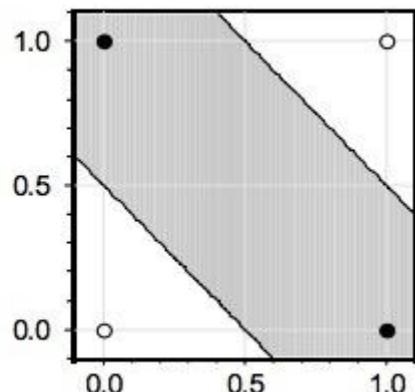
AND



OR



XOR(with $x_1 \cdot x_2$)



XOR

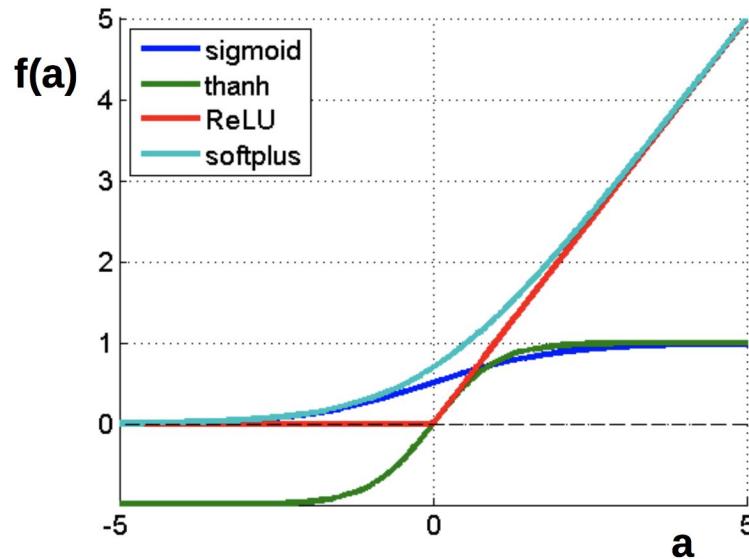
Activation functions: nonlinearities

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

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

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

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



Some generally accepted terms

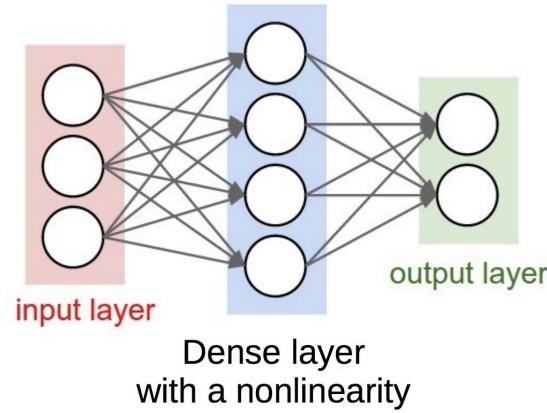
- Layer – a building block for NNs :

- Dense layer: $f(x) = Wx + b$
- Nonlinearity layer: $f(x) = \sigma(x)$
- Input layer, output layer
- A few more we will cover later

- Activation function – function applied to layer output

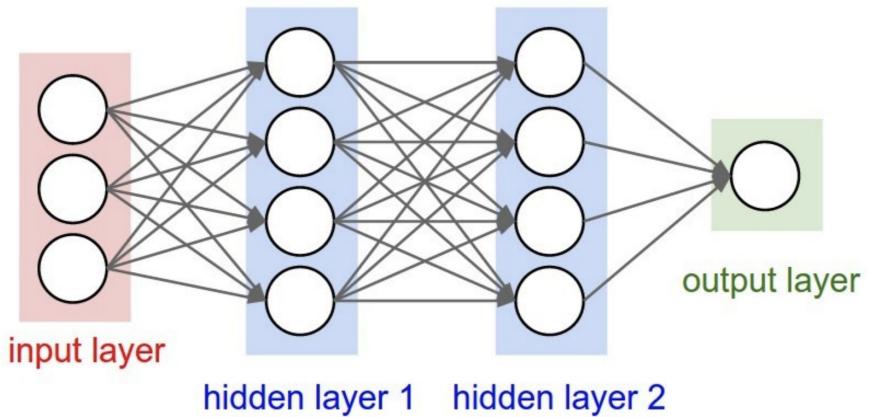
- Sigmoid
- \tanh
- ReLU
- Any other function to get nonlinear intermediate signal in NN

- Backpropagation – a fancy word for “chain rule”

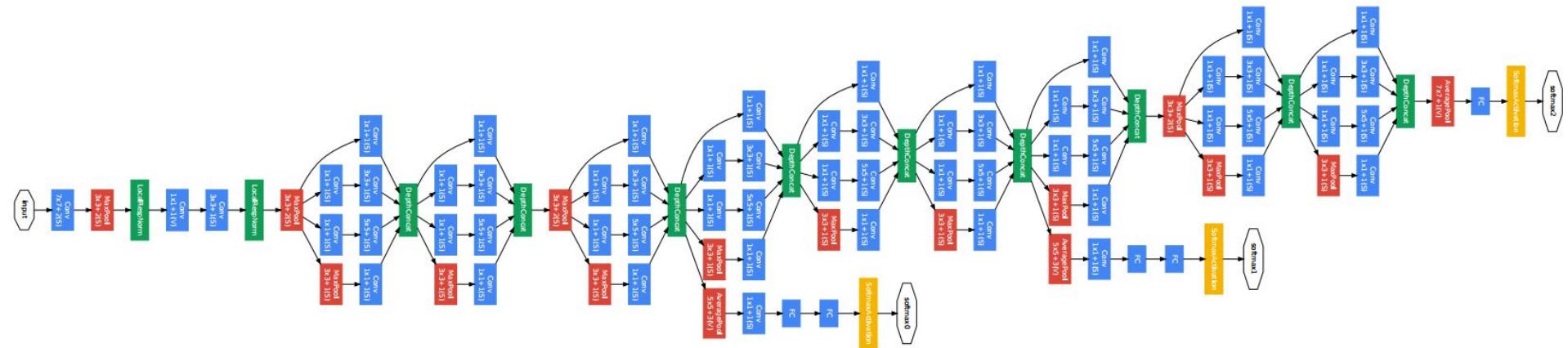


“Train it via backprop!”

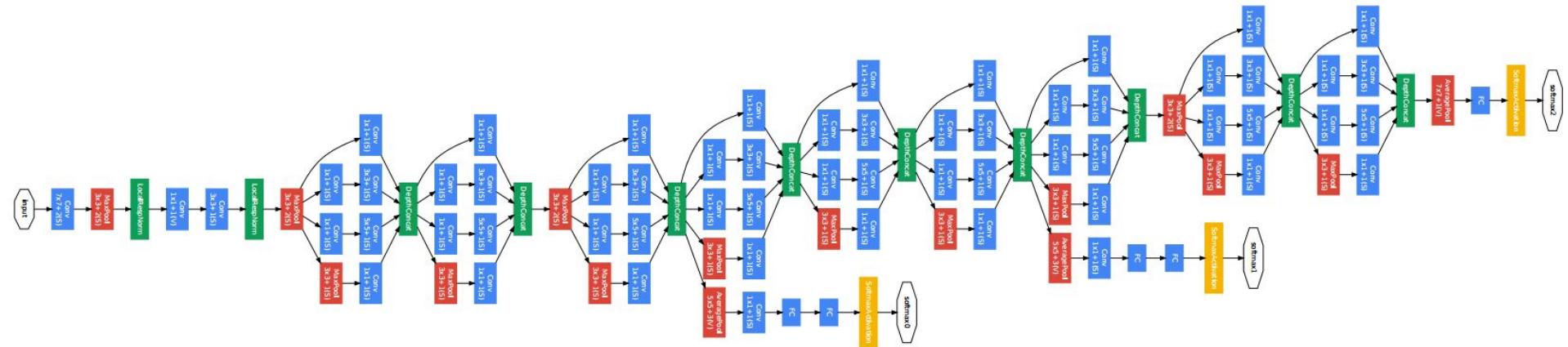
Actually, it can be deeper



Much deeper...



Much deeper...



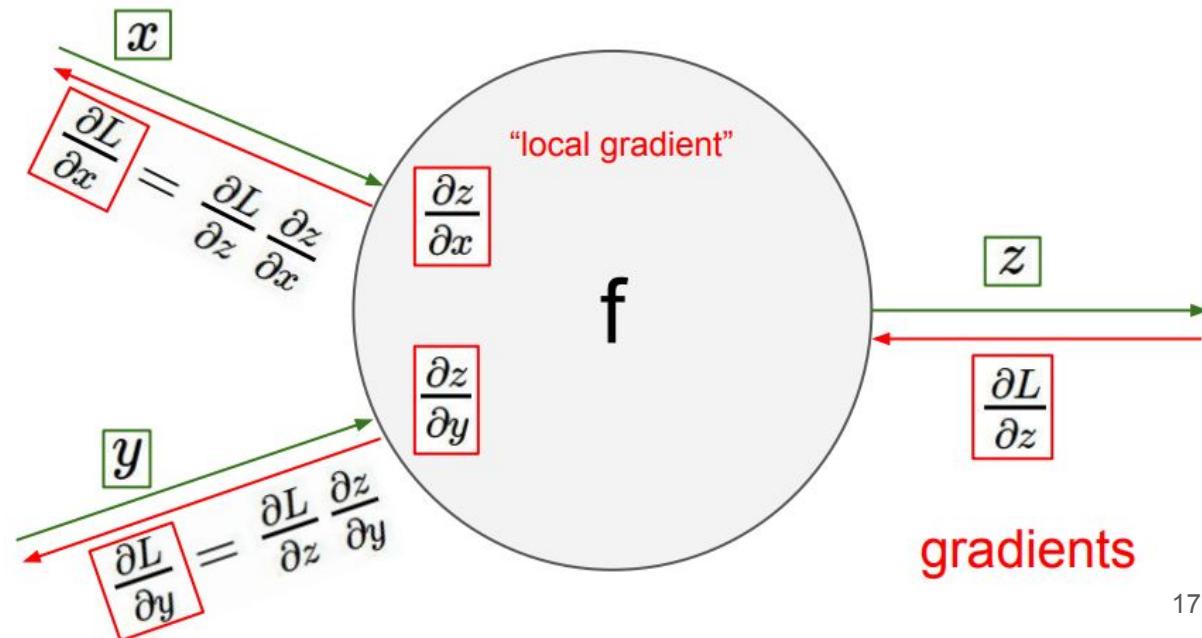
How to train it?

Backpropagation and chain rule

Chain rule is just simple math:

$$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z} \frac{\partial z}{\partial x}$$

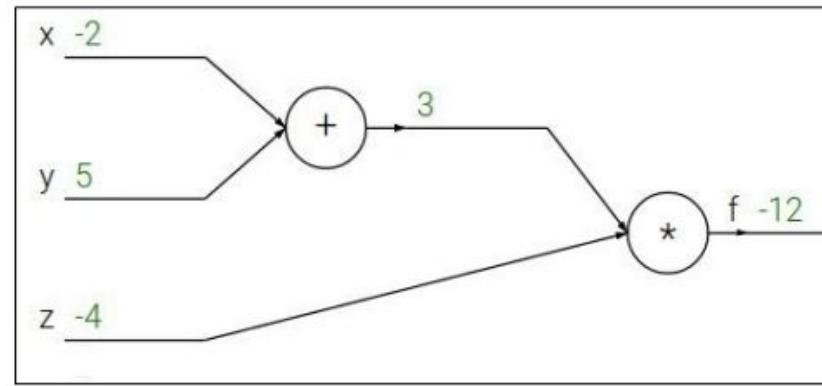
Backprop is just
way to use it in NN
training.



Backpropagation example

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

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



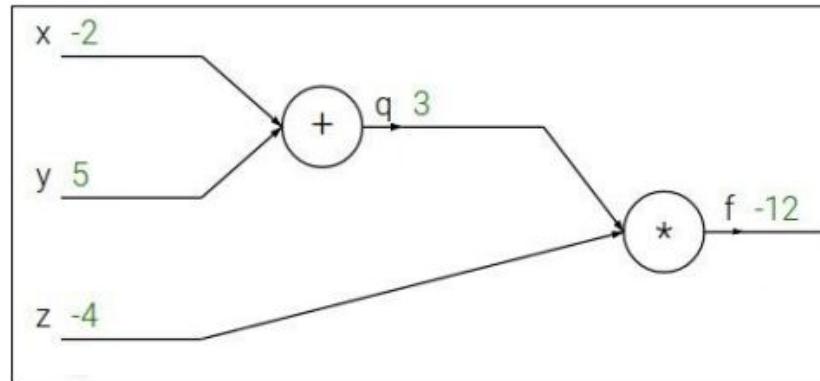
Backpropagation example

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$$q = x + y \quad \frac{\partial q}{\partial x} = 1, \frac{\partial q}{\partial y} = 1$$

$$f = qz \quad \frac{\partial f}{\partial q} = z, \frac{\partial f}{\partial z} = q$$



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

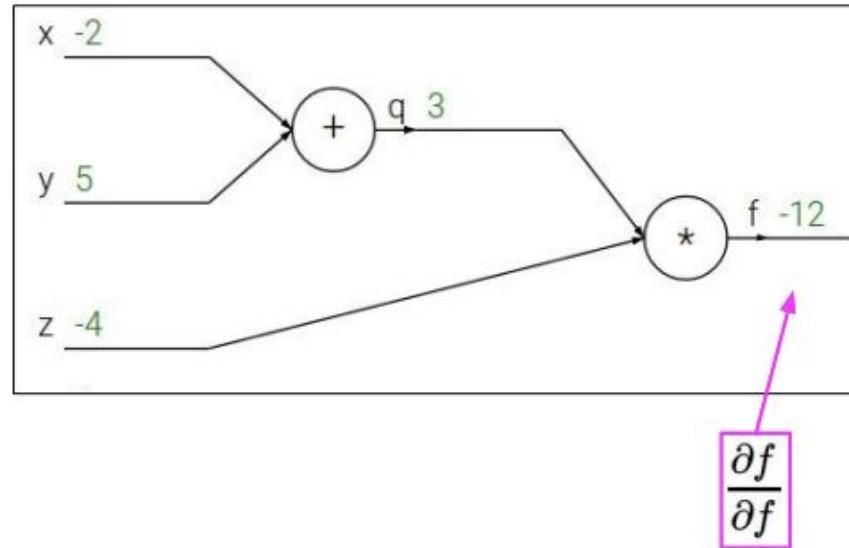
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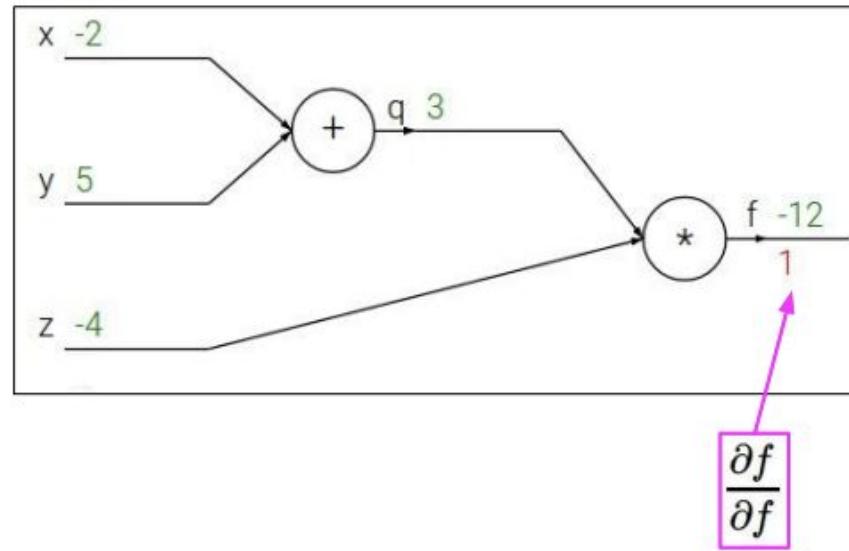
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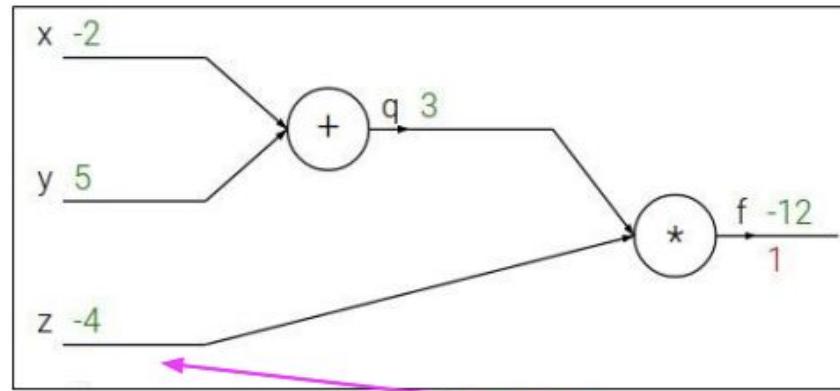
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$$\frac{\partial f}{\partial z}$$

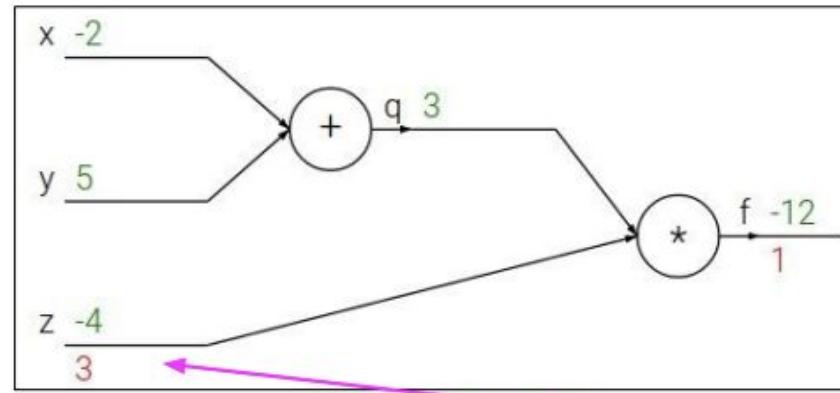
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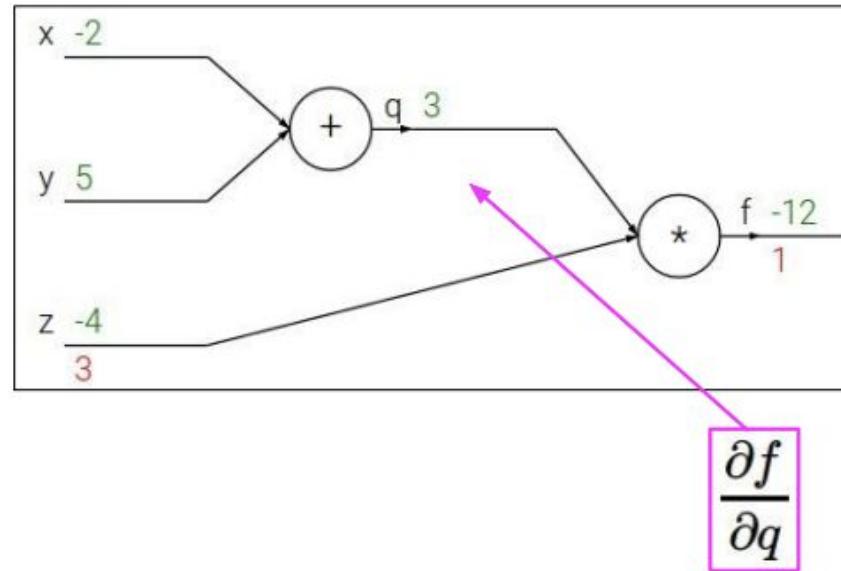
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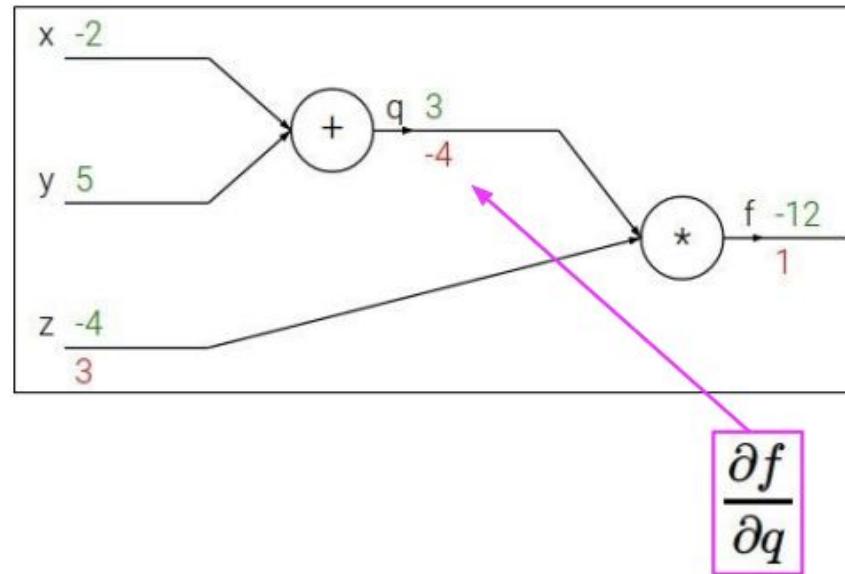
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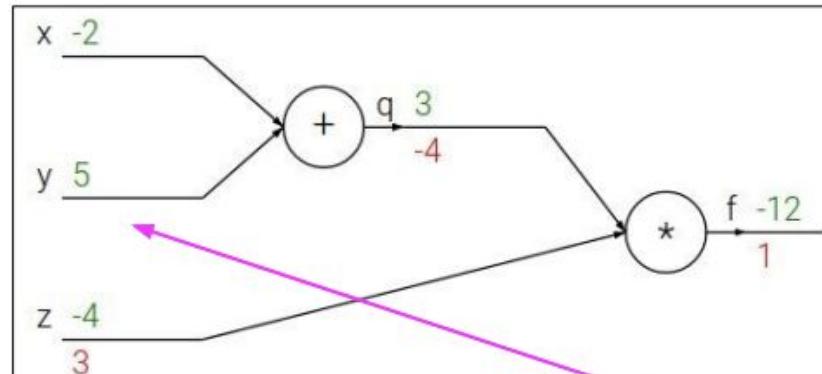
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Backpropagation example

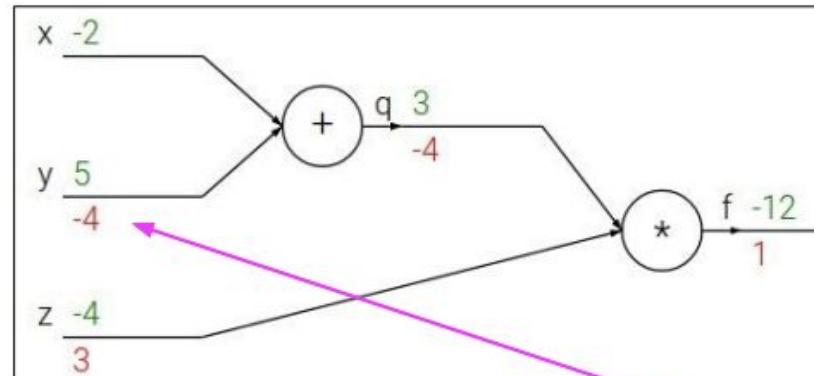
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Want: $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$



Chain rule:

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

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

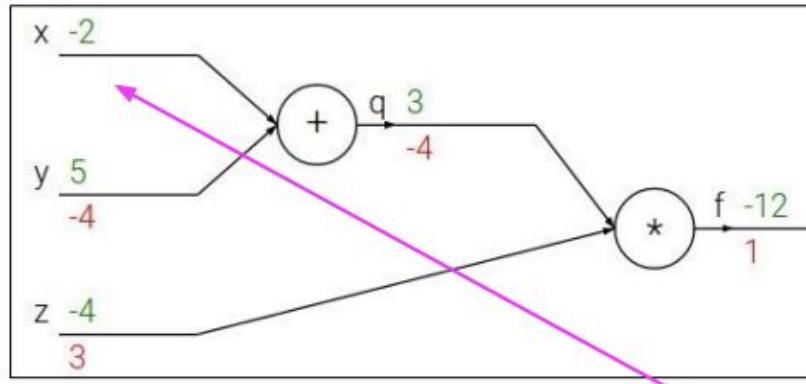
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$$\frac{\partial f}{\partial x}$$

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

Backpropagation example

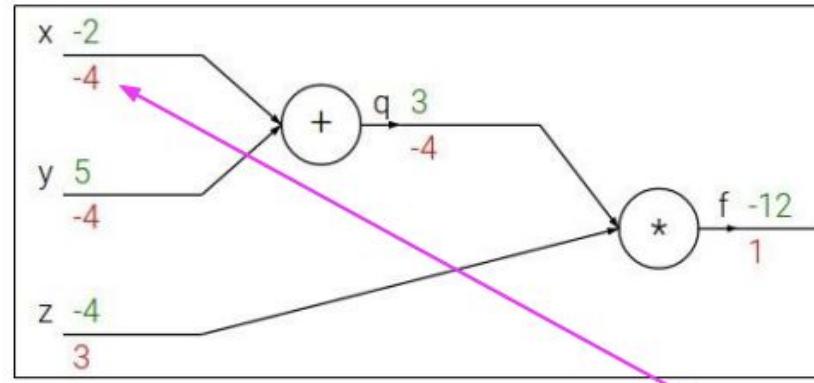
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Chain rule:

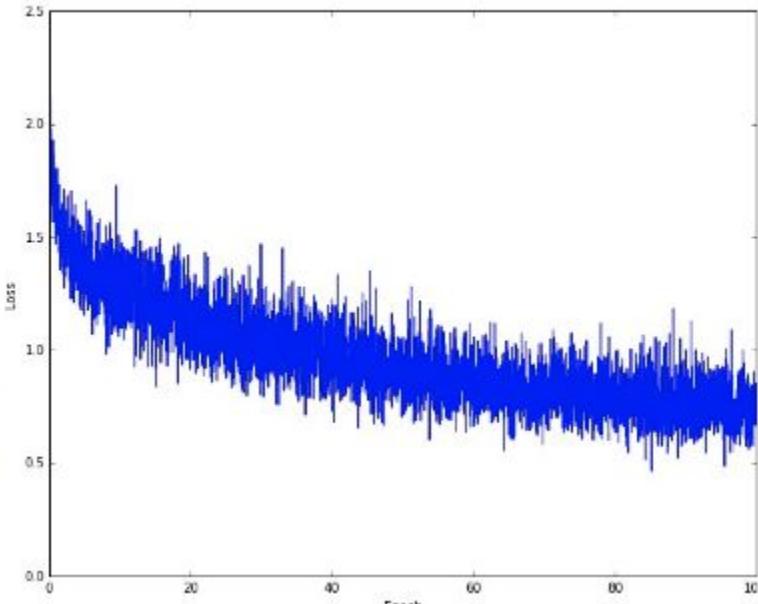
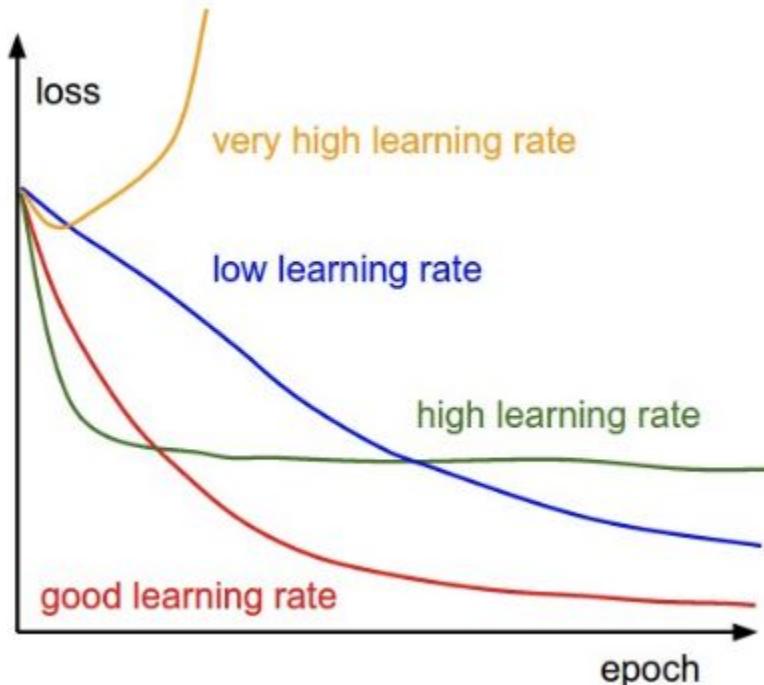
$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial q} \frac{\partial q}{\partial x}$$

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

Gradient optimization

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

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



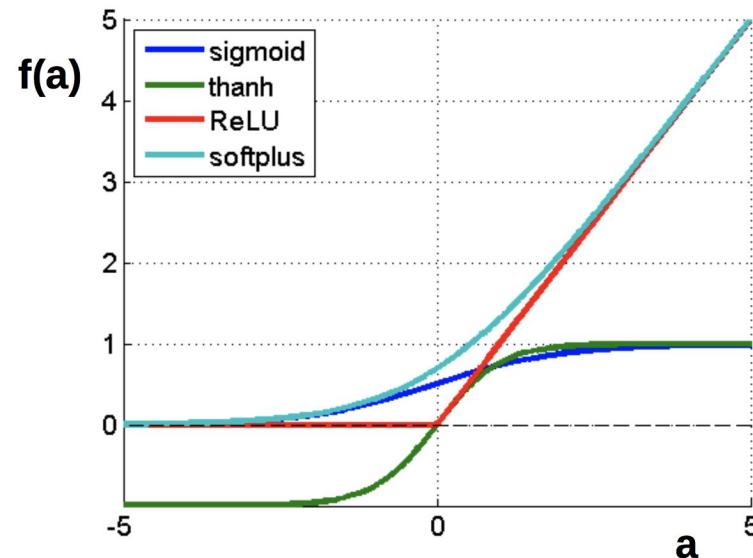
Once more: nonlinearities

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

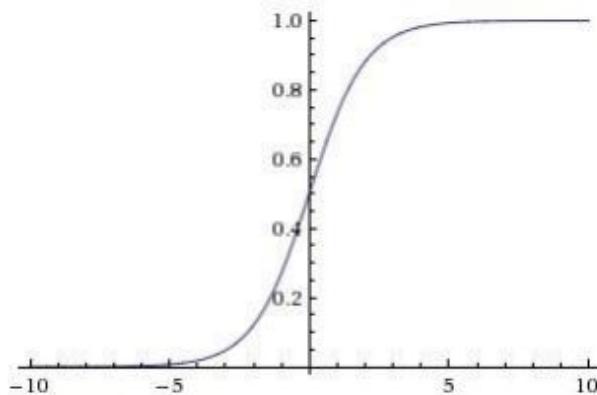
$$f(a) = \tanh(a)$$

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

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



Activation functions



Sigmoid

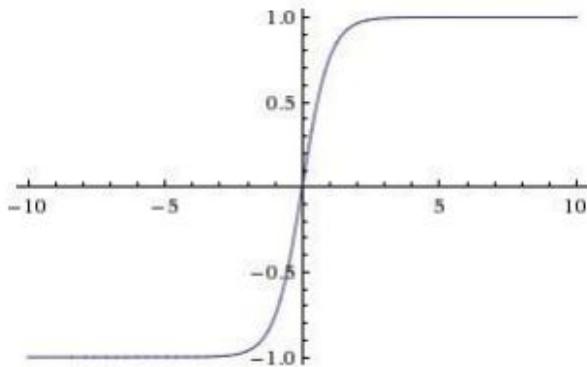
$$f(a) = \frac{1}{1 + e^a}$$

- 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

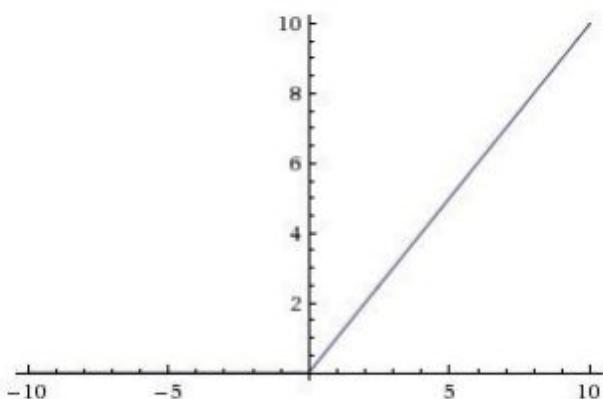


tanh(x)

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

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

Activation functions



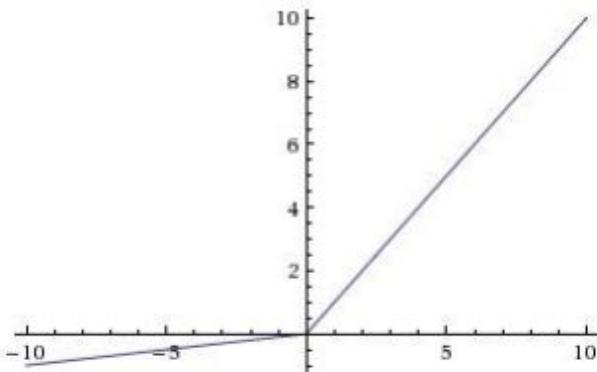
ReLU
(Rectified Linear Unit)

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

- 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

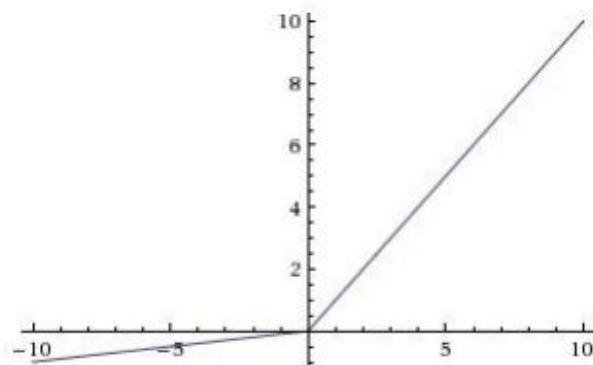


- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- **will not “die”.**

Leaky ReLU

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

Activation functions



Leaky ReLU

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

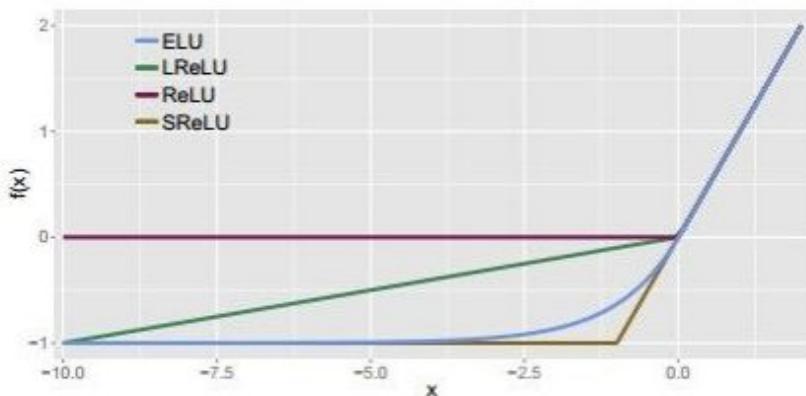
- Does not saturate
- Computationally efficient
- Converges much faster than sigmoid/tanh in practice! (e.g. 6x)
- will not “die”.

Parametric Rectifier (PReLU)

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

backprop into α
(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

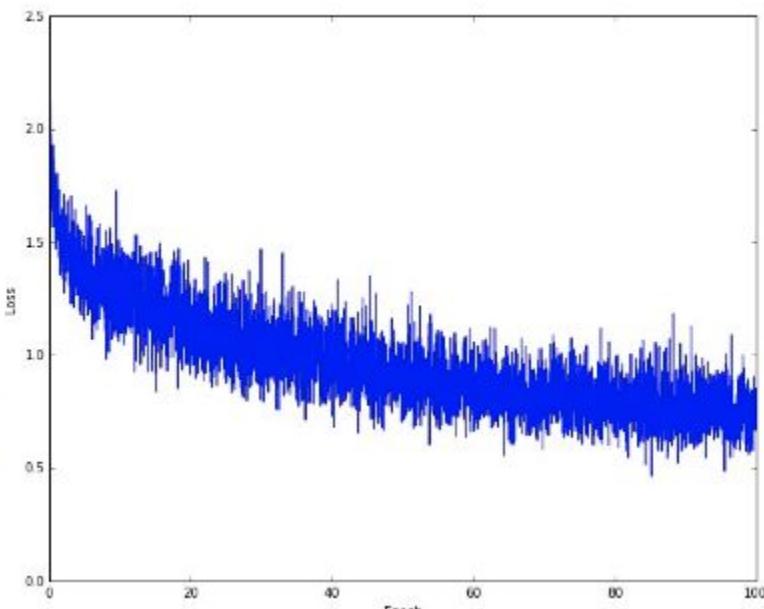
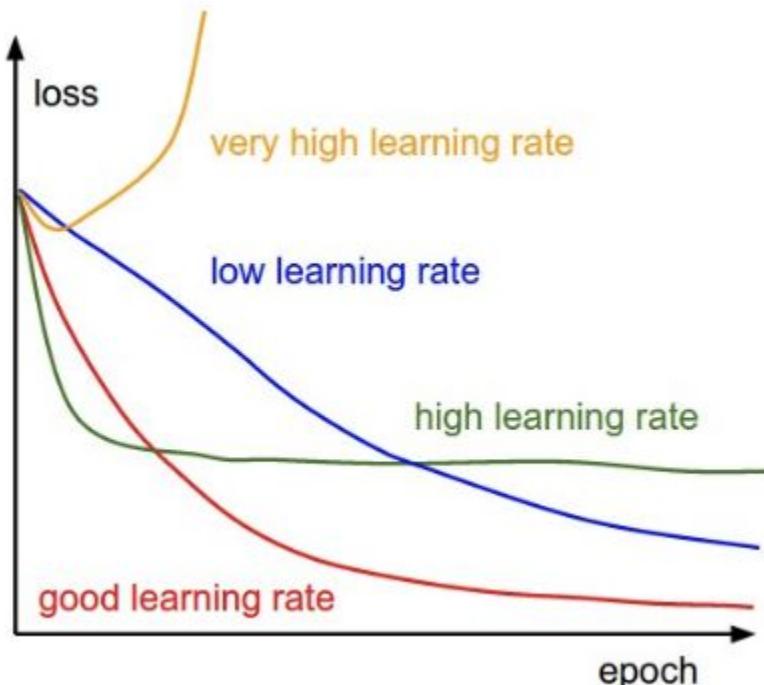
- Use **ReLU** as baseline approach
- Be careful with the learning rates
- Try out **Leaky ReLU** or **ELU**
- Try out **tanh** but do not expect much from it
- Do not use **Sigmoid**

Optimization in DL

Optimizers

Stochastic gradient descent is used to optimize NN parameters.

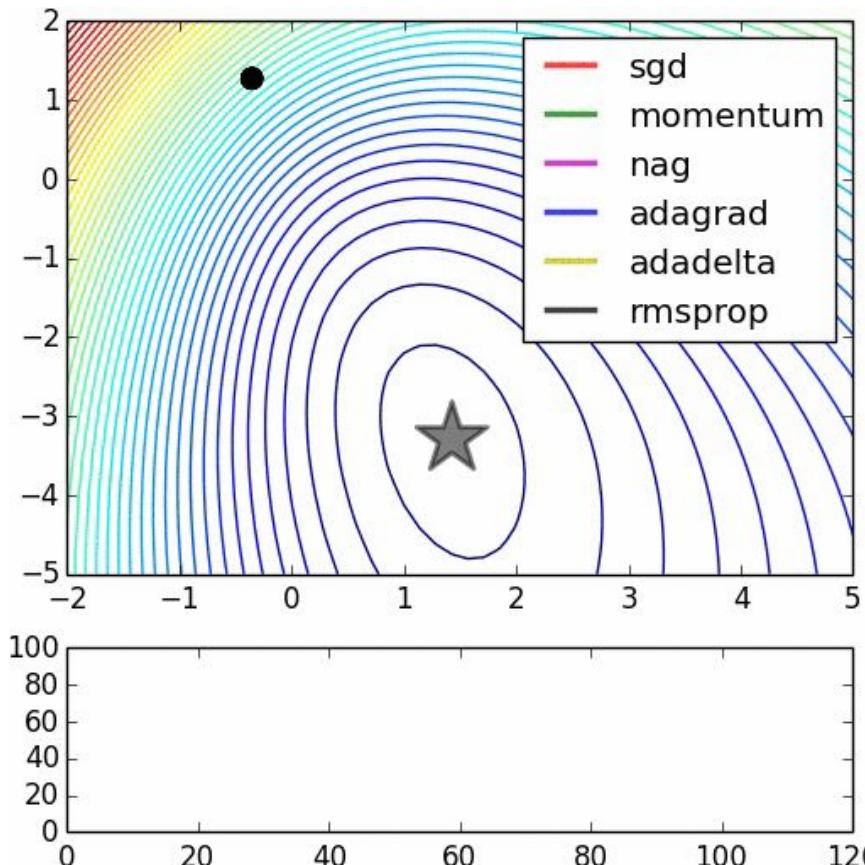
$$x_{t+1} = x_t - \text{learning rate} \cdot dx$$



Optimizers

There are much more optimizers:

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

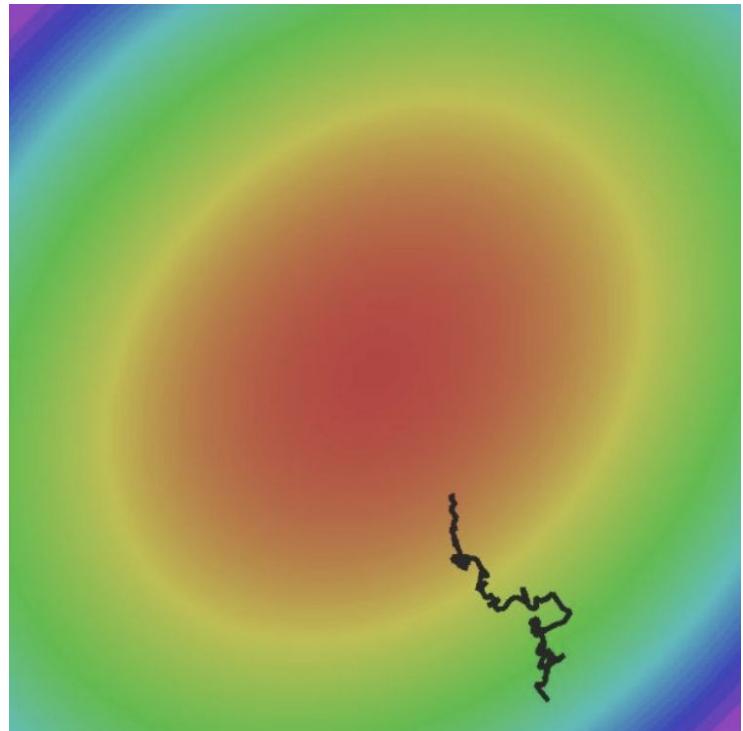


Optimization: SGD

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

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

Averaging over minibatches ---> noisy gradient



First idea: momentum

Simple SGD

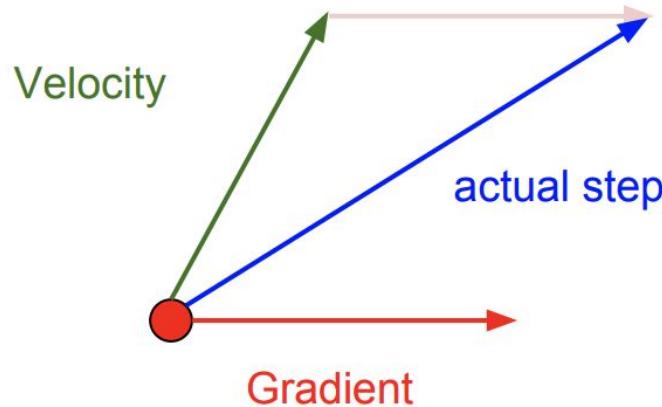
$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$

SGD with momentum

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

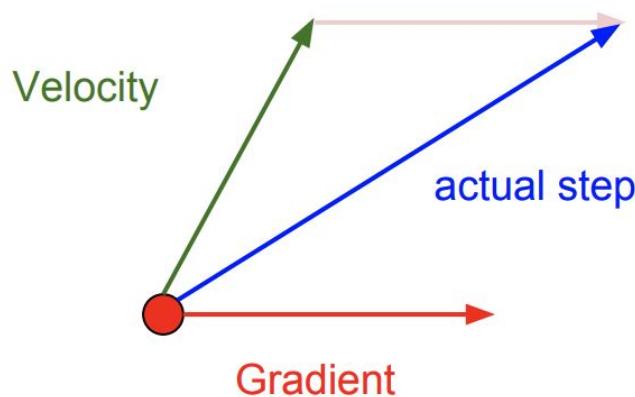
$$x_{t+1} = x_t - \alpha v_{t+1}$$

Momentum update:



Nesterov momentum

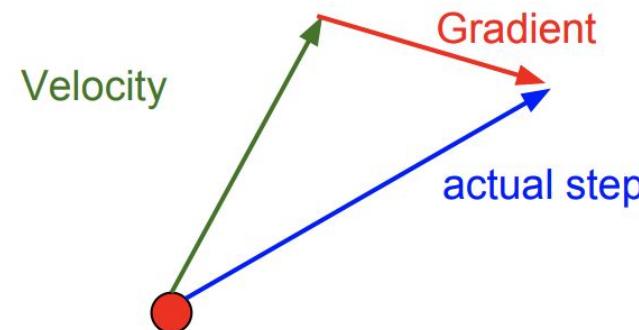
Momentum update:



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

$$x_{t+1} = x_t - \alpha v_{t+1}$$

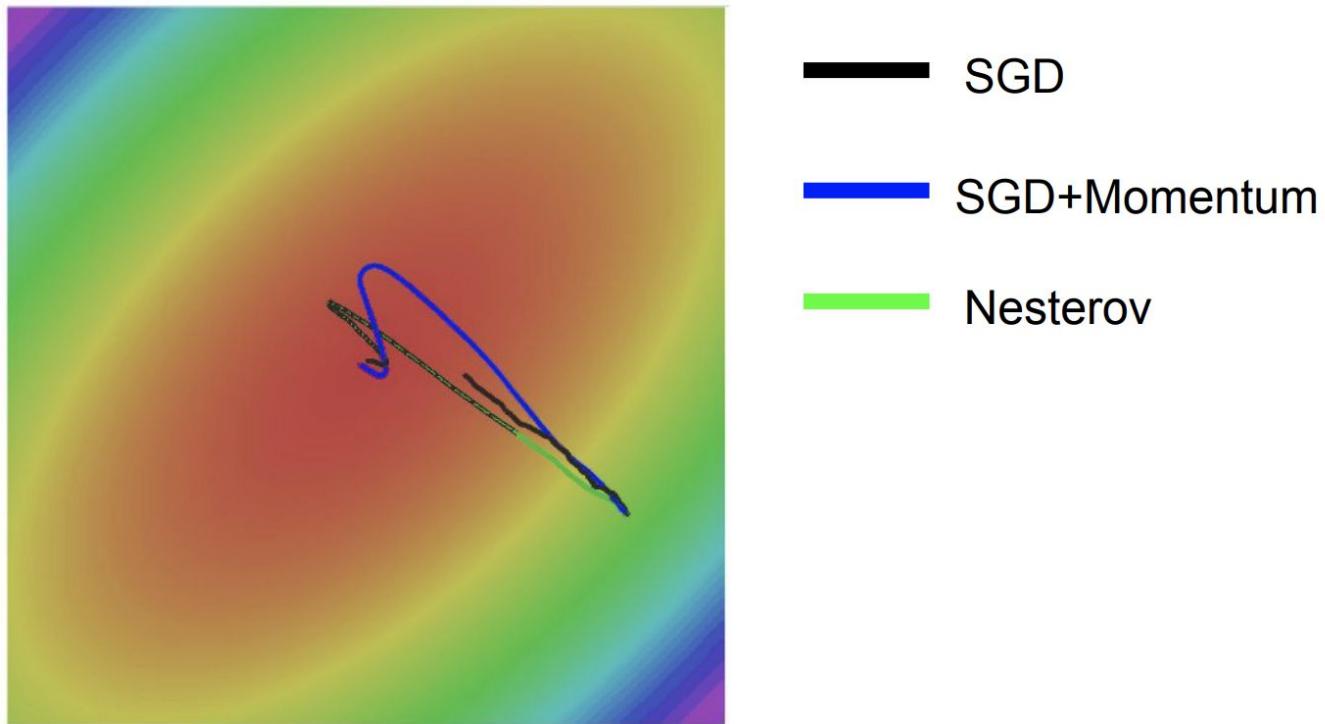
Nesterov Momentum



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

$$x_{t+1} = x_t + v_{t+1}$$

Comparing momentums



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

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

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



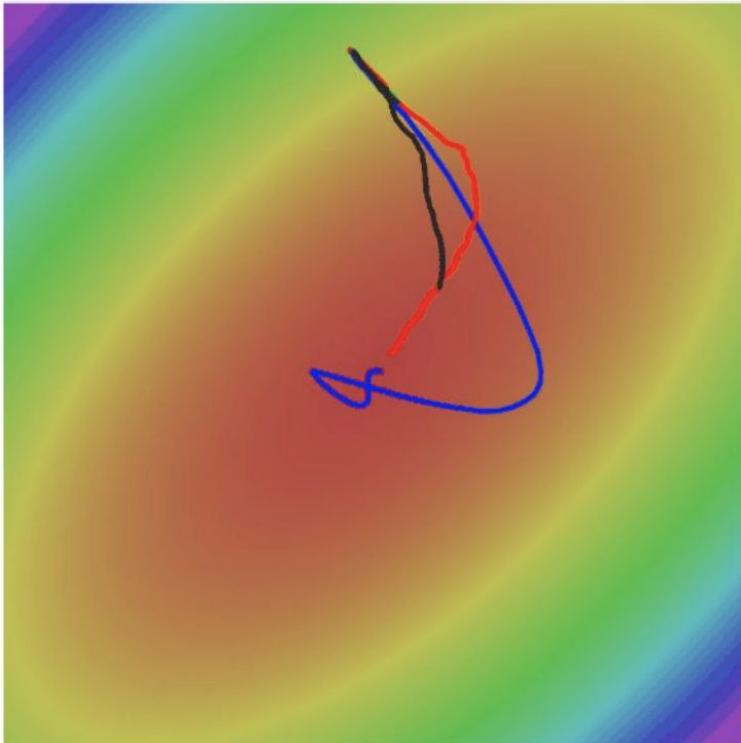
RMSProp: SGD with cache with exp. Smoothing

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

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

Slide 29 Lecture 6 of Geoff Hinton's Coursera class

http://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_lec6.pdf



- SGD
- SGD+Momentum
- RMSProp

Let's combine the momentum idea and RMSProp normalization:

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

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

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

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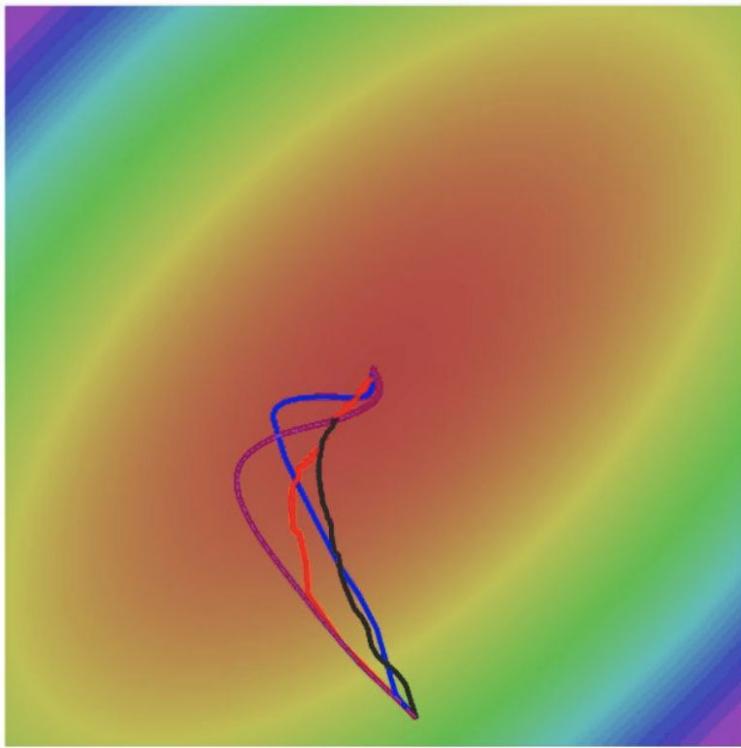
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$$x_{t+1} = x_t - \alpha \frac{v_{t+1}}{\text{cache}_{t+1} + \varepsilon}$$

Actually, that's not quite Adam.

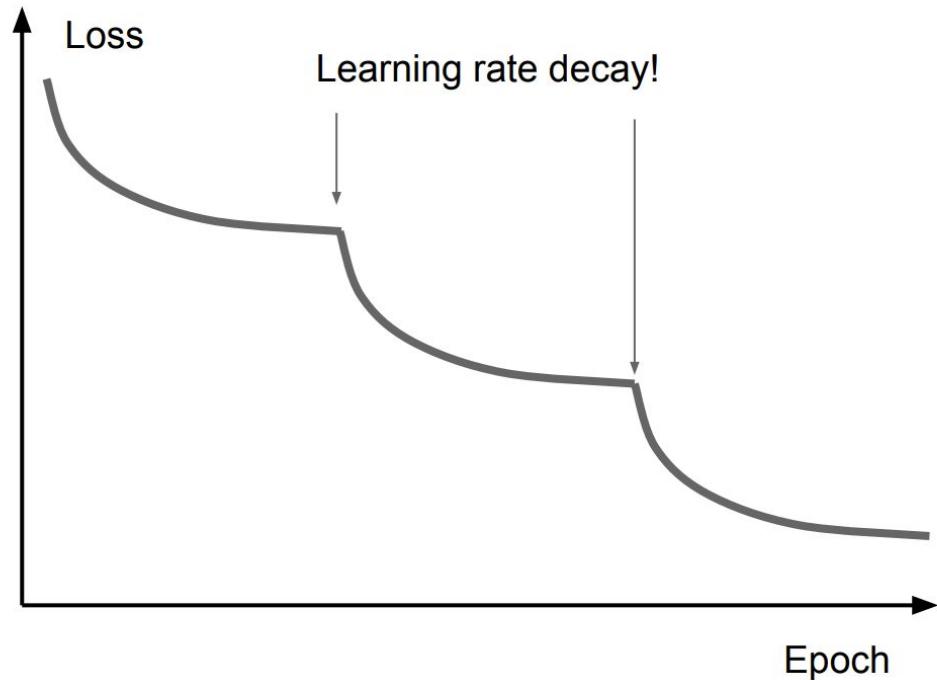
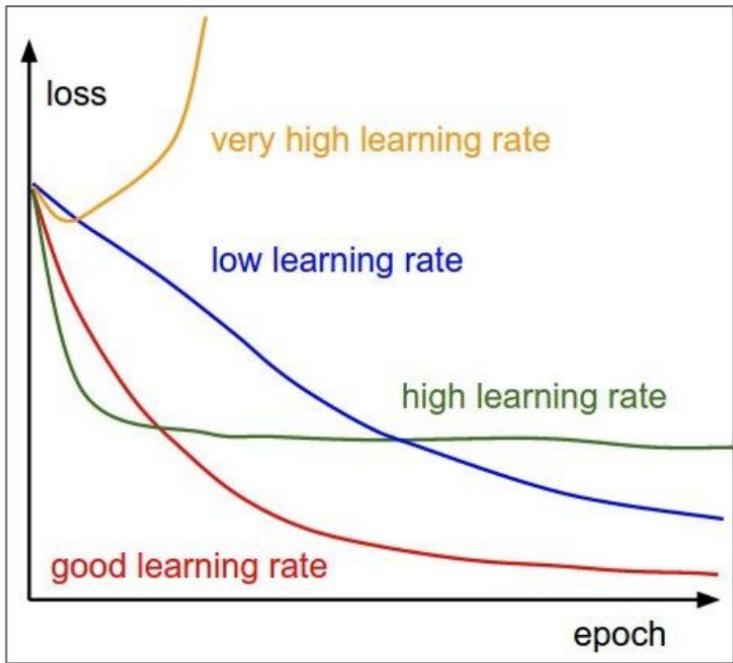
Adam full form involves bias correction term. See <http://cs231n.github.io/neural-networks-3/> for more info.

Comparing optimizers



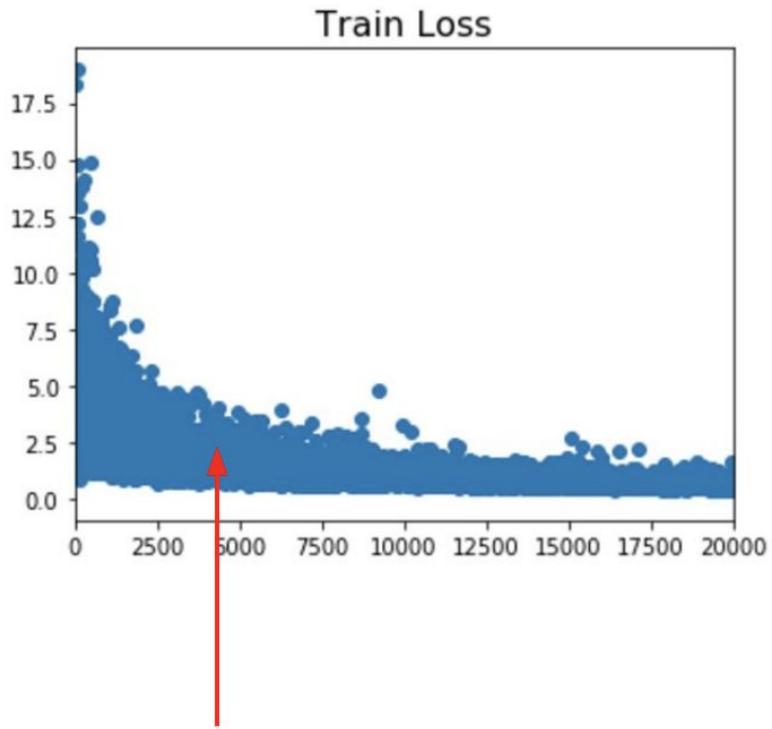
- SGD
- SGD+Momentum
- RMSProp
- Adam

Once more: learning rate

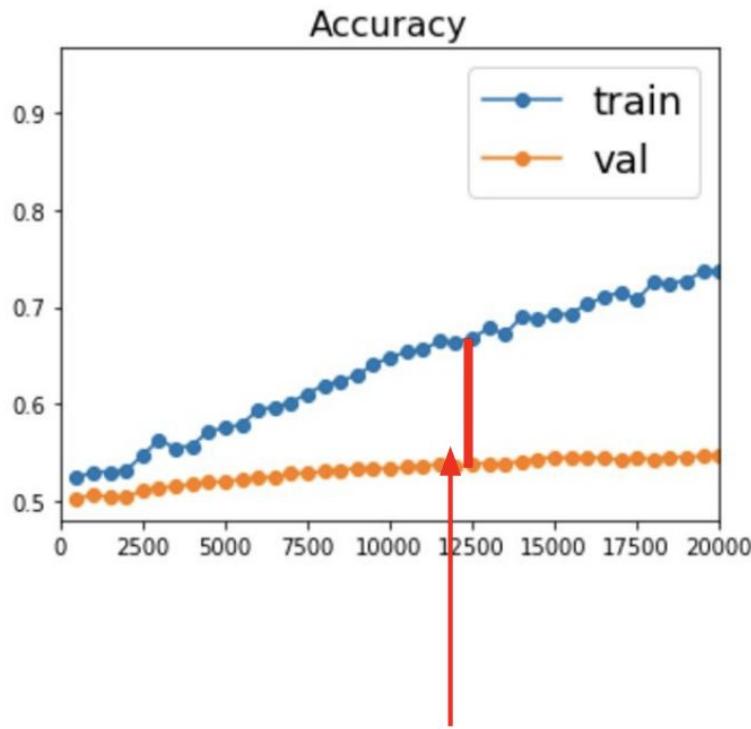


Sum up: optimization

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

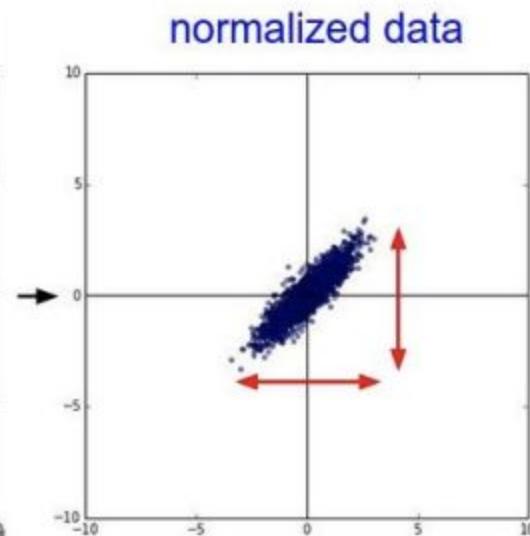
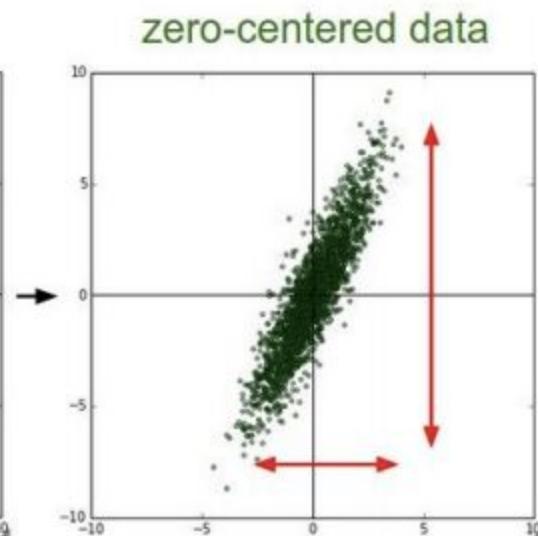
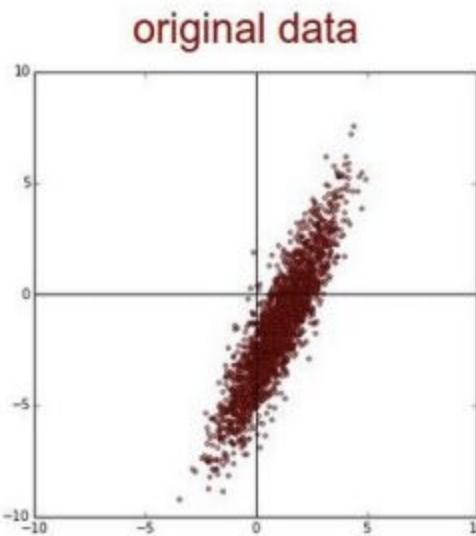


Better optimization algorithms
help reduce training loss



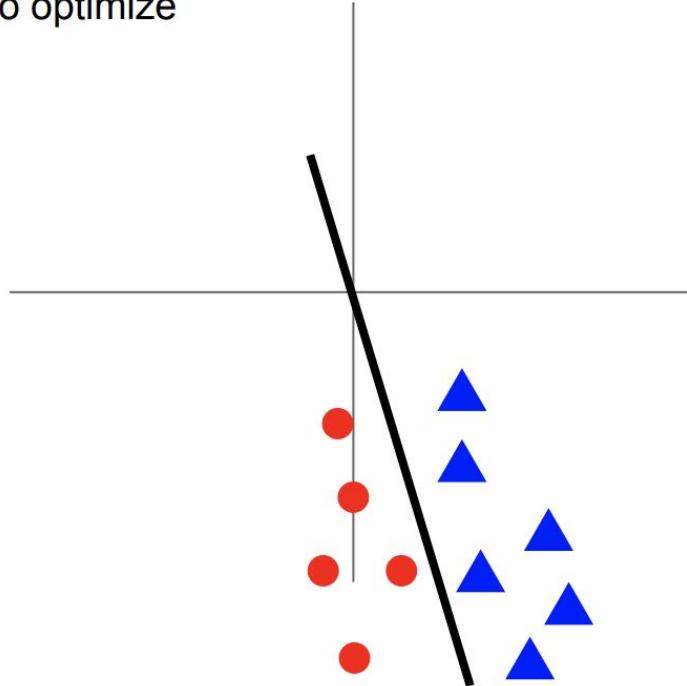
But we really care about error on new
data - how to reduce the gap?

Data normalization

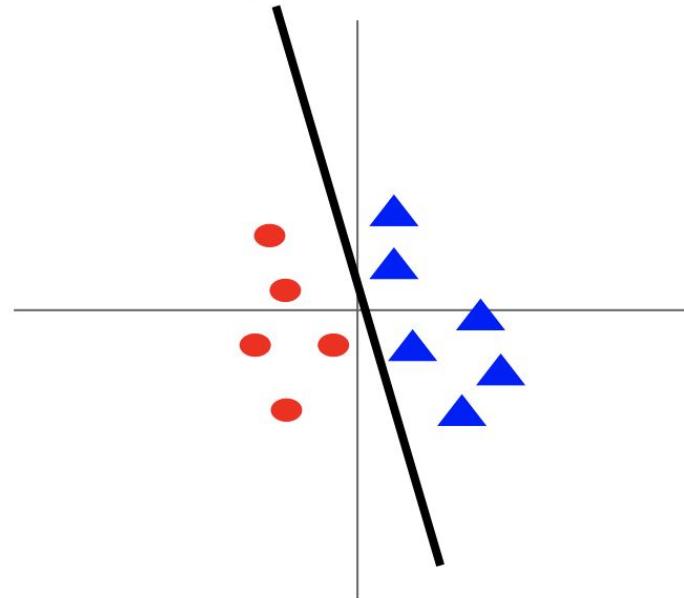


Data normalization

Before normalization: classification loss very sensitive to changes in weight matrix; hard to optimize



After normalization: less sensitive to small changes in weights; easier to optimize



Weights initialization

- Pitfall: all zero initialization.

Weights initialization

- Pitfall: all zero initialization.
- Small random numbers.

Weights initialization

- Pitfall: all zero initialization.
- Small random numbers.
- Calibrated random numbers.

$$s = \sum_i^n w_i x_i$$

$$\text{Var}(s) = \text{Var}\left(\sum_i^n w_i x_i\right)$$

$$= \sum_i^n \text{Var}(w_i x_i)$$

$$= \sum_i^n [E(w_i)]^2 \text{Var}(x_i) + E[(x_i)]^2 \text{Var}(w_i) + \text{Var}(x_i) \text{Var}(w_i)$$

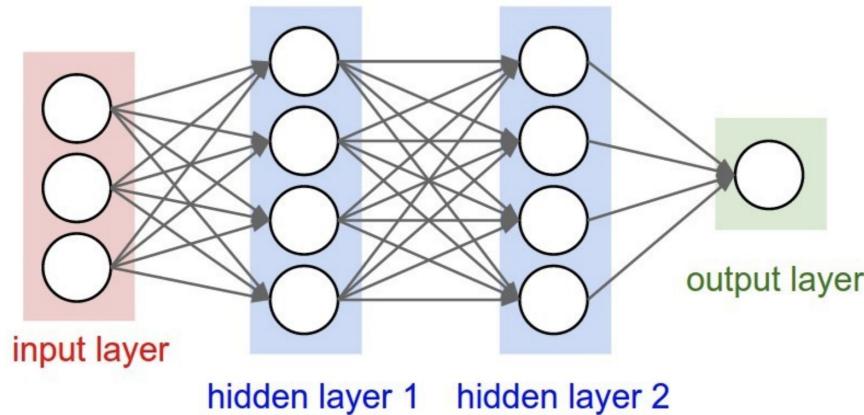
$$= \sum_i^n \text{Var}(x_i) \text{Var}(w_i)$$

$$= (n \text{Var}(w)) \text{Var}(x)$$

Batch normalization

Problem:

- Consider a neuron in any layer beyond first
- At each iteration we tune it's weights towards better loss function
- But we also tune it's inputs. Some of them become larger, some – smaller
- Now the neuron needs to be re-tuned for it's new inputs



Batch normalization

TL; DR:

- It's usually a good idea to normalize linear model inputs
 - (c) Every machine learning lecturer, ever

Batch normalization

- Normalize activation of a hidden layer
(zero mean unit variance)

$$h_i = \frac{h_i - \mu_i}{\sqrt{\sigma_i^2}}$$

- Update μ_i, σ_i^2 with moving average while training

$$\mu_i := \alpha \cdot \text{mean}_{batch} + (1 - \alpha) \cdot \mu_i$$

$$\sigma_i^2 := \alpha \cdot \text{variance}_{batch} + (1 - \alpha) \cdot \sigma_i^2$$

Batch normalization

Original algorithm
(2015)

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1\dots m}\}$;

Parameters to be learned: γ, β

Output: $\{y_i = \text{BN}_{\gamma, \beta}(x_i)\}$

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^m x_i \quad // \text{mini-batch mean}$$

$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2 \quad // \text{mini-batch variance}$$

$$\hat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \quad // \text{normalize}$$

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What is this?

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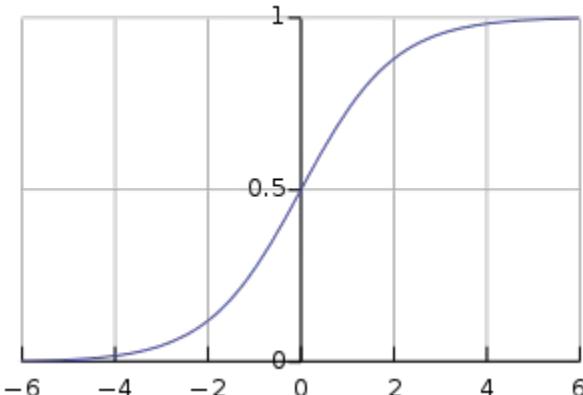
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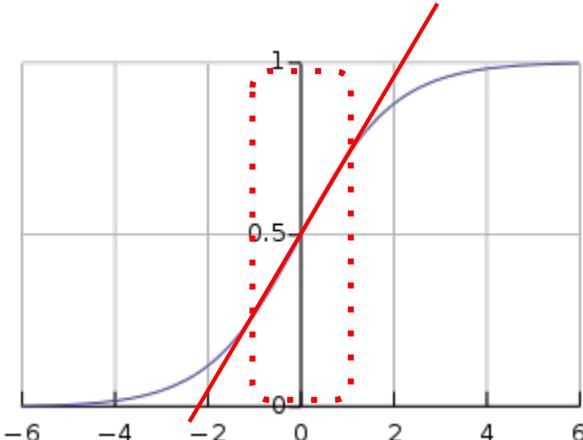
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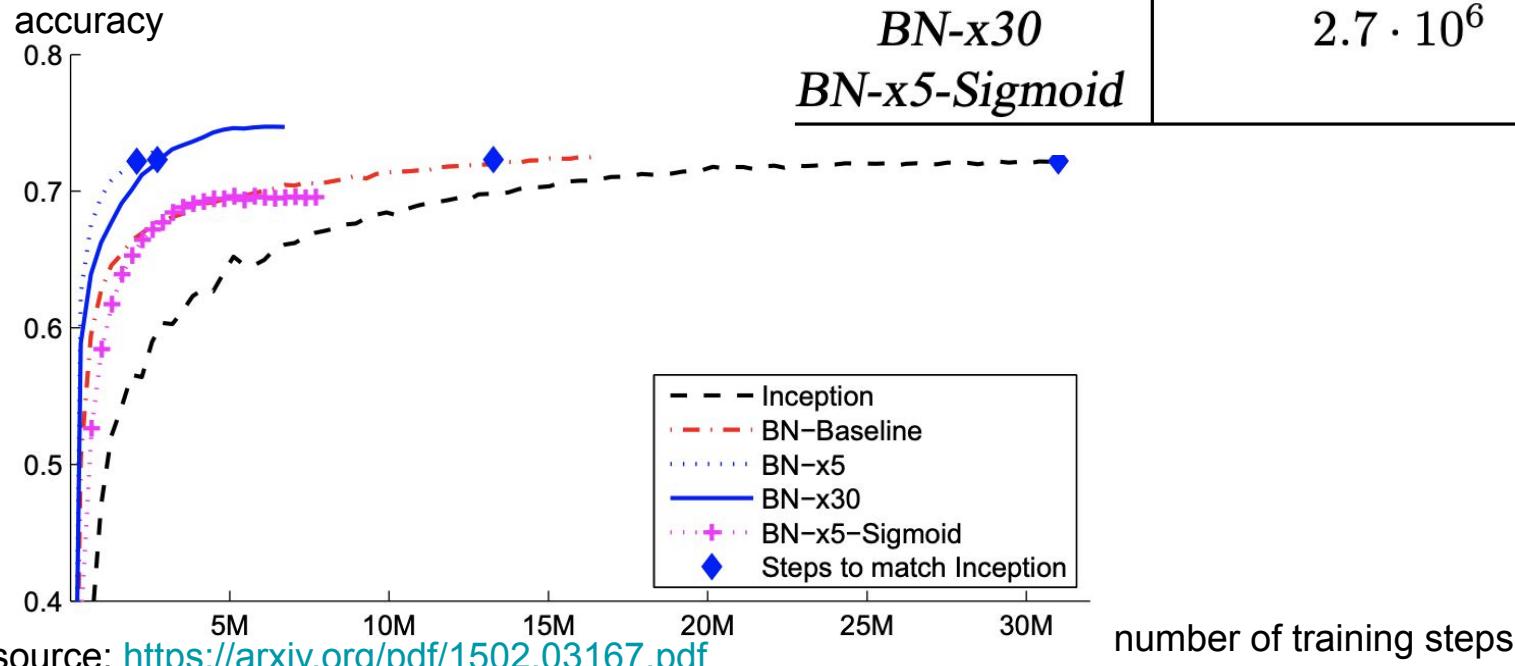
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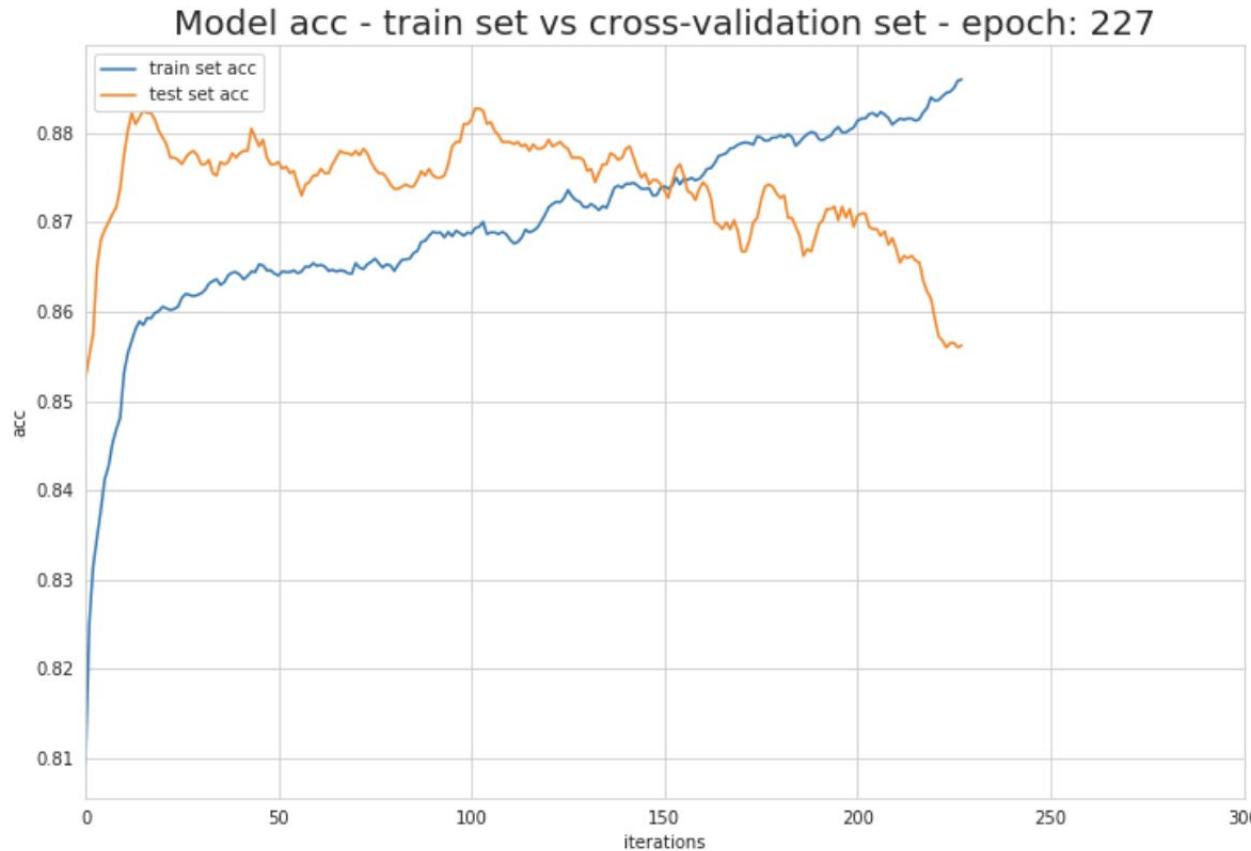
What is this?

This transformation
should be able to
represent the identity
transform.

Batch normalization



Problem: overfitting



Regularization

$$L = \frac{1}{N} \sum_{i=1}^N \sum_{j \neq y_i} \max(0, f(x_i; W)_j - f(x_i; W)_{y_i} + 1) + \boxed{\lambda R(W)}$$

Adding some extra term to the loss function.

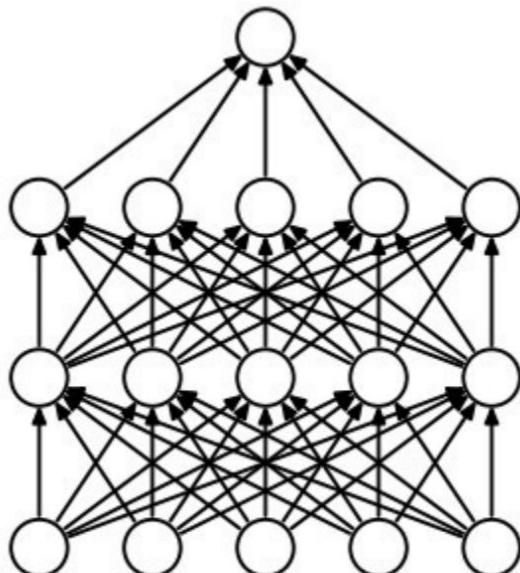
Common cases:

- L2 regularization: $R(W) = \|W\|_2^2$
- L1 regularization: $R(W) = \|W\|_1$
- Elastic Net (L1 + L2): $R(W) = \beta \|W\|_2^2 + \|W\|_1$

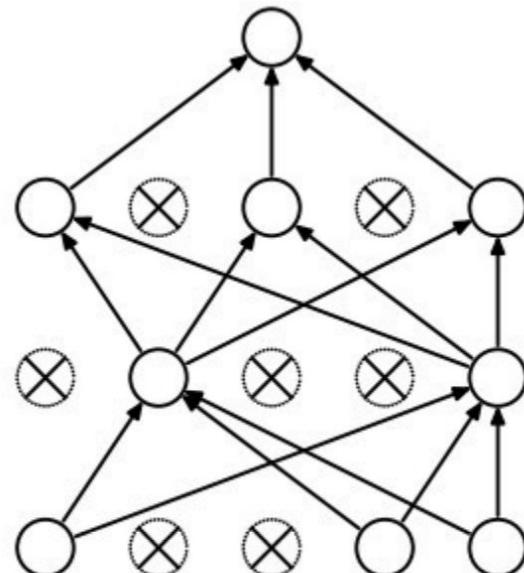
Regularization: Dropout

Some neurons are “dropped” during training.

Prevents overfitting.



(a) Standard Neural Net

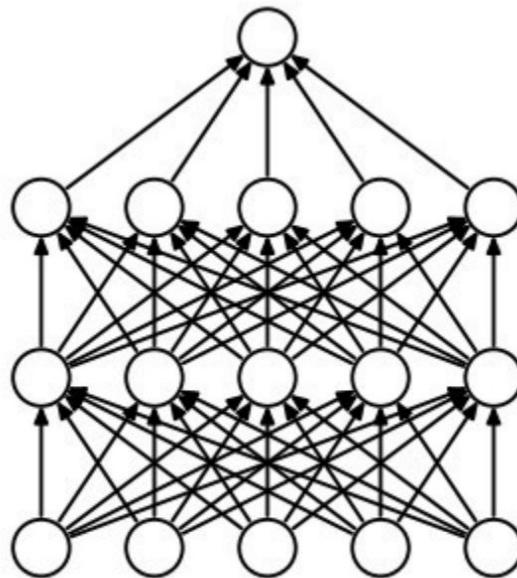


(b) After applying dropout.

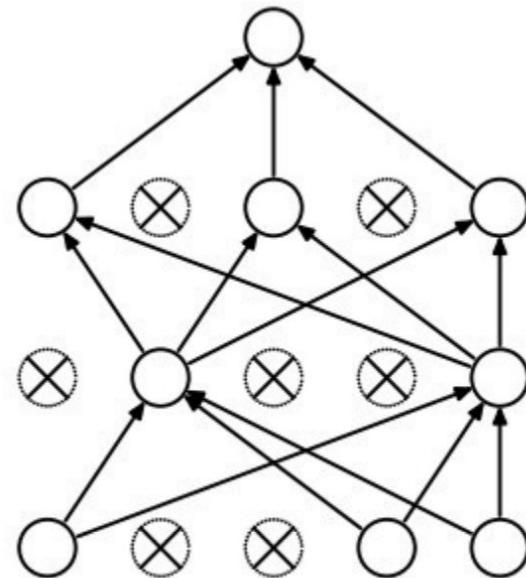
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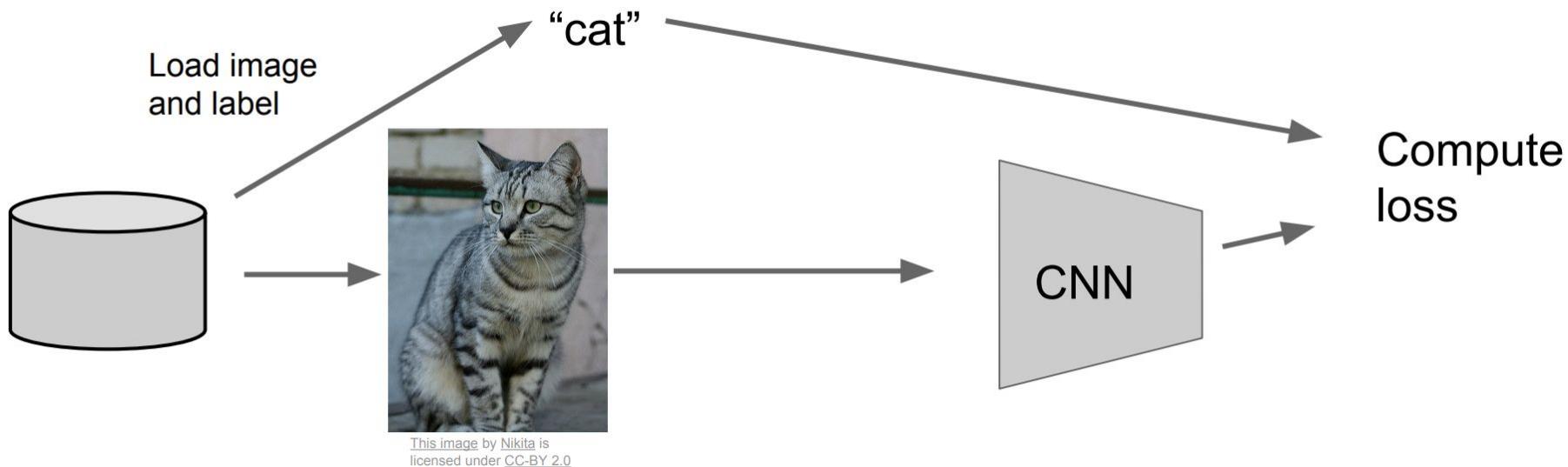
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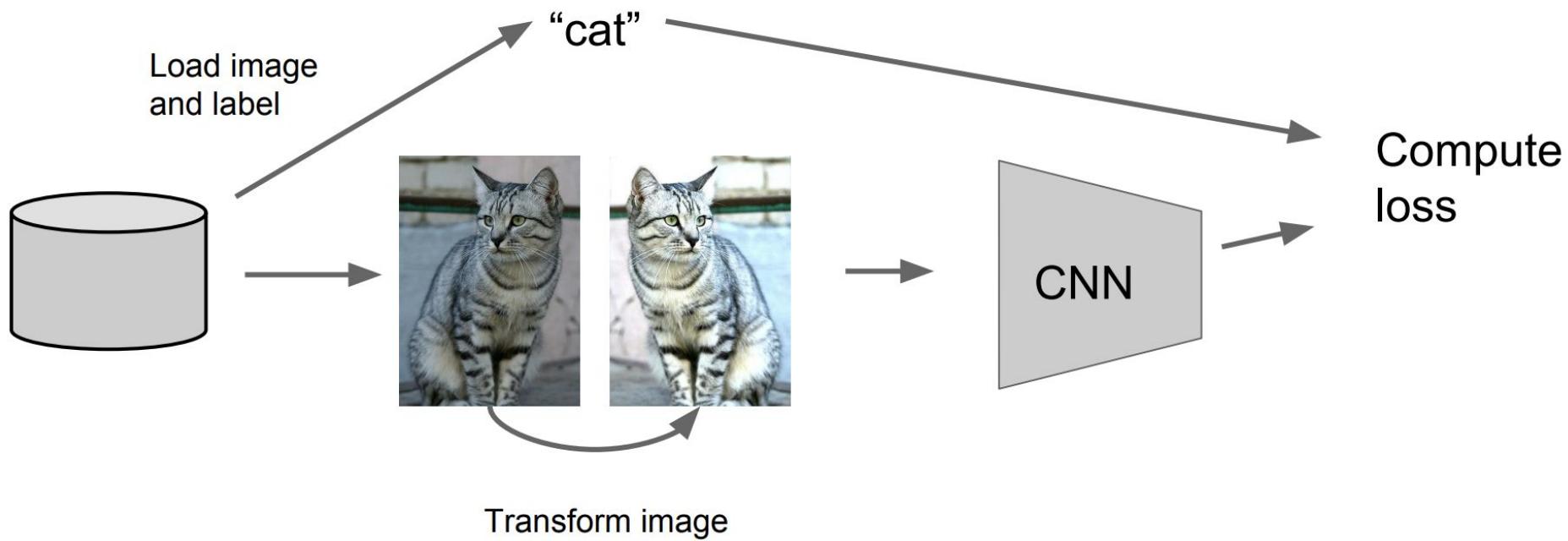
(b) After applying dropout.

Actually, on test case output should be normalized. See sources for more info.

Regularization: data augmentation



Regularization: data augmentation



Sum up: regularization

Regularization:

- Add some weight constraints
- Add some random noise during train and marginalize it during test
- Add some prior information in appropriate form

That's all. Feel free to ask any questions.