

Lecture 4

Optimisation & Regularization for Neural Networks

Goncharenko Vladislav

Moscow, 2021

1. Previous lecture recap: backpropagation, activations, intuition
2. Optimizers
3. Data normalization
4. Regularization
5. PyTorch practice
6. Q & A

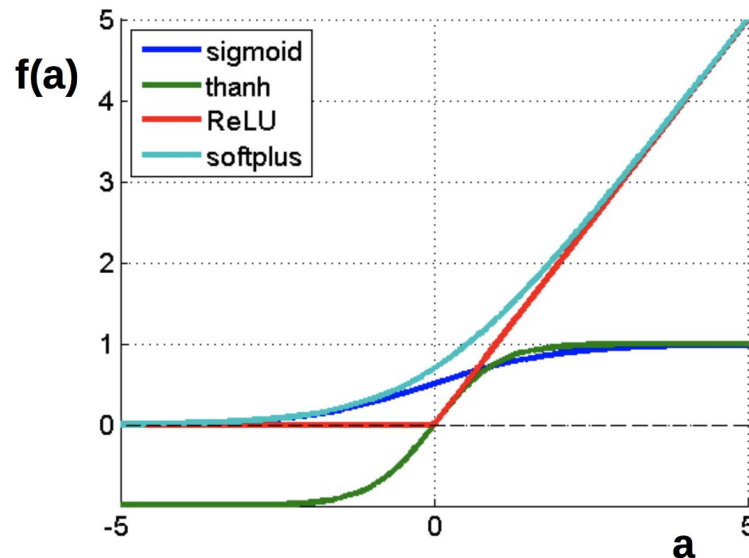
Once more: nonlinearities

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

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

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

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

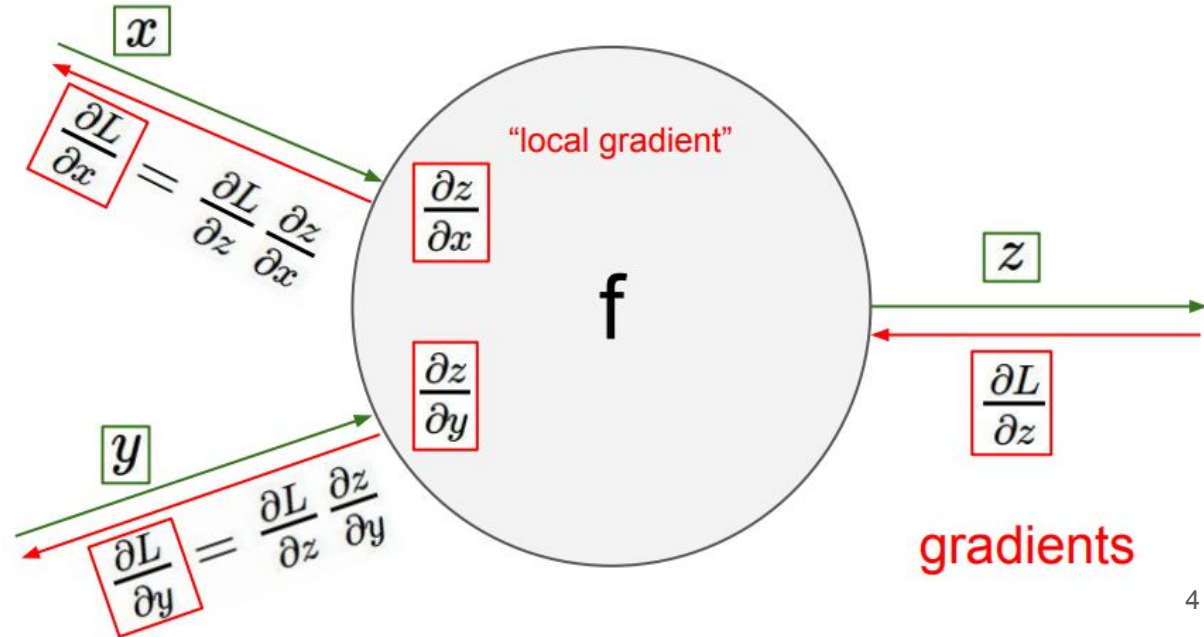


Backpropagation and chain rule

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.



- Layers
 - a. Dense layer (*done*)
 - b. Convolutional layer (*next lecture*)
 - c. Pooling layer (*next lecture*)
 - d. Dropout layer (*today*)
 - e. Batchnorm layer (batch normalization) (*today*)
 - f. Embeddings (aka word2vec, GloVe) (*last lecture*)
 - g. Recurrent layers (*last lecture*)

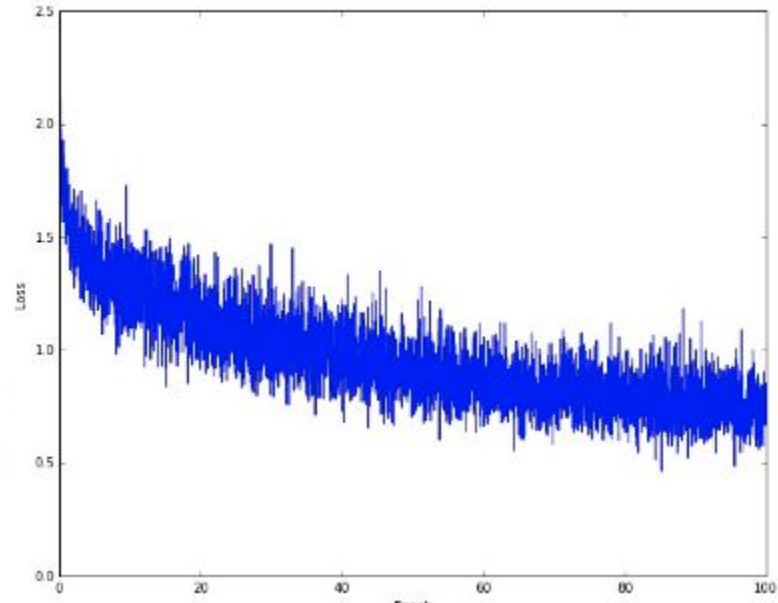
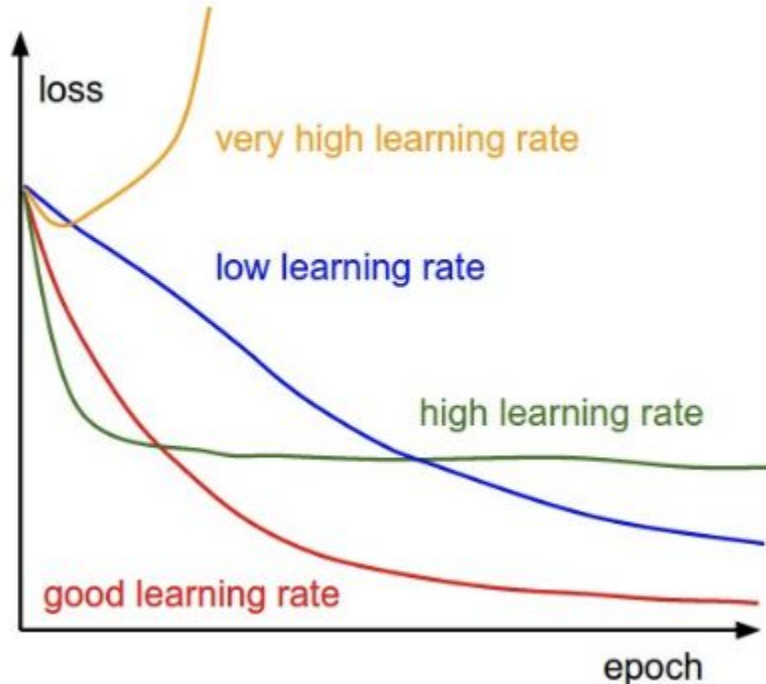
Different layers

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Optimizers

Stochastic gradient descent is used to optimize NN parameters.

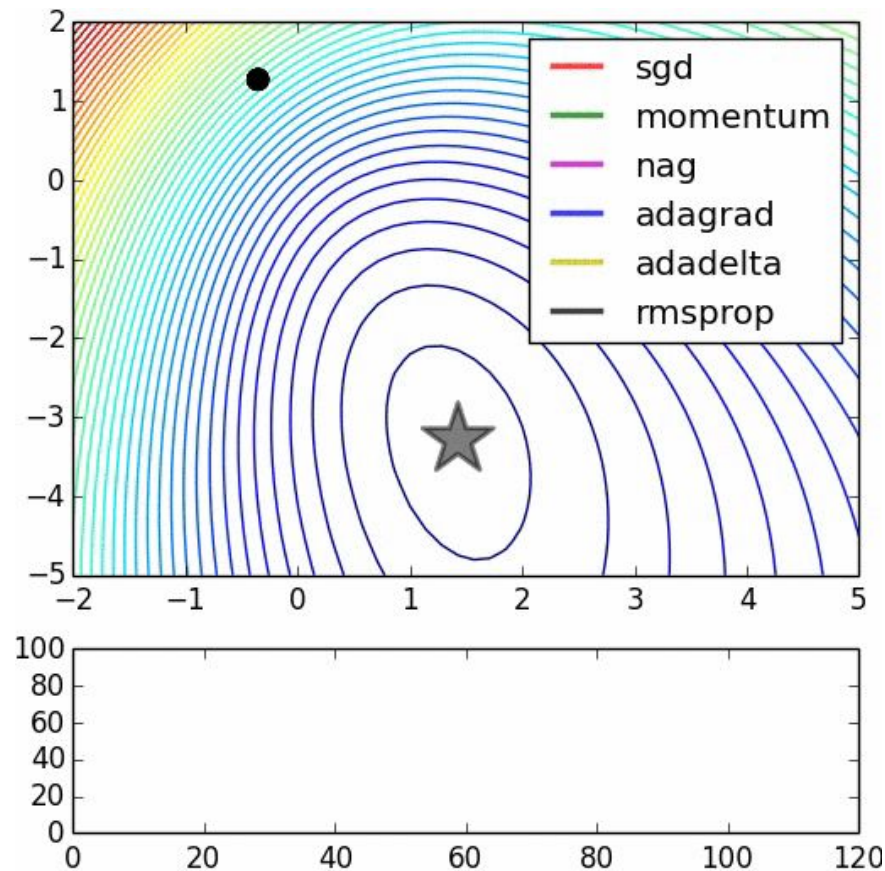
$$x_{t+1} = x_t - \text{learning rate} \cdot dx$$



Optimizers

There are much more optimizers:

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

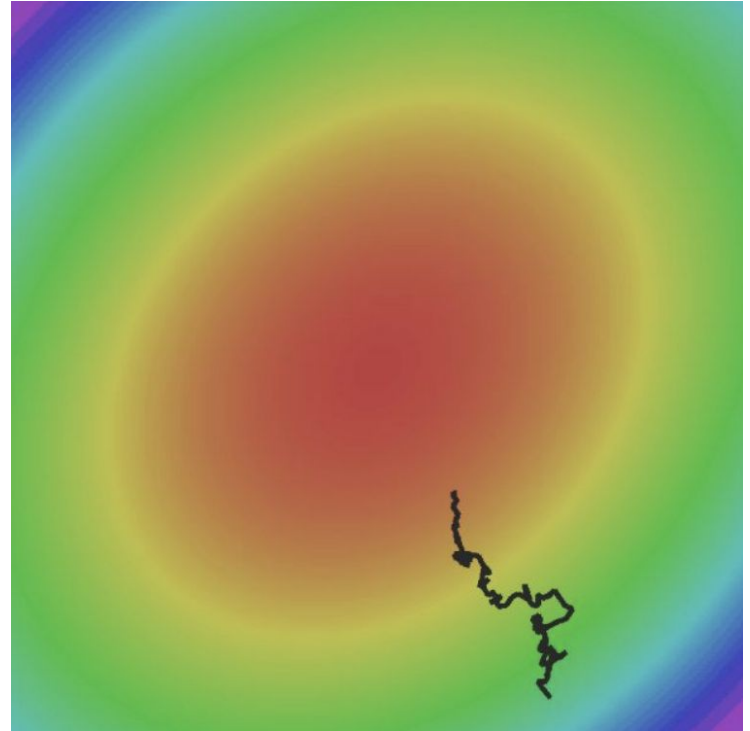


Optimization: SGD

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

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

Averaging over minibatches ---> noisy gradient



First idea: momentum

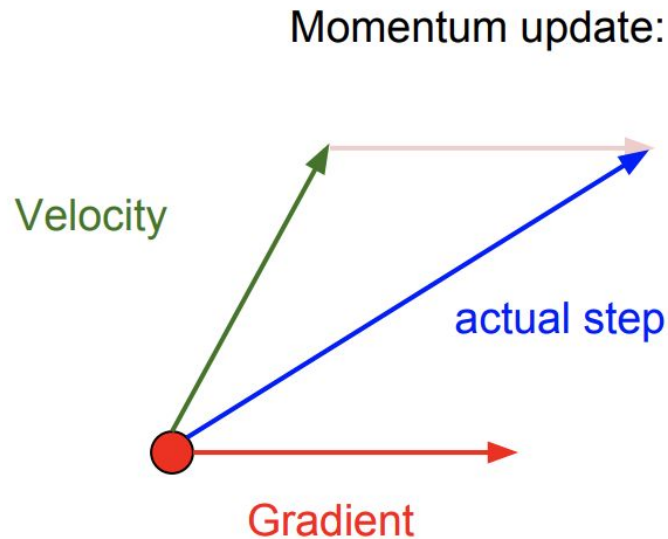
Simple SGD

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

SGD with momentum

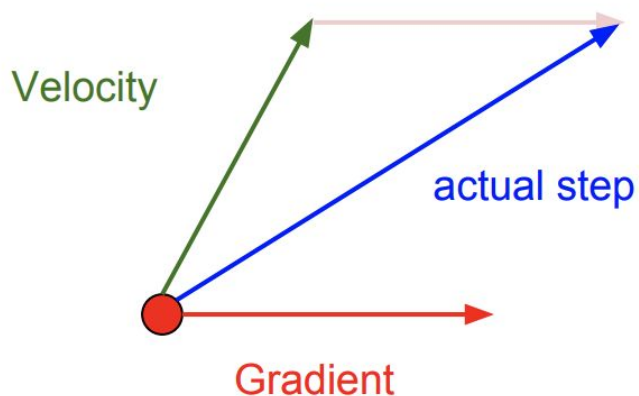
$$v_{t+1} = \rho v_t + \nabla f(x_t)$$

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



Nesterov momentum

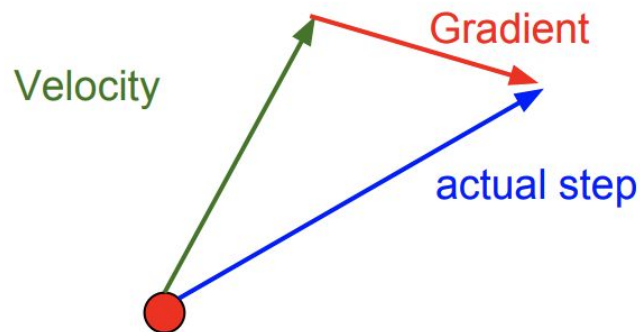
Momentum update:



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

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

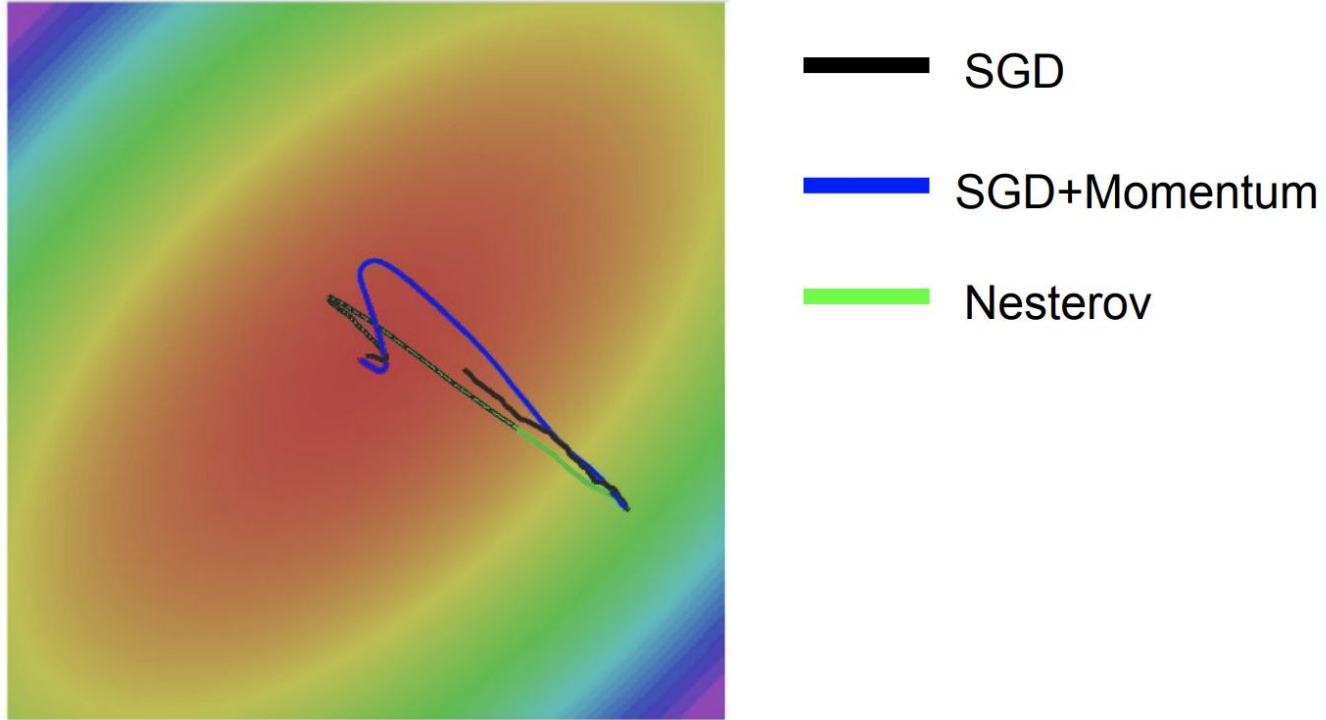
Nesterov Momentum



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

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

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

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Problem: gradient fades with time

Second idea: different dimensions are different

Adagrad: SGD with cache

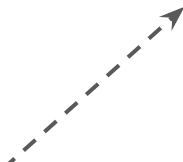
$$\text{cache}_{t+1} = \text{cache}_t + (\nabla f(x_t))^2$$

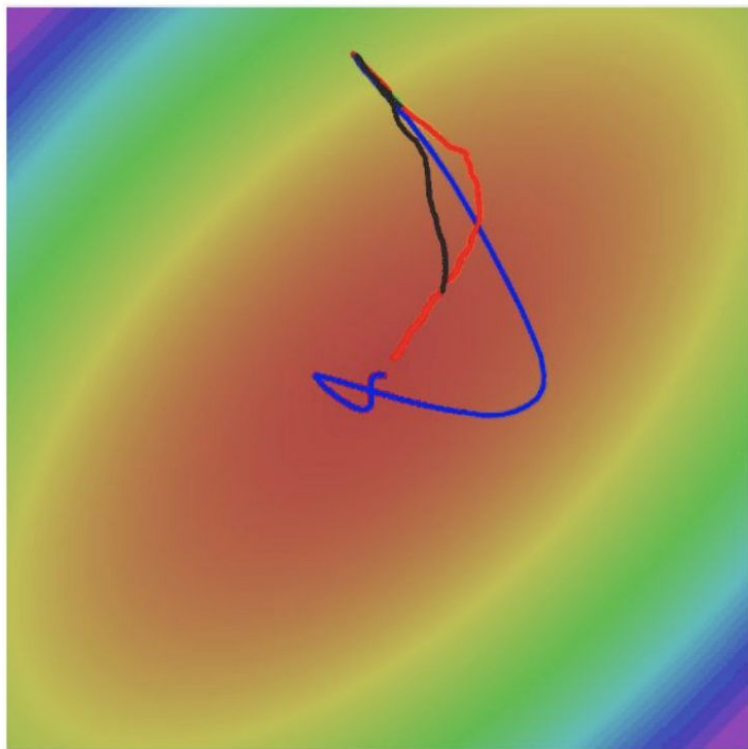
$$x_{t+1} = x_t - \alpha \frac{\nabla f(x_t)}{\text{cache}_{t+1} + \varepsilon}$$



RMSProp: SGD with cache with exp. Smoothing

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

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




- SGD
- SGD+Momentum
- RMSProp

Let's combine the momentum idea and RMSProp normalization:

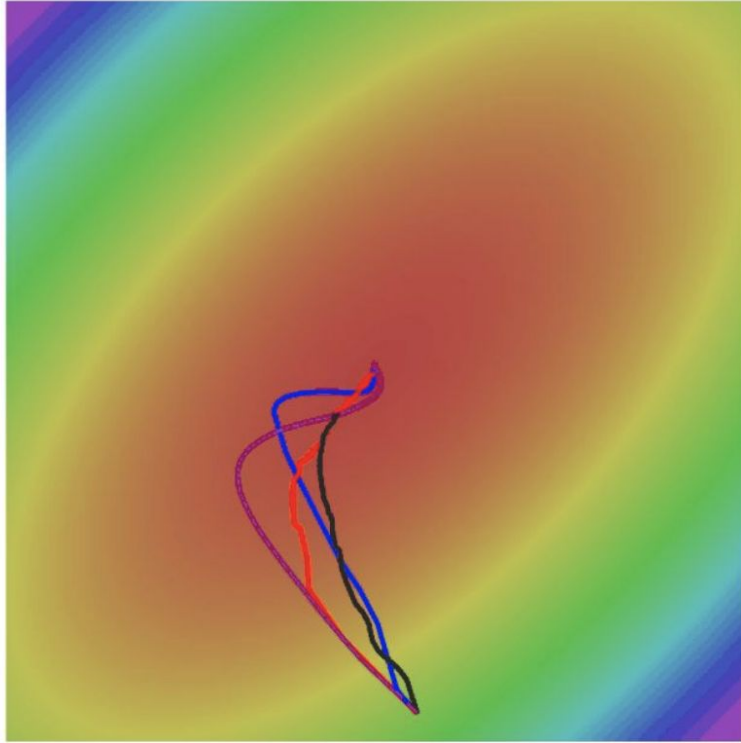
$$\begin{aligned}v_{t+1} &= \gamma v_t + (1 - \gamma) \nabla f(x_t) \\ \text{cache}_{t+1} &= \beta \text{cache}_t + (1 - \beta) (\nabla f(x_t))^2 \\ x_{t+1} &= x_t - \alpha \frac{v_{t+1}}{\text{cache}_{t+1} + \varepsilon}\end{aligned}$$

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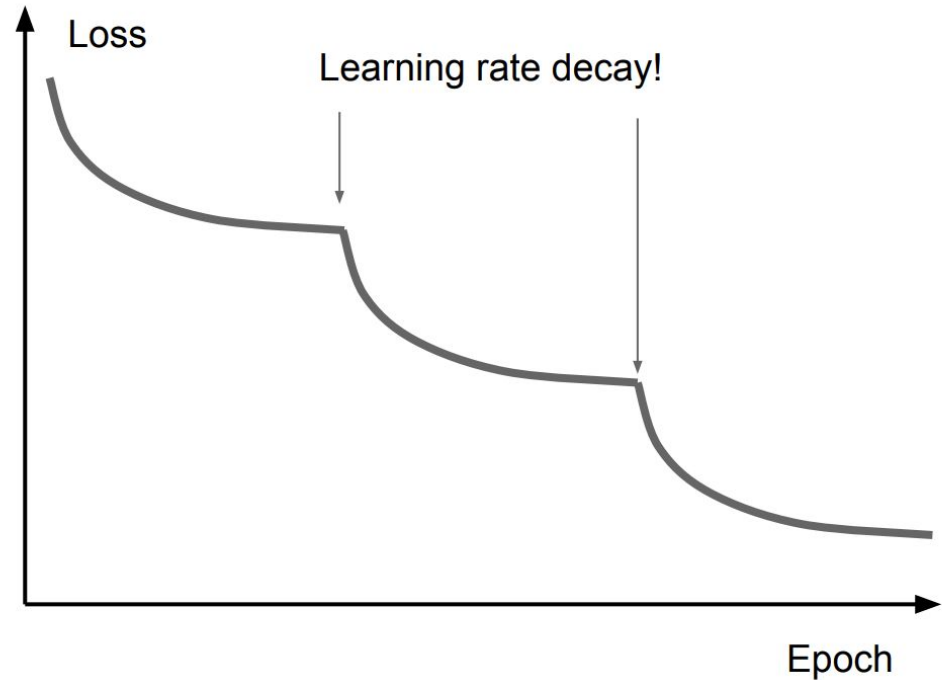
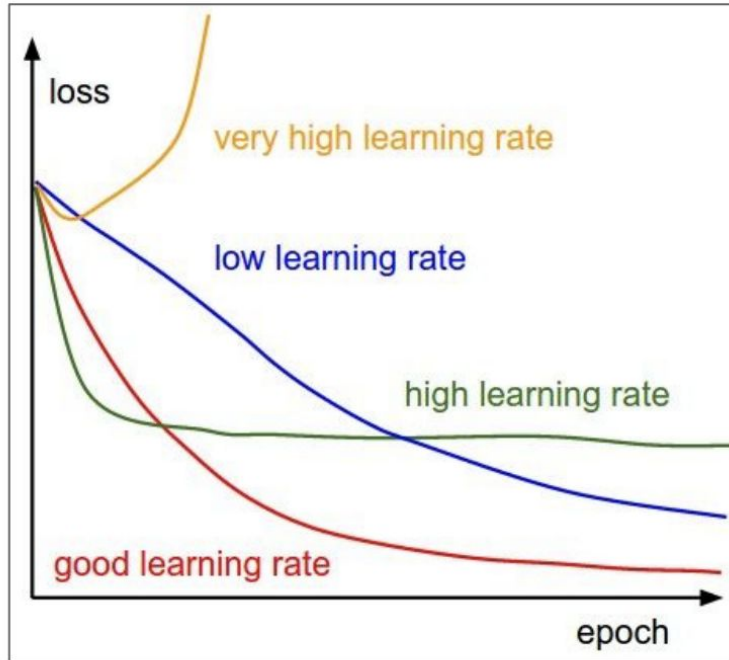
Actually, that's not quite Adam.

Comparing optimizers



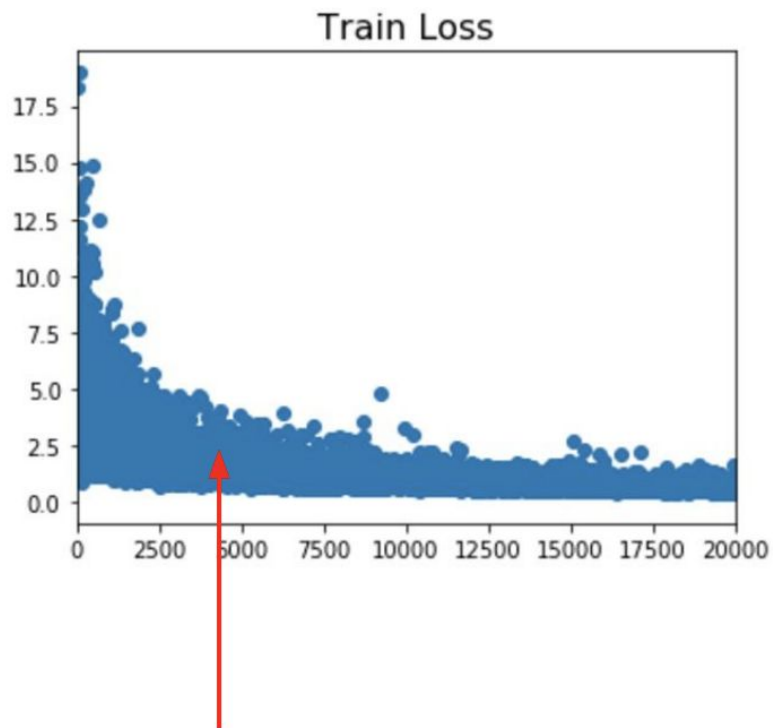
- SGD
- SGD+Momentum
- RMSProp
- Adam

Once more: learning rate

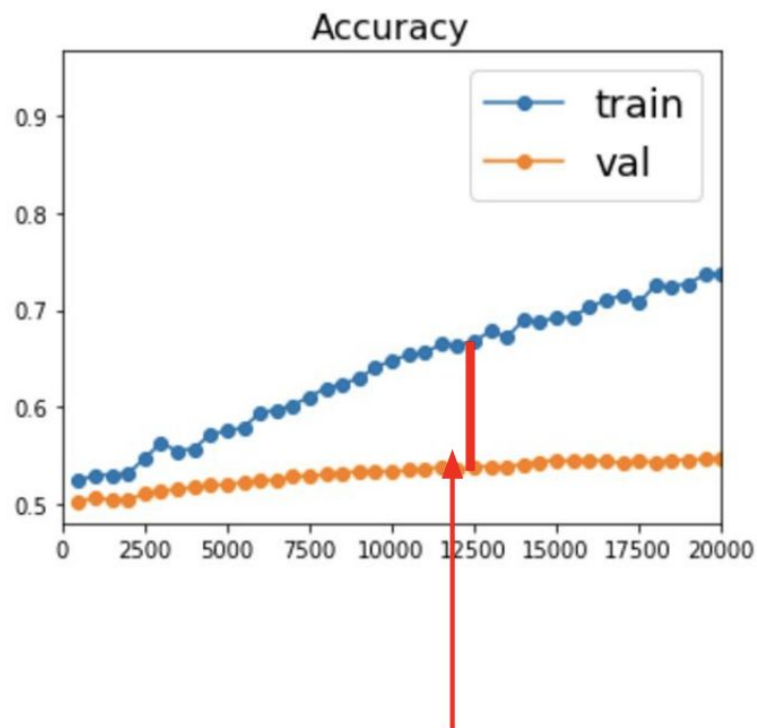


Sum up: optimization

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

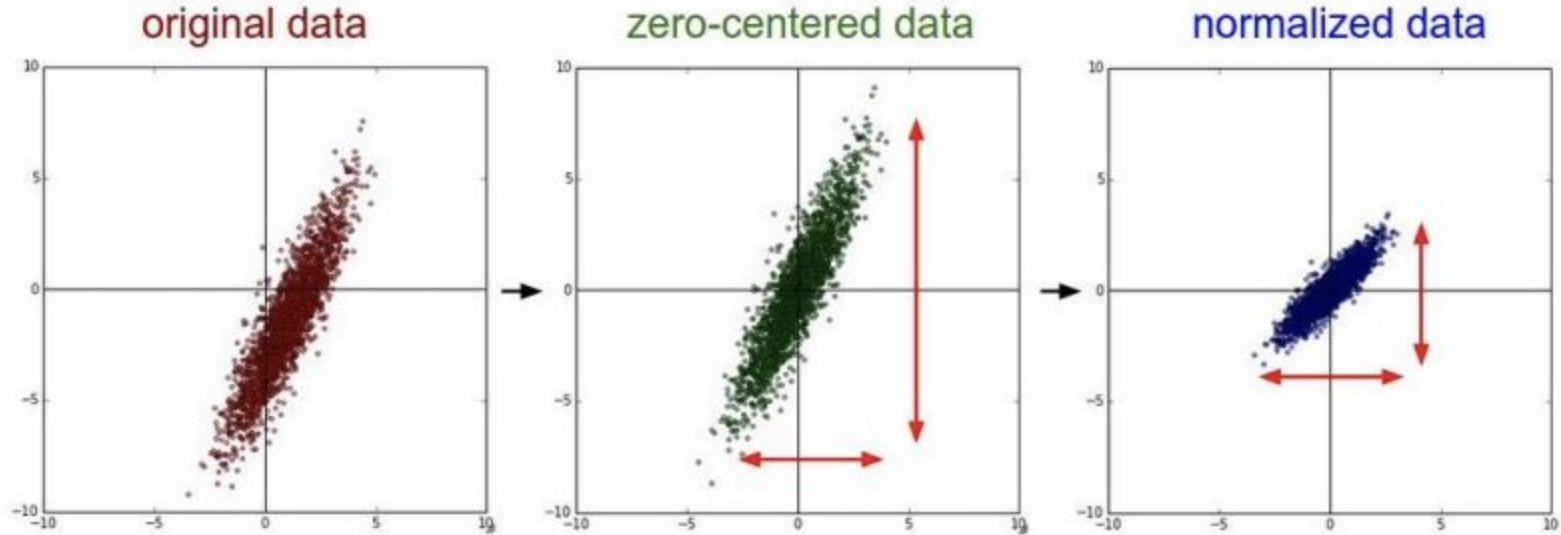


Better optimization algorithms
help reduce training loss



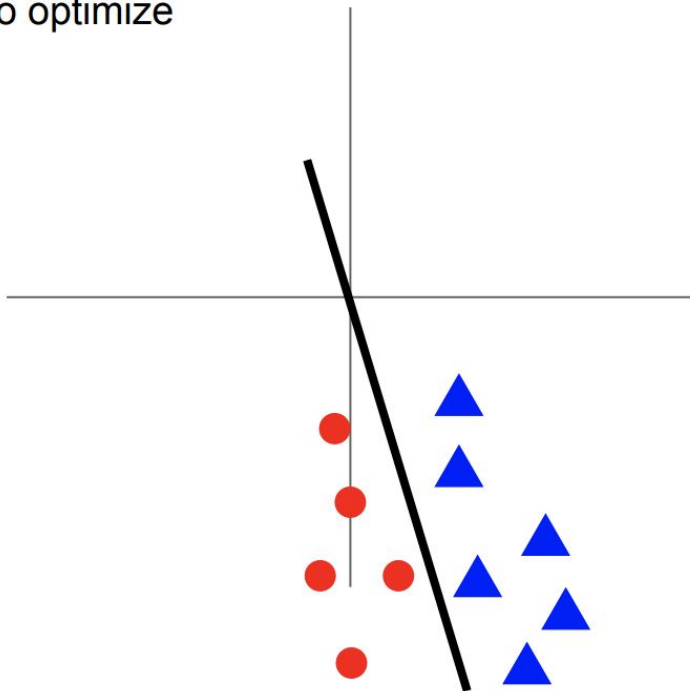
But we really care about error on new
data - how to reduce the gap?

Data normalization

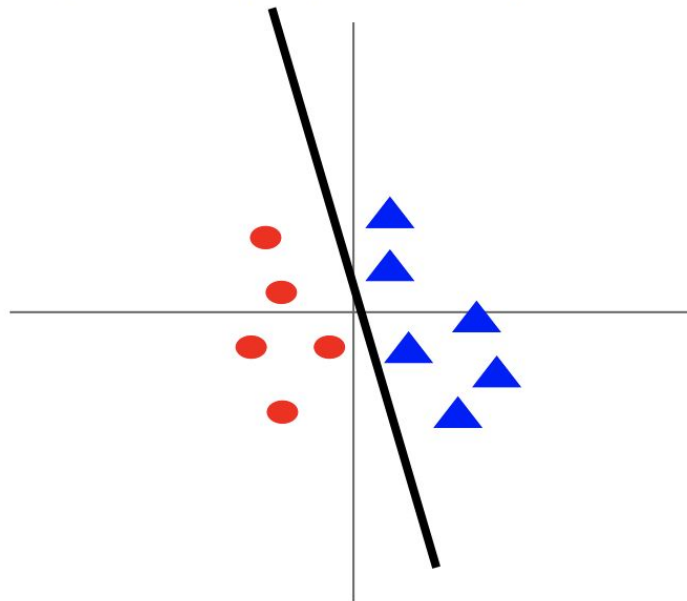


Data normalization

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

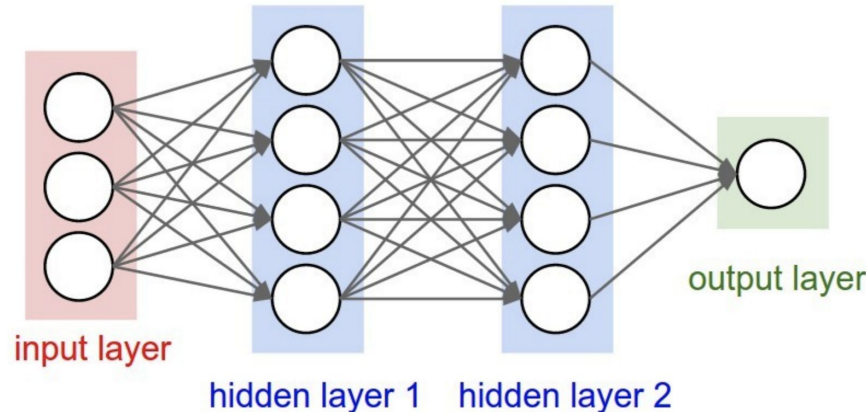
- Pitfall: all zero initialization.
- Small random numbers.
- Calibrated random numbers.

$$\begin{aligned} s &= \sum_i^n w_i x_i \\ \text{Var}(s) &= \text{Var}\left(\sum_i^n w_i x_i\right) \\ &= \sum_i^n \text{Var}(w_i x_i) \\ &= \sum_i^n [E(w_i)]^2 \text{Var}(x_i) + E[(x_i)]^2 \text{Var}(w_i) + \text{Var}(x_i) \text{Var}(w_i) \\ &= \sum_i^n \text{Var}(x_i) \text{Var}(w_i) \\ &= (n \text{Var}(w)) \text{Var}(x) \end{aligned}$$

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: $\mathcal{B} = \{x_1 \dots x_m\}$;

Parameters to be learned: γ, β

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

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

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

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

$$y_i \leftarrow \gamma \hat{x}_i + \beta \equiv \text{BN}_{\gamma, \beta}(x_i) \quad // \text{ scale and shift}$$

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What is this?

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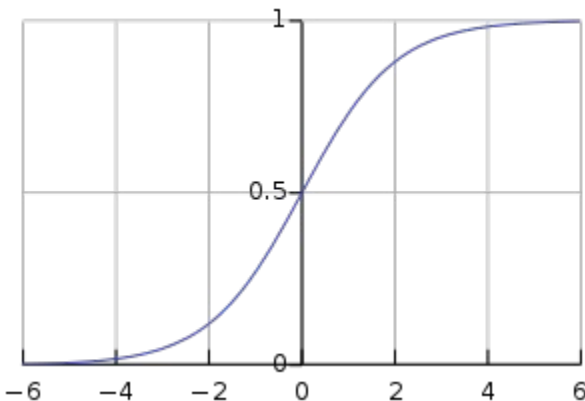
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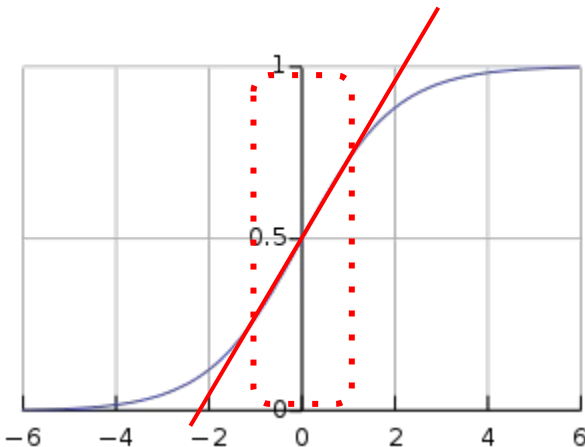
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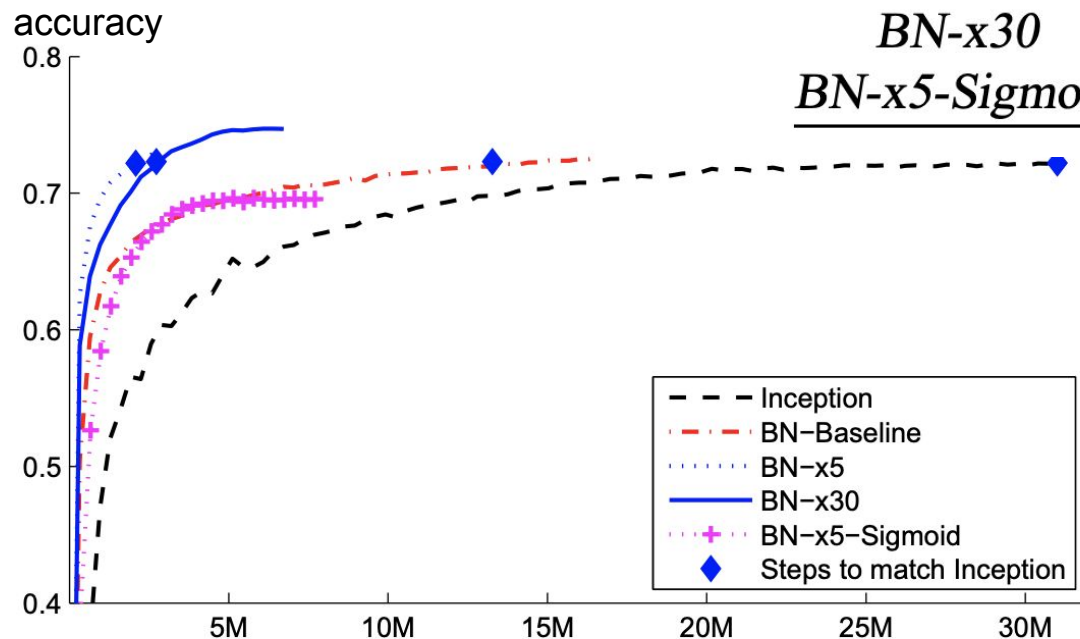
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What is this?

This transformation should be able to represent the identity transform.

Batch normalization

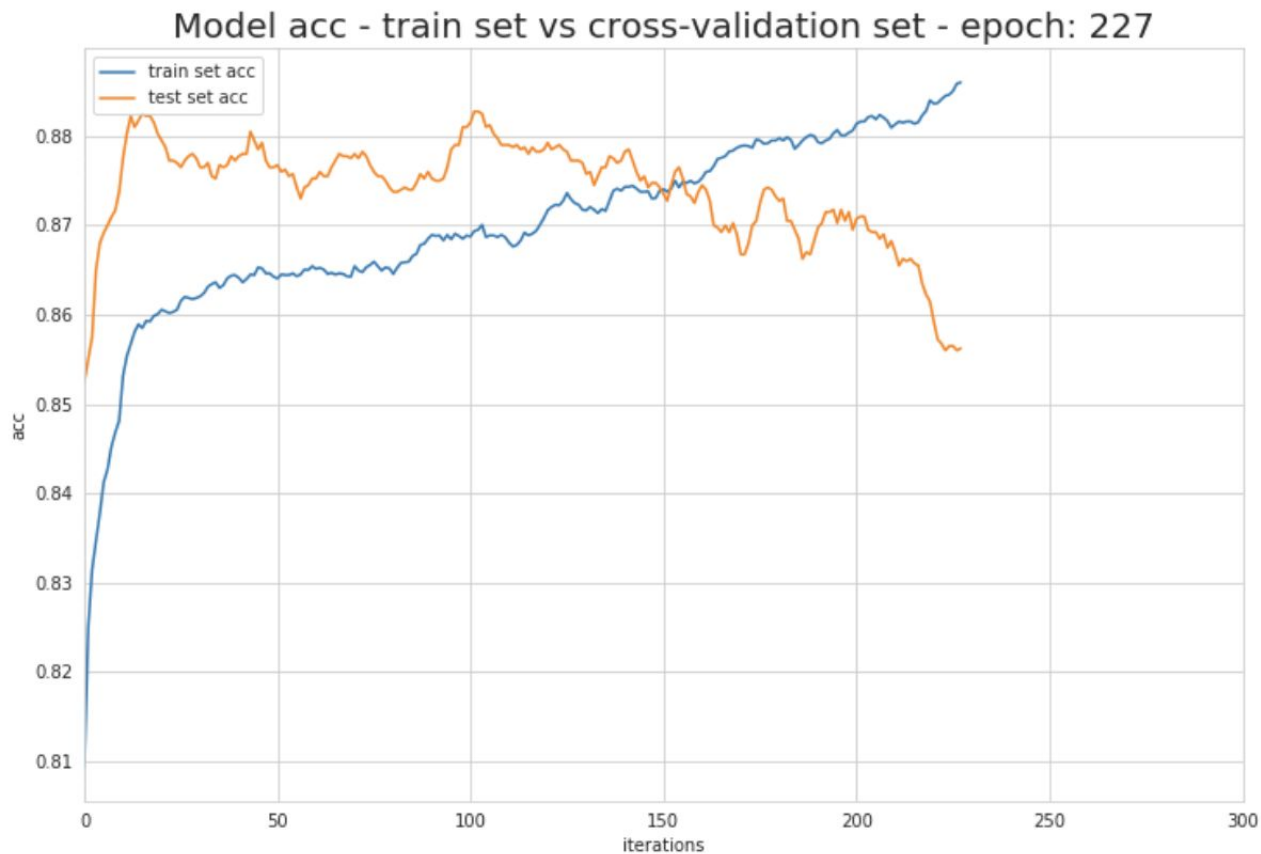
Model	Steps to 72.2%	Max accuracy
Inception	$31.0 \cdot 10^6$	72.2%
<i>BN-Baseline</i>	$13.3 \cdot 10^6$	72.7%
<i>BN-x5</i>	$2.1 \cdot 10^6$	73.0%
<i>BN-x30</i>	$2.7 \cdot 10^6$	74.8%
<i>BN-x5-Sigmoid</i>		69.8%



source: <https://arxiv.org/pdf/1502.03167.pdf>

number of training steps

Problem: overfitting



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

Adding some extra term to the loss function.

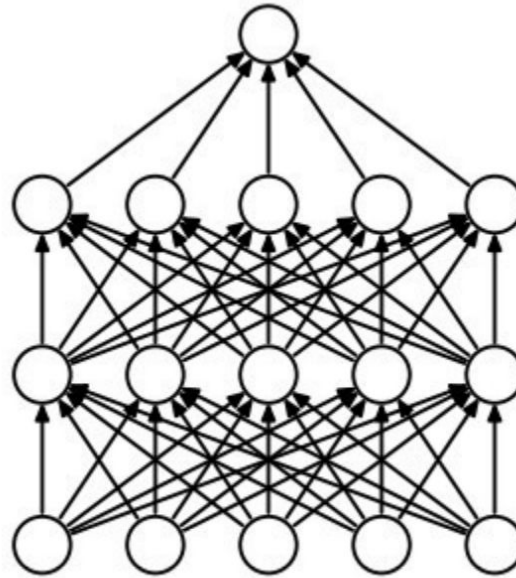
Common cases:

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

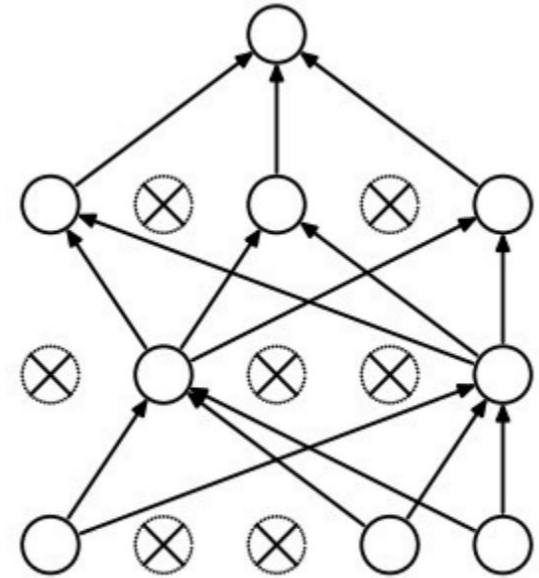
Regularization: Dropout

Some neurons are “dropped” during training.

Prevents overfitting.



(a) Standard Neural Net

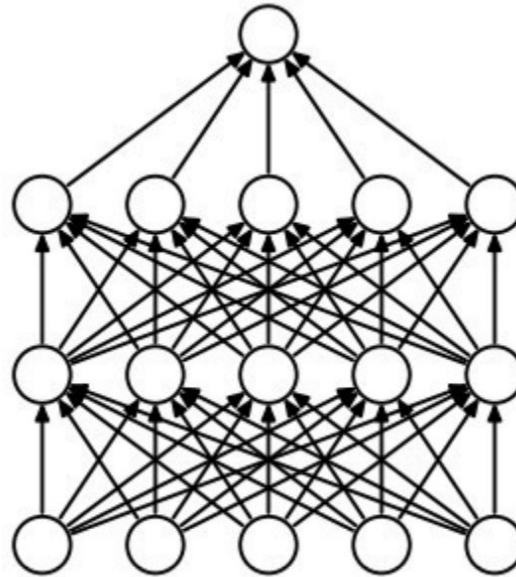


(b) After applying dropout.

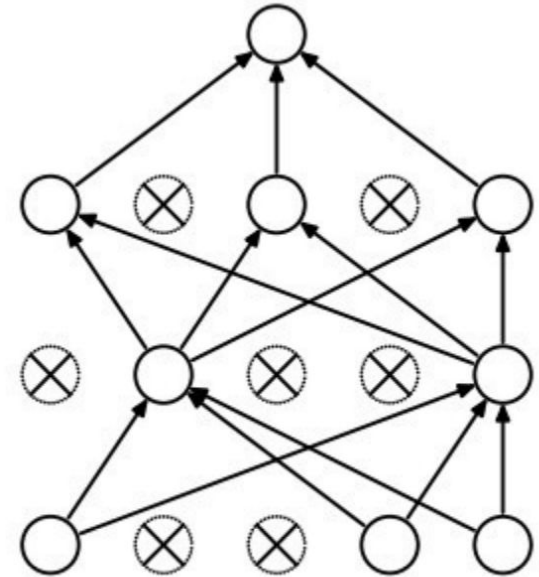
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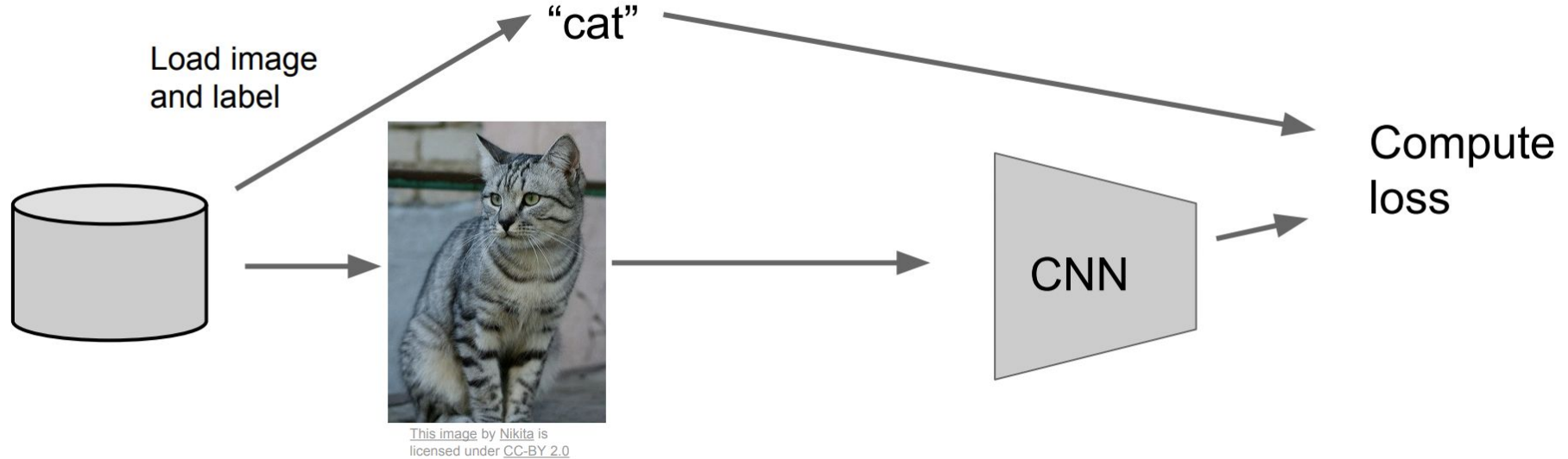
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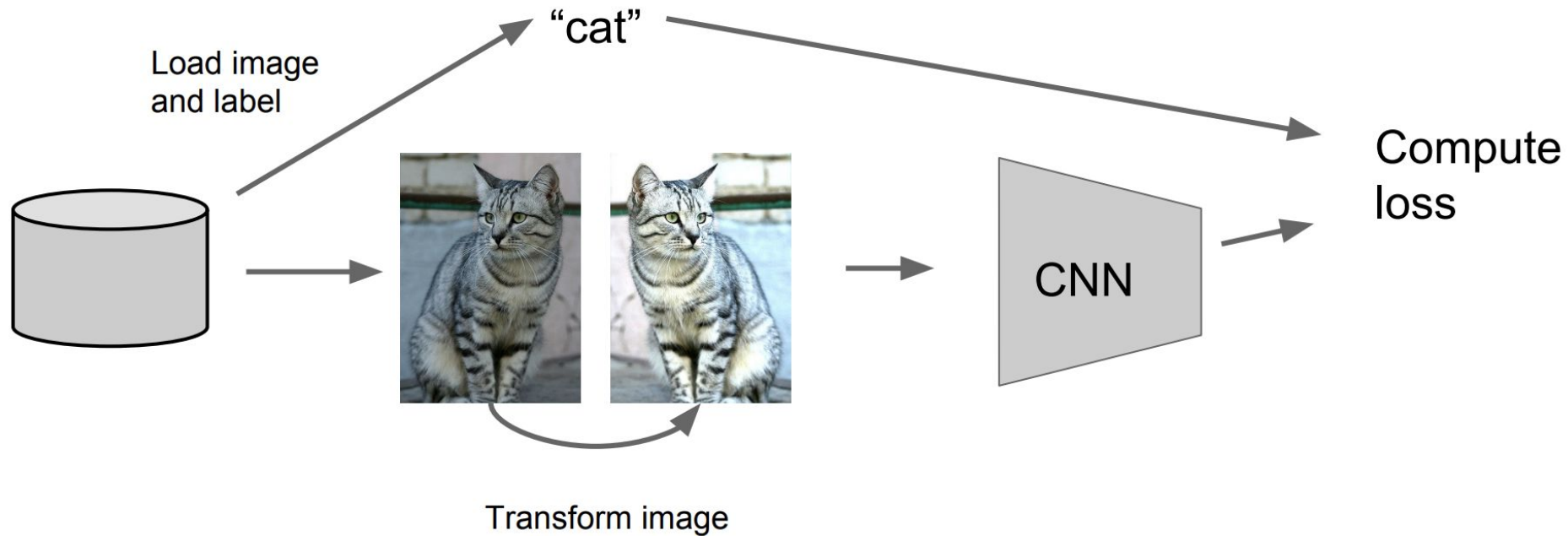
(b) After applying dropout.

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.