# 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

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

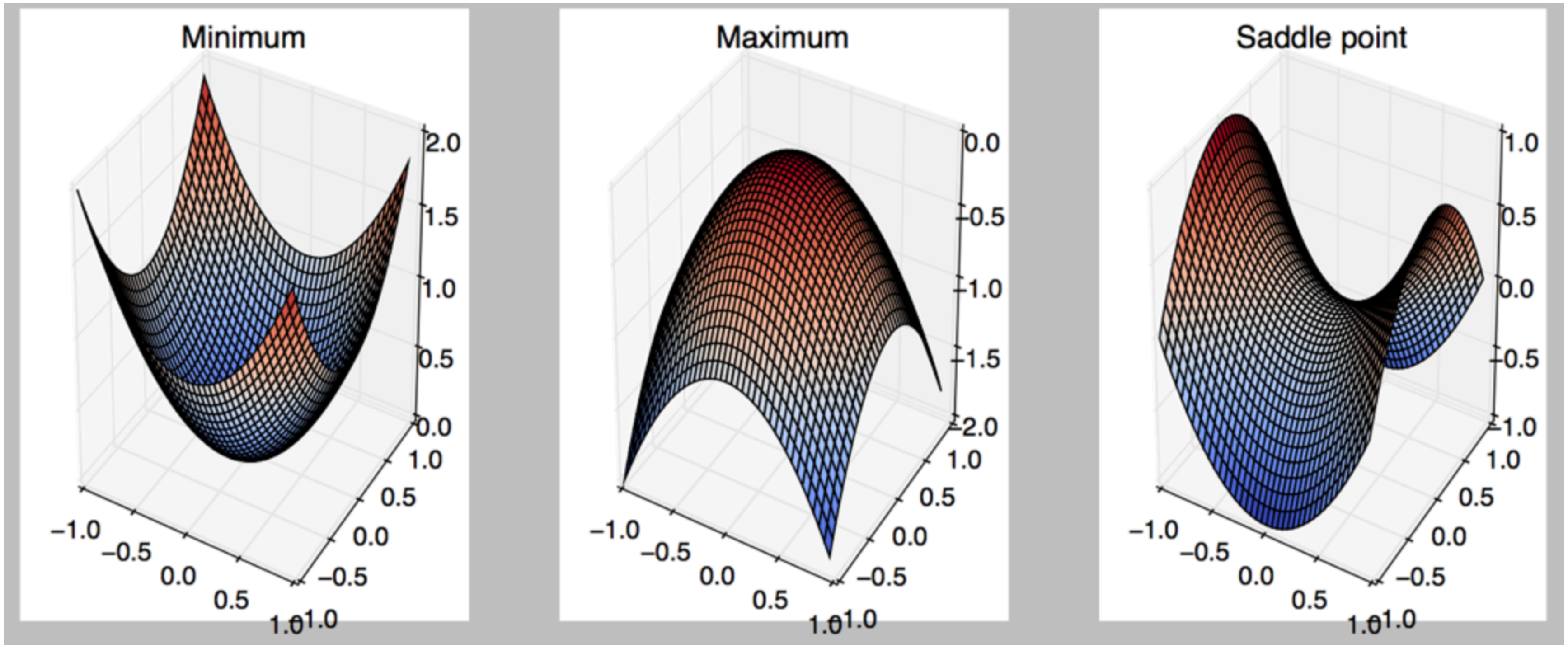
*Large mini-batch*: gradient computation expensive

*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:

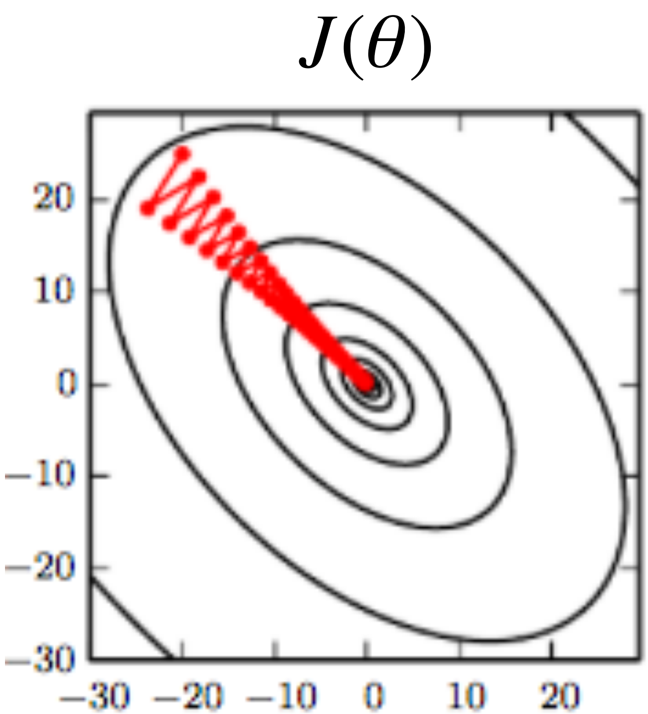
$$g = \frac{1}{m} \sum_i \nabla L(f(x^{(i)};\theta), y^{(i)})$$

- Update parameters:

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

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

# Stochastic Gradient Descent



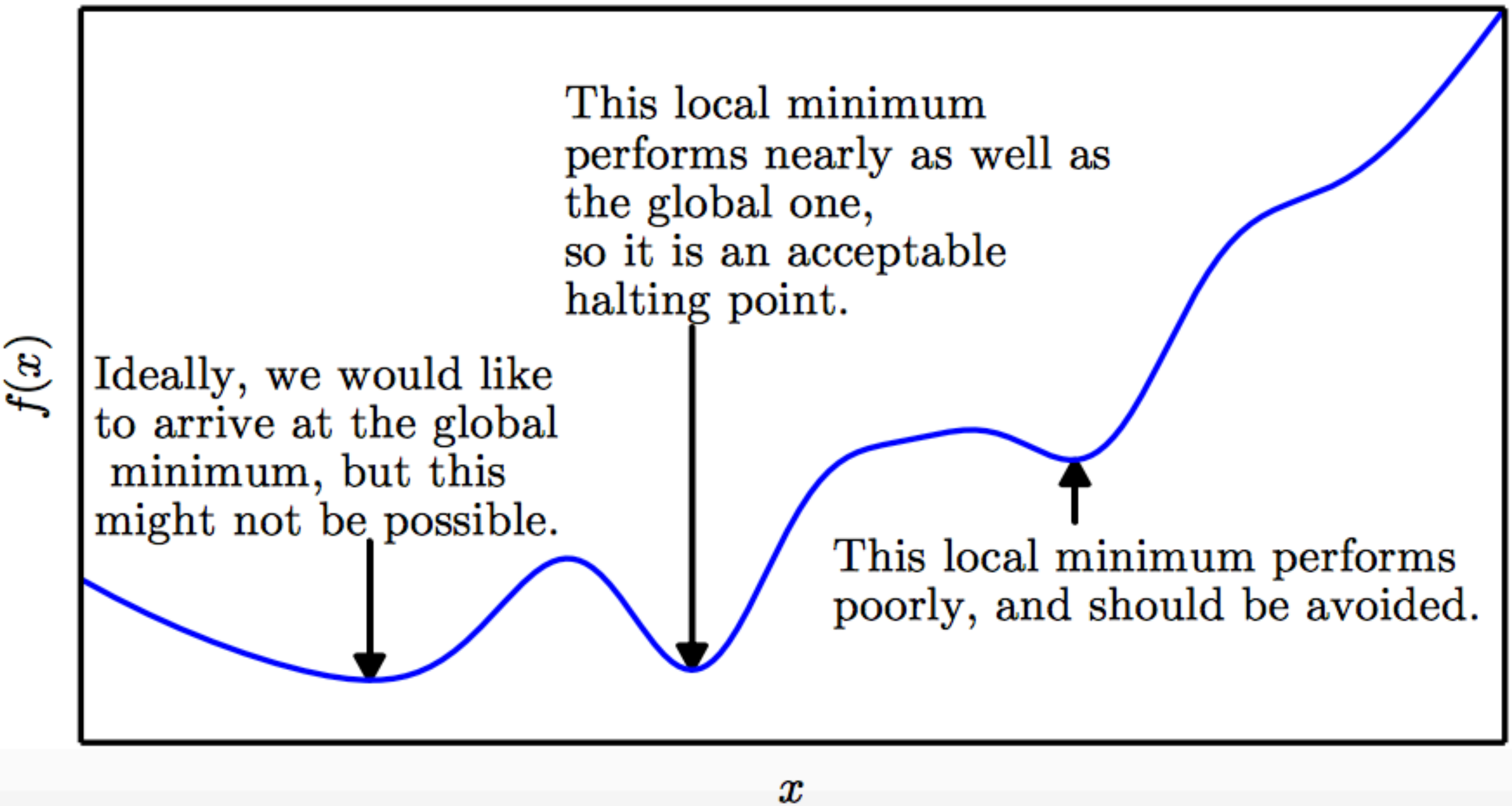

Oscillations because updates do not exploit curvature information

Goodfellow et al. (2016)

# Outline

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

# Local Minima

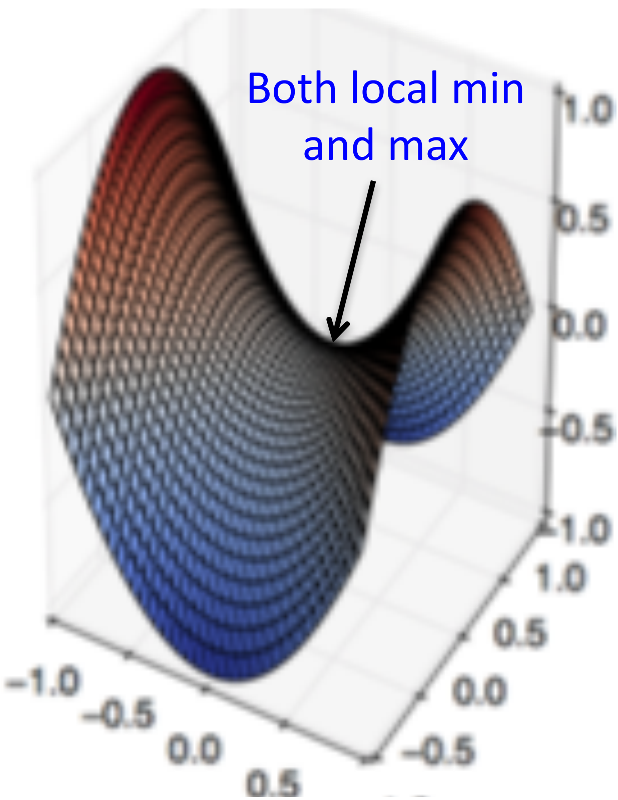



Goodfellow et al. (2016)

# 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

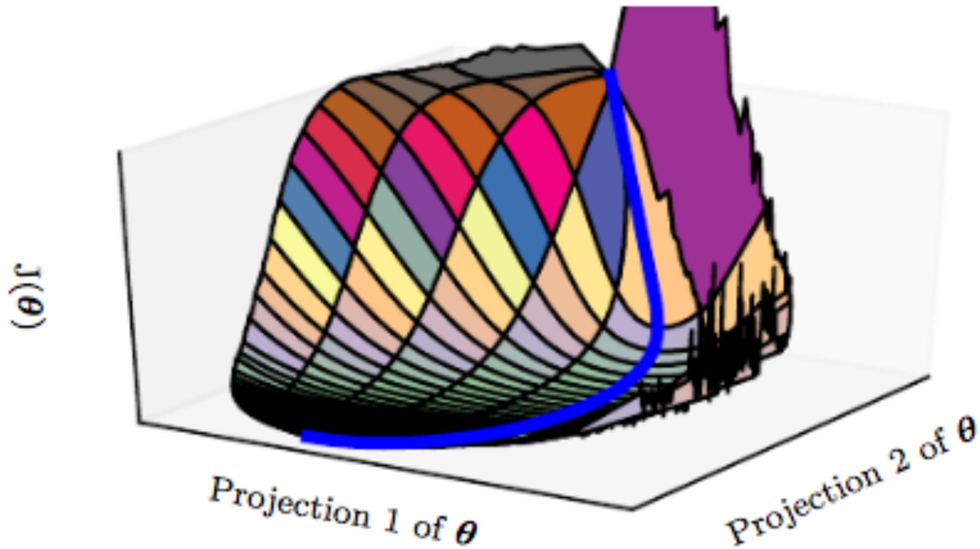



- Recent studies indicate that in high dim, saddle points are more likely than local min
- Gradient can be very small near saddle points

Goodfellow et al. (2016)

# Saddle Points

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



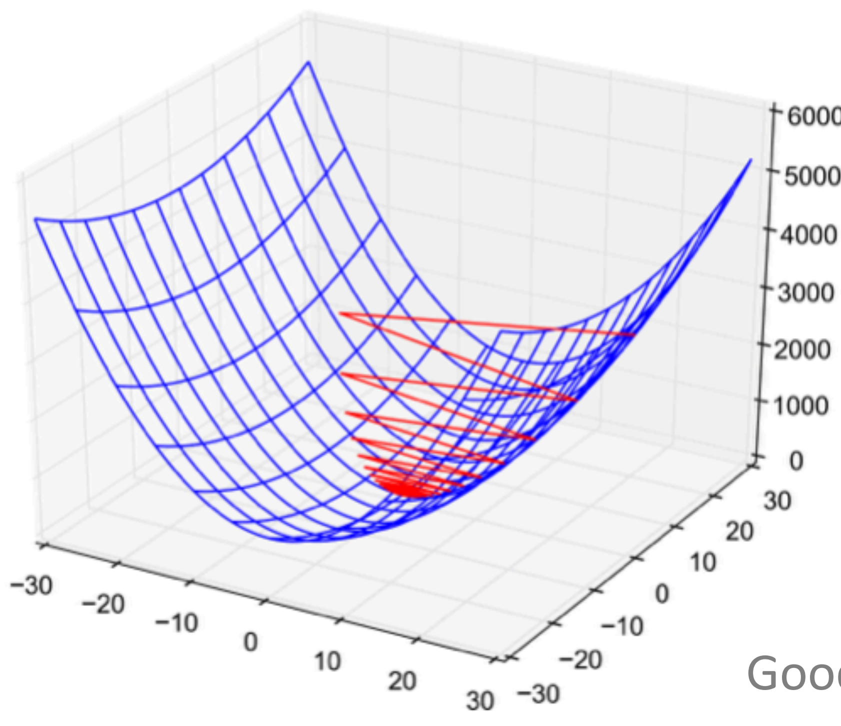

- Second-order methods get stuck
  - solves for a point with zero gradient

Goodfellow et al. (2016)

# Poor Conditioning

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

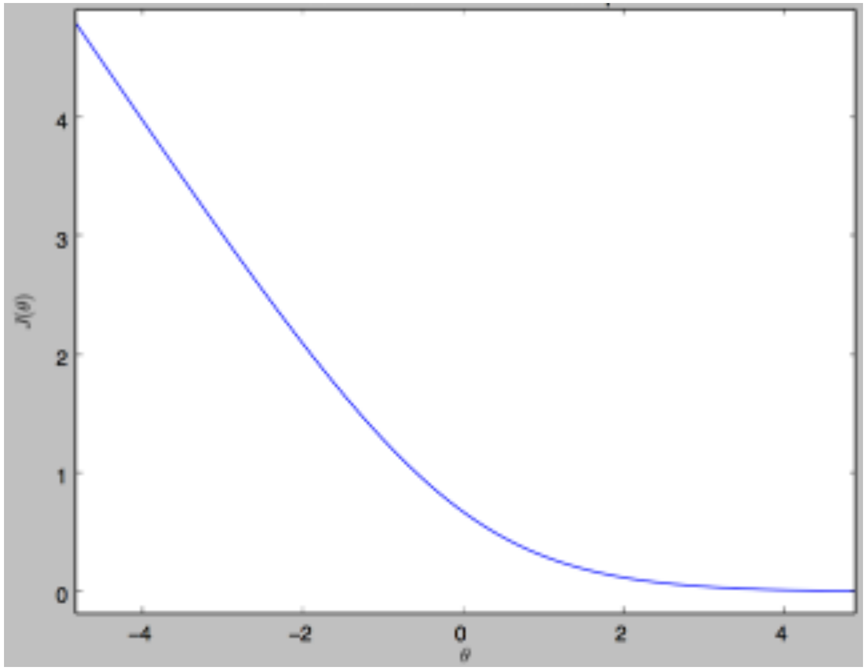
Oscillations slow down progress




Goodfellow et al. (2016)

# No Critical Points

- Some cost functions do not have critical points

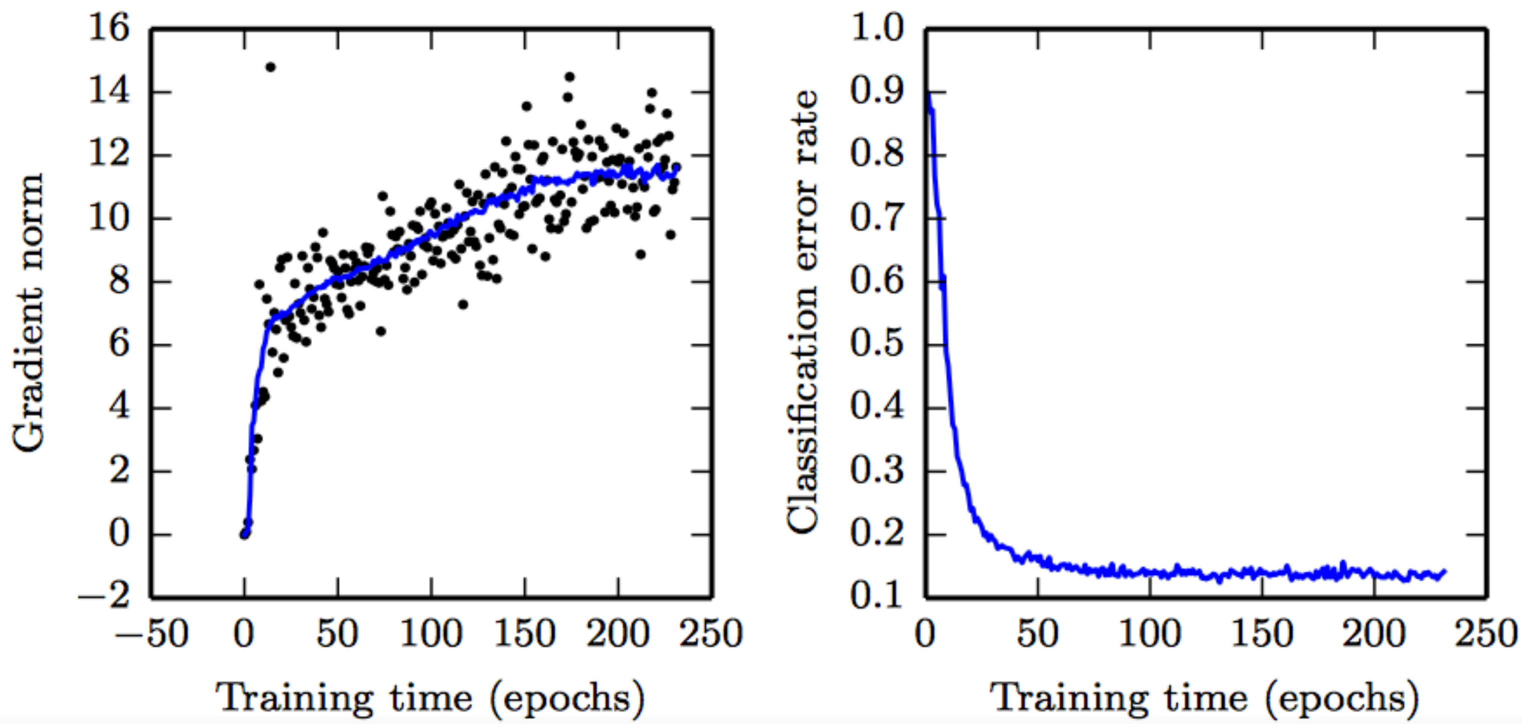



Early stopping works well

Goodfellow et al. (2016)

# No Critical Points

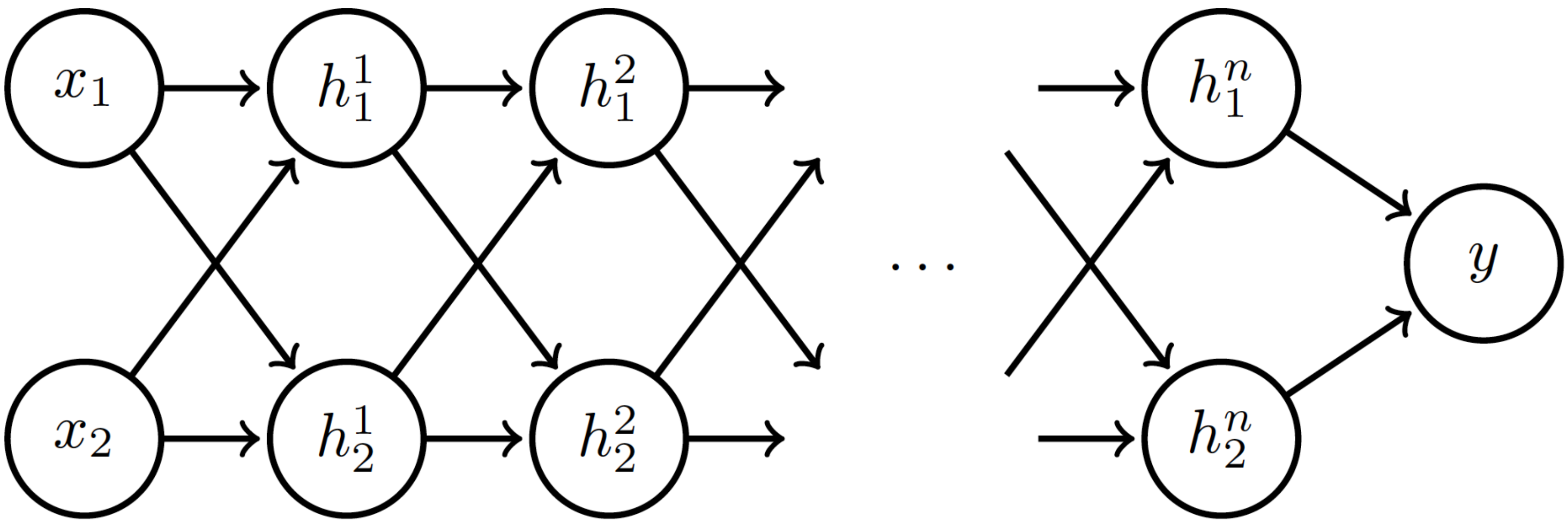
Gradient norm increases, but validation error decreases




*Convolution Nets for Object Detection*

Goodfellow et al. (2016)

# Exploding and Vanishing Gradients




Early stopping not useful if convergence before it

Linear activation

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

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

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

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

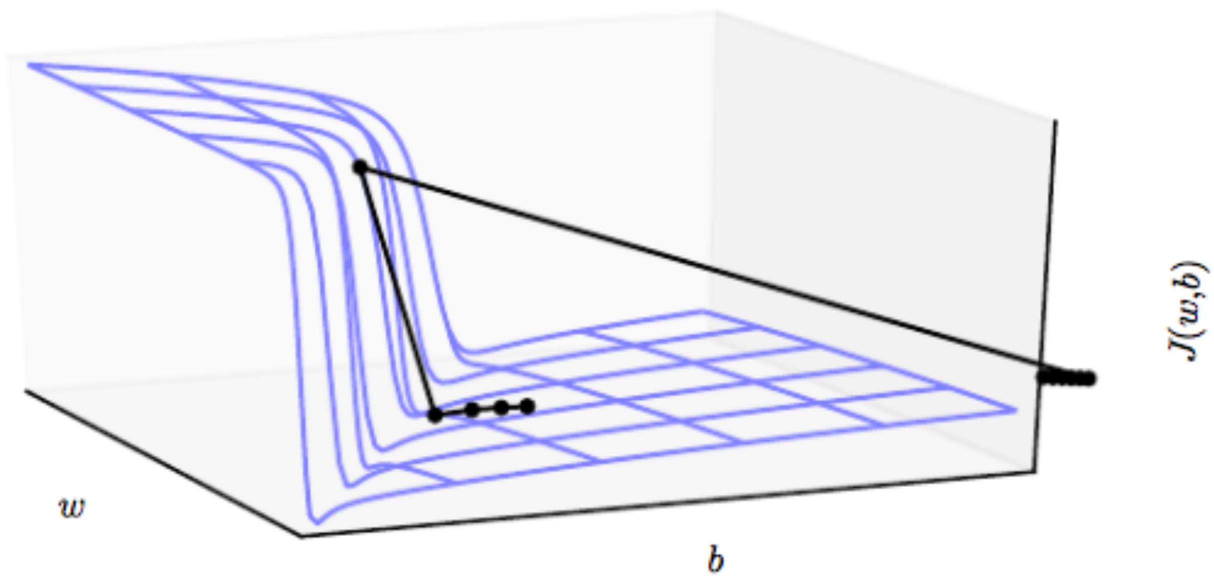
$$y \to 1, \quad \nabla y \to \begin{bmatrix} n \\ n2^{n-1} \end{bmatrix}$$ Explodes!

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

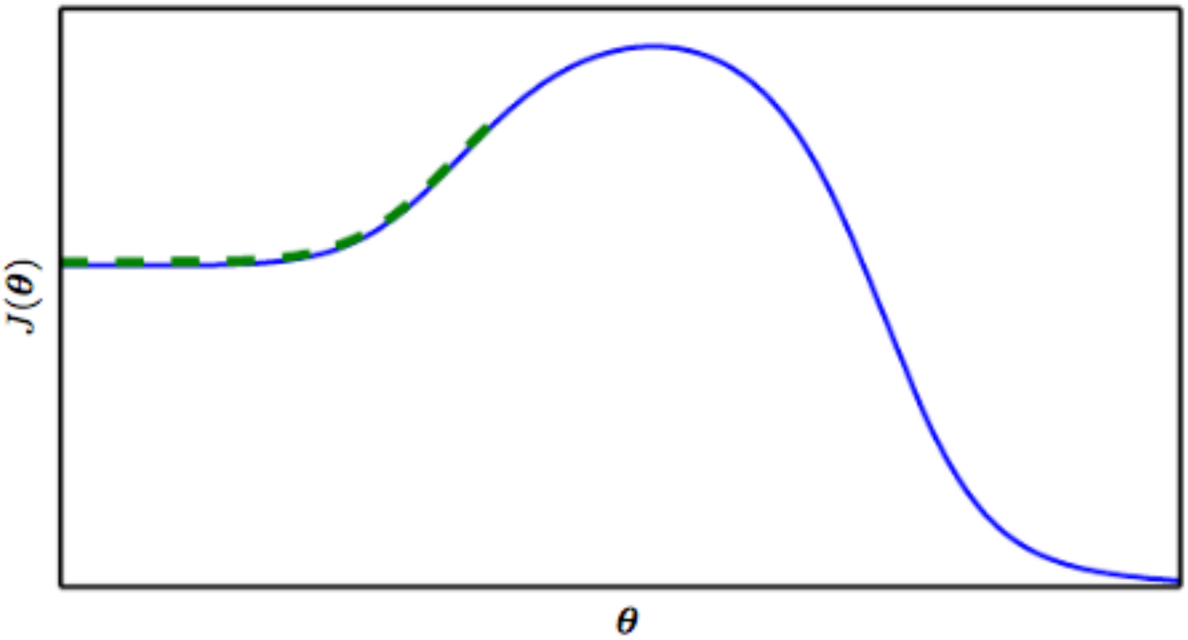
- Exploding gradients lead to cliffs
- Can be mitigated using gradient clipping




Goodfellow et al. (2016)

# Poor correspondence between local and global structure

It is really difficult to train large neural networks



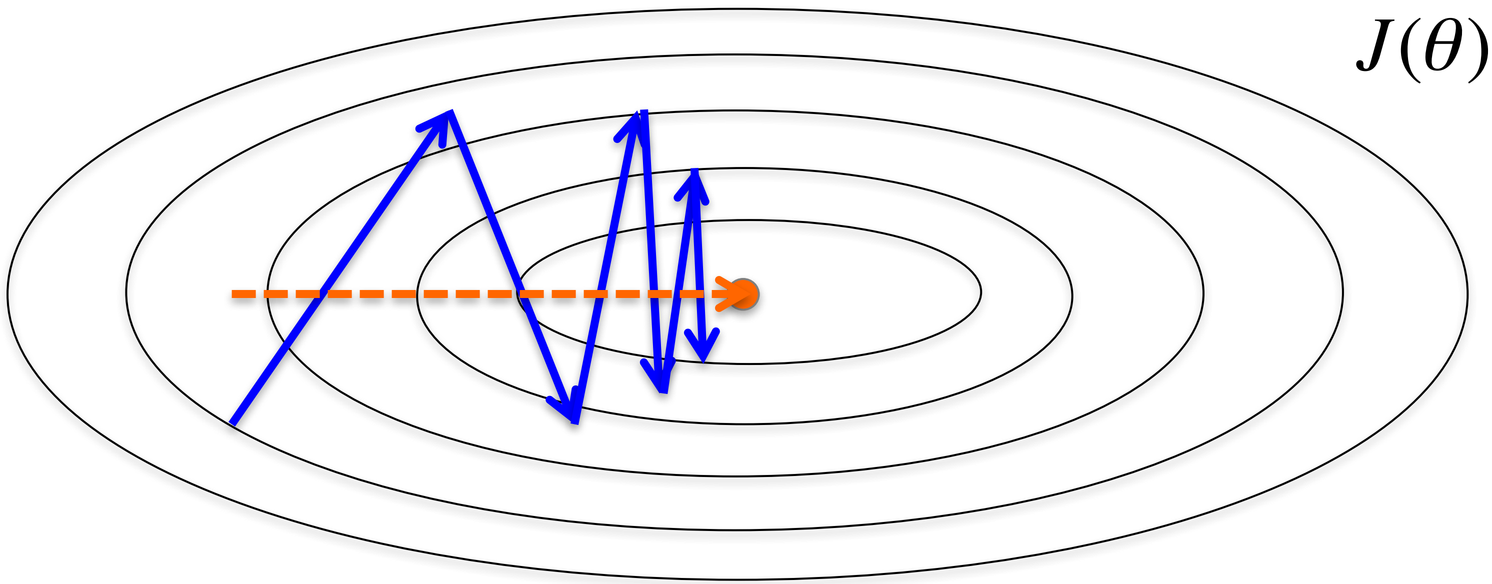

Goodfellow et al. (2016)

# Outline

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

# 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:

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

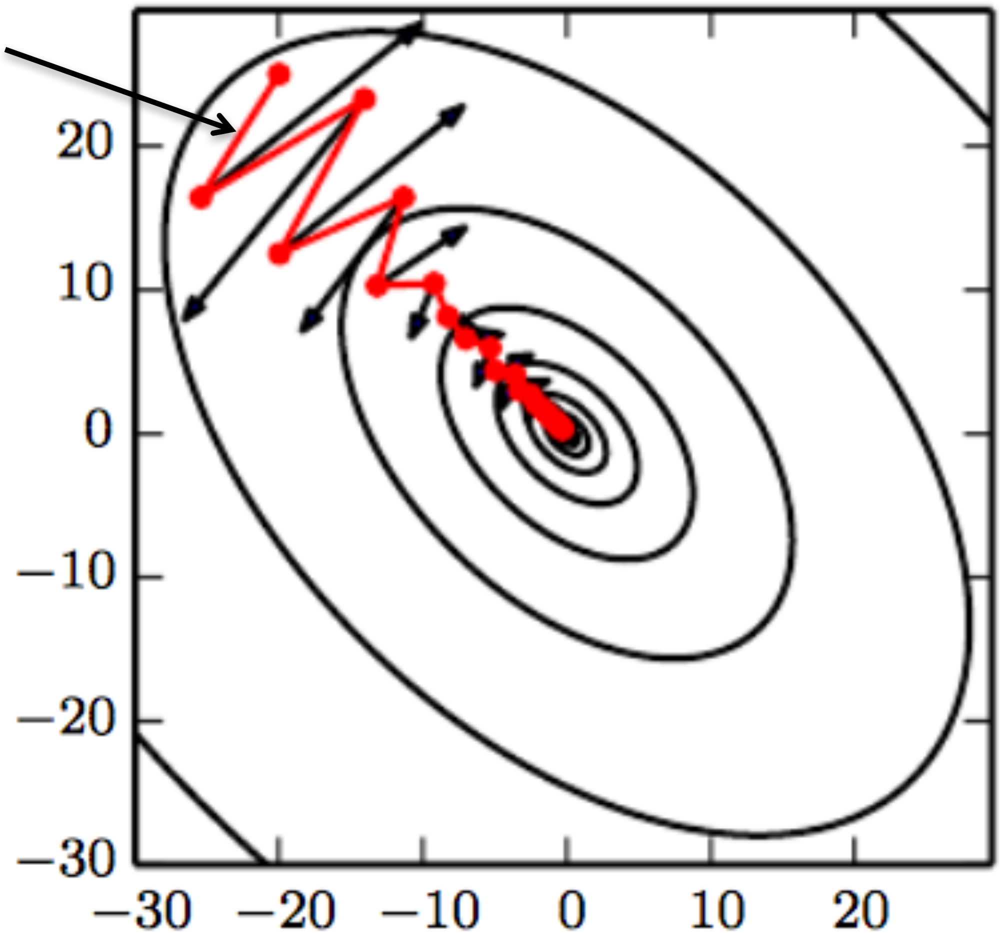
- Update parameters:

$$\theta = \theta + v$$

# Momentum

$J(\theta)$

*Damped oscillations:* gradients in opposite directions get cancelled out




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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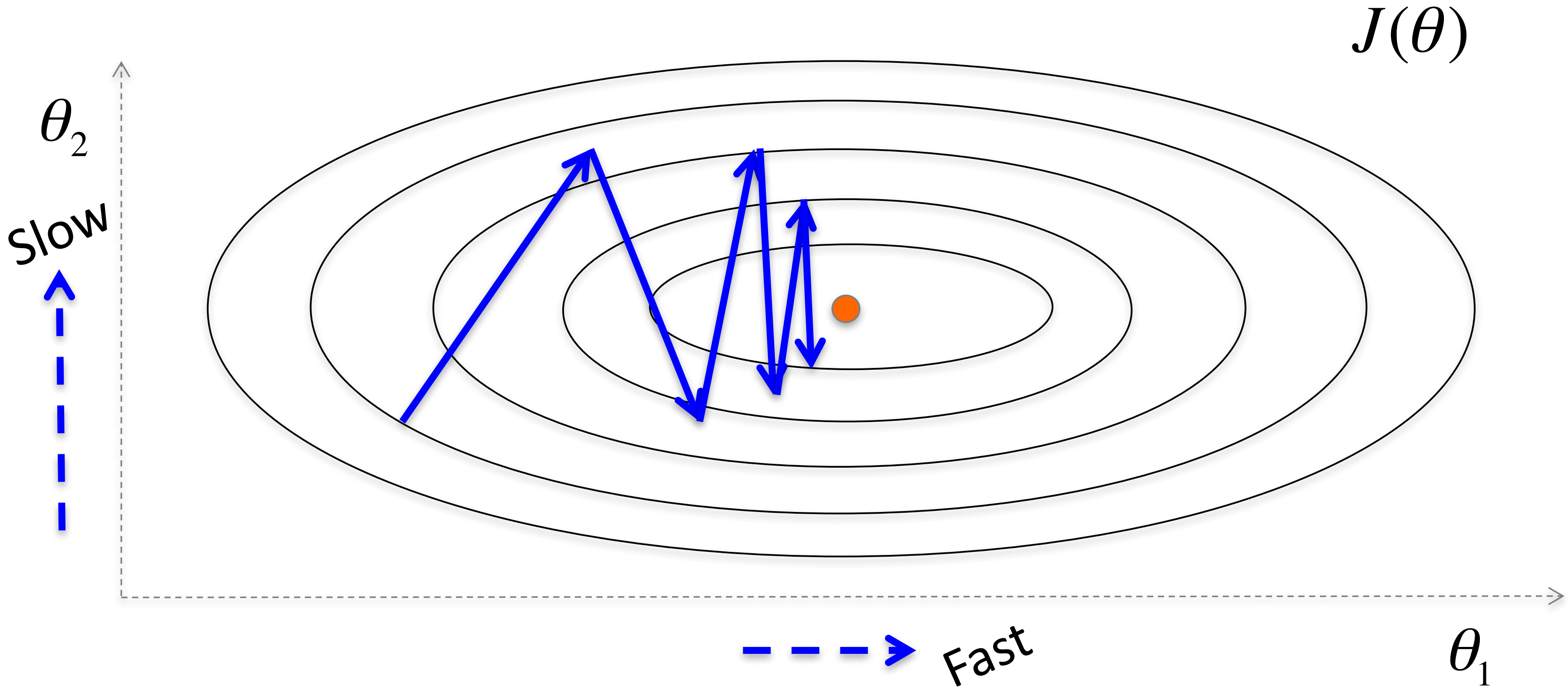
# Adaptive Learning Rates




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

# 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

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# Feature Normalization

- Good practice to normalize features before applying learning algorithm:

Feature vector

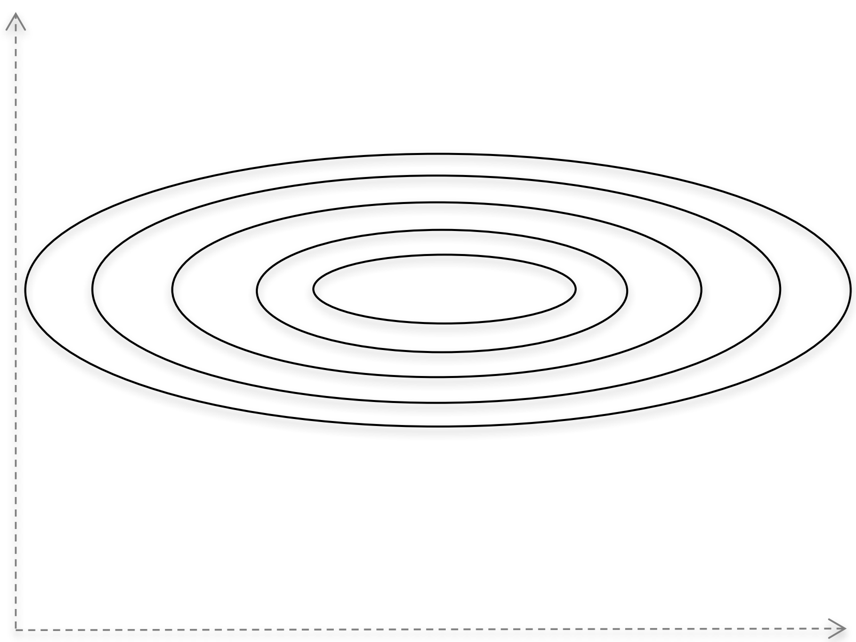
Vector of mean feature values

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

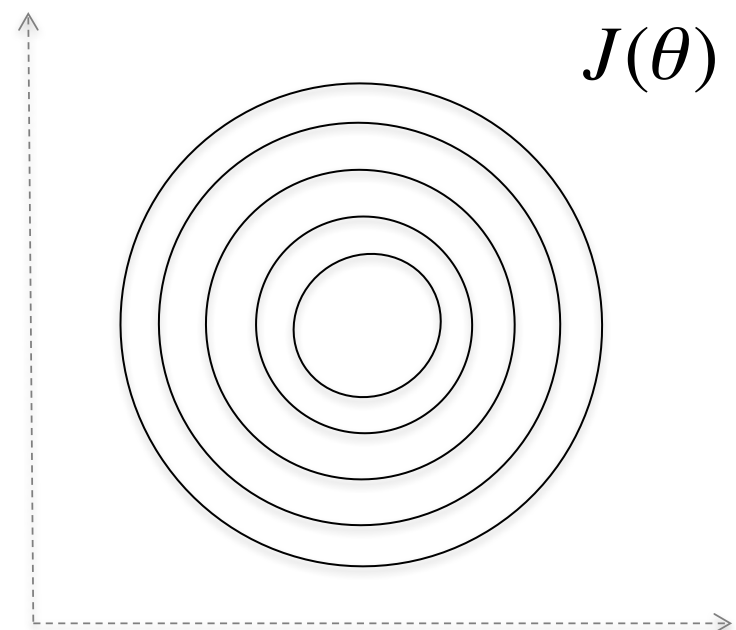
Vector of SD of feature values

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

# Feature Normalization



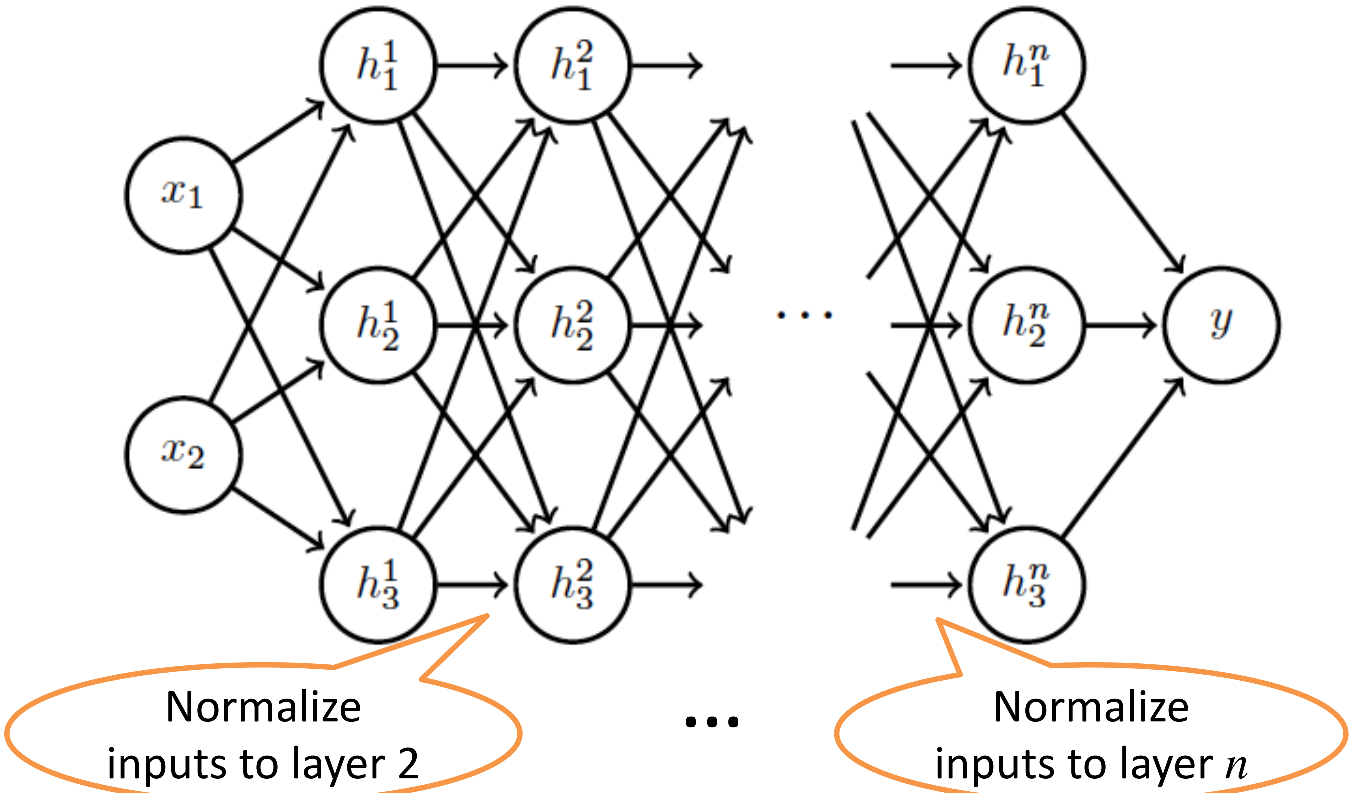
Before normalization




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

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

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:

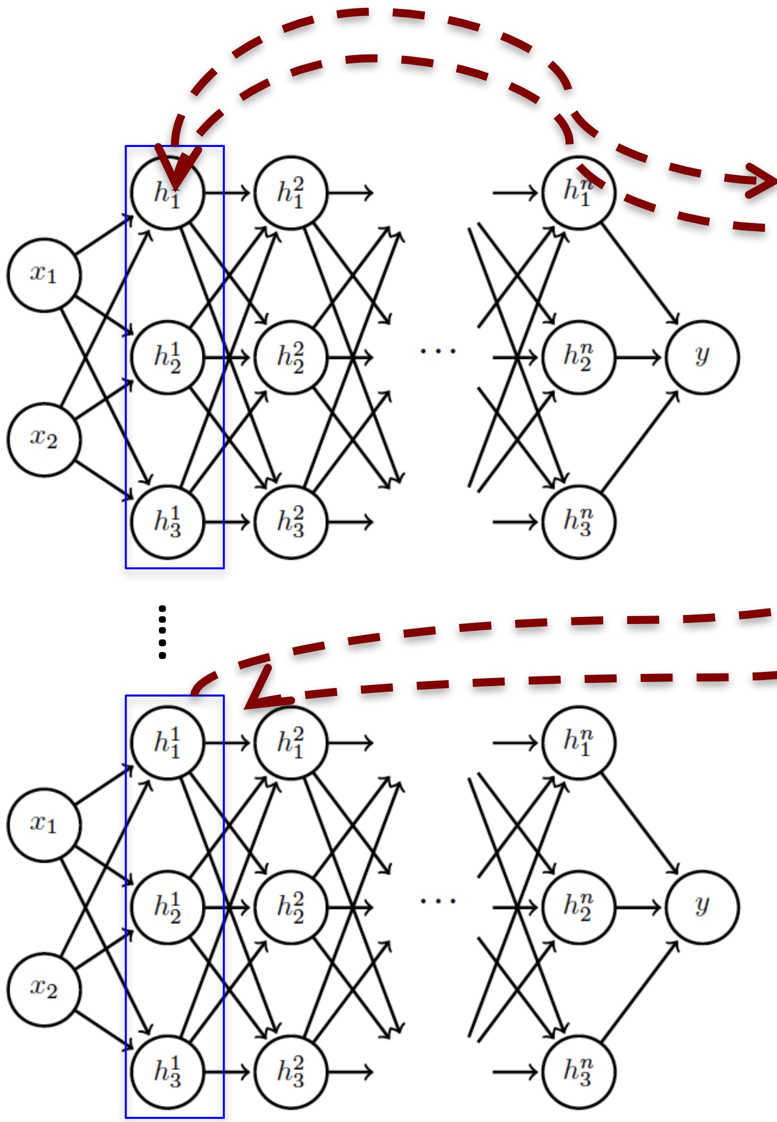
$$\underbrace{\gamma}_{\text{Learnable parameters}} H' + \underbrace{\beta}_{\text{Learnable parameters}}$$

Learnable parameters

  - Allows network to control range of normalization

# Batch Normalization

Batch 1




Batch $N$

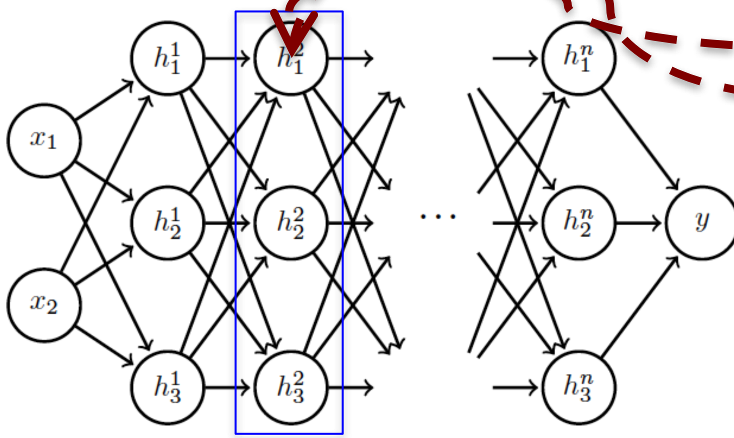
$$\mu^1 = \frac{1}{m}\sum_i H_{i,:}$$

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

Add normalization operations for layer 1

# Batch Normalization

Batch 1

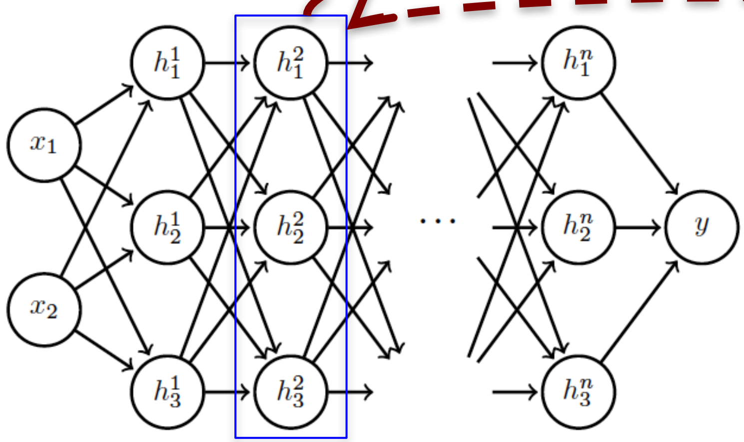



$$\mu^2 = \frac{1}{m}\sum_i H_{i,:}$$

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

⋮

Batch *N*




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 $\mu$ and $\sigma$ with running averages collected during training