CS 6501 Natural Language Processing

Optimization for Deep Learning

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Overview

1. Stochastic Gradient Descent

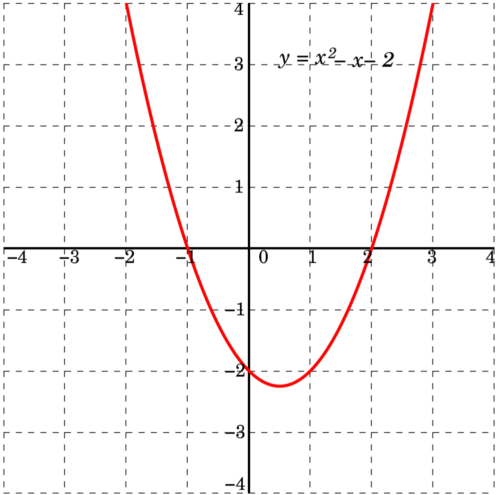
2. Adaptive Learning Rates

3. Other Tricks

4. Learning via Optimization

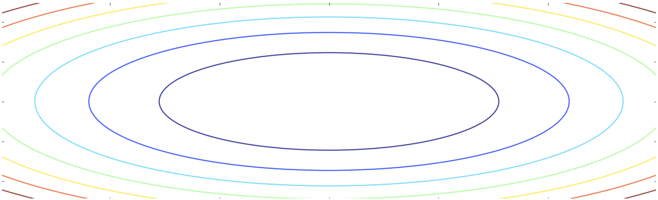
Stochastic Gradient Descent

Warmup: Gradient of a 1-D Function



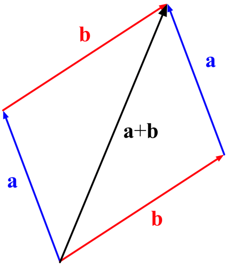
Warmup: Gradient of a 2-D Function

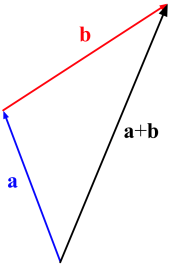
$$y = x_1^2 + 10x_2^2$$



Warmup: Vector Addition

The parallelogram law





Loss Function

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

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

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

Some examples of $L(\cdot, \cdot)$

- Negative log-likelihood
- Cross entropy

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

$$\boldsymbol{\theta}^{(t)} \leftarrow \boldsymbol{\theta}^{(t-1)} - \eta_t \cdot \boldsymbol{g}^{(t-1)} \tag{2}$$

where

- t: timestep
- $\boldsymbol{g}^{(t-1)} = \nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^{(t-1)})$ is the gradient of the single-example loss L
- η_t is the learning rate

Learning Rate

The usual conditions on the learning rates are

$$\sum_{t=1}^{\infty} \eta_t = \infty \tag{3}$$

$$\sum_{t=1}^{\infty} \eta_t^2 \leq \infty \tag{4}$$

A simplest function that satisfies these conditions is

$$\eta_t = \frac{1}{t} \tag{5}$$

[Bottou, 1998]

SGD with Momentum

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

$$\begin{aligned} \boldsymbol{v}^{(t)} &= \mu \boldsymbol{v}^{(t-1)} + \boldsymbol{g}^{(t-1)} \quad (6) \\ \boldsymbol{\theta}^{(t)} &= \boldsymbol{\theta}^{(t-1)} - \eta_t \boldsymbol{v}^{(t)} \quad (7) \end{aligned}$$

where

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

Intuitive Explanation

The effect of momentum in SGD: reduce the fluctuation

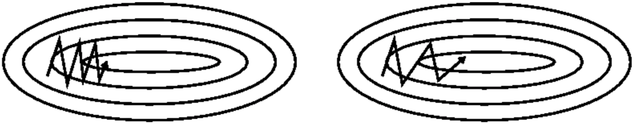


Figure: Left: SGD without momentum. Right: SGD with momentum.
(Credit: Genevieve B. Orr)

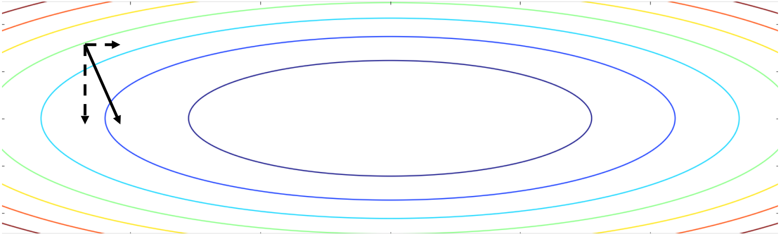
Note: the arrow show the opposite direction of the gradient

Another Example with Contour Plot

$$y = x_1^2 + 10x_2^2 \tag{8}$$

$$\frac{\partial y}{\partial x_1} = 2x_1 \tag{9}$$

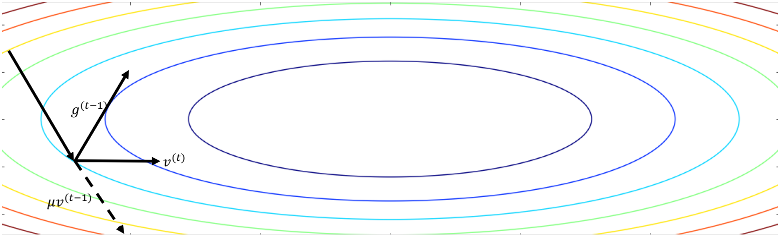
$$\frac{\partial y}{\partial x_2} = 20x_2 \tag{10}$$



Note: the arrow show the opposite direction of the gradient

Another Example with Contour Plot (Cont.)

$$v^{(t)} = \mu v^{(t-1)} + g^{(t-1)} \tag{11}$$



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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 $\partial_{\boldsymbol{\theta}_k} L$

$$\boldsymbol{\theta}_k^{(t)} = \boldsymbol{\theta}_k^{(t-1)} - \frac{\eta_0}{\sqrt{G_{k,k}^{(t-1)} + \epsilon}} \boldsymbol{g}_k^{(t-1)} \qquad (12)$$

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- $\boldsymbol{g}_k^{(t-1)} = [\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^{(t-1)})]_k$ is the k-th component of $\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^{(t-1)})$

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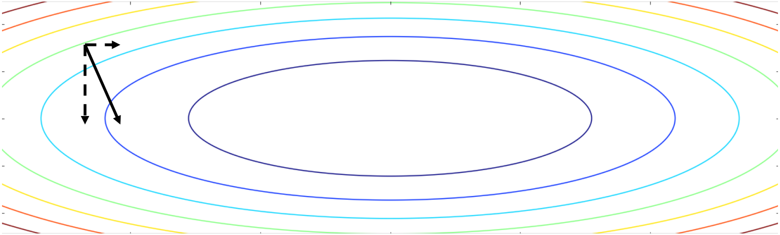
where

- $\boldsymbol{g}_k^{(t-1)} = [\nabla_{\boldsymbol{\theta}} L(\boldsymbol{\theta}^{(t-1)})]_k$ 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
- ϵ is a smoothing parameter usually with order 10^{-6}

AdaGrad: Intuitive Explanation

$$\theta_k^{(t)} = \theta_k^{(t-1)} - \frac{\eta_0}{\sqrt{G_{k,k}^{(t-1)} + \epsilon}} g_k^{(t-1)} \tag{13}$$



RMSProp

RMSProp uses a moving average over the past gradients

$$\boldsymbol{\theta}_k^{(t)} = \boldsymbol{\theta}_k^{(t-1)} - \frac{\eta_0}{\sqrt{\boldsymbol{r}_k^{(t)} + \epsilon}} \boldsymbol{g}_k^{(t-1)} \tag{14}$$

where

$$\boldsymbol{r}_k^{(t)} = \rho \boldsymbol{r}_k^{(t-1)} + (1 - \rho)[\boldsymbol{g}_k^{(t-1)}]^2 \tag{15}$$

and $\rho \in (0, 1)$

[Hinton et al., 2012]

Adam

$$
\begin{aligned}
\boldsymbol{v}_k^{(t)} &= \mu \boldsymbol{v}_k^{(t-1)} + (1-\mu)\boldsymbol{g}_k^{(t-1)} && (16)\\
\boldsymbol{r}_k^{(t)} &= \rho \boldsymbol{r}_k^{(t-1)} + (1-\rho)[\boldsymbol{g}_k^{(t-1)}]^2 && (17)\\
\hat{\boldsymbol{v}}_k^{(t)} &= \frac{\boldsymbol{v}_k^{(t)}}{1-\mu^t} && (18)\\
\hat{\boldsymbol{r}}_k^{(t)} &= \frac{\boldsymbol{r}_k^{(t)}}{1-\rho^t} && (19)\\
\boldsymbol{\theta}_k^{(t)} &= \boldsymbol{\theta}_k^{(t-1)} - \eta_0 \frac{\hat{\boldsymbol{v}}_k^{(t)}}{\sqrt{\hat{\boldsymbol{r}}_k^{(t)} + \epsilon}} && (20)
\end{aligned}
$$

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

How to Choose a Optimization Algorithm?

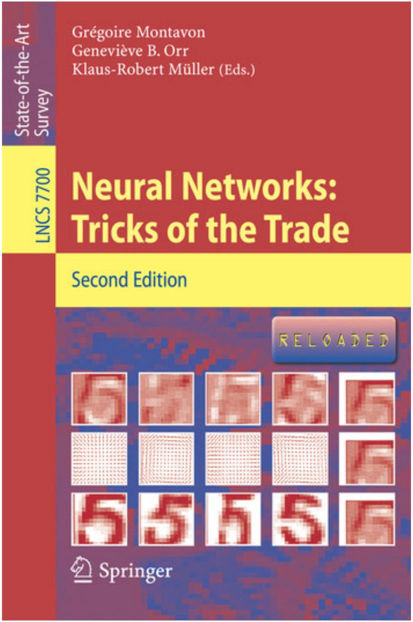
- User's familiarity with the algorithms [Goodfellow et al., 2016]
- Start from SGD first (my opinion)

Other Tricks

Other Tricks

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

Further Reference



Learning via Optimization

Expected Loss

For a distribution of $\mathcal{D}$ 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 $E(f) = \int_{\mathcal{D}} L(f(\boldsymbol{x}), y)$

$$f^* = \operatorname*{argmin}_f E(f) \tag{21}$$

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

However, $\mathcal{D}$ is unknown.

Empirical Loss

Instead of minimizing the expected loss in Equation 21, which is also impossible, we can minimize the empirical loss

$$E_n(f) = \frac{1}{n} \sum_{i=1}^{n} L(f(\boldsymbol{x}^{(i)}), y^{(i)}), \tag{22}$$

as

$$f_n = \operatorname*{argmin}_f E_n(f) \tag{23}$$

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

Question

How far from f_n to f^*

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Three steps in machine learning

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

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How far from f_n to f^*

Three steps in machine learning

1. collect data: *Do we have enough data?*
2. design a model: *Does the model have enough data?*
3. optimize an objective function: *Is the objective fully optimized?*

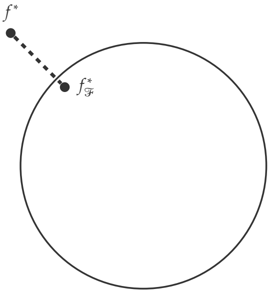
Errors (the difference between f_n and f^*) can be introduced in any of these three steps.

Approximation Error

Due to the model design: since we do not know the actual f^*, our starting point with all learnable function class $\mathcal{F}$ is predefined, such as logistic regression models or neural network models

$$f^* = \operatorname*{argmin}_{f} E(f) \tag{24}$$

$$f^*_{\mathcal{F}} = \operatorname*{argmin}_{f \in \mathcal{F}} E(f) \tag{25}$$



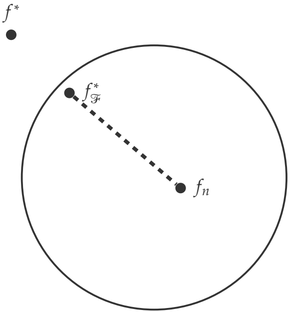
[Kearns et al., 1994, Agnostic ML]

Estimation Error

Due to the data collection: we can only have finite number of training examples and we have no idea about the real data distribution $\mathcal{D}$

$$f^*_{\mathcal{F}} = \operatorname*{argmin}_{f\in\mathcal{F}} E(f) \quad (26)$$

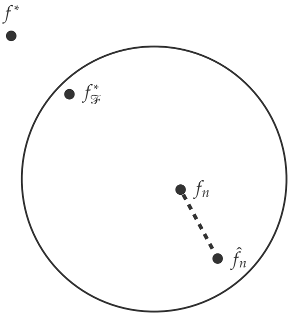
$$f_n = \operatorname*{argmin}_{f\in\mathcal{F}} E_n(f) \quad (27)$$



Optimization Error

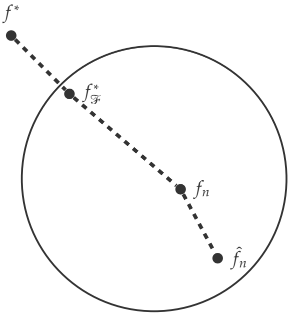
Due to the limited power of optimization methods

$$f_n = \operatorname{argmin} f \in \mathcal{F} E_n(f) \tag{28}$$



Error Decomposition

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

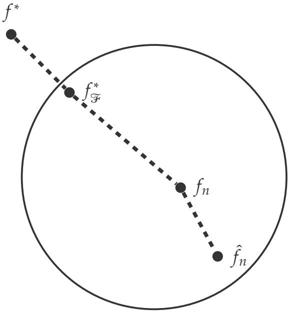


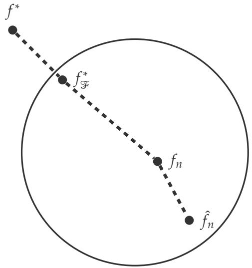
[Bottou, 2012, Sec. 18.3.1]

For a given machine learning problem,

- there is no way to know the oracle function f^* or $f^*_{\mathcal{F}}$, 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 this 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.

Summary

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

Reference

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