CS 6501 Natural Language Processing

Optimization for Deep Learning

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Overview

1. Learning via Optimization
2. Stochastic Gradient Descent
3. Adaptive Learning Rates
4. Other Tricks

Learning via Optimization

Expected Loss

For a distribution of $\mathscr{D}$ over $(\boldsymbol{x}, y)$, where $\boldsymbol{x}$ denotes the input and y is the corresponding output/label, the ideal prediction function is the one that minimize the expected loss $E(f) = \int_{\mathscr{D}} L(f(\boldsymbol{x}), y)$

$$f^* = \arg\min_f E(f) \tag{1}$$

where $L(\cdot, \cdot)$ is the loss function.

Empirical Loss

Instead of minimizing the expected loss in Equation 1, which is also impossible, we can minimize the empirical loss $E_n(f) = \frac{1}{n}\sum_{i=1}^{n} L(f(\boldsymbol{x}^{(i)}), y^{(i)})$,

$$f_n = \arg\min_f E_n(f) \tag{2}$$

where $\{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{n} \sim \mathcal{D}$ is the training set.

Question

How far from f_n to f^*

Question

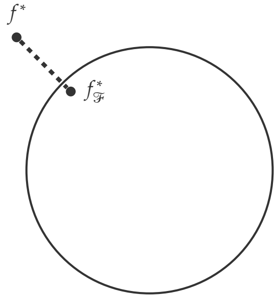
How far from f_n to f^*

Three steps in machine learning

1. collect data
2. design a model
3. optimize an objective function

Approximation Error

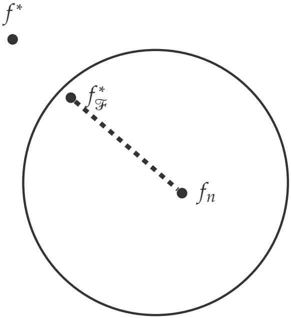
$$
\begin{aligned}
f^* &= \arg\min_{f} E(f) \qquad (3)\\
f^*_{\mathcal{F}} &= \arg\min_{f \in \mathcal{F}} E(f) \qquad (4)
\end{aligned}
$$



[Kearns et al., 1994, Agnostic ML]

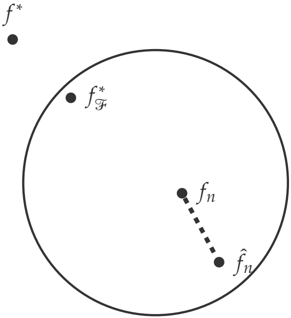
Estimation Error

$$
\begin{aligned}
f_{\mathcal{F}}^{*} &= \arg\min_{f \in \mathcal{F}} E(f) && (5)\\
f_n &= \arg\min_{f \in \mathcal{F}} E_n(f) && (6)
\end{aligned}
$$



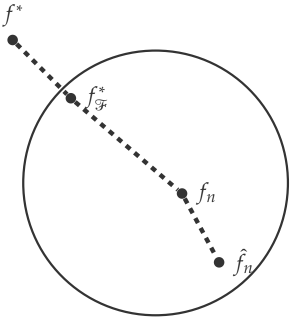
Optimization Error

$$f_n = \arg\min_{f \in \mathcal{F}} E_n(f) \tag{7}$$



Error Decomposition

$$\underbrace{E[E(f^*_{\mathcal{F}}) - E(f^*)]}_{\text{approximation error}} + \underbrace{E[E(f_n) - E(f^*_{\mathcal{F}})]}_{\text{estimation error}} + \underbrace{E[E(\hat{f}_n) - E(f_n)]}_{\text{optimization error}}$$

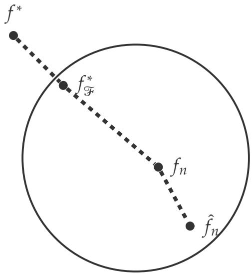


[Bottou, 2012, Sec. 18.3.1]

For a given machine learning problem,

- there is no way to know the oracle function f^* and $f^*_{\mathcal{F}}$, and
- it is difficult to get f_n, especially when $\mathcal{F}$ is a collection of deep neural networks

But it is useful to think about the decomposition.



For example, in the context of neural network learning,

- to reduce the approximation error is the motivation to design your neural network model carefully;
- to reduce the estimation error is the reason we should have enough data;
- to reduce the optimization error is why we need to know the optimization algorithms.

Stochastic Gradient Descent

Given a training set $\{(\boldsymbol{x}^{(i)}, y^{(i)})\}_{i=1}^{n}$, the empirical loss is defined as

$$\ell(\boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} L(f(\boldsymbol{x}^{(i)}; \boldsymbol{\theta}), y^{(i)}) \tag{8}$$

where $L(\cdot, \cdot)$ is the loss function for a single example and $\boldsymbol{\theta}$ denotes the parameters in f.

SGD

To learn the parameter $\boldsymbol{\theta}$, we can compute the gradient with respect to one training example and then use stochastic gradient descent as

$$\boldsymbol{\theta}^{(t)} \leftarrow \boldsymbol{\theta}^{(t-1)} - \eta \cdot \boldsymbol{g}^{(t-1)} \tag{9}$$

where $\boldsymbol{g}^{(t-1)} = \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^{(t-1)})$ is the gradient of the single-example loss L.

Learning Rate

The usual conditions on the learning rates are

$$\sum_{t=1}^{\infty} \eta_t = \infty \tag{10}$$

$$\sum_{t=1}^{\infty} \eta_t^2 \leq \infty \tag{11}$$

A simplest function that satisfies these conditions is $\eta_t = \frac{1}{t}$.

[Bottou, 1998]

SGD with Momentum

Given the loss function $L(\boldsymbol{\theta})$ to be minimized, SGD with momentum is given by

$$\boldsymbol{v}^{(t)} = \mu \boldsymbol{v}^{(t-1)} + \boldsymbol{g}^{(t-1)} \quad (12)$$

$$\boldsymbol{\theta}^{(t)} = \boldsymbol{\theta}^{(t-1)} - \eta \boldsymbol{v}^{(t)} \quad (13)$$

where η is still the learning rate and $\mu \in [0, 1]$ is the momentum coefficient. Usually, $\mu = 0.99$ or 0.999.

Intuitive Explanation

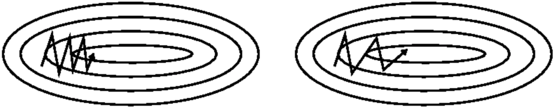
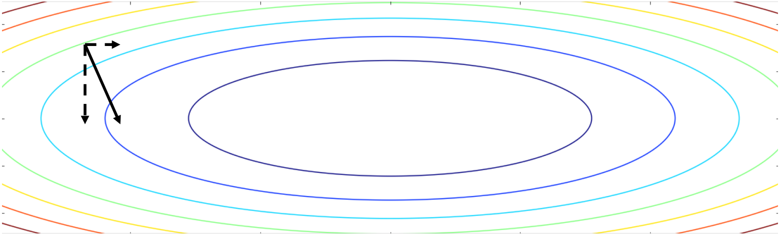


Figure: The effect of momentum in SGD. Left: SGD without momentum. Right: SGD with momentum. (Credit: Genevieve B. Orr)

$$y = x_1^2 + 10x_2^2 \tag{14}$$

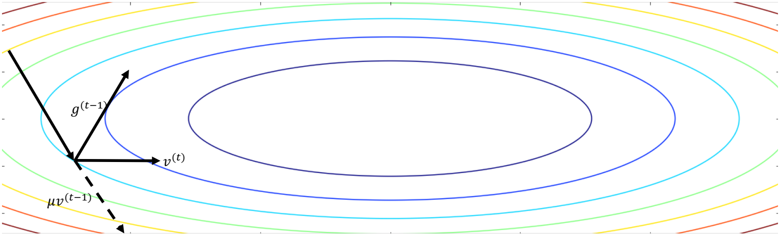
$$\frac{\partial y}{\partial x_1} = 2x_1 \tag{15}$$

$$\frac{\partial y}{\partial x_2} = 20x_2 \tag{16}$$



$$v^{(t)} = \mu v^{(t-1)} + g^{(t-1)} \tag{17}$$

$$\theta^{(t)} = \theta^{(t-1)} - \eta v^{(t)} \tag{18}$$



Adaptive Learning Rates

Basic Idea

For neural networks, the motivation of picking a different learning rate for each θ_k (the k-th component of parameter θ) is not new [LeCun et al., 2012] (the article was originally published in 1998).

- The basic idea is to make sure that all θ_k's converge roughly at the same speed.
- Depending on the curvature of the error surface, some θ_k's may require a small learning rate in order to avoid divergence, while others may require a large learning rate in order to converge fast.

AdaGrad

The basic idea of **AdaGrad** is to modify the learning rate η for $\boldsymbol{\theta}_k$ by using the history of $\partial_{\boldsymbol{\theta}_k} L$

$$\boldsymbol{\theta}_k^{(t)} = \boldsymbol{\theta}_k^{(t-1)} - \frac{\eta_0}{\sqrt{G_{k,k}^{(t-1)} + \epsilon}} \boldsymbol{g}_k^{(t-1)} \tag{19}$$

where $\boldsymbol{g}_k^{(t-1)} = [\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^{(t-1)})]_k$ is the k-th component of $\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^{(t-1)})$, $G_{k,k}^{(t-1)} = \sum_{i=1}^{t-1} (\boldsymbol{g}_k^{(i)})^2$, η_0 is the initial learning rate and ϵ is a smoothing parameter usually with order 10^{-6}.

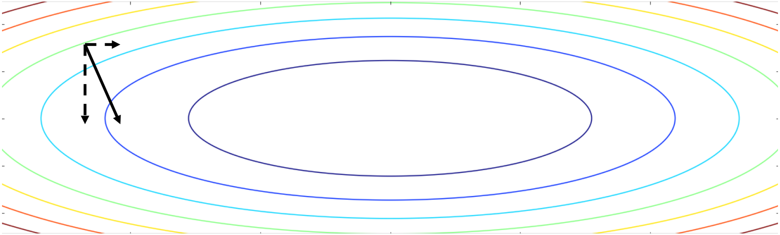
AdaGrad (II)

$$\theta_k^{(t)} = \theta_k^{(t-1)} - \frac{\eta_0}{\sqrt{G_{k,k}^{(t-1)} + \epsilon}} g_k^{(t-1)} \tag{20}$$

The accumulation of squared gradients from the beginning of training can result in a a premature and excessive decrease in the effective learning rate.

AdaGrad (III)

$$\theta_k^{(t)} = \theta_k^{(t-1)} - \frac{\eta_0}{\sqrt{G_{k,k}^{(t-1)} + \epsilon}} g_k^{(t-1)} \tag{21}$$



RMSProp

RMSProp uses a moving average over the past

$$r_k^{(t)} = \rho r_k^{(t-1)} + (1-\rho)[g_k^{(t-1)}]^2 \tag{22}$$

$$\theta_k^{(t)} = \theta_k^{(t-1)} - \frac{\eta_0}{\sqrt{r_k^{(t)} + \epsilon}} g_k^{(t-1)} \tag{23}$$

[Hinton et al., 2012]

Adam

$$
\begin{aligned}
\boldsymbol{v}_k^{(t)} &= \mu \boldsymbol{v}_k^{(t-1)} + (1-\mu)\boldsymbol{g}_k^{(t-1)} && (24) \\
\boldsymbol{r}_k^{(t)} &= \rho \boldsymbol{r}_k^{(t-1)} + (1-\rho)[\boldsymbol{g}_k^{(t-1)}]^2 && (25) \\
\hat{\boldsymbol{v}}_k^{(t)} &= \frac{\boldsymbol{v}_k^{(t)}}{1-\mu^t} && (26) \\
\hat{\boldsymbol{r}}_k^{(t)} &= \frac{\boldsymbol{r}_k^{(t)}}{1-\rho^t} && (27) \\
\boldsymbol{\theta}_k^{(t)} &= \boldsymbol{\theta}_k^{(t-1)} - \eta_0 \frac{\hat{\boldsymbol{v}}_k^{(t)}}{\sqrt{\hat{\boldsymbol{r}}_k^{(t)} + \epsilon}} && (28)
\end{aligned}
$$

The default values of μ and ρ are 0.9 and 0.999 respectively.

Adam (II)

Recent theoretical work [Reddi et al., 2018] shows that, for any constant $\mu, \rho \in [0, 1)$, if $\mu < \sqrt{\rho}$, there is a stochastic convex optimization problem for which Adam does not converge to the optimal solution.

How to Choose a Optimization Algorithm?

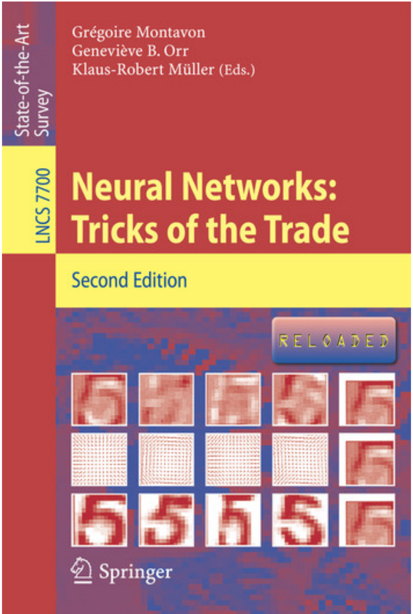
- User's familiarity with the algorithms [Goodfellow et al., 2016]
- Start from SGD first (My opinion)

Other Tricks

Other Tricks

1. Shuffle training examples in each epoch
2. Normalize inputs
3. Initialization

Further Reference



Summary

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Reference

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