Outline

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



Once again: nonlinearities

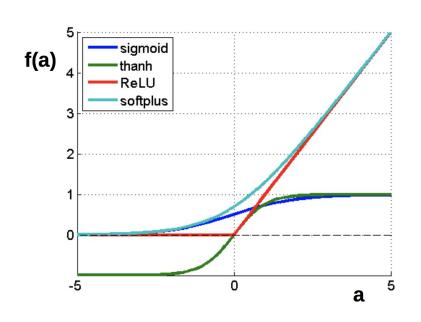


$$f(a) = \frac{1}{1 + e^{-a}}$$
$$f(a) = \tanh(a)$$

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

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

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



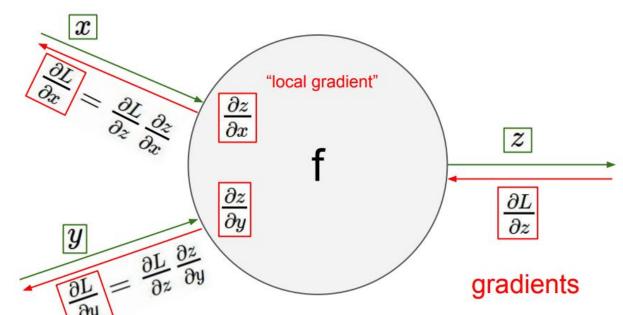
Backpropagation and chain rule



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.

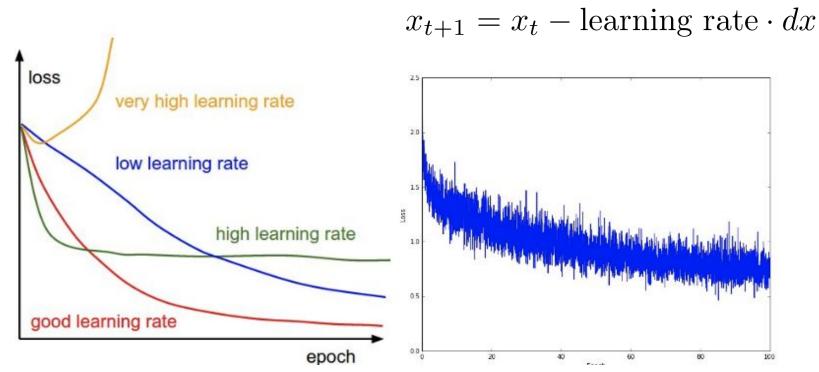


source: http://cs231n.github.

Optimizers



Stochastic gradient descent is used to optimize NN parameters.

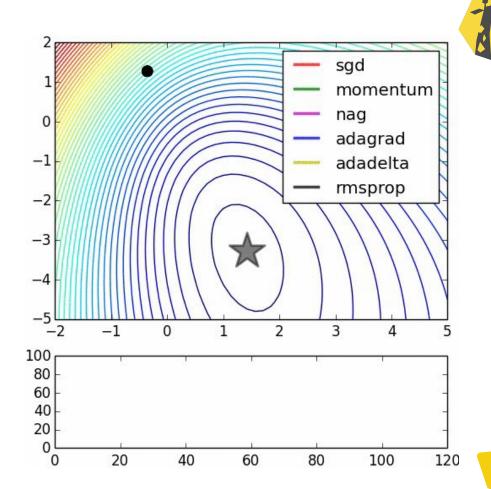


source: http://cs231n.github.io/neural-networks-3/

Optimizers

There are much more optimizers:

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





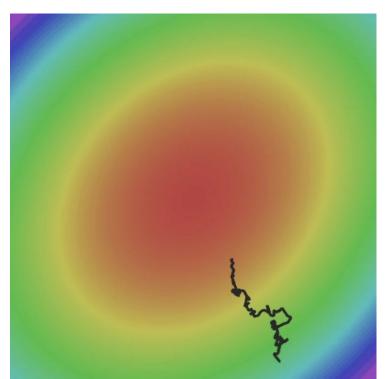
Optimization: SGD



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

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

Averaging over mini batches => noisy gradient



First idea: momentum



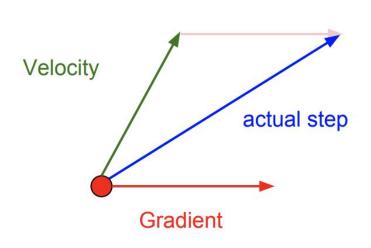
Simple SGD

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

SGD with momentum

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

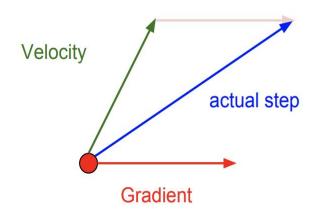
Momentum update:



Nesterov momentum

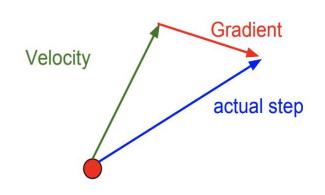


Momentum update:



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

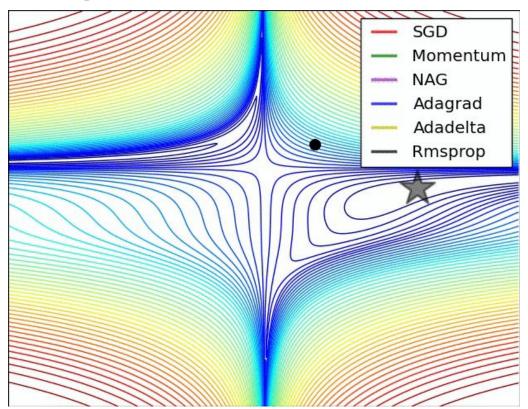
Nesterov Momentum



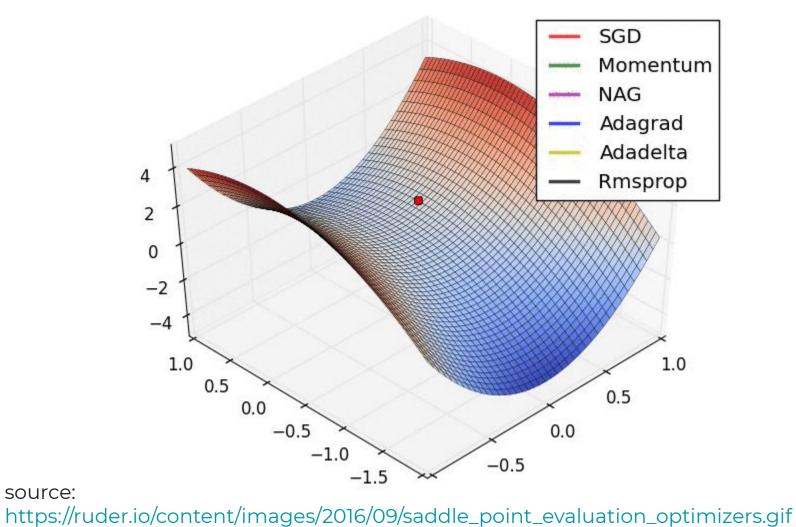
$$v_{t+1} = \rho v_t - \alpha \nabla f(x_t + \rho v_t)$$
$$x_{t+1} = x_t + v_{t+1}$$

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

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

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

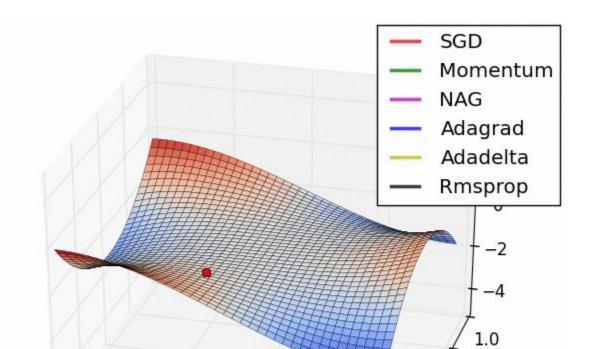
RMSProp: SGD with cache with exp. Smoothing

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

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

Slide 29 Lecture 6 of Geoff Hinton's Coursera class

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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:

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

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

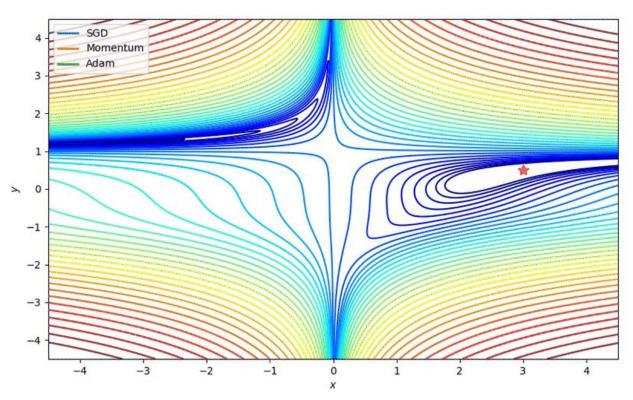
$$x_{t+1} = x_t - \alpha \frac{v_{t+1}}{\operatorname{cache}_{t+1} + \varepsilon}$$

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:

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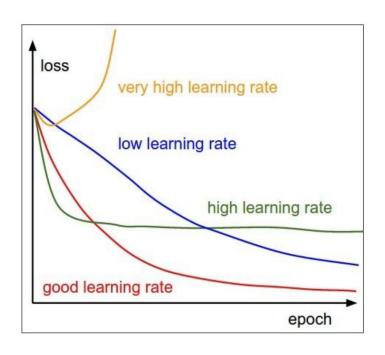
3e-4 is the best learning rate for Adam, hands down.

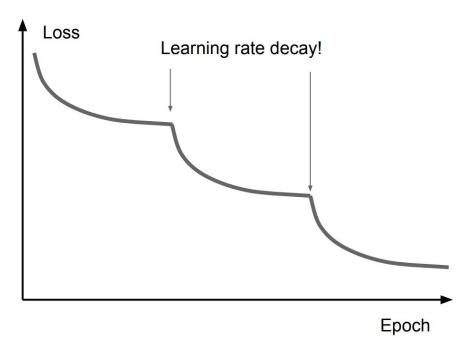
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108 Ret	weets 461	Likes			
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Once more: learning rate





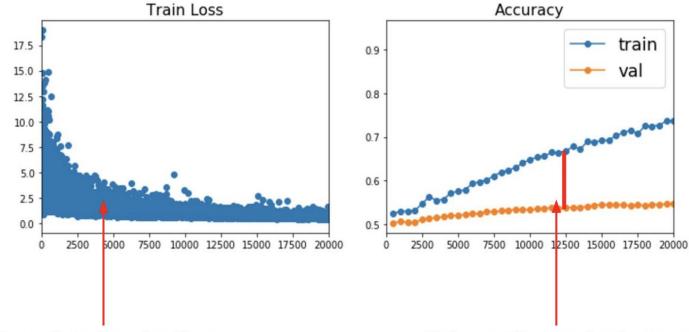


Sum up: optimization



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



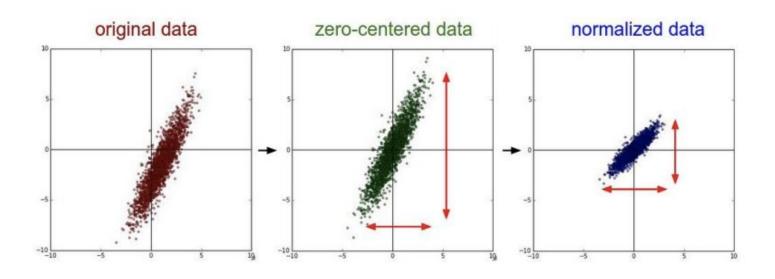


Better optimization algorithms help reduce training loss

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

Data normalization

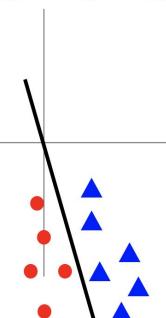




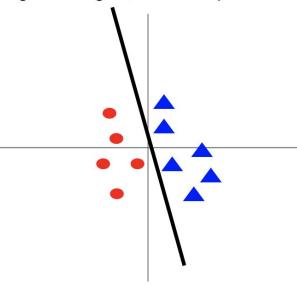
Data normalization



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.

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

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

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

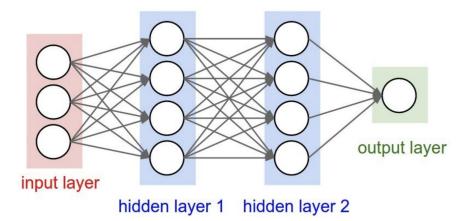
$$= \sum_{i}^{n} \operatorname{Var}(x_{i}) \operatorname{Var}(w_{i})$$

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



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 μ_i , σ_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
```

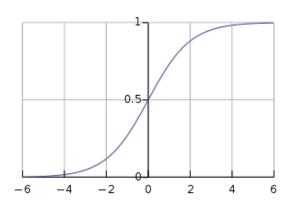


Original algorithm (2015)

What is this?

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

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

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

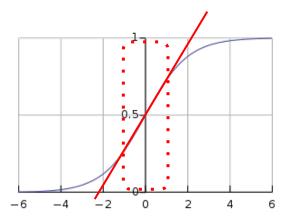
$$\sigma_{\mathcal{B}}^2 \leftarrow \frac{1}{m} \sum_{i=1}^m (x_i - \mu_{\mathcal{B}})^2$$
 // mini-batch variance

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

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



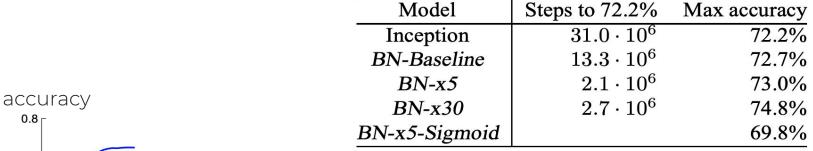
Original algorithm (2015)

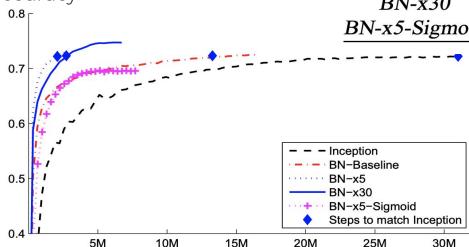
What is this?

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: γ , β 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



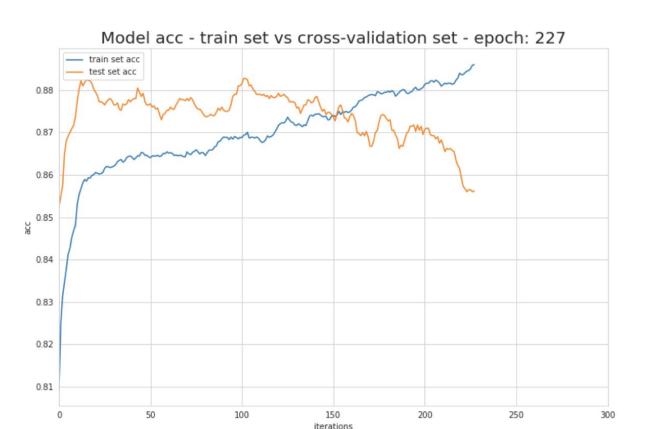




number of training steps

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):

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

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

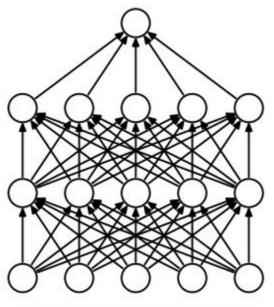
$$R(W) = \beta ||W||_2^2 + ||W||_1$$

Regularization: Dropout

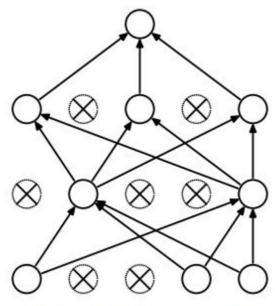


Some neurons are "drop training.

Prevents overfitting.



(a) Standard Neural Net



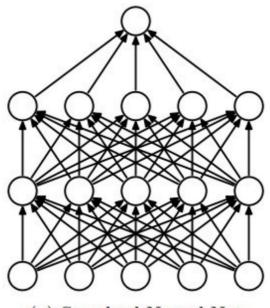
(b) After applying dropout.

Regularization: Dropout

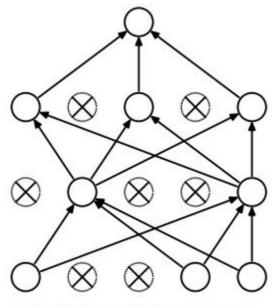


Some neurons are "dropped" during training.

Prevents overfitting.



(a) Standard Neural Net

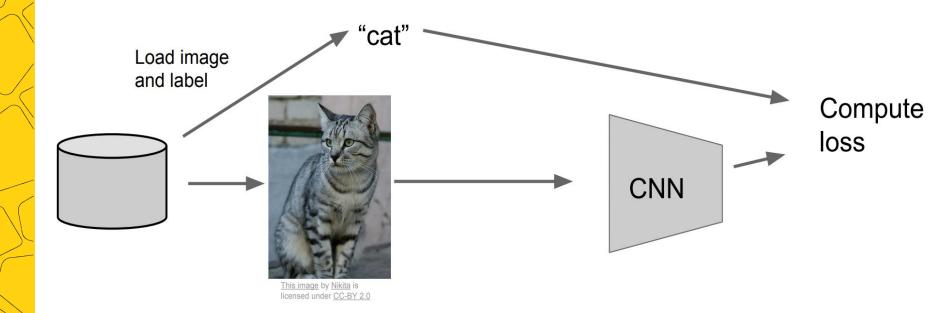


(b) After applying dropout.

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

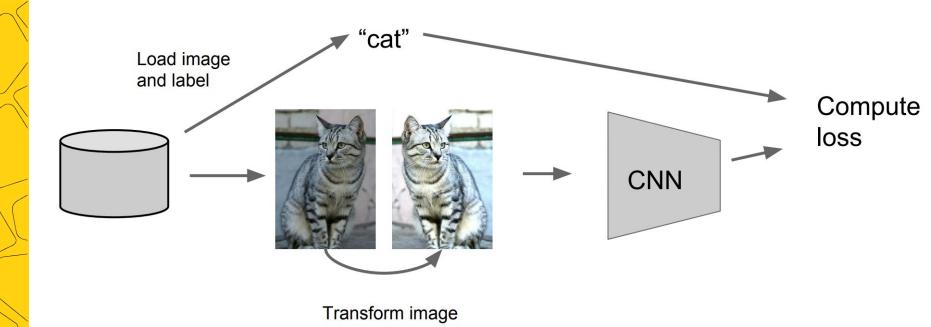
Regularization: data augmentation





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?



