Lecture 05:
DL recap: optimization, regularization, vanishing gradient problem

Sber RL course
Spring 2022

Radoslav Neychev

Outline

1. Recap: backpropagation, activations, intuition.
2. Optimizers.
3. Data normalization.
4. Regularization.
5. Vanishing gradient in RNNs
6. Vanishing gradient in deep neural networks
7. Q & A.

Advanced Machine Learning
Lecture 1:
Deep Learning recap

Radoslav Neychev

Outline

1. Recap: backpropagation, activations, intuition
2. Optimizers
3. Data normalization
4. Regularization

Recap: Deep Learning basics

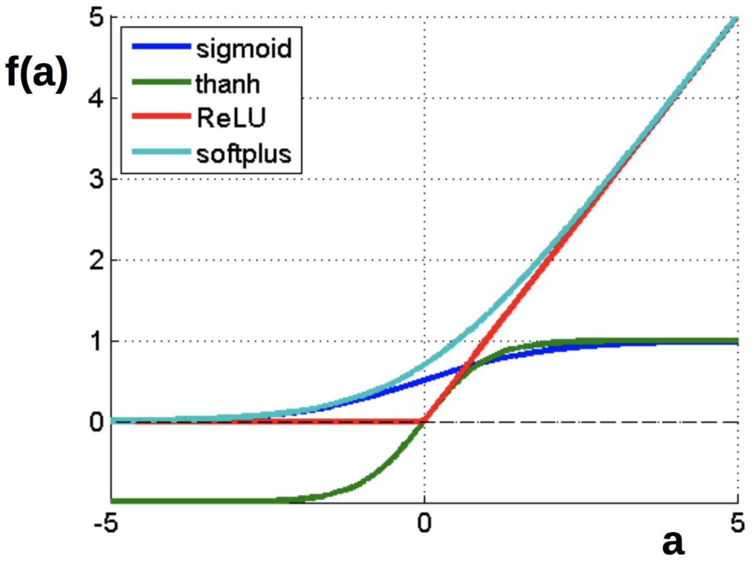
Once more: nonlinearities

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

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

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

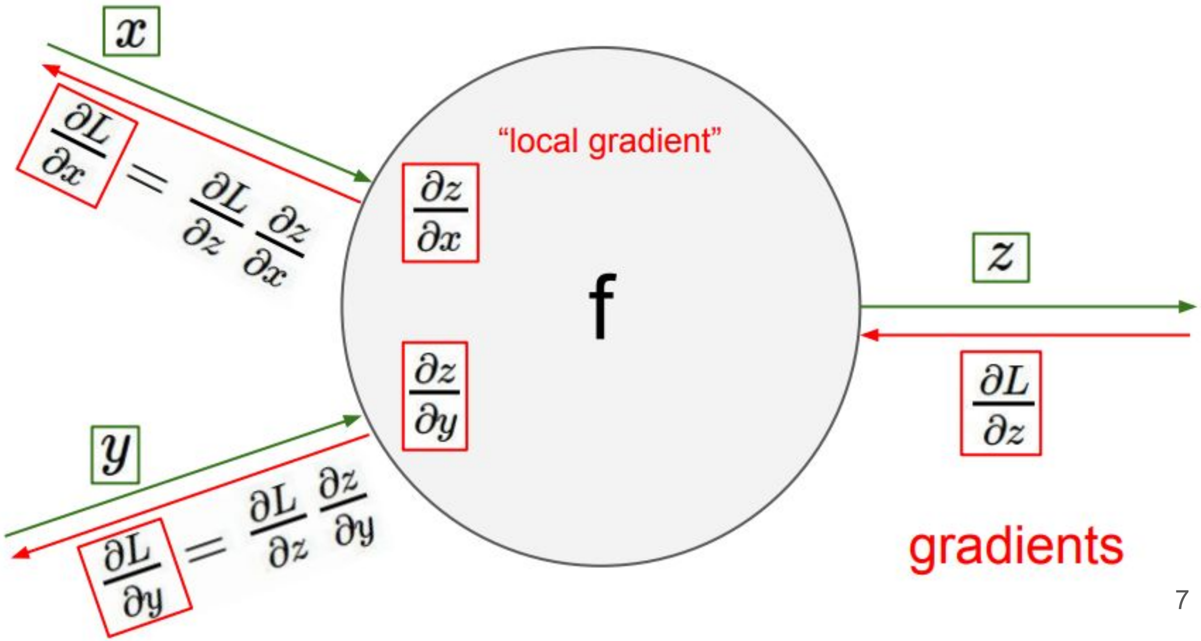
$$f(a) = \log(1 + e^{a})$$



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.

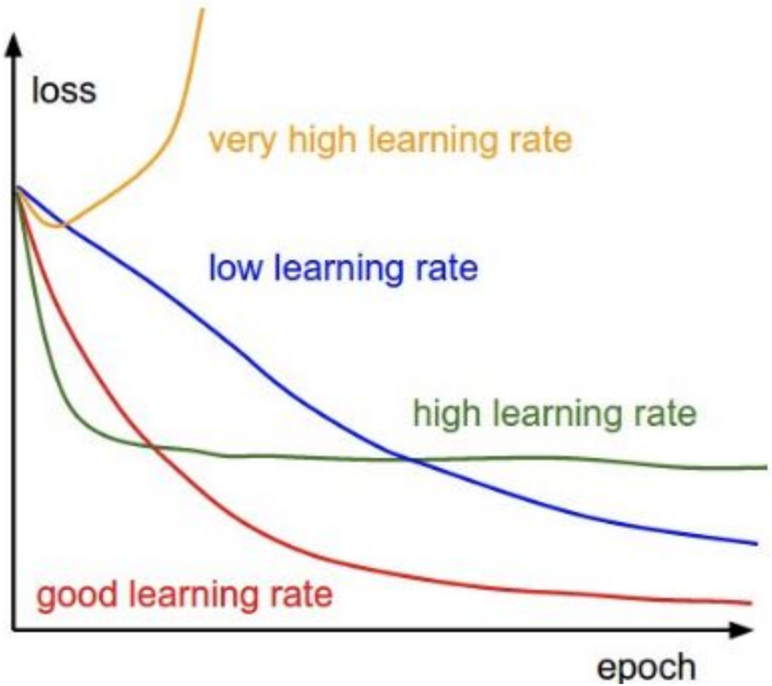


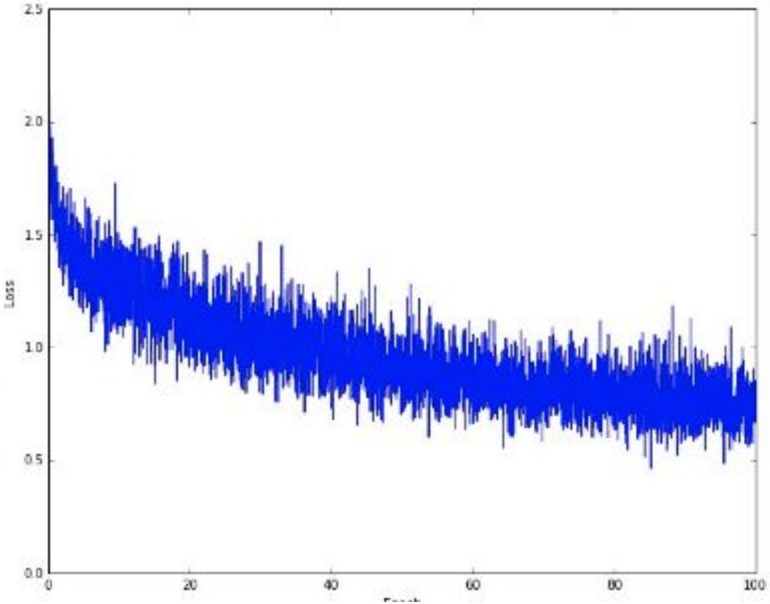
source: http://cs231n.github.io

Optimizers

Stochastic gradient descent is used to optimize NN parameters.

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





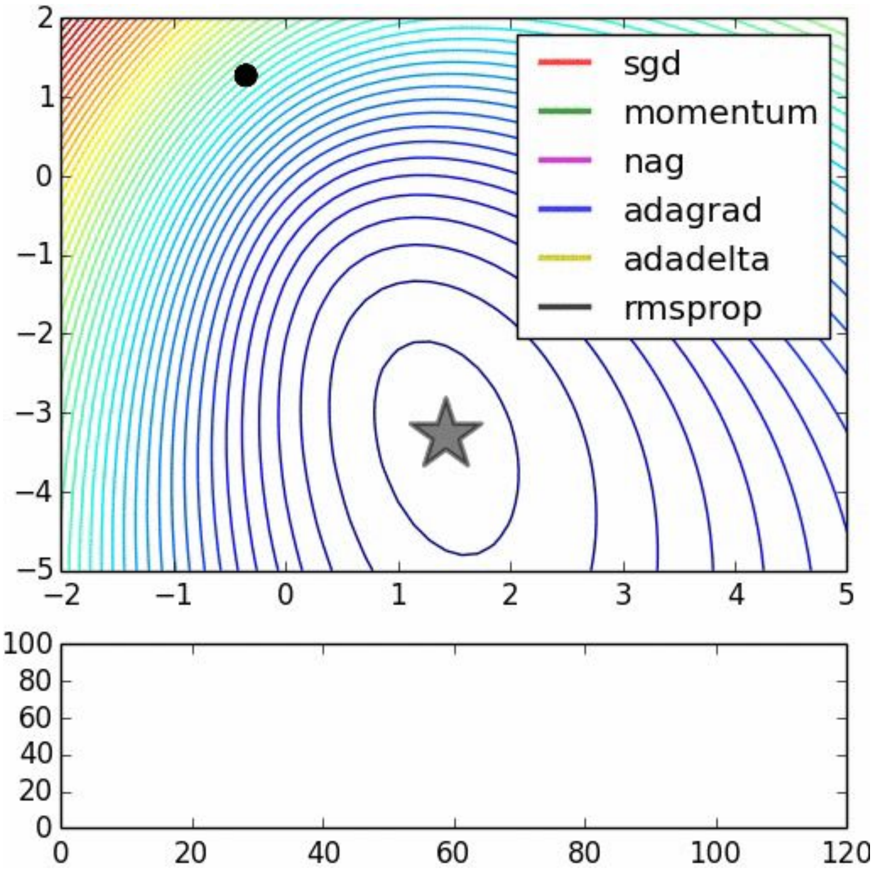
source: http://cs231n.github.io/neural-networks-3/

Optimization: SGD upgrades

Optimizers

There are much more optimizers:

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



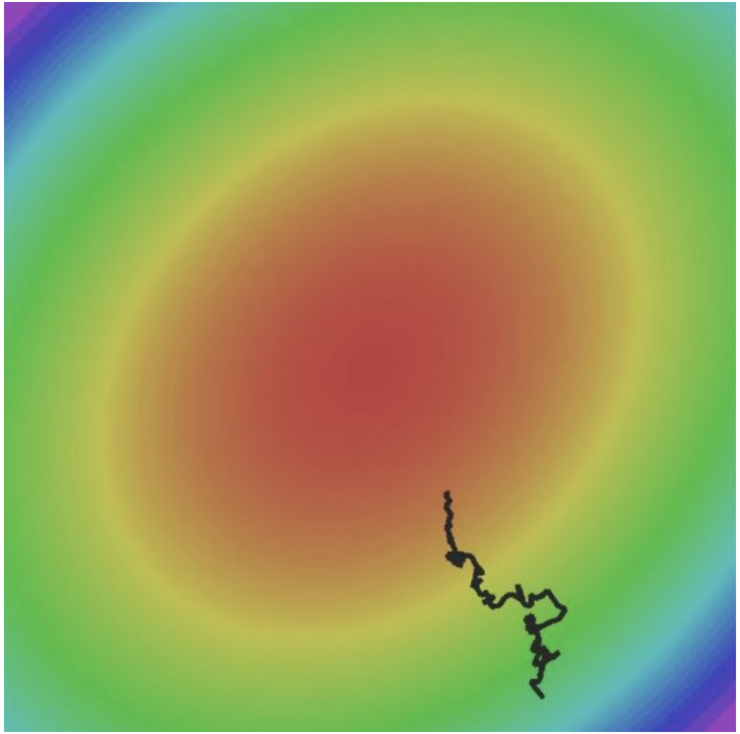
source: link

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 too small batches leads to noisy gradient



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

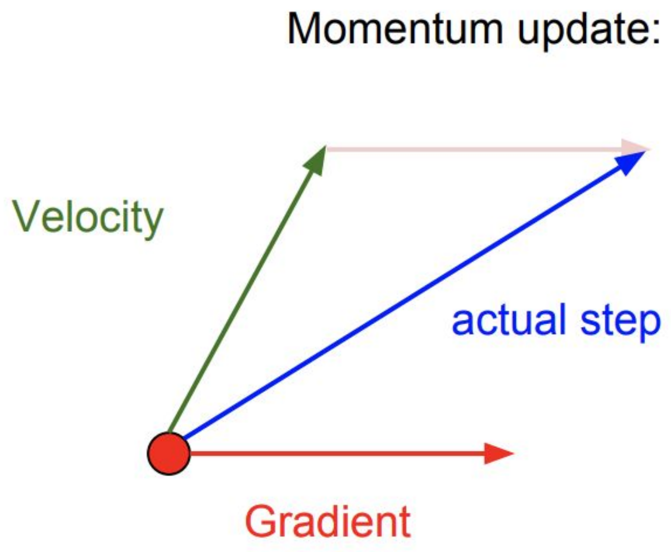
First idea: momentum

Simple SGD

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

SGD with momentum

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



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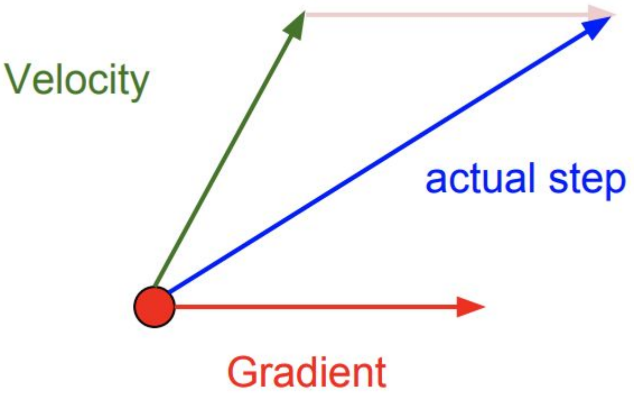
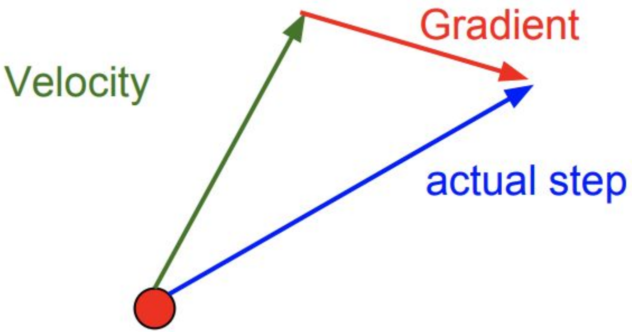
Nesterov momentum

Momentum update:



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

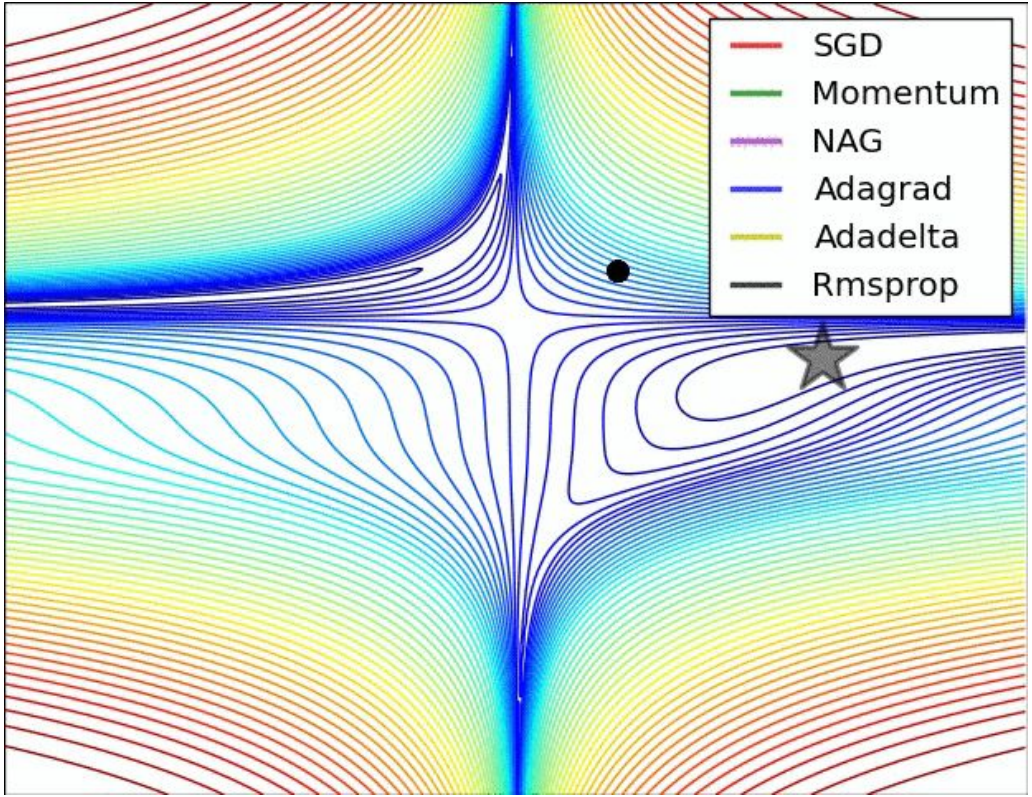
Nesterov Momentum



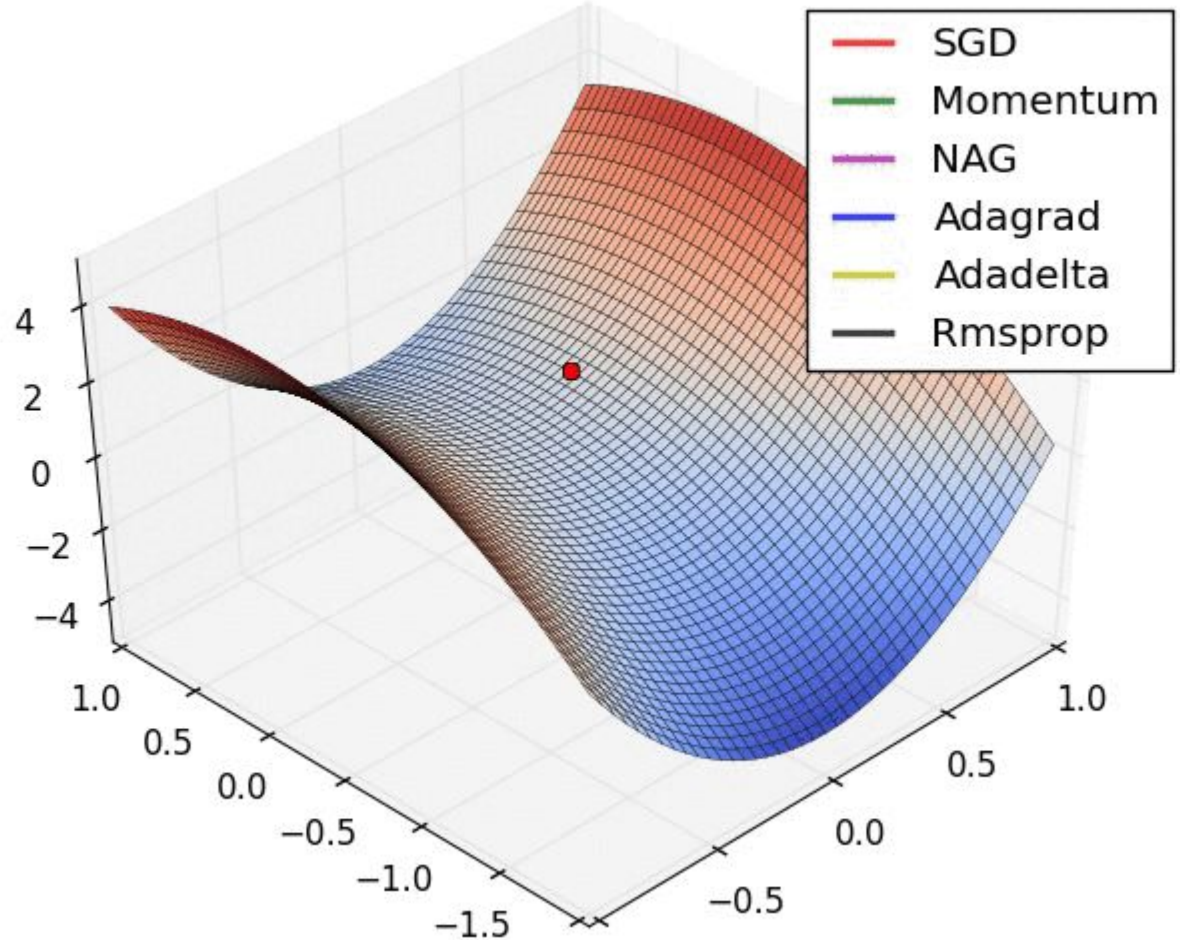
$$v_{t+1} = \rho v_t - \alpha \nabla f(\boxed{x_t + \rho v_t})$$
$$x_{t+1} = x_t + v_{t+1}$$

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

Comparing momentums



source: https://ruder.io/content/images/2016/09/contours_evaluation_optimizers.gif



source: https://ruder.io/content/images/2016/09/saddle_point_evaluation_optimizers.gif

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

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

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

Problem: gradient fades with time

Second idea: different dimensions are different

Adagrad: SGD with cache

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

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

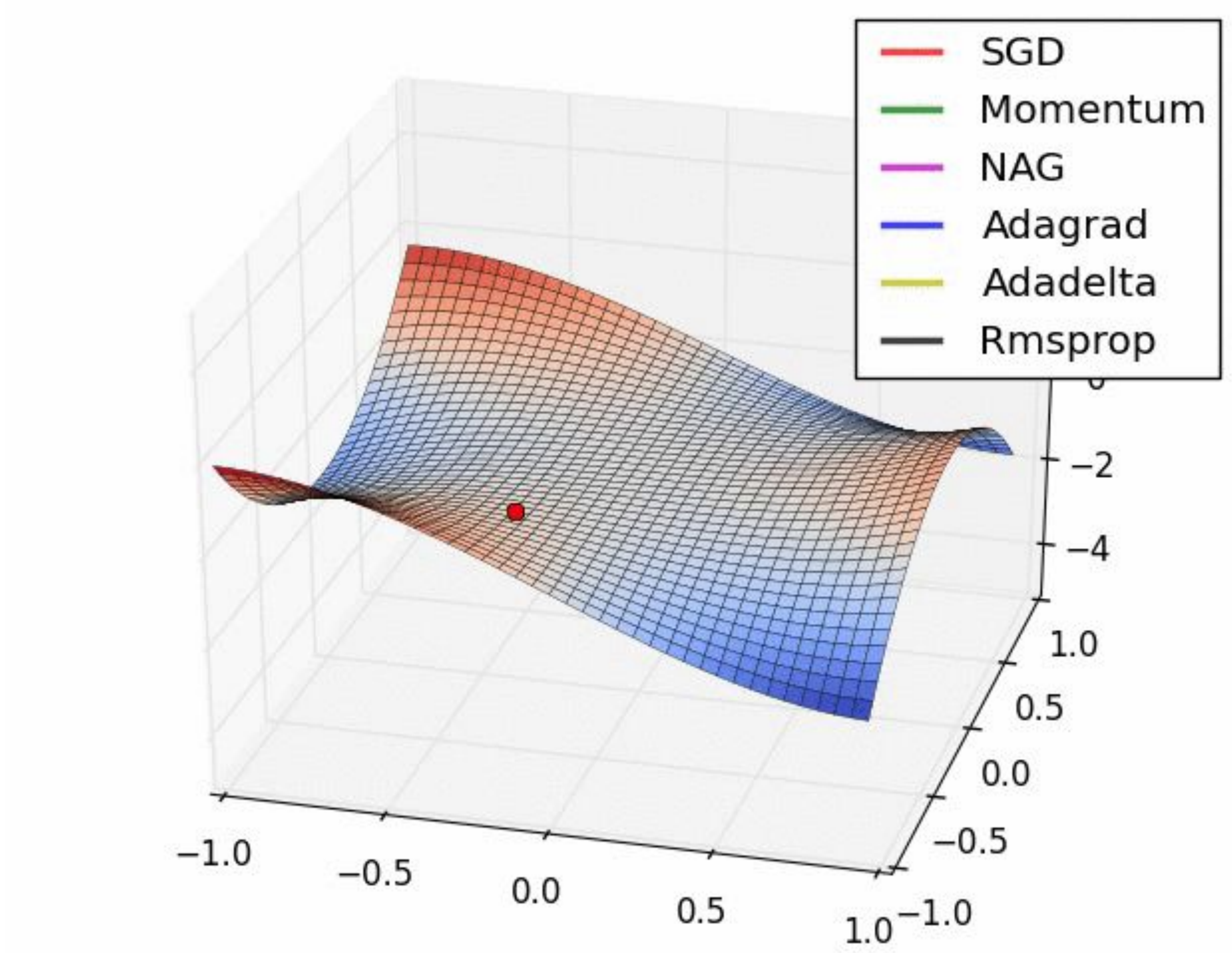
RMSProp: SGD with cache with exp. Smoothing

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

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

Slide 29 Lecture 6 of Geoff Hinton's Coursera class

http://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_lec6.pdf



source: https://imgur.com/a/Hqolp#NKsFHJb

Adam

Let's combine the momentum idea and RMSProp normalization:

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

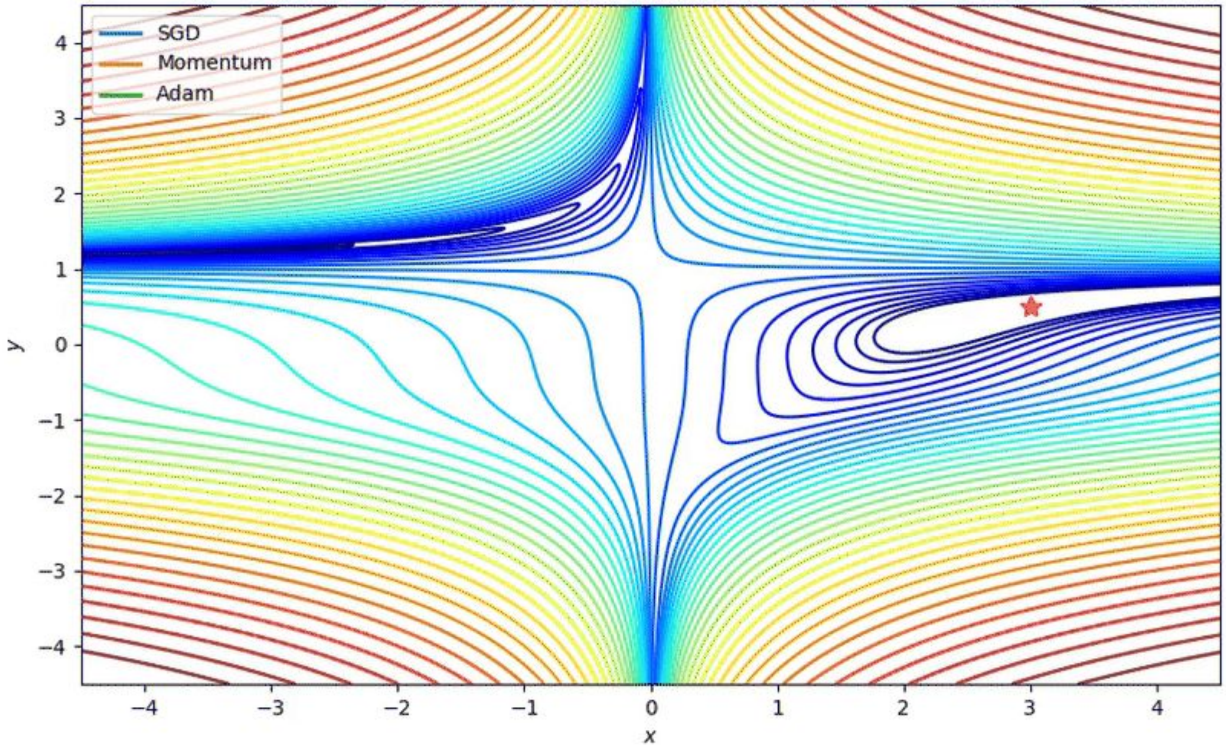
$$\text{cache}_{t+1} = \beta \text{cache}_t + (1-\beta)(\nabla f(x_t))^2$$

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

Actually, that's not quite Adam.

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

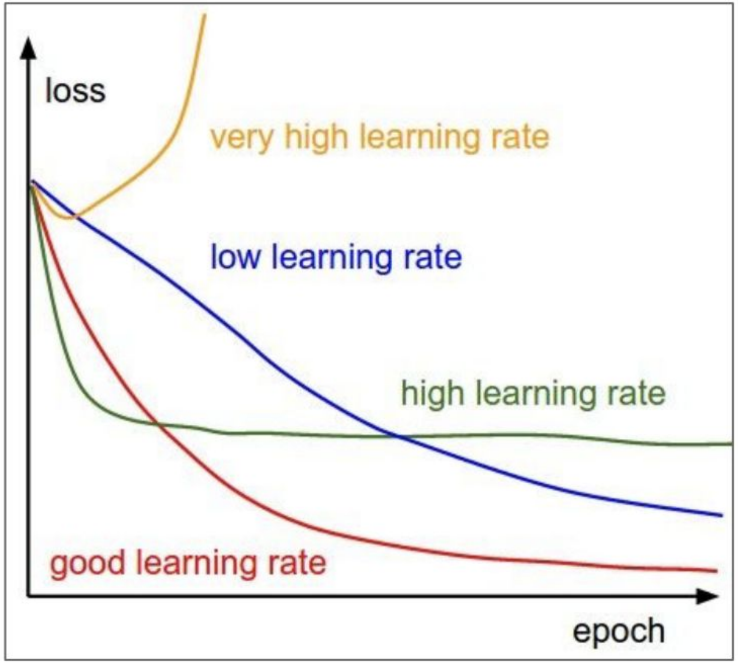
Comparing optimizers

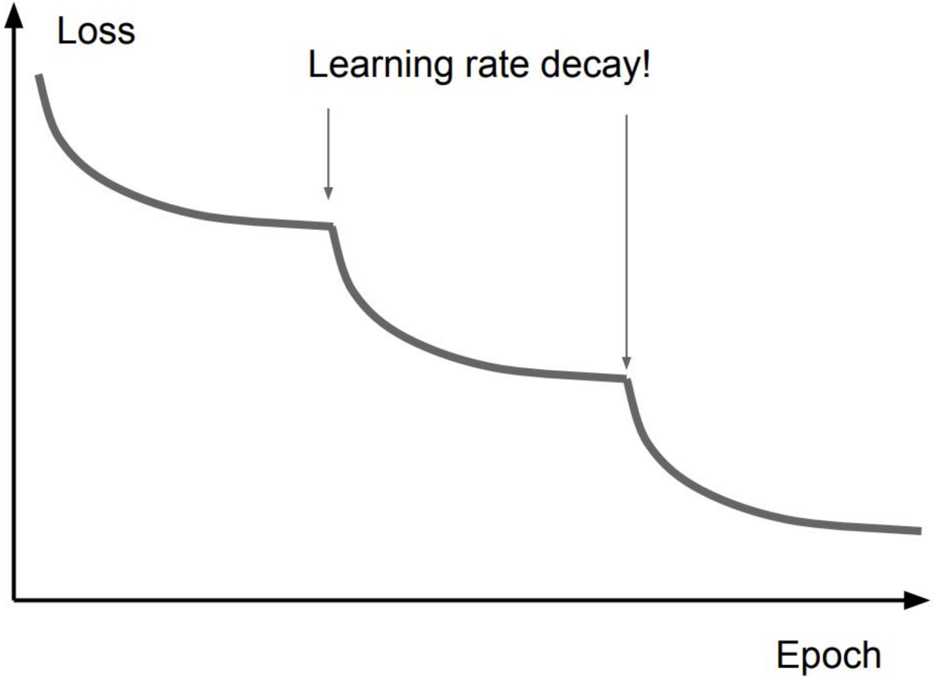


source: https://joshvarty.com/2018/02/27/ltfn-7-a-quick-look-at-tensorflow-optimizers/

source: https://twitter.com/karpathy/status/801621764144971776

Once more: learning rate





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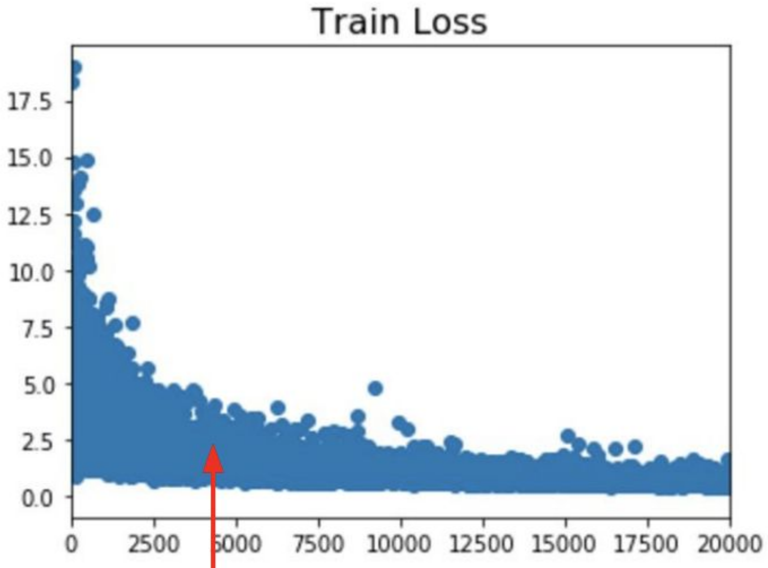
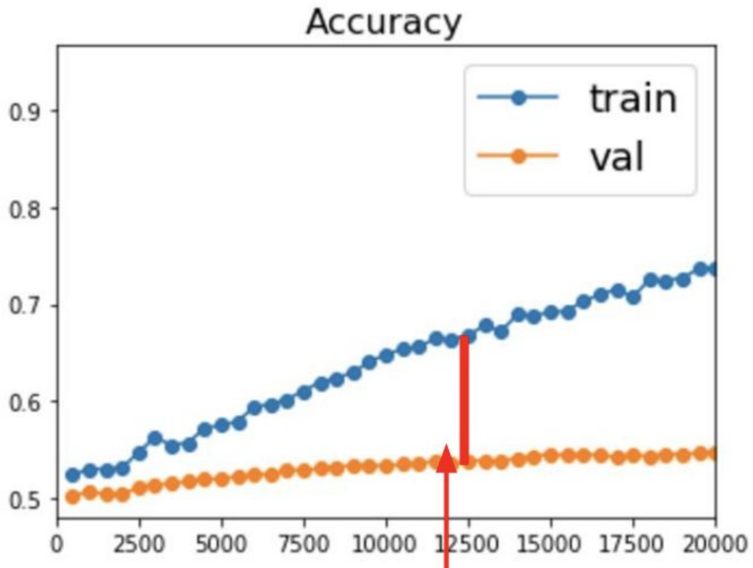
Sum up: optimization

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

Regularization in DL



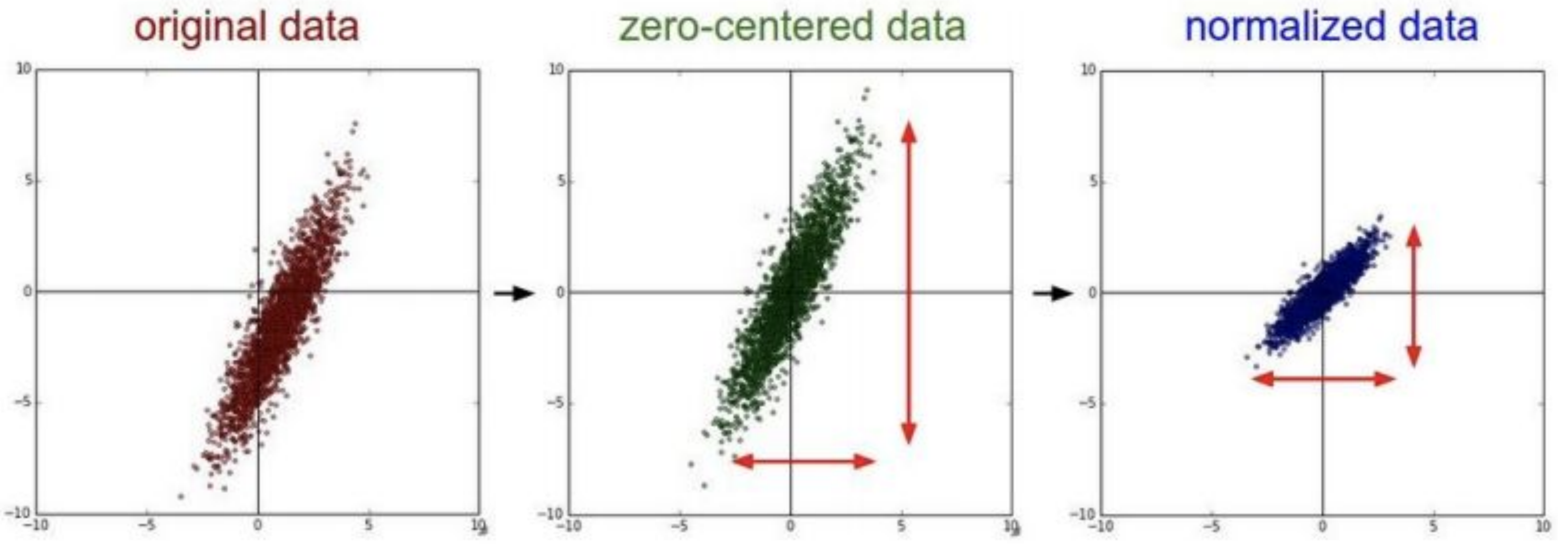


Better optimization algorithms
help reduce training loss

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

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

Data normalization



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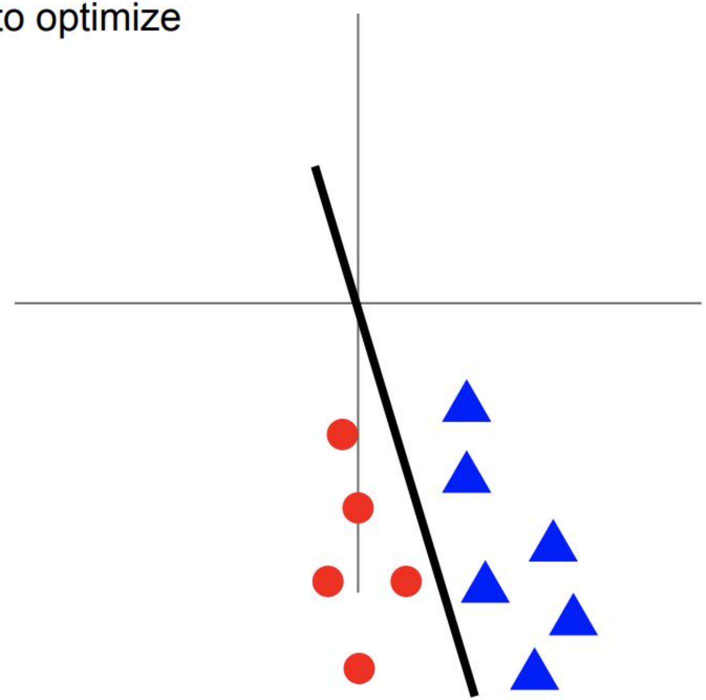
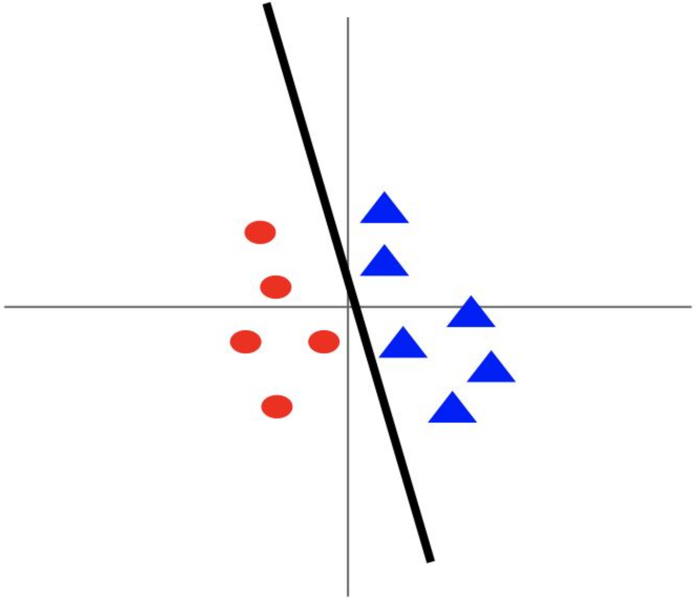
Data normalization

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



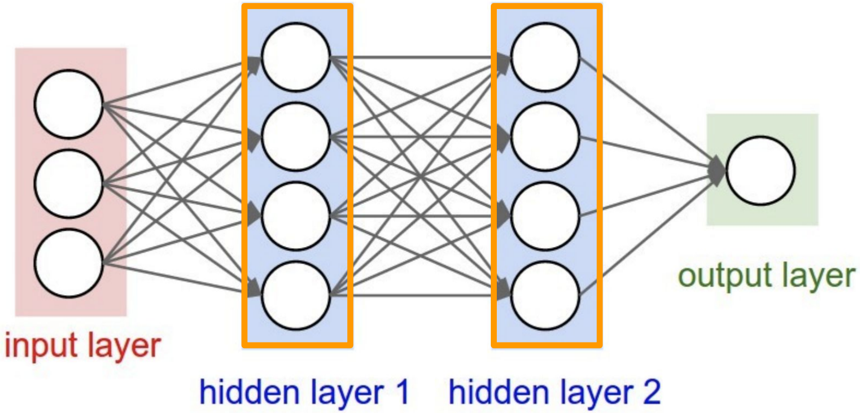
After normalization: less sensitive to small changes in weights; easier to optimize



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

Problem:

- Consider a neuron in any layer beyond first
- At each iteration its weights are tuned to reduce loss
- Its inputs are tuned as well. 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 la $h_i = \frac{h_i - \mu_i}{\sqrt{\sigma_i^2}}$

  (zero mean unit variance)

- 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)

What is this?

This transformation should be able to represent the identity transform.

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

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

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

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

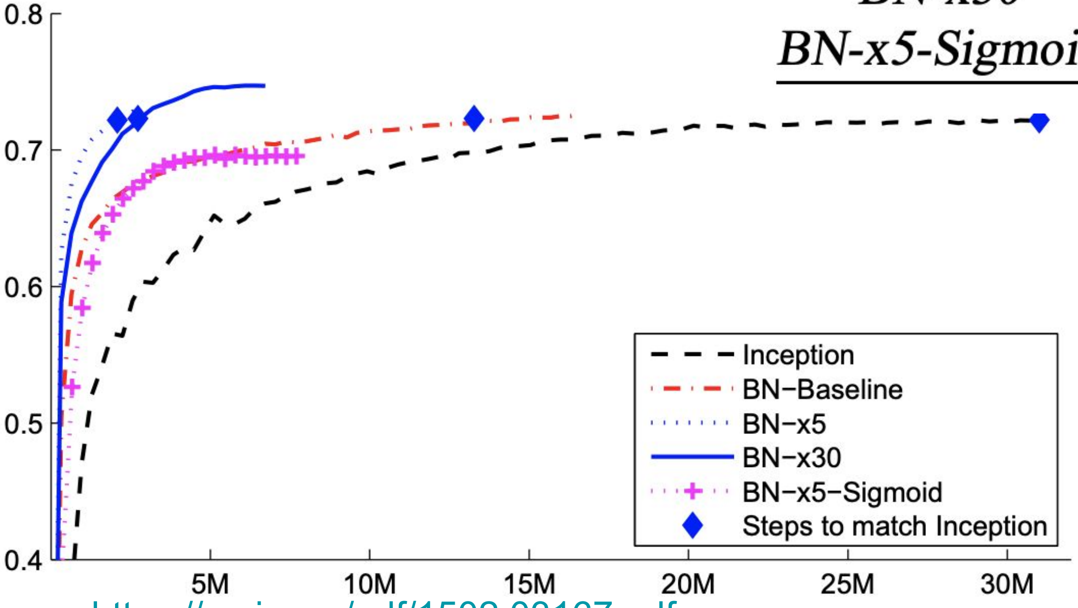
$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma_{\mathcal{B}}^2 + \epsilon}} \qquad \text{// normalize}$$

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

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%

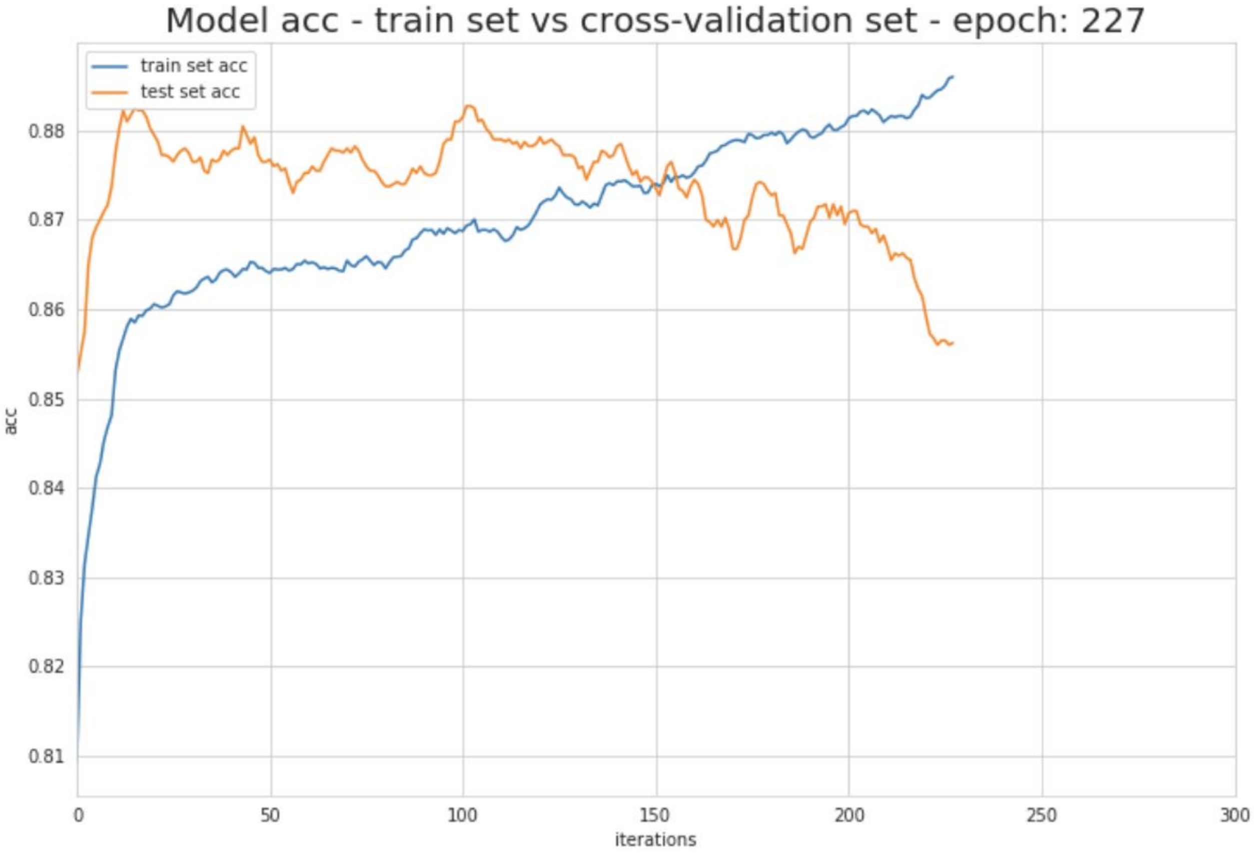
accuracy



number of training steps

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:

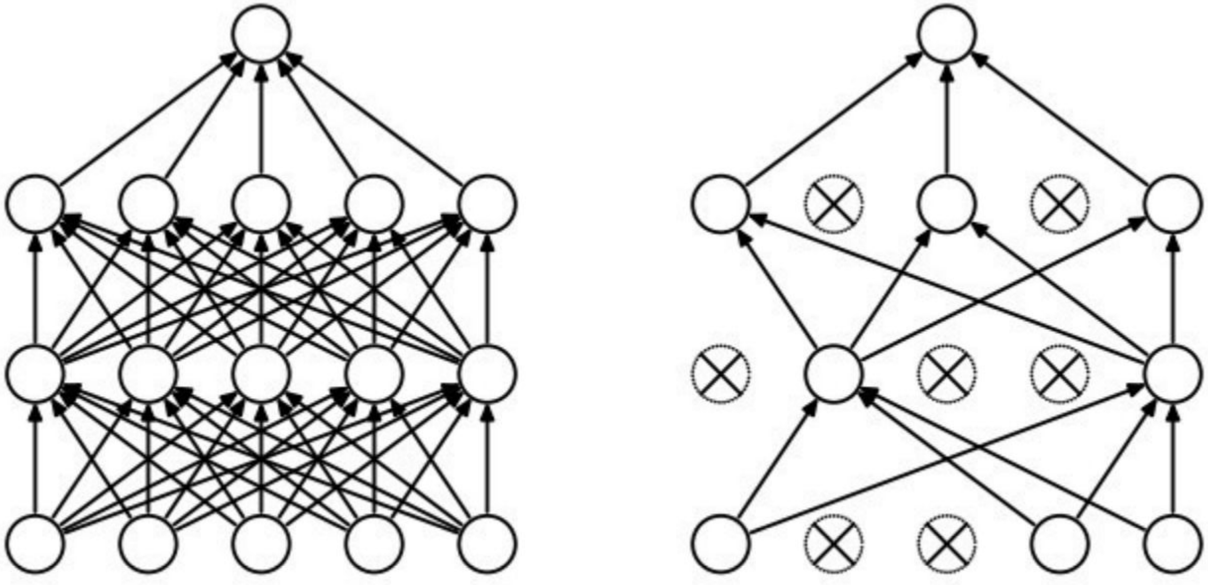
- L2 regularization: $R(W) = \|W\|_2^2$
- L1 regularization: $R(W) = \|W\|_1$
- Elastic Net (L1 + L2): $R(W) = \beta\|W\|_2^2 + \|W\|_1$

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

Regularization: Dropout

Some neurons are "dropped" during training.

Prevents overfitting.

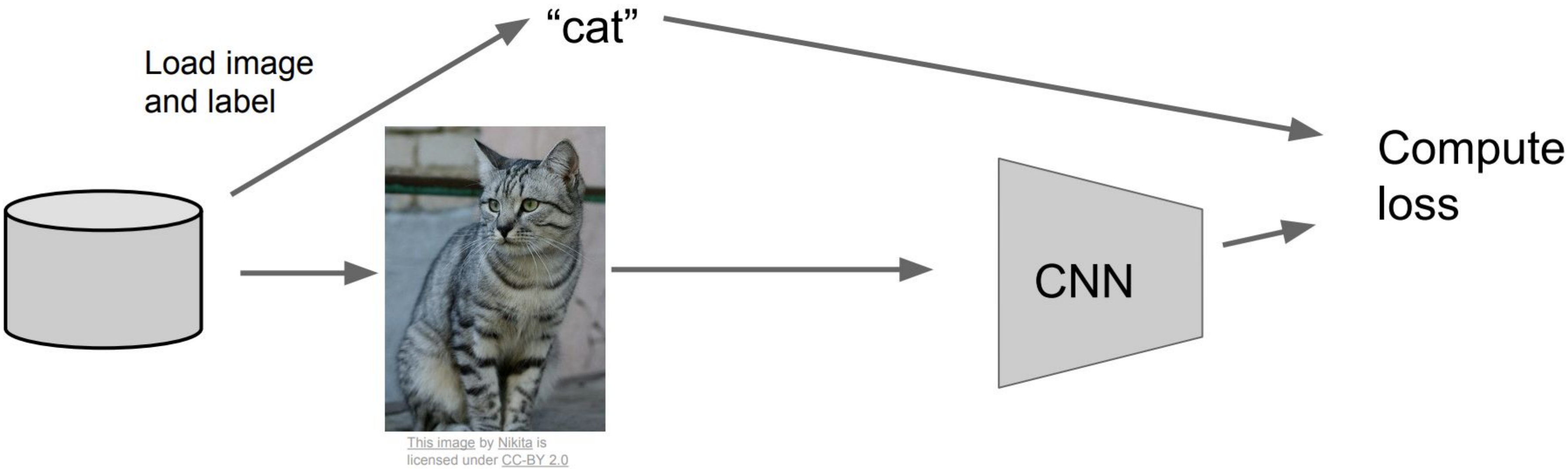


(a) Standard Neural Net (b) After applying dropout.

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

source: https://jmlr.org/papers/v15/srivastava14a.html

Regularization: data augmentation



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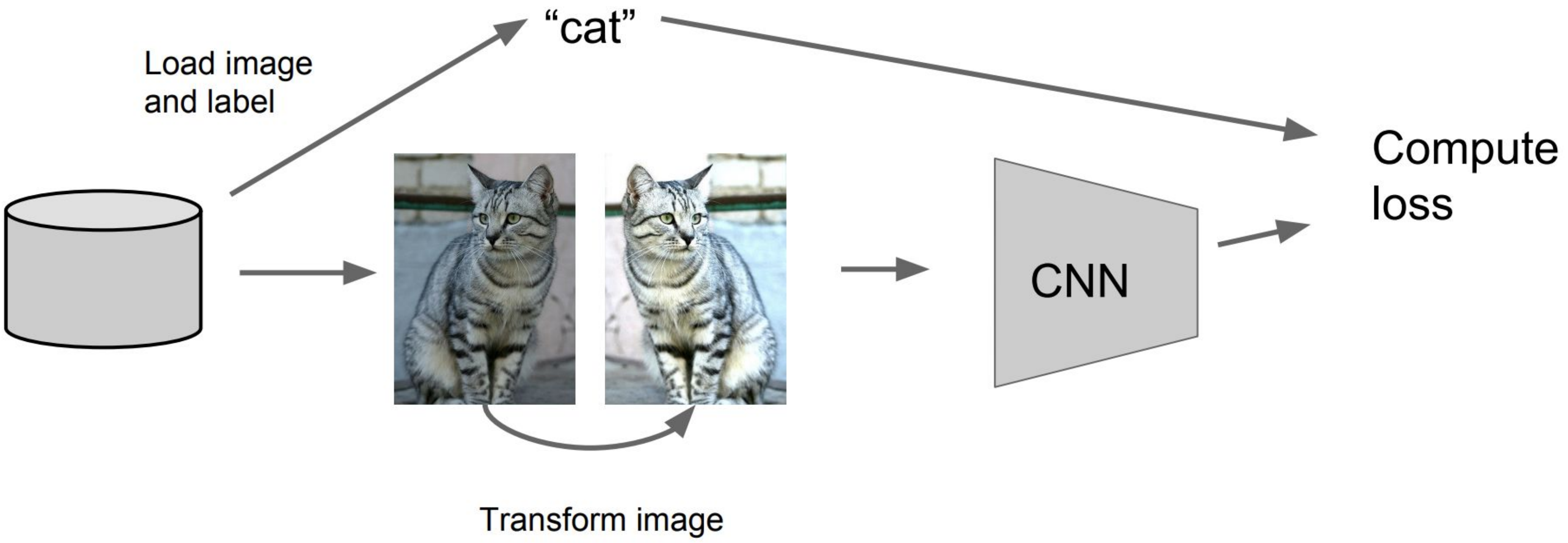
Regularization: data augmentation



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Optimization:

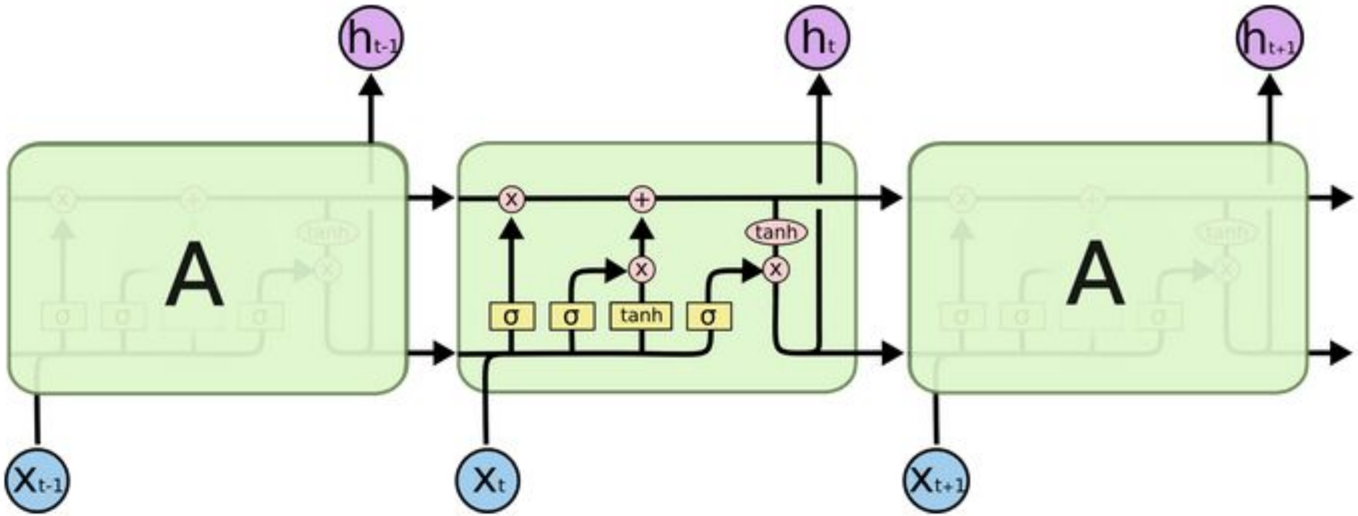
- Adam is great basic choice
- Even for Adam/RMSProp learning rate matters
- Use learning rate decay
- Monitor your model quality

Regularization:

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

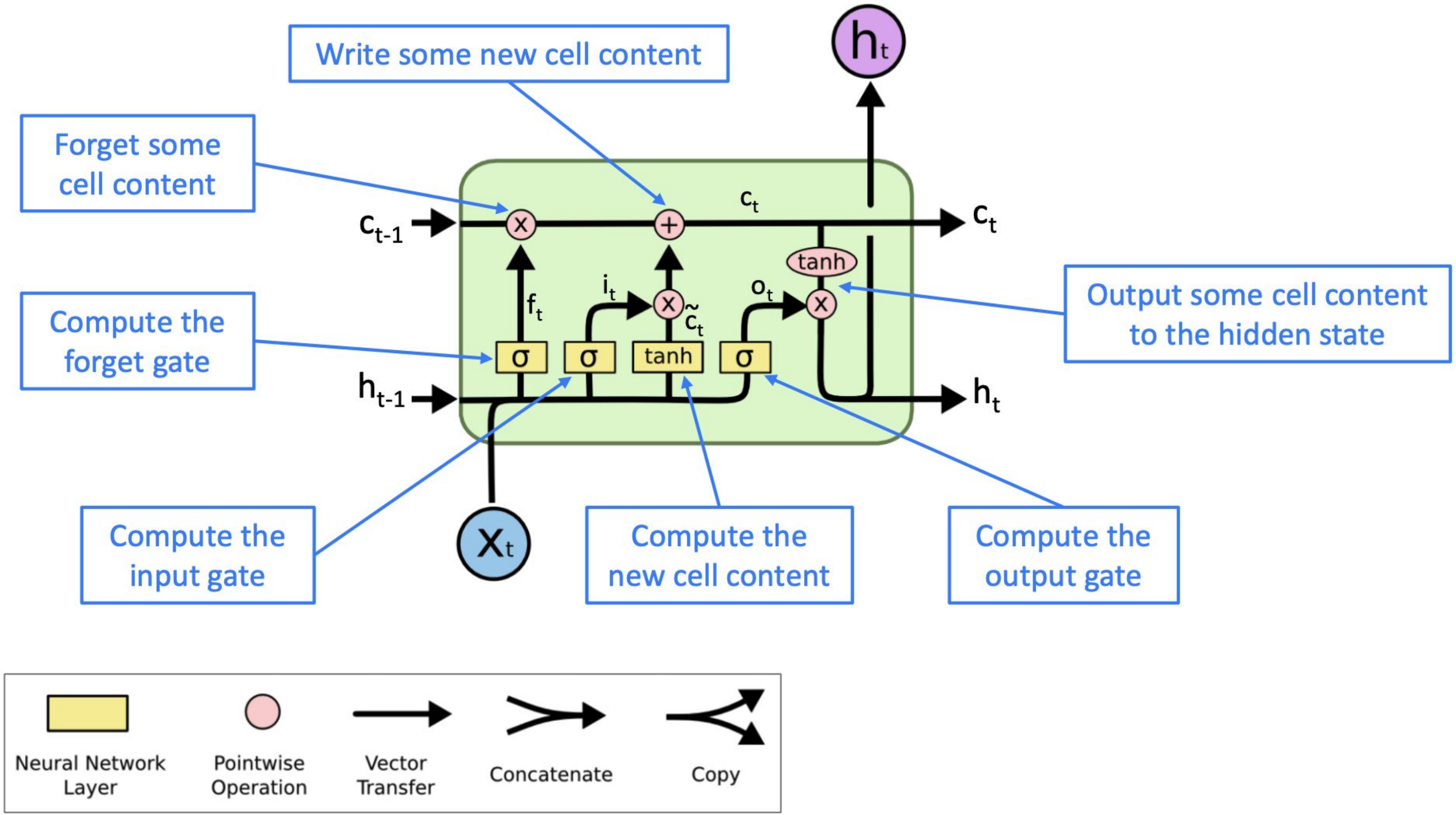
Further readings available here

LSTM



Source: https://colah.github.io/posts/2015-08-Understanding-LSTMs/

LSTM: quick overview



Source: Lecture by Abigail See, [CS224n Lecture 7]

LSTM: quick overview

Forget gate: controls what is kept vs forgotten, from previous cell state

Input gate: controls what parts of the new cell content are written to cell

Output gate: controls what parts of cell are output to hidden state

Sigmoid function: all gate values are between 0 and 1

$$f^{(t)} = \boxed{\sigma}\left(W_f h^{(t-1)} + U_f x^{(t)} + b_f\right)$$

$$i^{(t)} = \boxed{\sigma}\left(W_i h^{(t-1)} + U_i x^{(t)} + b_i\right)$$

$$o^{(t)} = \boxed{\sigma}\left(W_o h^{(t-1)} + U_o x^{(t)} + b_o\right)$$

New cell content: this is the new content to be written to the cell

Cell state: erase ("forget") some content from last cell state, and write ("input") some new cell content

Hidden state: read ("output") some content from the cell

$$\tilde{c}^{(t)} = \tanh\left(W_c h^{(t-1)} + U_c x^{(t)} + b_c\right)$$

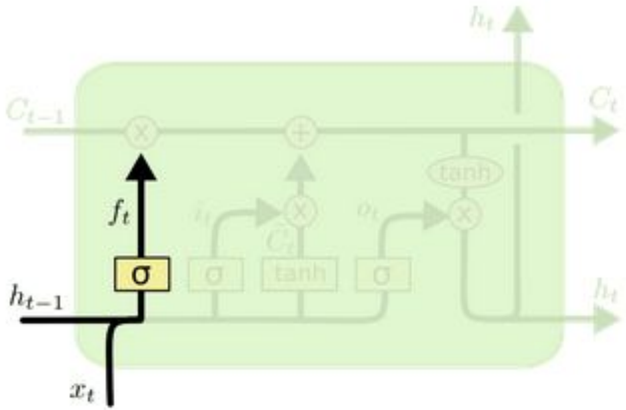
$$c^{(t)} = f^{(t)} \circ c^{(t-1)} + i^{(t)} \circ \tilde{c}^{(t)}$$

$$h^{(t)} = o^{(t)} \circ \tanh c^{(t)}$$

All these are vectors of same length n

Gates are applied using element-wise product

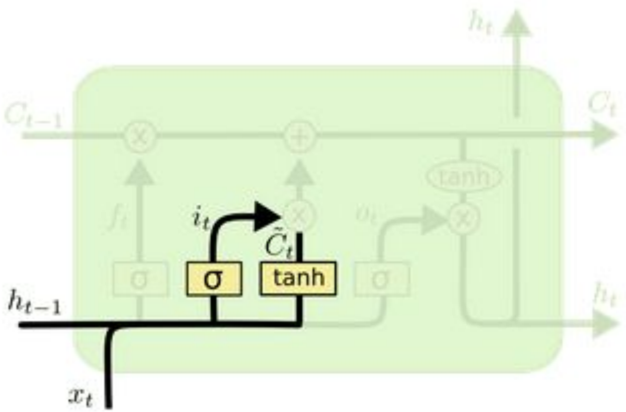
LSTM: quick overview



$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] + b_f\right)$$

Source: https://colah.github.io/posts/2015-08-Understanding-LSTMs/

LSTM: quick overview

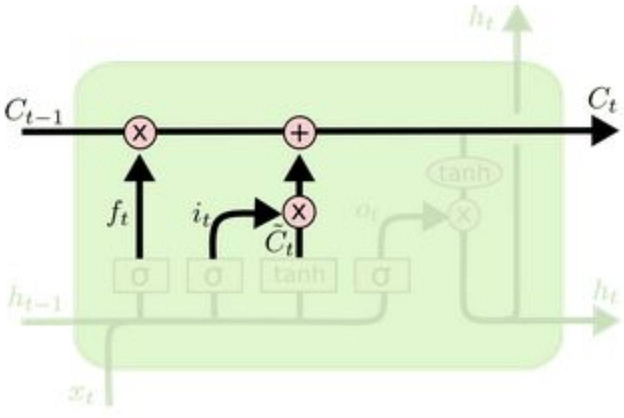


$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \ + \ b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \ + \ b_C)$$

Source: https://colah.github.io/posts/2015-08-Understanding-LSTMs/

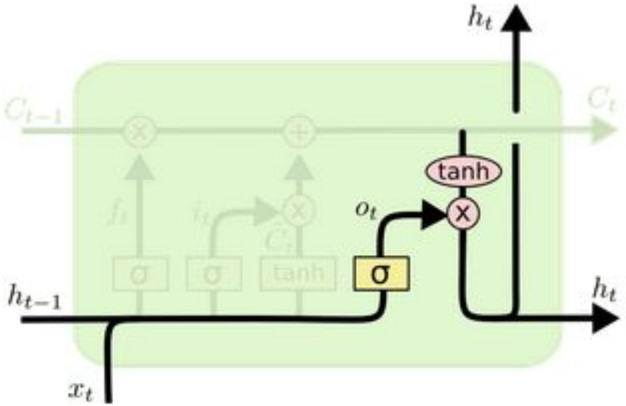
LSTM: quick overview



$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

Source: https://colah.github.io/posts/2015-08-Understanding-LSTMs/

LSTM: quick overview



$$o_t = \sigma\left(W_o \left[h_{t-1}, x_t\right] + b_o\right)$$

$$h_t = o_t * \tanh\left(C_t\right)$$

Source: https://colah.github.io/posts/2015-08-Understanding-LSTMs/

LSTM: with formulas

Forget gate: controls what is kept vs forgotten, from previous cell state

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Output gate: controls what parts of cell are output to hidden state

Sigmoid function: all gate values are between 0 and 1

$$\boldsymbol{f}^{(t)} = \sigma\left(\boldsymbol{W}_f \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_f \boldsymbol{x}^{(t)} + \boldsymbol{b}_f\right)$$

$$\boldsymbol{i}^{(t)} = \sigma\left(\boldsymbol{W}_i \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_i \boldsymbol{x}^{(t)} + \boldsymbol{b}_i\right)$$

$$\boldsymbol{o}^{(t)} = \sigma\left(\boldsymbol{W}_o \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_o \boldsymbol{x}^{(t)} + \boldsymbol{b}_o\right)$$

New cell content: this is the new content to be written to the cell

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$$\tilde{\boldsymbol{c}}^{(t)} = \tanh\left(\boldsymbol{W}_c \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_c \boldsymbol{x}^{(t)} + \boldsymbol{b}_c\right)$$

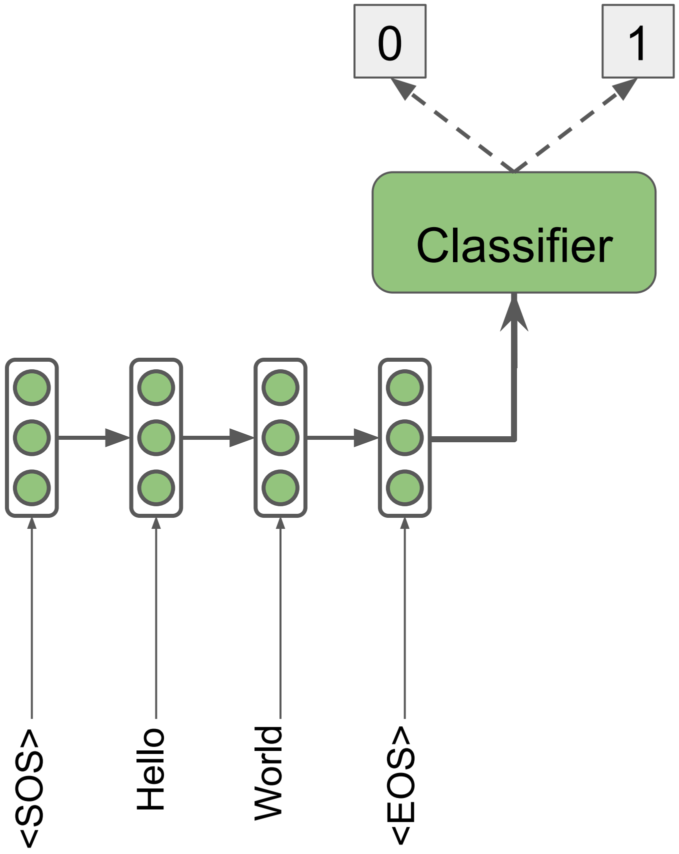
$$\boldsymbol{c}^{(t)} = \boldsymbol{f}^{(t)} \circ \boldsymbol{c}^{(t-1)} + \boldsymbol{i}^{(t)} \circ \tilde{\boldsymbol{c}}^{(t)}$$

$$\boldsymbol{h}^{(t)} = \boldsymbol{o}^{(t)} \circ \tanh \boldsymbol{c}^{(t)}$$

All these are vectors of same length *n*

Gates are applied using element-wise product

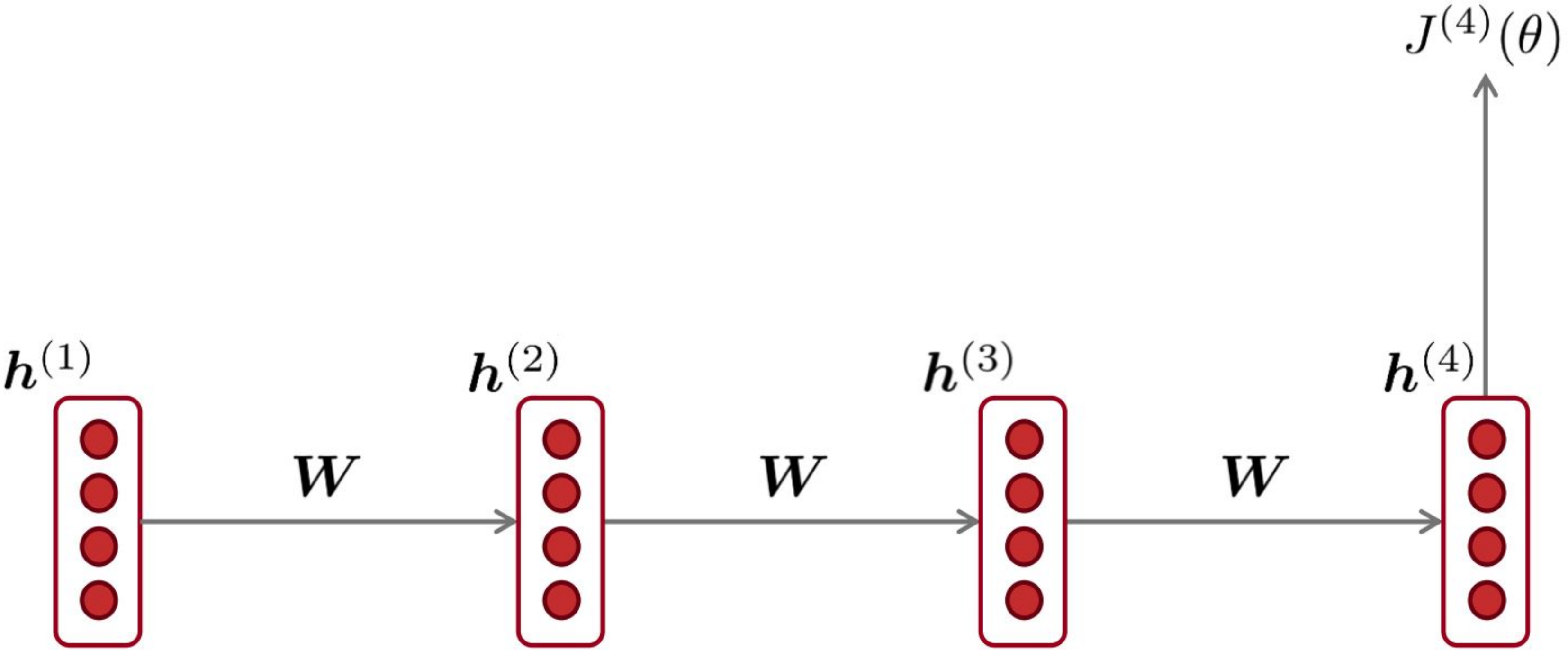
RNN as encoder for sequential data



RNNs can be used to encode an input sequence in a fixed size vector.

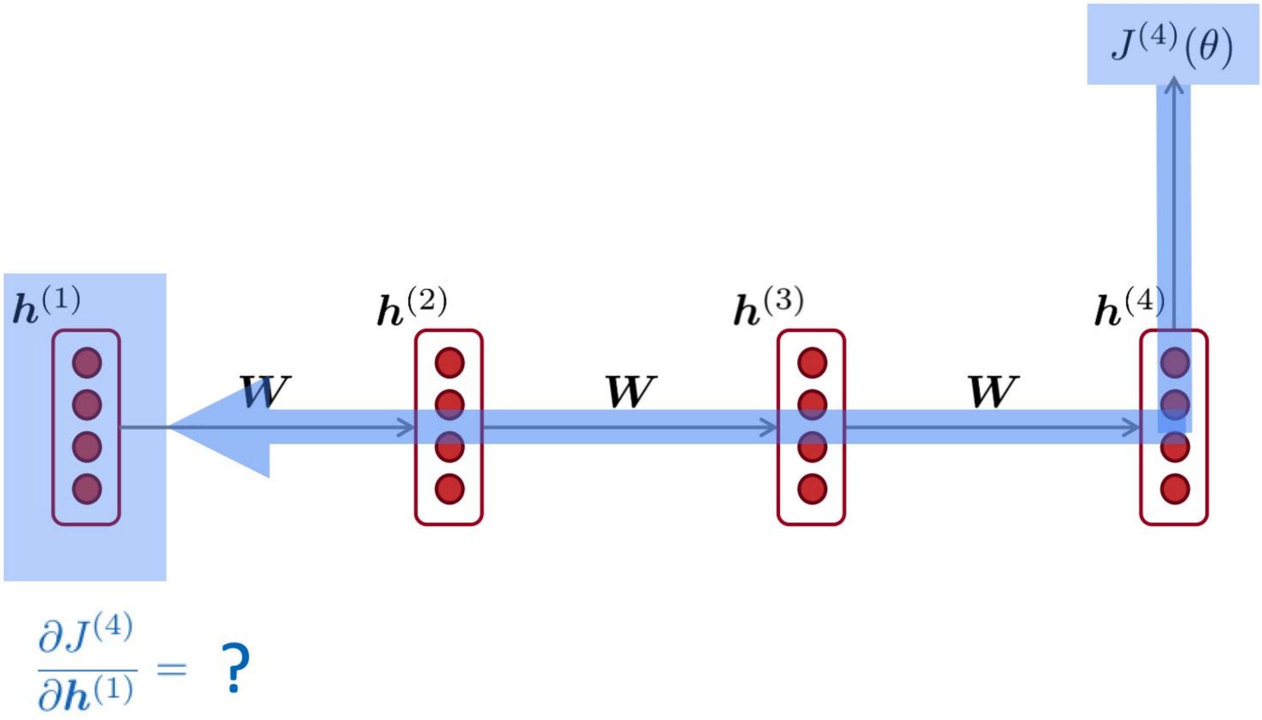
This vector can be treated as a representation of input sequence.

Vanishing gradient problem



Based on: Lecture by Abigail See, [CS224n Lecture 7]

Vanishing gradient problem



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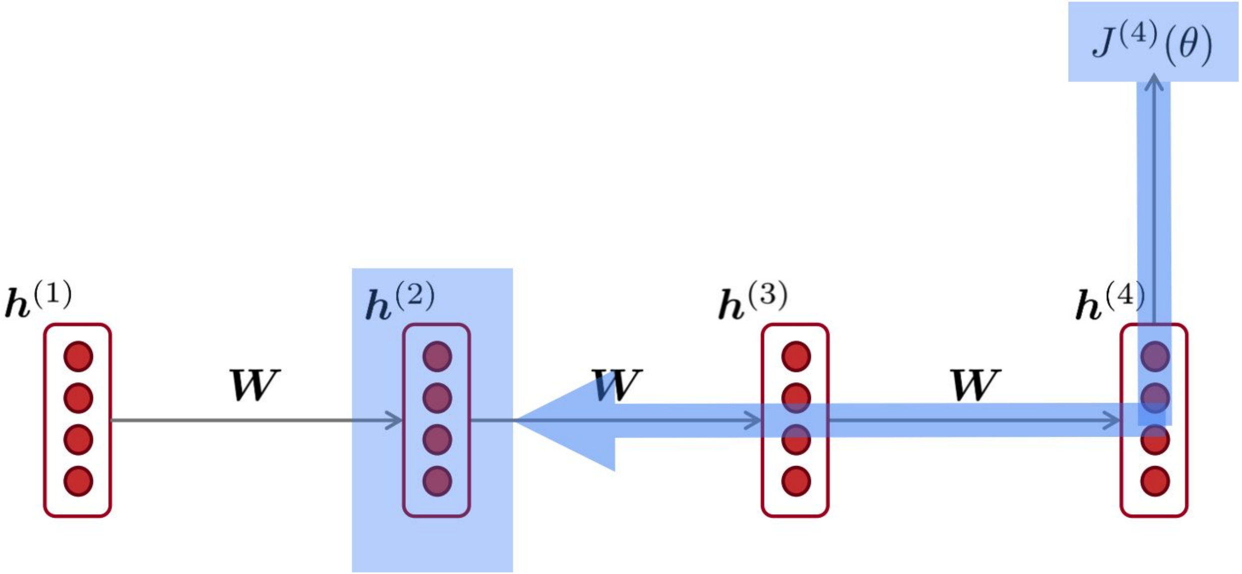
Vanishing gradient problem

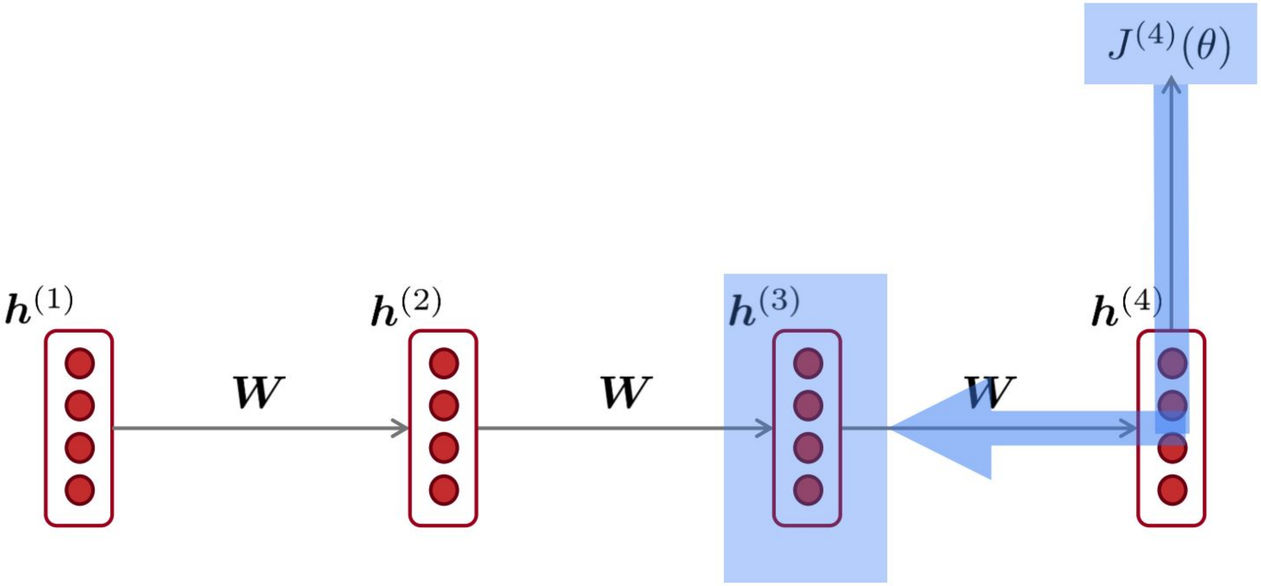


$$\frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(1)}} = \frac{\partial \boldsymbol{h}^{(2)}}{\partial \boldsymbol{h}^{(1)}} \times \frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(2)}}$$

chain rule!

Based on: Lecture by Abigail See, [CS224n Lecture 7]

Vanishing gradient problem

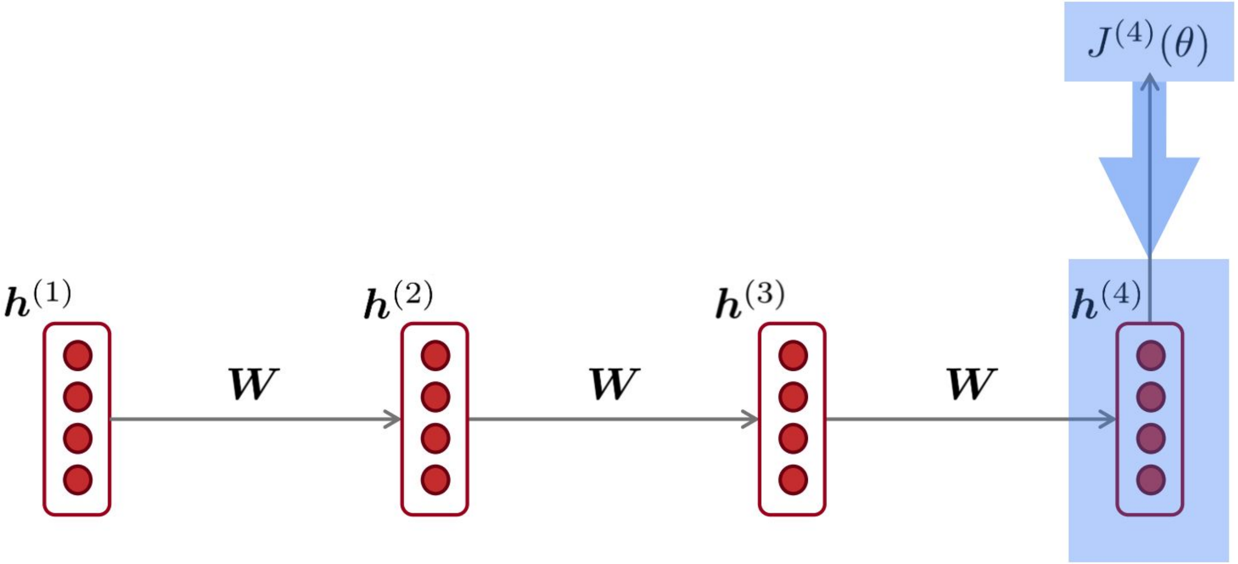


$$\frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(1)}} = \frac{\partial \boldsymbol{h}^{(2)}}{\partial \boldsymbol{h}^{(1)}} \times \qquad \frac{\partial \boldsymbol{h}^{(3)}}{\partial \boldsymbol{h}^{(2)}} \times \frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(3)}}$$

chain rule!

Based on: Lecture by Abigail See, [CS224n Lecture 7]

Vanishing gradient problem



$$\frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(1)}} = \frac{\partial \boldsymbol{h}^{(2)}}{\partial \boldsymbol{h}^{(1)}} \times \frac{\partial \boldsymbol{h}^{(3)}}{\partial \boldsymbol{h}^{(2)}} \times \frac{\partial \boldsymbol{h}^{(4)}}{\partial \boldsymbol{h}^{(3)}} \times \frac{\partial J^{(4)}}{\partial \boldsymbol{h}^{(4)}}$$

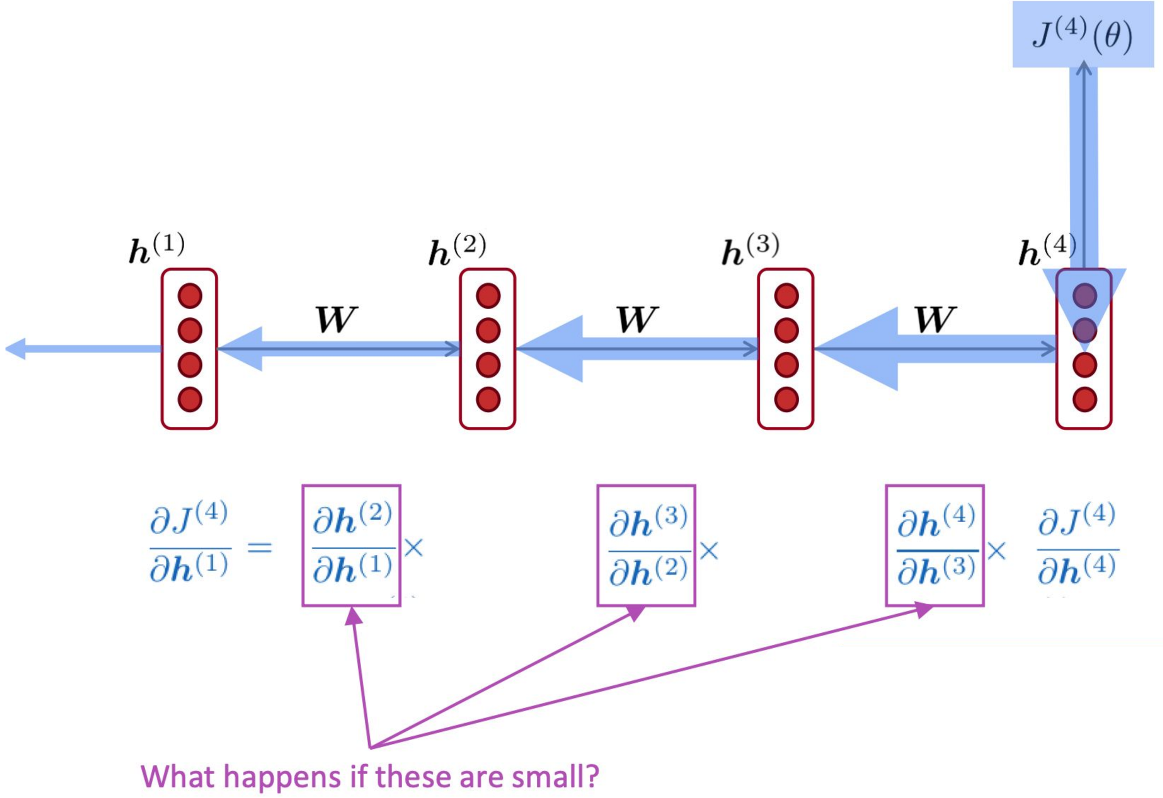
chain rule!

Based on: Lecture by Abigail See, CS224n Lecture 7

Vanishing gradient problem

Vanishing gradient problem:

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

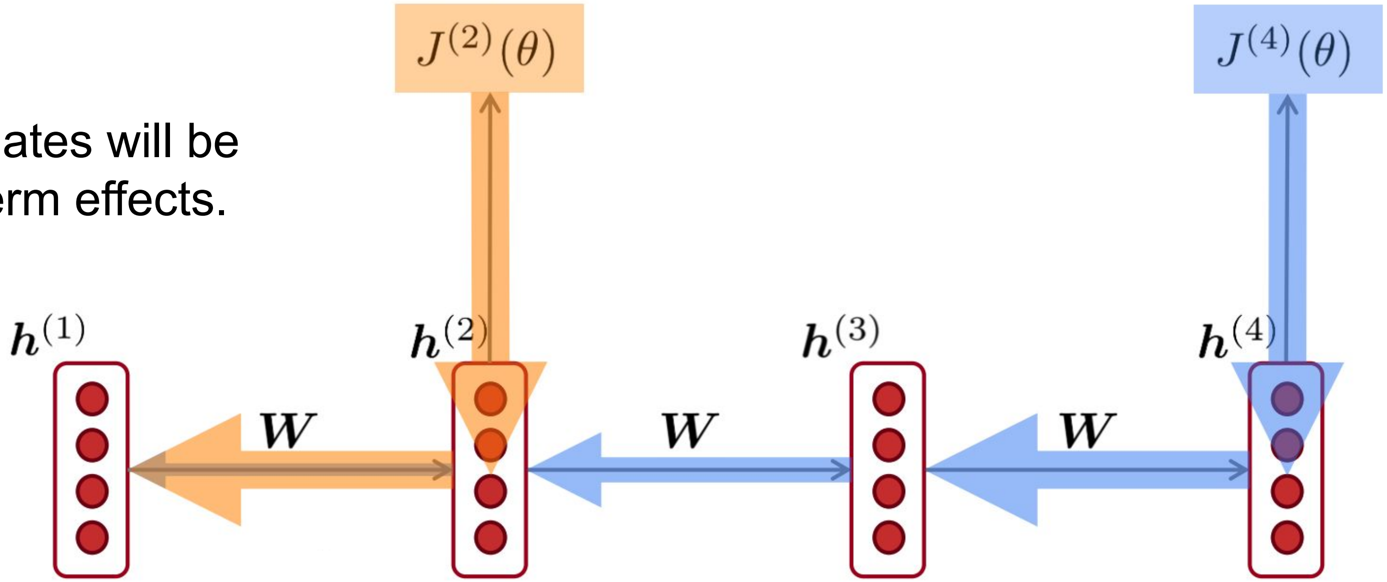


More info: “On the difficulty of training recurrent neural networks”, Pascanu et al, 2013
http://proceedings.mlr.press/v28/pascanu13.pdf

Vanishing gradient problem

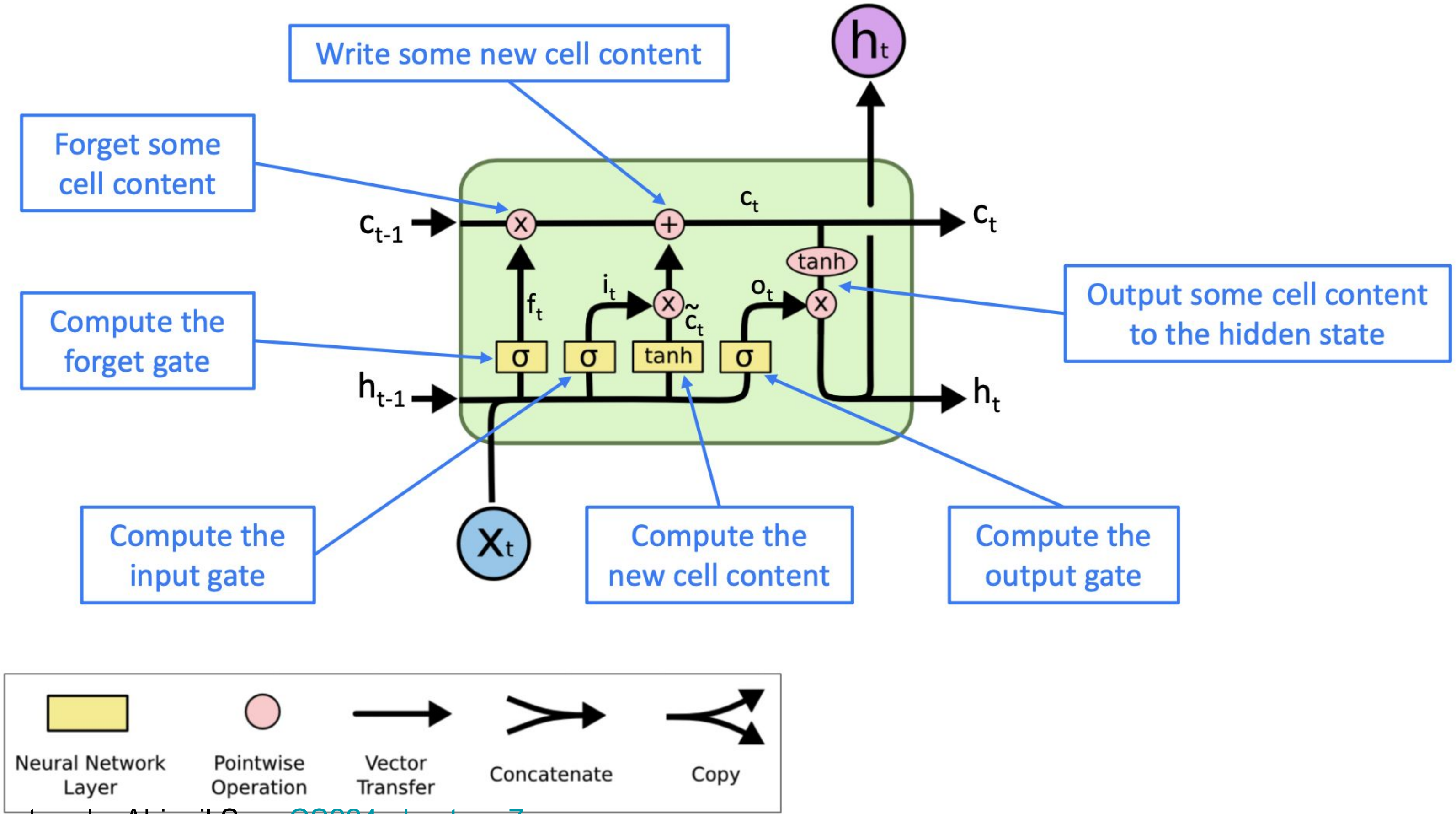
Gradient signal from far away is lost because it's much smaller than from close-by.

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



Based on: Lecture by Abigail See, CS224n Lecture 7

Vanishing gradient: LSTM



Based on: Lecture by Abigail See, [CS224n Lecture 7]

Vanishing gradient: LSTM

Sigmoid function: all gate values are between 0 and 1

Forget gate: controls what is kept vs forgotten, from previous cell state

Input gate: controls what parts of the new cell content are written to cell

Output gate: controls what parts of cell are output to hidden state

$$\boldsymbol{f}^{(t)} = \boxed{\sigma}\left(\boldsymbol{W}_f \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_f \boldsymbol{x}^{(t)} + \boldsymbol{b}_f\right)$$
$$\boldsymbol{i}^{(t)} = \boxed{\sigma}\left(\boldsymbol{W}_i \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_i \boldsymbol{x}^{(t)} + \boldsymbol{b}_i\right)$$
$$\boldsymbol{o}^{(t)} = \boxed{\sigma}\left(\boldsymbol{W}_o \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_o \boldsymbol{x}^{(t)} + \boldsymbol{b}_o\right)$$

New cell content: this is the new content to be written to the cell

Cell state: erase ("forget") some content from last cell state, and write ("input") some new cell content

Hidden state: read ("output") some content from the cell

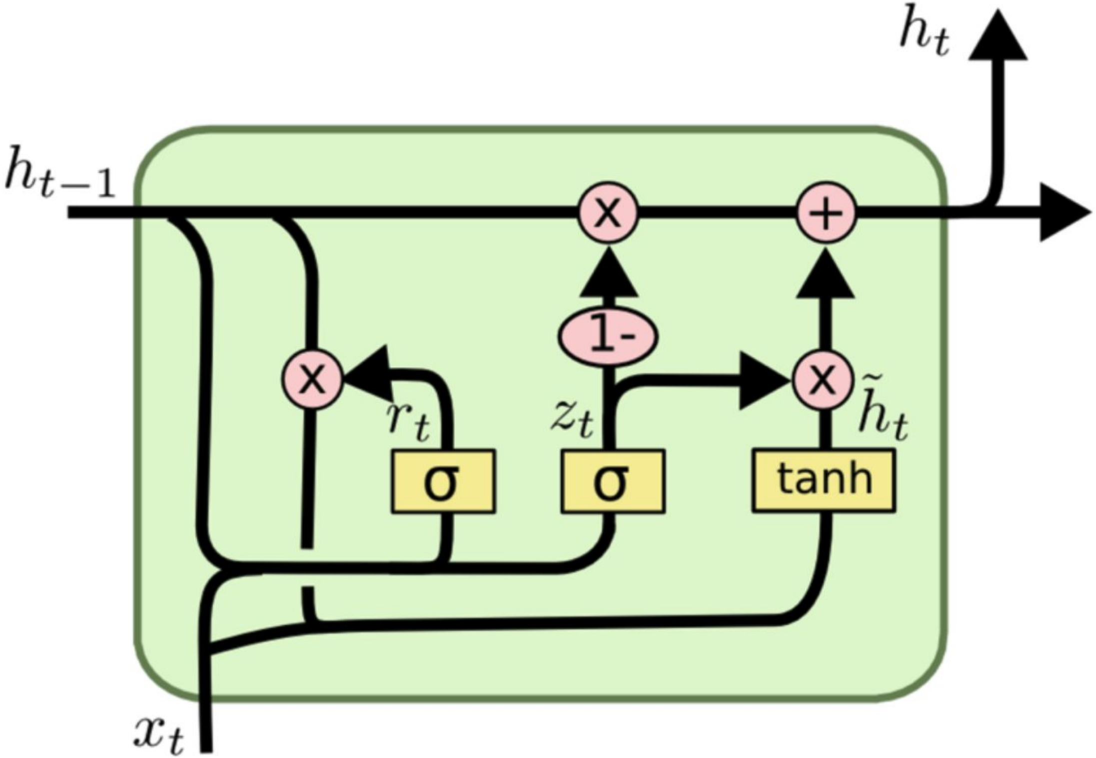
$$\tilde{\boldsymbol{c}}^{(t)} = \tanh\left(\boldsymbol{W}_c \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_c \boldsymbol{x}^{(t)} + \boldsymbol{b}_c\right)$$
$$\boldsymbol{c}^{(t)} = \boldsymbol{f}^{(t)} \circ \boldsymbol{c}^{(t-1)} + \boldsymbol{i}^{(t)} \circ \tilde{\boldsymbol{c}}^{(t)}$$
$$\boldsymbol{h}^{(t)} = \boldsymbol{o}^{(t)} \circ \tanh \boldsymbol{c}^{(t)}$$

All these are vectors of same length *n*

Gates are applied using element-wise product

Based on: Lecture by Abigail See, [CS224n Lecture 7]

Vanishing gradient: GRU



Vanishing gradient: GRU

Update gate: controls what parts of hidden state are updated vs preserved

Reset gate: controls what parts of previous hidden state are used to compute new content

$$\boldsymbol{u}^{(t)} = \sigma\left(\boldsymbol{W}_u \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_u \boldsymbol{x}^{(t)} + \boldsymbol{b}_u\right)$$

$$\boldsymbol{r}^{(t)} = \sigma\left(\boldsymbol{W}_r \boldsymbol{h}^{(t-1)} + \boldsymbol{U}_r \boldsymbol{x}^{(t)} + \boldsymbol{b}_r\right)$$

New hidden state content: reset gate selects useful parts of prev hidden state. Use this and current input to compute new hidden content.

Hidden state: update gate simultaneously controls what is kept from previous hidden state, and what is updated to new hidden state content

$$\tilde{\boldsymbol{h}}^{(t)} = \tanh\left(\boldsymbol{W}_h (\boldsymbol{r}^{(t)} \circ \boldsymbol{h}^{(t-1)}) + \boldsymbol{U}_h \boldsymbol{x}^{(t)} + \boldsymbol{b}_h\right)$$

$$\boldsymbol{h}^{(t)} = (1 - \boldsymbol{u}^{(t)}) \circ \boldsymbol{h}^{(t-1)} + \boldsymbol{u}^{(t)} \circ \tilde{\boldsymbol{h}}^{(t)}$$

How does this solve vanishing gradient?
Like LSTM, GRU makes it easier to retain info long-term (e.g. by setting update gate to 0)

Vanishing gradient: LSTM vs GRU

- LSTM and GRU are both great
    - GRU is quicker to compute and has fewer parameters than LSTM
    - There is no conclusive evidence that one consistently performs better than the other
    - LSTM is a good default choice (especially if your data has particularly long dependencies, or you have lots of training data)

Vanishing gradient in non-RNN

Vanishing gradient is present in **all** deep neural network architectures.

- Due to chain rule / choice of nonlinearity function, gradient can become vanishingly small during backpropagation
- Lower levels are hard to train and are trained slower
- **Potential solution**: direct (or skip-) connections (just like in ResNet)

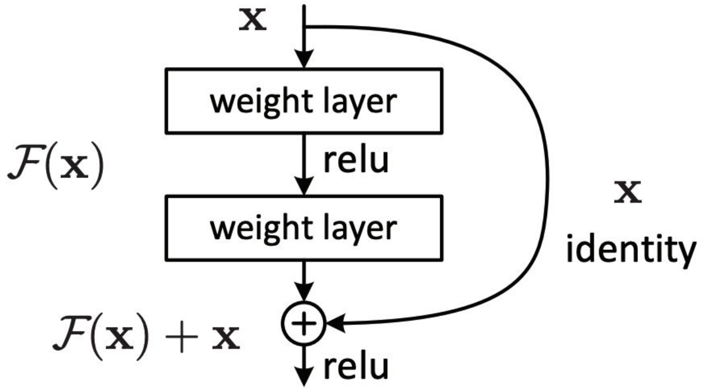


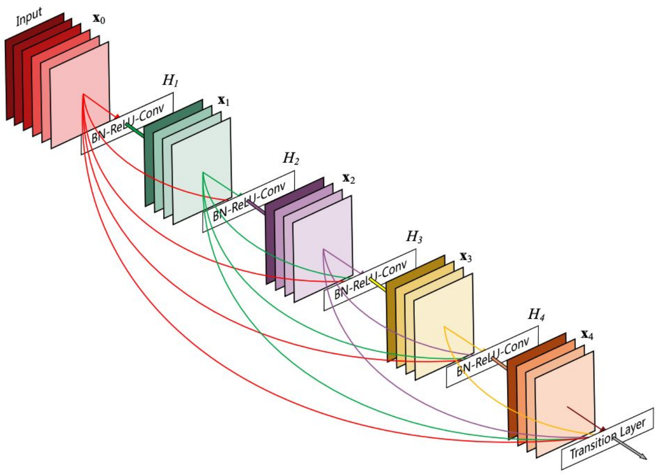
Figure 2. Residual learning: a building block.

Source: "Deep Residual Learning for Image Recognition", He et al, 2015. https://arxiv.org/pdf/1512.03385.pdf

Vanishing gradient in non-RNN

Vanishing gradient is present in **all** deep neural network architectures.

- Due to chain rule / choice of nonlinearity function, gradient can become vanishingly small during backpropagation
- Lower levels are hard to train and are trained slower
- **Potential solution**: dense connections (just like in DenseNet)

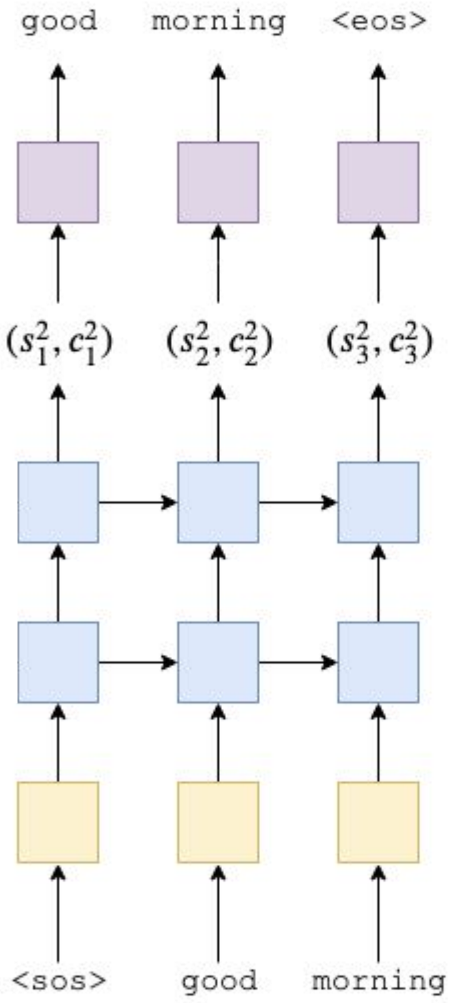


Source: ”Densely Connected Convolutional Networks", Huang et al, 2017 https://arxiv.org/pdf/1608.06993.pdf

Tips

- RNN is a great choice for data with sequential structure
- Multi-layer RNN can also be of great use

- **Rule of thumb**: start with LSTM, but switch to GRU if you want something more efficient



Q & A