

OPTIMIZATION FOR DEEP LEARNING



Stochastic Gradient Descent

Stochastic gradient descent (SGD) and its variants are probably the most used optimization algorithms for machine learning in general and for deep learning in particular.

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Optimization algorithms use only a single example at a time are sometimes called **stochastic** or sometimes **online** methods.

Most algorithms using more than one but less than all of the training examples. **minibatch** or **minibatch** stochastic methods and common to simply call them **stochastic** methods.

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

Require: Learning rate ϵ_k .

Require: Initial parameter θ

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

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

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

end while

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

Stochastic gradient descent (SGD) with momentum

method of momentum is designed to accelerate learning

momentum algorithm accumulates an exponentially decaying moving average of past gradients and continues to move in their direction

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A hyperparameter $\alpha \in [0,1)$ determines how quickly the contributions of previous gradients exponentially decay

The larger α is relative to e , the more previous gradients affect the current direction.

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


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

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 $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ 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

Nesterov Momentum

a variant of the momentum algorithm that was inspired by Nesterov's accelerated gradient method

difference between Nesterov momentum and standard momentum is where the gradient is evaluated.

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

Algorithm 8.3 Stochastic gradient descent (SGD) with Nesterov 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 $\{\boldsymbol{x}^{(1)}, \dots, \boldsymbol{x}^{(m)}\}$ with corresponding labels $\boldsymbol{y}^{(i)}$.

 Apply interim update: $\tilde{\boldsymbol{\theta}} \leftarrow \boldsymbol{\theta} + \alpha \boldsymbol{v}$

 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

Algorithms with Adaptive Learning Rates

- ❑ cost is often highly sensitive to some directions in parameter space and insensitive to others.
- ❑ use a separate learning rate for each parameter, and automatically adapt these learning rates

AdaGrad

- ❖ individually adapts the learning rates of all model parameters by scaling them inversely proportional to the square root of the sum of all of their historical squared values
- ❖ The parameters with the largest partial derivative of the loss have a correspondingly rapid decrease in their learning rate, while parameters with small partial derivatives have a relatively small decrease in their learning rate.

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 $\mathbf{r} = \mathbf{0}$

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

 Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\boldsymbol{\theta}} \sum_i L(f(\mathbf{x}^{(i)}; \boldsymbol{\theta}), \mathbf{y}^{(i)})$

 Accumulate squared gradient: $\mathbf{r} \leftarrow \mathbf{r} + \mathbf{g} \odot \mathbf{g}$

 Compute update: $\Delta \boldsymbol{\theta} \leftarrow -\frac{\epsilon}{\delta + \sqrt{\mathbf{r}}} \odot \mathbf{g}$. (Division and square root applied element-wise)

 Apply update: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \Delta \boldsymbol{\theta}$

end while

empirically it has been found that—for training deep neural network models—the accumulation of squared gradients *from the beginning of training* can result in a premature and excessive decrease in the effective learning rate.

RMSProp

RMSProp algorithm modifies AdaGrad to perform better in the non-convex setting by changing the gradient accumulation into an exponentially weighted moving average.

Algorithm 8.5 The RMSProp algorithm

Require: Global learning rate ϵ , decay rate ρ .

Require: Initial parameter θ

Require: Small constant δ , usually 10^{-6} , used to stabilize division by small numbers.

Initialize accumulation variables $r = 0$

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

 Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

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

 Compute parameter update: $\Delta \theta = -\frac{\epsilon}{\sqrt{\delta + \mathbf{r}}} \odot \mathbf{g}$. ($\frac{1}{\sqrt{\delta + \mathbf{r}}}$ applied element-wise)

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

end while

Adam

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 θ

Initialize 1st and 2nd moment variables $\mathbf{s} = \mathbf{0}$, $\mathbf{r} = \mathbf{0}$

Initialize time step $t = 0$

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

 Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

$t \leftarrow t + 1$

 Update biased first moment estimate: $\mathbf{s} \leftarrow \rho_1 \mathbf{s} + (1 - \rho_1) \mathbf{g}$

 Update biased second moment estimate: $\mathbf{r} \leftarrow \rho_2 \mathbf{r} + (1 - \rho_2) \mathbf{g} \odot \mathbf{g}$

 Correct bias in first moment: $\hat{\mathbf{s}} \leftarrow \frac{\mathbf{s}}{1 - \rho_1^t}$

 Correct bias in second moment: $\hat{\mathbf{r}} \leftarrow \frac{\mathbf{r}}{1 - \rho_2^t}$

 Compute update: $\Delta \theta = -\epsilon \frac{\hat{\mathbf{s}}}{\sqrt{\hat{\mathbf{r}} + \delta}}$ (operations applied element-wise)

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

end while
