Optimization

Optimization difficulties, Minibatch optimization, Momentum, Nesterov’s Momentum, Parameter initialization, Algorithms (SGD, Adam, AdaGrad)

How learning is different from pure *optimization*?

While training the model

$$J(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{x},\mathrm{y})\sim \hat{p}_{\text{data}}} L(f(\boldsymbol{x};\boldsymbol{\theta}), y),$$

$\hat{p}_{data}$ distribution of training data

What we actually want

$$J^*(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{x},\mathrm{y})\sim p_{\text{data}}} L(f(\boldsymbol{x};\boldsymbol{\theta}), y).$$

p_{data} distribution of actual data

Empirical risk minimization

$$\mathbb{E}_{\boldsymbol{x},\mathrm{y}\sim \hat{p}_{\text{data}}(\boldsymbol{x},y)}[L(f(\boldsymbol{x};\boldsymbol{\theta}), y)] = \frac{1}{m}\sum_{i=1}^{m} L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}), y^{(i)})$$

*Slide courtesy, Ian Goodfellow et al., deep learning book

Batch and Minibatch algorithms

Loss function

$$J(\boldsymbol{\theta}) = \mathbb{E}_{(\boldsymbol{x},y)\sim\hat{p}_{\text{data}}} L(f(\boldsymbol{x};\boldsymbol{\theta}), y),$$

Training by backpropagation

$$\nabla_\theta J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \nabla_\theta L(f(x_i;\theta), y_i)$$

It requires you to evaluate gradients w.r.t all the training examples for gradient estimation

Is this efficient?

- Variance in the estimation with m samples - $\sigma/\sqrt{m}$
- By calculating grads over all samples, we get only sub-linear performance

*Slide courtesy, Ian Goodfellow et al., deep learning book

Batch and Minibatch algorithms

Loss function

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Training by backpropagation

$$\nabla_\theta J(\theta) = \frac{1}{m}\sum_{i=1}^{m} \nabla_\theta L(f(x_i;\theta), y_i)$$

By calculating grads over all samples, we get only **sub-linear** performance

What is the alternative?

- Simple solution, don't use all the samples for gradient estimation
- At each update iteration, randomly chose B samples and use them for estimating gradients **Minibatch training**
- Also, does as unbiased estimate of gradients

$$\nabla_\theta J(\theta) = \frac{1}{B}\sum_{i=1}^{B} \nabla_\theta L(f(x_i;\theta), y_i)$$

*Slide courtesy, Ian Goodfellow et al., deep learning book

Algorithms for optimization

Stochastic Gradient Descent (SGD)

Algorithm 8.1 Stochastic gradient descent (SGD) update at training iteration k

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Require: Learning rate ϵ_k.
Require: Initial parameter $\boldsymbol{\theta}$
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient estimate: $\hat{\boldsymbol{g}} \leftarrow +\frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon \hat{\boldsymbol{g}}$
  end while

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*Slide courtesy, Ian Goodfellow et al., deep learning book

Algorithms for optimization

Stochastic Gradient Descent (SGD) with momentum

Parameter update step of SGD

$$\text{Apply update: } \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \epsilon \hat{\boldsymbol{g}}$$

- Depending on $\boldsymbol{\epsilon}$, learning can be very slow or have drastic oscillations
- Momentum is designed to accelerate SGD
- The momentum algorithm accumulates a weighted avg. of past gradients and continues to move in their direction.

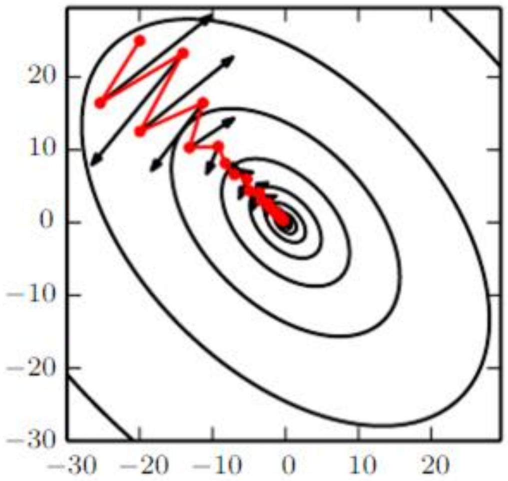

Figure showing effect of momentum
----- path with momentum
→ direction that SGD would take

$$\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \epsilon \nabla_{\boldsymbol{\theta}} \left(\frac{1}{m} \sum_{i=1}^{m} L(\boldsymbol{f}(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)}) \right),$$

Velocity $\boldsymbol{v}$ accumulates the past gradients

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}.$$

The larger α is relative to $\boldsymbol{\epsilon}$, the effect of past gradients is more

*Slide courtesy, Ian Goodfellow et al., deep learning book

Algorithms for optimization

Stochastic Gradient Descent (SGD) with momentum

Parameter update step now

$$v \leftarrow \alpha v - \epsilon \nabla_{\theta} \left(\frac{1}{m} \sum_{i=1}^{m} L(f(x^{(i)}; \theta), y^{(i)}) \right),$$

$$\theta \leftarrow \theta + v.$$

- In SGD, update step size was ϵ ||g||
- With momentum, depends on how large and how aligned a *sequence* of gradients are
- Its largest, when successive gradients are same

If momentum repeatedly observes gradient as ***g***, it accelerates by a factor of $\frac{1}{1-\alpha}$, resulting in $\frac{\epsilon ||g||}{1 - \alpha}$.

For α = 0.9, the descent is 10 times normal SGD

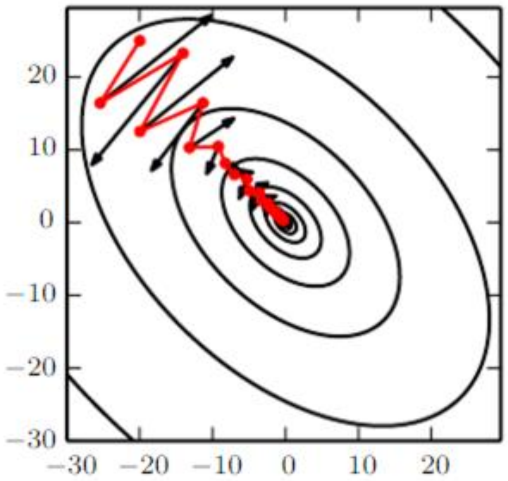

Figure showing effect of momentum
----- path with momentum
→ direction that SGD would take

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Algorithms for optimization

Stochastic Gradient Descent (SGD) with momentum

Algorithm 8.2 Stochastic gradient descent (SGD) with momentum

Require: Learning rate ϵ, momentum parameter α.
Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$.
while stopping criterion not met **do**
Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
Compute gradient estimate: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
Compute velocity update: $\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \epsilon \boldsymbol{g}$
Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
end while

*Slide courtesy, Ian Goodfellow et al., deep learning book

Algorithms for optimization

Nesterov momentum

Parameter update

$$v \leftarrow \alpha v - \epsilon \nabla_{\theta} \left[\frac{1}{m} \sum_{i=1}^{m} L\left(f(x^{(i)}; \boxed{\theta + \alpha v}), y^{(i)} \right) \right],$$

Look ahead

$$\theta \leftarrow \theta + v,$$

*Slide courtesy, Ian Goodfellow et al., deep learning book

Algorithms for optimization

Nesterov momentum

Algorithm 8.3 Stochastic gradient descent (SGD) with Nesterov momentum

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Require: Learning rate ϵ, momentum parameter α.
Require: Initial parameter $\boldsymbol{\theta}$, initial velocity $\boldsymbol{v}$.
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ with corresponding labels $\boldsymbol{y}^{(i)}$.
    Apply interim update: $\tilde{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta} + \alpha \boldsymbol{v}$ ***Look ahead step***
    Compute gradient (at interim point): $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\tilde{\boldsymbol{\theta}}} \sum_i L(f(\boldsymbol{x}^{(i)}; \tilde{\boldsymbol{\theta}}), \boldsymbol{y}^{(i)})$
    Compute velocity update: $\boldsymbol{v} \leftarrow \alpha \boldsymbol{v} - \epsilon \boldsymbol{g}$
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \boldsymbol{v}$
  end while

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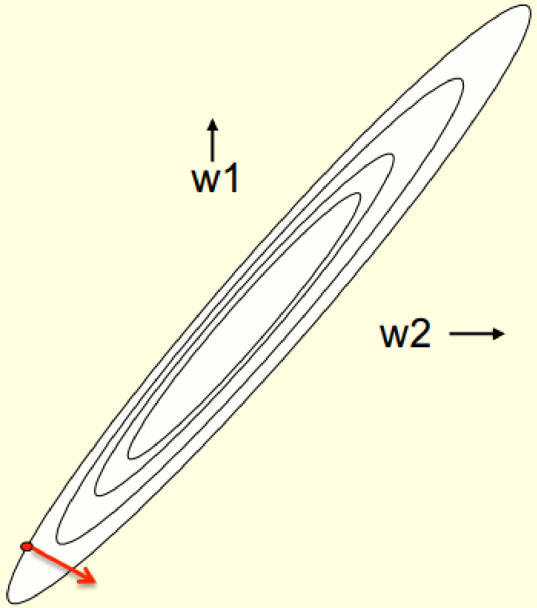
*Slide courtesy, Ian Goodfellow et al., deep learning book

Algorithms for optimization

Why learning can be slow

- If the ellipse is very elongated, the direction of steepest descent is almost perpendicular to the direction towards the minimum!
  - The red gradient vector has a large component along the short axis of the ellipse and a small component along the long axis of the ellipse.
  - This is just the opposite of what we want.



*Slide courtesy, G. Hinton's course on cousera week 3

Algorithms for optimization - adaptive learning rate

AdaGrad (Duchi et al., 2011)

Parameter update

Scales the learning rate with square root of sum of past gradients

- Larger partial derivatives - reduced learning rates (viceversa)

Algorithm 8.4 The AdaGrad algorithm

Require: Global learning rate ϵ
Require: Initial parameter $\boldsymbol{\theta}$
Require: Small constant δ, perhaps 10^{-7}, for numerical stability
  Initialize gradient accumulation variable $\boldsymbol{r} = \boldsymbol{0}$
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m}\nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)};\boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Accumulate squared gradient: $\boldsymbol{r} \leftarrow \boldsymbol{r} + \boldsymbol{g} \odot \boldsymbol{g}$
    Compute update: $\Delta\boldsymbol{\theta} \leftarrow -\frac{\epsilon}{\delta+\sqrt{\boldsymbol{r}}} \odot \boldsymbol{g}$. (Division and square root applied element-wise)
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta\boldsymbol{\theta}$
  end while

Algorithms for optimization - adaptive learning rate

RMSProp(Hinton et al., 2012)

Parameter update

Scales the learning rate with weighted average of square of past gradients

Algorithm 8.5 The RMSProp algorithm

Require: Global learning rate ϵ, decay rate ρ.
Require: Initial parameter $\boldsymbol{\theta}$
Require: Small constant δ, usually 10^{-6}, used to stabilize division by small numbers.
  Initialize accumulation variables $\boldsymbol{r} = 0$
  while stopping criterion not met **do**
    Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
    Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
    Accumulate squared gradient: $\boldsymbol{r} \leftarrow \rho \boldsymbol{r} + (1 - \rho) \boldsymbol{g} \odot \boldsymbol{g}$
    Compute parameter update: $\Delta \boldsymbol{\theta} = -\frac{\epsilon}{\sqrt{\delta + \boldsymbol{r}}} \odot \boldsymbol{g}$. ($\frac{1}{\sqrt{\delta + \boldsymbol{r}}}$ applied element-wise)
    Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta \boldsymbol{\theta}$
  end while

Algorithms for optimization - adaptive learning rate

Adam (Kingma et al., 2014)

Parameter update

Combines RMSProp and momentum methods

Algorithm 8.7 The Adam algorithm

Require: Step size ϵ (Suggested default: 0.001)
Require: Exponential decay rates for moment estimates, ρ_1 and ρ_2 in $[0, 1)$. (Suggested defaults: 0.9 and 0.999 respectively)
Require: Small constant δ used for numerical stabilization. (Suggested default: 10^{-8})
Require: Initial parameters $\boldsymbol{\theta}$
Initialize 1st and 2nd moment variables $\boldsymbol{s} = \boldsymbol{0}$, $\boldsymbol{r} = \boldsymbol{0}$
Initialize time step $t = 0$
while stopping criterion not met **do**
Sample a minibatch of m examples from the training set $\{\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(m)}\}$ with corresponding targets $\boldsymbol{y}^{(i)}$.
Compute gradient: $\boldsymbol{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), \boldsymbol{y}^{(i)})$
$t \leftarrow t + 1$
Update biased first moment estimate: $\boldsymbol{s} \leftarrow \rho_1 \boldsymbol{s} + (1 - \rho_1)\boldsymbol{g}$
Update biased second moment estimate: $\boldsymbol{r} \leftarrow \rho_2 \boldsymbol{r} + (1 - \rho_2)\boldsymbol{g} \odot \boldsymbol{g}$
Correct bias in first moment: $\hat{\boldsymbol{s}} \leftarrow \frac{\boldsymbol{s}}{1-\rho_1^t}$
Correct bias in second moment: $\hat{\boldsymbol{r}} \leftarrow \frac{\boldsymbol{r}}{1-\rho_2^t}$
Compute update: $\Delta \boldsymbol{\theta} = -\epsilon \frac{\hat{\boldsymbol{s}}}{\sqrt{\hat{\boldsymbol{r}}}+\delta}$ (operations applied element-wise)
Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta \boldsymbol{\theta}$
end while

*Slide courtesy, Ian Goodfellow et al., deep learning book

END