Machine Learning Course
basic track

Into the depth of the Deep Learning

Radoslav Neychev

11.11.2019, MIPT
Moscow, Russia

Outline

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

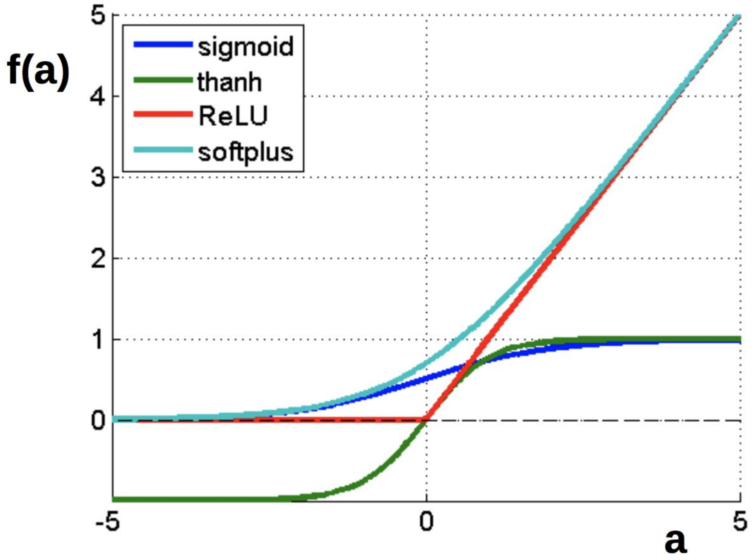
Once more: nonlinearities

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

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

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

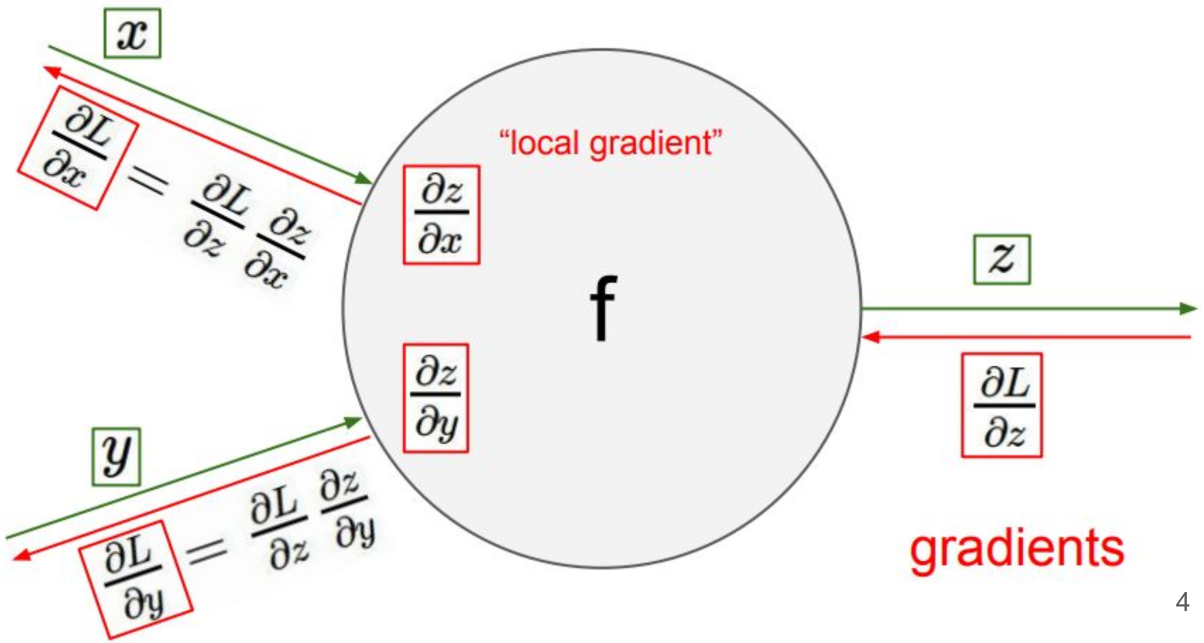
$$f(a) = \log(1 + e^{a})$$



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.



x
$\frac{\partial L}{\partial x} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial x}$
“local gradient”
$\frac{\partial z}{\partial x}$
f
z
$\frac{\partial z}{\partial y}$
$\frac{\partial L}{\partial z}$
y
$\frac{\partial L}{\partial y} = \frac{\partial L}{\partial z}\frac{\partial z}{\partial y}$
gradients

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 layer~~s~~ *(last lecture)*

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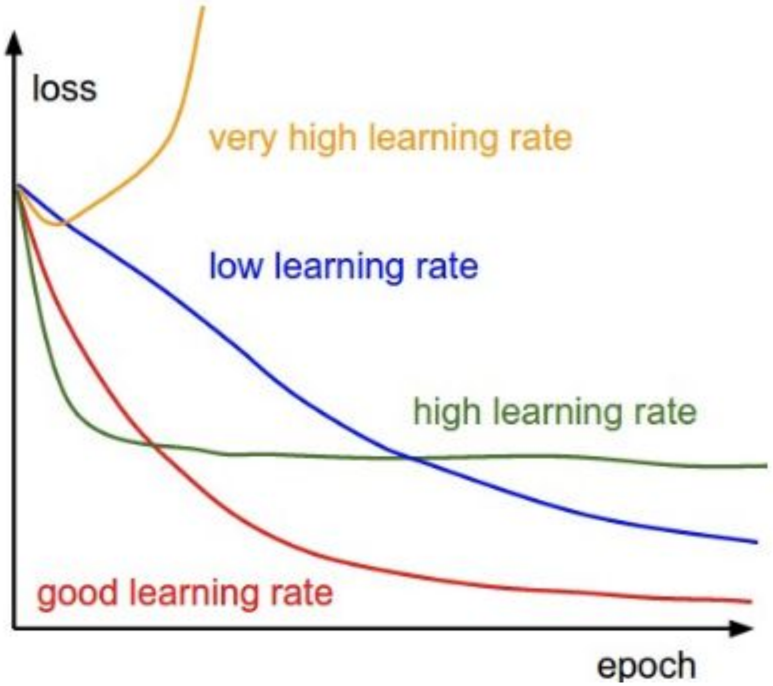
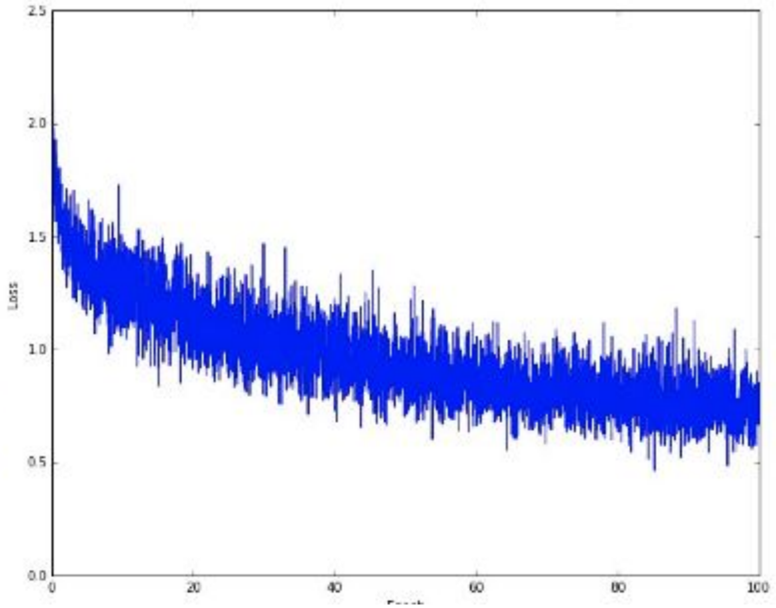
Optimizers

Stochastic gradient descent is used to optimize NN parameters.

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



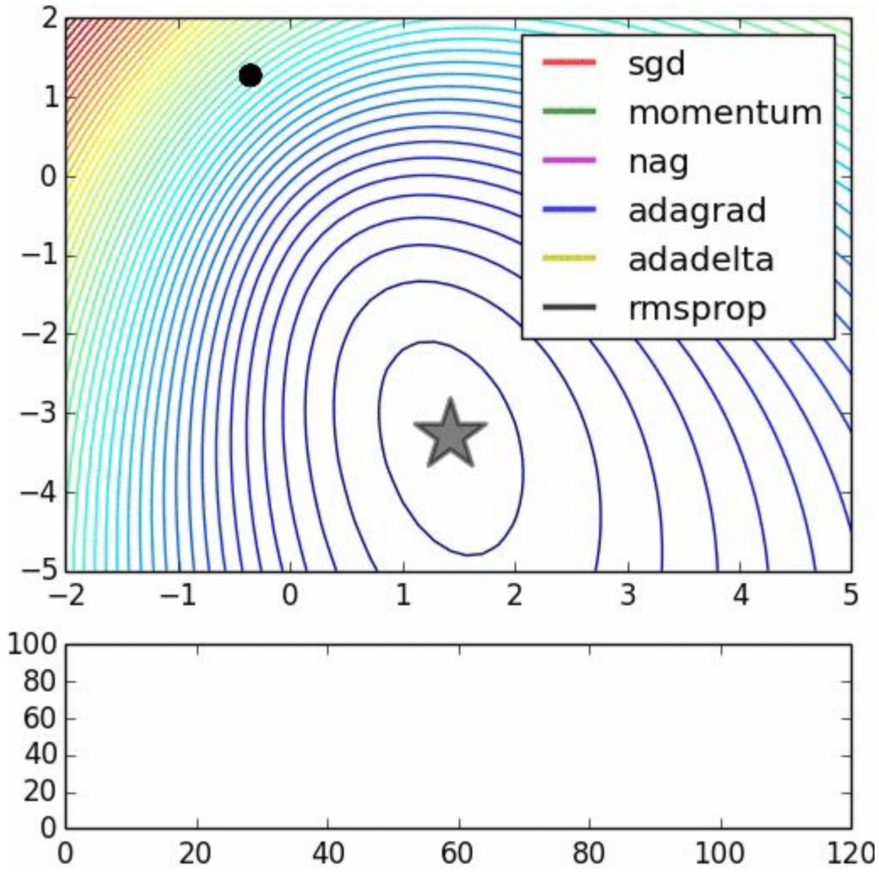


source: http://cs231n.github.io/neural-networks-3/

Optimizers

There are much more optimizers:

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

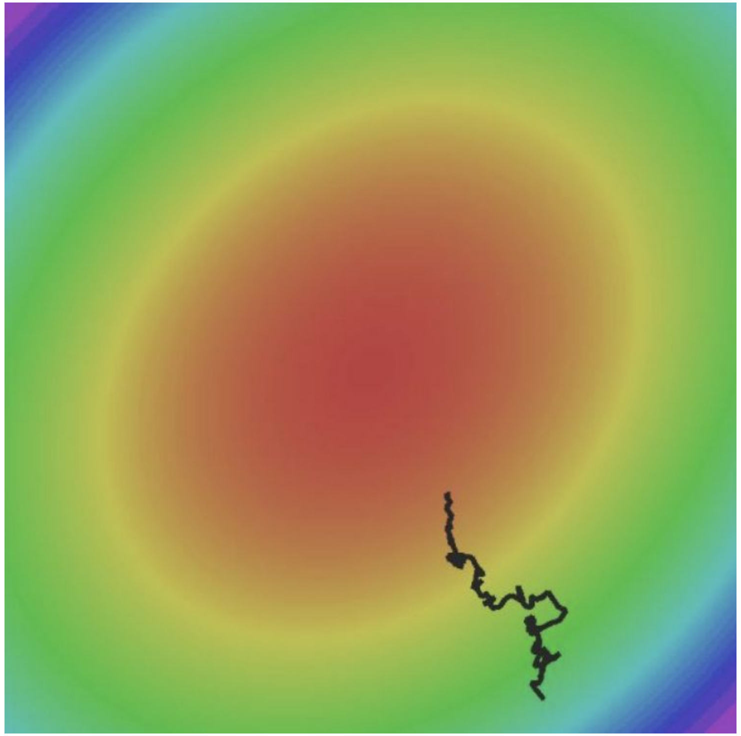


Optimization: SGD

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

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

Averaging over minibatches ---> noisy gradient



source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

First idea: momentum

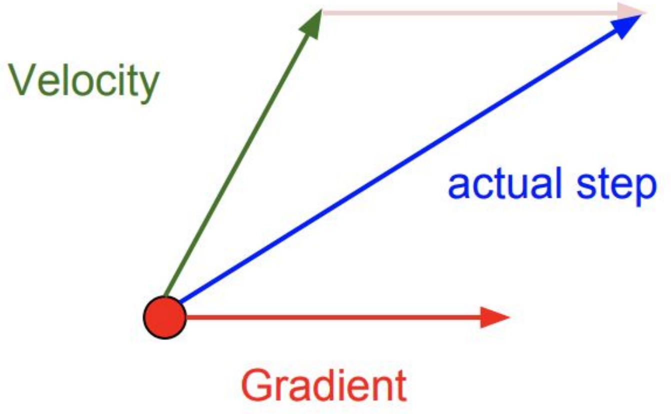
Simple SGD

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

SGD with momentum

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

Momentum update:



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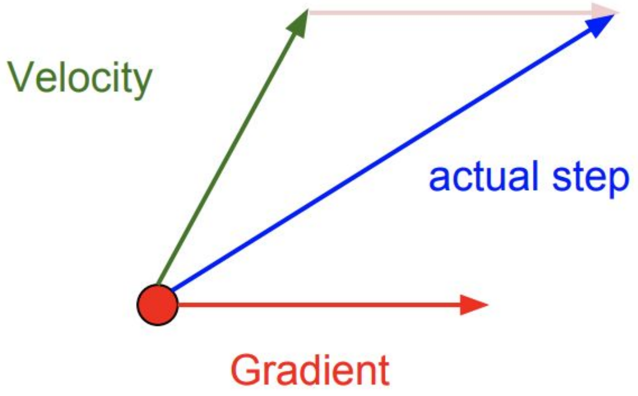
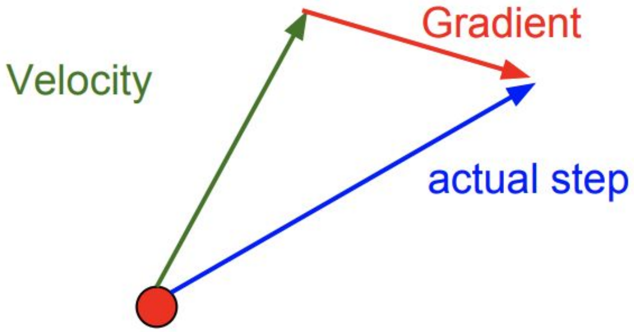
Nesterov momentum

Momentum update:



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

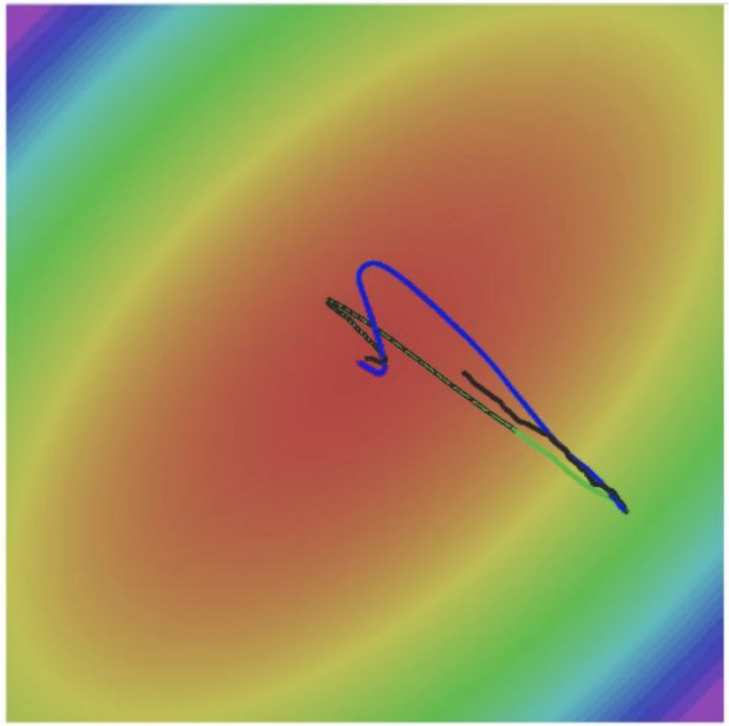
Nesterov Momentum

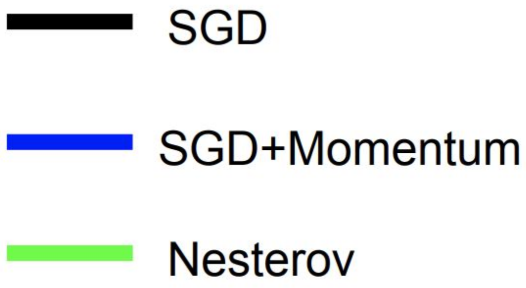


$$v_{t+1} = \rho v_t - \alpha \nabla f(\boxed{x_t + \rho v_t})$$
$$x_{t+1} = x_t + v_{t+1}$$

source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

Comparing momentums





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Second idea: different dimensions are different

Adagrad: SGD with cache

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

Second idea: different dimensions are different

Adagrad: SGD with cache

$$\text{cache}_{t+1} = \text{cache}_t + (\nabla f(x_t))^2$$
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Problem: gradient fades with time

Second idea: different dimensions are different

Adagrad: SGD with cache

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

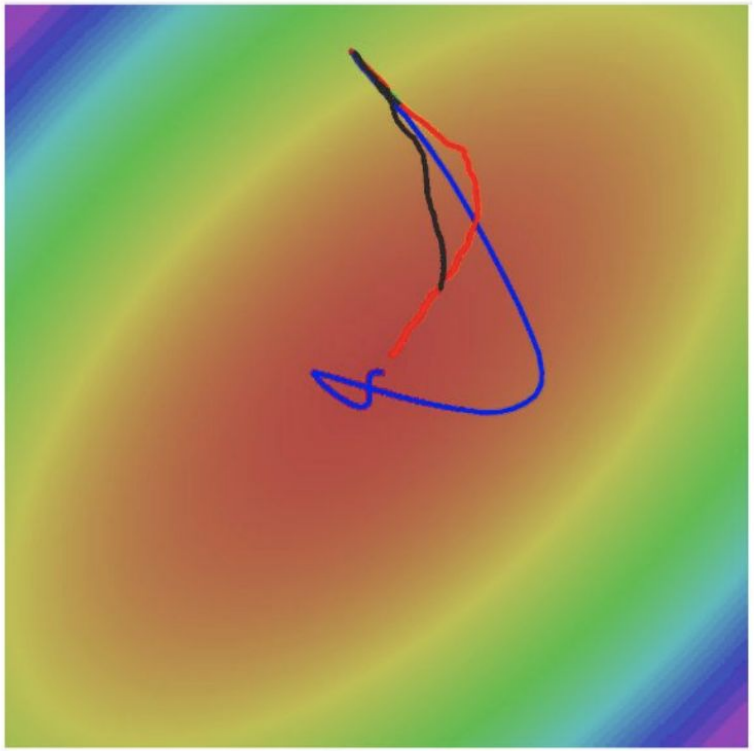
$$x_{t+1} = x_t - \alpha \frac{\nabla f(x_t)}{\text{cache}_{t+1} + \varepsilon}$$

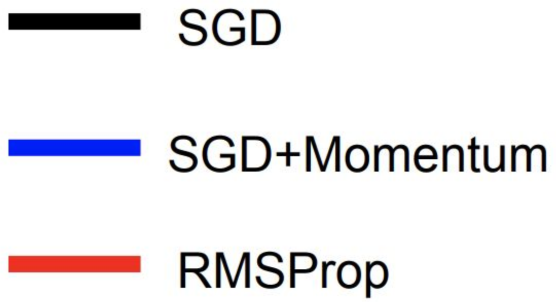
RMSProp: SGD with cache with exp. Smoothing

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

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

Slide 29 Lecture 6 of Geoff Hinton’s Coursera class
http://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_lec6.pdf





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Adam

Let’s combine the momentum idea and RMSProp normalization:

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

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

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

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

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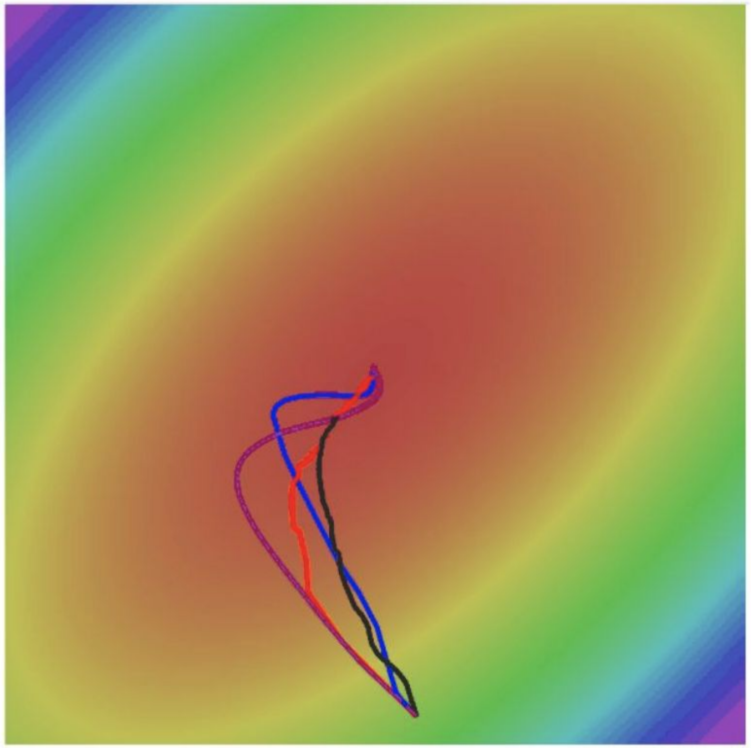
Actually, that’s not quite Adam.

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

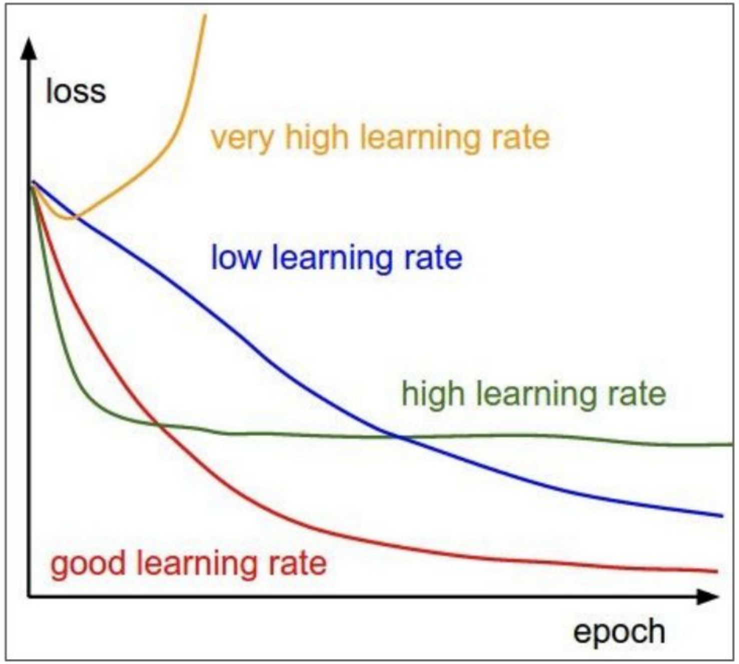
Comparing optimizers

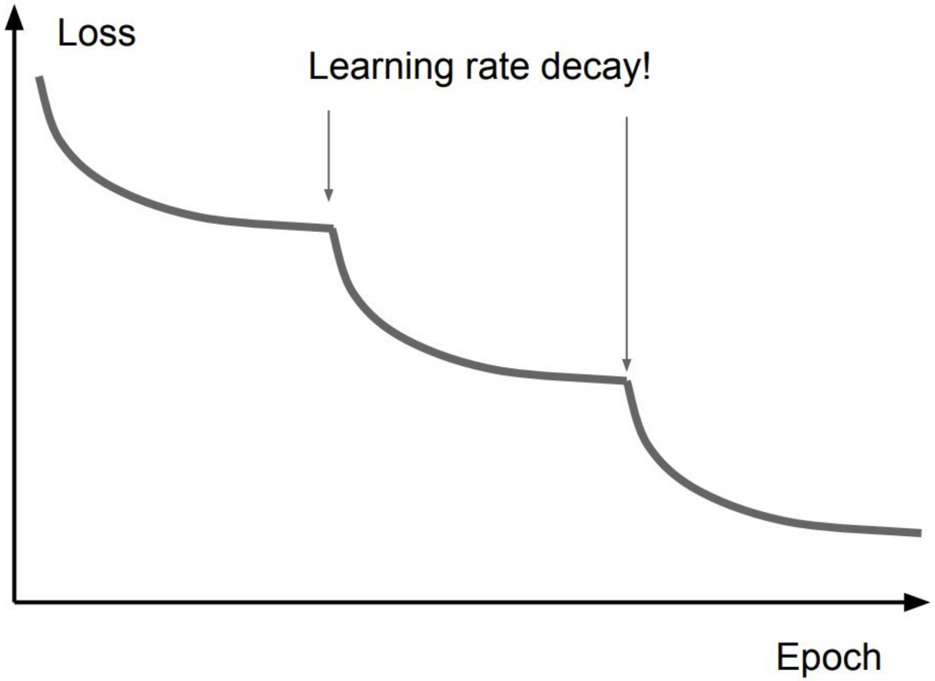


▬	SGD
▬	SGD+Momentum
▬	RMSProp
▬	Adam

source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

Once more: learning rate





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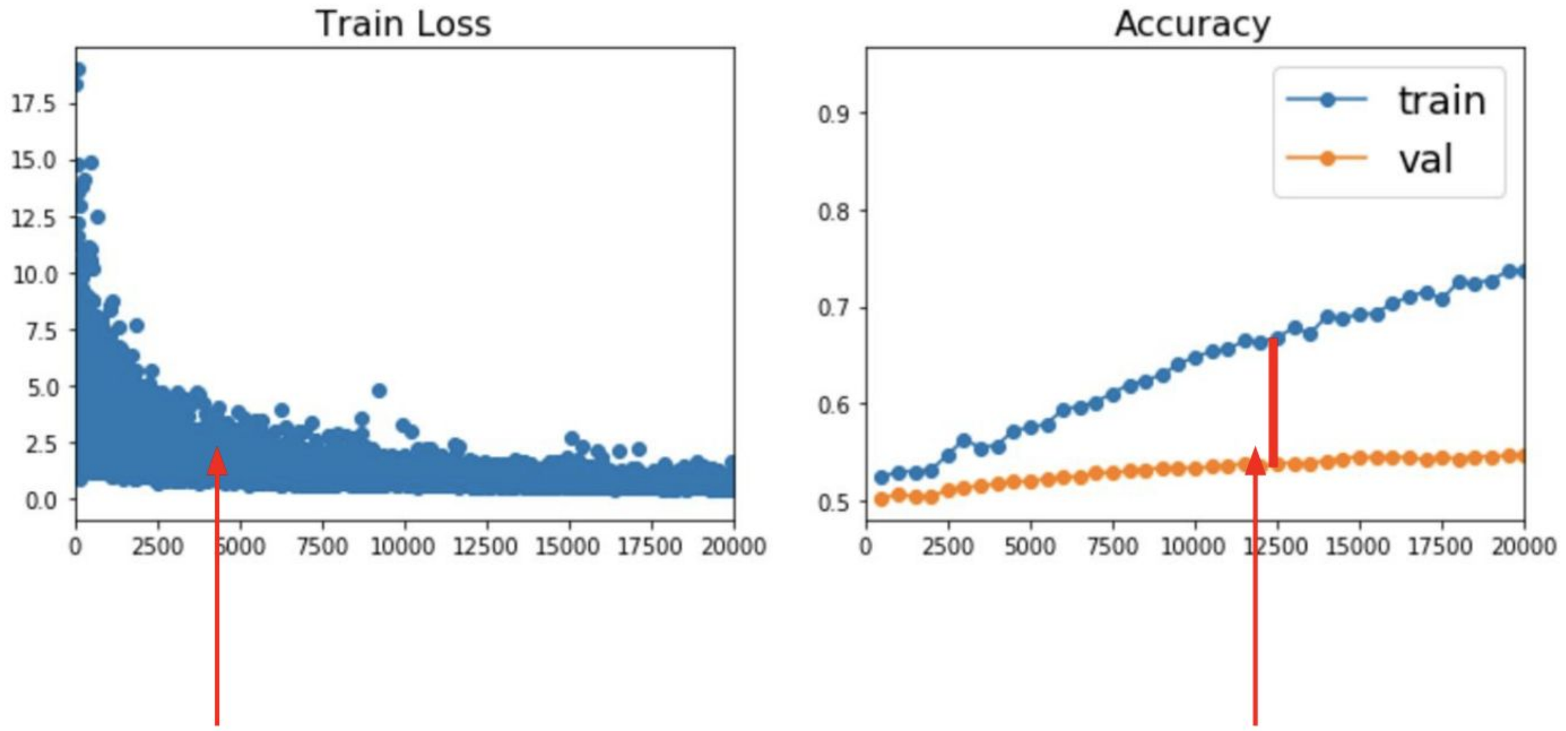
Sum up: optimization

- 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?

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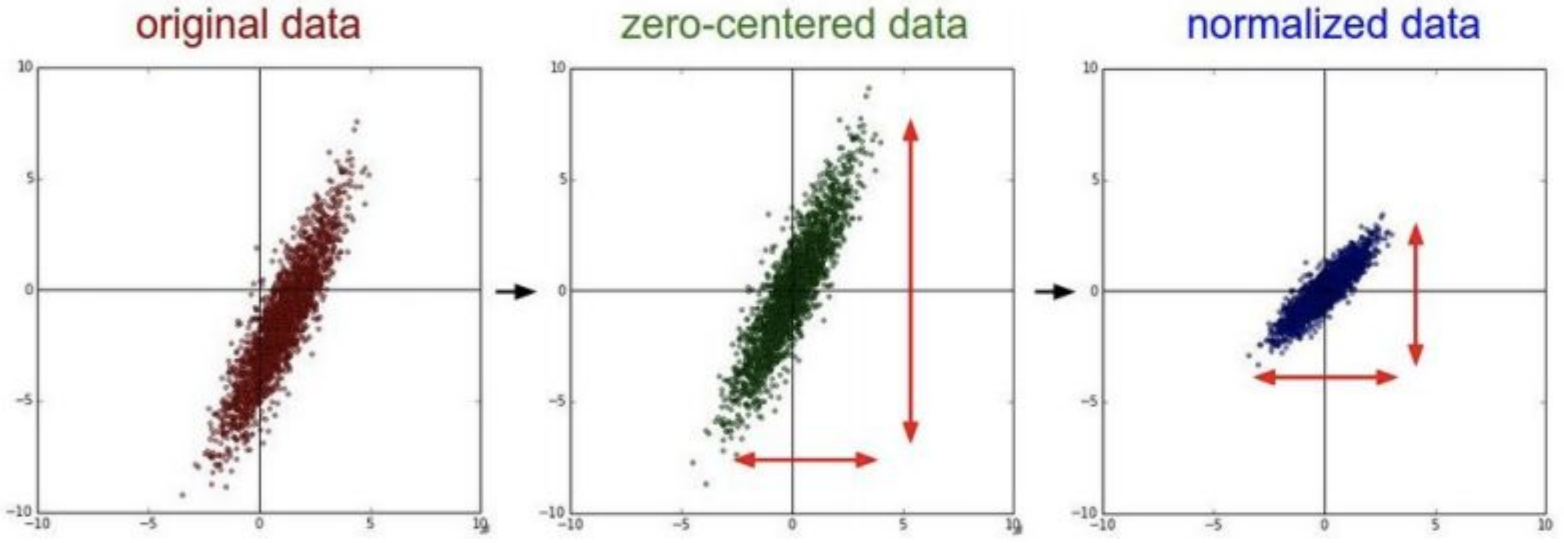
Data normalization



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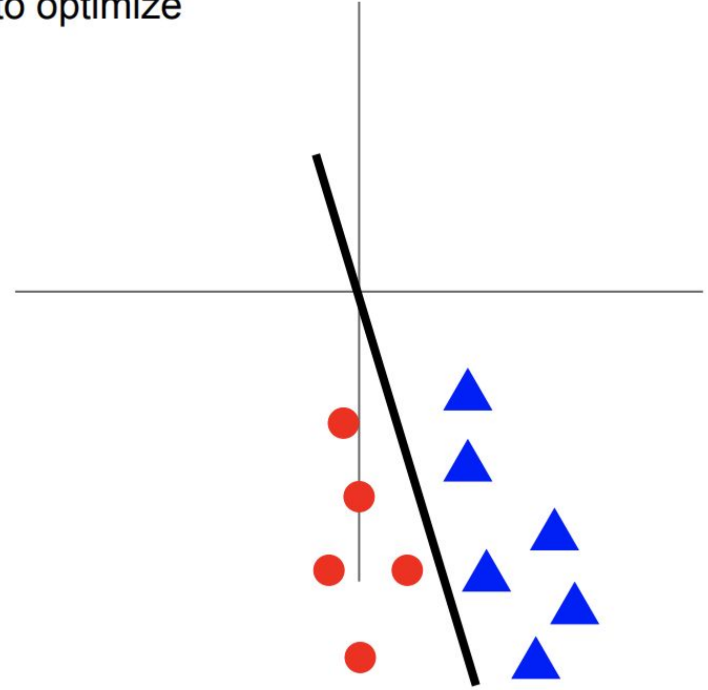
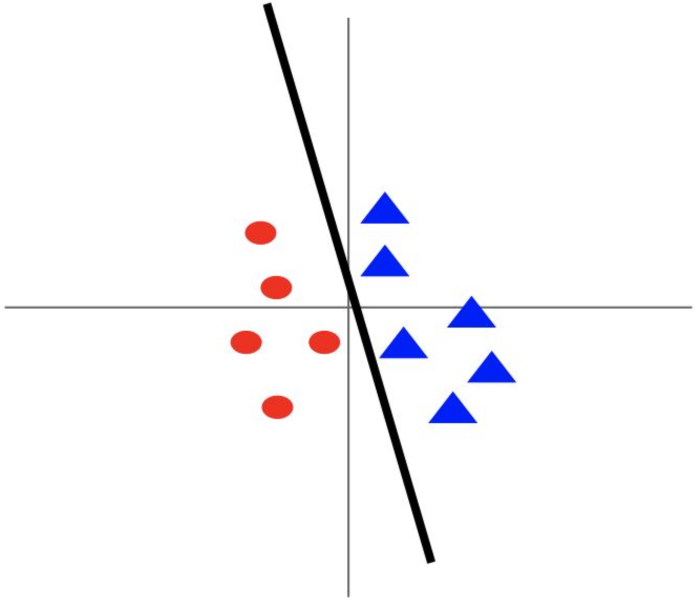
Data normalization

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



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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.

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

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

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

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

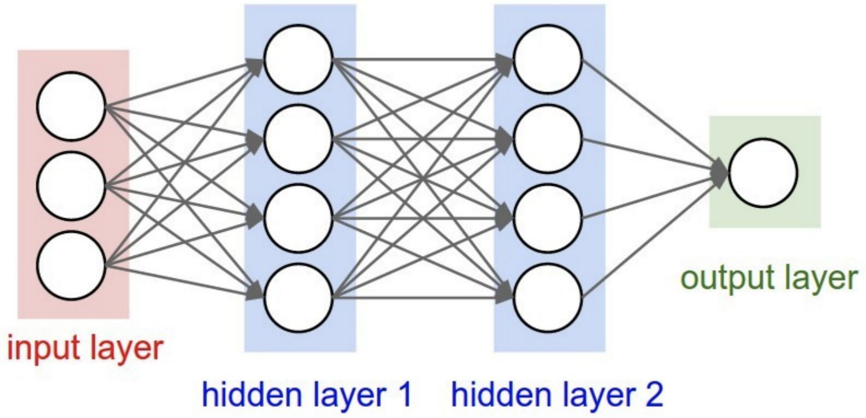
$$= \sum_i^n \mathrm{Var}(x_i)\mathrm{Var}(w_i)$$

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

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)

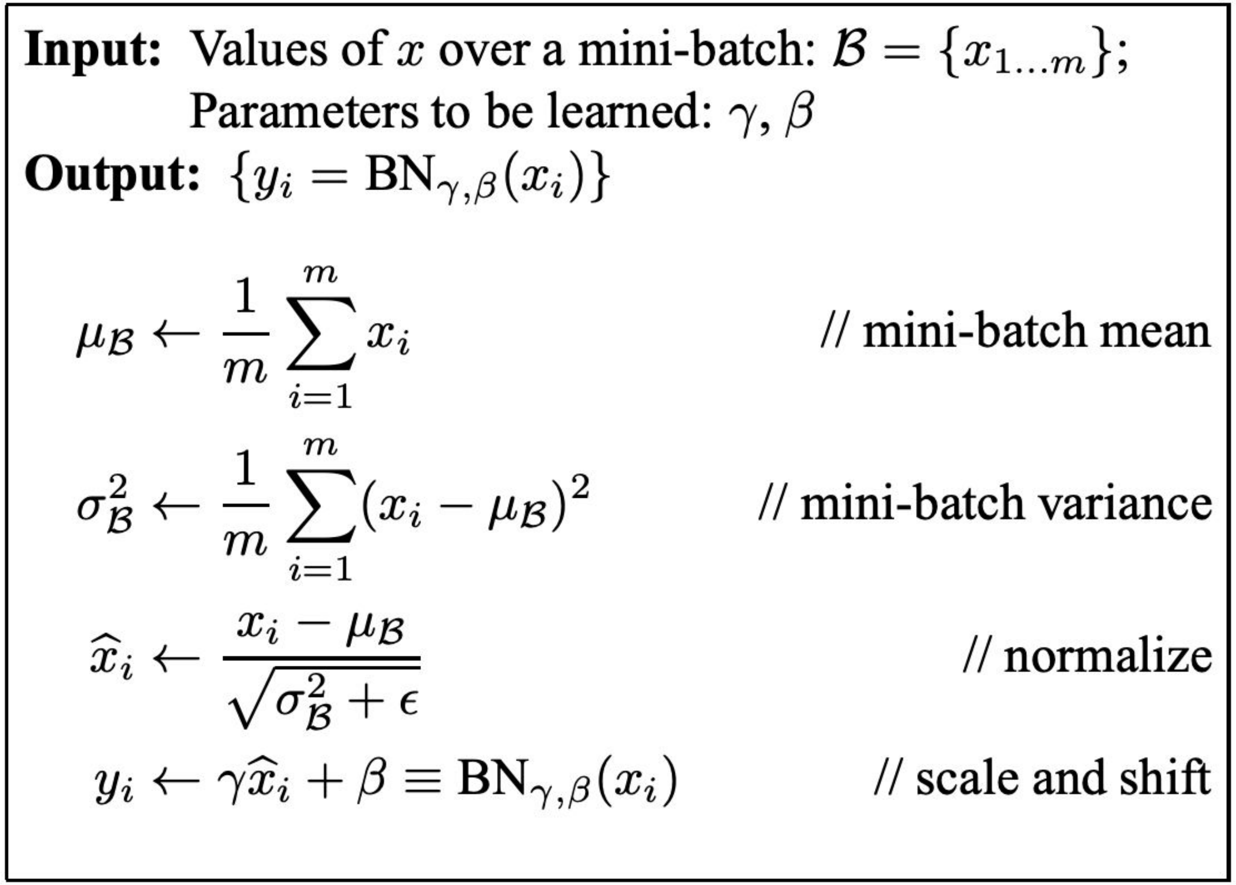
$$h_i = \frac{h_i - \mu_i}{\sqrt{\sigma_i^2}}$$

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

$$\mu_i := \alpha \cdot mean_{batch} + (1-\alpha) \cdot \mu_i$$
$$\sigma_i^2 := \alpha \cdot variance_{batch} + (1-\alpha) \cdot \sigma_i^2$$

Batch normalization

Original algorithm (2015)



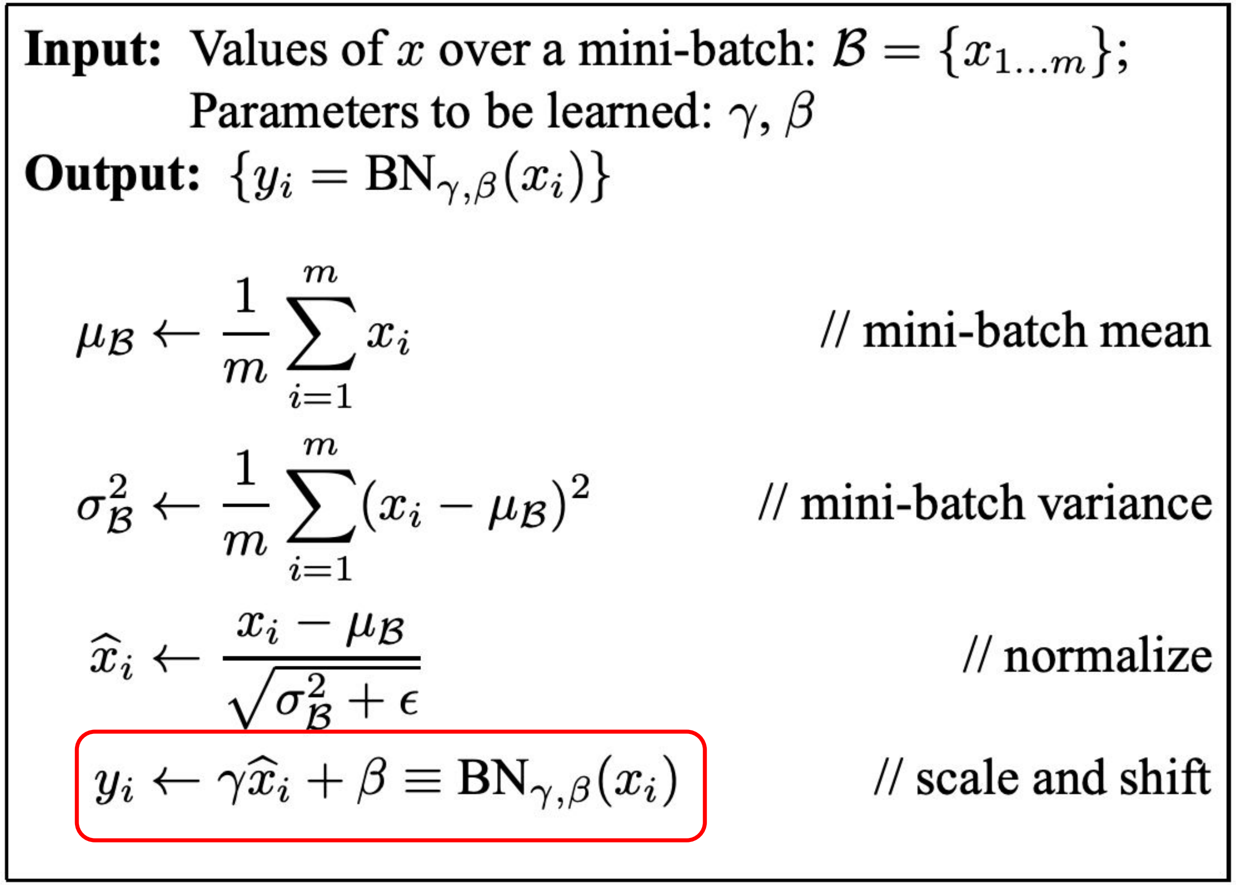
```
Input: Values of $x$ over a mini-batch: $\mathcal{B} = \{x_{1\ldots m}\}$;
       Parameters to be learned: $\gamma$, $\beta$
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

Batch normalization

Original algorithm (2015)

What is this?



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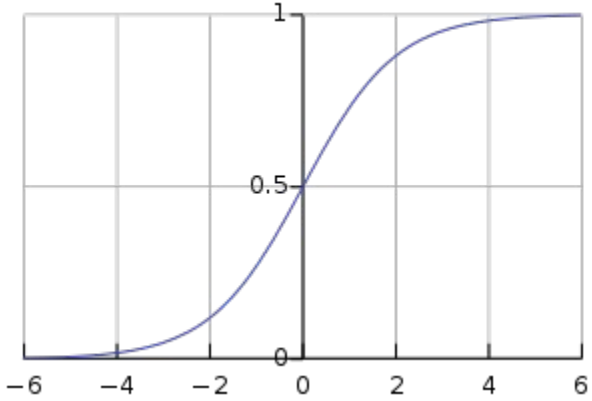
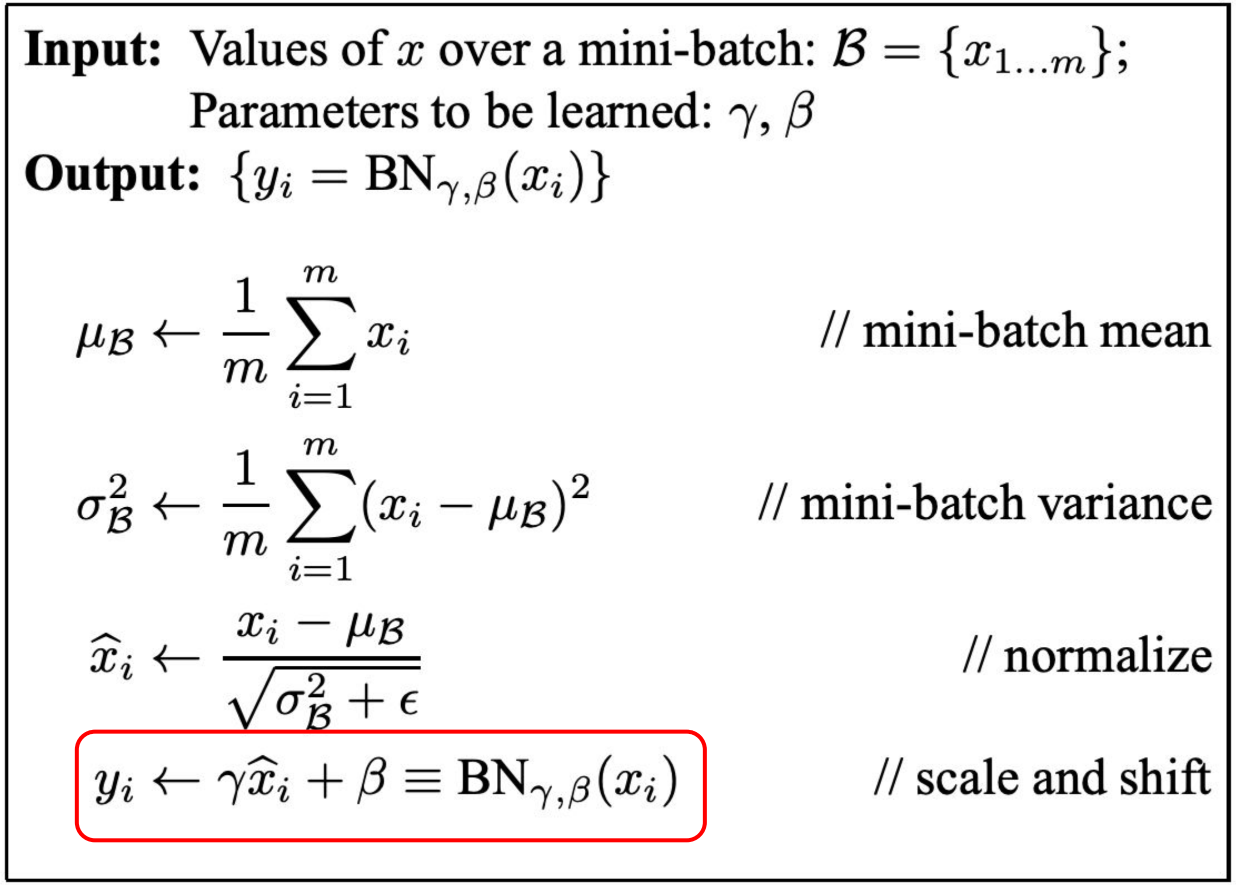
Batch normalization





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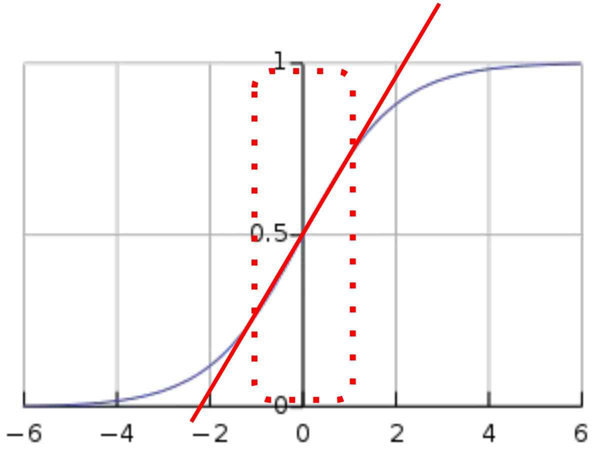
Batch normalization



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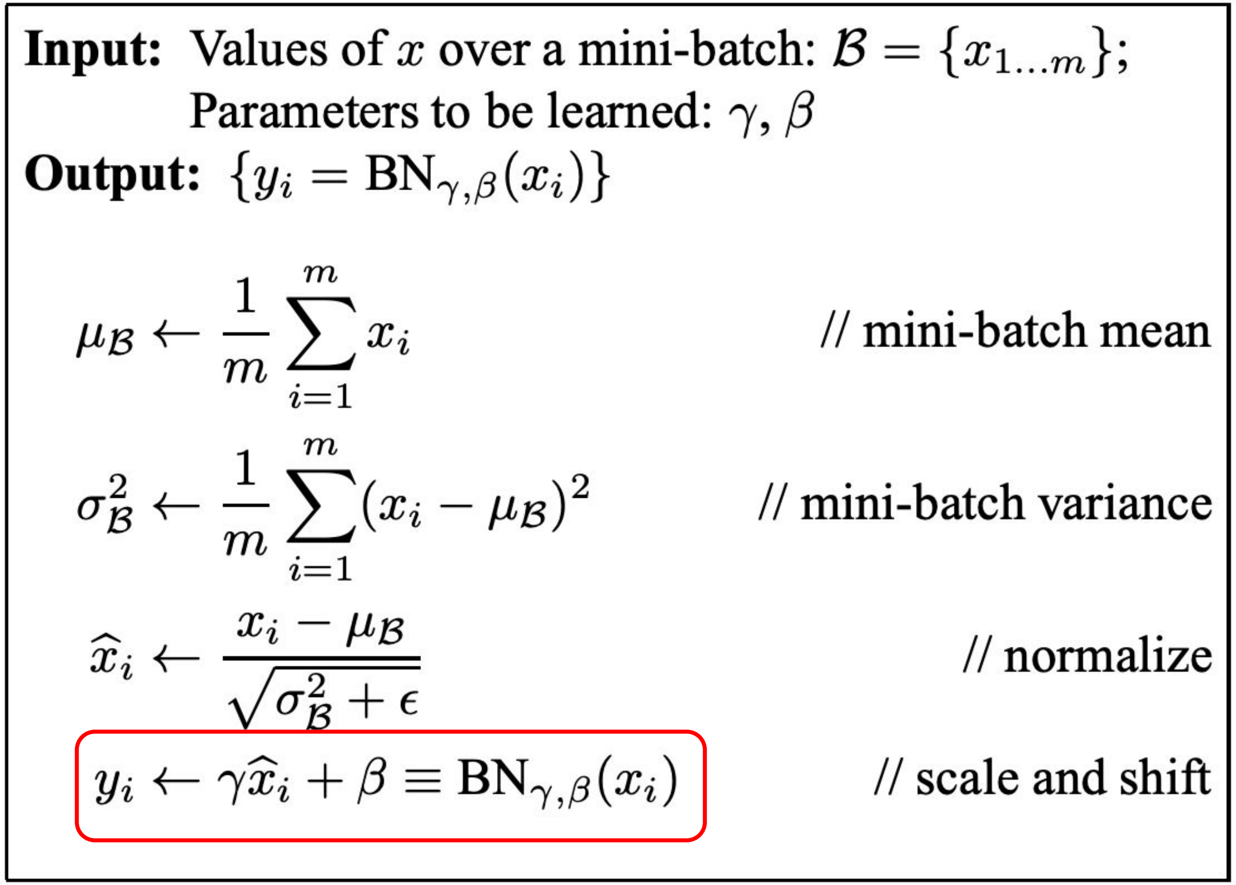
Batch normalization

Original algorithm (2015)

What is this?

This transformation should be able to represent the identity transform.



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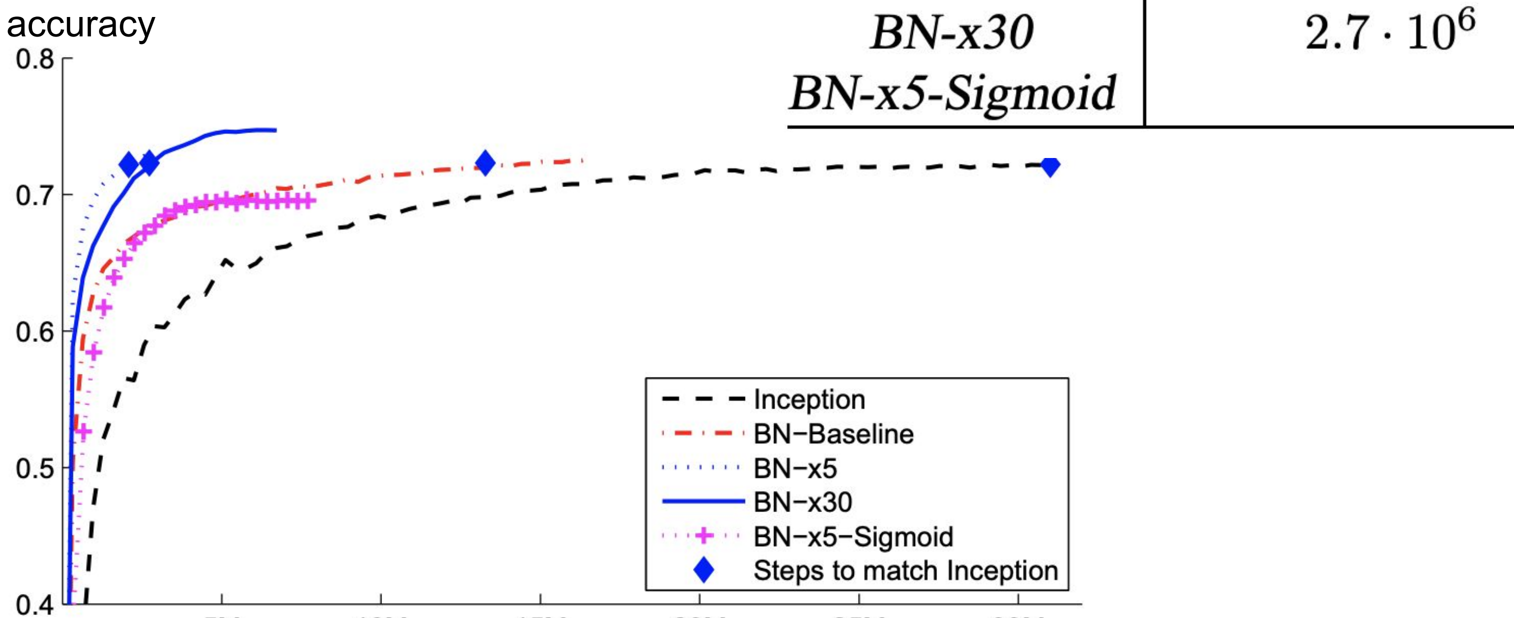
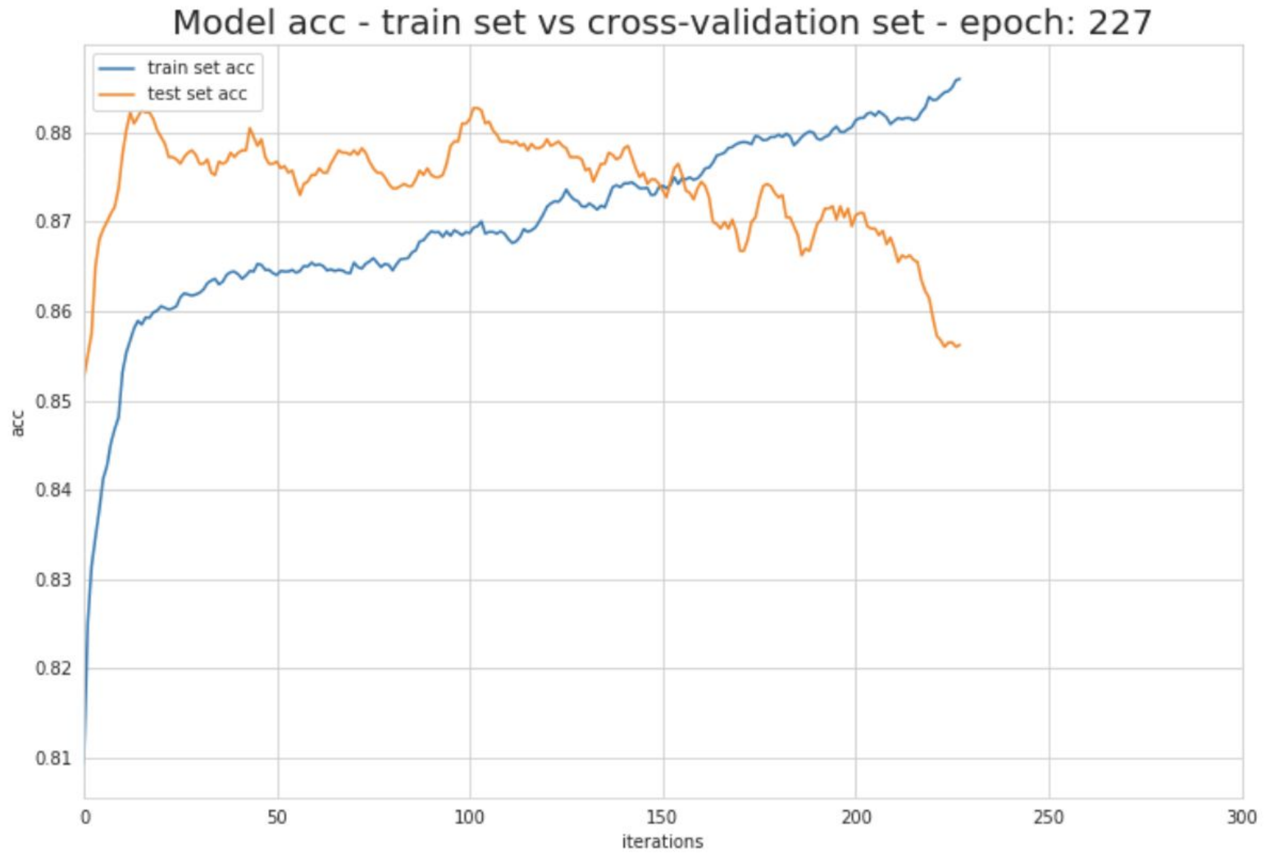
Batch normalization

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%
BN-x30	$2.7 \cdot 10^6$	74.8%
BN-x5-Sigmoid		69.8%



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

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:

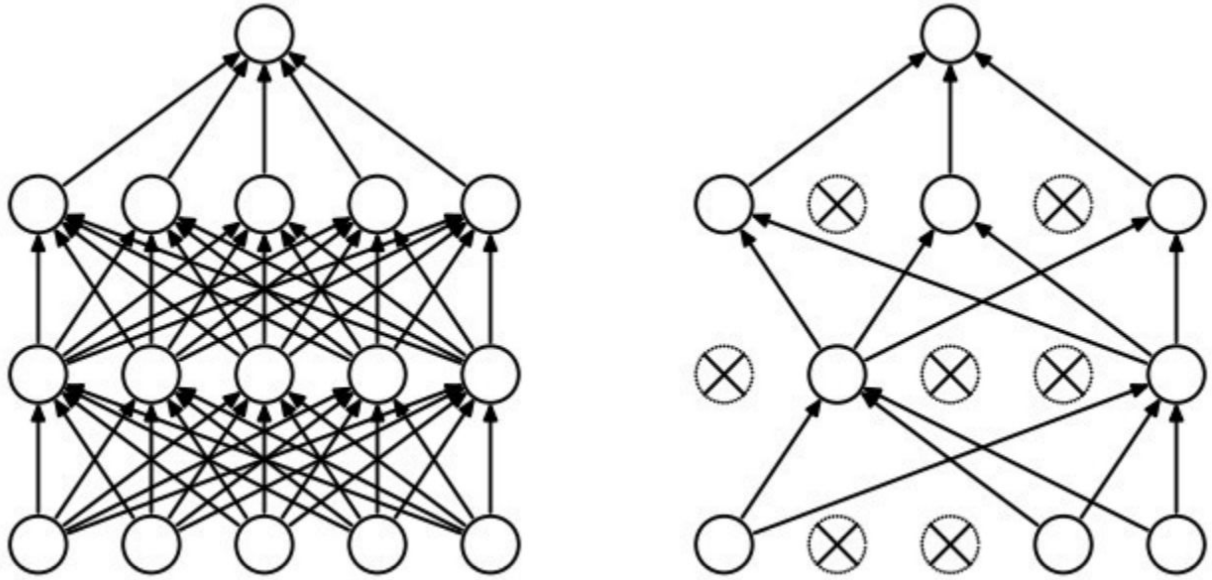
- L2 regularization: $R(W) = \|W\|_2^2$
- L1 regularization: $R(W) = \|W\|_1$
- Elastic Net (L1 + L2): $R(W) = \beta\|W\|_2^2 + \|W\|_1$

source: http://cs231n.stanford.edu/slides/2017/cs231n_2017_lecture7.pdf

Regularization: Dropout

Some neurons are “dropped” during training.

Prevents overfitting.

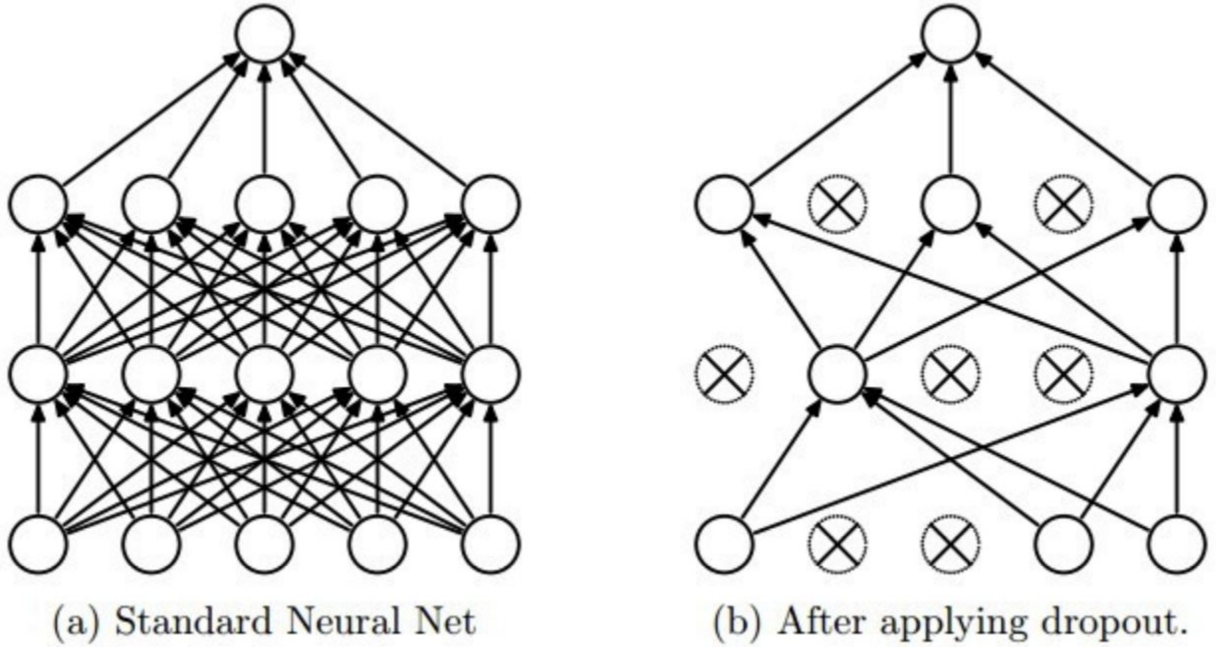


(a) Standard Neural Net (b) After applying dropout.

Regularization: Dropout

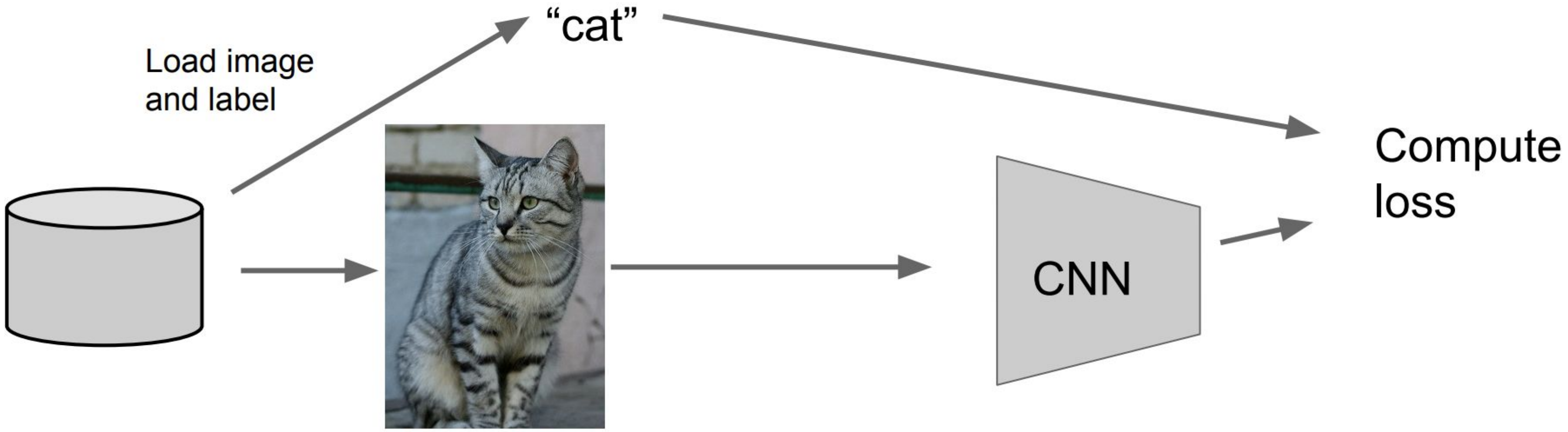
Some neurons are “dropped” during training.

Prevents overfitting.



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

Regularization: data augmentation



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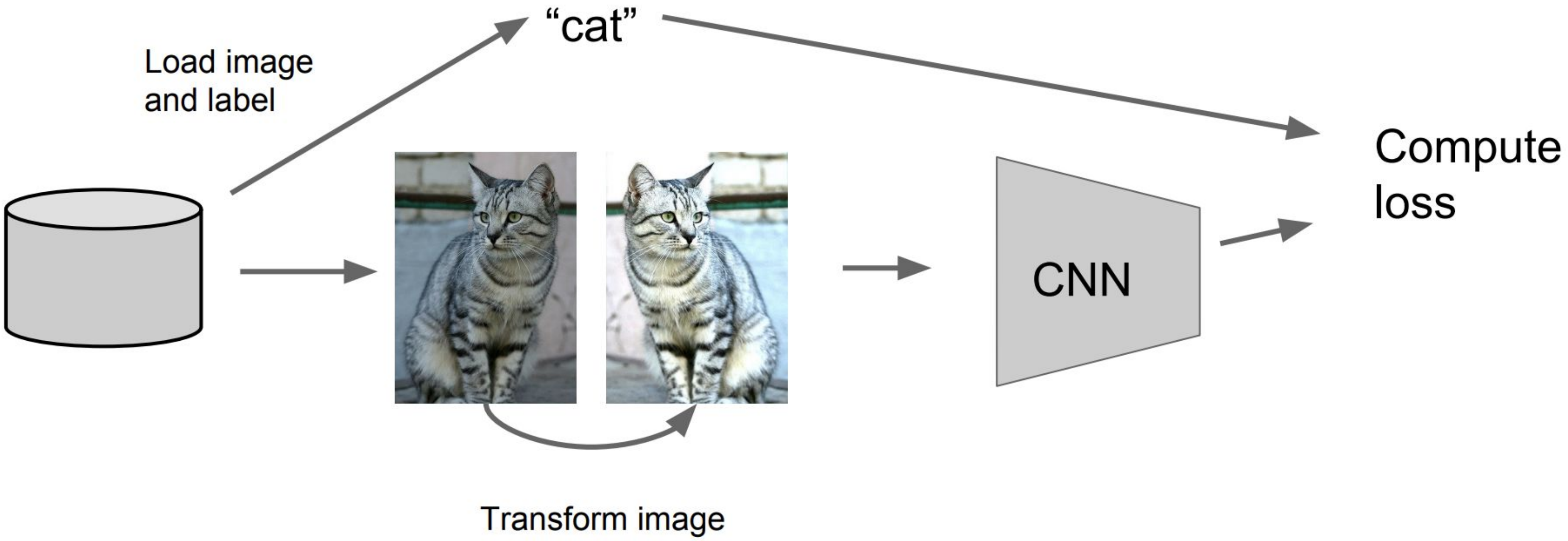
Regularization: data augmentation



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Sum up: regularization

Regularization:

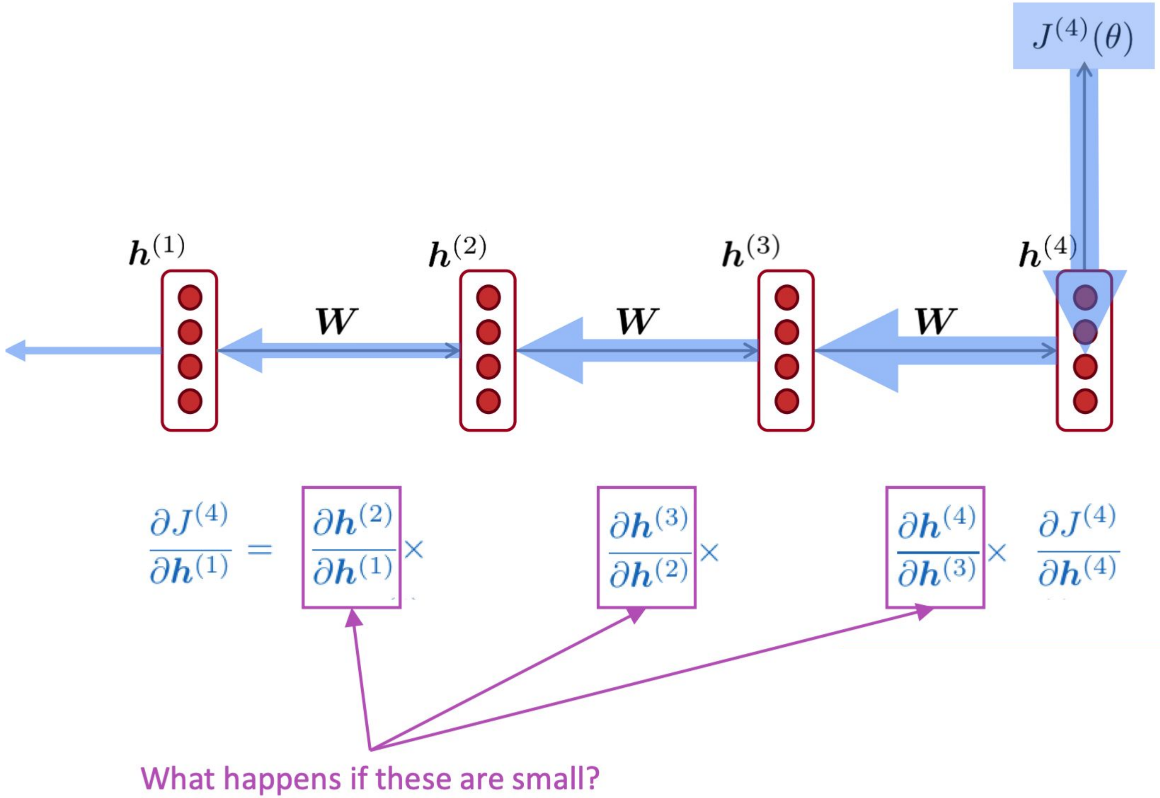
- Add some weight constraints
- Add some random noise during train and marginalize it during test
- Add some prior information in appropriate form

Q & A

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

Backup

Vanishing gradient problem


$J^{(4)}(\theta)$
$\boldsymbol{h}^{(1)}$
$\boldsymbol{h}^{(2)}$
$\boldsymbol{h}^{(3)}$
$\boldsymbol{h}^{(4)}$
$\boldsymbol{W}$
$\boldsymbol{W}$
$\boldsymbol{W}$
$\frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(1)}} = \boxed{\frac{\partial \boldsymbol{h}^{(2)}}{\partial \boldsymbol{h}^{(1)}}} \times \boxed{\frac{\partial \boldsymbol{h}^{(3)}}{\partial \boldsymbol{h}^{(2)}}} \times \boxed{\frac{\partial \boldsymbol{h}^{(4)}}{\partial \boldsymbol{h}^{(3)}}} \times \frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(4)}}$
What happens if these are small?

Vanishing gradient problem:

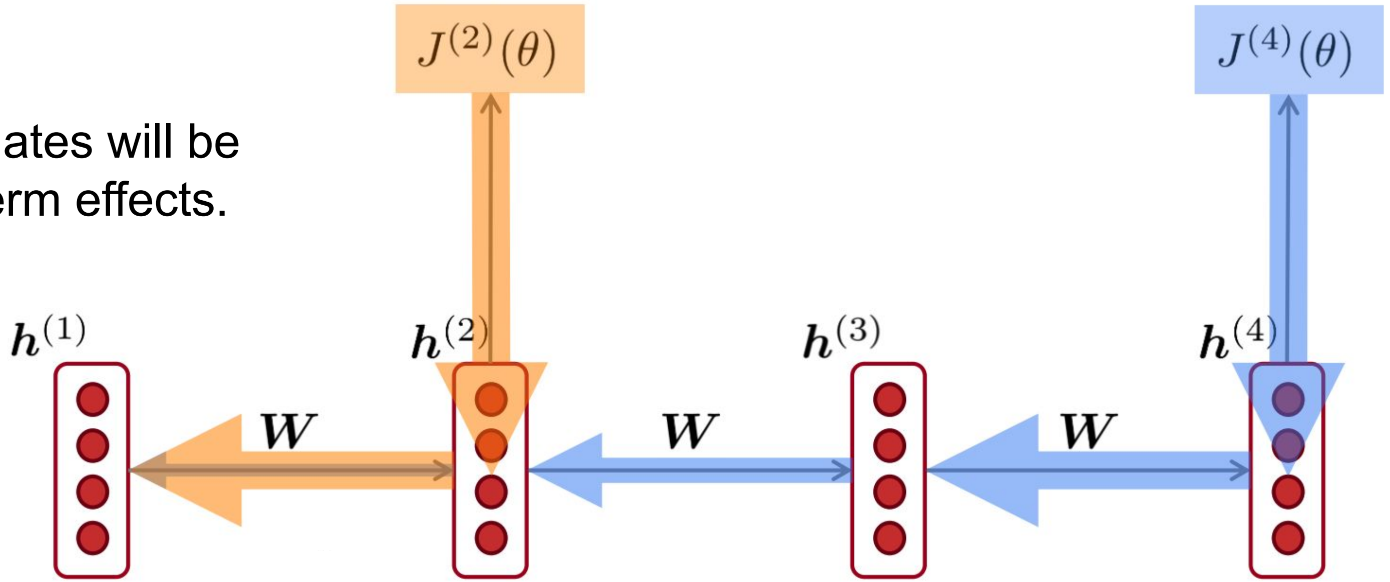
When the derivatives are small, the gradient signal gets smaller and smaller as it backpropagates further

More info: “On the difficulty of training recurrent neural networks”, Pascanu et al, 2013
http://proceedings.mlr.press/v28/pascanu13.pdf

Vanishing gradient problem

Gradient signal from far away is lost because it's much smaller than from close-by.

So model weights updates will be based only on short-term effects.



Based on: Lecture by Abigail See, CS224n Lecture 7

Exploding gradient problem

- If the gradient becomes too big, then the SGD update step becomes too big:

$$\theta^{new} = \theta^{old} - \overbrace{\alpha}^{\text{learning rate}} \underbrace{\nabla_\theta J(\theta)}_{\text{gradient}}$$

- This can cause bad updates: we take too large a step and reach a bad parameter configuration (with large loss)

- In the worst case, this will result in Inf or NaN in your network (then you have to restart training from an earlier checkpoint)

Based on: Lecture by Abigail See, CS224n Lecture 7

Exploding gradient solution

- Gradient clipping: if the norm of the gradient is greater than some threshold, scale it down before applying SGD update

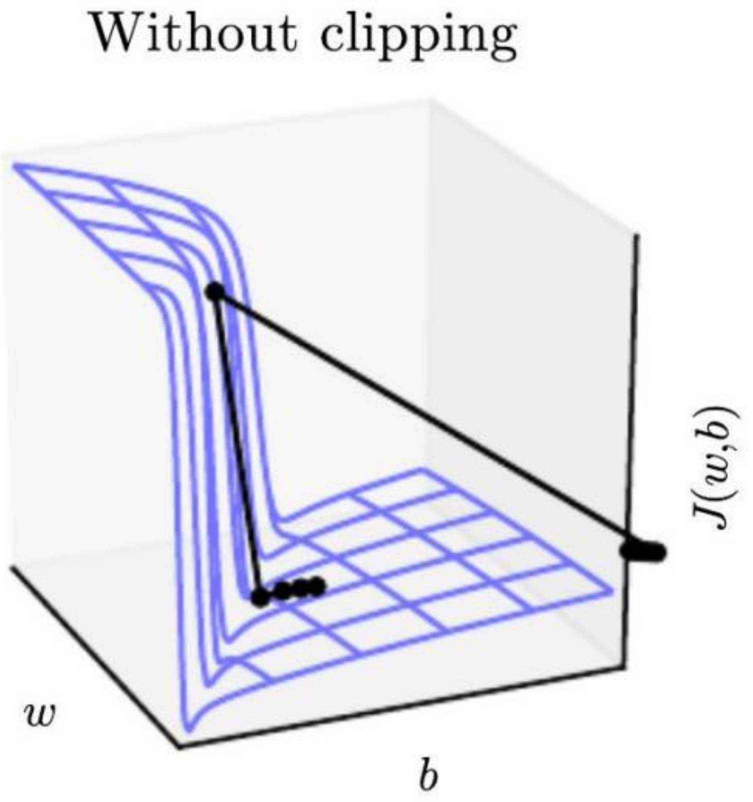
Algorithm 1 Pseudo-code for norm clipping

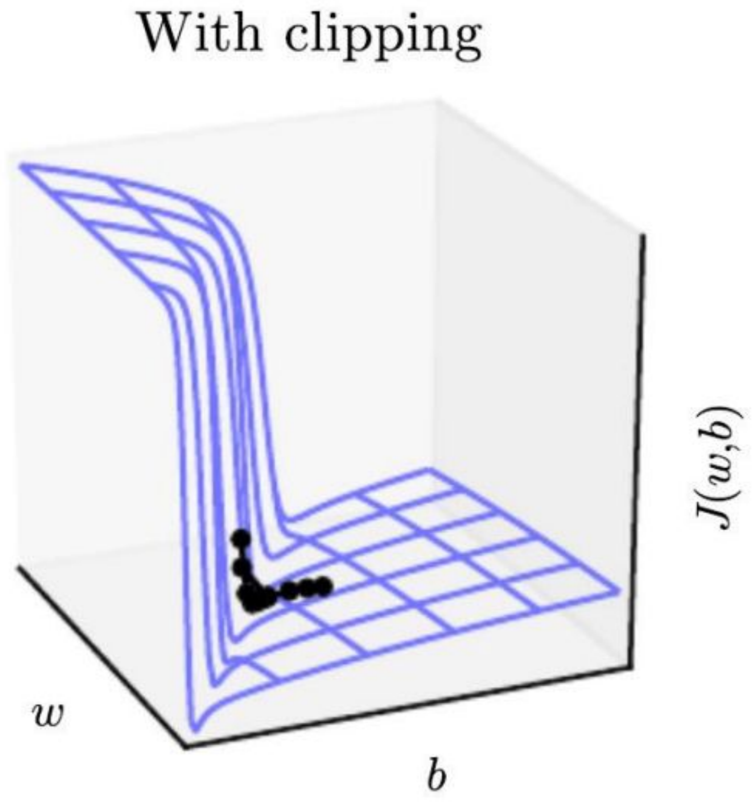
```
$\hat{\mathbf{g}} \leftarrow \frac{\partial \mathcal{E}}{\partial \theta}$
if $\|\hat{\mathbf{g}}\| \geq threshold$ then
    $\hat{\mathbf{g}} \leftarrow \frac{threshold}{\|\hat{\mathbf{g}}\|} \hat{\mathbf{g}}$
end if
```

- Intuition: take a step in the same direction, but a smaller step

Based on: Lecture by Abigail See, CS224n Lecture 7

Exploding gradient solution





Based on: Lecture by Abigail See, CS224n Lecture 7