Lecture 15: Optimization

CS 109B, STAT 121B, AC 209B, CSE 109B

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Learning vs. Optimization

- Goal of learning: minimize generalization error

$$J(\theta) = \mathbf{E}_{(x,y)\sim p_{data}}\left[L(f(x;\theta),y)\right]$$

- In practice, empirical risk minimization:

$$\hat{J}(\theta) = \frac{1}{m}\sum_{i=1}^{m} L(f(x^{(i)};\theta),y^{(i)})$$

Quantity optimized different from the quantity we care about

Batch vs. Stochastic Algorithms

Shuffle the data before mini-batch

- Batch algorithms
  - Optimize empirical risk using exact gradients
- Stochastic algorithms
  - Estimates gradient from a small random sample

$$\nabla J(\theta) = \mathbf{E}_{(x,y)\sim p_{data}}\left[\nabla L(f(x;\theta), y)\right]$$

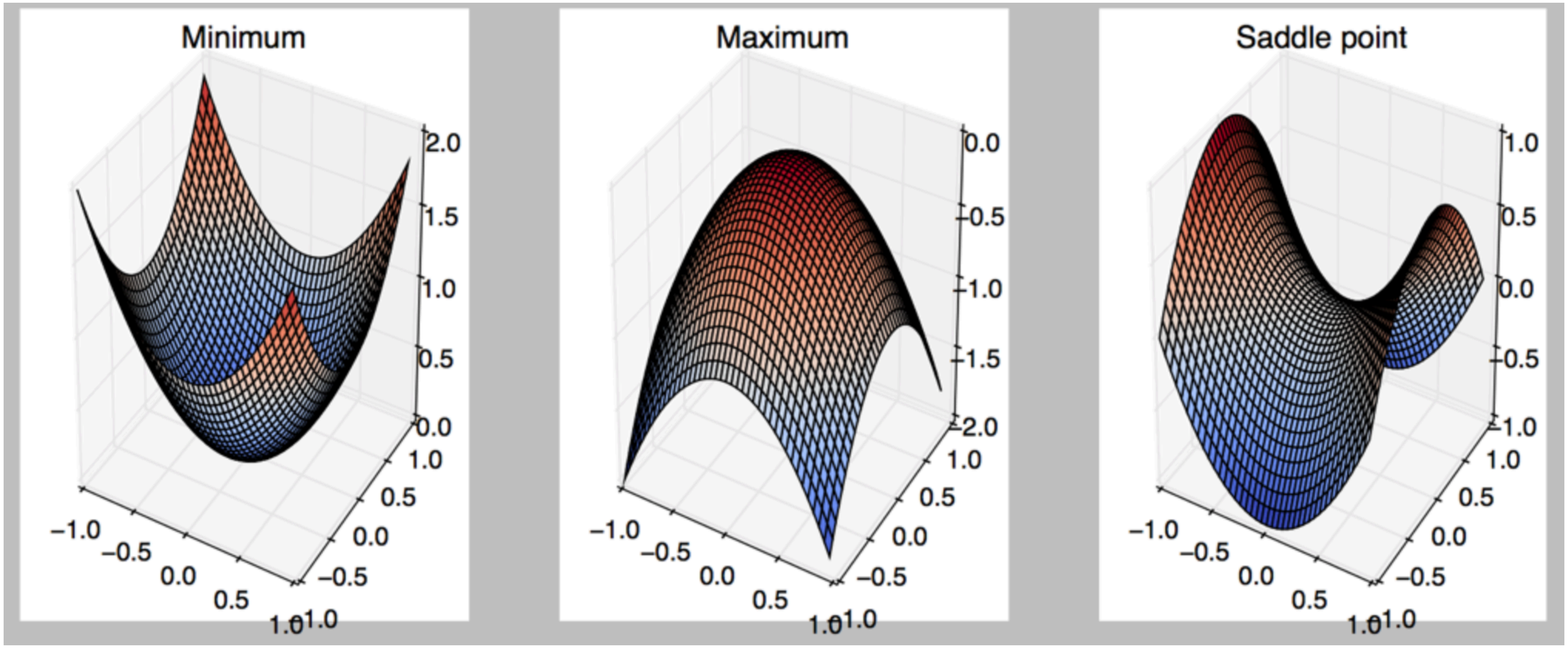
Large mini-batch: gradient computation expensive

Small mini-batch: greater variance in estimate, longer steps for convergence

Critical Points

- Points with zero gradient
- 2nd-derivate (Hessian) determines curvature

- Saddle point and min and max
- Derivative may be 0 but point is max



Goodfellow et al. (2016)

Stochastic Gradient Descent

- Take small steps in direction of negative gradient
- Sample *m* examples from training set and compute:

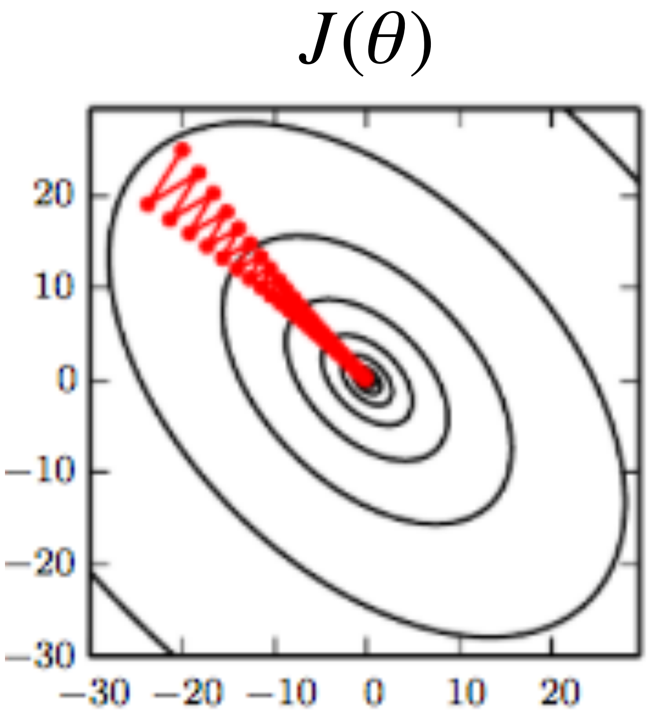
$$g = \frac{1}{m} \sum_i \nabla L(f(x^{(i)};\theta), y^{(i)})$$

- Update parameters:

$$\theta = \theta - \varepsilon_k g$$

In practice: shuffle training set once and pass through multiple times

Stochastic Gradient Descent



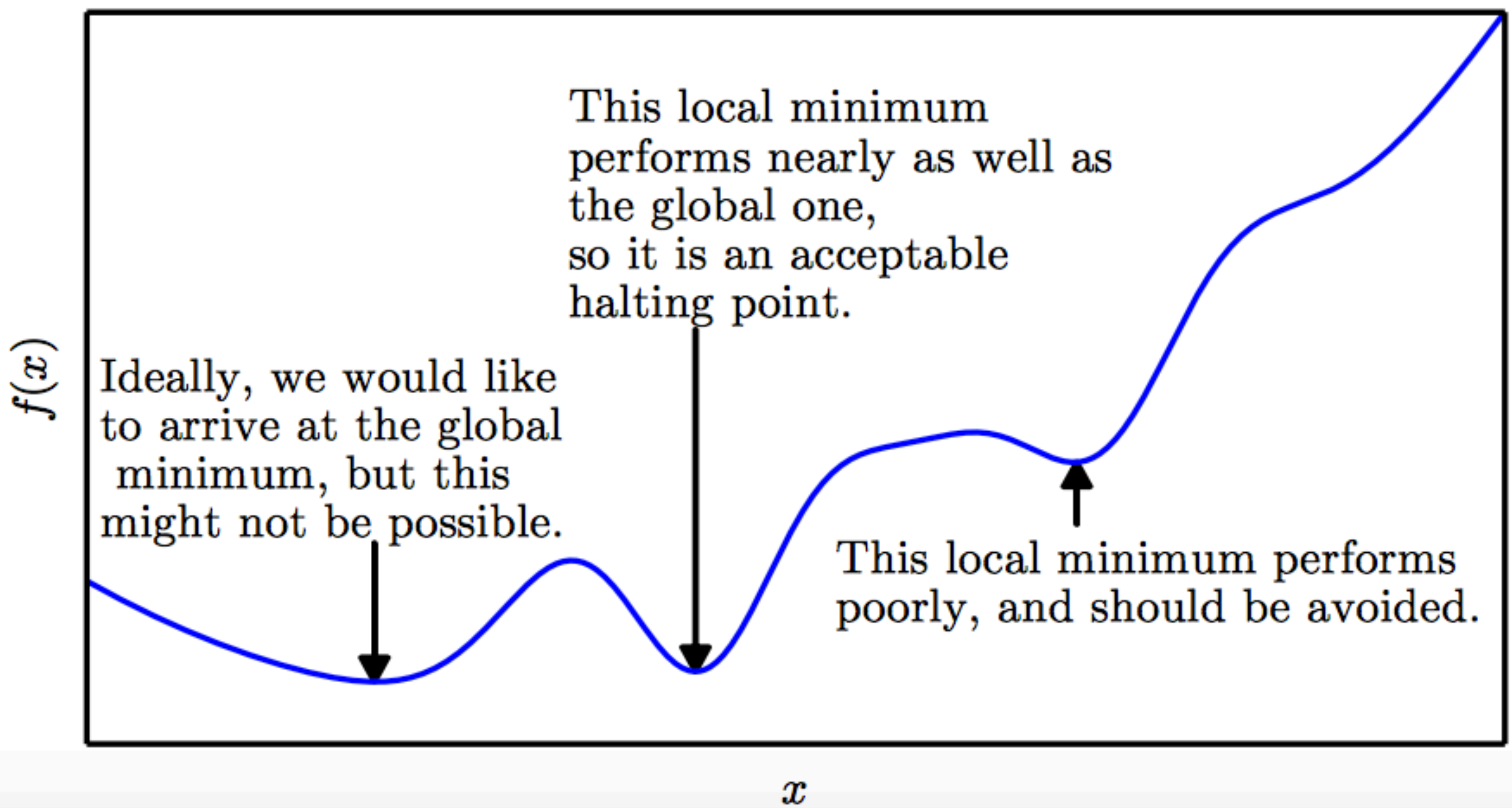
Oscillations because updates do not exploit curvature information

Goodfellow et al. (2016)

Outline

- Challenges in Optimization
- Momentum
- Adaptive Learning Rate
- Parameter Initialization
- Batch Normalization

Local Minima

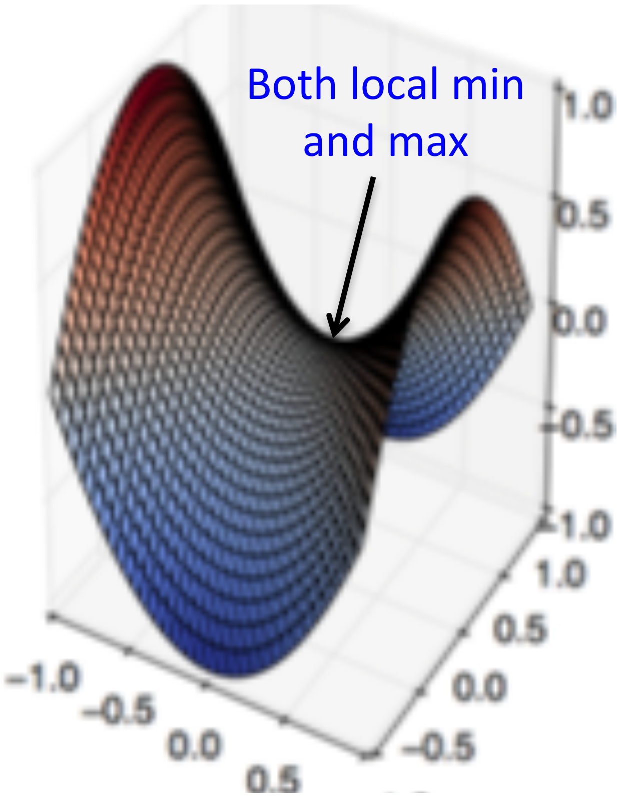


Goodfellow et al. (2016)

Local Minima

- Old view: local minima is major problem in neural network training
- Recent view:
  - For sufficiently large neural networks, most local minima incur low cost
  - Not important to find true global minimum

Saddle Points

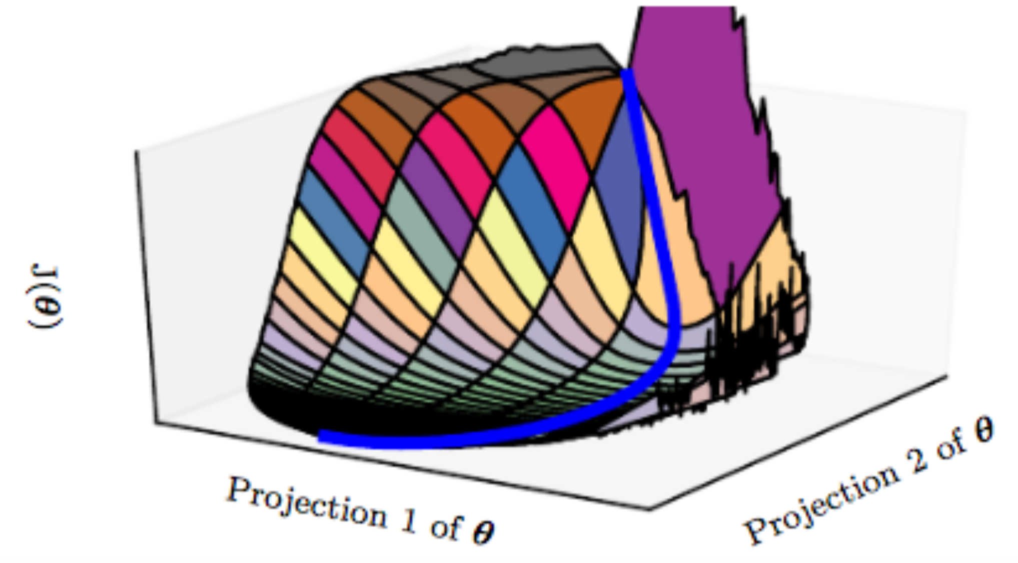


- Recent studies indicate that in high dim, saddle points are more likely than local min
- Gradient can be very small near saddle points

Goodfellow et al. (2016)

Saddle Points

- SGD is seen to escape saddle points
  - Moves down-hill, uses noisy gradients



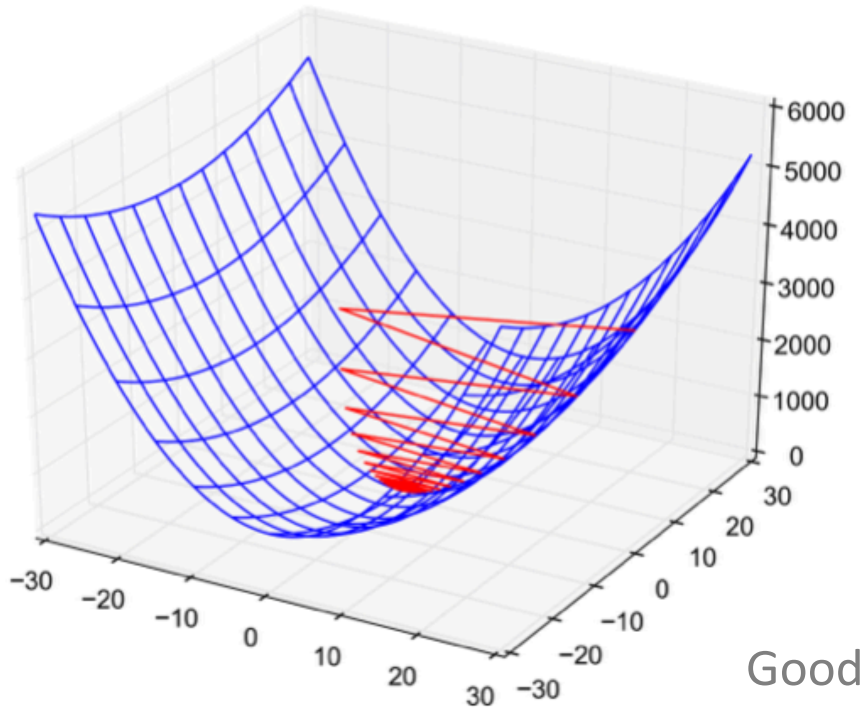
- Second-order methods get stuck
  - solves for a point with zero gradient

Goodfellow et al. (2016)

Poor Conditioning

- Poorly conditioned Hessian matrix
  - High curvature: small steps leads to huge increase
- Learning is slow despite strong gradients

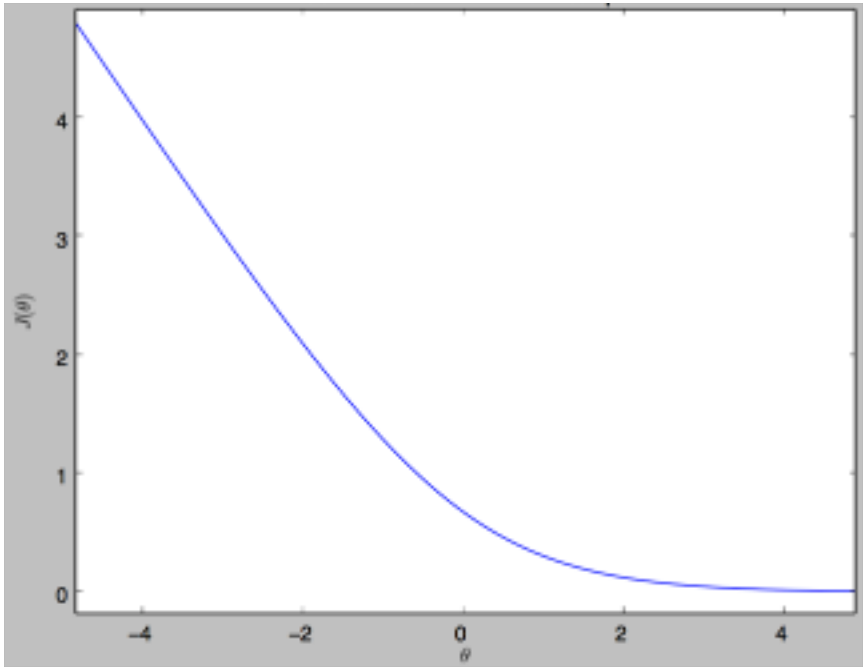
Oscillations slow down progress



Goodfellow et al. (2016)

No Critical Points

- Some cost functions do not have critical points

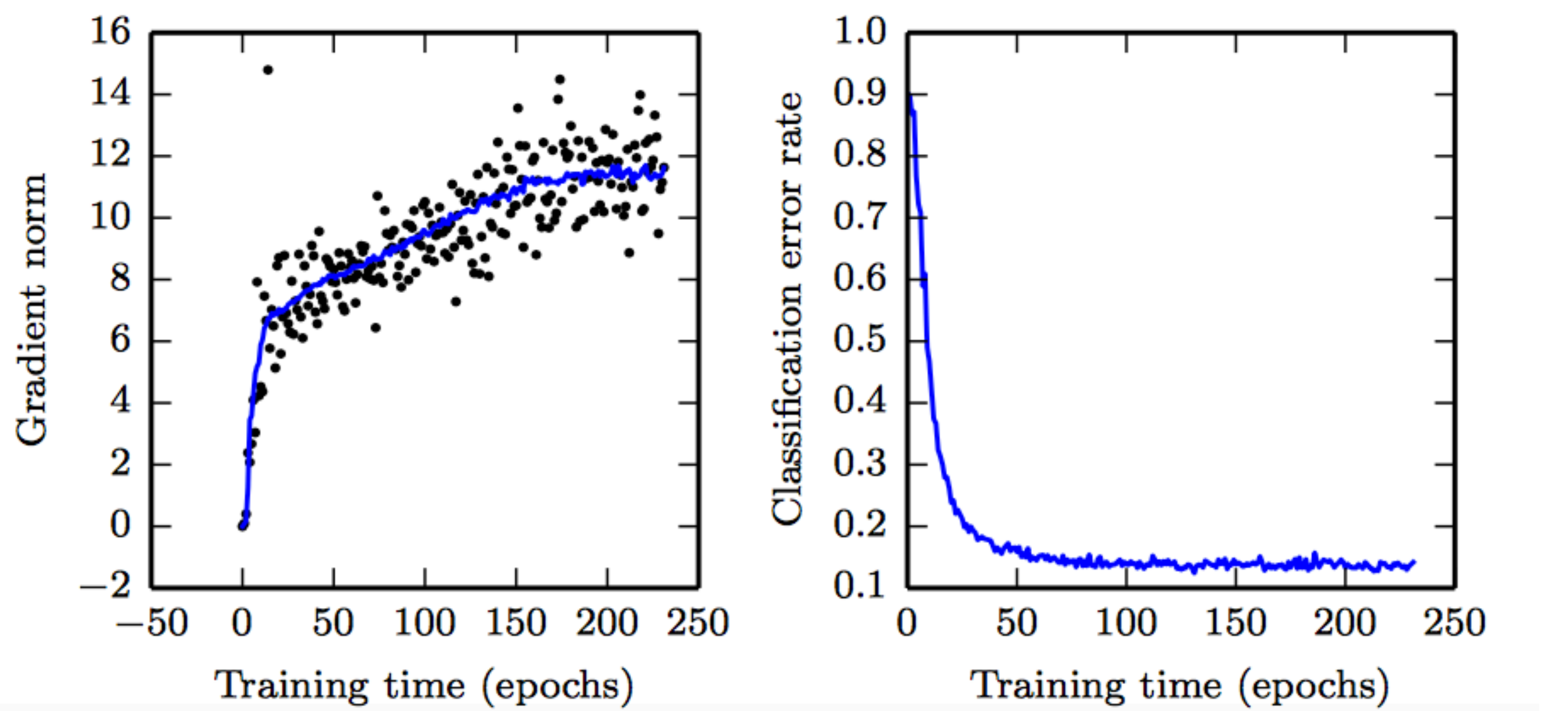


Early stopping works well

Goodfellow et al. (2016)

No Critical Points

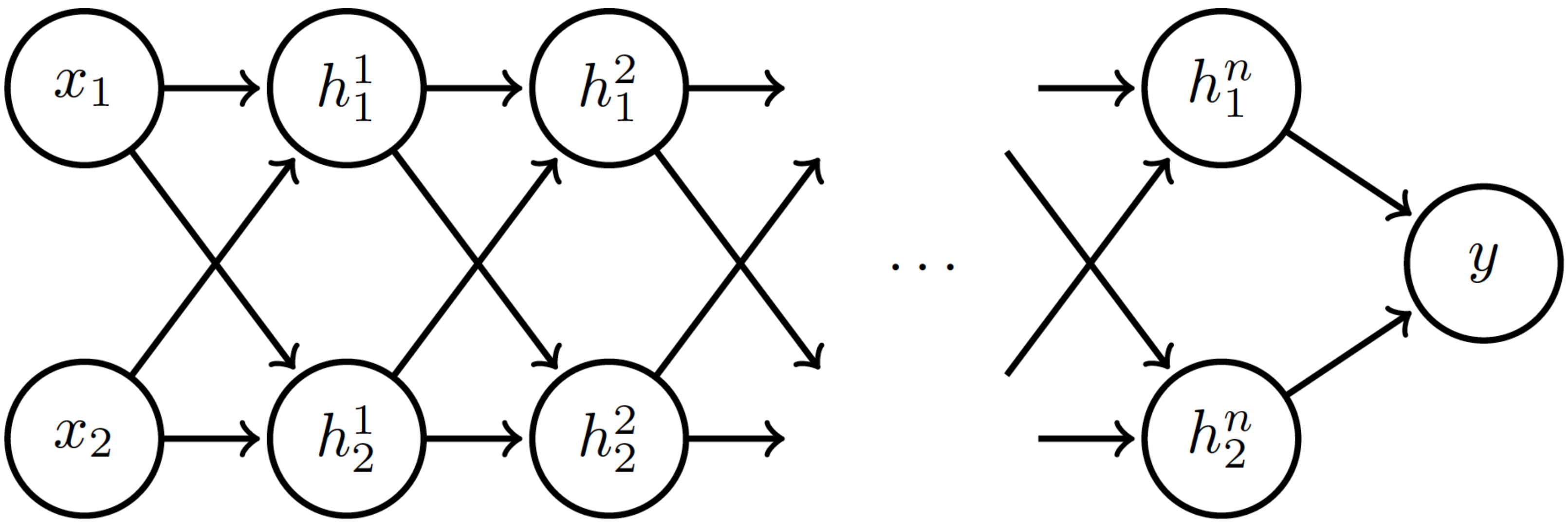
Gradient norm increases, but validation error decreases



Convolution Nets for Object Detection

Goodfellow et al. (2016)

Exploding and Vanishing Gradients



Early stopping not useful if convergence before it

Linear activation

$$\mathbf{h}_1 = \mathbf{W}\mathbf{x}$$

$$\mathbf{h}_i = \mathbf{W}\mathbf{h}_{i-1}, \quad i = 2\ldots n$$

$$y = \sigma(h_1^n + h_2^n), \quad \text{where } \sigma(s) = \frac{1}{1+e^{-s}}$$

Exploding and Vanishing Gradients

Suppose $\mathbf{W} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}$:

$$\begin{bmatrix} h_1^1 \\ h_2^1 \end{bmatrix} = \begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \qquad \cdots \qquad \begin{bmatrix} h_1^n \\ h_2^n \end{bmatrix} = \begin{bmatrix} a^n & 0 \\ 0 & b^n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$y = \sigma(a^n x_1 + b^n x_2)$$

$$\nabla y = \sigma'(a^n x_1 + b^n x_2) \begin{bmatrix} n a^{n-1} x_1 \\ n b^{n-1} x_2 \end{bmatrix}$$

Exploding and Vanishing Gradients

Suppose $x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

Case 1: $a = 1,\ b = 2:$

$$y \to 1, \quad \nabla y \to \begin{bmatrix} n \\ n2^{n-1} \end{bmatrix}$$

Explodes!

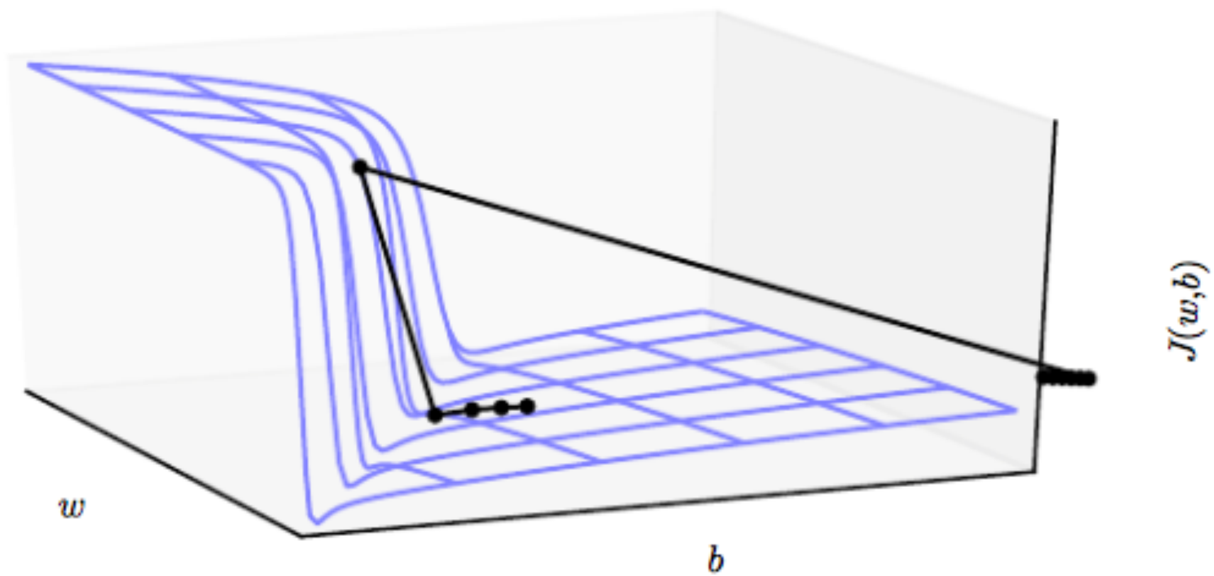
Case 2: $a = 0.5,\ b = 0.9:$

$$y \to 0, \quad \nabla y \to \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Vanishes!

Exploding and Vanishing Gradients

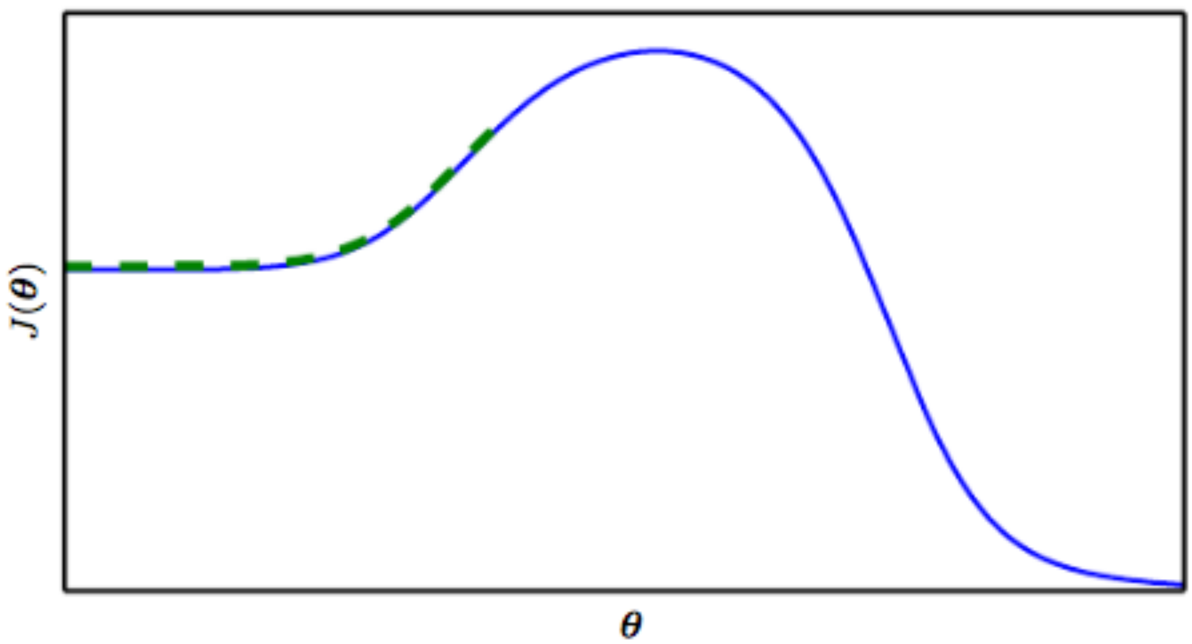
- Exploding gradients lead to cliffs
- Can be mitigated using gradient clipping



Goodfellow et al. (2016)

Poor correspondence between local and global structure

It is really difficult to train large neural networks



Goodfellow et al. (2016)

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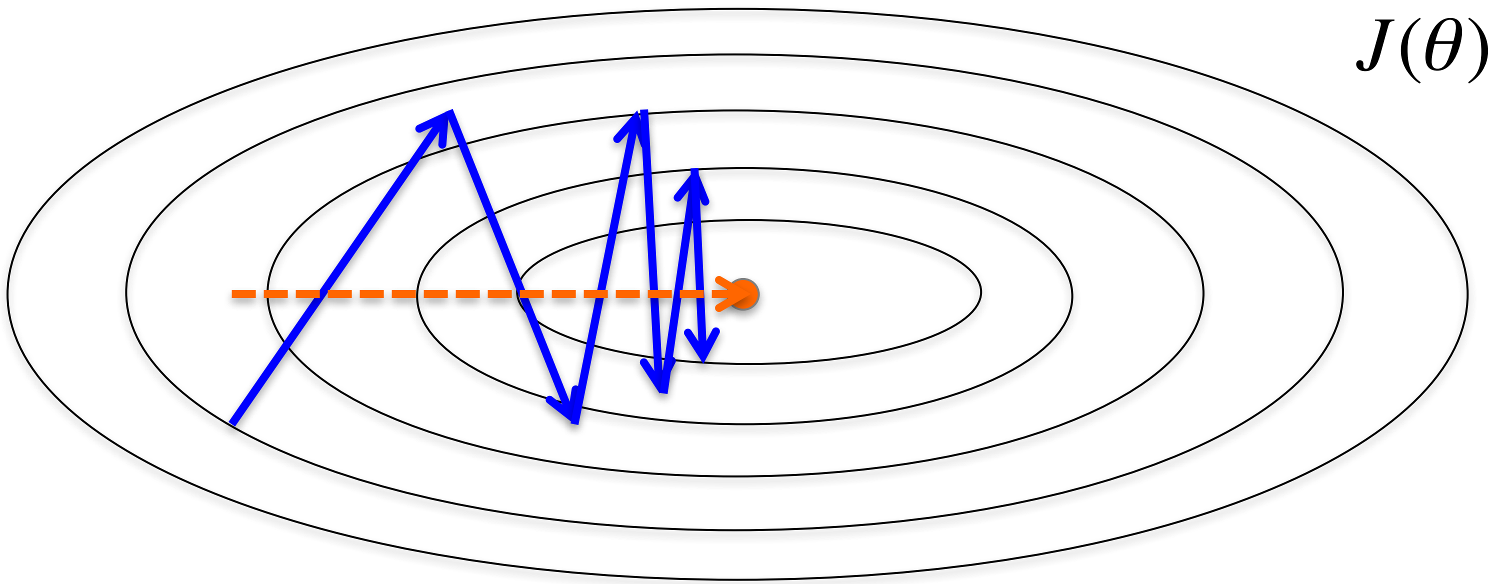
Momentum

- SGD is slow when there is high curvature



- Average gradient presents faster path to opt:
  - vertical components cancel out

Momentum

- Uses past gradients for update
- Maintains a new quantity: ‘velocity’
- *Exponentially decaying average* of gradients:

Current gradient update

$$v = \alpha v + (-\varepsilon g)$$

$\alpha \in [0,1)$ controls how quickly effect of past gradients decay

Momentum

- Compute gradient estimate:

$$g = \frac{1}{m} \sum_i \nabla_\theta L(f(x^{(i)};\theta), y^{(i)})$$

- Update velocity:

$$v = \alpha v - \varepsilon g$$

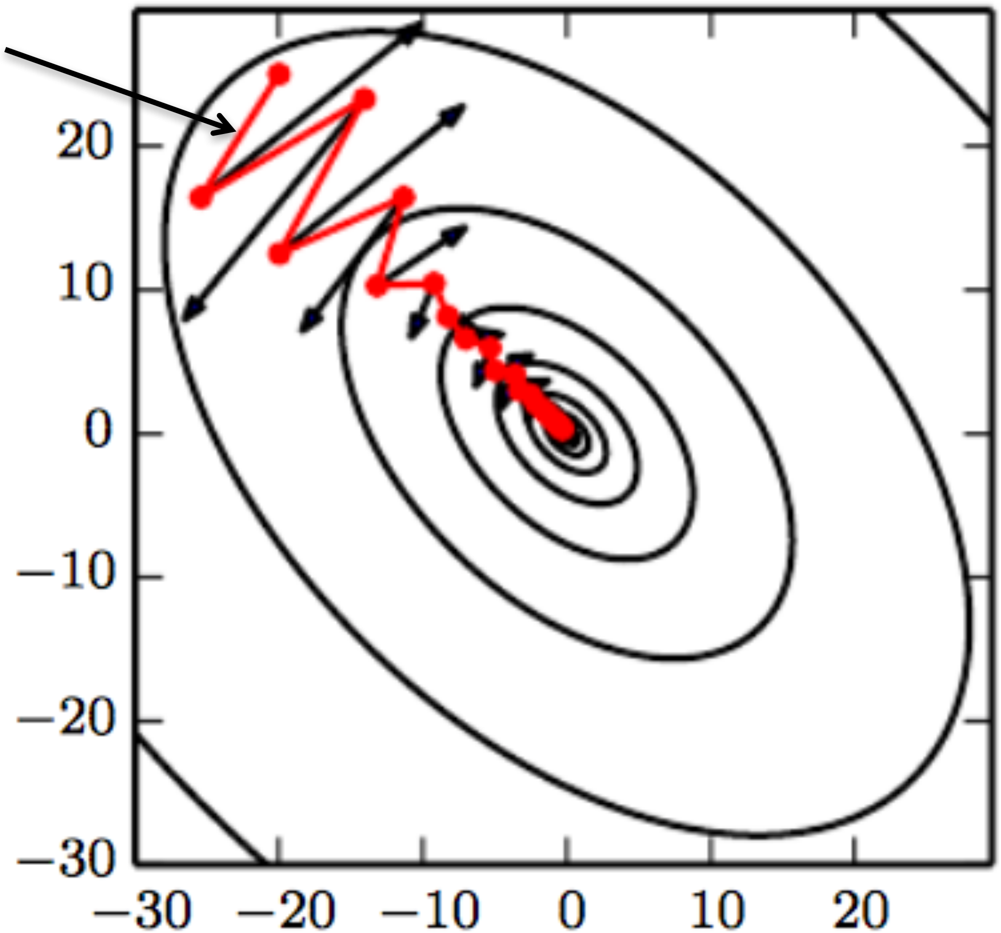
- Update parameters:

$$\theta = \theta + v$$

Momentum

Damped oscillations: gradients in opposite directions get cancelled out

$J(\theta)$



Goodfellow et al. (2016)

Nesterov Momentum

- Apply an interim update:

$$\tilde{\theta} = \theta + v$$

- Perform a correction based on gradient at the interim point:

$$g = \frac{1}{m} \sum_i \nabla_\theta L(f(x^{(i)}; \tilde{\theta}), y^{(i)})$$

$$v = \alpha v - \varepsilon g$$

$$\theta = \theta + v$$

Momentum based on look-ahead slope

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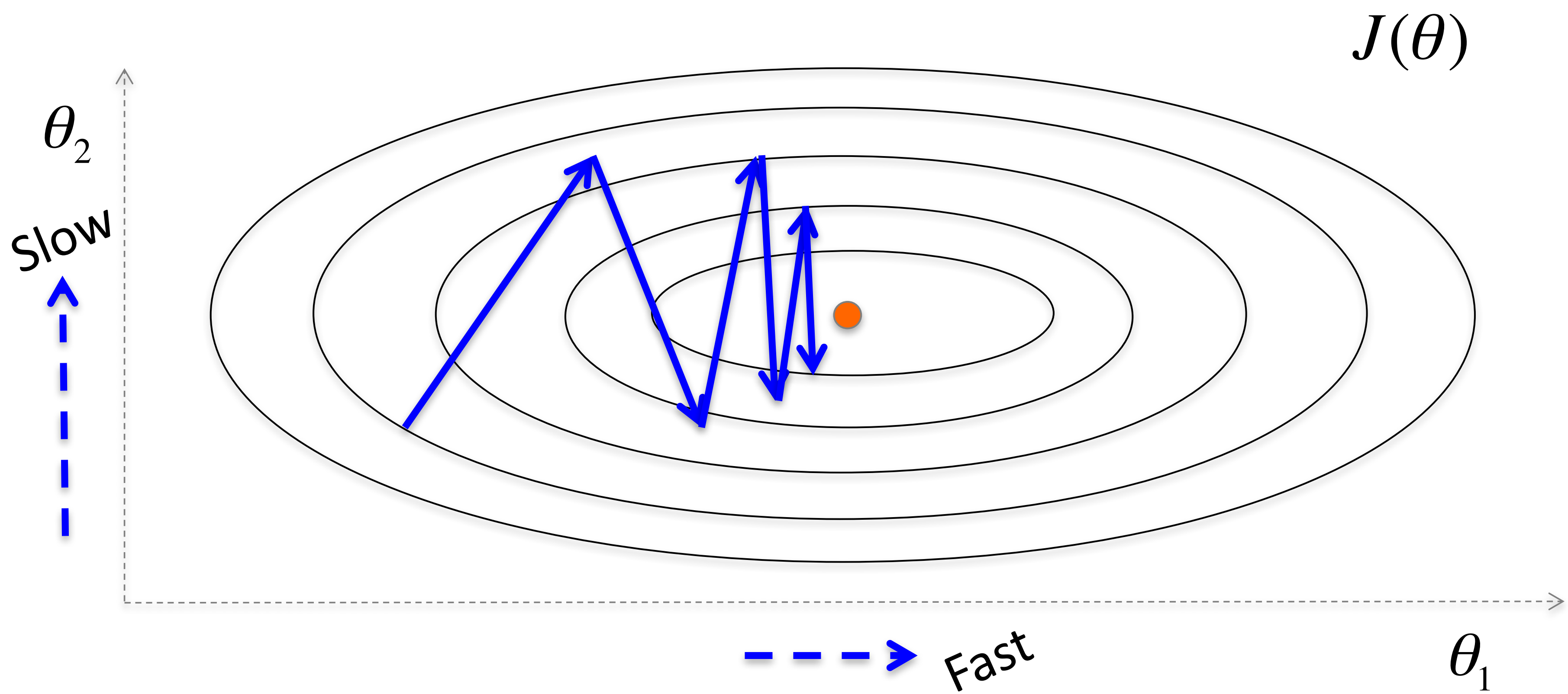
Adaptive Learning Rates



- Oscillations along vertical direction
  - Learning must be slower along parameter 2
- Use a different learning rate for each parameter?

- Derivative v. steep,
- If learning rate too large, bounces around

AdaGrad

- Accumulate squared gradients:

$$r_i = r_i + g_i^2$$

- Update each parameter:

$$\theta_i = \theta_i - \frac{\varepsilon}{\delta + \sqrt{r_i}} g_i$$

Inversely proportional to cumulative squared gradient

- Greater progress along gently sloped directions

RMSProp

- For non-convex problems, AdaGrad can prematurely decrease learning rate
- Use exponentially weighted average for gradient accumulation

$$r_i = \rho r_i + (1-\rho) g_i^2$$

$$\theta_i = \theta_i - \frac{\varepsilon}{\delta + \sqrt{r_i}} g_i$$

Adam

- RMSProp + Momentum
- Estimate first moment:

$$v_i = \rho_1 v_i + (1-\rho_1) g_i$$

- Estimate second moment:

$$r_i = \rho_2 r_i + (1-\rho_2) g_i^2$$

- Update parameters:

$$\theta_i = \theta_i - \frac{\varepsilon}{\delta + \sqrt{r_i}} v_i$$

Also applies bias correction to v and r

Works well in practice, is fairly robust to hyper-parameters

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Parameter Initialization

- Goal: break symmetry between units
  - so that each unit computes a different function
- Initialize all weights (not biases) randomly
  - Gaussian or uniform distribution
- Scale of initialization?
  - *Large* -> grad explosion, *Small* -> grad vanishing

Xavier Initialization

- Heuristic for all outputs to have unit variance
- For a fully-connected layer with m inputs:

$$W_{ij} \sim N\left(0,\ \frac{1}{m}\right)$$

- For ReLU units, it is recommended:

$$W_{ij} \sim N\left(0,\ \frac{2}{m}\right)$$

Normalized Initialization

- Fully-connected layer with m inputs, n outputs:

$$W_{ij} \sim U\left(-\sqrt{\frac{6}{m+n}},\ \sqrt{\frac{6}{m+n}}\right)$$

- Heuristic trades off between initialize all layers have same activation and gradient variance
- Sparse variant when m is large
  - Initialize k nonzero weights in each unit

Bias Initialization

- Output unit bias
  - Marginal statistics of the output in the training set
- Hidden unit bias
  - Avoid saturation at initialization
  - E.g. in ReLU, initialize bias to 0.1 instead of 0
- Units controlling participation of other units
  - Set bias to allow participation at initialization

- If initialised with only W=0, we want biases to be as close to std dev, mean as possible.

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Feature Normalization

- Good practice to normalize features before applying learning algorithm:

- NW: all nodes interconnected

Feature vector

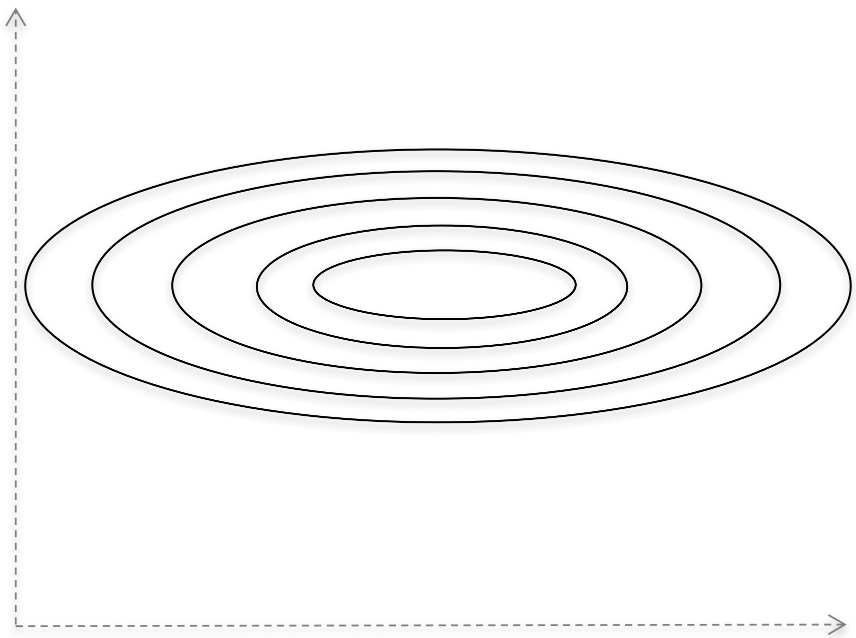
Vector of mean feature values

$$x' = \frac{x - \mu}{\sigma}$$

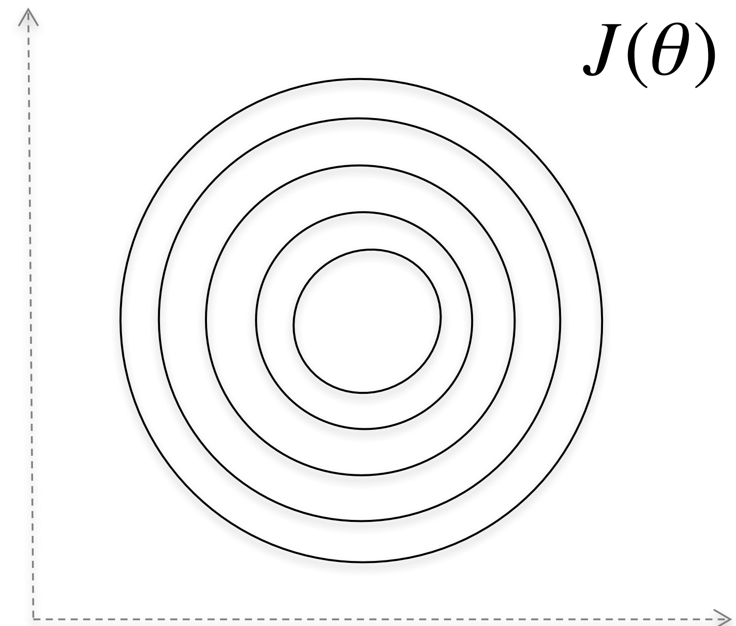
Vector of SD of feature values

- Features in same scale: mean 0 and variance 1
  - Speeds up learning

Feature Normalization



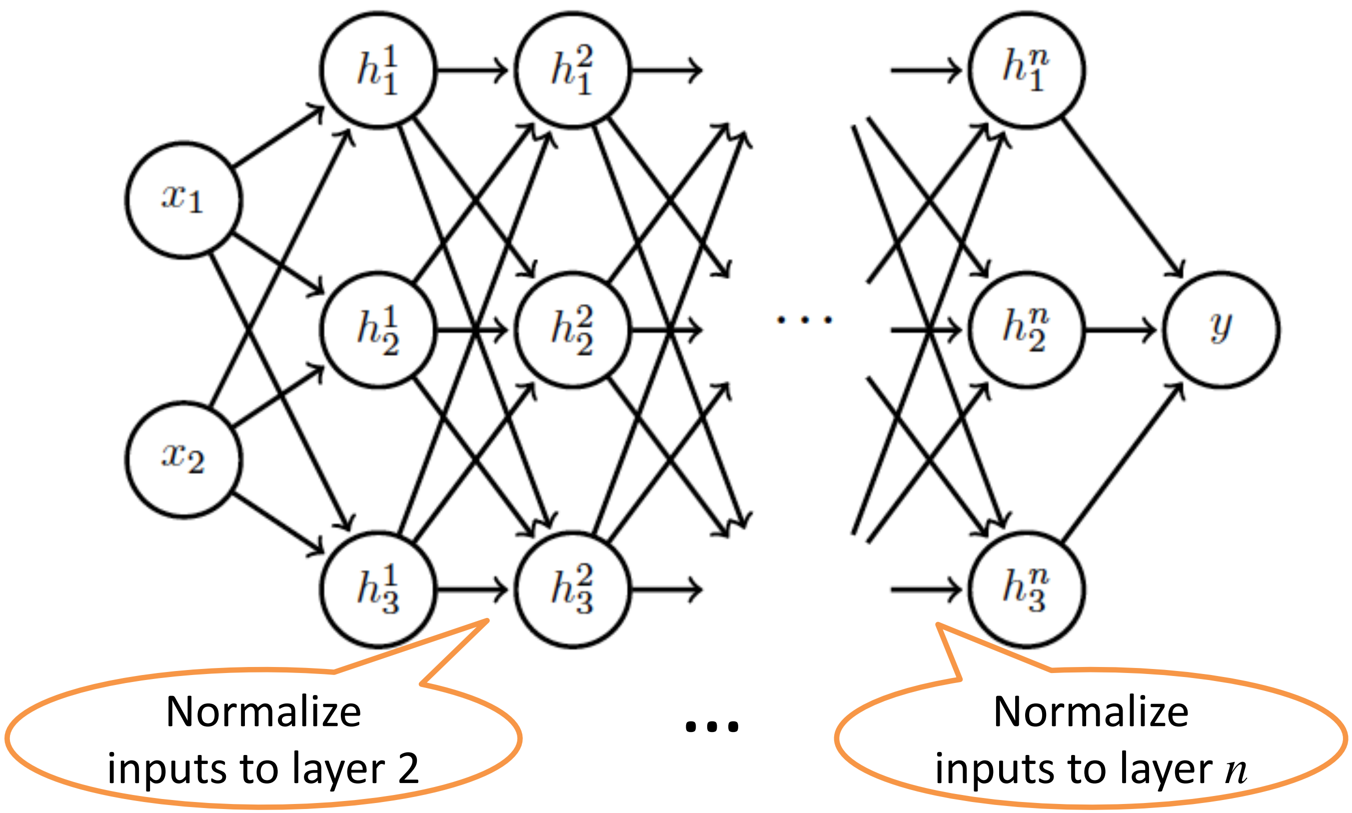
Before normalization



After normalization

Internal Covariance Shift

Each hidden layer changes distribution of inputs to next layer: *slows down learning*



Batch Normalization

- Training time:
  - Mini-batch of activations for layer to normalize

$$H = \begin{bmatrix} H_{11} & \cdots & H_{1K} \\ \vdots & \ddots & \vdots \\ H_{N1} & \cdots & H_{NK} \end{bmatrix}$$

K hidden layer activations

N data points in mini-batch

Batch Normalization

- Training time:
  - Mini-batch of activations for layer to normalize

=Loss of expressiveness with normalization

-

$$H' = \frac{H - \mu}{\sigma}$$

where

$$\mu = \frac{1}{m} \sum_i H_{i,:} \qquad \sigma = \sqrt{\frac{1}{m} \sum_i (H - \mu)_i^2 + \delta}$$

Vector of mean activations across mini-batch

Vector of SD of each unit across mini-batch

Batch Normalization

- Training time:
  - Normalization can reduce expressive power
  - Instead use:

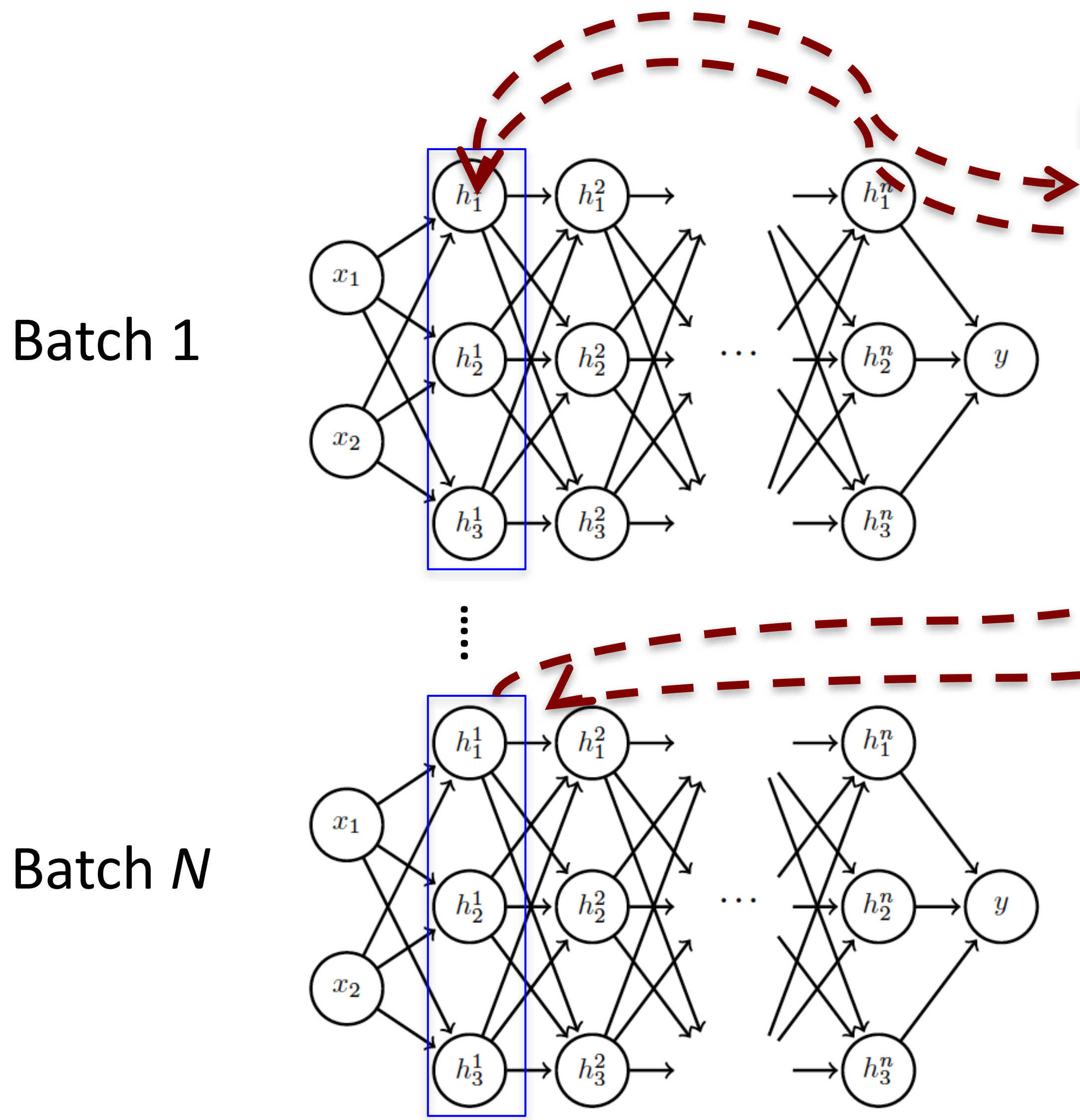
$$\gamma H' + \beta$$

- We get mu and sigma back.

Learnable parameters

  - Allows network to control range of normalization

Batch Normalization



$$\mu^1 = \frac{1}{m}\sum_i H_{i,:}$$

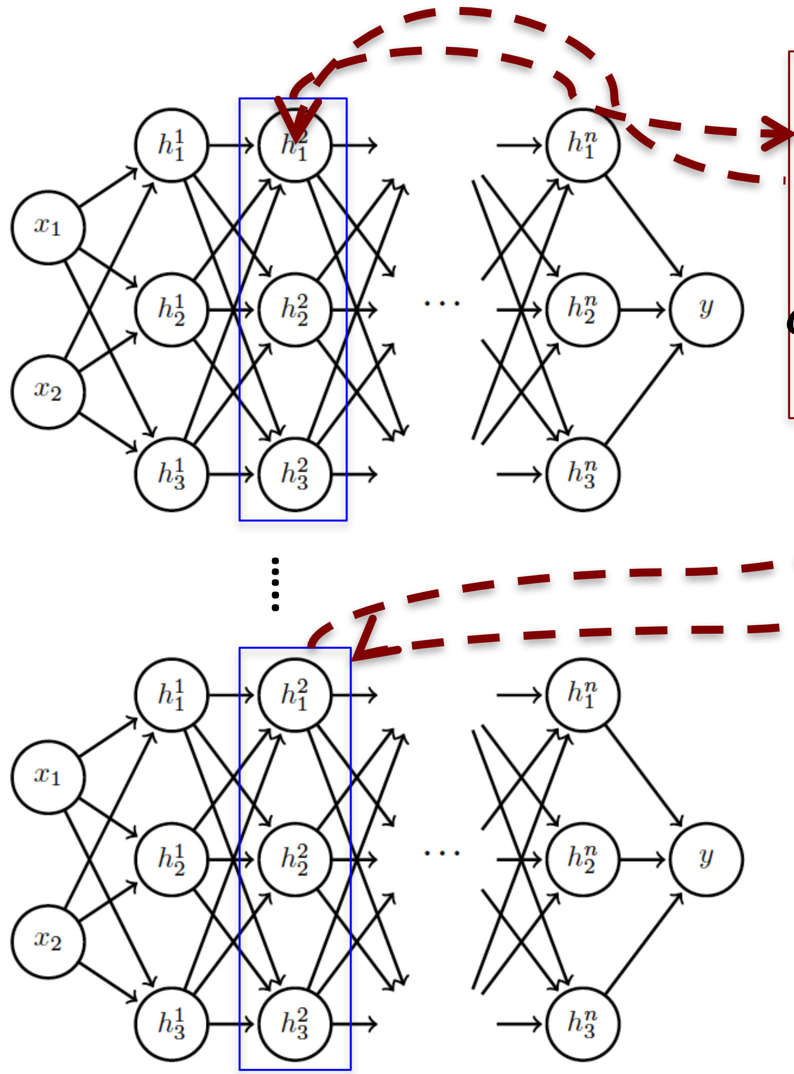
$$\sigma^1 = \sqrt{\frac{1}{m}\sum_i (H-\mu)_i^2 + \delta}$$

Add normalization operations for layer 1

Batch Normalization

Batch 1

Batch N



$$\mu^2 = \frac{1}{m}\sum_i H_{i,:}$$

$$\sigma^2 = \sqrt{\frac{1}{m}\sum_i (H-\mu)_i^2 + \delta}$$

Add normalization operations for layer 2 and so on ...

Batch Normalization

- Differentiate the joint loss for *N* mini-batches
- Back-propagate *through* the norm operations

- Test time:
  - Model needs to be evaluated on a *single example*
  - Replace μ and σ with running averages collected during training