Momentum-based Optimization Techniques in Machine Learning and Deep Learning

Pham Viet Hung



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But before digging into the topic...

https://www.youtube.com/watch?v=dQ4jUFmp7hQ

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Overview

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Estimation/Learning vs. Pure Optimization

- ► Stats: Estimation; CS: Learning Meaning: using data to estimate an unknown quantity. (Wasserman, 2004)
- In Machine Learning (ML) / Deep Learning (DL), optimization is a tool to achieve the best possible P (some performance metric) defined w.r.t the test set; hard to track it \Longrightarrow optimize P indirectly through a cost function $J(\theta)$.
- ▶ In pure optimization, we care about only $J(\theta)$.
- ▶ Cost Function: $J(\theta) = \mathbb{E}_{(x,y) \sim \hat{p}_{\mathsf{data}}} [L(f(x;\theta),y)]; \quad \hat{p}_{\mathsf{data}}$: empirical distro
- Empirical Risk Minimization (ERM):

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

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Gradient-based Optimization

- ► First-order optimization algorithms: Using flavours of gradient-only algorithm. Mostly some variants of gradient descent algorithms.
- ➤ Second-order optimization algorithms: Algorithms that make use of Hessian matrix (a.k.a second derivatives). *Problem*: Poor conditioning of the Hessian matrix.
- ► The above-mentioned optimization techniques are mostly used in convex optimization. In DL, mostly as a subroutine of some DL algorithms.
- ▶ Usually variants of Stochastic Gradient Descent optimization (usually with minibatch) are used in ML and DL.

Vanilla SGD SGD with Polyak Momentum SGD with Nesterov Momentum

Momentum-based methods

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Vanilla SGD (1)

- SGD (with minibatch) and its flavours are the most used optimization methods for ML tasks.
- ▶ The step length/learning rate is defined as fixed in SGD, but in practice, we need a gradually decreasing value \Longrightarrow denote it as ϵ_k .
- ▶ The two sufficient conditions to guarantee the convergence of SGD:

$$\sum_{k=1}^{\infty} \epsilon_k = \infty \tag{2}$$

$$\sum_{k=1}^{\infty} \epsilon_k^2 \le \infty \tag{3}$$

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Vanilla SGD (2)

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

```
Require: Learning rate \epsilon_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)}, \dots, \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

Figure: Algorithm of the Vanilla SGD (Goodfellow et al., 2016)

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SGD with Polyak Momentum (1)

- Sometimes learning with SGD is slow.
- ▶ Polyak (1964) proposes a method to accelerate learning in a high curvature, small and consistent/noisy gradient environment.
- ▶ The key driver is the **velocity** variable v.

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SGD with Polyak Momentum (2)

Algorithm 8.2 Stochastic gradient descent (SGD) with momentum

Require: Learning rate ϵ , momentum parameter α

Require: Initial parameter θ , initial velocity v

while stopping criterion not met do

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

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

Compute velocity update: $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \mathbf{g}$.

Apply update: $\theta \leftarrow \theta + v$.

end while

Figure: Algorithm of the SGD w/ Polyak Momentum (Goodfellow et al., 2016)

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SGD with Nesterov Momentum (1)

- ▶ Based on Nesterov's (1983, 2004) accelerated method, Sutskever (2013) in his PhD thesis proposed a variant of momentum-based SGD optimization technique.
- ▶ Difference between Nesterov and Polyak momentum is the evaluation point of the gradient.
- ▶ With Nesterov momentum, the evaluation of the the gradient occurs after the current velocity is applied.

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SGD with Nesterov Momentum (2)

```
Algorithm 8.3 Stochastic gradient descent (SGD) with Nesterov momentum
```

Require: Learning rate ϵ , momentum parameter α

Require: Initial parameter θ , initial velocity v

while stopping criterion not met do

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

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

Compute gradient (at interim point): $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\tilde{\boldsymbol{\theta}}} \sum_{i} L(f(\mathbf{x}^{(i)}; \tilde{\boldsymbol{\theta}}), \mathbf{y}^{(i)}).$

Compute velocity update: $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \mathbf{g}$.

Apply update: $\theta \leftarrow \theta + v$.

end while

Figure: Algorithm of the SGD w/ Nesterov Momentum (Goodfellow et al., 2016)

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Vanilla SGD SGD with Polyak Momentum SGD with Nesterov Momentum

Thank you very much for your attention!

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References 1

- Wasserman, L. (2004). All of statistics: a concise course in statistical inference (Vol. 26). New York: Springer.
- Goodfellow, I., Bengio, Y., Courville, A. (2016). Deep Learning. MIT Press.
- Melville, J. (2016). *Nesterov Accelerated Gradient and Momentum*. https://jlmelville.github.io/mize/nesterov.html#Sutskever_Nesterov_Momentum
- Li, F-F. et al. (2022). *CS231n: Deep Learning for Computer Vision*. Stanford University. https://cs231n.github.io/neural-networks-3/

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References 2

- Polyak, B. T. (1964). Some methods of speeding up the convergence of iteration methods. USSR Computational Mathematics and Mathematical Physics, 4(5), 1–17.
- Nesterov, Y. (1983). A method of solving a convex programming problem with convergence rate $O(1/k^2)$. Soviet Mathematics Doklady, 27(2):372–376
- Nesterov, Y. (2004). *Introductory lectures on convex optimization: A basic course*. Kluwer Academic Publishers
- Sutskever, I. (2013). *Training Recurrent Neural Networks*. University of Toronto. https://tspace.library.utoronto.ca/bitstream/1807/36012/6/Ilya_Sutskever_201306 PhD thesis.pdf

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