10-05/10-805: Machine Learning with Large Datasets

Fall 2022

Optimization for Deep Learning

Announcements

- HW4b due on Thursday
- Recitation this week will be a discussion on step size/learning rate tuning

Key course topics

Data preparation
- Data cleaning
- Data summarization
- Visualization
- Dimensionality reduction

Training
- Distributed ML
- **Large-scale optimization**
- **Scalable deep learning**
- Efficient data structures
- Hyperparameter tuning

Inference
- Hardware for ML
- Techniques for low-latency inference (compression, pruning, distillation)

Infrastructure / Frameworks
- Apache Spark
- TensorFlow
- AWS / Google Cloud / Azure

Advanced topics
- Federated learning
- Neural architecture search
- Productionizing ML

MOVING FORWARD

What makes deep learning expensive?

Training requires lots of computation

- Specialized hardware (GPUs, TPUs) can help with matrix computations
- Can use advanced iterative optimization methods
- Can parallelize training

Hyperparameter tuning and neural architecture search (NAS) make this worse

- Lots of knobs to tune!

Resulting models can be large!

- Can be expensive to store model, perform inference

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Outline

1. Optimization review
2. DL Optimization: adaptive learning rates, momentum
3. Other tricks: early stopping, batch norm

RECALL

Empirical risk minimization

$$\hat{f}_n = \arg\min_{f \in F} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i)$$

- A popular approach in supervised ML
- Given a loss ℓ and data (x_1, y_1), … (x_n, y_n), we estimate a predictor *f* by minimizing the *empirical risk*
- We typically restrict this predictor to lie in some class, *F*
  - Could reflect our prior knowledge about the task
  - Or may be for computational convenience

Question: how should we select our function class, *F*, and our loss function, ℓ ??

RECALL

Previous assumption: linear models

$$\hat{f}_n = \arg\min_{f \in F} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i)$$

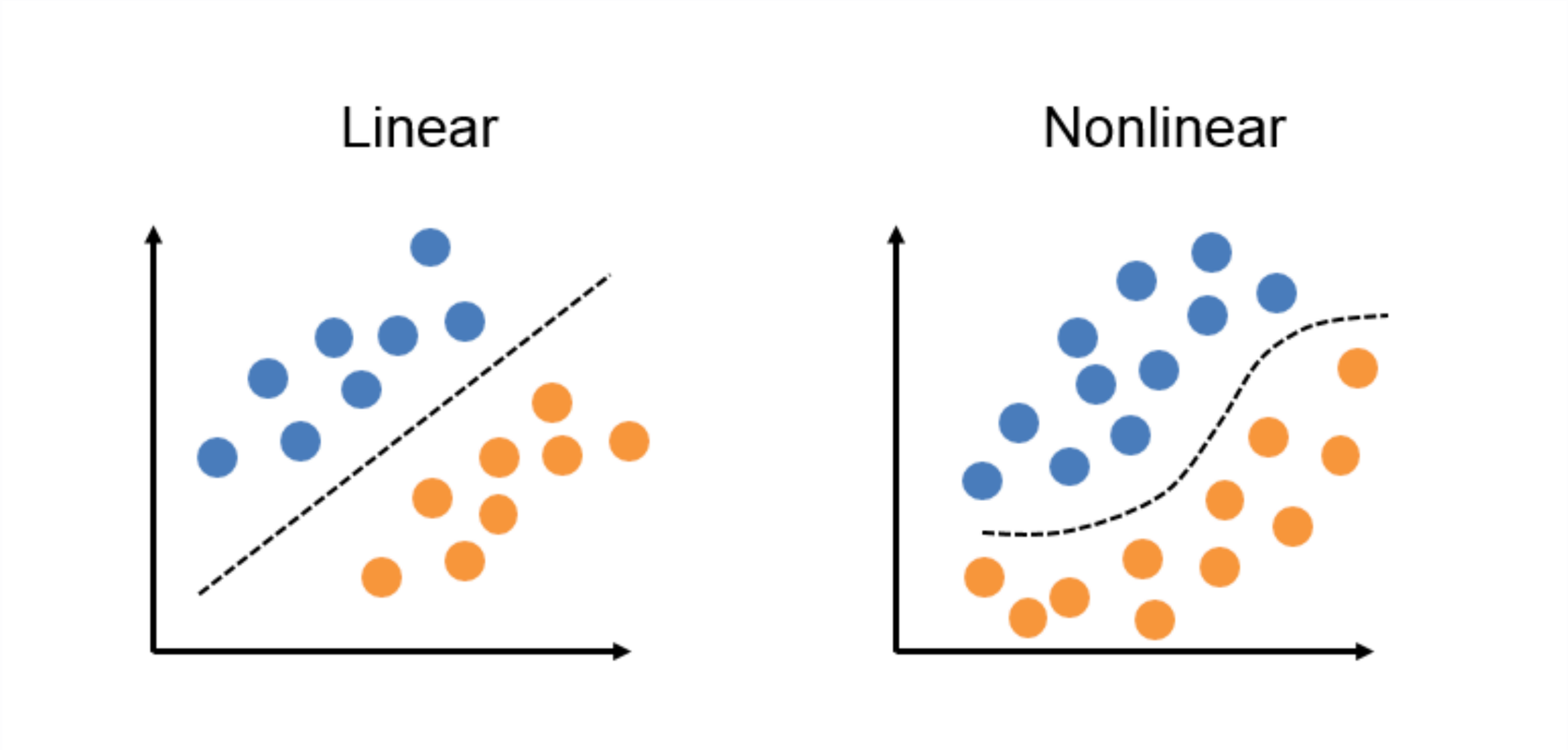
Assume: $f(\mathbf{x}) = \mathbf{w}^\top \mathbf{x}$

Losses:

- Square loss: linear regression $\min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^{n} (\mathbf{w}^\top \mathbf{x}_i - y_i)^2$
- Log loss: logistic regression $\min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^{n} \ell_{log}(y_i \cdot \mathbf{w}^\top \mathbf{x}_i)$
- Hinge loss: SVMs $\min_{\mathbf{w}} \frac{1}{n} \sum_{i=1}^{n} \max\{0, 1 - y_i \cdot \mathbf{w}^\top \mathbf{x}_i\}$

RECALL

Not all data is linear …



How can we learn more complicated hypotheses?

ONE APPROACH

Neural networks

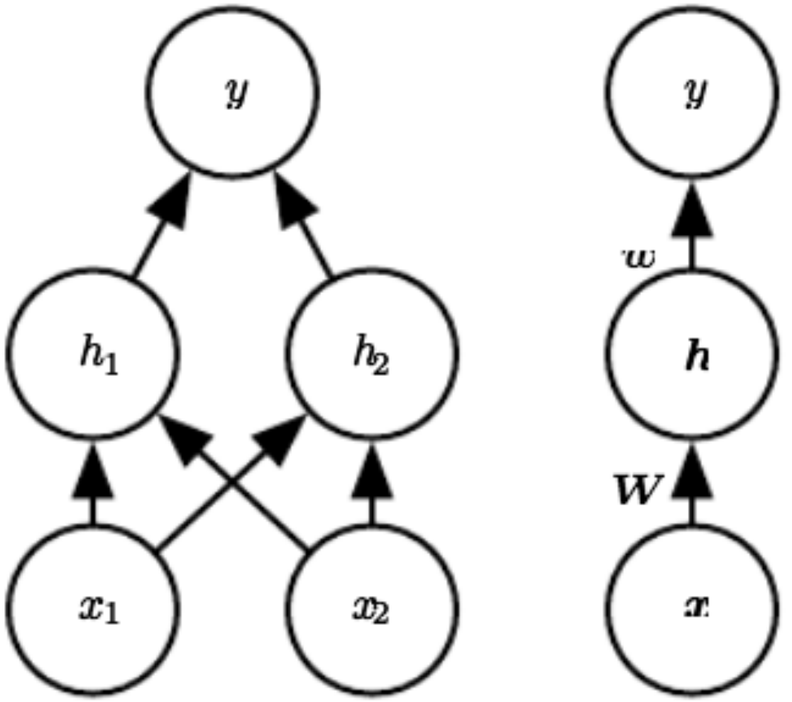
Goal: apply a nonlinear transformation to our input data: $f(\mathbf{x}) = \mathbf{w}^\top \phi(\mathbf{x}; \theta)$

Neural networks provide a way to learn such a transformation

Simple approach: feedforward neural networks

- E.g., suppose we have: $\phi(\mathbf{x}; \mathbf{W}) = \sigma(\mathbf{W}^\top \mathbf{x})$
- Then: $f(\mathbf{x}) = \mathbf{w}^\top \sigma(\mathbf{W}^\top \mathbf{x})$

$\sigma(\cdot)$ is referred to as an *activation function*



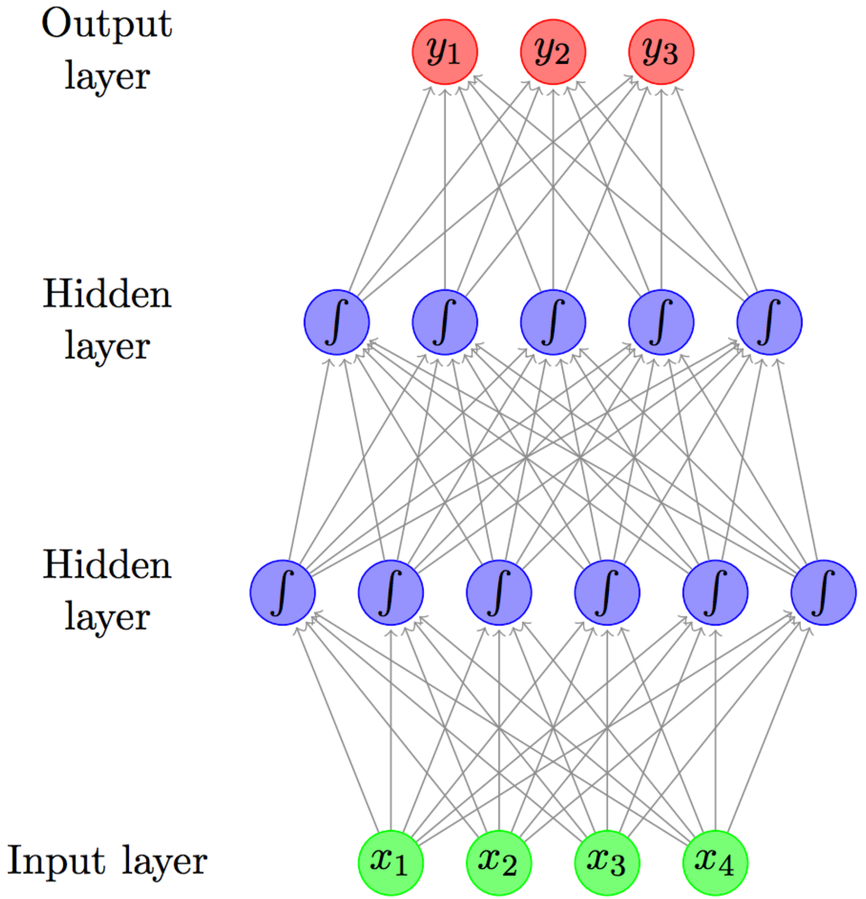
an example of a feedforward network with *one* hidden layer containing *two* units

MORE GENERALLY

Feedforward neural networks

We can consider adding L hidden layers, each with their own activation functions σ_l and corresponding weights $\mathbf{W}_l$

Using this layering technique, the resulting model becomes:



$$f(\mathbf{x}) = \mathbf{w}^\top \sigma_L(\mathbf{W}_L^\top(\sigma_{L-1}(\mathbf{W}_{L-1}^\top \ldots \sigma_2(\mathbf{W}_2^\top \sigma_1(\mathbf{W}_1^\top \mathbf{x}))\ldots)$$

QUESTION

How do we train neural networks?

$$\hat{f}_n = \arg\min_{f \in F} \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), y_i)$$

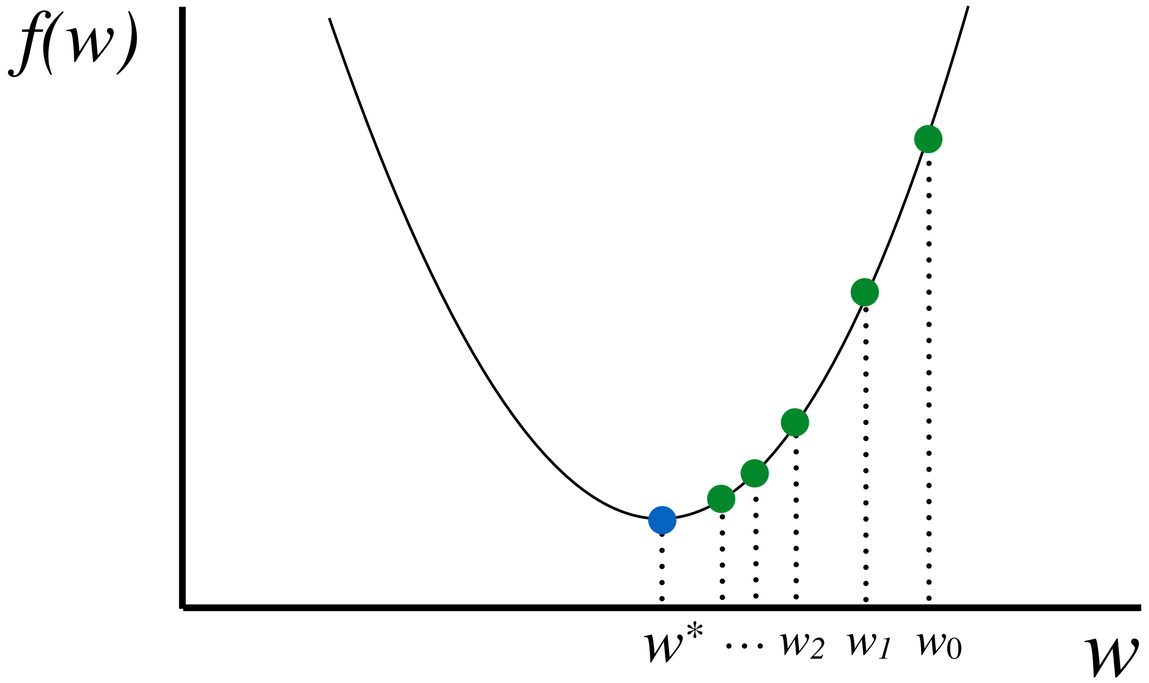
- A popular approach in supervised ML
- Given a loss ℓ and data (x_1, y_1), … (x_n, y_n), we estimate a predictor *f* by minimizing the *empirical risk*
- We typically restrict this predictor to lie in some class, *F*
  - Could reflect our prior knowledge about the task
  - Or may be for computational convenience

To train: solve the ERM objective via an iterative optimization method

RECALL

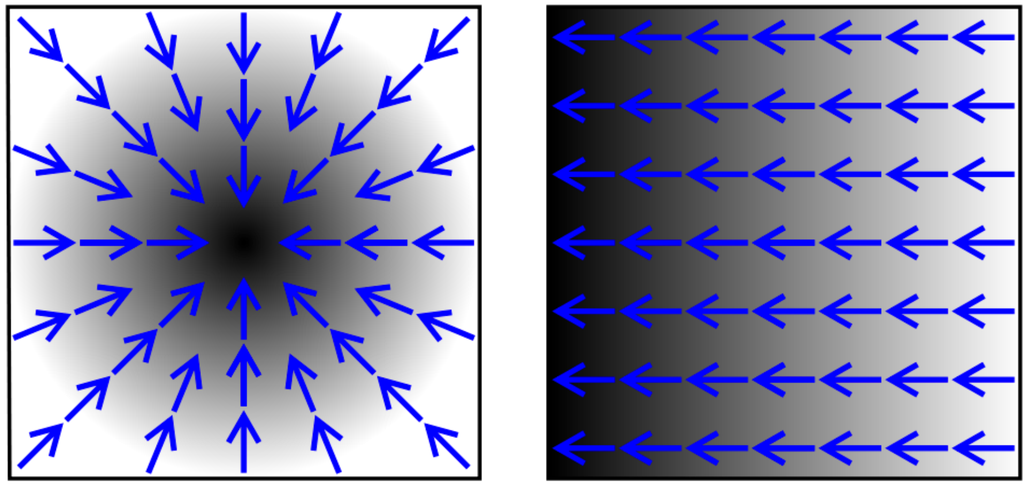
Gradient descent

Start at a random point
Repeat
    Determine a descent direction
    Choose a step size
    Update
Until stopping criterion is satisfied



RECALL

Choosing a descent direction



"Gradient2" by Sarang. Licensed under CC BY-SA 2.5 via Wikimedia Commons
http://commons.wikimedia.org/wiki/File:Gradient2.svg#/media/File:Gradient2.svg

2D Example:

- Function values are in black/white and black represents higher values
- Arrows are gradients

We can move anywhere in $\mathbb{R}^d$

Negative gradient is direction of *steepest* descent!

Step Size

Update Rule: $\mathbf{w}_{i+1} = \mathbf{w}_i - \alpha_i \nabla f(\mathbf{w}_i)$

Negative Slope

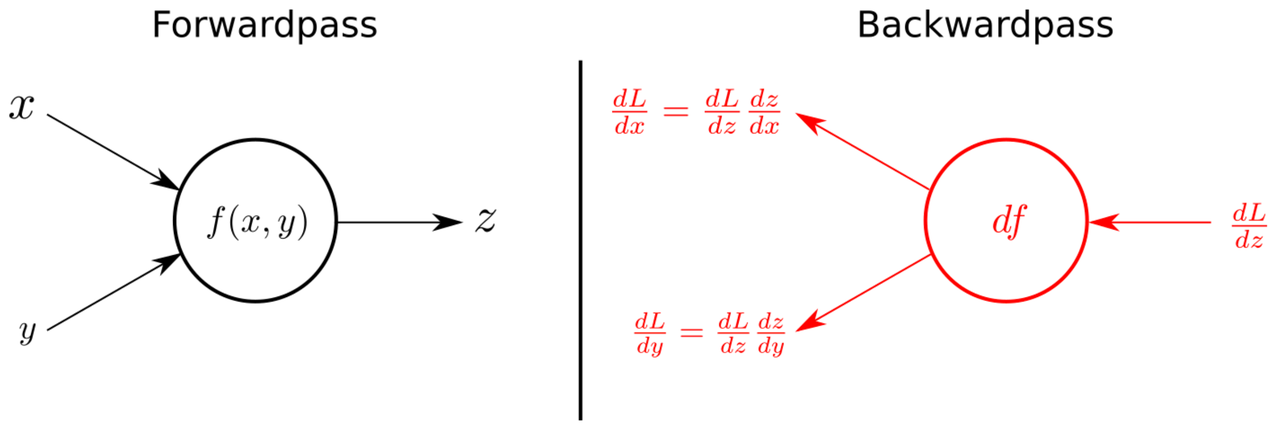
RECALL

How are gradients computed for NNs?

Backpropagation: efficiently computes the gradient of a feedforward neural network

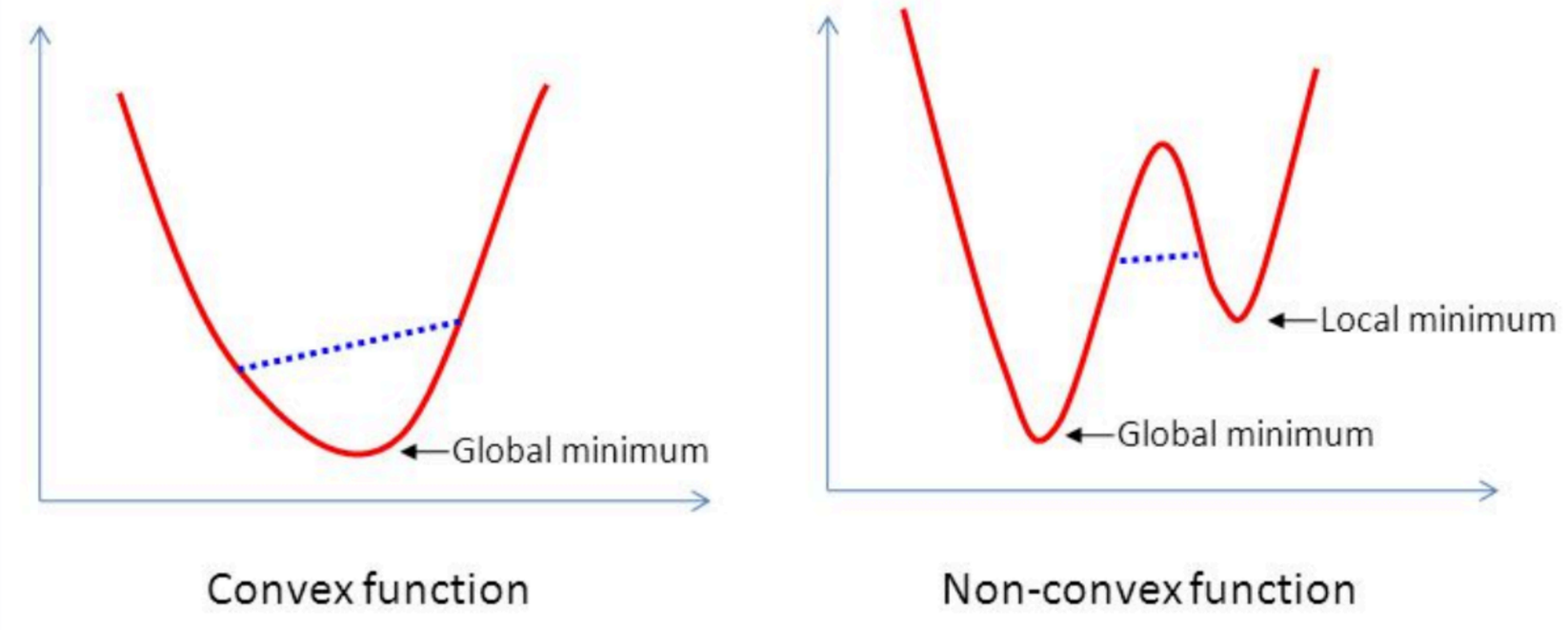
Two main steps:

- *forward pass*: traverse through the network normally, as if we were computing the function value, and save all intermediate values
- *backward pass*: proceed backwards through the network, computing gradients of the function value with respect to intermediates



CHALLENGE

Non-convexity



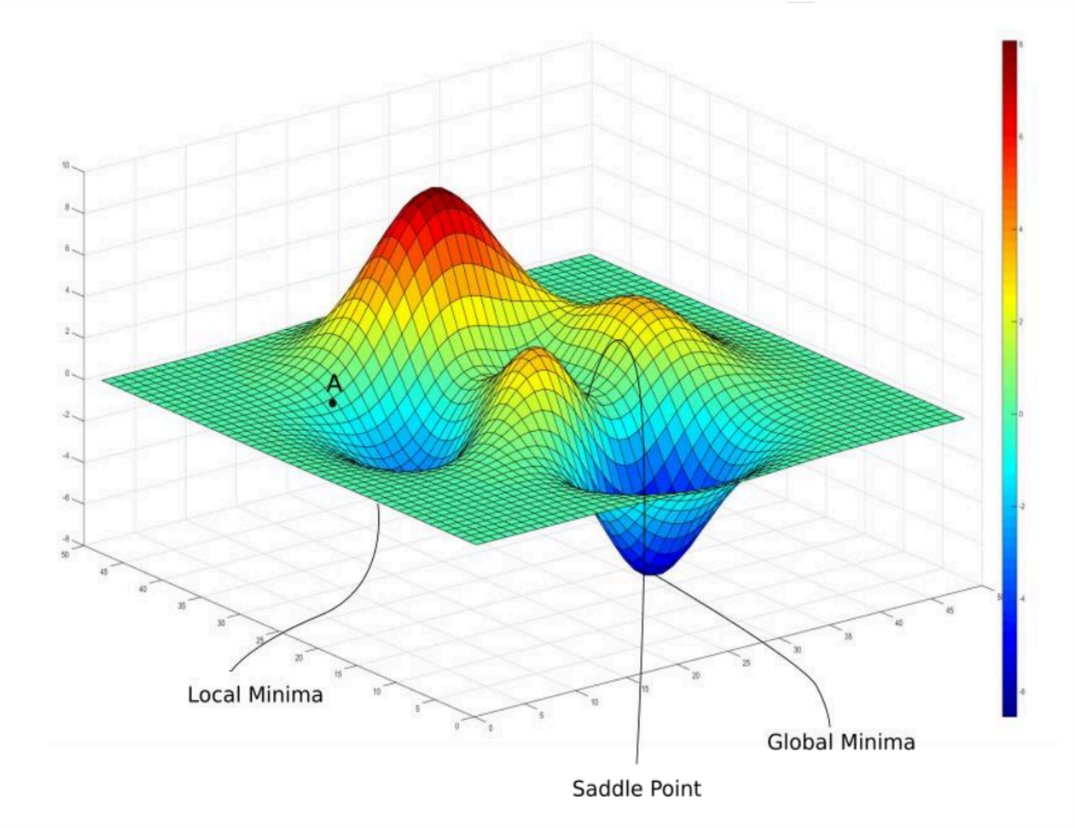
Deep neural networks are non-convex

How would a method like gradient descent work on non-convex objectives?

Can find *stationary points,* i.e., points where $\nabla f(x) \approx 0$

CHALLENGE

Non-convexity

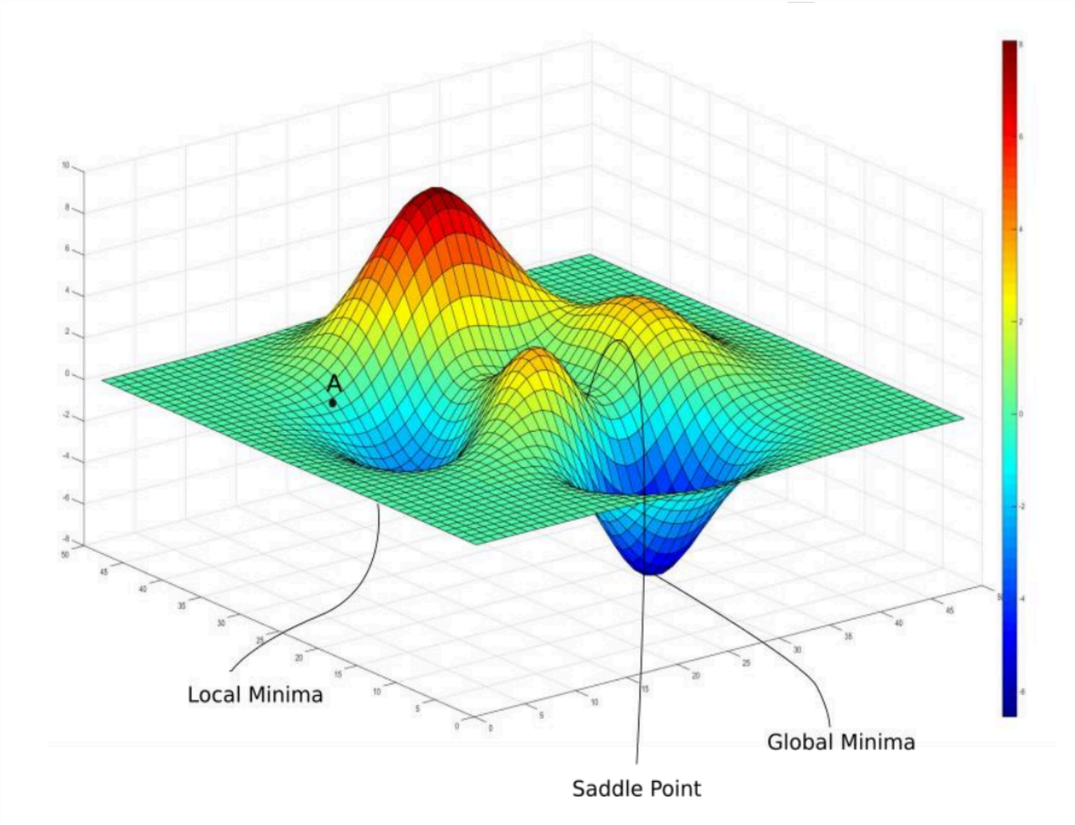


Types of stationary points:

- Global minimum: actual minimizer, i.e., $f(\hat{\mathbf{x}}) \leq f(\mathbf{x}) \;\; \forall\, \mathbf{x} \in \mathbb{R}^k$
- Local minimum: $f(\hat{\mathbf{x}}) \leq f(\mathbf{x}) \;\; \forall\, \mathbf{x} \in \mathbb{R}^k : \;\; \|\mathbf{x} - \hat{\mathbf{x}}\| \leq \epsilon$
- Local maximum: $f(\hat{\mathbf{x}}) \geq f(\mathbf{x}) \;\; \forall\, \mathbf{x} \in \mathbb{R}^k : \;\; \|\mathbf{x} - \hat{\mathbf{x}}\| \leq \epsilon$
- Saddle point: a stationary point that is not a local minimum or maximum

CHALLENGE

Non-convexity

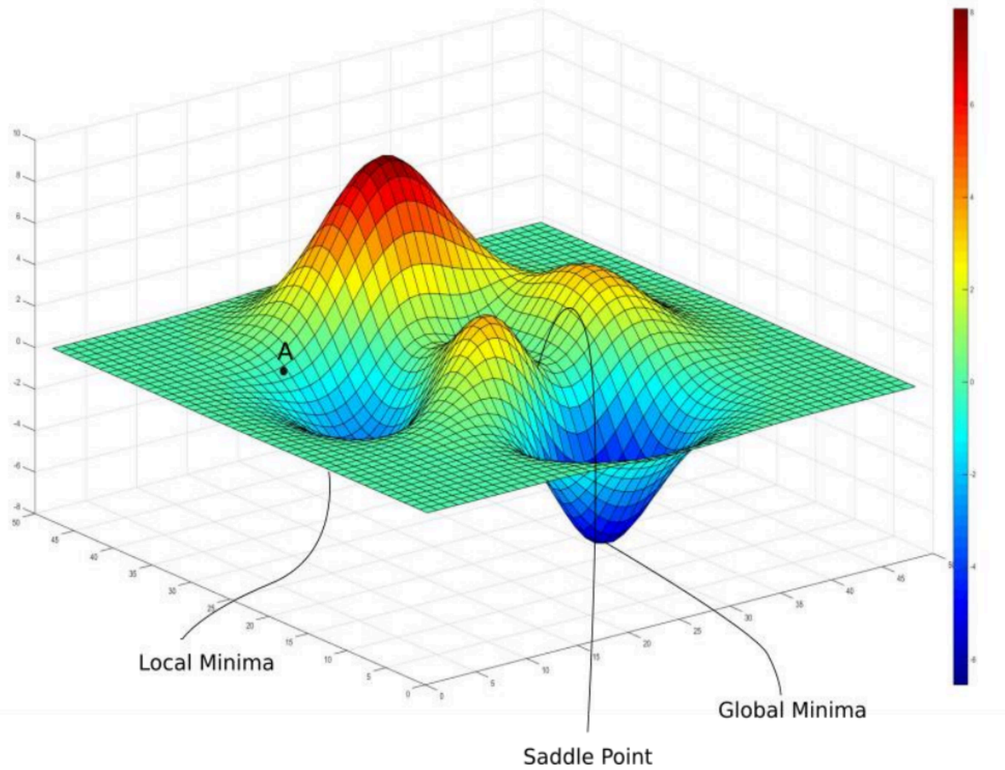


Types of stationary points:

- Global minimum: finding these is hard (both in theory [NP-hard] and in practice)
- Local minimum: can often still provide reasonable solutions
- Saddle point: want to avoid these

CHALLENGE

Non-convexity



What makes non-convex optimization difficult?

- Potentially many local minima
- Saddle points
- Very flat regions
- Widely varying curvature

RECALL

Techniques for large-scale optimization

Reduce computation:

- Parallelize/distribute computation
- Use stochastic methods
- Use first-order methods (i.e., no 2nd-order or higher gradients)

***Reduce communication*:**

- Keep large objects local
- Reduce iterations

RECALL

Techniques for large-scale optimization

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will talk about parallel/ distributed DL next lecture

***Reduce communication*:**

- Keep large objects local
- Reduce iterations

this is particularly important for DL, since the models are very large

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Techniques for large-scale optimization

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***Reduce communication*:**

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Reducing iterations

We are interested in optimization techniques that reduce the total number of iterations until convergence

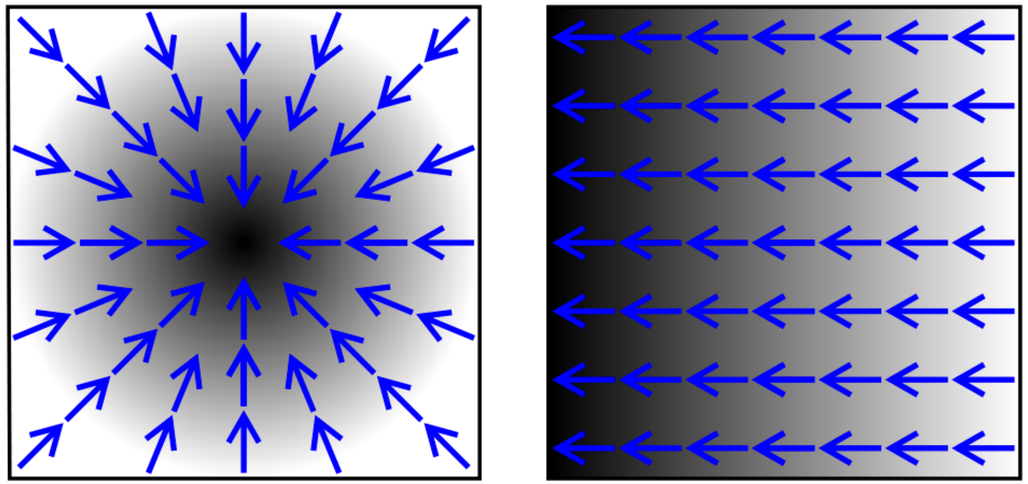
However, these techniques often come at a price: *more computation*

Will discuss two popular techniques for DL that aim to reduce iterations with little additional computation:

- Adaptive learning rate methods
- Momentum-based methods

RECALL

Gradient descent



"Gradient2" by Sarang. Licensed under CC BY-SA 2.5 via Wikimedia Commons
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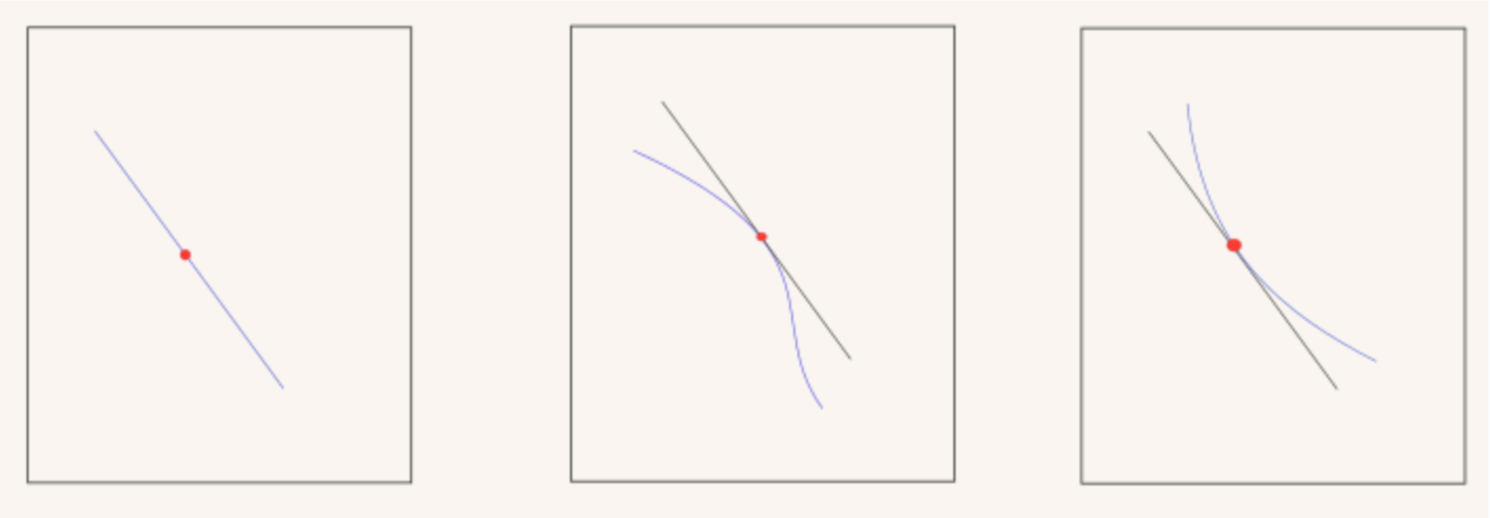
Step Size

Update Rule: $\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla f(\mathbf{w}_t)$

Negative Slope

Motivation: Newton's method

issue: gradient may be the same despite varying curvature



Newton's method uses second order information to estimate the curvature of the function being minimized (i.e., the ERM objective)

Motivation: Newton's method

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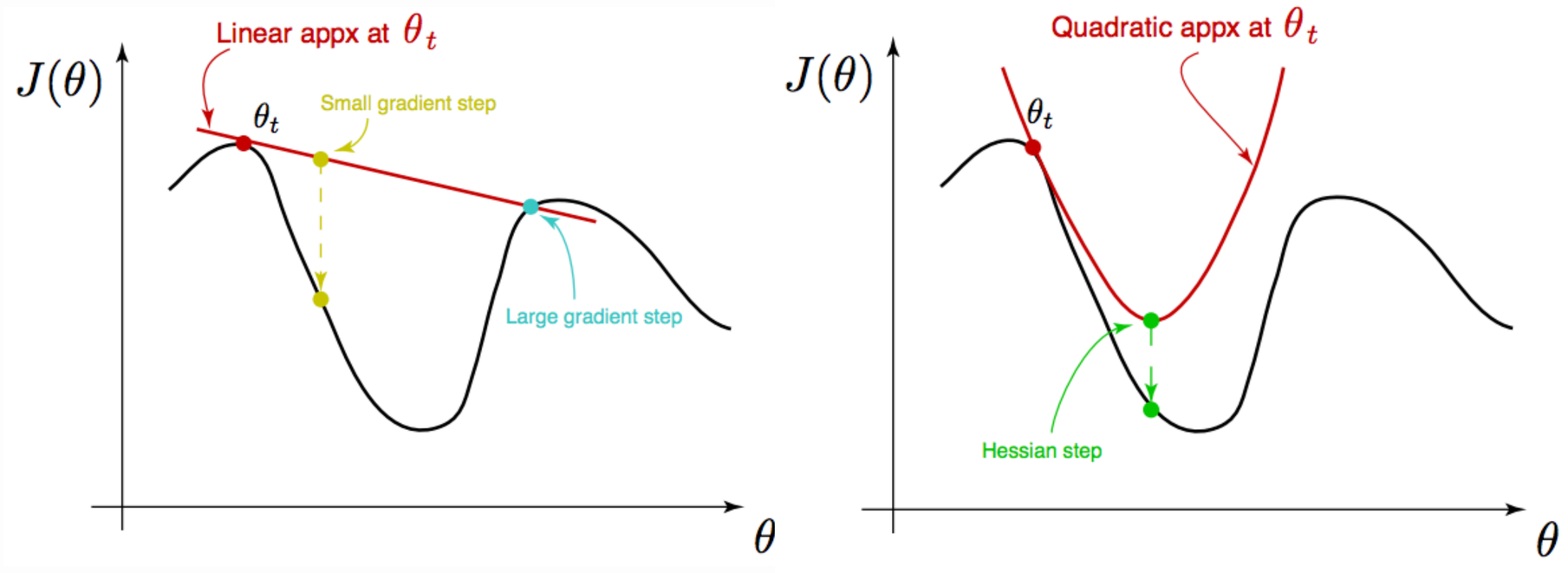

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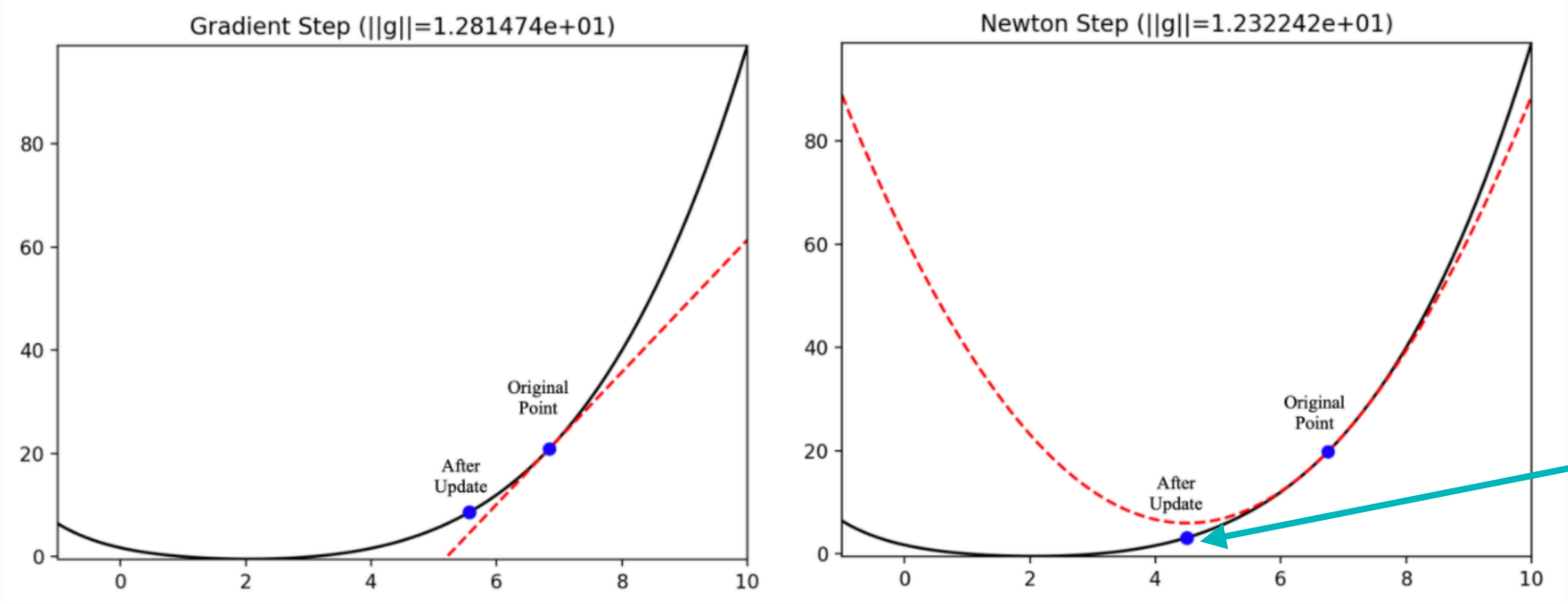
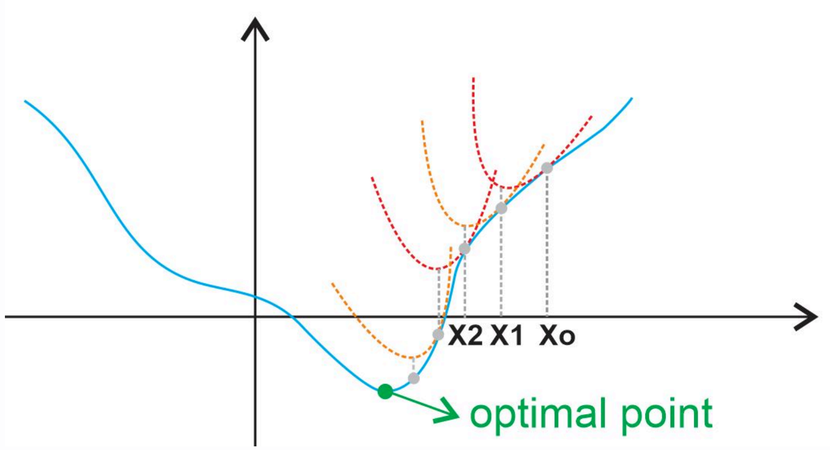


Newton step makes more progress

Newton's method uses second order information to estimate the curvature of the function being minimized (i.e., the ERM objective)

Motivation: Newton's method

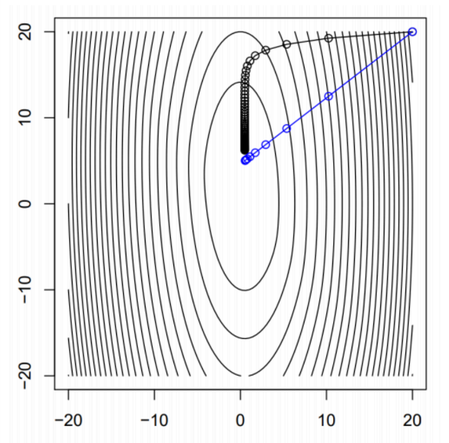


RECALL

Gradient descent $\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla f(\mathbf{w}_t)$

can we do better? idea: use second order information (i.e., the hessian)

Newton's method $\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \left(\nabla^2 f(\mathbf{w}_t) \right)^{-1} \nabla f(\mathbf{w}_t)$



can significantly reduce number of iterations needed for convergence

however, comes at a cost: need to invert $k \times k$ matrix → $O(k^3)$

often too expensive for neural networks (k can be in the millions)

A CHEAPER APPROACH

AdaGrad

AdaGrad: $$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha G_t^{-1} \nabla f(\mathbf{w}_t)$$

where $$\left(G_t\right)_{ii} = \sqrt{\sum_{j=1}^{t} \nabla f(\mathbf{w}_j)_i^2} \quad , \quad \textit{else} \quad 0$$

- A cheap approximation of the Hessian: only estimate the diagonal elements
- Enforces a separate step size / learning rate for every coordinate of the weight vector
  - Decreases the step size for coordinates with high gradient magnitudes
- Why does this make sense when the model is large?
  - There may be high variability across the coordinates
- Potential issue: step size can become very small in some directions

Duchi et al, 2011

AN ALTERNATIVE TO ADAGRAD

RMSProp

RMSProp: $$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha G_t^{-1} \nabla f(\mathbf{w}_t)$$

where $$\left(G_t\right)_{ii} = \sqrt{(g_t)_i} \;, \quad \textit{else} \quad 0$$

$$\left(g_t\right)_i = \beta(g_{t-1})_i + (1-\beta)(\nabla f(\mathbf{w}_t)_i)^2$$

- Take a moving average of the coordinates of the gradient, instead of a sum
- Puts more of an emphasis on the current gradients than the gradient history
- Can be more effective for DNNs
- Also see: AdaDelta

Hinton [Coursera], 2012

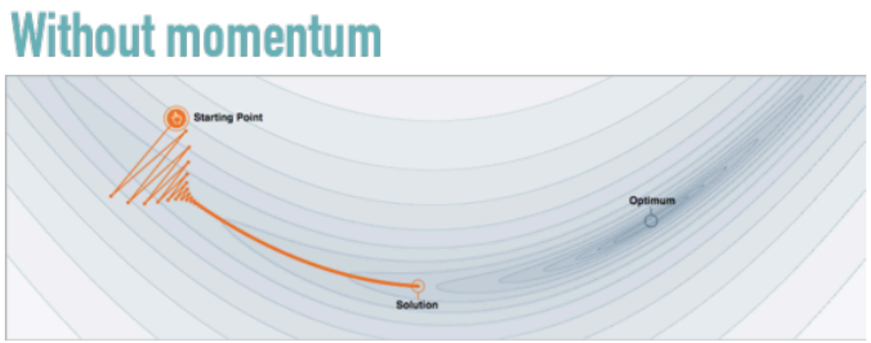
ANOTHER APPROACH

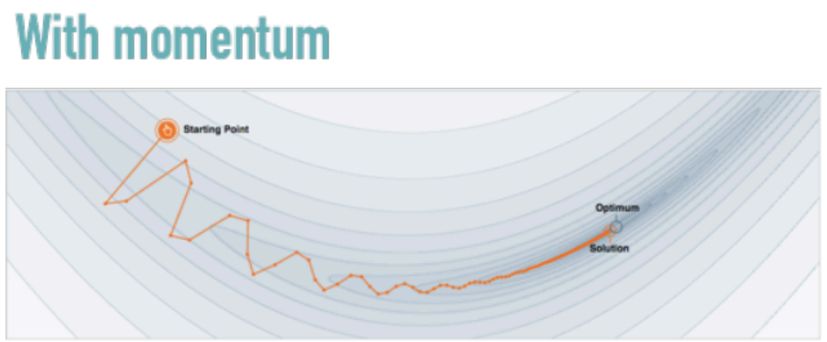
Momentum

Polyak momentum

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla f(\mathbf{w}_t) + \beta(\mathbf{w}_t - \mathbf{w}_{t-1})$$

- Another cheap way to potentially improve gradient descent: use momentum
- Intuition: if current gradient step is in same direction as previous step, then move a little further in that direction; if not, move less far
- Also known as the heavy ball method





Polyak ‘64

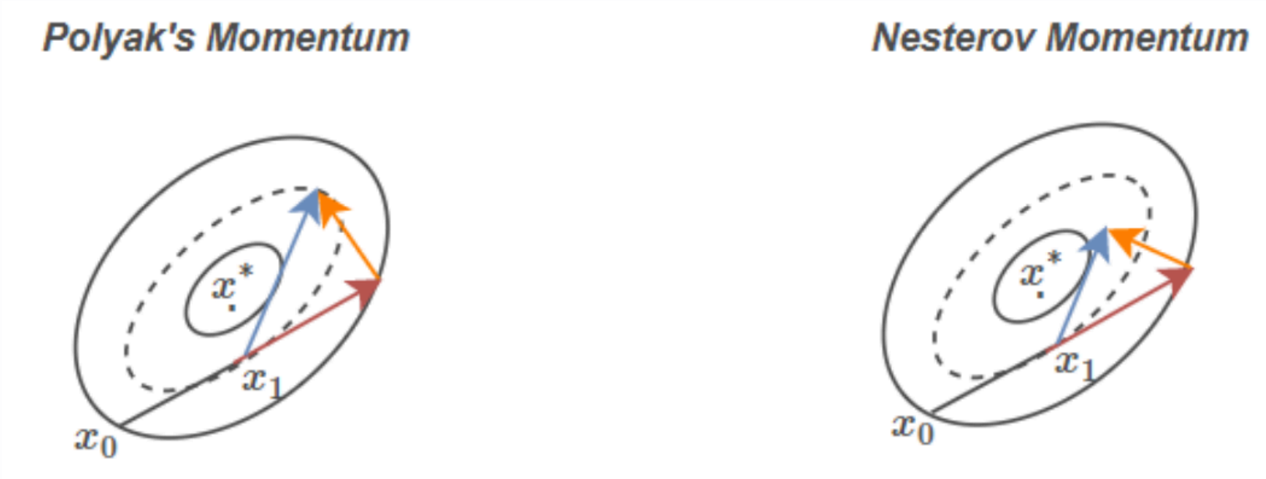
Nesterov accelerated gradient

evaluate gradient at 'look-ahead' point

Nesterov momentum

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha \nabla f(\mathbf{w}_t + \beta(\mathbf{w}_t - \mathbf{w}_{t-1})) + \beta(\mathbf{w}_t - \mathbf{w}_{t-1})$$

- A "look-ahead" variant of momentum
- Provably faster convergence than GD for any convex function



Nesterov '83

ONE LAST METHOD: COMBINE EVERYTHING!

Adam

Adam:

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \alpha G_t^{-1} \mathbf{v}_t$$

where

$$\left(G_t\right)_{ii} = \sqrt{(g_t)_i} \quad , \quad \textit{else} \quad 0$$

$$\left(g_t\right)_i = \beta_1 (g_{t-1})_i + (1-\beta_1)(\nabla f(\mathbf{w}_t)_i)^2$$

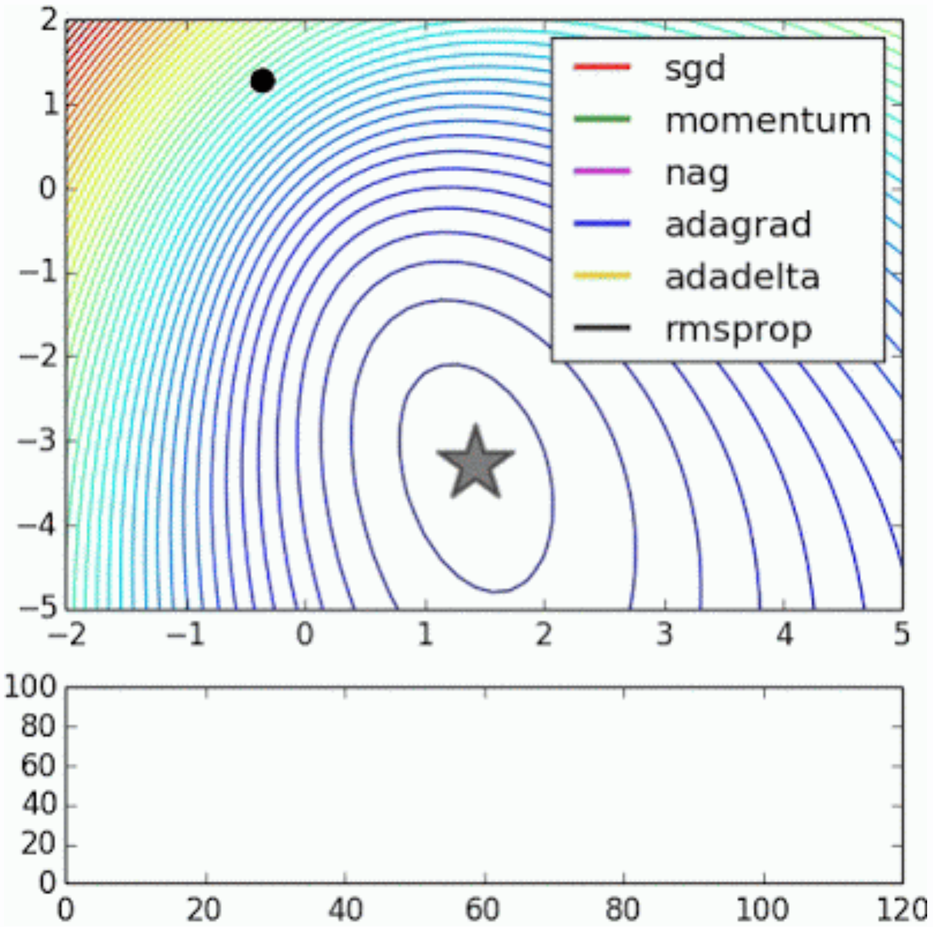
$$\mathbf{v}_t = \beta_2 \mathbf{v}_{t-1} + (1-\beta_2)\nabla f(\mathbf{w}_t)$$

RMSProp update

Momentum

- Combines momentum and RMSprop
- Default choice in most DL frameworks
- However, does not converge (even for convex problems) without modifications
  - [*Reddi, Kale, Kumar, ICLR '19 best paper*]

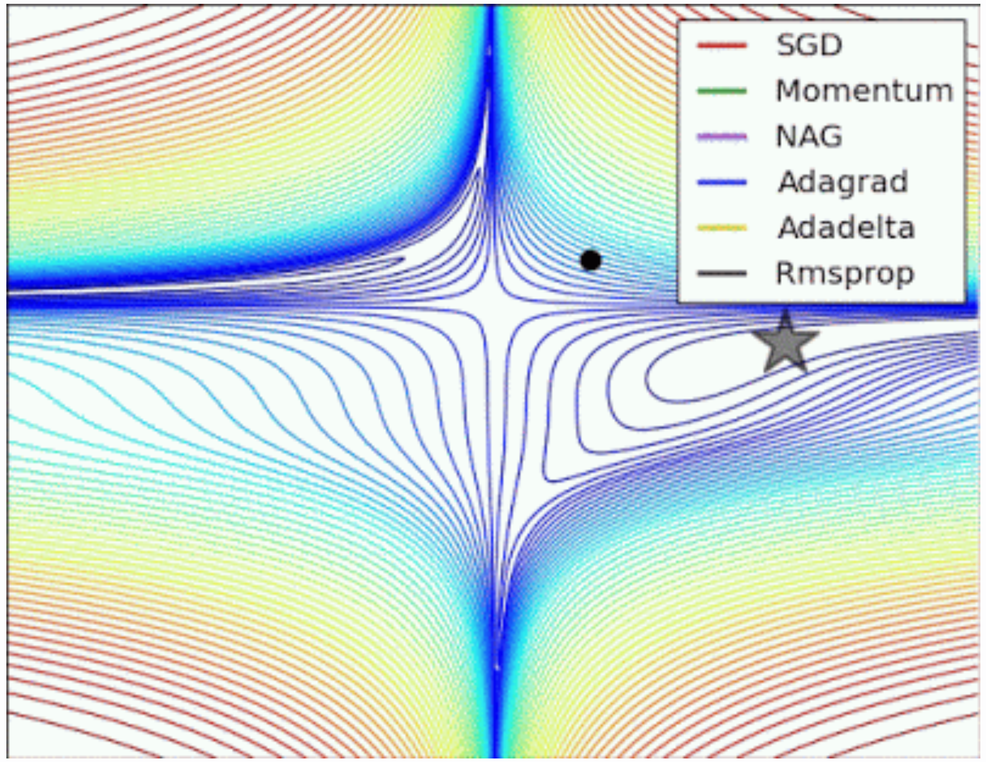
Performance on toy examples



- Logistic regression model (convex)
- All methods improve upon SGD
- AdaGrad converges the fastest
- Momentum methods have smoothing effect

https://imgur.com/a/Hqolp

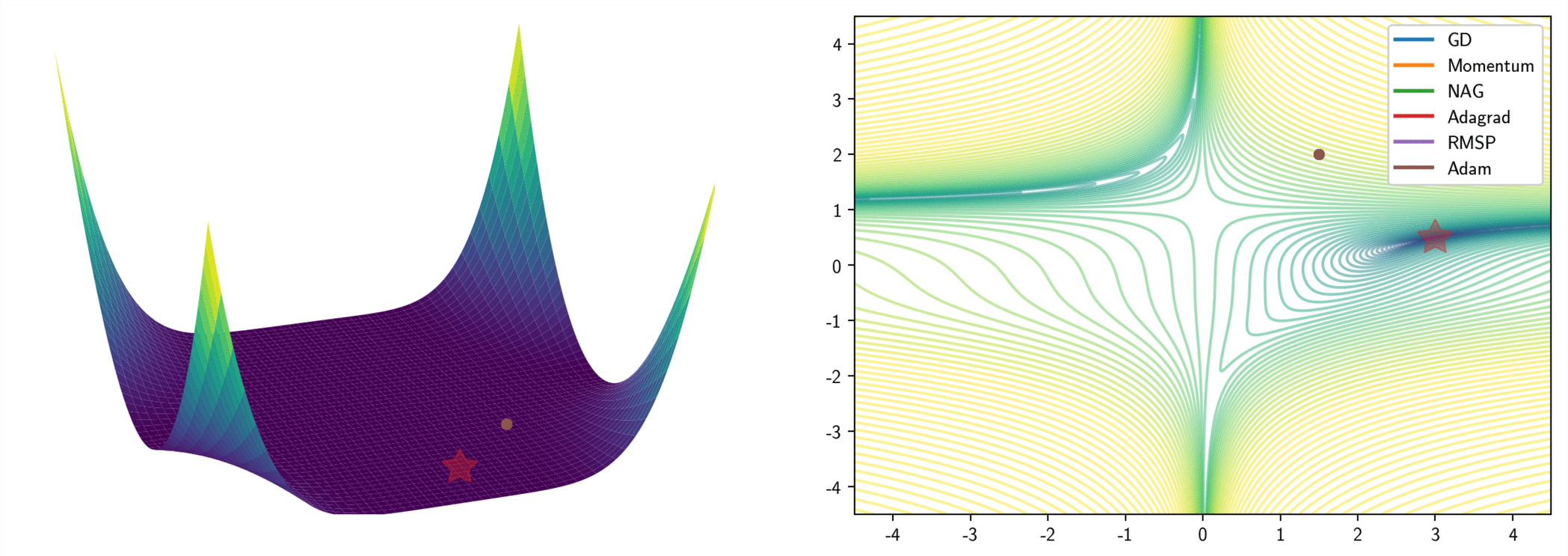
Performance on toy examples



- Beale's function (nonconvex): high variability in terms of gradients (initial gradient is very large)
- AdaGrad & momentum methods are unstable
- RMSProp/AdaDelta perform the best

https://imgur.com/a/Hqolp

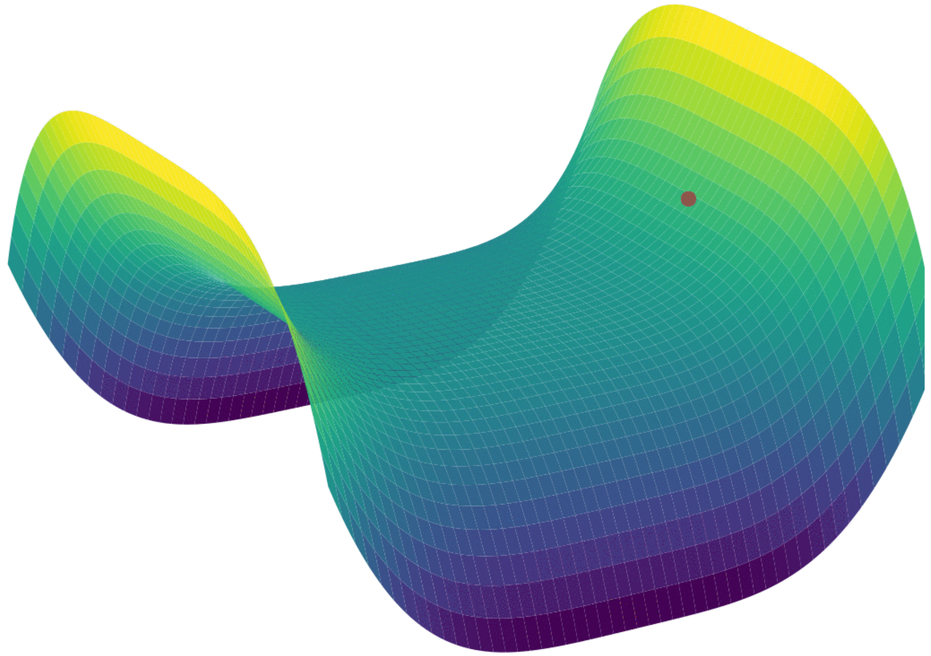
Performance on toy examples

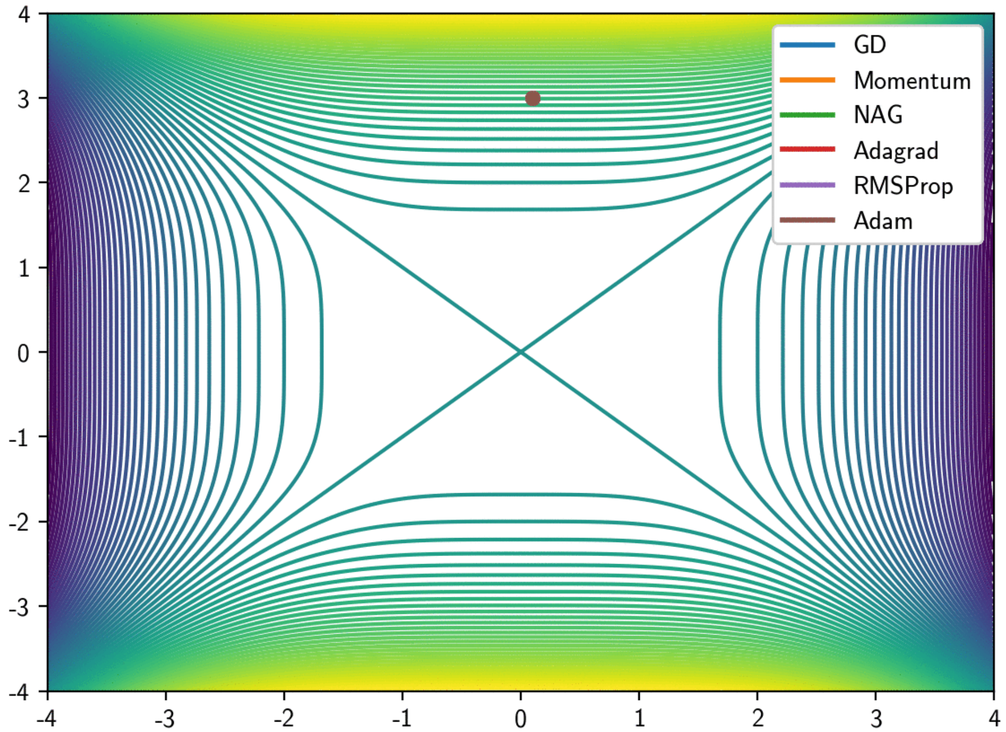


- Beale's function (nonconvex): this time including Adam
- Minimized at (3,0)

https://tangbinh.github.io/01/04/Optimizers.html

Performance on toy examples

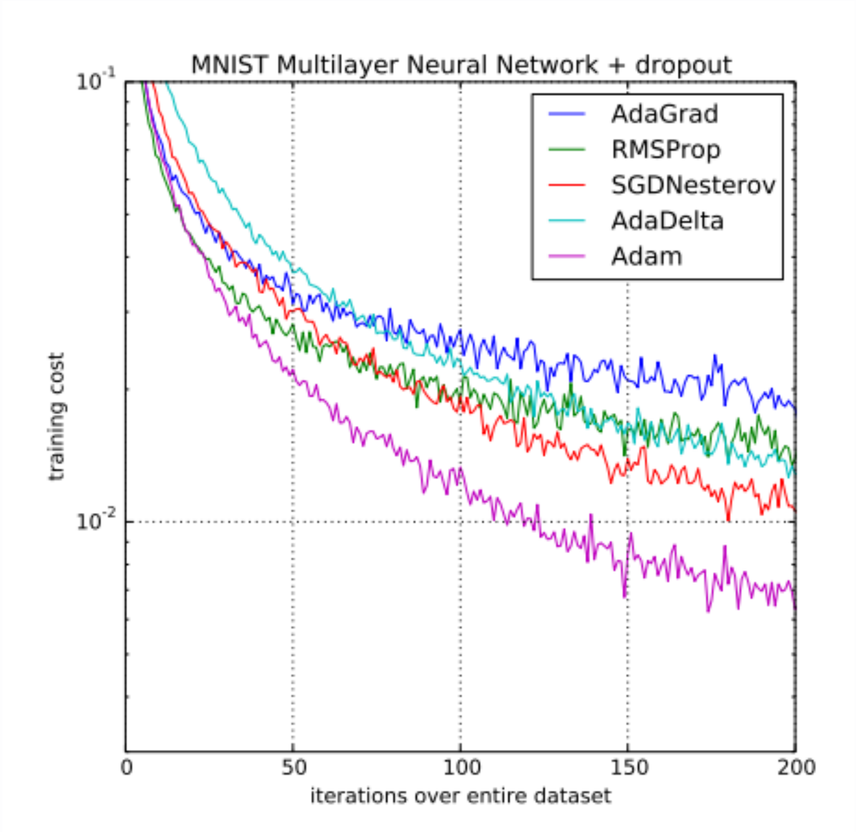


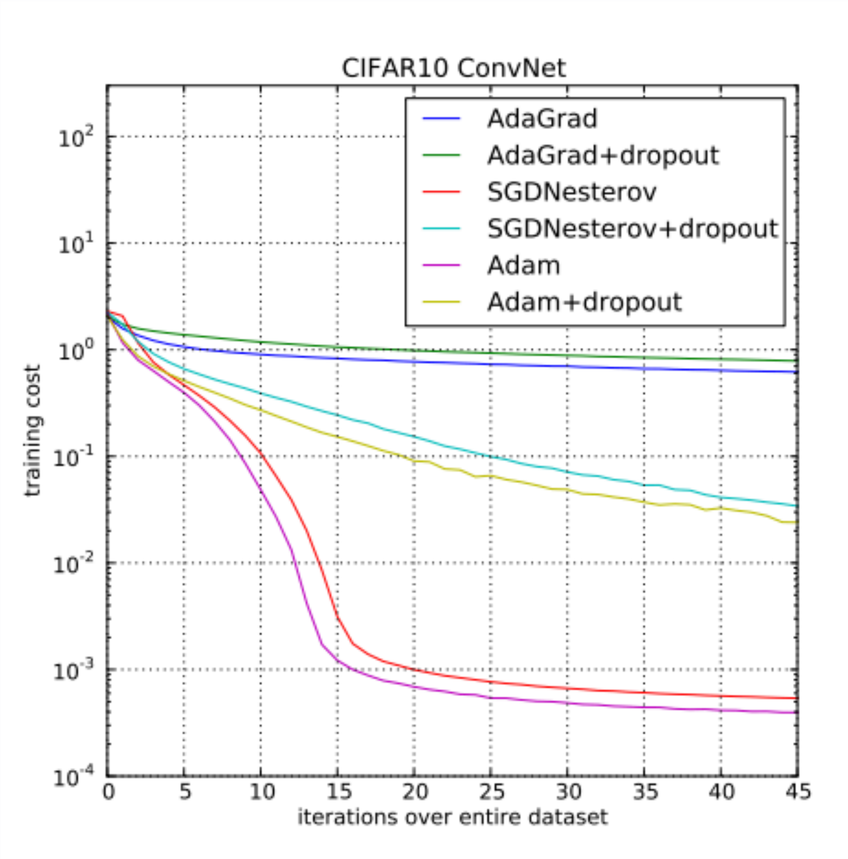


- Loss function: $f(x) = y^4 - x^4$
- Saddle point at (0,0), minimized at $(0, \infty)$

https://tangbinh.github.io/01/04/Optimizers.html

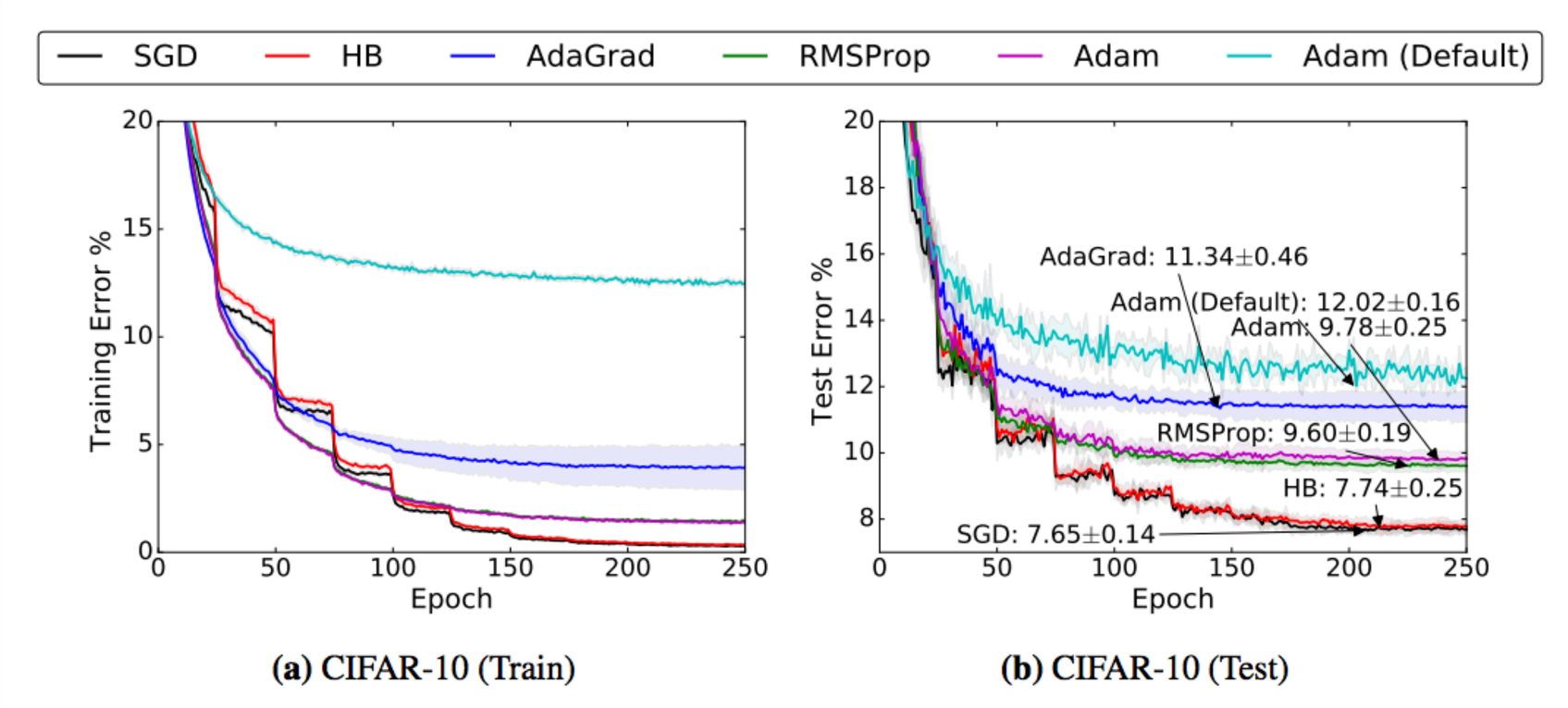
Performance on DL benchmarks





- Initial results: “Adam: A Method for Stochastic Optimization”, Kingma & Ba, ICLR 2015

Performance on DL benchmarks



(a) CIFAR-10 (Train)

(b) CIFAR-10 (Test)

- More recently: “The Marginal Value of Adaptive Gradient Methods in Machine Learning”, Wilson et al., NeurIPS 2017
- Performance can particularly drop for test error (i.e., what we actually care about!)

Outline

1. Optimization review
2. DL Optimization: adaptive learning rates, momentum
3. Other tricks: early stopping, batch norm

Batch normalization

- Motivation: Normalizing/whitening (mean = 0, variance = 1) the inputs speeds up training [LeCun et al, 1998]
  - *Could normalization at the hidden layers also be useful?*
- Batch normalization is an attempt to do this [Ioffe and Szegedy, 2014]
  - each unit's pre-activation is normalized (subtract mean, divide by standard deviation)
  - during training, mean and standard deviation computed for each minibatch
  - backpropagation takes into account the normalization
  - at test time, the global mean and standard deviation are used

Batch normalization

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

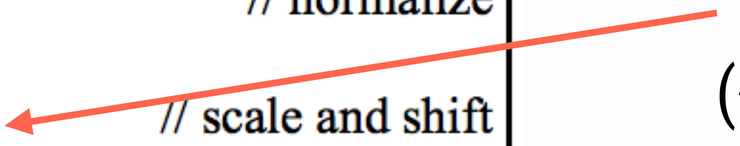
Output: $\{y_i = \mathrm{BN}_{\gamma,\beta}(x_i)\}$

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

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

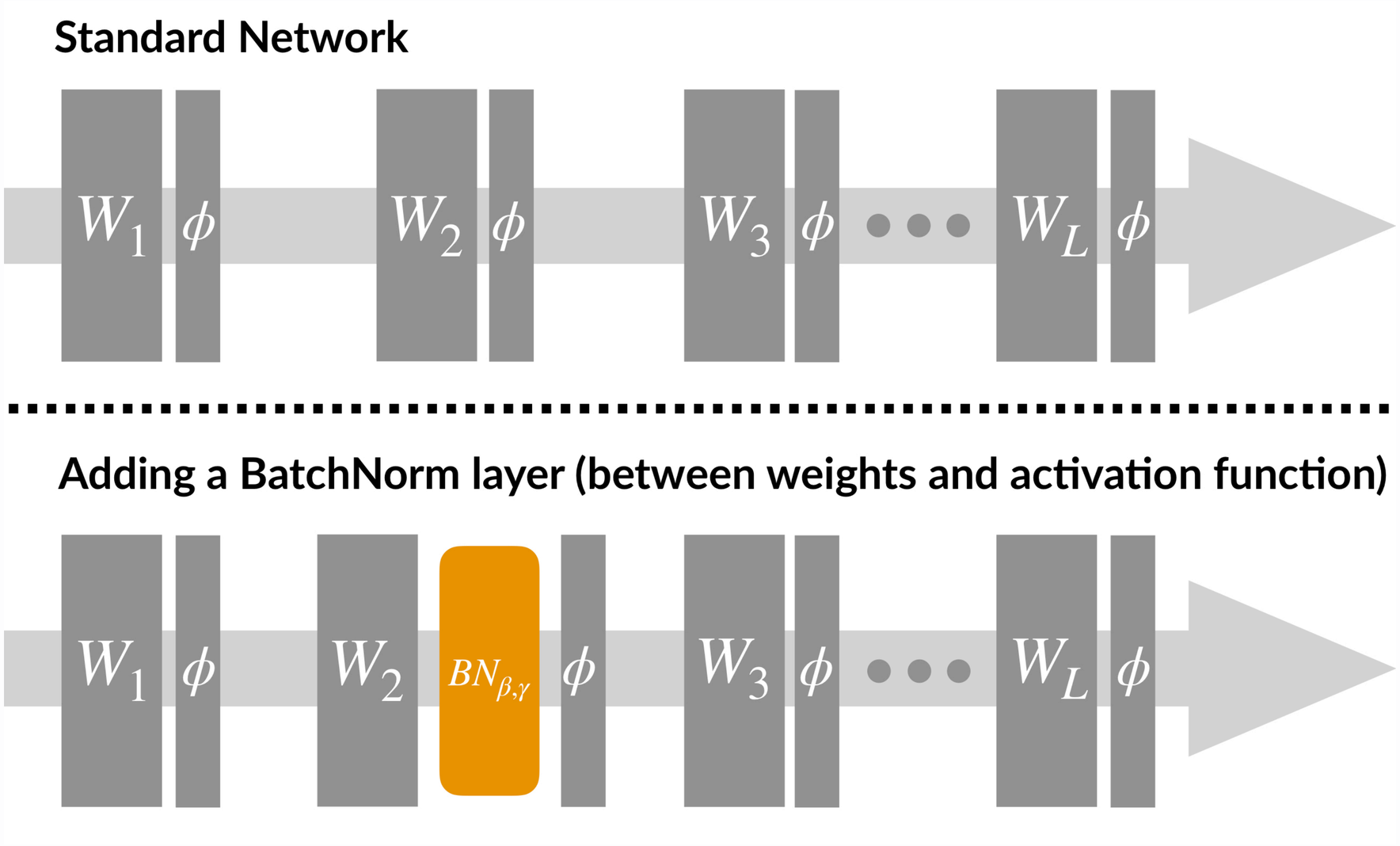
$$\widehat{x}_i \leftarrow \frac{x_i - \mu_{\mathcal{B}}}{\sqrt{\sigma^2_{\mathcal{B}} + \epsilon}} \qquad \text{// normalize}$$

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



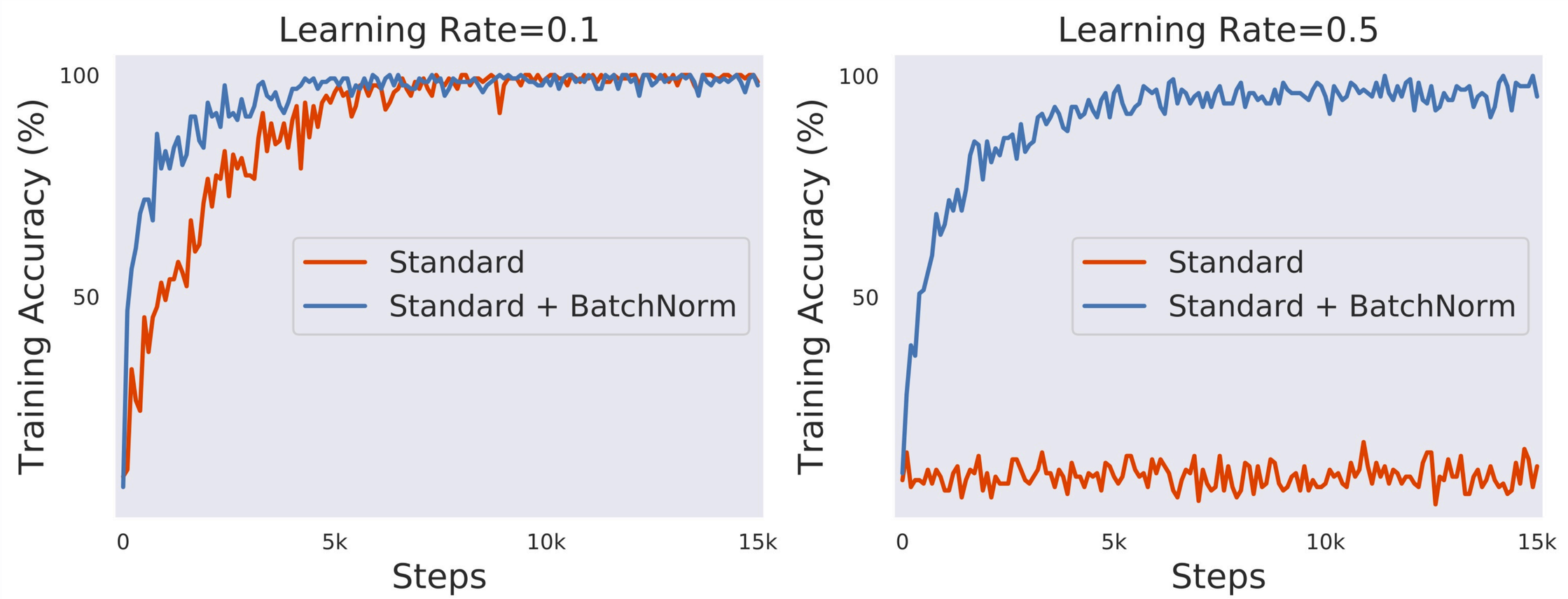
Learned linear transformation (γ and β are trained)

Batch normalization



http://gradientscience.org/batchnorm/

Batch normalization



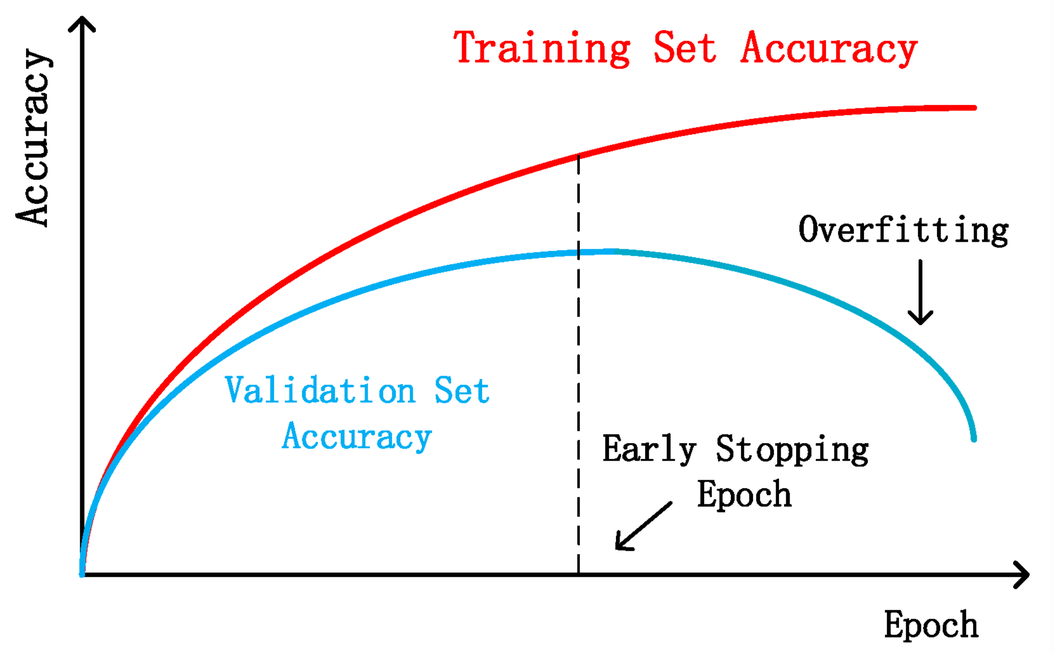
http://gradientscience.org/batchnorm/

ONE LAST TRICK …

Early stopping

- Recall: what we actually care about is generalization performance (i.e., how will the trained model perform on new, unseen data?)
- Many techniques to regularize DNNs and prevent overfitting
- Early stopping is a simple (and cheap!) way to improve generalization and prevent overfitting

- Idea: stop training when validation accuracy starts to reduce



Additional Resources

Optimization for DL

- Deep Learning Book, Chapter 8: https://www.deeplearningbook.org/
- AdaGrad:
    - https://arxiv.org/abs/1002.4908
    - http://www.jmlr.org/papers/volume12/duchi11a/duchi11a.pdf
- Adam: https://arxiv.org/pdf/1412.6980.pdf

Batch normalization

- http://gradientscience.org/batchnorm/