Lecture 6
Optimization for Deep Neural Networks
CMSC 35246: Deep Learning

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Things we will look at today

- Stochastic Gradient Descent
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- Momentum Method and the Nesterov Variant
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- Polyak Averaging

On Slides but for self study: Newton and Quasi Newton Methods (BFGS, L-BFGS, Conjugate Gradient)
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We’ve seen backpropagation as a method for computing gradients
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Assignment: Was about implementation of SGD in conjunction with backprop
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Assignment: Was about implementation of SGD in conjunction with backprop.
Let’s see a family of first order methods.
Batch Gradient Descent

**Algorithm 1** Batch Gradient Descent at Iteration $k$

**Require:** Learning rate $\epsilon_k$

**Require:** Initial Parameter $\theta$

1: while stopping criteria not met do
2: Compute gradient estimate over $N$ examples:
3: $\hat{g} \leftarrow +\frac{1}{N} \nabla_{\theta} \sum_{i} L(f(x^{(i)}; \theta), y^{(i)})$
4: Apply Update: $\theta \leftarrow \theta - \epsilon \hat{g}$
5: end while

- Positive: Gradient estimates are stable
- Negative: Need to compute gradients over the entire training for one update
Gradient Descent
Gradient Descent
Gradient Descent
Gradient Descent
Gradient Descent
Gradient Descent
Algorithm 2: Stochastic Gradient Descent at Iteration $k$

Require: Learning rate $\epsilon_k$

Require: Initial Parameter $\theta$

1: while stopping criteria not met do
2: Sample example $(x^{(i)}, y^{(i)})$ from training set
3: Compute gradient estimate:
4: $\hat{g} \leftarrow +\nabla_\theta L(f(x^{(i)}; \theta), y^{(i)})$
5: Apply Update: $\theta \leftarrow \theta - \epsilon \hat{g}$
6: end while
Stochastic Gradient Descent

Algorithm 2 Stochastic Gradient Descent at Iteration $k$

Require: Learning rate $\epsilon_k$

Require: Initial Parameter $\theta$

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$\epsilon_k$ is learning rate at step $k$
Algorithm 2 Stochastic Gradient Descent at Iteration $k$

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5: Apply Update: $\theta \leftarrow \theta - \epsilon \hat{g}$
6: end while

- $\epsilon_k$ is learning rate at step $k$
- Sufficient condition to guarantee convergence:

$$
\sum_{k=1}^{\infty} \epsilon_k = \infty \text{ and } \sum_{k=1}^{\infty} \epsilon_k^2 < \infty
$$
In practice the learning rate is decayed linearly till iteration $\tau$

\[ \epsilon_k = (1 - \alpha) \epsilon_0 + \alpha \epsilon_{\tau} \]

$\alpha$ is usually set to the number of iterations needed for a large number of passes through the data.

$\epsilon_0$ and $\epsilon_{\tau}$ should roughly be set to 1% of each other.

**Learning Rate Schedule**
In practice the learning rate is decayed linearly till iteration $\tau$

$$\epsilon_k = (1 - \alpha)\epsilon_0 + \alpha\epsilon_\tau \text{ with } \alpha = \frac{k}{\tau}$$
Learning Rate Schedule

In practice the learning rate is decayed linearly till iteration $\tau$

$$\epsilon_k = (1 - \alpha)\epsilon_0 + \alpha\epsilon_\tau \quad \text{with} \quad \alpha = \frac{k}{\tau}$$

$\tau$ is usually set to the number of iterations needed for a large number of passes through the data

$\epsilon_\tau$ should roughly be set to 1\% of $\epsilon_0$

How to set $\epsilon_0$?
Minibatching

- **Potential Problem:** Gradient estimates can be very noisy

See: Large Scale Learning with Stochastic Gradient Descent by Leon Bottou
Minibatching

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- **Obvious Solution:** Use larger mini-batches
Minibatching

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So far..

- **Batch Gradient Descent:**

\[ \hat{g} \leftarrow + \frac{1}{N} \nabla_{\theta} \sum_{i} L(f(x^{(i)}; \theta), y^{(i)}) \]

\[ \theta \leftarrow \theta - \epsilon \hat{g} \]
So far..

- **Batch Gradient Descent:**

\[
\hat{g} \leftarrow + \frac{1}{N} \nabla_\theta \sum_i L(f(x^{(i)}; \theta), y^{(i)})
\]

\[
\theta \leftarrow \theta - \epsilon \hat{g}
\]

- **SGD:**

\[
\hat{g} \leftarrow + \nabla_\theta L(f(x^{(i)}; \theta), y^{(i)})
\]

\[
\theta \leftarrow \theta - \epsilon \hat{g}
\]
Momentum

- The Momentum method is a method to accelerate learning using SGD.
Momentum

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In particular SGD suffers in the following scenarios:
  - Error surface has high curvature
Momentum

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  - We get small but consistent gradients
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In particular SGD suffers in the following scenarios:

- Error surface has high curvature
- We get small but consistent gradients
- The gradients are very noisy
Gradient Descent would move quickly down the walls, but very slowly through the valley floor.
Momentum

- How do we try and solve this problem?

\[ \text{Introduce a new variable } v \text{, the velocity} \]

We think of \( v \) as the direction and speed by which the parameters move as the learning dynamics progresses. The velocity is an exponentially decaying moving average of the negative gradients:

\[
\begin{align*}
v &\leftarrow \alpha v - \epsilon \nabla \theta (L(f(x(i); \theta), y(i))) \\
\alpha &\in [0, 1)
\end{align*}
\]

Update rule:
Momentum

- How do we try and solve this problem?
- Introduce a new variable $v$, the velocity

Update rule:

$$\theta \leftarrow \theta + v$$
Momentum

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- We think of \( v \) as the direction and speed by which the parameters move as the learning dynamics progresses

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\begin{align*}
\text{Update rule:} \\
\theta & \leftarrow \theta + v
\end{align*}
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\[
\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \nabla_{\theta} \left( L(f(x^{(i)}; \theta), y^{(i)}) \right)
\]

- $\alpha \in [0, 1)$ Update rule: $\theta \leftarrow \theta + \mathbf{v}$
Momentum

Let’s look at the velocity term:

\[ v \leftarrow \alpha v - \epsilon \nabla_{\theta} \left( L(f(x^{(i)}; \theta), y^{(i)}) \right) \]
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The velocity accumulates the previous gradients.
Momentum

Let’s look at the velocity term:

\[ \mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \nabla_{\theta} \left( L(f(x^{(i)}; \theta), y^{(i)}) \right) \]

The velocity accumulates the previous gradients

What is the role of \( \alpha \)?

- If \( \alpha \) is larger than \( \epsilon \) the current update is more affected by the previous gradients
Let's look at the velocity term:

$$v \leftarrow \alpha v - \epsilon \nabla_\theta \left( L(f(x^{(i)}; \theta), y^{(i)}) \right)$$

The velocity accumulates the previous gradients.

What is the role of $\alpha$?

- If $\alpha$ is larger than $\epsilon$ the current update is more affected by the previous gradients.
- Usually values for $\alpha$ are set high $\approx 0.8, 0.9$.
Momentum

Gradient Step

Gradient Step
Momentum

Momentum Step

Gradient Step
Momentum

Momentum Step

Gradient Step

Actual Step
In SGD, the step size was the norm of the gradient scaled by the learning rate $\epsilon \|g\|$. Why?
Momentum: Step Sizes

- In SGD, the step size was the norm of the gradient scaled by the learning rate $\epsilon \|g\|$. Why?
- While using momentum, the step size will also depend on the norm and alignment of a sequence of gradients.
In SGD, the step size was the norm of the gradient scaled by the learning rate $\epsilon \|g\|$. Why?

While using momentum, the step size will also depend on the norm and alignment of a sequence of gradients.

For example, if at each step we observed $\mathbf{g}$, the step size would be (exercise!): 

$$
\epsilon \frac{\|\mathbf{g}\|}{1 - \alpha}
$$
Momentum: Step Sizes

- In SGD, the step size was the norm of the gradient scaled by the learning rate $\epsilon \| g \|$. Why?
- While using momentum, the step size will also depend on the norm and alignment of a sequence of gradients.
- For example, if at each step we observed $g$, the step size would be (exercise!):

$$
\epsilon \frac{\| g \|}{1 - \alpha}
$$

- If $\alpha = 0.9 \implies$ multiply the maximum speed by 10 relative to the current gradient direction.
Momentum

Illustration of how momentum traverses such an error surface better compared to Gradient Descent
Algorithm 2 Stochastic Gradient Descent with Momentum

Require: Learning rate $\epsilon_k$
Require: Momentum Parameter $\alpha$
Require: Initial Parameter $\theta$
Require: Initial Velocity $v$

1: while stopping criteria not met do
2: Sample example $(x^{(i)}, y^{(i)})$ from training set
3: Compute gradient estimate:
4: $\hat{g} \leftarrow +\nabla_\theta L(f(x^{(i)}; \theta), y^{(i)})$
5: Compute the velocity update:
6: $v \leftarrow \alpha v - \epsilon \hat{g}$
7: Apply Update: $\theta \leftarrow \theta + v$
8: end while
Nesterov Momentum

- Another approach: First take a step in the direction of the accumulated gradient
- Then calculate the gradient and make a correction
Nesterov Momentum

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Nesterov Momentum

Next Step
Nesterov Momentum

Next Step
Nesterov Momentum

Next Step
Nesterov Momentum

Next Step
Let’s Write it out..

- Recall the velocity term in the Momentum method:

\[
v \leftarrow \alpha v - \epsilon \nabla_{\theta} \left( L(f(x^{(i)}; \theta), y^{(i)}) \right)
\]
Let’s Write it out..

- Recall the velocity term in the Momentum method:

  \[ \mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \nabla_{\theta} \left( L(f(x^{(i)}; \theta), y^{(i)}) \right) \]

- Nesterov Momentum:

  \[ \mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \nabla_{\theta} \left( L(f(x^{(i)}; \theta + \alpha \mathbf{v}), y^{(i)}) \right) \]
Let’s Write it out..

- Recall the velocity term in the Momentum method:

\[
v \leftarrow \alpha v - \epsilon \nabla_{\theta} \left( L(f(x^{(i)}; \theta), y^{(i)}) \right)
\]

- Nesterov Momentum:

\[
v \leftarrow \alpha v - \epsilon \nabla_{\theta} \left( L(f(x^{(i)}; \theta + \alpha v), y^{(i)}) \right)
\]

- Update: \( \theta \leftarrow \theta + v \)
SGD with Nesterov Momentum

Algorithm 3 SGD with Nesterov Momentum

Require: Learning rate $\epsilon$
Require: Momentum Parameter $\alpha$
Require: Initial Parameter $\theta$
Require: Initial Velocity $\mathbf{v}$

1: while stopping criteria not met do
2: Sample example $(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})$ from training set
3: Update parameters: $\tilde{\theta} \leftarrow \theta + \alpha \mathbf{v}$
4: Compute gradient estimate:
5: $\hat{\mathbf{g}} \leftarrow +\nabla_{\tilde{\theta}} L(f(\mathbf{x}^{(i)}; \tilde{\theta}), \mathbf{y}^{(i)})$
6: Compute the velocity update: $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \hat{\mathbf{g}}$
7: Apply Update: $\theta \leftarrow \theta + \mathbf{v}$
8: end while
Adaptive Learning Rate Methods
Motivation

- Till now we assign the same learning rate to all features
Motivation

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- If the features vary in importance and frequency, why is this a good idea?
Motivation

- Till now we assign the same learning rate to all features
- If the features vary in importance and frequency, why is this a good idea?
- It’s probably not!
Motivation

Nice (all features are equally important)
Motivation

Harder!
AdaGrad

- **Idea:** Downscale a model parameter by square-root of sum of squares of all its historical values.
AdaGrad

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- Parameters that have large partial derivative of the loss – learning rates for them are rapidly declined.
AdaGrad

- **Idea**: Downscale a model parameter by square-root of sum of squares of all its historical values.
- Parameters that have large partial derivative of the loss – learning rates for them are rapidly declined.
- Some interesting theoretical properties.
Algorithm 4 AdaGrad

Require: Global Learning rate $\epsilon$, Initial Parameter $\theta$, $\delta$

Initialize $r = 0$

1: while stopping criteria not met do
2: Sample example $(x^{(i)}, y^{(i)})$ from training set
3: Compute gradient estimate: $\hat{g} \leftarrow +\nabla_{\theta} L(f(x^{(i)}; \theta), y^{(i)})$
4: Accumulate: $r \leftarrow r + \hat{g} \odot \hat{g}$
5: Compute update: $\Delta\theta \leftarrow -\frac{\epsilon}{\delta + \sqrt{r}} \odot \hat{g}$
6: Apply Update: $\theta \leftarrow \theta + \Delta\theta$

7: end while
RMSProp

- AdaGrad is good when the objective is convex.
RMSProp

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- AdaGrad might shrink the learning rate too aggressively, we want to keep the history in mind.
RMSProp

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- AdaGrad might shrink the learning rate too aggressively, we want to keep the history in mind
- We can adapt it to perform better in non-convex settings by accumulating an exponentially decaying average of the gradient
AdaGrad is good when the objective is convex.

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We can adapt it to perform better in non-convex settings by accumulating an exponentially decaying average of the gradient.

This is an idea that we use again and again in Neural Networks.
RMSProp

- AdaGrad is good when the objective is convex.
- AdaGrad might shrink the learning rate too aggressively, we want to keep the history in mind.
- We can adapt it to perform better in non-convex settings by accumulating an exponentially decaying average of the gradient.
- This is an idea that we use again and again in Neural Networks.
- Currently has about 500 citations on scholar, but was proposed in a slide in Geoffrey Hinton’s Coursera course.
Algorithm 5 RMSProp

Require: Global Learning rate $\epsilon$, decay parameter $\rho$, $\delta$

Initialize $r = 0$

1: while stopping criteria not met do
2: Sample example $(x^{(i)}, y^{(i)})$ from training set
3: Compute gradient estimate: $\hat{g} \leftarrow +\nabla_{\theta} L(f(x^{(i)}; \theta), y^{(i)})$
4: Accumulate: $r \leftarrow \rho r + (1 - \rho) \hat{g} \odot \hat{g}$
5: Compute update: $\Delta \theta \leftarrow -\frac{\epsilon}{\delta + \sqrt{r}} \odot \hat{g}$
6: Apply Update: $\theta \leftarrow \theta + \Delta \theta$
7: end while
RMSProp with Nesterov

Algorithm 6 RMSProp with Nesterov

**Require:** Global Learning rate $\epsilon$, decay parameter $\rho$, $\delta$, $\alpha$, $v$

Initialize $r = 0$

1: while stopping criteria not met do
2: Sample example $(x^{(i)}, y^{(i)})$ from training set
3: Compute Update: $\tilde{\theta} \leftarrow \theta + \alpha v$
4: Compute gradient estimate: $\hat{g} \leftarrow \nabla_{\tilde{\theta}} L(f(x^{(i)}; \tilde{\theta}), y^{(i)})$
5: Accumulate: $r \leftarrow \rho r + (1 - \rho) \hat{g} \odot \hat{g}$
6: Compute Velocity: $v \leftarrow \alpha v - \frac{\epsilon}{\sqrt{r}} \odot \hat{g}$
7: Apply Update: $\theta \leftarrow \theta + v$
8: end while
We could have used RMSProp with momentum
Adam

- We could have used RMSProp with momentum
- Use of Momentum with rescaling is not well motivated
Adam

- We could have used RMSProp with momentum
- Use of Momentum with rescaling is not well motivated
- Adam is like RMSProp with Momentum but with bias correction terms for the first and second moments
Adam: ADAdptive Moments

Algorithm 7 RMSProp with Nesterov

Require: $\epsilon$ (set to 0.0001), decay rates $\rho_1$ (set to 0.9), $\rho_2$ (set to 0.9), $\theta$, $\delta$

Initialize moments variables $s = 0$ and $r = 0$, time step $t = 0$

1: while stopping criteria not met do
2: Sample example $(x^{(i)}, y^{(i)})$ from training set
3: Compute gradient estimate: $\hat{g} \leftarrow + \nabla_{\theta} L(f(x^{(i)}; \theta), y^{(i)})$
4: $t \leftarrow t + 1$
5: Update: $s \leftarrow \rho_1 s + (1 - \rho_1) \hat{g}$
6: Update: $r \leftarrow \rho_2 r + (1 - \rho_2) \hat{g} \odot \hat{g}$
7: Correct Biases: $\hat{s} \leftarrow \frac{s}{1 - \rho_1^t}$, $\hat{r} \leftarrow \frac{r}{1 - \rho_2^t}$
8: Compute Update: $\Delta \theta = -\epsilon \frac{\hat{s}}{\sqrt{\hat{r} + \delta}}$
9: Apply Update: $\theta \leftarrow \theta + \Delta \theta$
10: end while
All your GRADs are belong to us!

**SGD:** \( \theta \leftarrow \theta - \epsilon \hat{g} \)

**Momentum:** \( v \leftarrow \alpha v - \epsilon \hat{g} \) then \( \theta \leftarrow \theta + v \)

**Nesterov:** \( v \leftarrow \alpha v - \epsilon \nabla \theta \left( L(f(x^{(i)}; \theta + \alpha v), y^{(i)}) \right) \) then \( \theta \leftarrow \theta + v \)

**AdaGrad:** \( r \leftarrow r + g \odot g \) then \( \Delta \theta - \leftarrow \frac{\epsilon}{\delta + \sqrt{r}} \odot g \) then \( \theta \leftarrow \theta + \Delta \theta \)

**RMSProp:** \( r \leftarrow \rho r + (1 - \rho)\hat{g} \odot \hat{g} \) then \( \Delta \theta \leftarrow -\frac{\epsilon}{\delta + \sqrt{r}} \odot \hat{g} \) then \( \theta \leftarrow \theta + \Delta \theta \)

**Adam:** \( \hat{s} \leftarrow \frac{s}{1 - \rho_1^t}, \hat{r} \leftarrow \frac{r}{1 - \rho_2^t} \) then \( \Delta \theta = -\epsilon \frac{\hat{s}}{\sqrt{\hat{r}} + \delta} \) then \( \theta \leftarrow \theta + \Delta \theta \)
Batch Normalization
A Difficultly in Training Deep Neural Networks

A deep model involves composition of several functions

\[ \hat{y} = W_4^T (\tanh(W_3^T (\tanh(W_2^T (\tanh(W_1^T x + b_1) + b_2) + b_3)))) \]
A Difficulty in Training Deep Neural Networks

- We have a recipe to compute gradients (Backpropagation), and update every parameter (we saw half a dozen methods)
A Difficulty in Training Deep Neural Networks

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- Implicit Assumption: Other layers don't change i.e. other functions are fixed.
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- In Practice: We update all layers simultaneously.
A Difficulty in Training Deep Neural Networks

- We have a recipe to compute gradients (Backpropagation), and update every parameter (we saw half a dozen methods)
- **Implicit Assumption:** Other layers don’t change i.e. other functions are fixed
- **In Practice:** We update all layers simultaneously
- This can give rise to unexpected difficulties
A Difficulty in Training Deep Neural Networks

- We have a recipe to compute gradients (Backpropagation), and update every parameter (we saw half a dozen methods).
- Implicit Assumption: Other layers don't change i.e. other functions are fixed.
- In Practice: We update all layers simultaneously.
- This can give rise to unexpected difficulties.
- Let’s look at two illustrations.
Consider a second order approximation of our cost function (which is a function composition) around current point $\theta^{(0)}$:

$$J(\theta) \approx J(\theta^{(0)}) + (\theta - \theta^{(0)})^T g + \frac{1}{2}(\theta - \theta^{(0)})^T H(\theta - \theta^{(0)})$$
Intuition

- Consider a second order approximation of our cost function (which is a function composition) around current point $\theta^{(0)}$:

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- $g$ is gradient and $H$ the Hessian at $\theta^{(0)}$
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- $g$ is gradient and $H$ the Hessian at $\theta^{(0)}$
- If $\epsilon$ is the learning rate, the new point

$$\theta = \theta^{(0)} - \epsilon g$$
Plugging our new point, $\theta = \theta^{(0)} - \epsilon g$ into the approximation:

$$J(\theta^{(0)} - \epsilon g) = J(\theta^{(0)}) - \epsilon g^T g + \frac{1}{2} g^T H g$$
Intuition

- Plugging our new point, $\theta = \theta^{(0)} - \epsilon g$ into the approximation:
  
  $$J(\theta^{(0)} - \epsilon g) = J(\theta^{(0)}) - \epsilon g^T g + \frac{1}{2}g^T H g$$

- There are three terms here:
Intuition

- Plugging our new point, $\theta = \theta^{(0)} - \epsilon g$ into the approximation:

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- There are three terms here:
  - Value of function before update
Intuition

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- There are three terms here:
  - Value of function before update
  - Improvement using gradient (i.e. first order information)
  - Correction factor that accounts for the curvature of the function
Intuition

- Plugging our new point, \( \theta = \theta^{(0)} - \epsilon g \) into the approximation:

\[
J(\theta^{(0)} - \epsilon g) = J(\theta^{(0)}) - \epsilon g^T g + \frac{1}{2}g^T H g
\]

- There are three terms here:
  - Value of function before update
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Intuition

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- **Observations:**
  - \( g^T H g \) too large: Gradient will start moving upwards
  - \( g^T H g = 0 \): \( J \) will decrease for even large \( \epsilon \)
  - Optimal step size \( \epsilon^* = g^T g \) for zero curvature, \( \epsilon^* = g^T g g^T H g \) to take into account curvature

Conclusion: Just neglecting second order effects can cause problems (remedy: second order methods). What about higher order effects?
Intuition

\[ J(\theta^{(0)} - \epsilon g) = J(\theta^{(0)}) - \epsilon g^T g + \frac{1}{2} g^T H g \]

Observations:
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\[ J(\theta^{(0)} - \epsilon g) = J(\theta^{(0)}) - \epsilon g^T g + \frac{1}{2} g^T H g \]

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Intuition

\[ J(\theta^{(0)} - \epsilon g) = J(\theta^{(0)}) - \epsilon g^T g + \frac{1}{2} g^T H g \]

- **Observations:**
  - \(g^T H g\) too large: Gradient will start moving upwards
  - \(g^T H g = 0\): \(J\) will decrease for even large \(\epsilon\)
  - Optimal step size \(\epsilon^* = g^T g\) for zero curvature,
    \(\epsilon^* = \frac{g^T g}{g^T H g}\) to take into account curvature

Conclusion: Just neglecting second order effects can cause problems (remedy: second order methods). What about higher order effects?
\[ J(\theta(0) - \epsilon g) = J(\theta(0)) - \epsilon g^T g + \frac{1}{2} g^T H g \]

- **Observations:**
  - \( g^T H g \) too large: Gradient will start moving upwards
  - \( g^T H g = 0 \): \( J \) will decrease for even large \( \epsilon \)
  - Optimal step size \( \epsilon^* = g^T g \) for zero curvature, \( \epsilon^* = \frac{g^T g}{g^T H g} \) to take into account curvature

- **Conclusion:** Just neglecting second order effects can cause problems (remedy: second order methods). What about higher order effects?
Higher Order Effects: Toy Model

\[ \hat{y} \]

\[ x \]

\[ w_1 \]

\[ h_1 \]

\[ w_2 \]

\[ h_2 \]

\[ \vdots \]

\[ w_l \]

\[ h_l \]

\[ y \]
Higher Order Effects: Toy Model

Just one node per layer, no non-linearity
Higher Order Effects: Toy Model

- Just one node per layer, no non-linearity
- $\hat{y}$ is linear in $x$ but non-linear in $w_i$
Suppose $\delta = 1$, so we want to decrease our output $\hat{y}$.
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Usual strategy:
- Using backprop find $g = \nabla_w (\hat{y} - y)^2$.
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Higher Order Effects: Toy Model

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  - Update weights $w := w - \epsilon g$
- The first order Taylor approximation (in previous slide) says the cost will reduce by $\epsilon g^T g$
- If we need to reduce cost by 0.1, then learning rate should be $\frac{0.1}{g^T g}$
Higher Order Effects: Toy Model

The new $\hat{y}$ will however be:

$$\hat{y} = x(w_1 - \epsilon g_1)(w_2 - \epsilon g_2) \ldots (w_l - \epsilon g_l)$$
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Contains terms like $\epsilon^3 g_1 g_2 g_3 w_4 w_5 \ldots w_l$
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**Conclusion:** Higher order terms make it very hard to choose the right learning rate
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**Conclusion:** Higher order terms make it very hard to choose the right learning rate

- Second Order Methods are already expensive, $n$th order methods are hopeless. Solution?

Lecture 6 Optimization for Deep Neural Networks CMSC 35246
Batch Normalization

- Method to reparameterize a deep network to reduce co-ordination of update across layers

Let $H$ be a design matrix having activations in any layer for $m$ examples in the mini-batch:

$$H = \begin{bmatrix}
    h_{11} & h_{12} & h_{13} & \ldots & h_{1k} \\
    h_{21} & h_{22} & h_{23} & \ldots & h_{2k} \\
    \vdots & \vdots & \vdots & \ddots & \vdots \\
    h_{m1} & h_{m2} & h_{m3} & \ldots & h_{mk}
\end{bmatrix}$$
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- Method to reparameterize a deep network to reduce co-ordination of update across layers
- Can be applied to input layer, or any hidden layer

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- Each row represents all the activations in layer for one example
Batch Normalization

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Idea: Replace $H$ by $H'$ such that:

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

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Idea: Replace $H$ by $H'$ such that:

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$\mu$ is mean of each unit and $\sigma$ the standard deviation
Batch Normalization

- $\mu$ is a vector with $\mu_j$ the column mean

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Batch Normalization

- $\mu$ is a vector with $\mu_j$ the column mean
- $\sigma$ is a vector with $\sigma_j$ the column standard deviation
- $H_{i,j}$ is normalized by subtracting $\mu_j$ and dividing by $\sigma_j$
Batch Normalization

During training we have:

\[ \mu = \frac{1}{m} \sum_{j} H_{:,j} \]

\[ \sigma = \sqrt{\frac{\sum_{j} (H_{:,j} - \mu)^2}{m}} \]
Batch Normalization

During training we have:

\[ \mu = \frac{1}{m} \sum_j H_{:,j} \]

\[ \sigma = \sqrt{\delta + \frac{1}{m} \sum_j (H - \mu)^2} \]

We then operate on \( H' \) as before \( \implies \) we backpropagate through the normalized activations.
Why is this good?

- The update will never act to only increase the mean and standard deviation of any activation
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- The update will never act to only increase the mean and standard deviation of any activation
- Previous approaches added penalties to cost or per layer to encourage units to have standardized outputs
- Batch normalization makes the reparameterization easier
- At test time: Use running averages of $\mu$ and $\sigma$ collected during training, use these for evaluating new input $x$
An Innovation

- Standardizing the output of a unit can limit the expressive power of the neural network.
An Innovation

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- Solution: Instead of replacing $H$ by $H'$, replace it with $\gamma H' + \beta$ and $\gamma$ and $\beta$ are also learned by backpropagation.
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An Innovation

- Standardizing the output of a unit can limit the expressive power of the neural network.
- Solution: Instead of replacing $H$ by $H'$, replace it with $\gamma H' + \beta$.
- $\gamma$ and $\beta$ are also learned by backpropagation.
- Normalizing for mean and standard deviation was the goal of batch normalization, why add $\gamma$ and $\beta$ again?
Initialization Strategies
In convex problems with good $\epsilon$ no matter what the initialization, convergence is guaranteed.
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In the non-convex regime initialization is much more important.
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What is known: Initialization should break symmetry (quiz!)

What is known: Scale of weights is important

Most initialization strategies are based on intuitions and heuristics.
Some Heuristics

For a fully connected layer with $m$ inputs and $n$ outputs, sample:

$$W_{ij} \sim U\left(-\frac{1}{\sqrt{m}}, \frac{1}{\sqrt{m}}\right)$$
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- For a fully connected layer with $m$ inputs and $n$ outputs, sample:

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- Xavier Initialization: Sample

  $$ W_{ij} \sim U\left(-\frac{6}{\sqrt{m+n}}, \frac{6}{\sqrt{m+n}}\right) $$
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- Xavier initialization is derived considering that the network consists of matrix multiplications with no nonlinearities
- Works well in practice!
More Heuristics

- Saxe *et al.* 2013, recommend initializing to random orthogonal matrices, with a carefully chosen gain $g$ that accounts for non-linearities
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- Saxe *et al*. 2013, recommend initializing to random orthogonal matrices, with a carefully chosen gain $g$ that accounts for non-linearities.
- If $g$ could be divined, it could solve the vanishing and exploding gradients problem (more later).
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- The idea of choosing $g$ and initializing weights accordingly is that we want norm of activations to increase, and pass back strong gradients.
- Martens 2010, suggested an initialization that was sparse: Each unit could only receive $k$ non-zero weights.
- **Motivation:** It is a bad idea to have all initial weights to have the same standard deviation $\frac{1}{\sqrt{m}}$. 

Lecture 6 Optimization for Deep Neural Networks
Polyak Averaging: Motivation

Consider gradient descent above with high step size $\epsilon$. Gradient points towards right.
Polyak Averaging: Motivation

Gradient points towards left
Polyak Averaging: Motivation

Gradient points towards right
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Gradient points towards right
A Solution: Polyak Averaging

Suppose in $t$ iterations you have parameters $\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(t)}$.
A Solution: Polyak Averaging

- Suppose in $t$ iterations you have parameters $\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(t)}$
- Polyak Averaging suggests setting $\hat{\theta}(t) = \frac{1}{t} \sum_i \theta^{(i)}$
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- Has strong convergence guarantees in convex settings.
A Solution: Polyak Averaging

Suppose in $t$ iterations you have parameters $\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(t)}$.

Polyak Averaging suggests setting $\hat{\theta}(t) = \frac{1}{t} \sum_i \theta^{(i)}$.

Has strong convergence guarantees in convex settings.

Is this a good idea in non-convex problems?
In non-convex surfaces the parameter space can differ greatly in different regions.
Simple Modification

- In non-convex surfaces the parameter space can differ greatly in different regions
- Averaging is not useful
In non-convex surfaces the parameter space can differ greatly in different regions.

Averaging is not useful.

Typical to consider the exponentially decaying average instead:

\[ \hat{\theta}(t) = \alpha \hat{\theta}(t-1) + (1 - \alpha) \hat{\theta}(t) \] with \( \alpha \in [0, 1] \)
Next time

- Convolutional Neural Networks