Lecture 19 Additional Material: Optimization

CS109A Introduction to Data Science

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Outline

Optimization

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

Learning vs. Optimization

Goal of learning: minimize generalization error

In practice, empirical risk minimization:

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

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

Quantity optimized different from the quantity we care about

Batch vs. Stochastic Algorithms

Batch algorithms

- Optimize empirical risk using exact gradients

Stochastic algorithms

- Estimates gradient from a small random sample

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

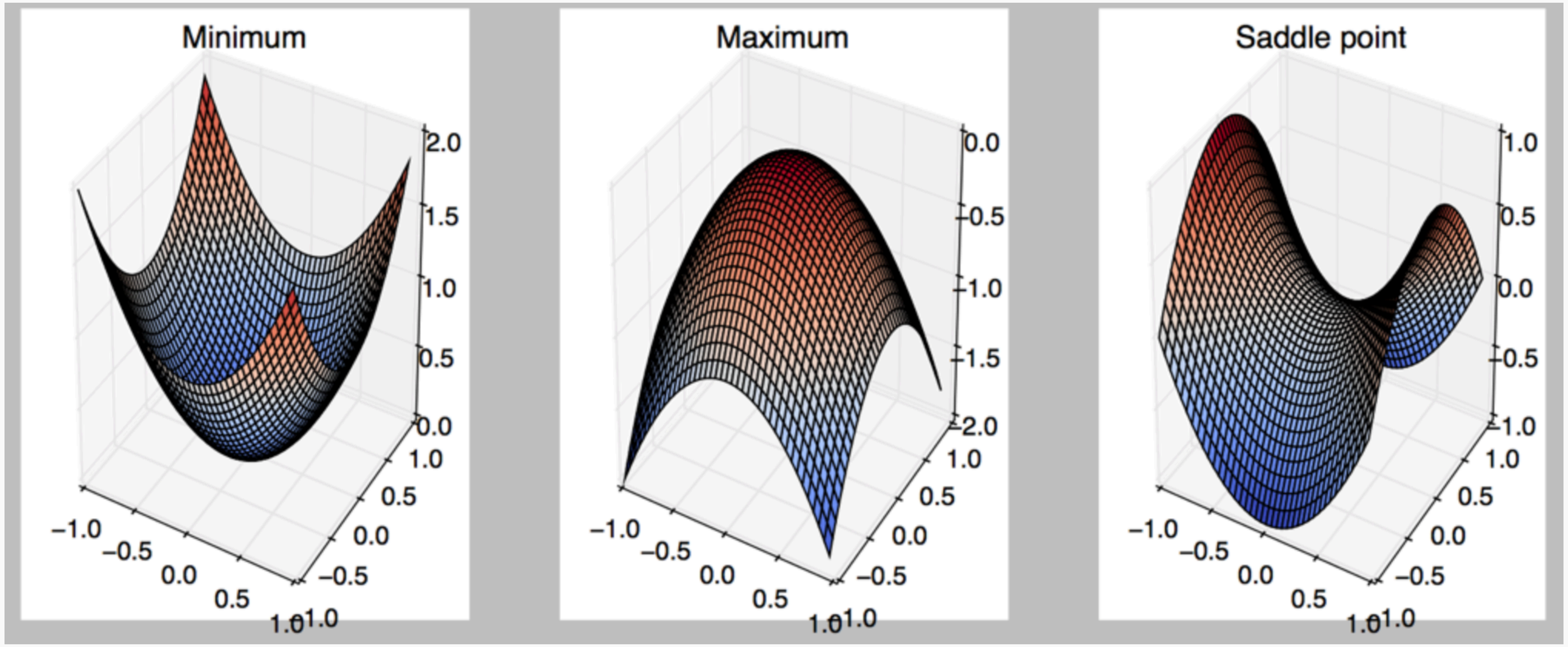
Large mini-batch: gradient computation expensive

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

Critical Points

Points with zero gradient

2nd-derivate (Hessian) determines curvature



Goodfellow et al. (2016)

Stochastic Gradient Descent

Take small steps in direction of negative gradient

Sample *m* examples from training set and compute:

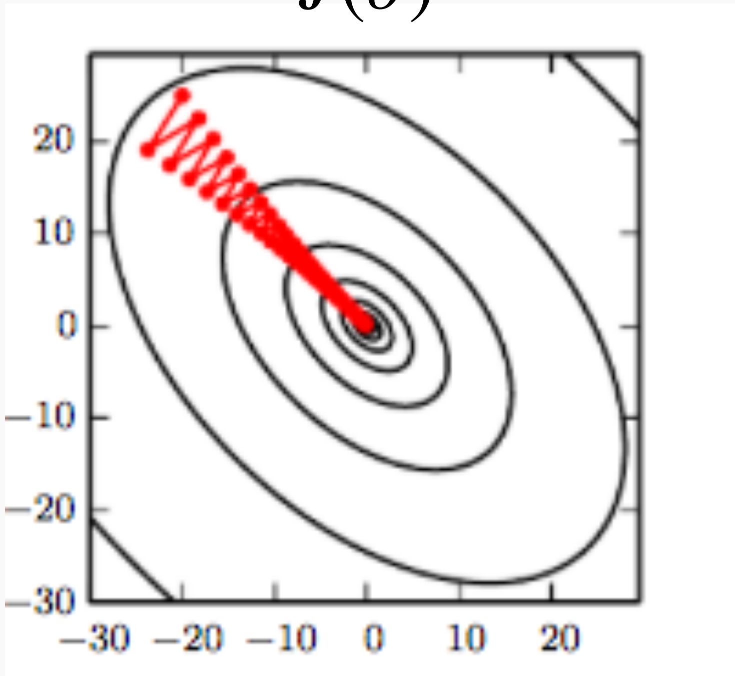
Update parameters: $$g = \frac{1}{m}\sum_i \nabla L(f(x^{(i)};\theta), y^{(i)})$$

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

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

Stochastic Gradient Descent

$J(\theta)$



Oscillations because updates do not exploit curvature information

Goodfellow et al. (2016)

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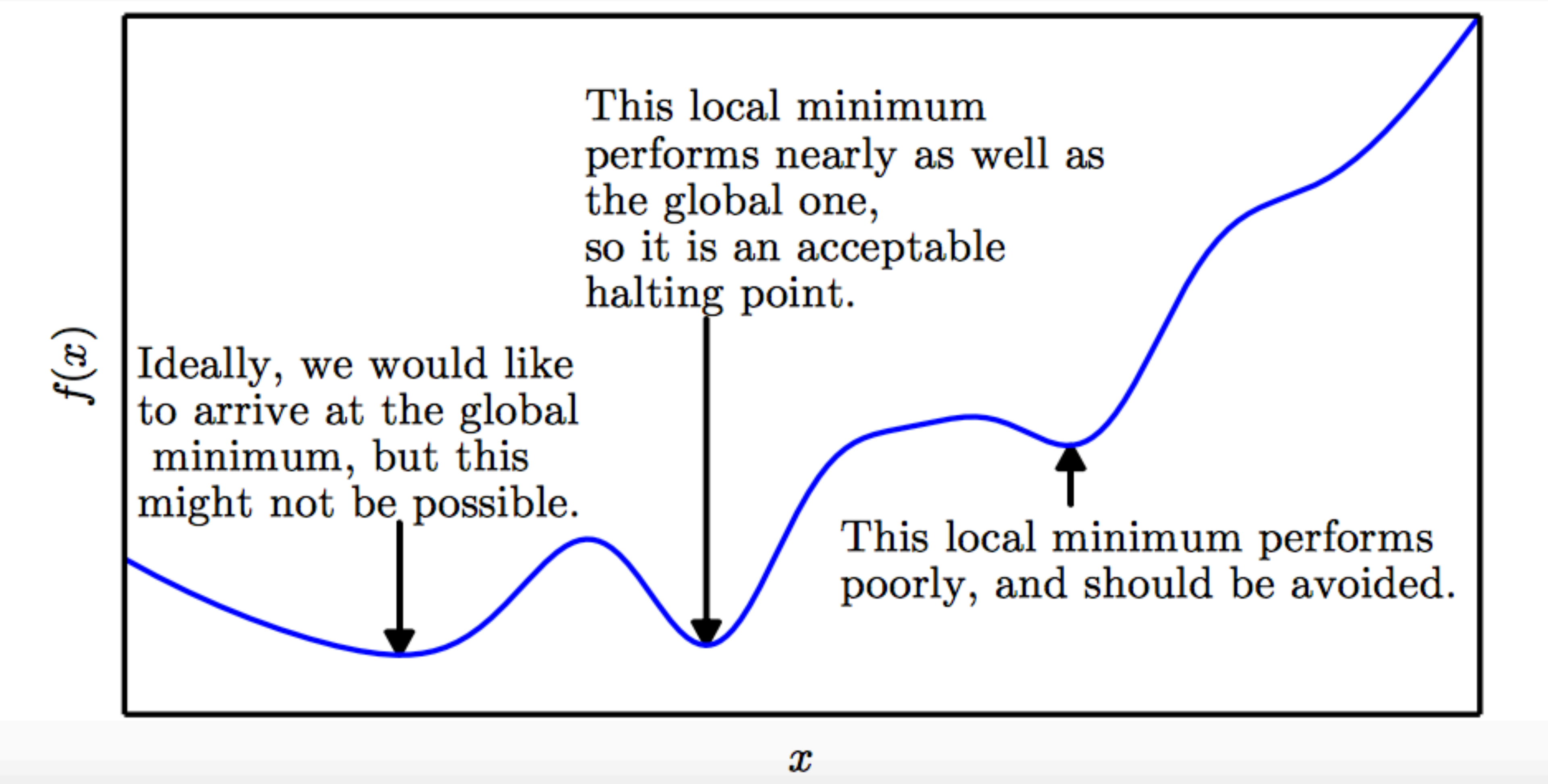
Local Minima



Goodfellow et al. (2016)

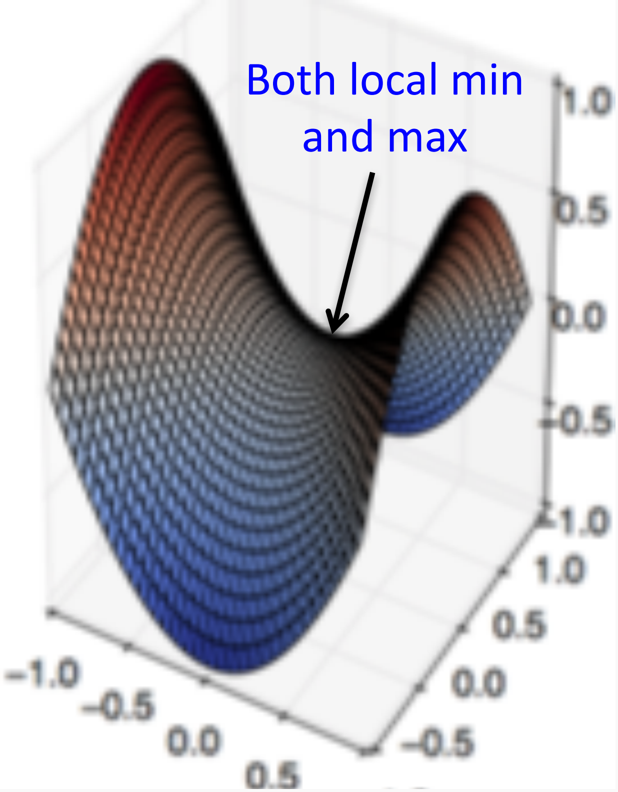
Local Minima

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

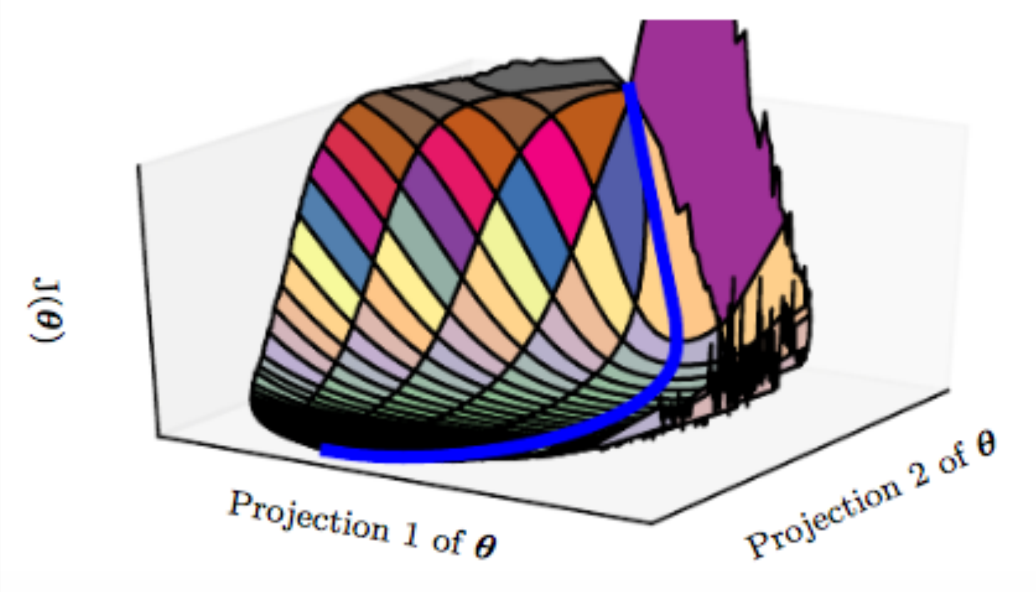
Gradient can be very small near saddle points

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)

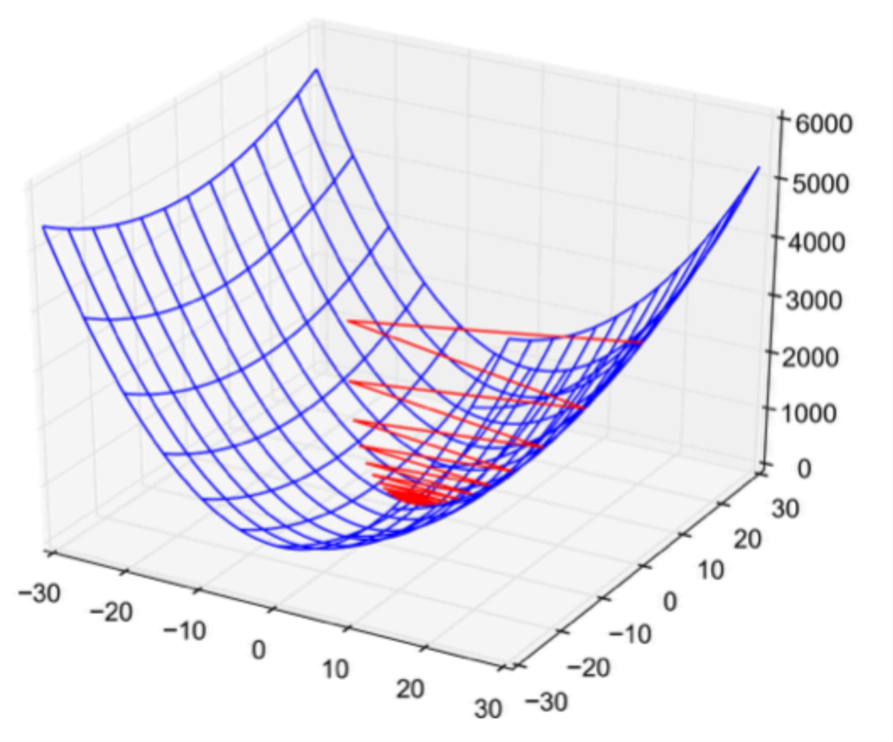
Poor Conditioning

Poorly conditioned Hessian matrix

- High curvature: small steps leads to huge increase

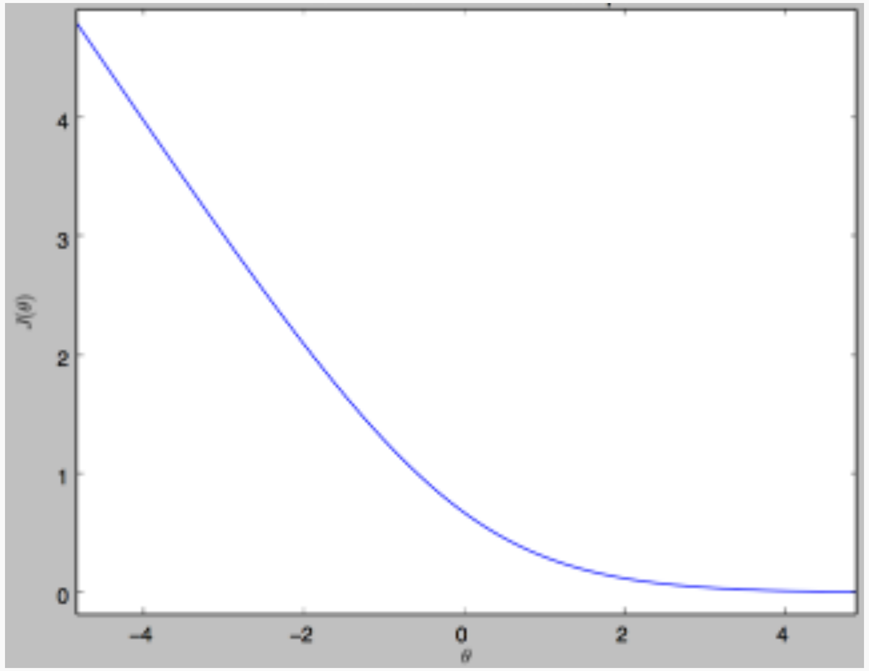
Learning is slow despite strong gradients

Oscillations slow down progress



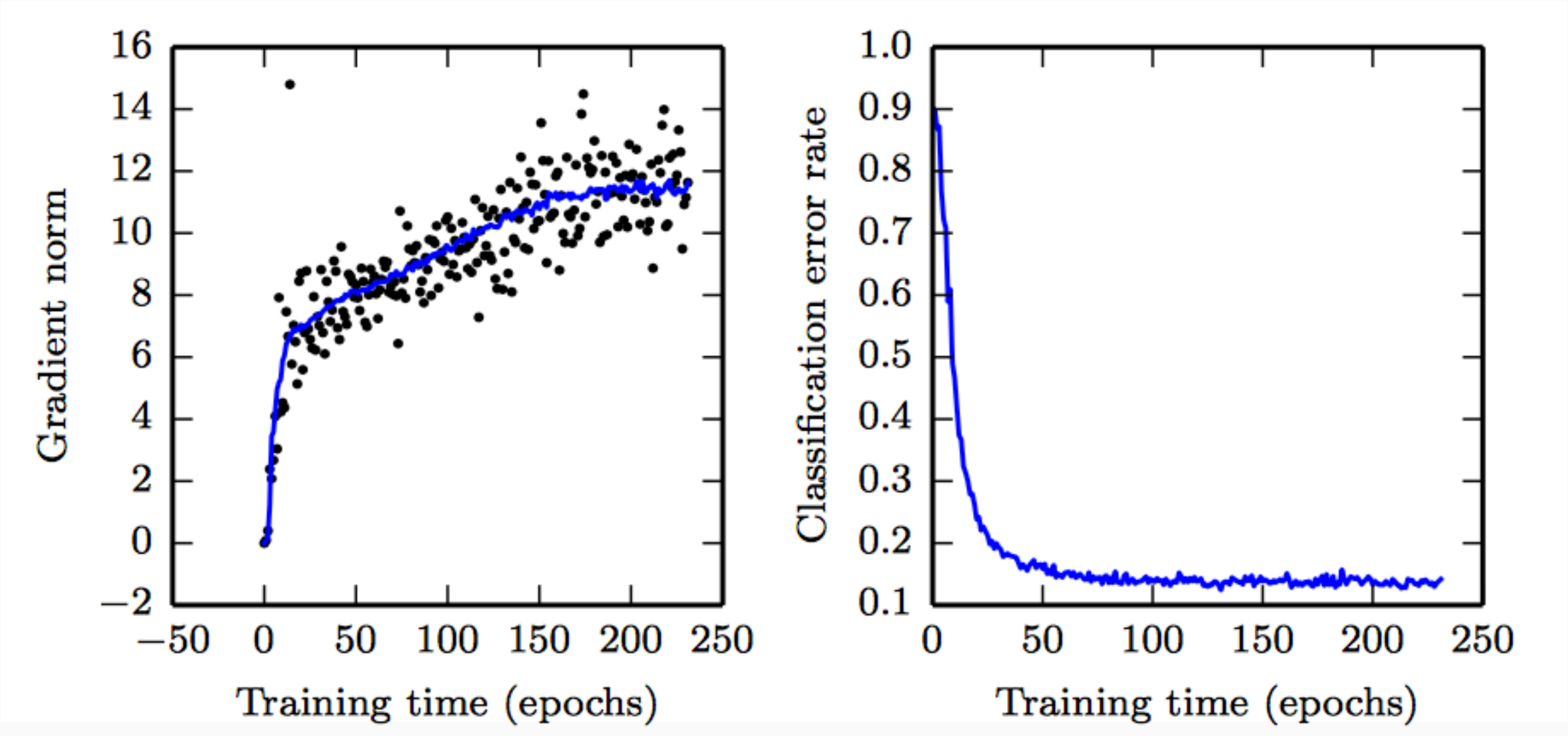
No Critical Points

Some cost functions do not have critical points. In particular classification.



No Critical Points

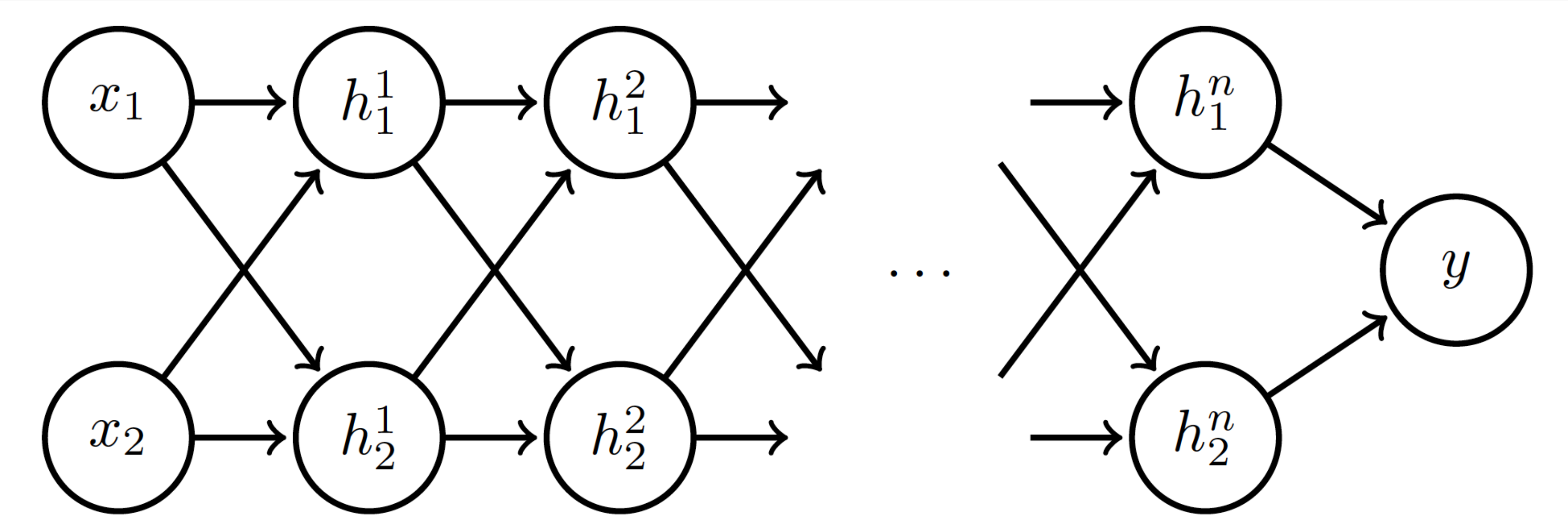
Gradient norm increases, but validation error decreases



Convolution Nets for Object Detection

Goodfellow et al. (2016)

Exploding and Vanishing Gradients



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

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

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

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

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

Exploding and Vanishing Gradients

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

$$\text{Case 1:} \;\; a = 1, \; b = 2:$$

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

Explodes!

$$\text{Case 2:} \;\; a = 0.5, \; b = 0.9:$$

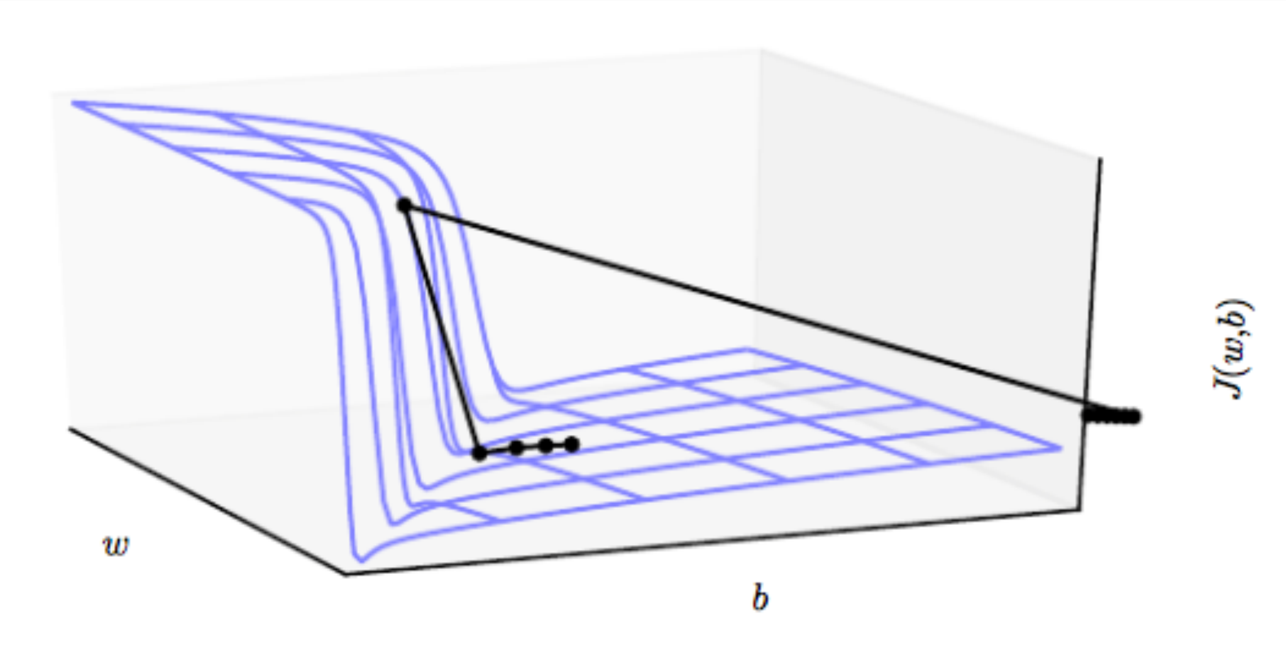
$$y \to 0, \quad \nabla y \to \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Vanishes!

Exploding and Vanishing Gradients

Exploding gradients lead to cliffs

Can be mitigated using gradient clipping



Goodfellow et al. (2016)

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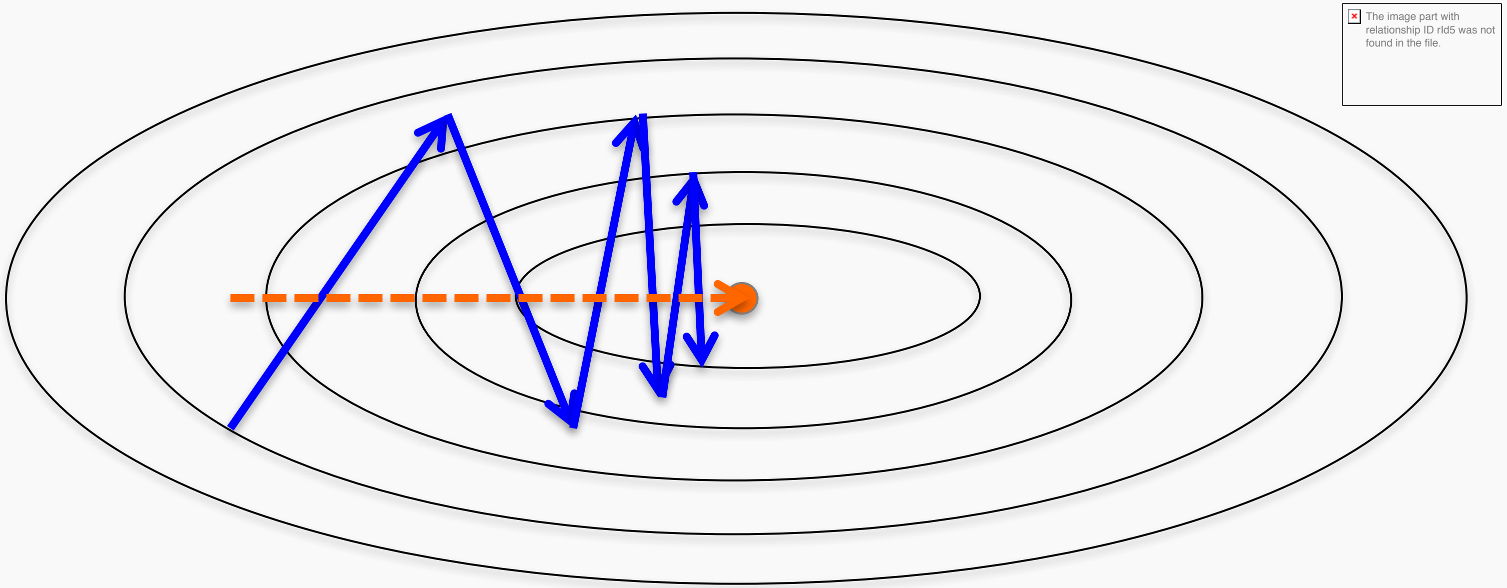
Momentum

SGD is slow when there is high curvature



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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

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

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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

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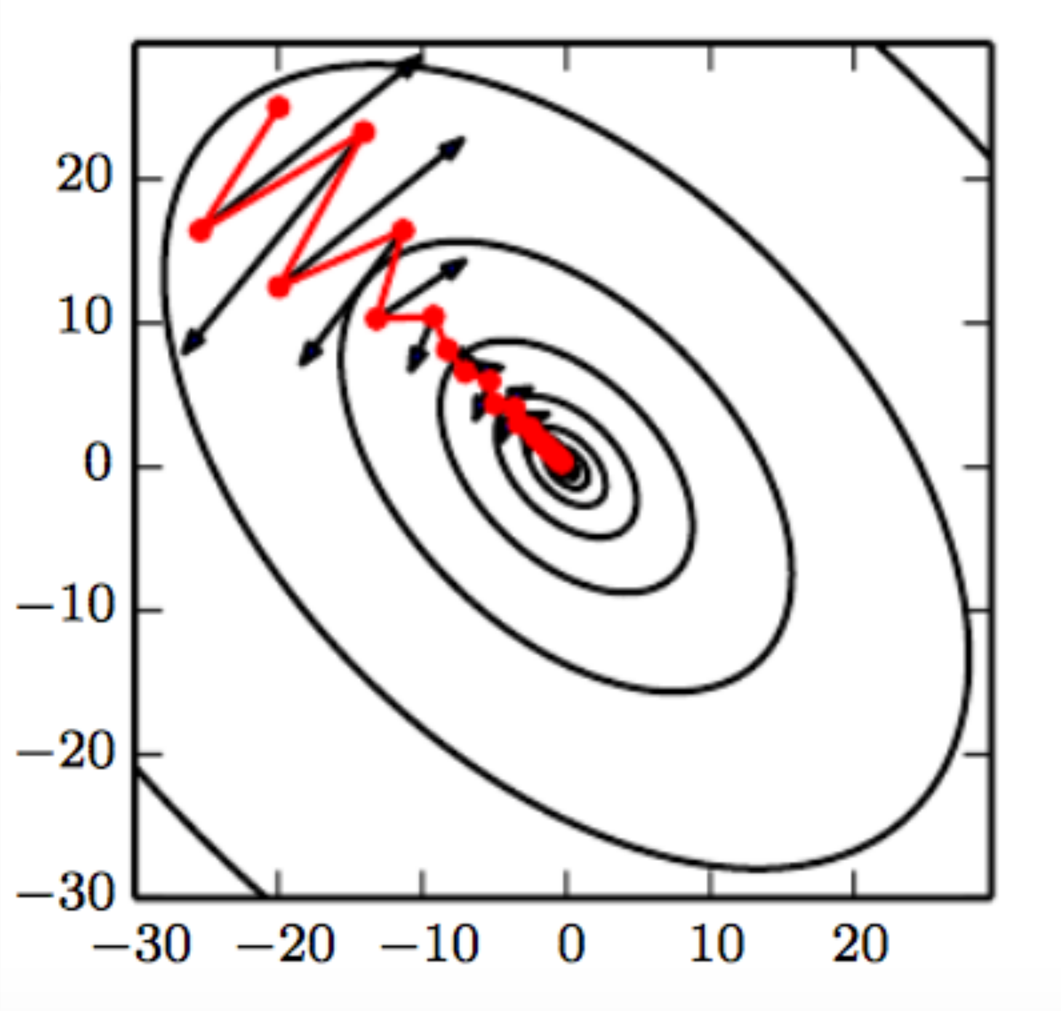
Damped oscillations: gradients in opposite directions get cancelled out



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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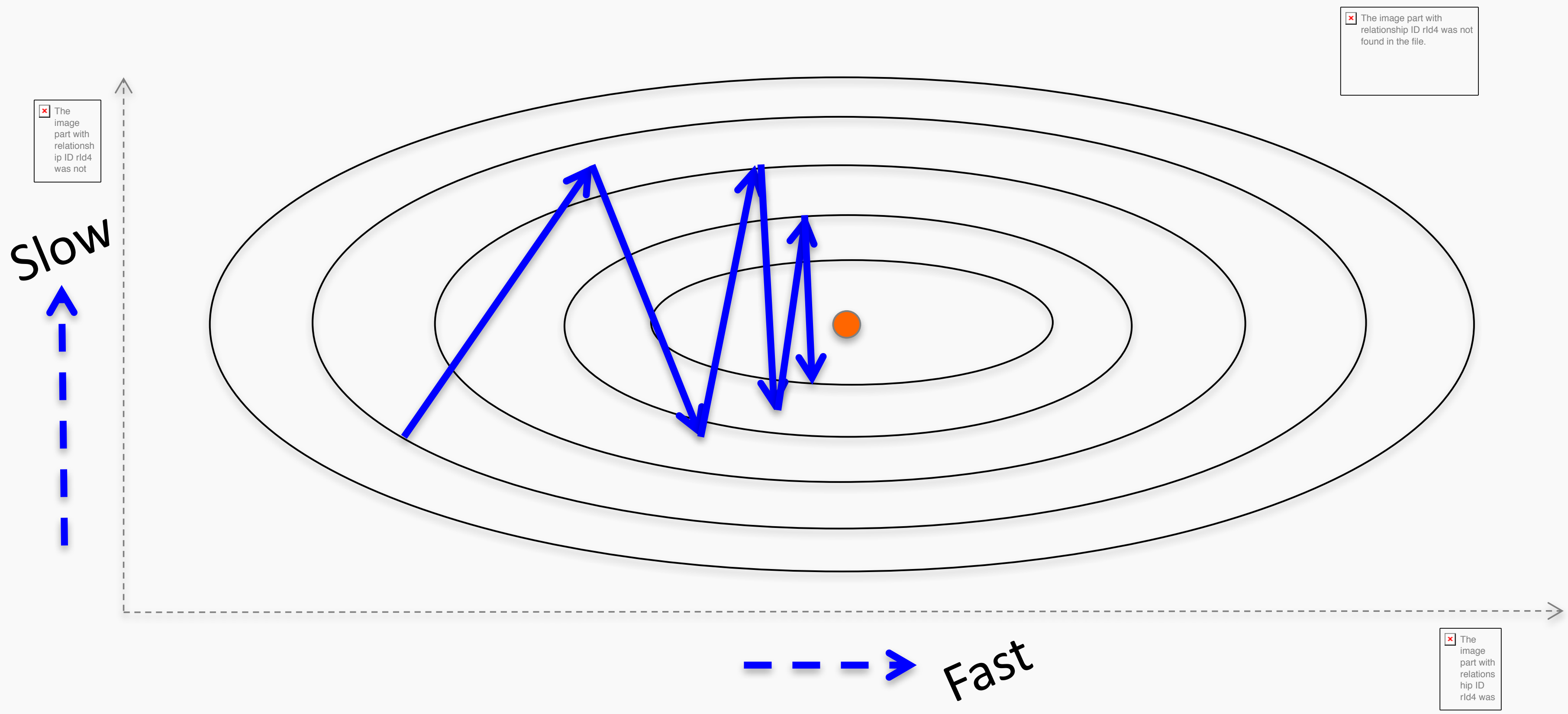
Adaptive Learning Rates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Slow
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Oscillations along vertical direction

– 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

Outline

Challenges in Optimization

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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

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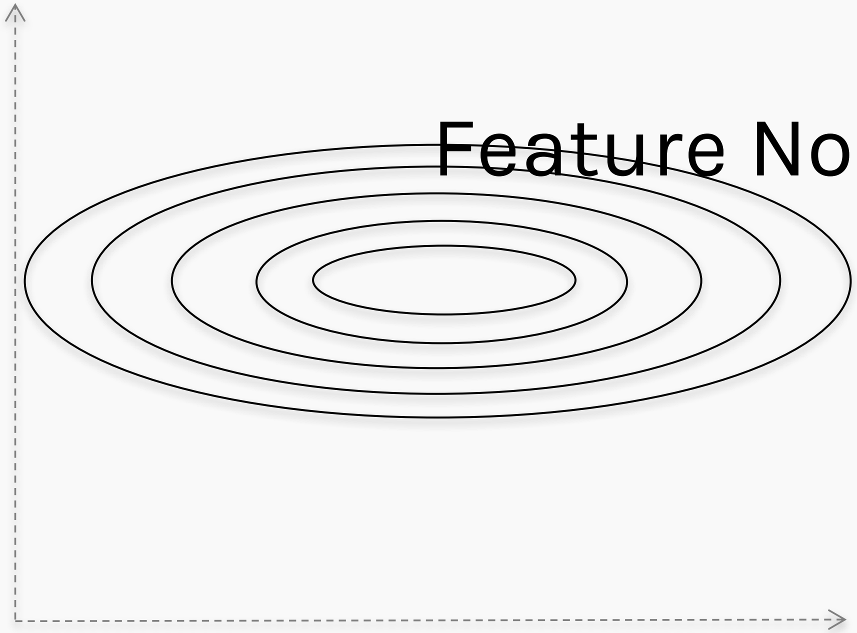
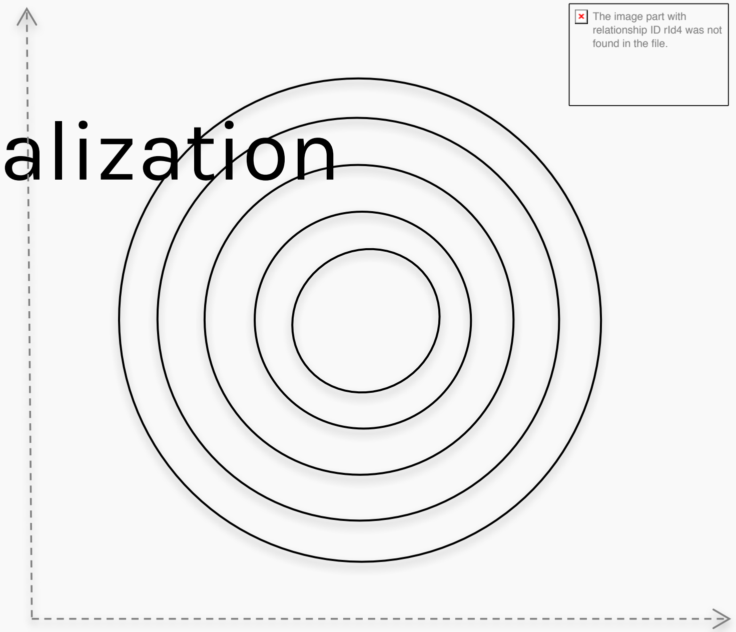


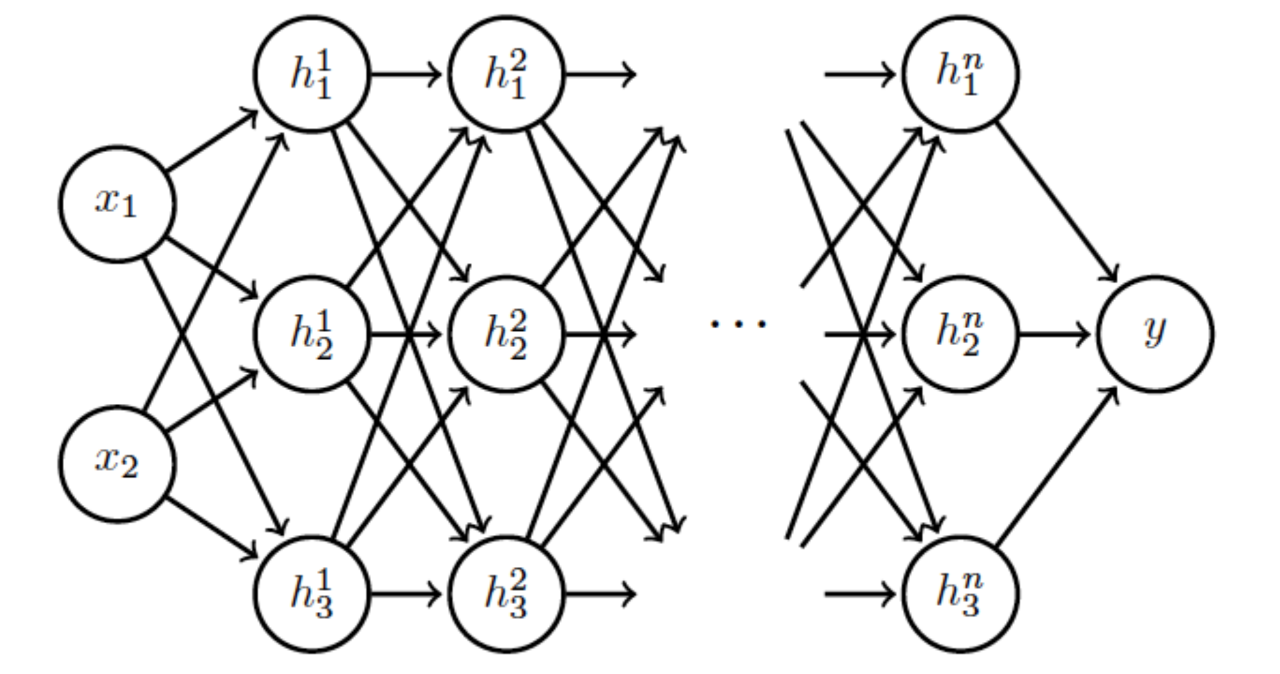
Before normalization



After normalization

Internal Covariance Shift

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



Normalize inputs to layer 2

...

Normalize inputs to layer n

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

where

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

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

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:

$$\gamma H' + \beta$$

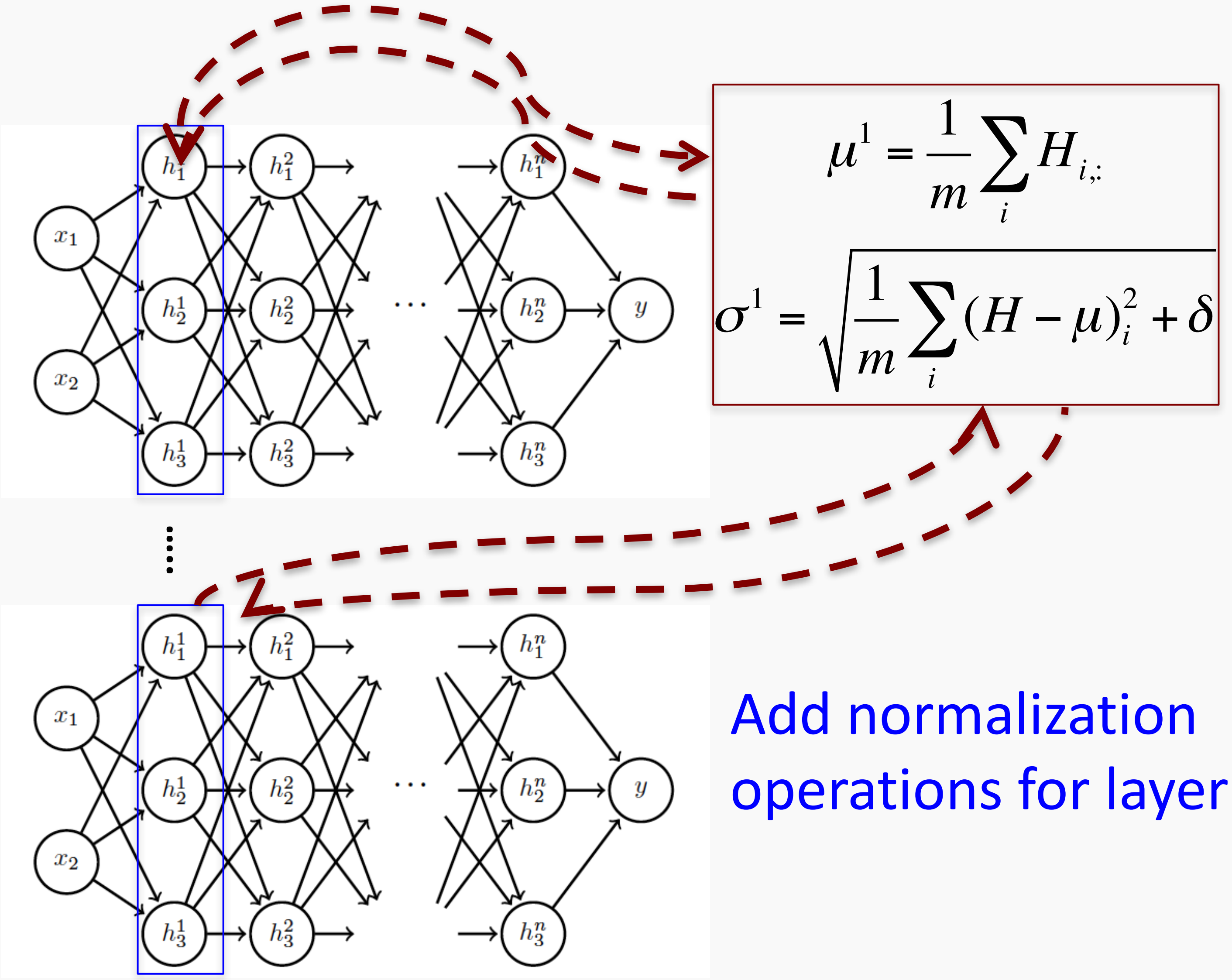
Learnable parameters

- Allows network to control range of normalization

Batch Normalization

Batch 1

Batch *N*



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

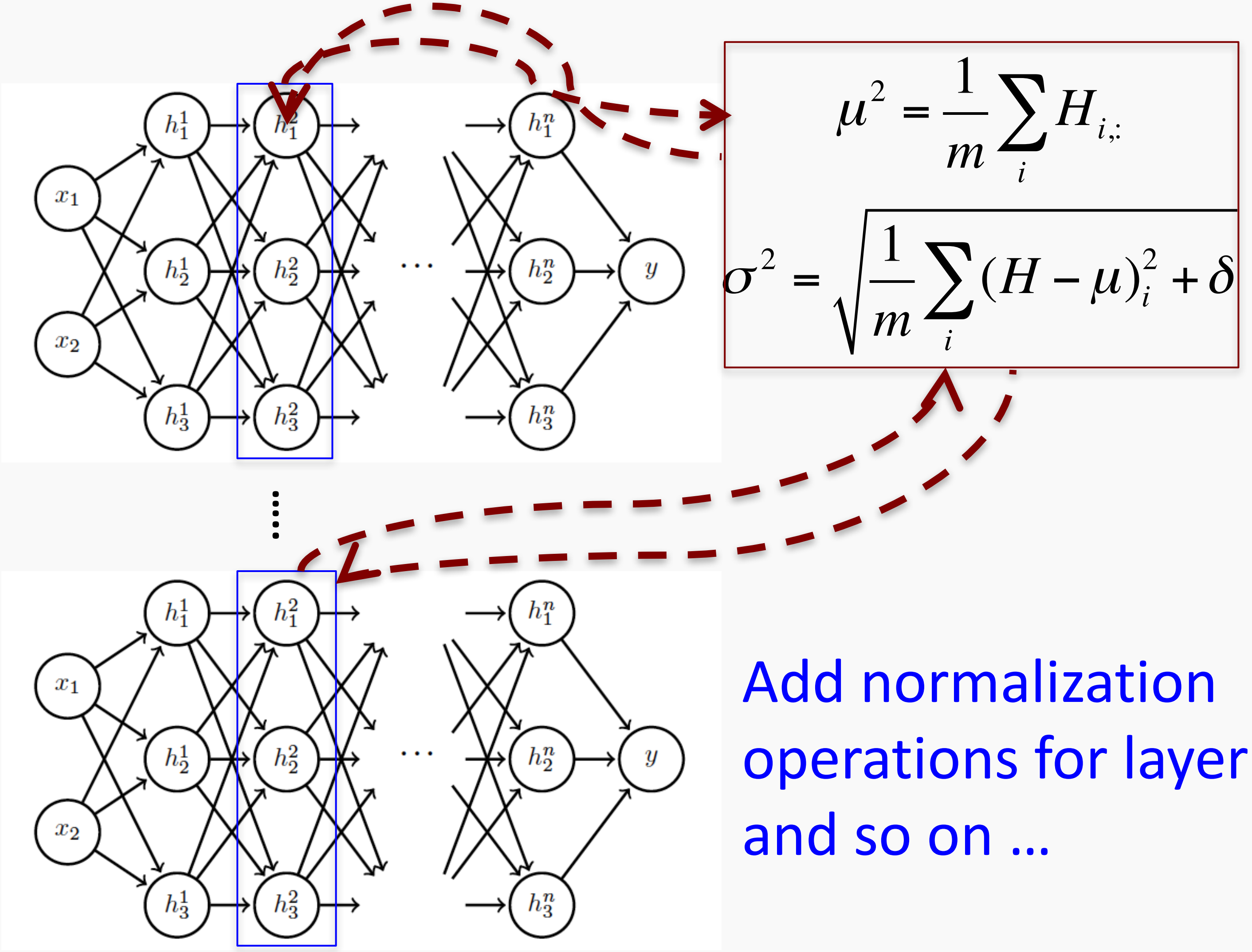
$$\sigma^1 = \sqrt{\frac{1}{m}\sum_i (H-\mu)_i^2 + \delta}$$

Add normalization operations for layer 1

Batch Normalization

Batch 1

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