Lecture 6
Optimization for Deep Neural Networks

CMSC 35246: Deep Learning

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  - Stochastic Gradient Descent

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  - On Slides but for self study: Newton and Quasi Newton Methods (BFGS, L-BFGS, Conjugate Gradient)

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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

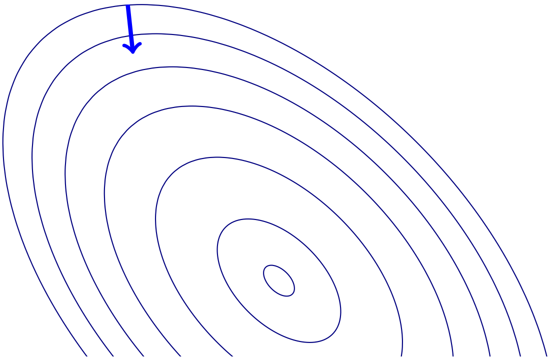
Algorithm 1 Batch Gradient Descent at Iteration k

Require: Learning rate ϵ_k
Require: Initial Parameter θ

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

- Positive: Gradient estimates are stable
- Negative: Need to compute gradients over the entire training for one update

Gradient Descent



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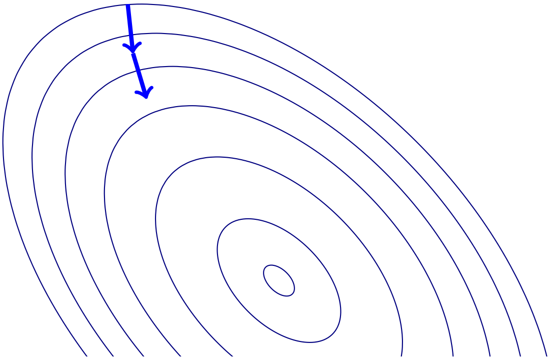

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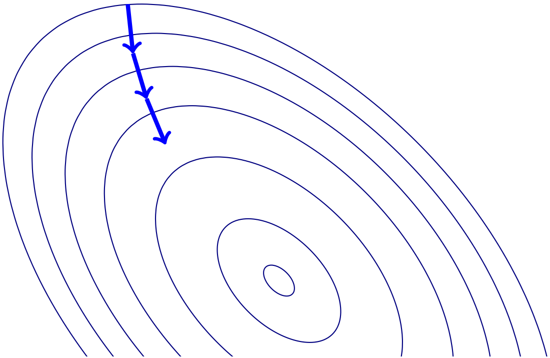

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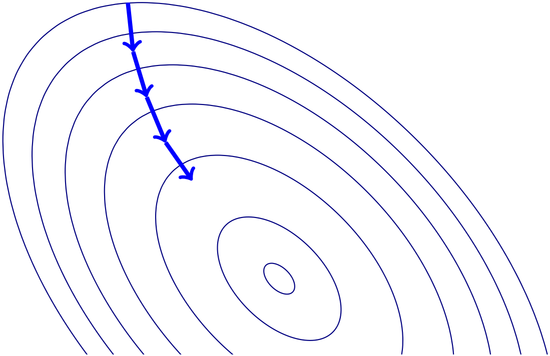

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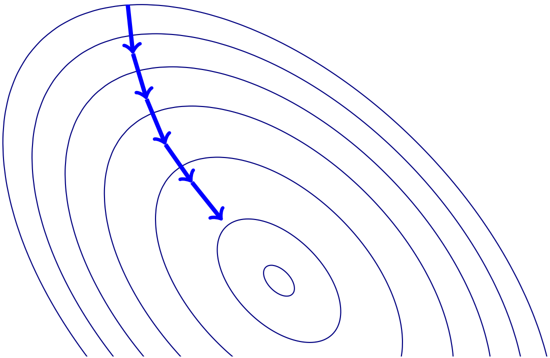

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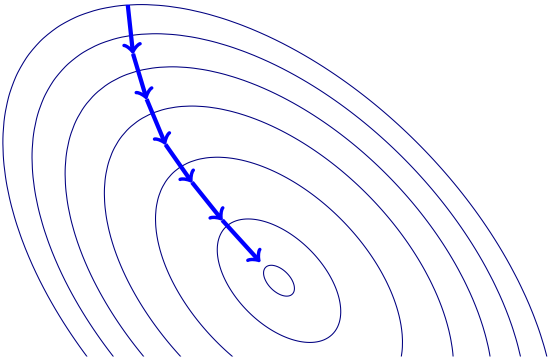

Stochastic Gradient Descent

Algorithm 2 Stochastic Gradient Descent at Iteration k

Require: Learning rate ϵ_k
Require: Initial Parameter θ

```
while stopping criteria not met do
    Sample example (x^(i), y^(i)) from training set
    Compute gradient estimate:
    ĝ ← +∇_θ L(f(x^(i); θ), y^(i))
    Apply Update: θ ← θ − εĝ
end while
```

- **while** stopping criteria not met **do**
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  - $\hat{\mathbf{g}} \leftarrow +\nabla_\theta L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$
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- **end while**

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- ϵ_k is learning rate at step k

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end while

- ϵ_k is learning rate at step k
- Sufficient condition to guarantee convergence:

$$\sum_{k=1}^{\infty} \epsilon_k = \infty \text{ and } \sum_{k=1}^{\infty} \epsilon_k^2 < \infty$$

Learning Rate Schedule

- In practice the learning rate is decayed linearly till iteration τ

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- τ is usually set to the number of iterations needed for a large number of passes through the data
- ϵ_τ should roughly be set to 1% of ϵ_0
- How to set ϵ_0?

Minibatching

- Potential Problem: Gradient estimates can be very noisy

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

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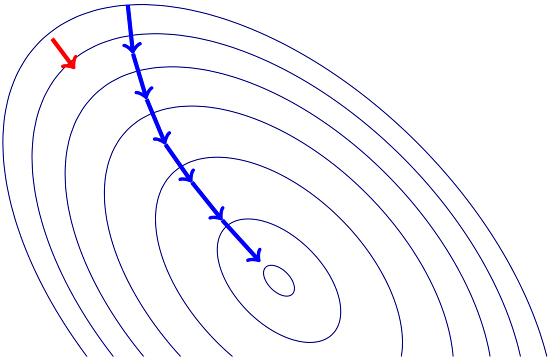

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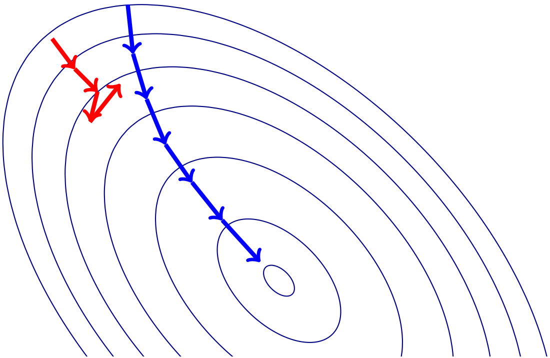

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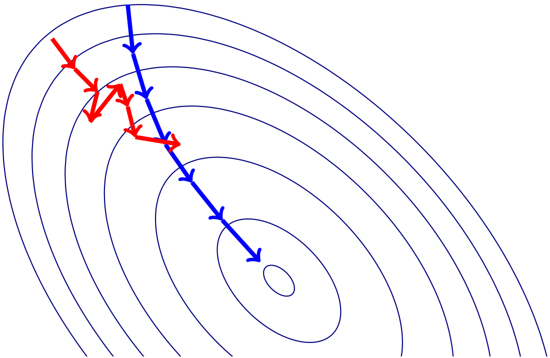

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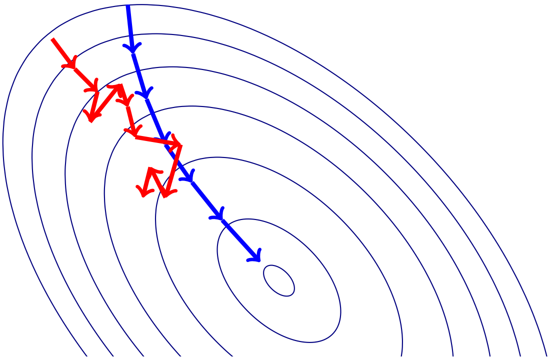

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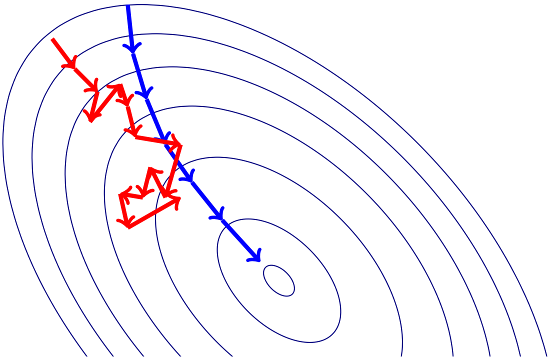

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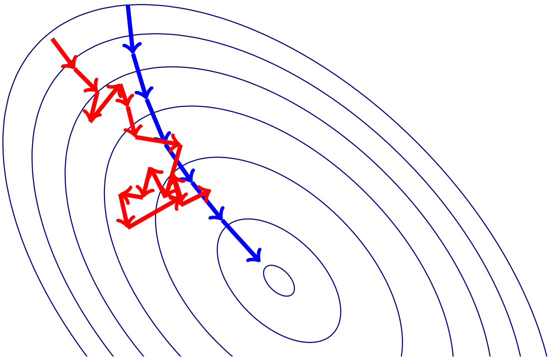

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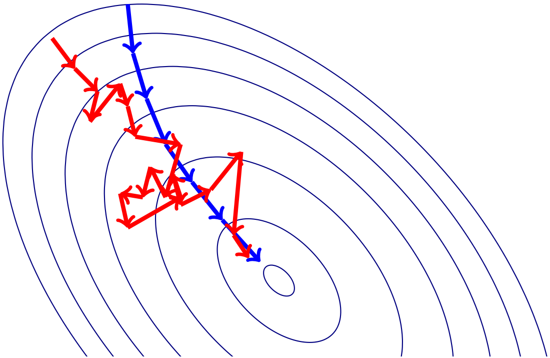

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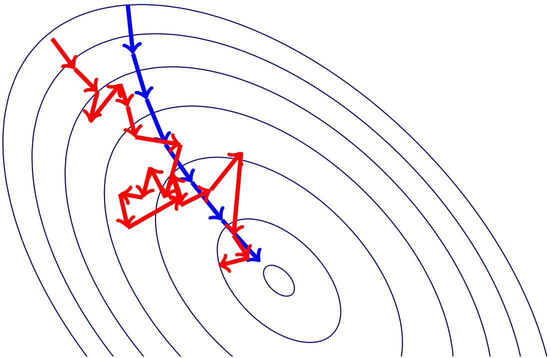

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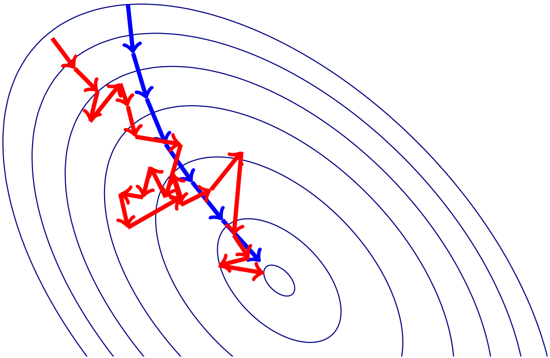

So far..

- Batch Gradient Descent:

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

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- SGD:

$$\hat{\mathbf{g}} \leftarrow +\nabla_\theta L(f(\mathbf{x}^{(i)};\theta),\mathbf{y}^{(i)})$$
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Momentum

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  - Error surface has high curvature

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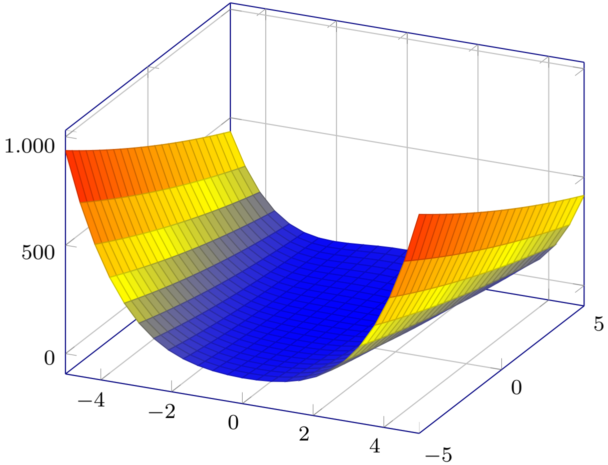
- In particular SGD suffers in the following scenarios:
  - Error surface has high curvature
  - We get small but consistent gradients
  - The gradients are very noisy

Momentum



- Gradient Descent would move quickly down the walls, but very slowly through the valley floor

Momentum

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- Introduce a new variable $\mathbf{v}$, the velocity
- We think of $\mathbf{v}$ 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

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

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

Momentum

- Let's look at the velocity term:

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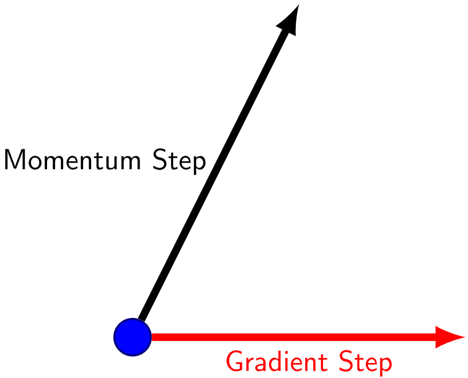
  - If α is larger than ϵ the current update is more affected by the previous gradients
  - Usually values for α are set high $\approx 0.8, 0.9$

Momentum

Momentum



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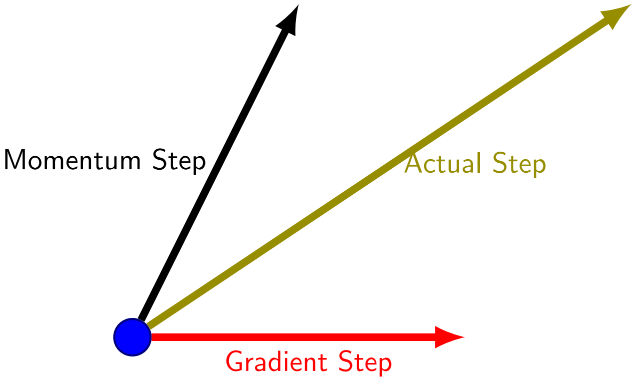

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- For example, if at each step we observed $\mathbf{g}$, the step size would be (exercise!):

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

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

Momentum

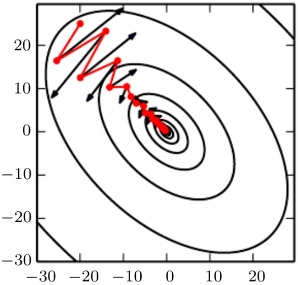

Illustration of how momentum traverses such an error surface better compared to Gradient Descent

SGD with Momentum

Algorithm 2 Stochastic Gradient Descent with Momentum

Require: Learning rate ϵ_k
Require: Momentum Parameter α
Require: Initial Parameter θ
Require: Initial Velocity $\mathbf{v}$

```
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    Sample example (x^(i), y^(i)) from training set
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    Compute the velocity update:
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```
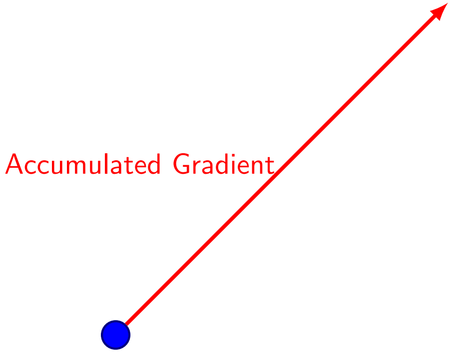

Nesterov Momentum

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



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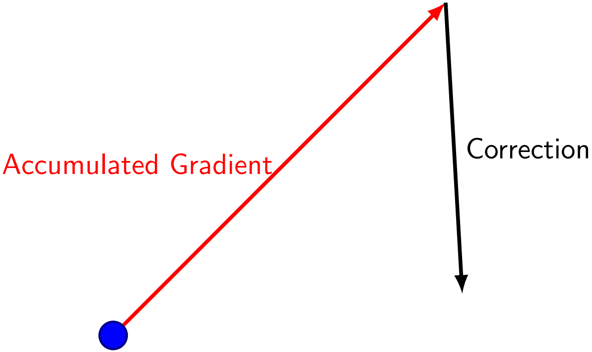

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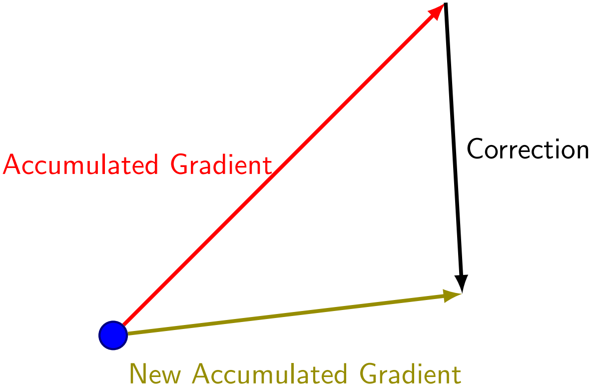

Nesterov Momentum

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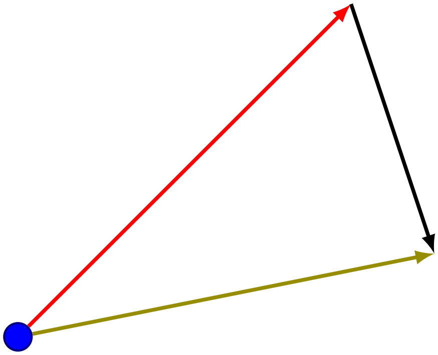

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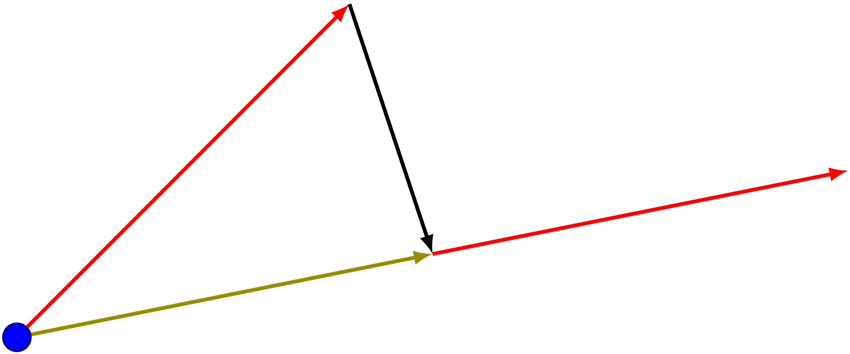

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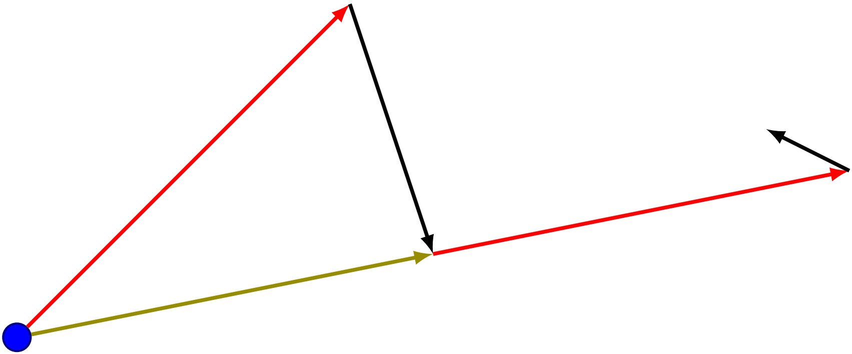

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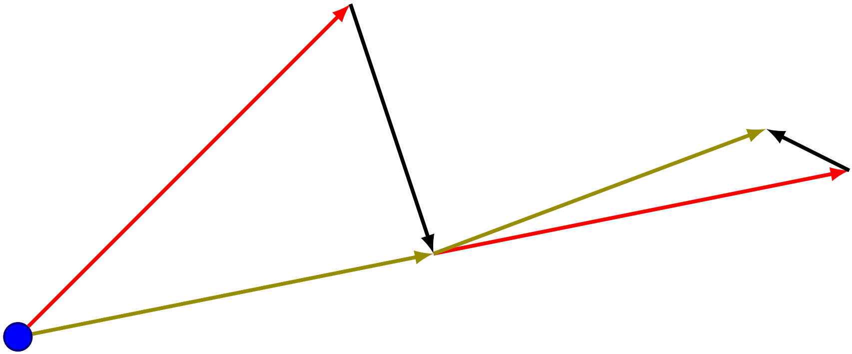

Let's Write it out..

- Recall the velocity term in the Momentum method:

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

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- Update: $\theta \leftarrow \theta + \mathbf{v}$

SGD with Nesterov Momentum

Algorithm 3 SGD with Nesterov Momentum

Require: Learning rate ϵ
Require: Momentum Parameter α
Require: Initial Parameter θ
Require: Initial Velocity $\mathbf{v}$

```
while stopping criteria not met do
    Sample example (x^(i), y^(i)) from training set
    Update parameters: θ̃ ← θ + αv
    Compute gradient estimate:
    ĝ ← +∇_θ̃ L(f(x^(i); θ̃), y^(i))
    Compute the velocity update: v ← αv − εĝ
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```

- **while** stopping criteria not met **do**
  - Sample example $(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})$ from training set
  - Update parameters: $\tilde{\theta} \leftarrow \theta + \alpha \mathbf{v}$
  - Compute gradient estimate:
  - $\hat{\mathbf{g}} \leftarrow +\nabla_{\tilde{\theta}} L(f(\mathbf{x}^{(i)}; \tilde{\theta}), \mathbf{y}^{(i)})$
  - Compute the velocity update: $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \hat{\mathbf{g}}$
  - Apply Update: $\theta \leftarrow \theta + \mathbf{v}$
- **end while**

Adaptive Learning Rate Methods

Motivation

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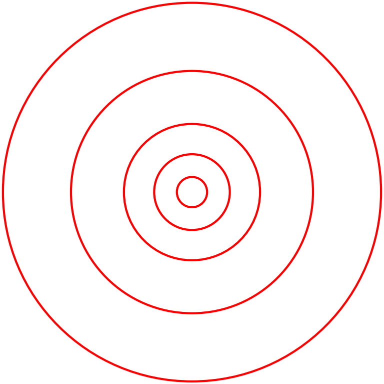
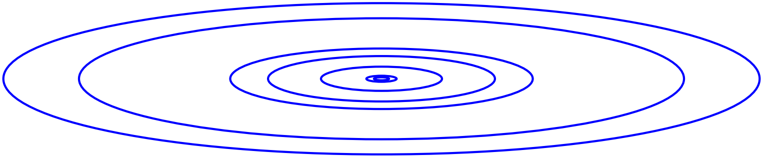
- Till now we assign the same learning rate to all features
- If the features vary in importance and frequency, why is this a good idea?
- It's probably not!

Motivation



Nice (all features are equally important)

Motivation



Harder!

AdaGrad

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- 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

AdaGrad

Algorithm 4 AdaGrad

Require: Global Learning rate ϵ, Initial Parameter θ, δ

Initialize $\mathbf{r} = 0$

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

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
- 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

RMSProp

Algorithm 5 RMSProp

Require: Global Learning rate ϵ, decay parameter ρ, δ

Initialize $\mathbf{r} = 0$

```
while stopping criteria not met do
    Sample example (x^(i), y^(i)) from training set
    Compute gradient estimate: ĝ ← +∇_θ L(f(x^(i); θ), y^(i))
    Accumulate: r ← ρr + (1 − ρ)ĝ ⊙ ĝ
    Compute update: Δθ ← −ε/(δ+√r) ⊙ ĝ
    Apply Update: θ ← θ + Δθ
end while
```

while stopping criteria not met **do**

- Sample example $(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})$ from training set
- Compute gradient estimate: $\hat{\mathbf{g}} \leftarrow +\nabla_\theta L(f(\mathbf{x}^{(i)};\theta), \mathbf{y}^{(i)})$
- Accumulate: $\mathbf{r} \leftarrow \rho\mathbf{r} + (1-\rho)\hat{\mathbf{g}} \odot \hat{\mathbf{g}}$
- Compute update: $\Delta\theta \leftarrow -\frac{\epsilon}{\delta+\sqrt{\mathbf{r}}} \odot \hat{\mathbf{g}}$
- Apply Update: $\theta \leftarrow \theta + \Delta\theta$

end while

RMSProp with Nesterov

Algorithm 6 RMSProp with Nesterov

Require: Global Learning rate ϵ, decay parameter ρ, δ, α, $\mathbf{v}$

Initialize $\mathbf{r} = 0$

while stopping criteria not met **do**

  Sample example $(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})$ from training set

  Compute Update: $\tilde{\theta} \leftarrow \theta + \alpha \mathbf{v}$

  Compute gradient estimate: $\hat{\mathbf{g}} \leftarrow +\nabla_{\tilde{\theta}} L(f(\mathbf{x}^{(i)}; \tilde{\theta}), \mathbf{y}^{(i)})$

  Accumulate: $\mathbf{r} \leftarrow \rho \mathbf{r} + (1 - \rho) \hat{\mathbf{g}} \odot \hat{\mathbf{g}}$

  Compute Velocity: $\mathbf{v} \leftarrow \alpha \mathbf{v} - \frac{\epsilon}{\sqrt{\mathbf{r}}} \odot \hat{\mathbf{g}}$

  Apply Update: $\theta \leftarrow \theta + \mathbf{v}$

end while

Adam

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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: ADAptive Moments

Algorithm 7 RMSProp with Nesterov

Require: ϵ (set to 0.0001), decay rates ρ_1 (set to 0.9), ρ_2 (set to 0.9), θ, δ

Initialize moments variables $\mathbf{s} = 0$ and $\mathbf{r} = 0$, time step t = 0

while stopping criteria not met **do**

  Sample example $(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})$ from training set

  Compute gradient estimate: $\hat{\mathbf{g}} \leftarrow +\nabla_\theta L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

  $t \leftarrow t + 1$

  Update: $\mathbf{s} \leftarrow \rho_1 \mathbf{s} + (1 - \rho_1)\hat{\mathbf{g}}$

  Update: $\mathbf{r} \leftarrow \rho_2 \mathbf{r} + (1 - \rho_2)\hat{\mathbf{g}} \odot \hat{\mathbf{g}}$

  Correct Biases: $\hat{\mathbf{s}} \leftarrow \frac{\mathbf{s}}{1-\rho_1^t}, \hat{\mathbf{r}} \leftarrow \frac{\mathbf{r}}{1-\rho_2^t}$

  Compute Update: $\Delta\theta = -\epsilon \frac{\hat{\mathbf{s}}}{\sqrt{\hat{\mathbf{r}}} + \delta}$

  Apply Update: $\theta \leftarrow \theta + \Delta\theta$

end while

All your GRADs are belong to us!

SGD: $\theta \leftarrow \theta - \epsilon \hat{\mathbf{g}}$

Momentum: $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \hat{\mathbf{g}}$ then $\theta \leftarrow \theta + \mathbf{v}$

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

AdaGrad: $\mathbf{r} \leftarrow \mathbf{r} + \mathbf{g} \odot \mathbf{g}$ then $\Delta\theta - \leftarrow \dfrac{\epsilon}{\delta + \sqrt{\mathbf{r}}} \odot \mathbf{g}$ then $\theta \leftarrow \theta + \Delta\theta$

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

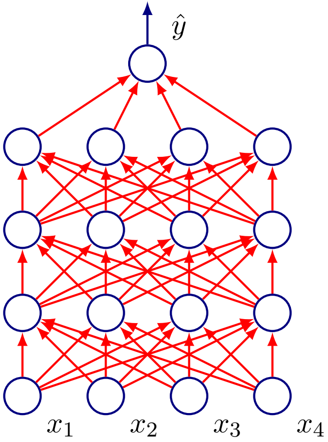
Adam: $\hat{\mathbf{s}} \leftarrow \dfrac{\mathbf{s}}{1 - \rho_1^t}, \hat{\mathbf{r}} \leftarrow \dfrac{\mathbf{r}}{1 - \rho_2^t}$ then $\Delta\theta = -\epsilon \dfrac{\hat{\mathbf{s}}}{\sqrt{\hat{\mathbf{r}}} + \delta}$ then $\theta \leftarrow \theta + \Delta\theta$

Batch Normalization

A Difficulty in Training Deep Neural Networks

A deep model involves composition of several functions

$$\hat{y} = W_4^T(\tanh(W_3^T(\tanh(W_2^T(\tanh(W_1^T\mathbf{x} + \mathbf{b}_1) + \mathbf{b}_2) + \mathbf{b}_3))))$$



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- This can give rise to unexpected difficulties
- Let's look at two illustrations

Intuition

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

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

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

$$\theta = \theta^{(0)} - \epsilon \mathbf{g}$$

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

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  - Correction factor that accounts for the curvature of the function

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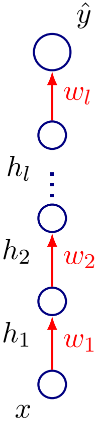
- Conclusion: Just neglecting second order effects can cause problems (remedy: second order methods). What about higher order effects?

Higher Order Effects: Toy Model



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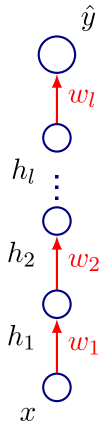

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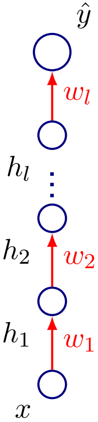

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- $\hat{y}$ is linear in x but non-linear in w_i

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- If we need to reduce cost by 0.1, then learning rate should be $\frac{0.1}{\mathbf{g}^T\mathbf{g}}$

Higher Order Effects: Toy Model

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

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- Second Order Methods are already expensive, nth order methods are hopeless. Solution?

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- μ is mean of each unit and σ the standard deviation

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

- We then operate on H' as before $\implies$ we backpropagate *through* the normalized activations

Why is this good?

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- At test time: Use running averages of μ and σ collected during training, use these for evaluating new input $\mathbf{x}$

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- Normalizing for mean and standard deviation was the goal of batch normalization, why add γ and β again?

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- Most initialization strategies are based on intuitions and heuristics

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- Works well in practice!

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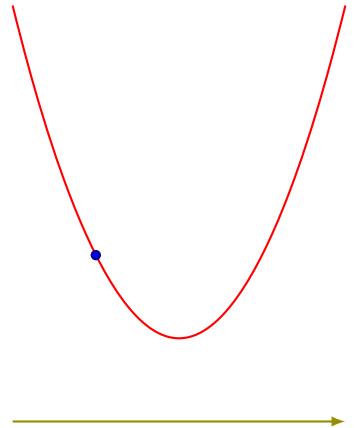
- The idea of choosing g and initializing weights accordingly is that we want norm of activations to increase, and pass back strong gradients
- Martens 2010, suggested an initialization that was sparse: Each unit could only receive k non-zero weights
- Motivation: Ir is a bad idea to have all initial weights to have the same standard deviation $\frac{1}{\sqrt{m}}$

Polyak Averaging: Motivation



- Consider gradient descent above with high step size ϵ

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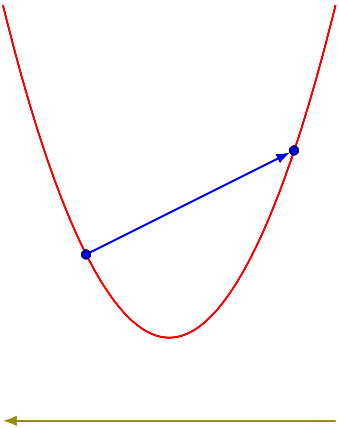

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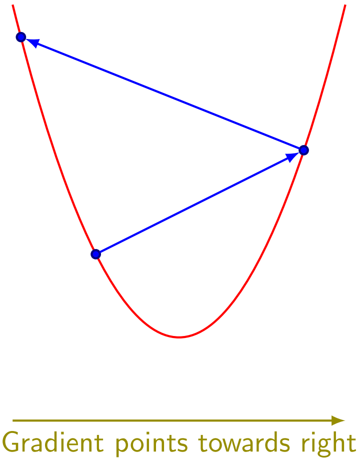
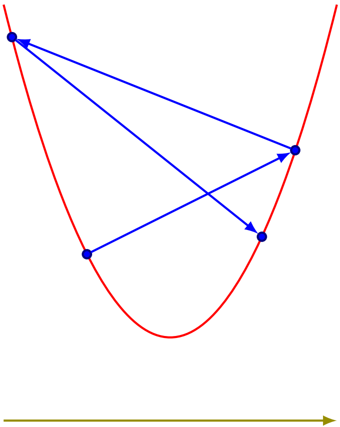


Polyak Averaging: Motivation



Gradient points towards left

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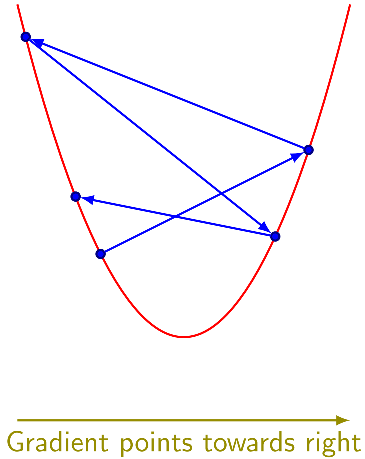

A Solution: Polyak Averaging

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- 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?

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- 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:

$$\hat{\theta}^{(t)} = \alpha\hat{\theta}^{(t-1)} + (1-\alpha)\hat{\theta}^{(t)} \text{ with } \alpha \in [0,1]$$

Next time

- Convolutional Neural Networks