Machine Learning Lecture 11: Into the depth of the Deep Learning

Harbour.Space University February 2021

Iurii Efimov

Outline

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

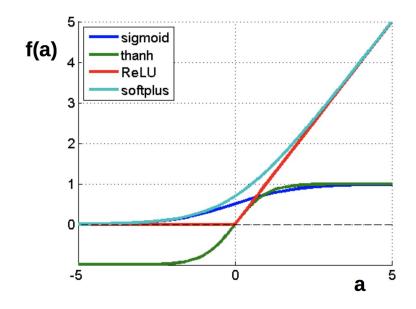
Once more: nonlinearities

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

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

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

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

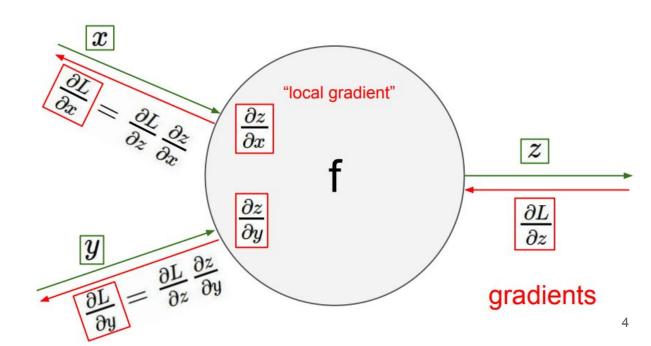


Backpropagation and chain rule

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.



source: http://cs231n.github.io

Different layers

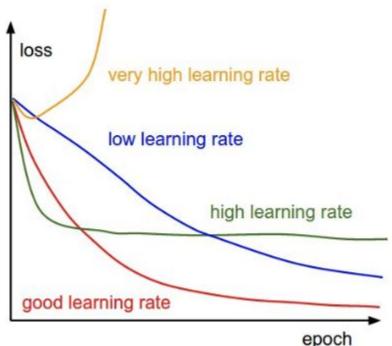
- Layers
 - a. Dense layer (done)
 - b. Convolutional layer (next lecture)
 - c. Pooling layer (next lecture)
 - d. Dropout layer (today)
 - e. Batchnorm layer (batch normalization) (today)
 - f. Embeddings (aka word2vec, GloVe) (last lecture)
 - g. Recurrent layers (last lecture)

Different layers

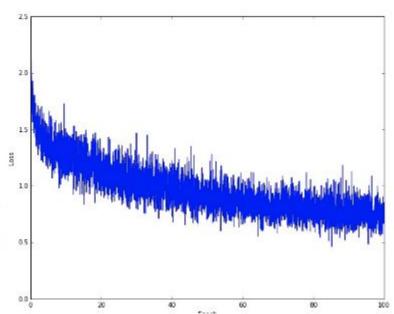
- Layers
 - a. Dense layer (done)
 - b. Convolutional layer (later)
 - c. Pooling layer (later)
 - d. Dropout layer (today)
 - e. Batchnorm layer (batch normalization) (today)
 - f. Embeddings (aka word2vec, GloVe) (later)
 - g. Recurrent layers (next lecture)

Optimizers

Stochastic gradient descent is used to optimize NN parameters.



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

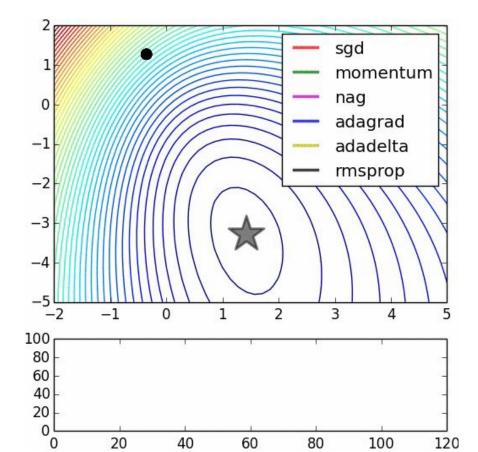


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Optimizers

There are much more optimizers:

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

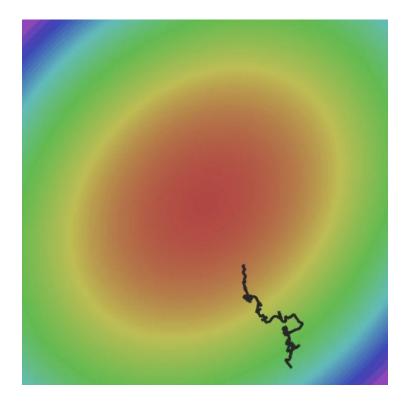


Optimization: SGD

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

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

Averaging over minibatches ---> noisy gradient



First idea: momentum

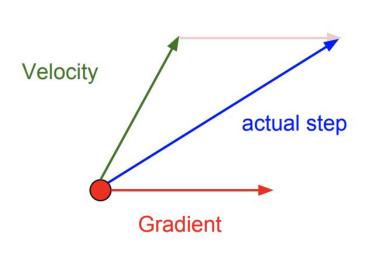
Simple SGD

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

SGD with momentum

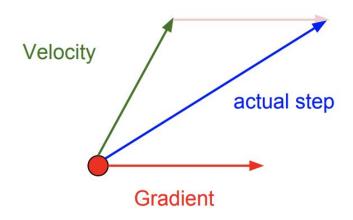
$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

Momentum update:



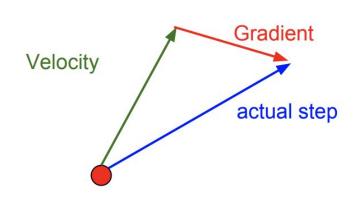
Nesterov momentum

Momentum update:



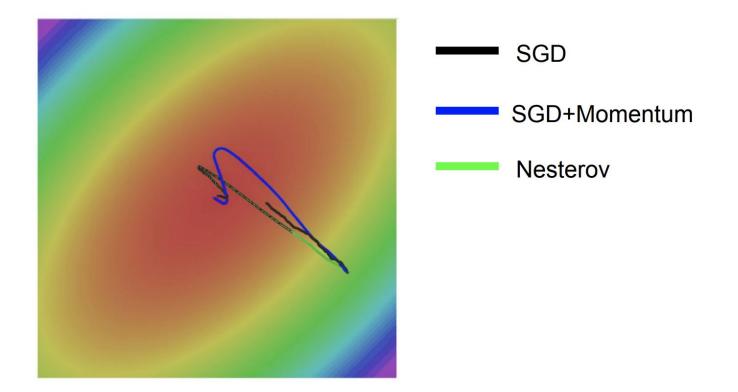
$$v_{t+1} = \rho v_t + \nabla f(x_t)$$
$$x_{t+1} = x_t - \alpha v_{t+1}$$

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

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

Second idea: different dimensions are different

Adagrad: SGD with cache

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

Problem: gradient fades with time

Second idea: different dimensions are different

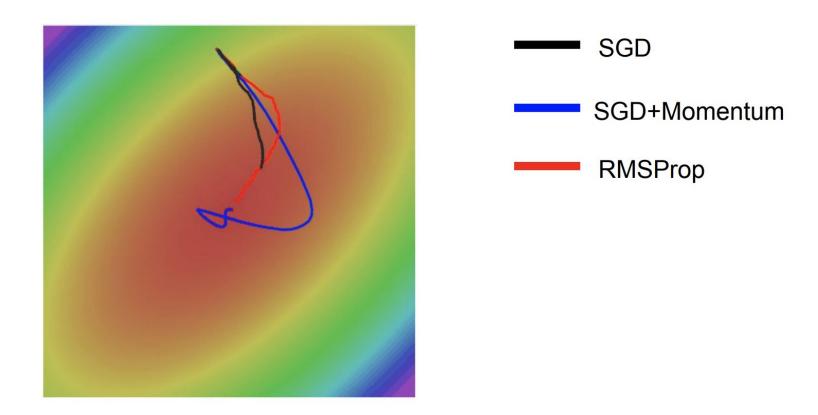
Adagrad: SGD with cache

$$cache_{t+1} = cache_t + (\nabla f(x_t))^2$$
$$x_{t+1} = x_t - \alpha \frac{\nabla f(x_t)}{cache_{t+1} + \varepsilon}$$

RMSProp: SGD with cache with exp. Smoothing
$$\operatorname{cache}_{t+1} = \beta \operatorname{cache}_t + (1 - \beta)(\nabla f(x_t))^2$$

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

Slide 29 Lecture 6 of Geoff Hinton's Coursera class



Adam

Let's combine the momentum idea and RMSProp normalization:

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

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

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

Let's combine the momentum idea and RMSProp normalization:

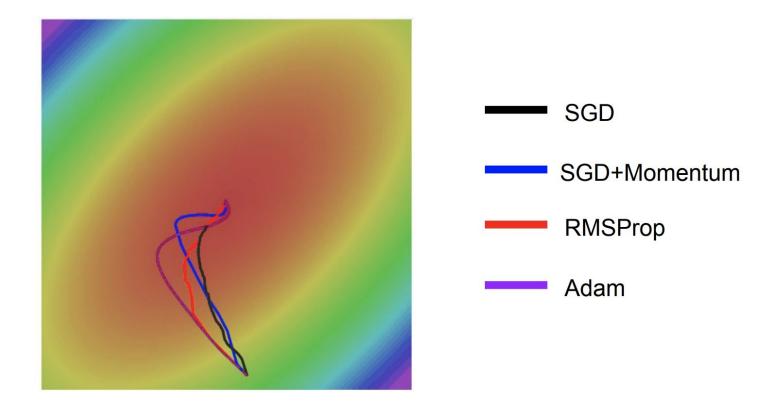
$$v_{t+1} = \gamma v_t + (1 - \gamma) \nabla f(x_t)$$

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

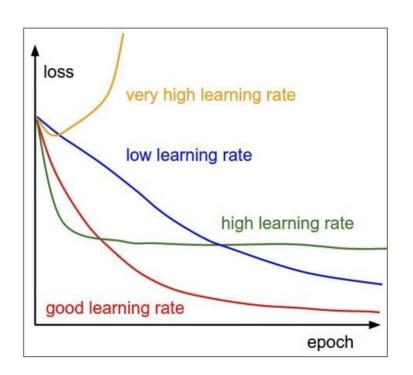
$$x_{t+1} = x_t - \alpha \frac{v_{t+1}}{\operatorname{cache}_{t+1} + \varepsilon}$$

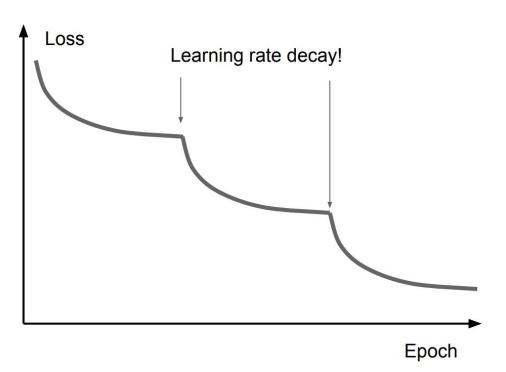
Actually, that's not quite Adam.

Comparing optimizers



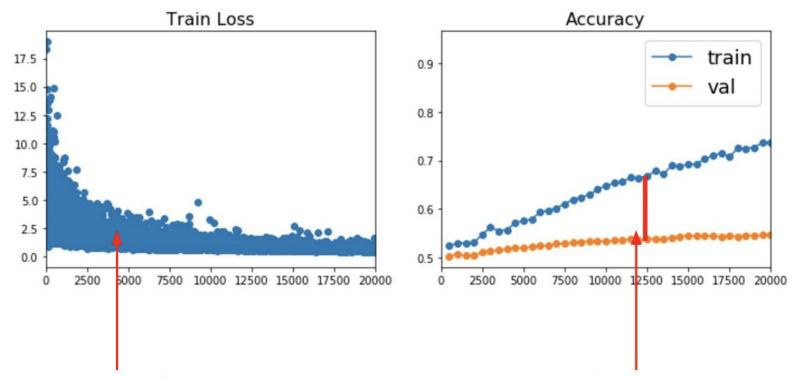
Once more: learning rate





Sum up: optimization

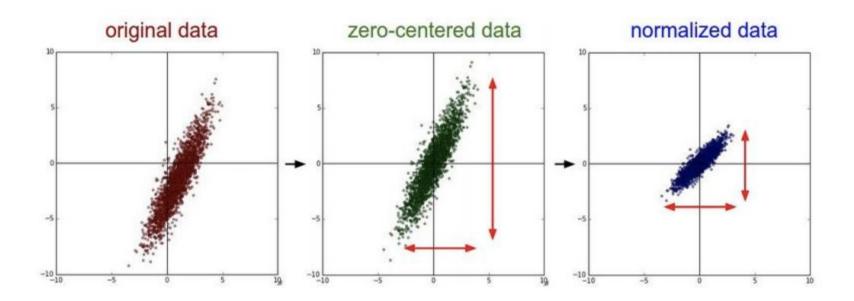
- Adam is great basic choice
- Even for Adam/RMSProp learning rate matters
- Use learning rate decay
- Monitor your model quality



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

After normalization: less sensitive to small Before normalization: classification loss changes in weights; easier to optimize very sensitive to changes in weight matrix; hard 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.

$$S = \sum_{i}^{n} w_{i}x_{i}$$

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

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

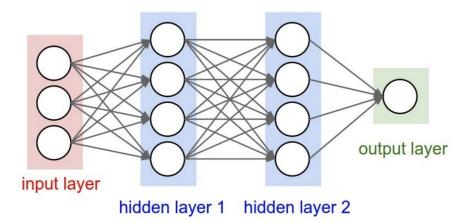
$$= \sum_{i}^{n} [E(w_{i})]^{2} Var(x_{i}) + E[(x_{i})]^{2} Var(w_{i}) + Var(x_{i}) Var(w_{i})$$

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

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

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: 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

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

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

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

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

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

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

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

$$\mu_{\mathcal{B}} \leftarrow \frac{1}{m} \sum_{i=1}^{m} x_i$$

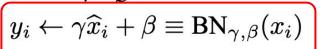
// mini-batch mean

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

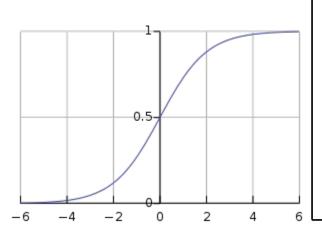
// mini-batch variance

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

// normalize



// 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

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

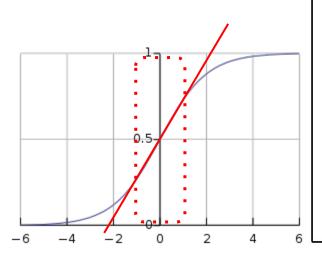
// mini-batch variance

$$\widehat{x}_i \leftarrow rac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}}$$

// normalize

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

// scale and shift



Original algorithm (2015)

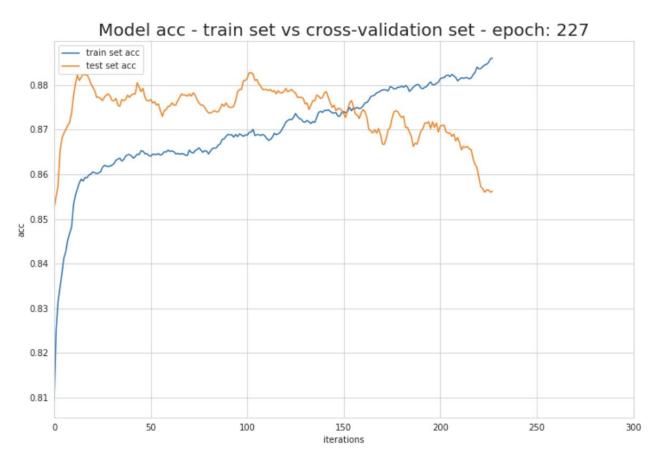
What is this?

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: \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
                                                      // mini-batch variance
                                                                     // normalize
    y_i \leftarrow \gamma \widehat{x}_i + \beta \equiv BN_{\gamma,\beta}(x_i)
                                                              // scale and shift
```

	Model	Steps to 72.2%	Max accuracy
	Inception	$31.0 \cdot 10^{6}$	72.2%
	BN-Baseline	$13.3\cdot 10^6$	72.7%
	BN-x5	$2.1\cdot 10^6$	73.0%
accuracy	BN-x30	$2.7\cdot 10^6$	74.8%
0.8	BN-x5-Sigmoid		69.8%
0.6			
	nception BN-Baseline		
0.5	BN-x5 BN-x30 BN-x5-Sigmoid		
	Steps to match Inception		
5M 10M 15M 20M cource: https://arxiv.org/pdf/1502.03167.pdf	^{25M} 30M n	umber of training steps	36

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

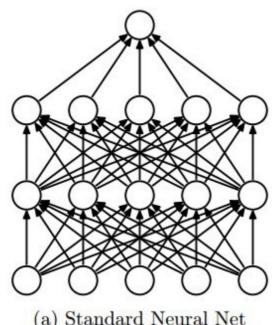
• L1 regularization:
$$R(W) = \|W\|_1$$

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

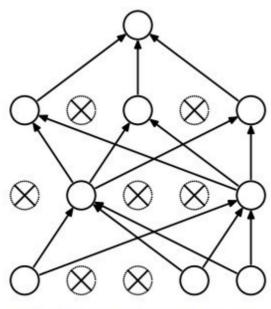
Regularization: Dropout

Some neurons are "dropped" during training.

Prevents overfitting.



(a) Standard Neural Net

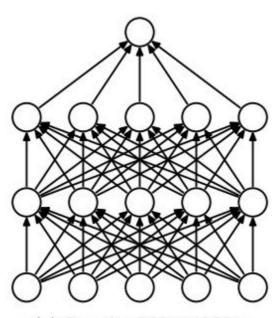


(b) After applying dropout.

Regularization: Dropout

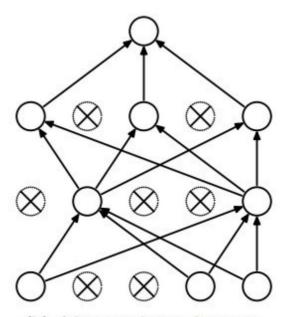
Some neurons are "dropped" during training.

Prevents overfitting.



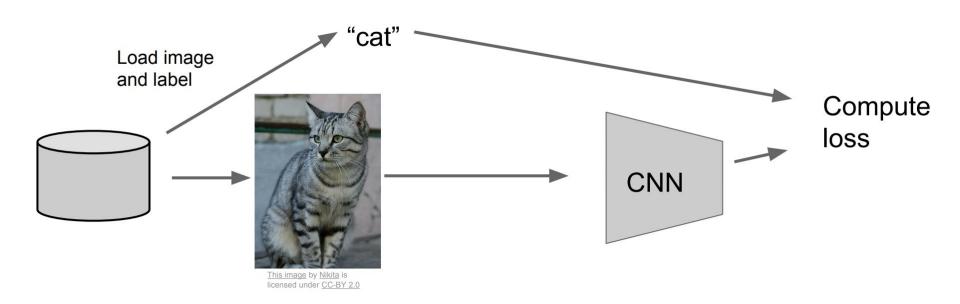
(a) Standard Neural Net

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

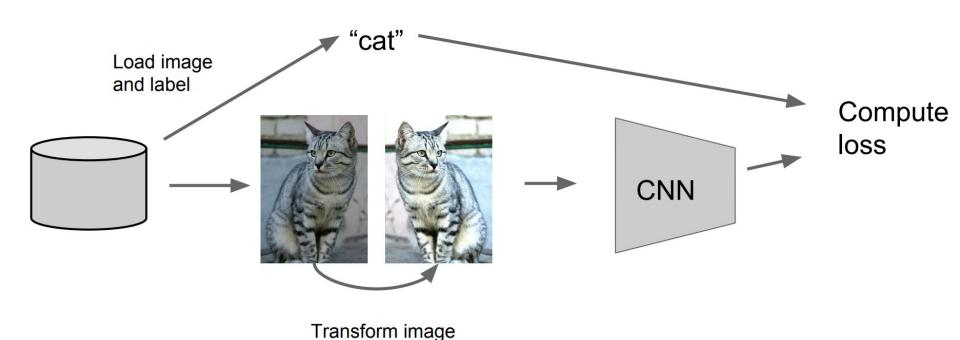


(b) After applying dropout.

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.