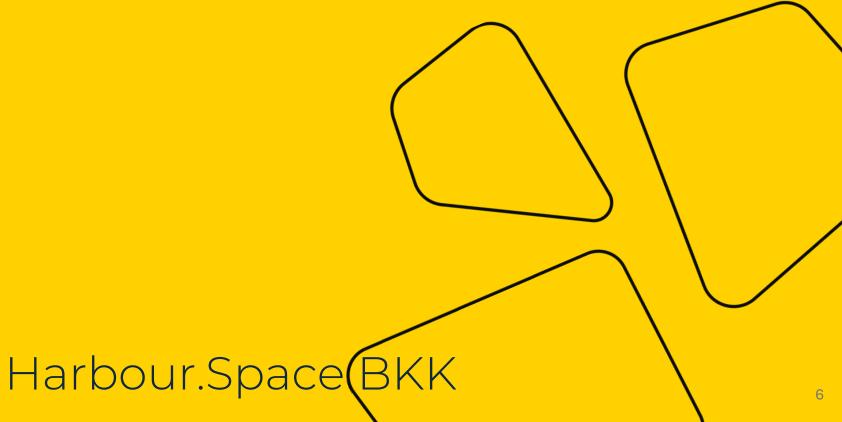
# Machine Learning. Lecture 9:

NN regularization.

Ivan Solomatin





# Outline

- Previous lecture recap: backpropagation, activations, intuition.
- 2. Optimizers.
- 3. Data normalization.
- 4. Regularization.



## Once again: nonlinearities

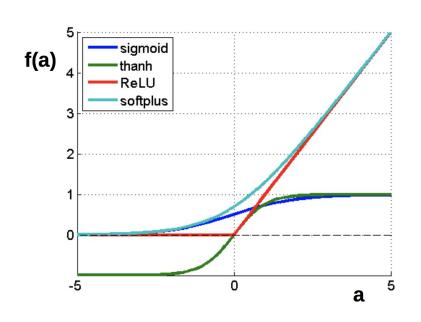


$$f(a) = \frac{1}{1 + e^{-a}}$$
$$f(a) = \tanh(a)$$

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

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

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



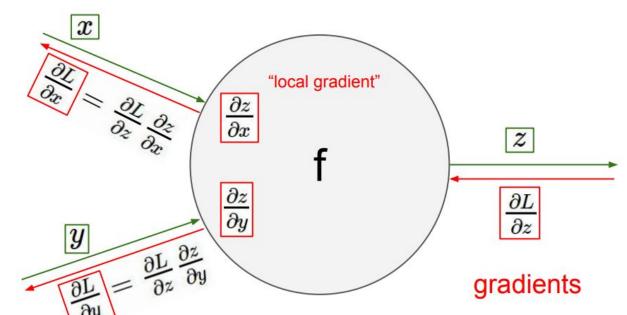
## **Backpropagation and chain rule**



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.

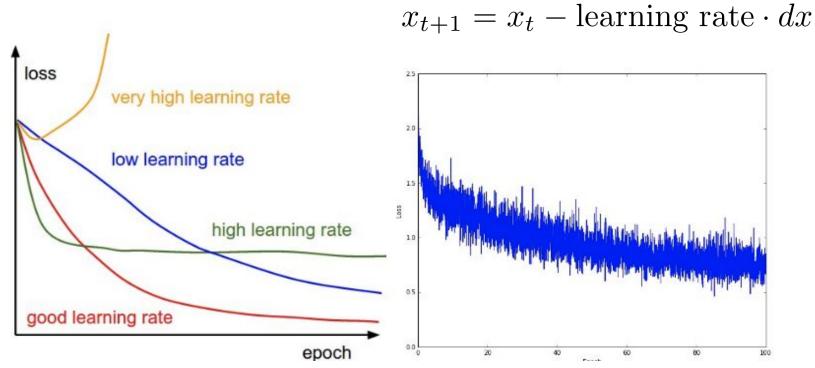


source: http://cs231n.github.

## **Optimizers**



Stochastic gradient descent is used to optimize NN parameters.

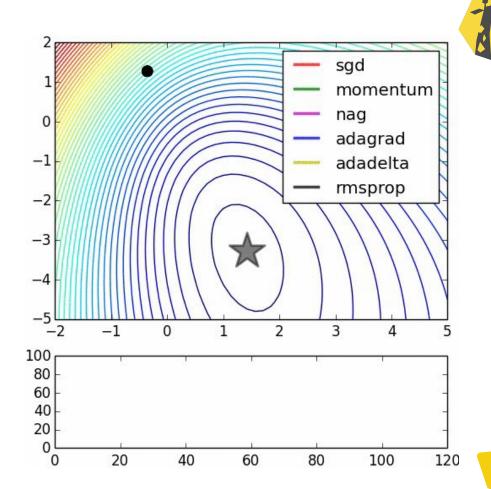


source: http://cs231n.github.io/neural-networks-3/

## **Optimizers**

There are much more optimizers:

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





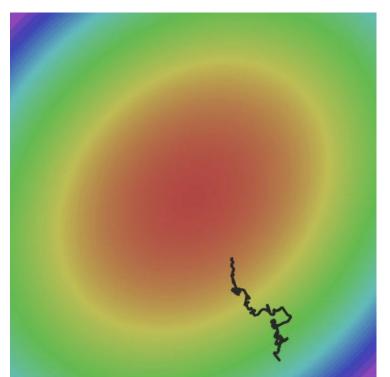
## **Optimization: SGD**



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

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

Averaging over mini batches => noisy gradient



#### First idea: momentum



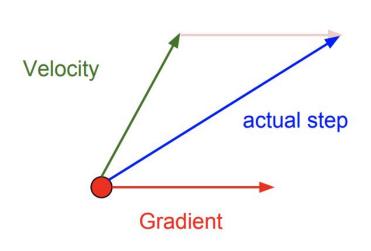
Simple SGD

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

SGD with momentum

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

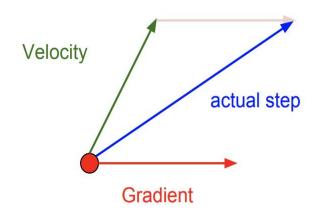
#### Momentum update:



#### **Nesterov momentum**

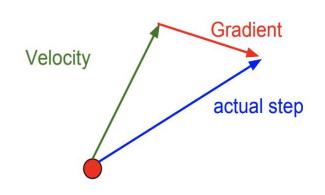


#### Momentum update:



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

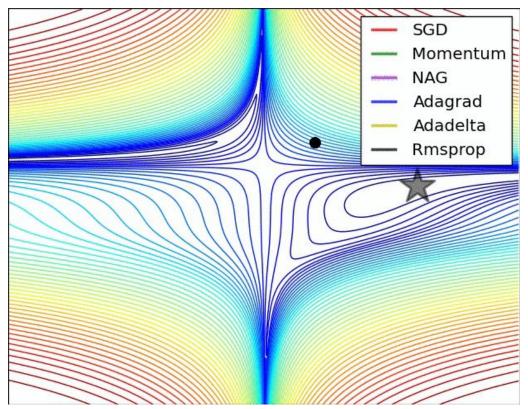
#### **Nesterov Momentum**



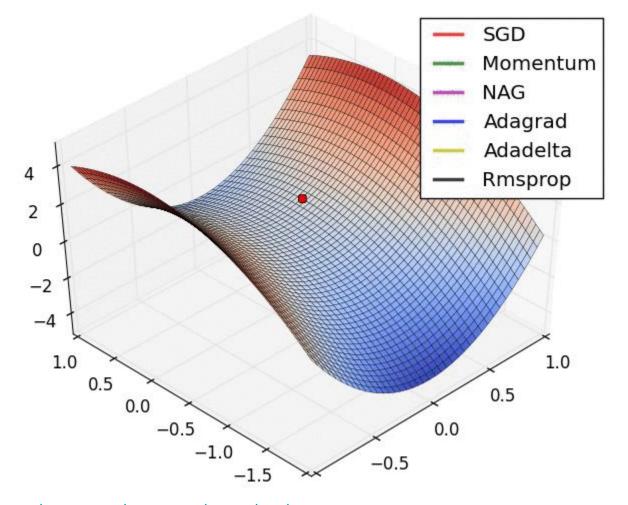
$$v_{t+1} = \rho v_t - \alpha \nabla f(x_t + \rho v_t)$$
$$x_{t+1} = x_t + v_{t+1}$$

## **Comparing momentums**





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Adagrad: SGD with cache

$$cache_{t+1} = cache_t + (\nabla f(x_t))^2$$

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





Adagrad: SGD with cache

$$cache_{t+1} = cache_t + (\nabla f(x_t))^2$$

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

Problem: gradient fades with time

# Second idea: different dimensions are different



Adagrad: SGD with cache

$$cache_{t+1} = cache_t + (\nabla f(x_t))^2$$

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

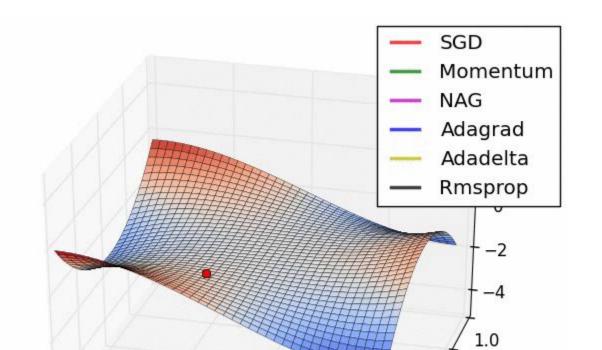
RMSProp: SGD with cache with exp. Smoothing

$$cache_{t+1} = \beta cache_t + (1 - \beta)(\nabla f(x_t))^2$$

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

Slide 29 Lecture 6 of Geoff Hinton's Coursera class

14



0.5

0.5

0.0

-0.5

 $1.0^{-1.0}$ 





-1.0

-0.5

0.0

#### **Adam**



Let's combine the momentum idea and RMSProp normalization:

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

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

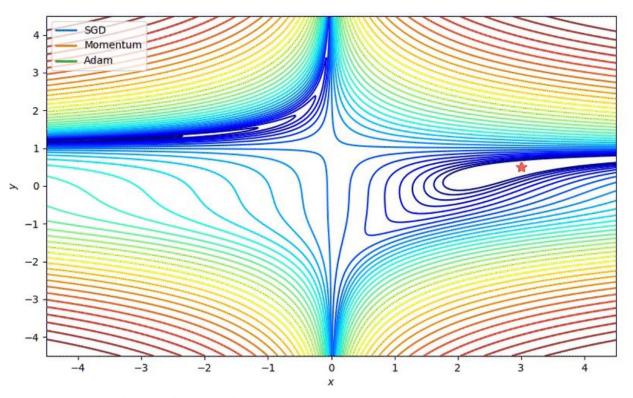
$$x_{t+1} = x_t - \alpha \frac{v_{t+1}}{\operatorname{cache}_{t+1} + \varepsilon}$$

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:

17



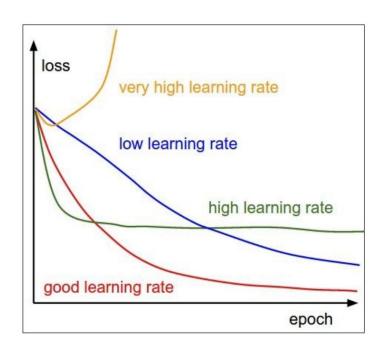


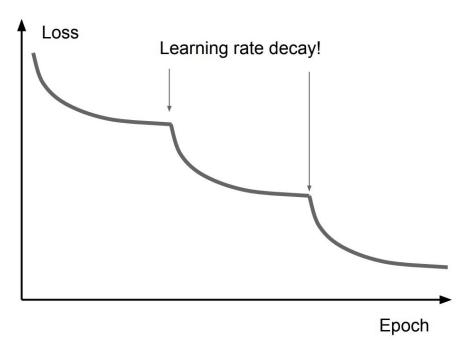
#### 3e-4 is the best learning rate for Adam, hands down.

6:01 AM · Nov 24, 2016 · Twitter Web Client					
<b>108</b> Ret	weets 461 l	Likes			
	9	t]	$\bigcirc$	$\triangle$	
	Andrej Karpathy @ @karpathy · Nov 24, 2016 Replying to @karpathy (i just wanted to make sure that people understand that this is a joke)				<b>V</b>
	Q 9	₹7 3	♡ 119	$\triangle$	

## Once more: learning rate





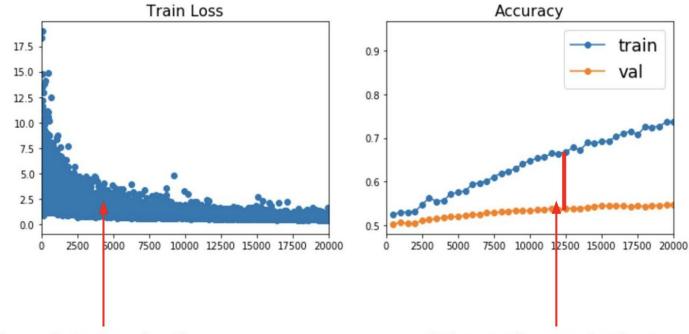


## Sum up: optimization



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



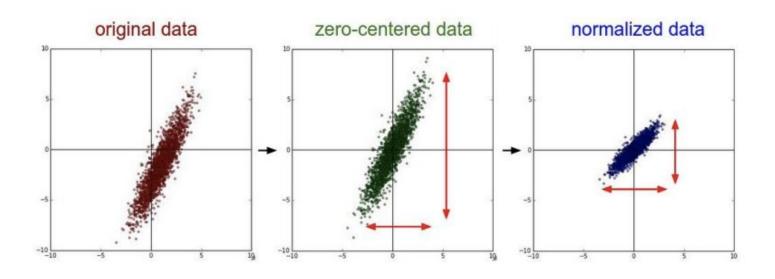


Better optimization algorithms help reduce training loss

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

## **Data normalization**



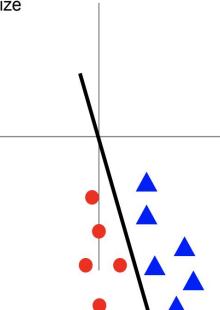


#### **Data normalization**

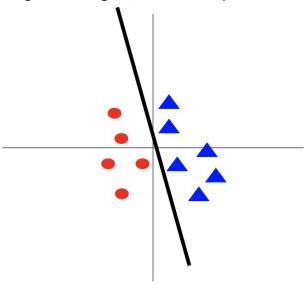


**Before normalization**: classification loss very sensitive to changes in weight matrix; hard to optimize

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.

$$Var(s) = Var(\sum_{i}^{n} w_{i}x_{i})$$

$$= \sum_{i}^{n} \operatorname{Var}(w_{i}x_{i})$$

$$= \sum_{i=1}^{n} [E(w_i)]^2 \operatorname{Var}(x_i) + E[(x_i)]^2 \operatorname{Var}(w_i) + \operatorname{Var}(x_i) \operatorname{Var}(w_i)$$

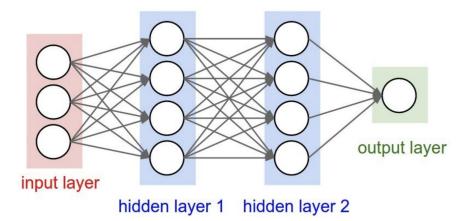
$$= \sum_{i}^{n} \operatorname{Var}(x_{i}) \operatorname{Var}(w_{i})$$

$$= (nVar(w)) Var(x)$$



#### 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





TL; DR:

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



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

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

• Update  $\mu_i, \sigma_i^2$  with moving average while training

$$\mu_{i} := \alpha \cdot mean_{batch} + (1 - \alpha) \cdot \mu_{i}$$

$$\sigma_{i}^{2} := \alpha \cdot variance_{batch} + (1 - \alpha) \cdot \sigma_{i}^{2}$$



Original algorithm (2015)

```
Input: Values of x over a mini-batch: \mathcal{B} = \{x_{1...m}\};
               Parameters to be learned: \gamma, \beta
Output: \{y_i = BN_{\gamma,\beta}(x_i)\}
  \mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i
                                                                         // mini-batch mean
   \sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2
                                                               // mini-batch variance
    \widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}
                                                                                       // normalize
     y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv BN_{\gamma,\beta}(x_i)
                                                                              // scale and shift
```

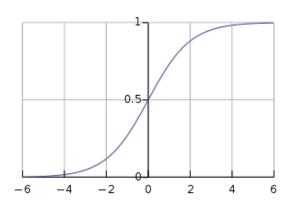


Original algorithm (2015)

What is this?

**Input:** Values of x over a mini-batch:  $\mathcal{B} = \{x_{1...m}\}$ ; Parameters to be learned:  $\gamma$ ,  $\beta$ **Output:**  $\{y_i = BN_{\gamma,\beta}(x_i)\}$  $\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i$ // mini-batch mean  $\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2$ // mini-batch variance  $\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}}$ // normalize  $y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv BN_{\gamma,\beta}(x_i)$ // scale and shift





Input: Values of x over a mini-batch:  $\mathcal{B} = \{x_{1...m}\}$ ; Parameters to be learned:  $\gamma$ ,  $\beta$ 

Output:  $\{y_i = BN_{\gamma,\beta}(x_i)\}$ 

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

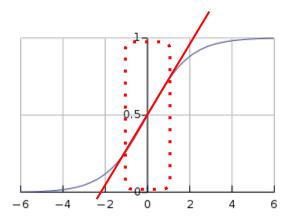
$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2$$
 // mini-batch variance

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

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i)$$

// scale and shift





**Input:** Values of x over a mini-batch:  $\mathcal{B} = \{x_{1...m}\}$ ; Parameters to be learned:  $\gamma$ ,  $\beta$ 

Output:  $\{y_i = BN_{\gamma,\beta}(x_i)\}$ 

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

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

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

$$y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv \mathrm{BN}_{\gamma,\beta}(x_i)$$
 // s

// scale and shift



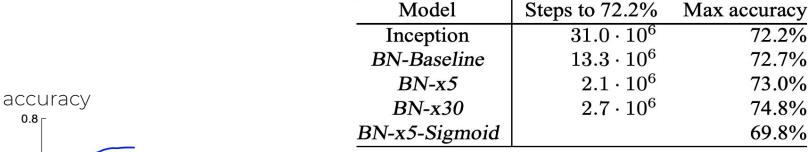
Original algorithm (2015)

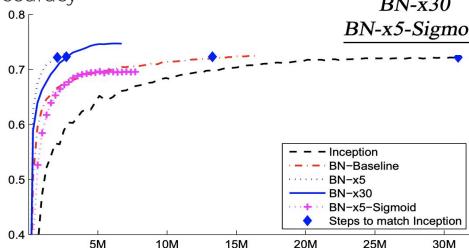
What is this?

This transformation should be able to represent the identity transform.

```
Input: Values of x over a mini-batch: \mathcal{B} = \{x_{1...m}\};
              Parameters to be learned: \gamma, \beta
Output: \{y_i = BN_{\gamma,\beta}(x_i)\}
   \mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i
                                                                       // mini-batch mean
   \sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2
                                                                 // mini-batch variance
    \widehat{x}_i \leftarrow \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}
                                                                                    // normalize
     y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv BN_{\gamma,\beta}(x_i)
                                                                            // scale and shift
```



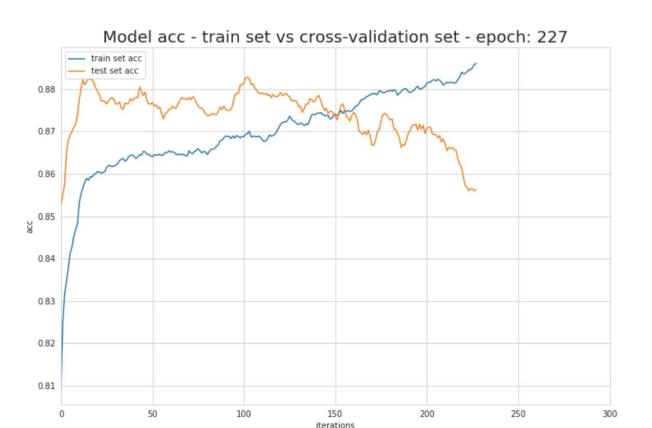




number of training steps

## **Problem: overfitting**





## Regularization



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

Adding some extra term to the loss function.

#### Common cases:

- L2 regularization:
- L1 regularization:
- Elastic Net (L1 + L2):

$$R(W) = ||W||_2^2$$

$$R(W) = ||W||_1$$

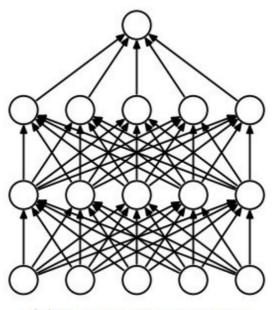
$$R(W) = \beta ||W||_2^2 + ||W||_1$$

## **Regularization: Dropout**

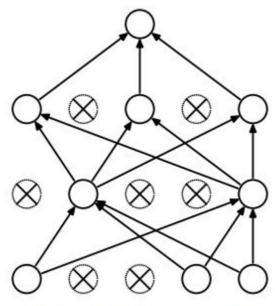


Some neurons are "drop training.

Prevents overfitting.



(a) Standard Neural Net



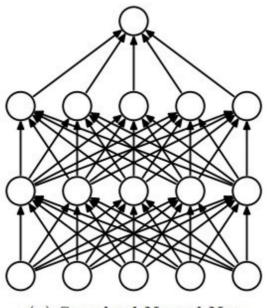
(b) After applying dropout.

## **Regularization: Dropout**

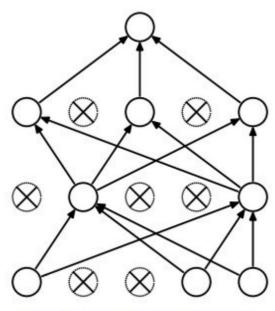


Some neurons are "dropped" during training.

Prevents overfitting.



(a) Standard Neural Net

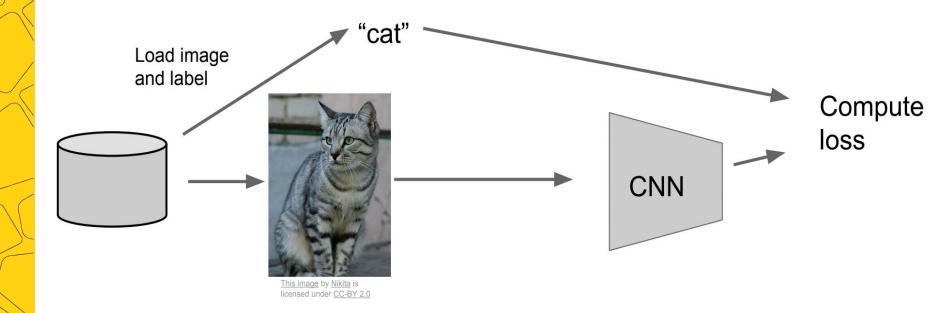


(b) After applying dropout.

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

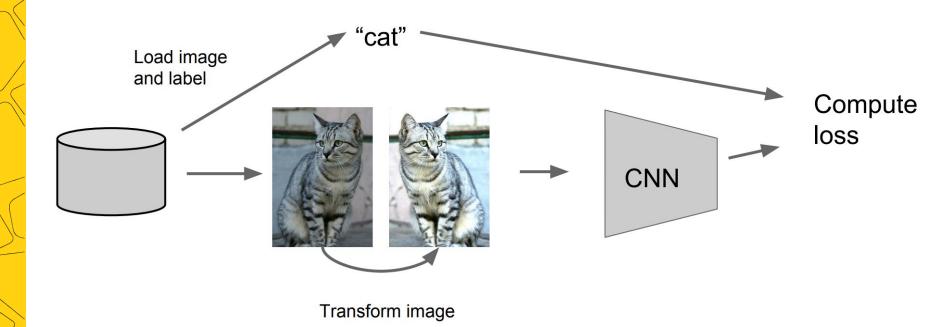
## Regularization: data augmentation





## Regularization: data augmentation





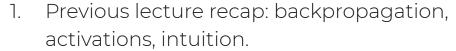
## Sum up: regularization



#### Regularization:

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

# Revise



- 2. Optimizers.
- 3. Data normalization.
- 4. Regularization.



# **Thanks for attention!**

Questions?



