Language Technologies Institute

Carnegie Mellon University

Multimodal Machine Learning

Lecture 2.2: Basic Concepts - Network Optimization

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* Original version co-developed with Tadas Baltrusaitis

Lecture Objectives

- Learning neural networks
  - Optimization
  - Gradient computation
- Practical Deep Model Optimization
  - Adaptive Optimization Methods
  - Regularization
  - Co-adaptation
  - Multimodal Optimization

Learning model parameters

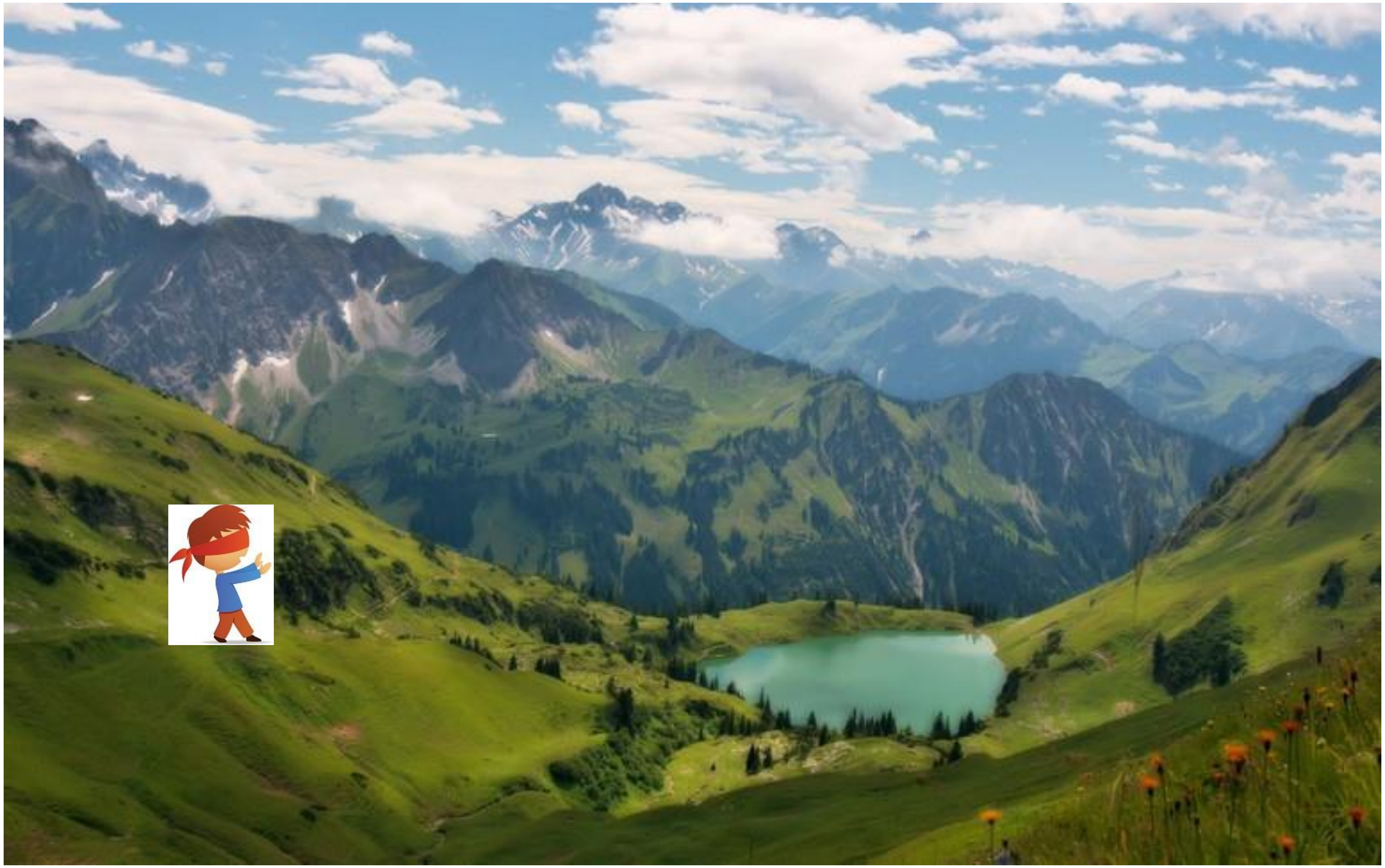
Learning model parameters

- We have our training data
  - $\mathrm{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_n\}$ (e.g. images, videos, text etc.)
  - $\mathrm{Y} = \{y_1, y_2, \dots, y_n\}$ (labels)
  - Fixed
- We want to learn the W (weights and biases) that leads to best loss

$$\underset{W}{\operatorname{argmin}}[L(\mathrm{X}, \mathrm{Y}, W)]$$

- The notation means find W for which $L(\mathrm{X}, \mathrm{Y}, W)$ has the lowest value

Optimization



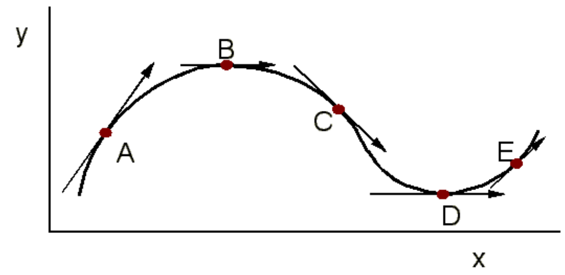
Optimizing a generic function

- We want to find a minimum of the loss function
- How do we do that?
  - Searching everywhere (global optimum) is computationally infeasible
  - We could search randomly from our starting point (mostly picked at random) and then refine the search region – impractical and not accurate
  - Instead we can follow the gradient

What is a gradient?

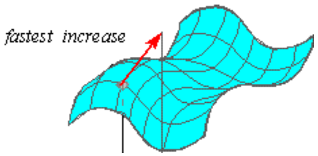
- Geometrically
  - Points in the direction of the greatest rate of increase of the function and its magnitude is the slope of the graph in that direction
- More formally in 1D

$$\frac{df(x)}{dx} = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$



- In higher dimensions

$$\frac{\partial f}{\partial x_i}(a_1, \ldots, a_n) = \lim_{h \to 0} \frac{f(a_1, \ldots, a_i + h, \ldots, a_n) - f(a_1, \ldots, a_i, \ldots, a_n)}{h}$$



➢ In multiple dimension, the **gradient** is the vector of (partial derivatives) and is called a **Jacobian**.

Numeric gradient

- Can set *h* to a very low number and compute:

$$\frac{df(x)}{dx} = \frac{f(x+h) - f(x)}{h}$$

- Slow and just an approximation
  - Need to compute score once (or even twice for central limit) for each parameter
  - Sensitive to choice of h
- h needs to be chosen as well - hyperparameter

Analytical gradient

- If we know the function and it is **differentiable**
  - Derivative/gradient is defined at every point in *f*
  - Sometimes use differentiable approximations
  - Some are locally differentiable
- Use Calculus (or Wikipedia)!
- Examples:

$$f(x) = \frac{1}{1+e^{-x}}; \frac{df}{dx} = (1 - f(x))f(x)$$

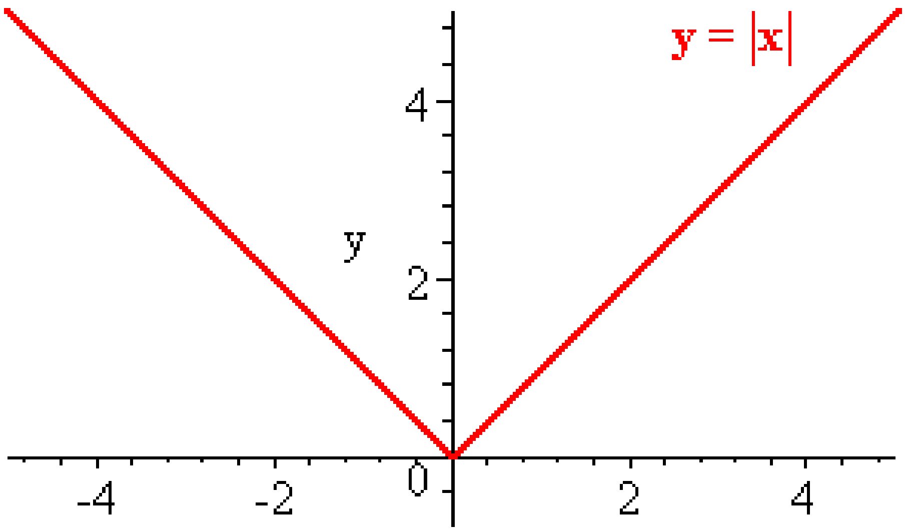
$$f(x) = (x-y)^2; \frac{df}{dx} = 2(x-y)$$

Analytical gradient

- If we know the function and it is **differentiable**
  - Derivative/gradient is defined at every point in *f*
  - Sometimes use differentiable approximations
  - Some are locally differentiable
- Use Cal
- Example

$f($ ... $x)$

$f($



Which one should we use?

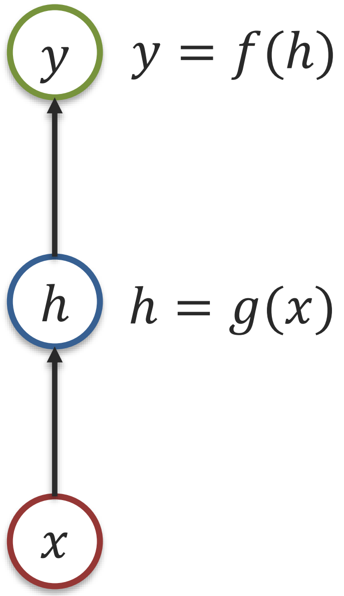
- Numeric
  - Slow
  - Approximate
- Analytical
  - More error prone to implement (need to get the gradient right)
  - Can use automated tools to help – Theano, autograd, Matlab symbolic toolbox
- Have both, use analytical for speed but check using numeric
- [Why you should understand gradient]

Neural Networks gradient

Gradient Computation

Chain rule:

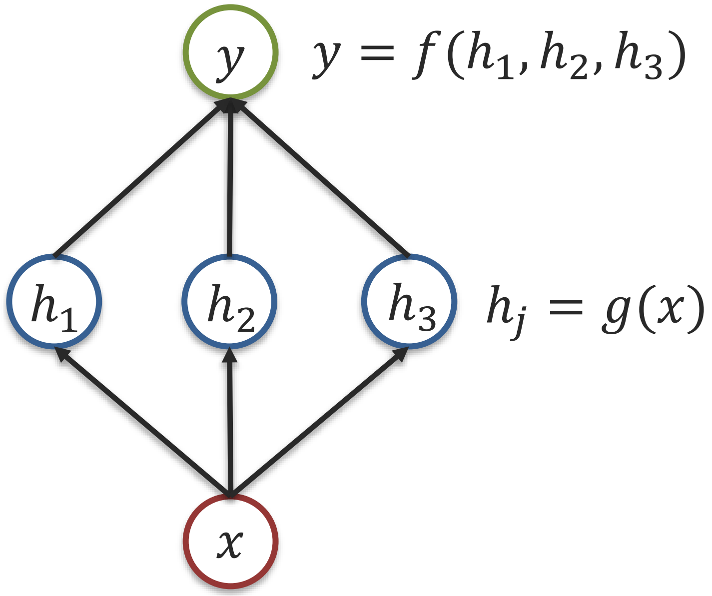
$$\frac{\partial y}{\partial x} = \frac{\partial y}{\partial h}\frac{\partial h}{\partial x}$$



Optimization: Gradient Computation

Multiple-path chain rule:

$$\frac{\partial y}{\partial x} = \sum_j \frac{\partial y}{\partial h_j}\frac{\partial h_j}{\partial x}$$



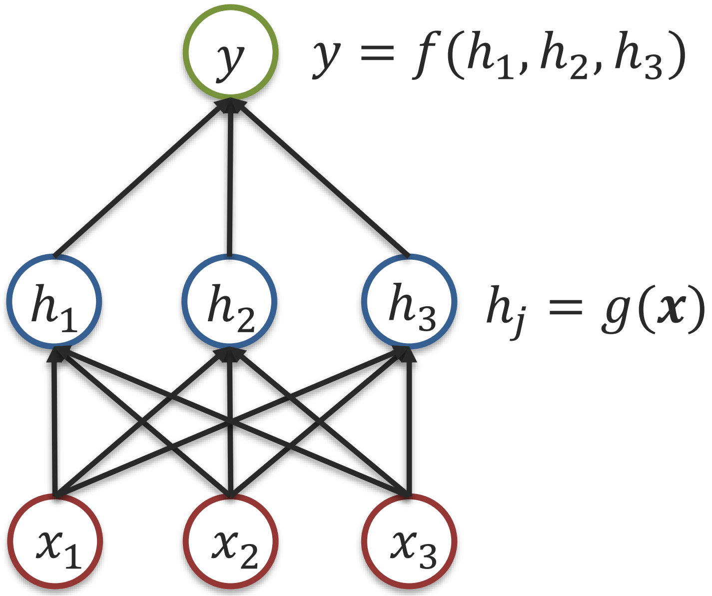
Optimization: Gradient Computation

Multiple-path chain rule:

$$\frac{\partial y}{\partial x_1} = \sum_j \frac{\partial y}{\partial h_j}\frac{\partial h_j}{\partial x_1}$$

$$\frac{\partial y}{\partial x_2} = \sum_j \frac{\partial y}{\partial h_j}\frac{\partial h_j}{\partial x_2}$$

$$\frac{\partial y}{\partial x_3} = \sum_j \frac{\partial y}{\partial h_j}\frac{\partial h_j}{\partial x_3}$$



Optimization: Gradient Computation

Vector representation:

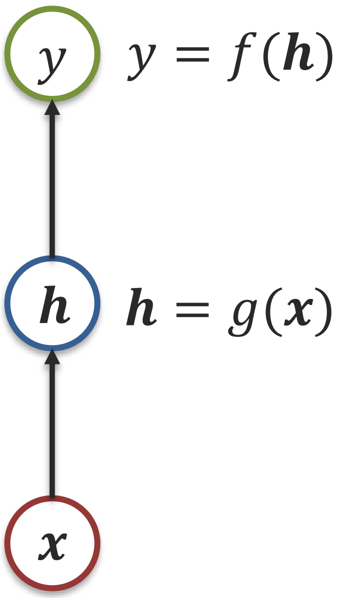
$$\nabla_{\boldsymbol{x}}\, y = \left[\frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2}, \frac{\partial y}{\partial x_3}\right]$$

Gradient

$$\nabla_{\boldsymbol{x}}\, y = \left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{x}}\right)^T \nabla_{\boldsymbol{h}}\, y$$

"local" Jacobian
(matrix of size $|h| \times |x|$ computed using partial derivatives)

"backprop" Gradient



Backpropagation Algorithm (efficient gradient)

Forward pass

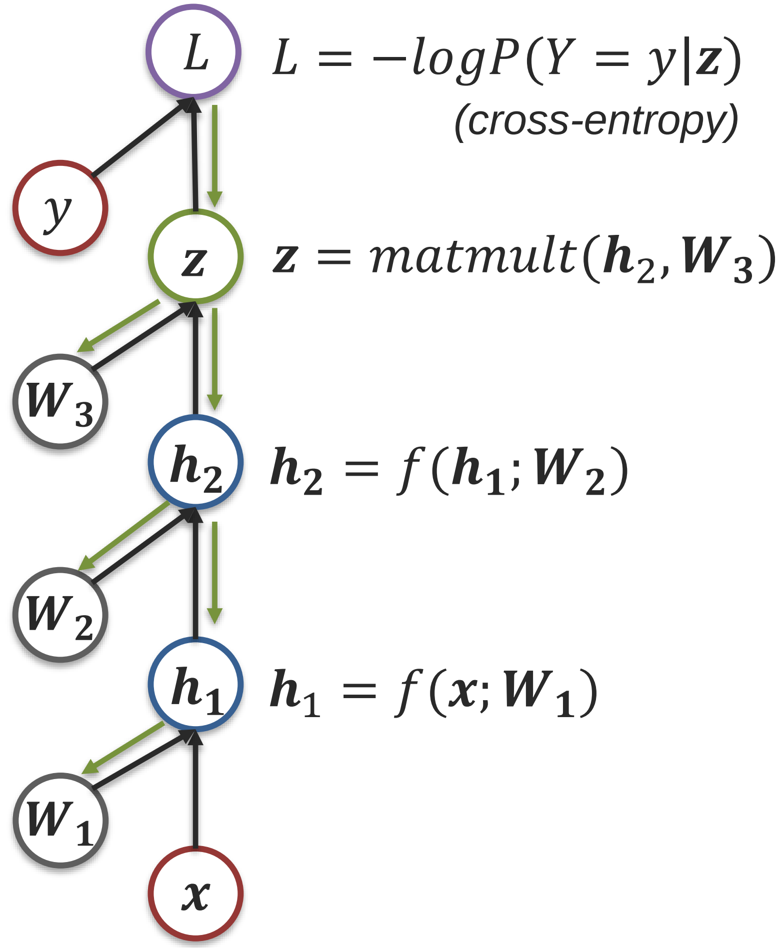
- Following the graph topology, compute value of each unit

Backpropagation pass

- Initialize output gradient = 1
- Compute "local" Jacobian matrix using values from forward pass
- Use the chain rule:

Gradient = "local" Jacobian x "backprop" gradient

- Why is this rule important?



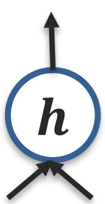
Computational Graph: Multi-layer Feedforward Network

Computational unit:

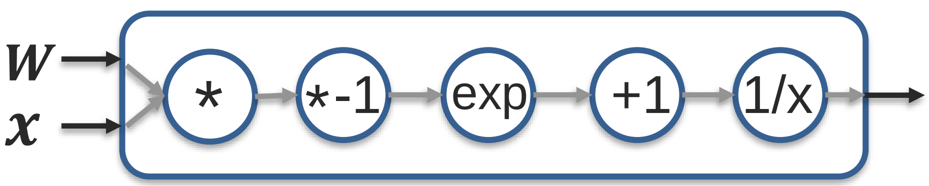
$\boldsymbol{h} = f(\boldsymbol{x}; \boldsymbol{W})$

- Multiple input
- One output
- Vector/tensor

- Sigmoid unit:

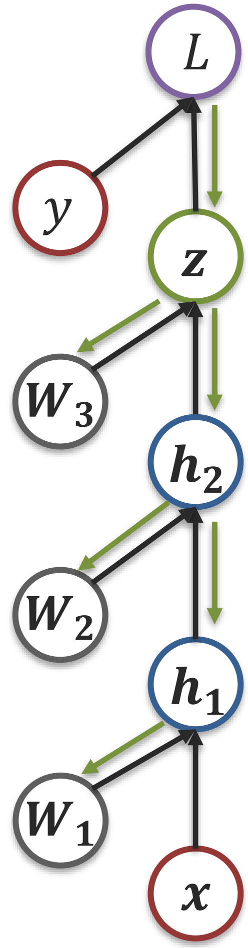


$$h_j = (1 + e^{-W_j \boldsymbol{x}})^{-1}$$



Differentiable "unit" function!

(or close approximation to compute "local Jacobian)



$L = -logP(Y = y|\boldsymbol{z})$

(cross-entropy)

$\boldsymbol{z} = matmult(\boldsymbol{h}_2, \boldsymbol{W}_3)$

$\boldsymbol{h}_2 = f(\boldsymbol{h}_1; \boldsymbol{W}_2)$

$\boldsymbol{h}_1 = f(\boldsymbol{x}; \boldsymbol{W}_1)$

Gradient descent

How to follow the gradient

- Many methods for optimization
  - **Gradient Descent (actually the "simplest" one)**
  - Newton methods (use Hessian – second derivative)
  - Quasi-Newton (use approximate Hessian)
    - BFGS
    - LBFGS
    - Don't require learning rates (fewer hyperparameters)
    - But, do not work with stochastic and batch methods so rarely used to train modern Neural Networks
- **All of them look at the gradient**
  - Very few non gradient based optimization methods

Parameter Update Strategies

Gradient descent:

$$\theta^{(t+1)} = \theta^t - \epsilon_k \nabla_\theta L$$

Gradient of our loss function

New model parameters

Previous parameters

Learning rate at iteration *k*

$$\epsilon_k = (1-\alpha)\epsilon_0 + \alpha\epsilon_\tau$$

Decay learning rate linearly until iteration τ

Learning rate at iteration *k*

Decay

Initial learning rate

Extensions:

- Stochastic (“batch”)
- with momentum
- AdaGrad
- RMSProp

Vanilla Gradient Descent

- Compute gradient with respect to loss and keep updating weights till convergence

```
while not converged:
        # compute gradients
        weights_grad = compute_gradient(loss_fun, data, weights)
        # perform parameter update
        weights += - step_size * weights_grad
       # (optionally update step size)
```

Batch (stochastic) gradient descent

- Using all of data points might be tricky when computing a gradient
  - Uses lots of memory and slow to compute
- Instead use batch gradient descent
  - Take a subset of data when computing the gradient

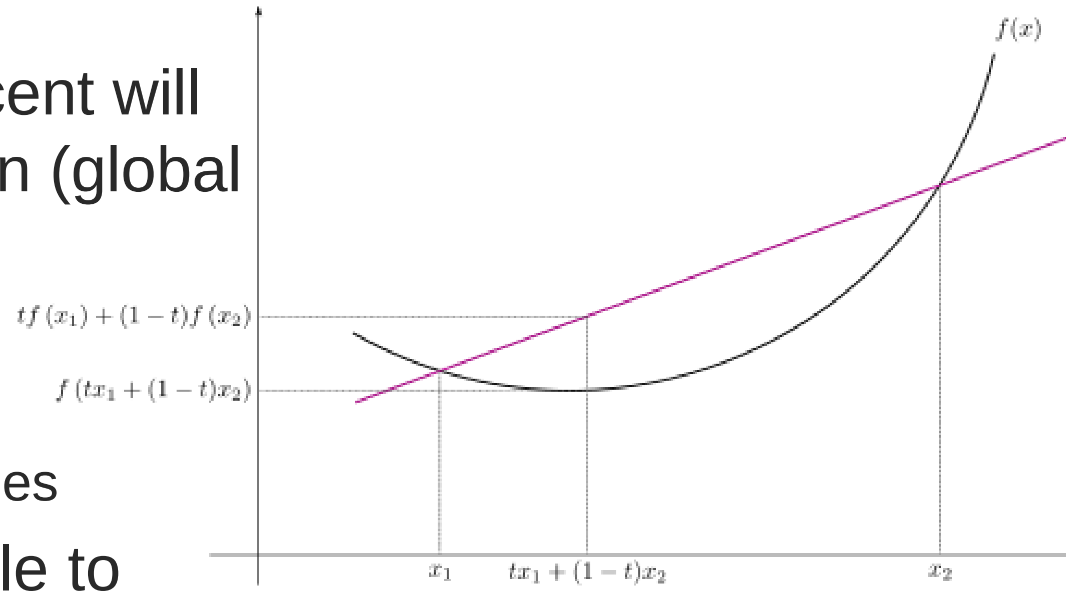
```
while not converged:
        # Shuffle data
        data = randomize(data)
        # Split data into batches and update each batch individual
        for data_batch in data:
                weights_grad = backpropagation(loss_fun, data_batch , weights)
                # perform parameter update
                weights += - step_size * weights_grad
```

Iteration

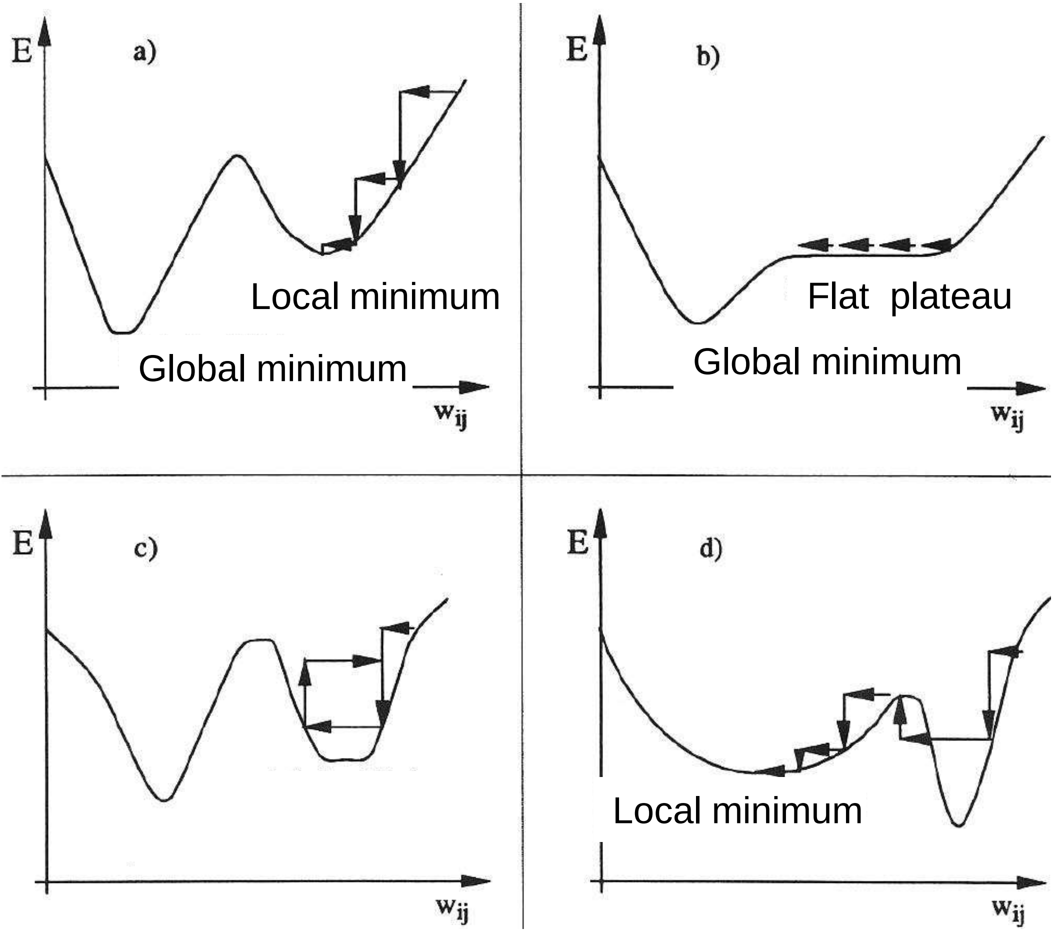
Epoch

Convex vs. non-convex functions and local minima

- Convex – gradient descent will lead to a perfect solution (global optimum)
  - Logistic regression
  - Least squares models
  - Support vector machines
- Non-convex – impossible to guarantee that the solution is the best – will lead to local-minima
  - Neural networks
  - Various graphical models



Potential issues

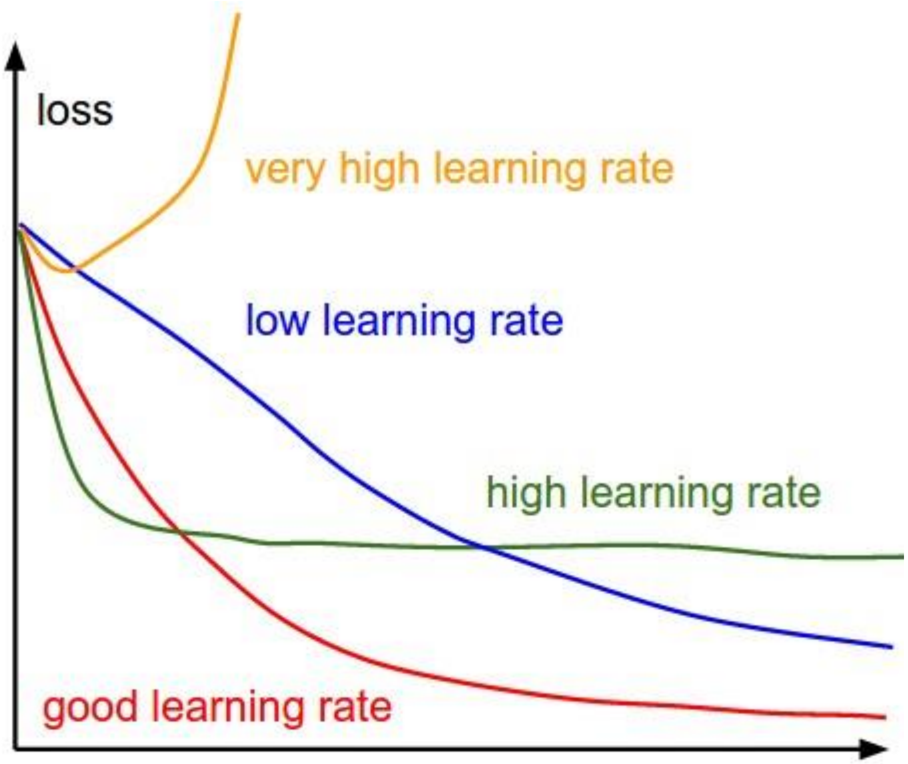


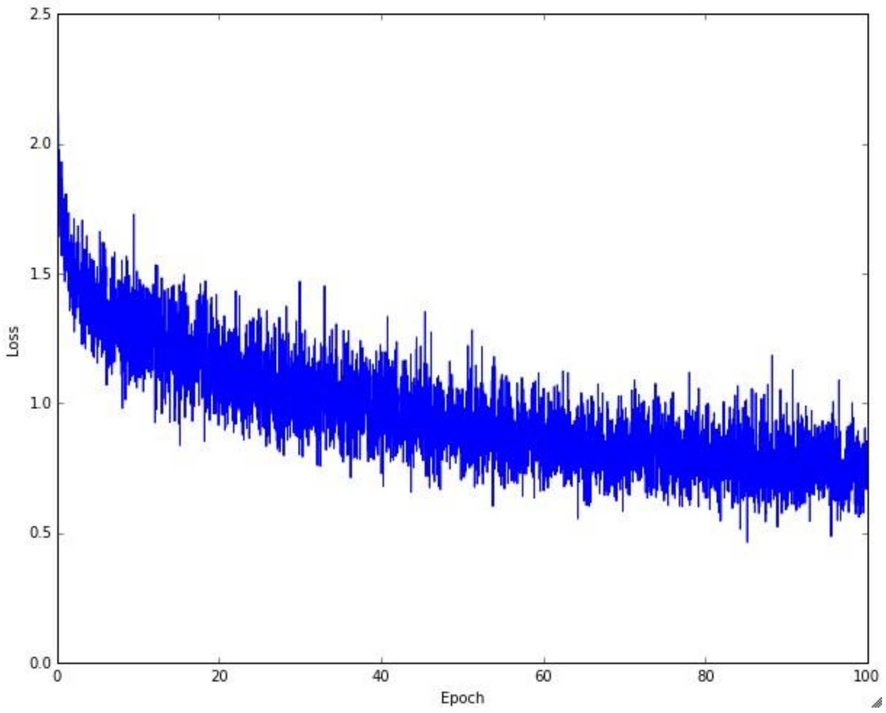
- Problems that can occur?
  - Getting stuck in local minima (global minimum is never found) (a)
  - Getting stuck on flat plateaus of the error-plane (b)
  - Oscillations in error rates (c)
  - Learning rate is critical (d)

Some observations:

- Small steps are likely to lead to consistent but slow progress.
- Large steps can lead to better progress but are more risky.
- Note that eventually, for a large step size we will overshoot and make the loss worse.

Interpreting learning rates





Optimization – Practical Guidelines

Optimization – Practical Guidelines

- Adaptive Optimization Methods
- Regularization
- Co-adaptation
- Multimodal Optimization

Adaptive Learning Rate

General Idea: Let neurons who just started learning have huge learning rate.

Adaptive Learning Rate is an active area of research:

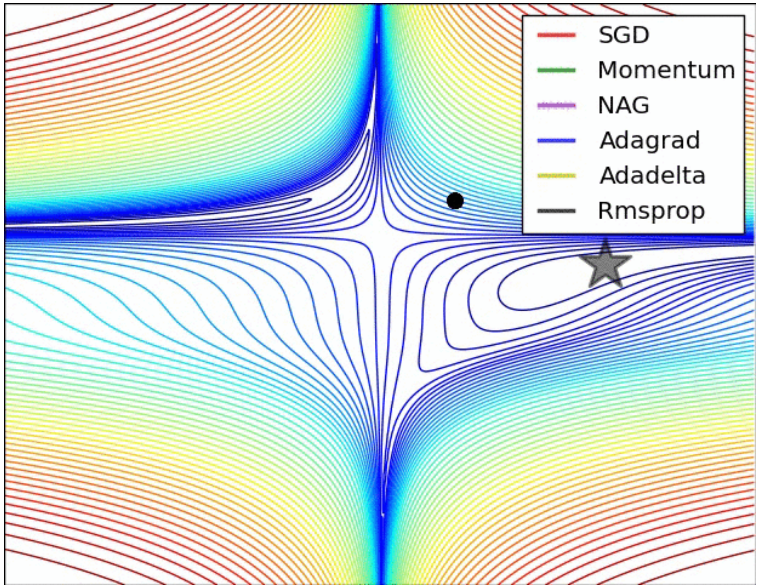
- Adadelta
- RMSProp

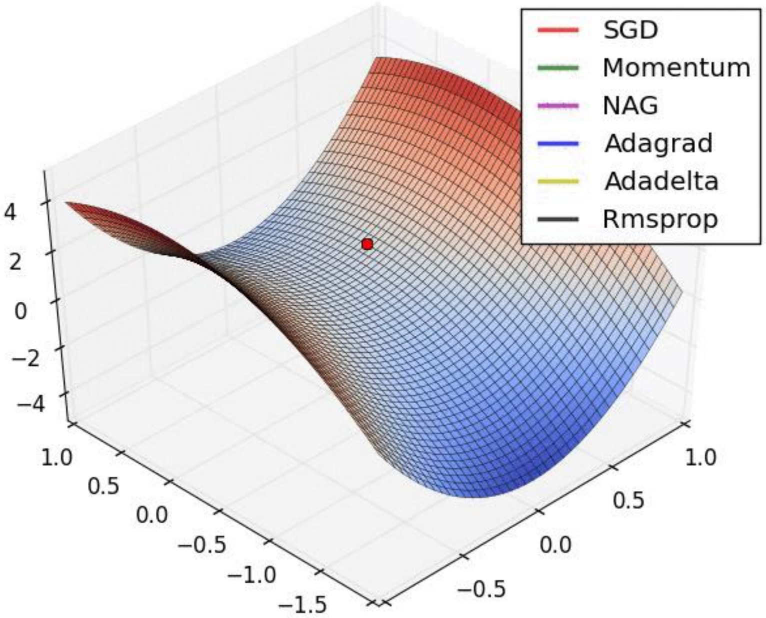
```
cache = decay_rate * cache + (1 - decay_rate) * dx**2
x += - learning_rate * dx / (np.sqrt(cache) + eps)
```

- Adam

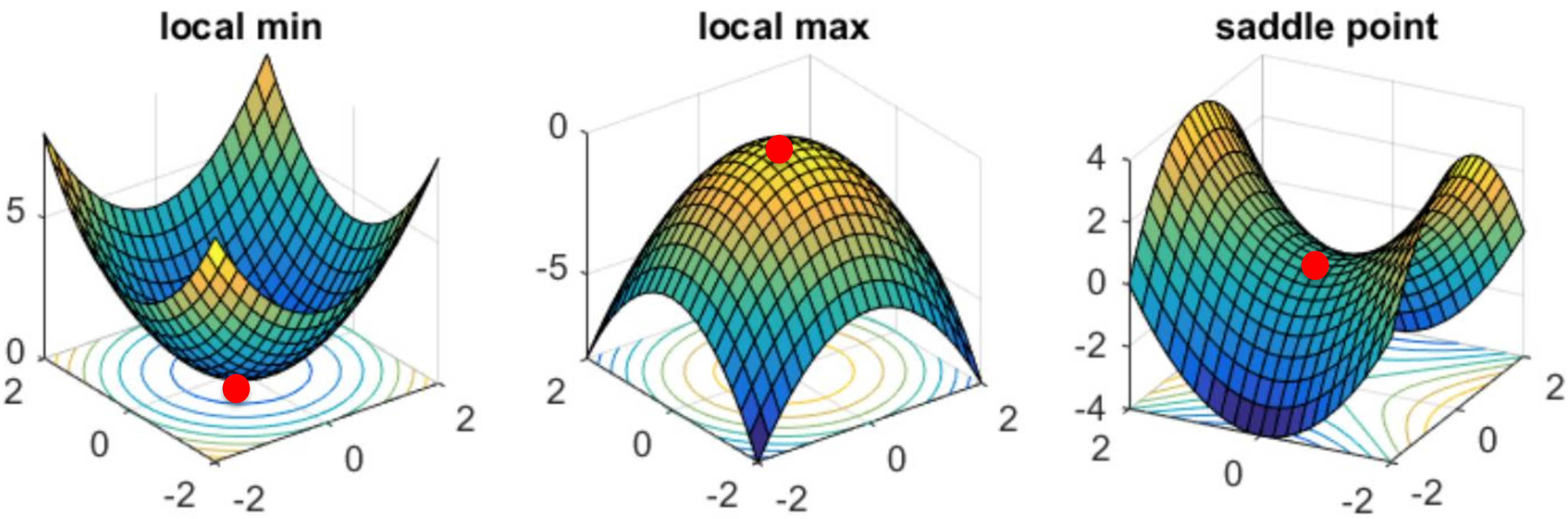
```
m = beta1*m + (1-beta1)*dx
v = beta2*v + (1-beta2)*(dx**2)
x += - learning_rate * m / (np.sqrt(v) + eps)
```

Comparison


SGD
Momentum
NAG
Adagrad
Adadelta
Rmsprop


SGD
Momentum
NAG
Adagrad
Adadelta
Rmsprop
4
2
0
−2
−4
1.0
0.5
0.0
−0.5
−1.0
−1.5
1.0
0.5
0.0
−0.5

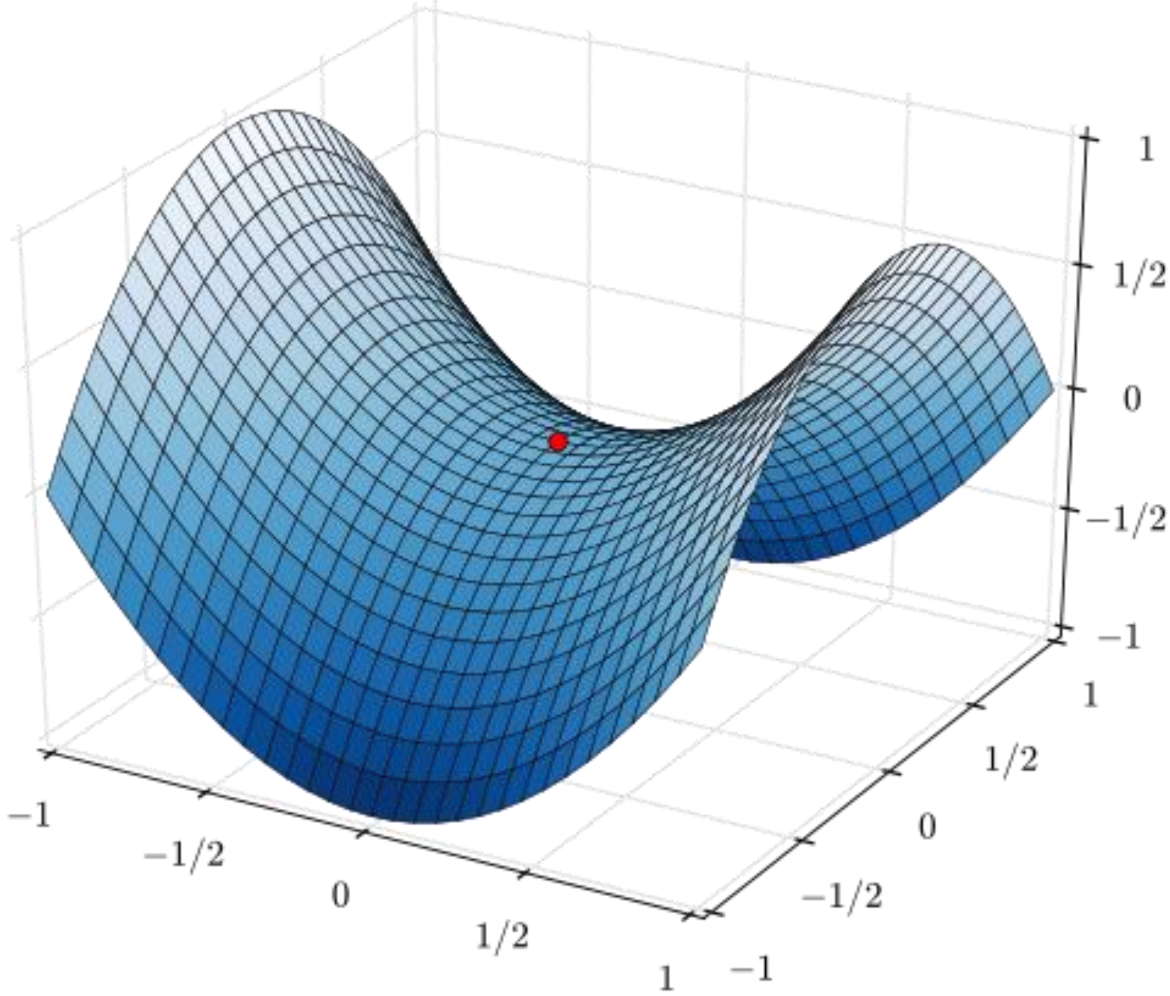
Critical Points



Saddle Points

- Deep Learning Optimization:
  - Deep Learning problems in general have many local minimas
  - Many (not all) of them are actually almost as good as global minima due to parameter permutation
  - However it is NP-hard to even find a local minima
- Lots and lots of saddles in many deep learning problems.

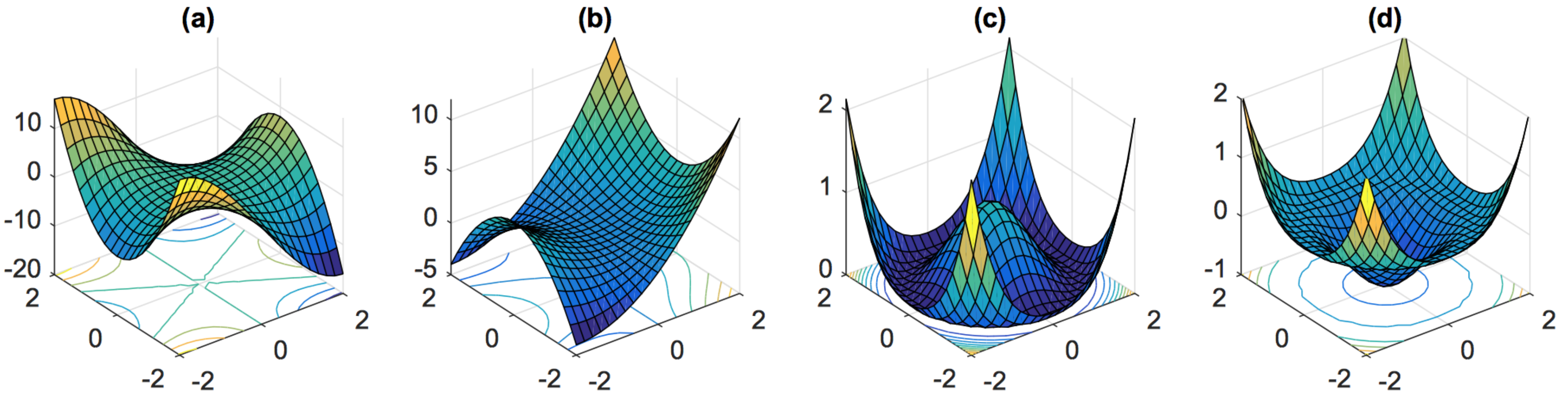
Why Saddles are Bad



Detecting Saddles

- One way to detect saddles:
  - Calculate Hessian at point x
  - If Hessian is indefinite you have a saddle for sure.
  - If Hessian is not indefinite you really can't tell.
- My loss isn't changing:
  - You are definitely close to a critical point
    - You may be in a saddle point
    - You may be in the local minima/maxima
  - One trick: quickly check the sorrounding
    - Best practical trick if Hessian is not indefinite.

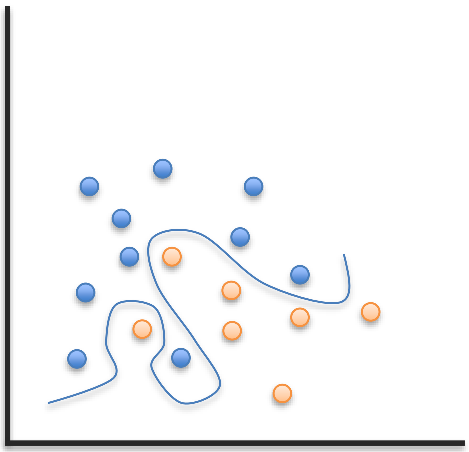
Bad Saddle Points



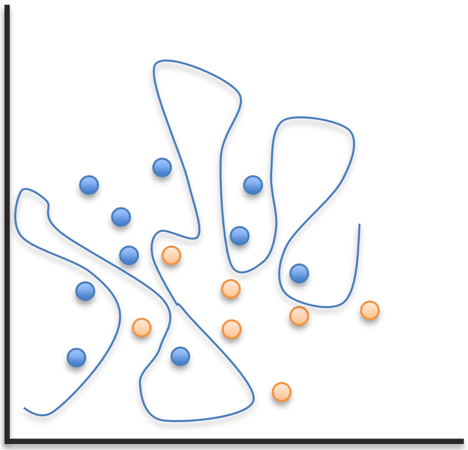
https://arxiv.org/pdf/1602.05908.pdf

Example

Real

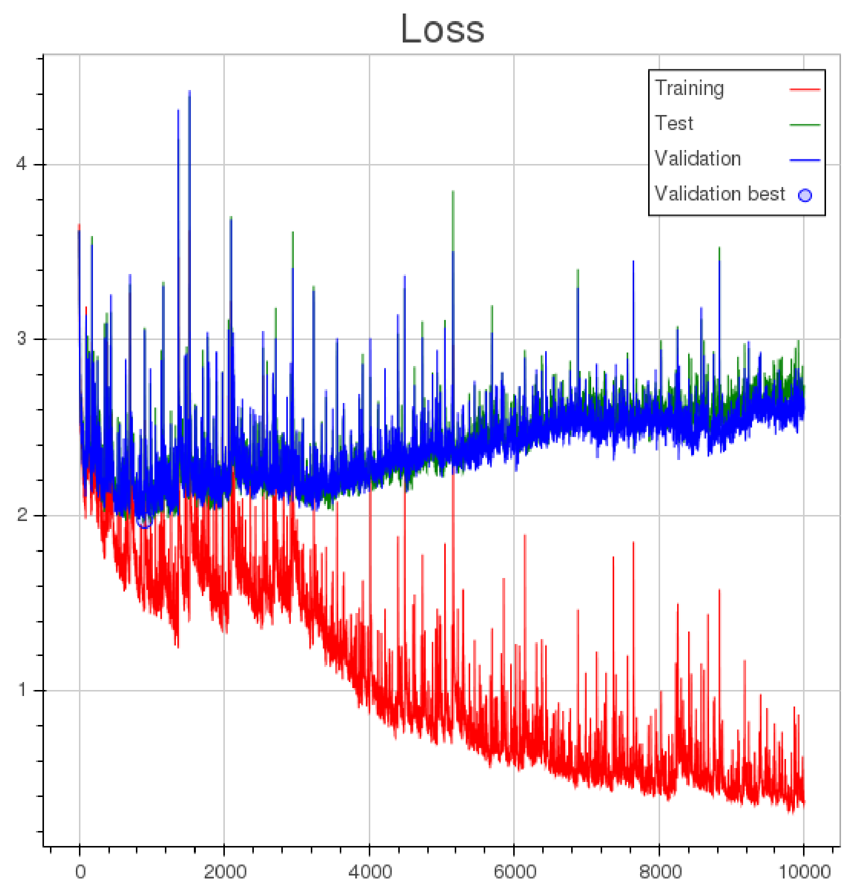


Our Model



Not the fault of learning rate or momentum

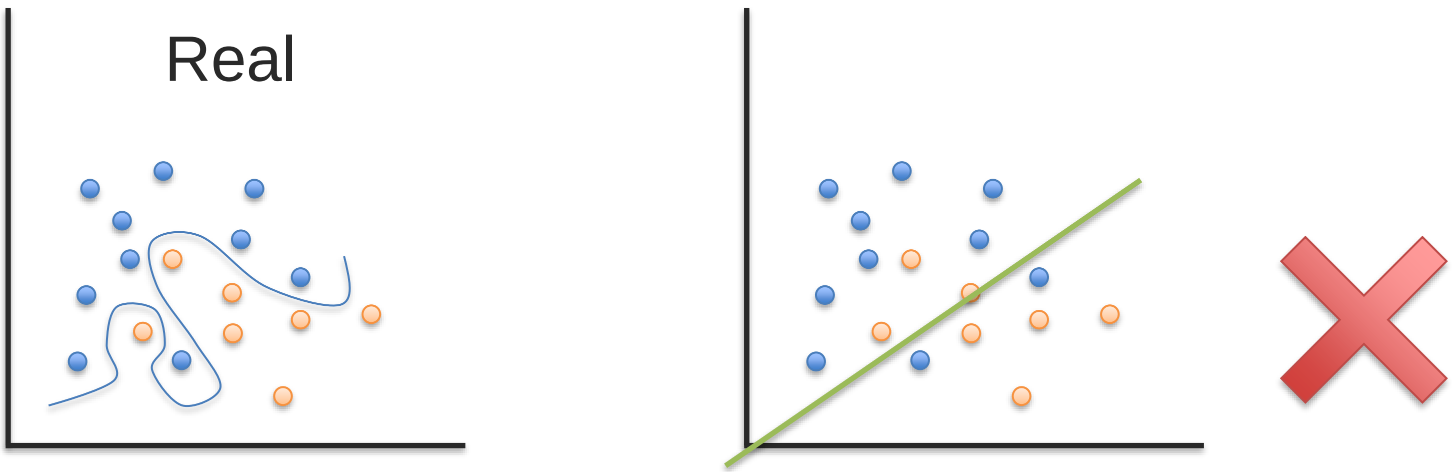
Example


Loss
Training
Test
Validation
Validation best
4
3
2
1
0
2000
4000
6000
8000
10000

Bias-Variance

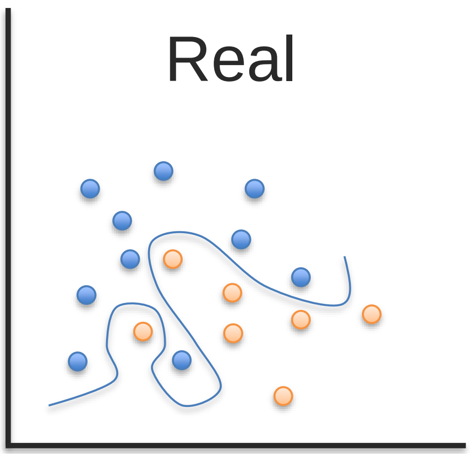
- Problem of bias and variance
  - Simple models are unlikely to find the solution to a hard problem, thus probability of finding the right model is low.

No longer SOT!

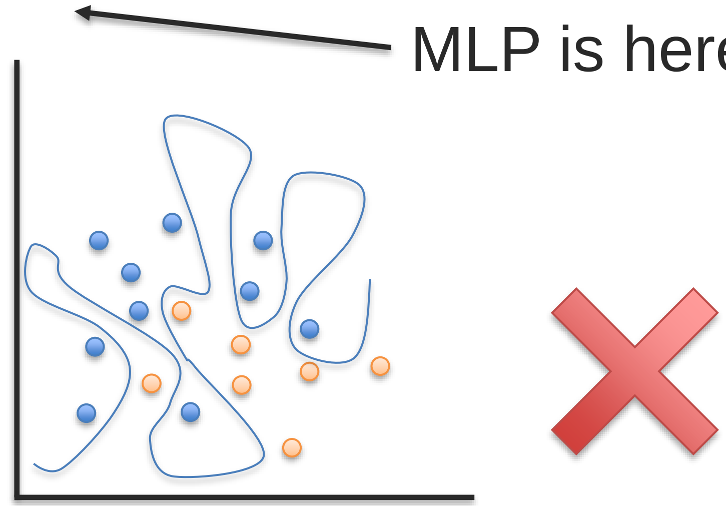


Bias-Variance

- Problem of bias and variance
  - Simple models are unlikely to find the solution to a hard problem, thus probability of finding the right model is low.
  - Complex models find many solutions to a problem, thus probability of finding the right model is again low.



MLP is here!



Optimization – Practical Guidelines

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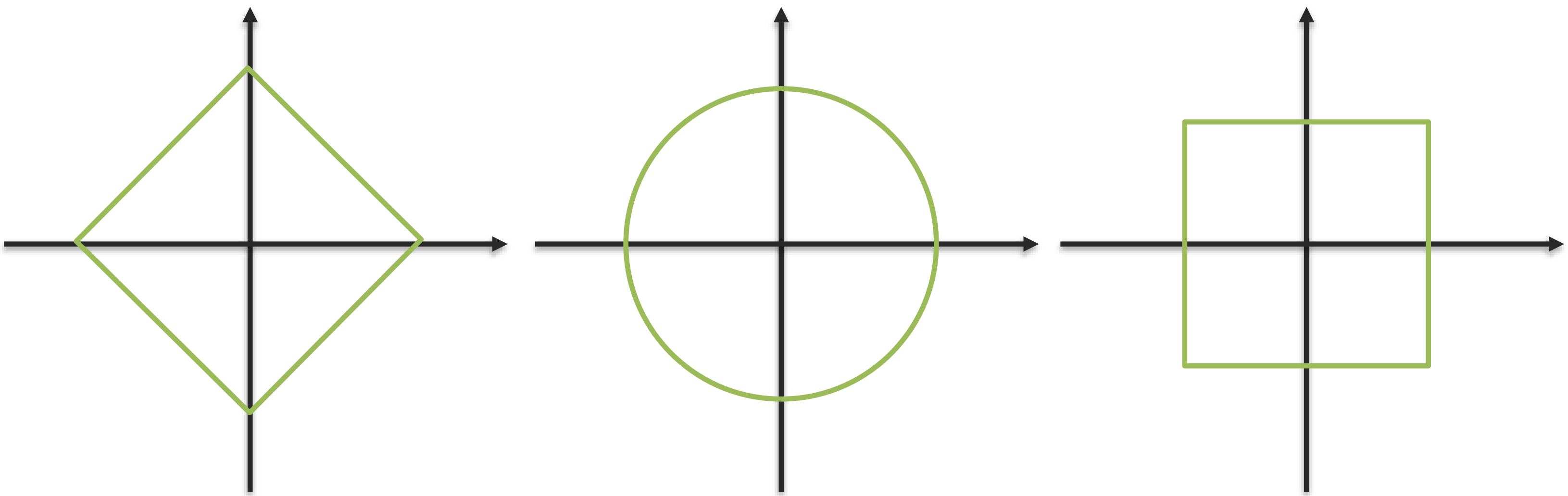
Regularization

- Parameter Regularization:
  - Adding prior to the network parameters
  - L^p Norms



L^1 L^2 L^∞

Minimize: $Loss(x;\theta) + \propto ||\theta||$

Parameter Regularization

- Parameter Regularization:
  - L^1(Lasso) and L^2 (Ridge) are the most famous norms used. Sometimes combined (Elastic)
  - Other norms are computationally ineffective.
- Maximum a posteriori (MAP) estimation:
  - Having priors one the model parameters
  - L^2 can be seen as a Gaussian prior on model parameters θ
  - A generalization of L^2 is called Tikhonov Regularization with Multivariate Gaussian prior on model parameters.
    - Assuming Correlation between parameters one can build a Mahalanobis variation of Tikhonov Regularization.

Structural Regularization

- Lots of models can learn everything.
- Go for simpler ones.
- Use task specific models:
  - CNNs
  - RecNNs
  - LSTMs
  - GRUs

Occam's razor

Optimization – Practical Guidelines

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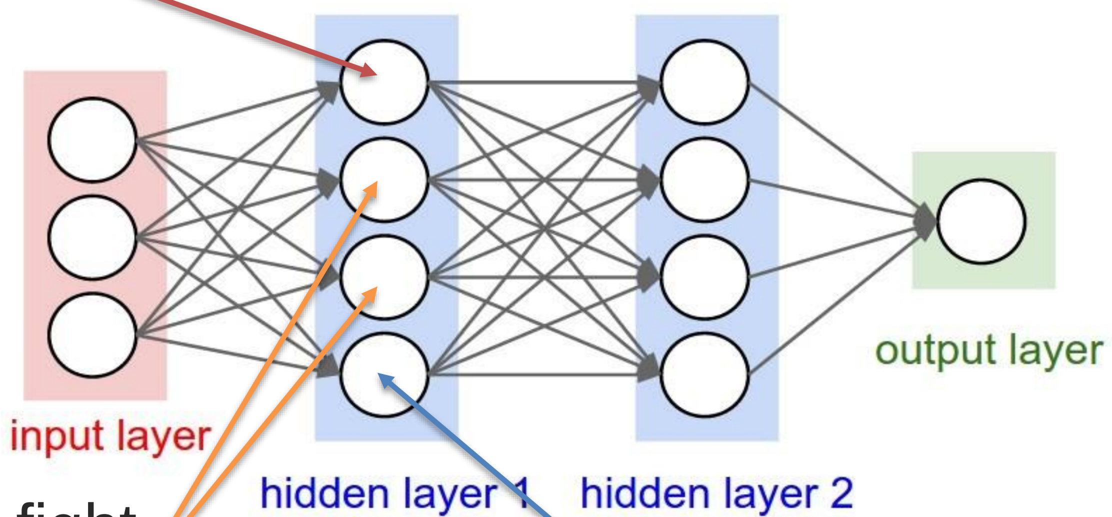
Example

- A neuron learns something that is not useful:
  1. Learn something useful
  2. Other neurons learn to mitigate it.

Useless neuron

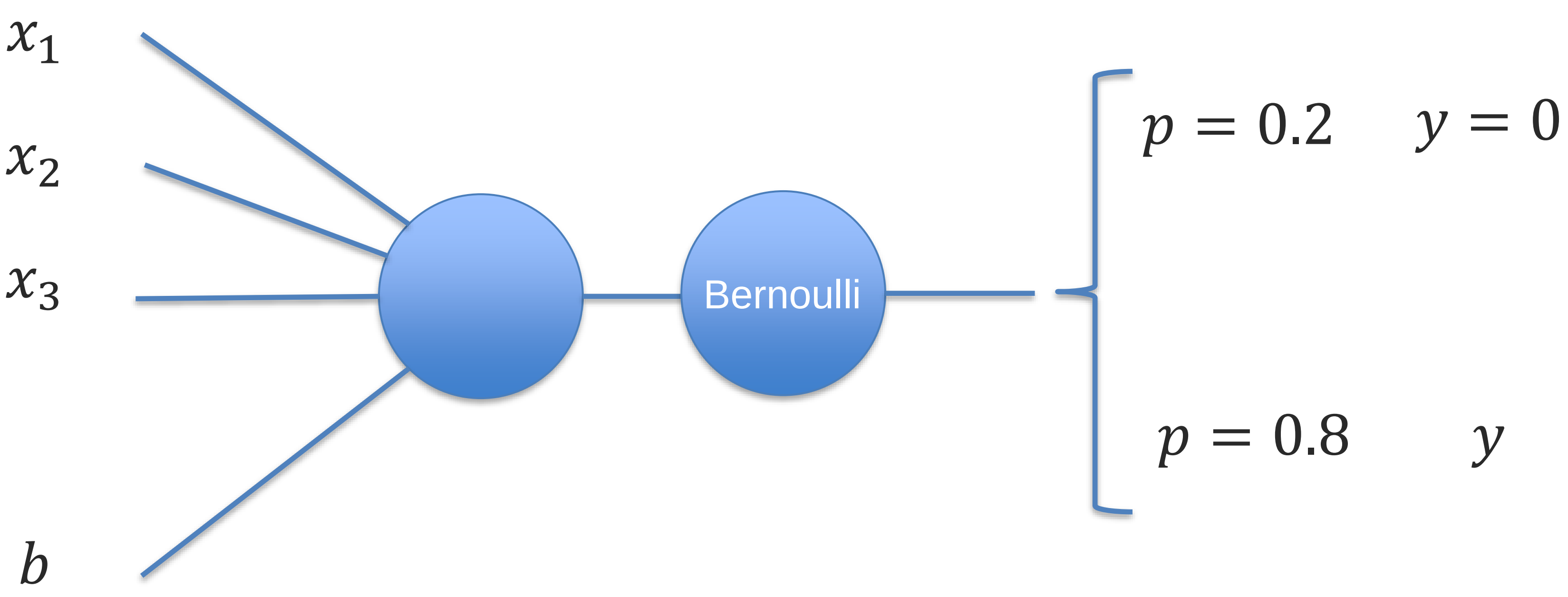


Learning to fight useless neuron

Actually learning something

Dropout

- Simply multiply the output of a hidden layer with a mask of 0s and 1s (Bernoulli)



Dropout

Forward step: multiply with a Bernoulli distribution per epoch, batch or sample point. Question: which one works better?

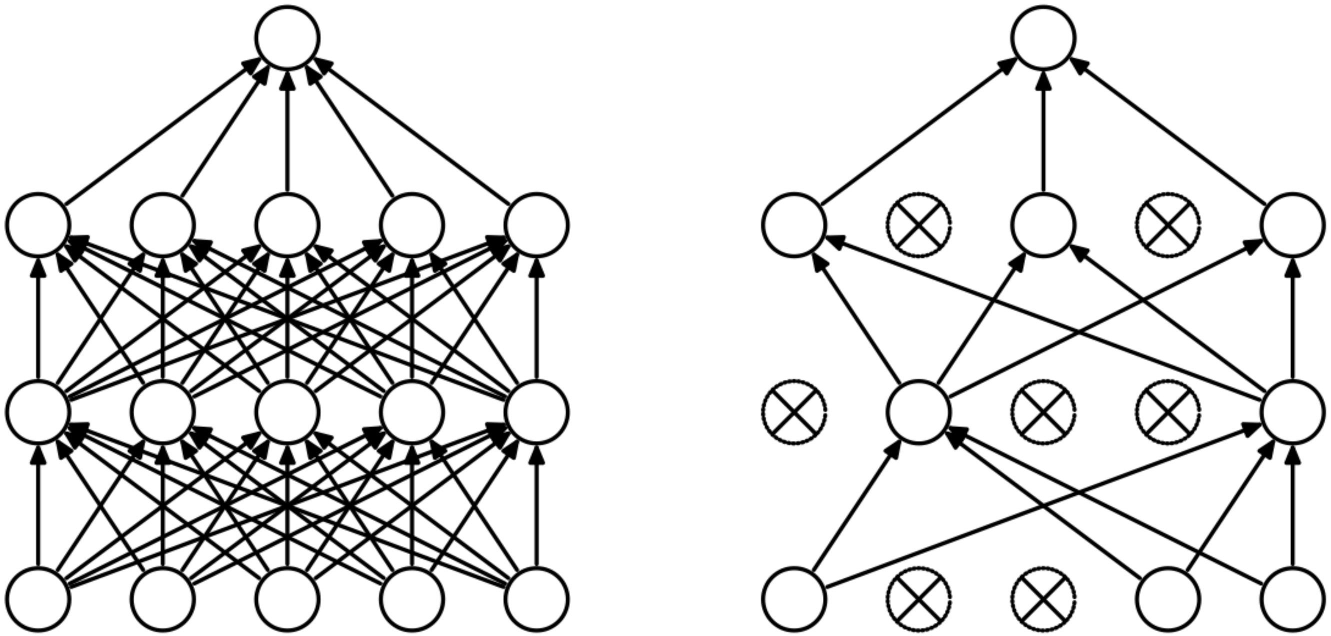
Backward step: just calculate the gradients same as before. Question: some neurons are out of the network, so how does this work?

All good? Nope

Multiply the weights by $1 - p_i$

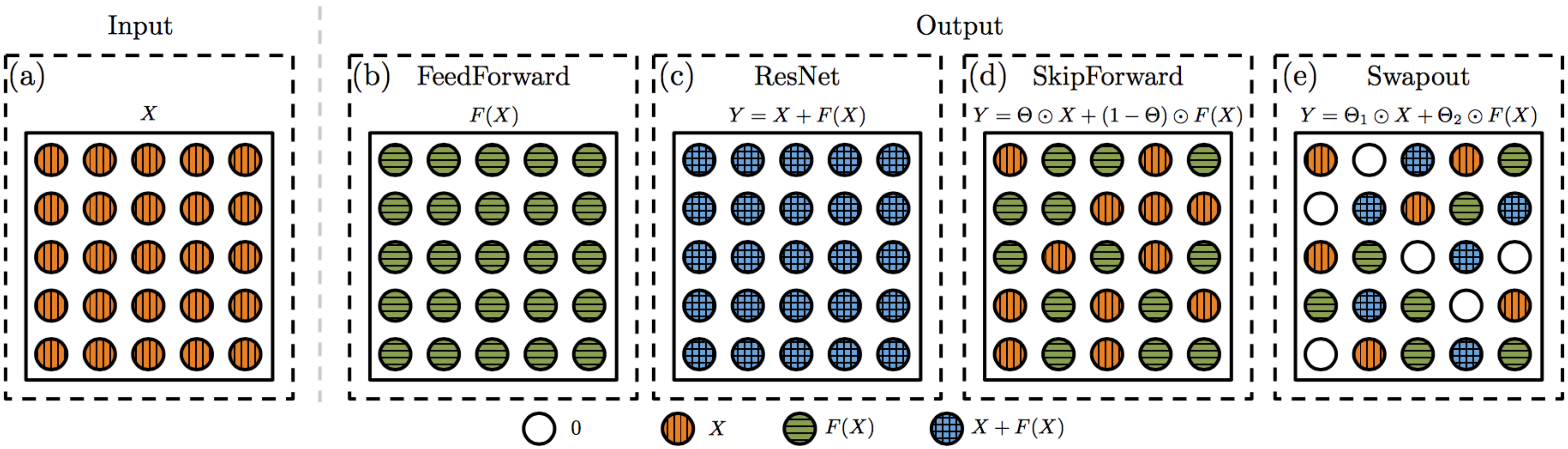
Dropout

Stop co-adaptation + learn ensemble



Other variations

- Gaussian dropout: instead of multiplying with a Bernoulli random variable, multiply with a Gaussian with mean 1.
- Swapout: Allow skip-connections to happen



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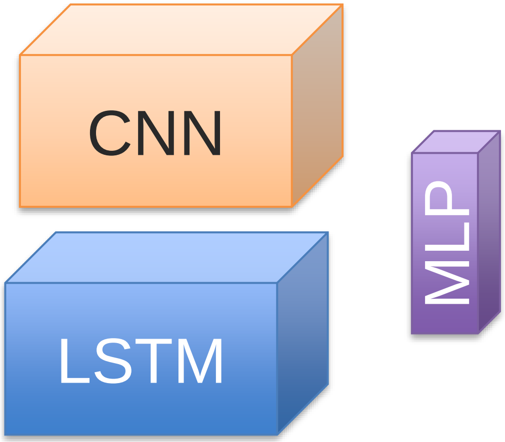
Multimodal Optimization

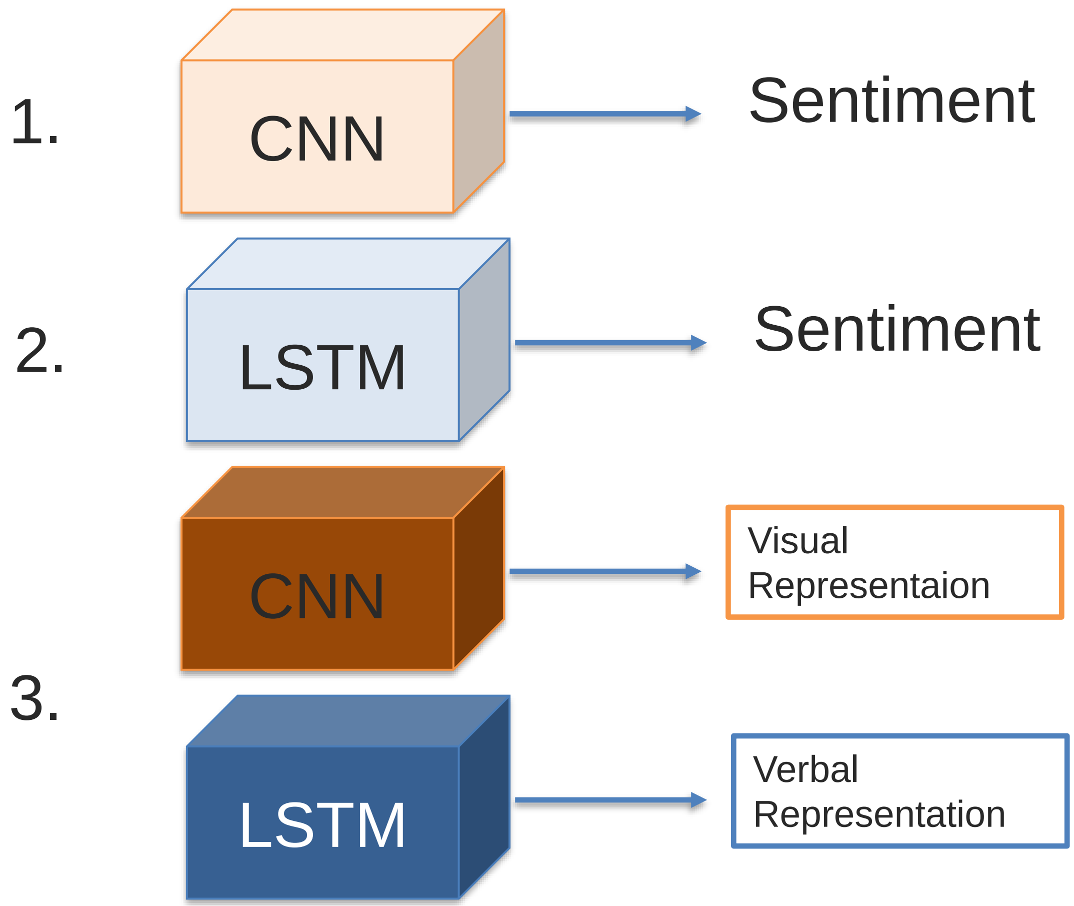


- Biggest Challenge:
  - Data from different sources
  - Different networks
- Example:
  - Question Answering: LSTM(s) connected to a CNN
  - Multimodal Sentiment: LSTM(s) fused with MLPs and 3D-CNNs
- CNNs work well with high decaying learning rate
- LSTMs work well with adaptive methods and normal SGD
- MLPs are very good with adaptive methods

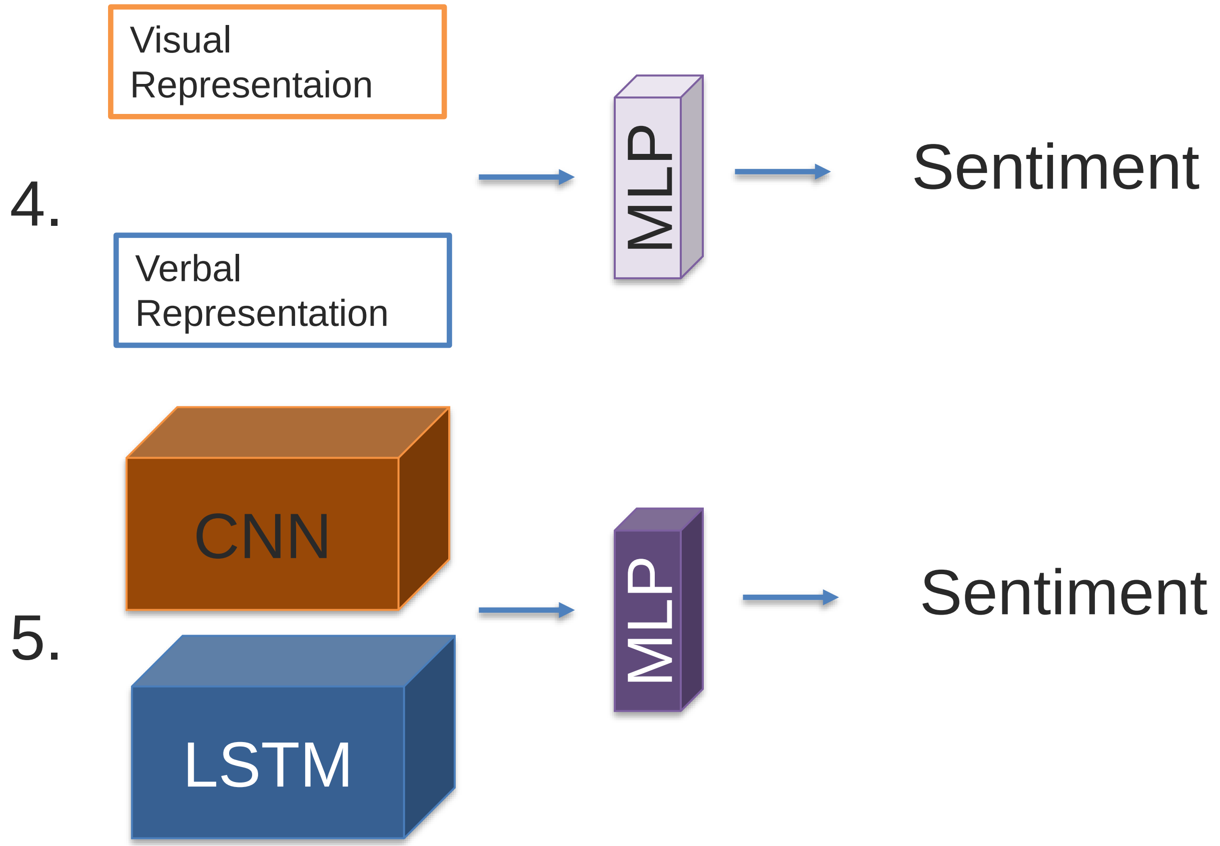
Multimodal Optimization

- How to work with all of them?
- Pre-training is the most straight forward way:
  - Train each individual component of the model separately
  - Put together and fine tune
- Example: Multimodal Sentiment Analysis

Pre-training



Pre-training



Pre-training Tricks

- In the final stage (5), it is better to not use adaptive methods such as Adam.
  - Adam starts with huge momentum on all the networks parameters and can destroy the effects of pretraining.
  - Simple SGD mostly helpful.
- Initialization from other pre-trained models:
  - VGG for CNNs
  - Language models for RNNs
  - Layer by layer training for MLPs