Newton Methods for Neural Networks: Introduction

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Outline

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Optimization Methods Other than Stochastic Gradient

- We have explained why stochastic gradient is popular for deep learning
- The same reasons may explain why other methods are not suitable for deep learning
- But we also notice that from the simplest SG to what people are using many modifications were made
- Can we extend other optimization methods to be suitable for deep learning?

Outline

Newton Method

- Consider an optimization problem

$$\min_{\boldsymbol{\theta}} f(\boldsymbol{\theta})$$

- Newton method solves the 2nd-order approximation to get a direction $\boldsymbol{d}$

$$\min_{\boldsymbol{d}} \quad \nabla f(\boldsymbol{\theta})^T \boldsymbol{d} + \frac{1}{2} \boldsymbol{d}^T \nabla^2 f(\boldsymbol{\theta}) \boldsymbol{d} \qquad (1)$$

- If $f(\boldsymbol{\theta})$ isn't strictly convex, (1) may not have a unique solution

Newton Method (Cont'd)

- We may use a positive-definite G to approximate $\nabla^2 f(\boldsymbol{\theta})$.
- Then (1) can be solved by

$$G\boldsymbol{d} = -\nabla f(\boldsymbol{\theta})$$

- The resulting direction is a descent one

$$\nabla f(\boldsymbol{\theta})^T \boldsymbol{d} = -\nabla f(\boldsymbol{\theta})^T G^{-1} \nabla f(\boldsymbol{\theta}) < 0$$

Newton Method (Cont'd)

The procedure:

while stopping condition not satisfied **do**

Let G be $\nabla^2 f(\boldsymbol{\theta})$ or its approximation

Exactly or approximately solve

$$G\boldsymbol{d} = -\nabla f(\boldsymbol{\theta})$$

Find a suitable step size α

Update

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha \boldsymbol{d}.$$

end while

Step Size I

- Selection of the step size α: usually two types of approaches
  - Line search
  - Trust region (or its predecessor: Levenberg-Marquardt algorithm)
- If using line search, details are similar to what we had for gradient descent
- We gradually reduce α such that

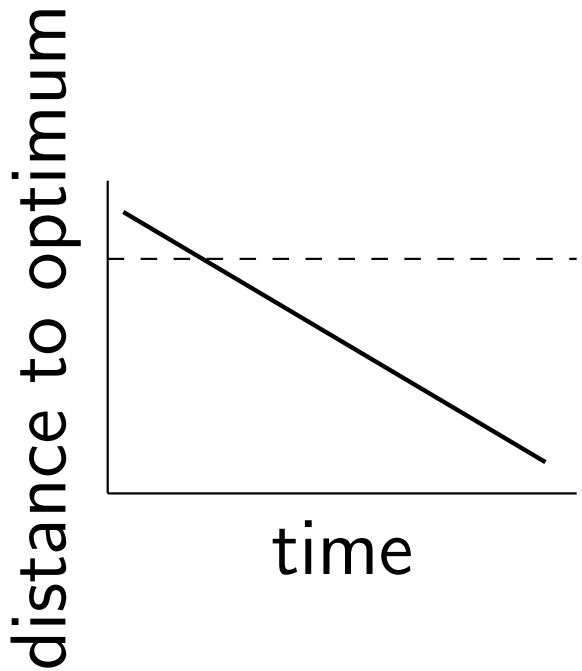
$$f(\boldsymbol{\theta} + \alpha \boldsymbol{d}) < f(\boldsymbol{\theta}) + \nu \nabla f(\boldsymbol{\theta})^T (\alpha \boldsymbol{d})$$

Newton versus Gradient Descent I

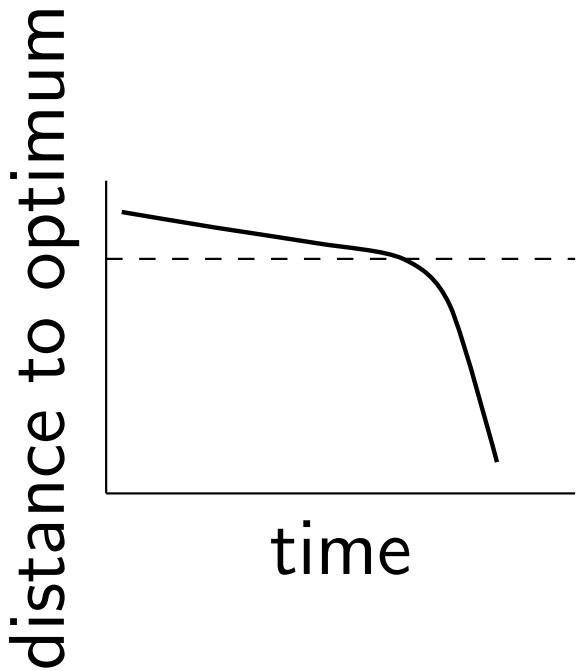
- We know they use second-order and first-order information respectively
- What are their special properties?
- It is known that using higher order information leads to faster final local convergence

Newton versus Gradient Descent II

- An illustration (modified from Tsai et al. (2014)) presented earlier



Slow final convergence



Fast final convergence

Newton versus Gradient Descent III

- But the question is for machine learning why we need fast local convergence?
- The answer is no
- However, higher-order methods tend to be more robust
- Their behavior may be more consistent across easy and difficult problems
- It's known that stochastic gradient is sometimes sensitive to parameters
- Thus what we hope to try here is if we can have a more robust optimization method

Difficulties of Newton for NN I

- The Newton linear system

$$G\boldsymbol{d} = -\nabla f(\boldsymbol{\theta}) \tag{2}$$

  can be large.

$$G \in R^{n \times n},$$

  where n is the total number of variables
- Thus G is often too large to be stored

Difficulties of Newton for NN II

- Evan if we can store G, calculating

$$\boldsymbol{d} = -G^{-1}\nabla f(\boldsymbol{\theta})$$

  is usually very expensive
- Thus a direct use of Newton for deep learning is hopeless

Existing Works Trying to Make Newton Practical I

- Many works tried to address this issue
- Their approaches significantly vary
- I roughly categorize them to two groups
  - Hessian-free (Martens, 2010; Martens and Sutskever, 2012; Wang et al., 2020; Henriques et al., 2018)
  - Hessian approximation (Martens and Grosse, 2015; Botev et al., 2017; Zhang et al., 2017) In particular, diagonal approximation

Existing Works Trying to Make Newton Practical II

- There are many others where I didn't put into the above two groups for various reasons (Osawa et al., 2019; Wang et al., 2018; Chen et al., 2019; Wilamowski et al., 2007)
- There are also comparisons (Chen and Hsieh, 2018)
- With the many possibilities it is difficult to reach conclusions
- We decide to first check the robustness of standard Newton methods on small-scale data

Existing Works Trying to Make Newton Practical III

- Thus in our discussion we try not to do approximations

Outline

Introduction

- We will check techniques to address the difficulty of storing or inverting the Hessian
- But before that let's derive the mathematical form

Hessian Matrix I

- For CNN, the gradient of $f(\boldsymbol{\theta})$ is

$$\nabla f(\boldsymbol{\theta}) = \frac{1}{C}\boldsymbol{\theta} + \frac{1}{l}\sum_{i=1}^{l}(J^i)^T \nabla_{\boldsymbol{z}^{L+1,i}} \xi(\boldsymbol{z}^{L+1,i}; \boldsymbol{y}^i, Z^{1,i}), \tag{3}$$

where

$$J^i = \begin{bmatrix} \frac{\partial z_1^{L+1,i}}{\partial \theta_1} & \cdots & \frac{\partial z_1^{L+1,i}}{\partial \theta_n} \\ \vdots & \vdots & \vdots \\ \frac{\partial z_{n_{L+1}}^{L+1,i}}{\partial \theta_1} & \cdots & \frac{\partial z_{n_{L+1}}^{L+1,i}}{\partial \theta_n} \end{bmatrix}_{n_{L+1} \times n}, \quad i = 1, \ldots, l, \tag{4}$$

Hessian Matrix II

is the Jacobian of $z^{L+1,i}(\theta)$.

- The Hessian matrix of $f(\theta)$ is

$$\nabla^2 f(\theta) = \frac{1}{C}\mathcal{I} + \frac{1}{l}\sum_{i=1}^{l}(J^i)^T B^i J^i$$

$$+ \frac{1}{l}\sum_{i=1}^{l}\sum_{j=1}^{n_L}\frac{\partial \xi(z^{L+1,i}; y^i, Z^{1,i})}{\partial z_j^{L+1,i}} \begin{bmatrix} \frac{\partial^2 z_j^{L+1,i}}{\partial\theta_1\partial\theta_1} & \cdots & \frac{\partial^2 z_j^{L+1,i}}{\partial\theta_1\partial\theta_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 z_j^{L+1,i}}{\partial\theta_n\partial\theta_1} & \cdots & \frac{\partial^2 z_j^{L+1,i}}{\partial\theta_n\partial\theta_n} \end{bmatrix},$$

Hessian Matrix III

where $\mathcal{I}$ is the identity matrix and B^i is the Hessian of $\xi(\cdot)$ with respect to $z^{L+1,i}$:

$$B^i = \nabla^2_{z^{L+1,i}, z^{L+1,i}} \xi(z^{L+1,i}; y^i, Z^{1,i})$$

- More precisely,

$$B^i_{ts} = \frac{\partial^2 \xi(z^{L+1,i}; y^i, Z^{1,i})}{\partial z^{L+1,i}_t \partial z^{L+1,i}_s}, \forall t, s = 1, \ldots, n_{L+1}. \quad (5)$$

- Usually B^i is very simple.

Hessian Matrix IV

- For example, if the squared loss is used,

$$\xi(z^{L+1,i}; y^i) = ||z^{L+1,i} - y^i||^2.$$

then

$$B^i = \begin{bmatrix} 2 & & \\ & \ddots & \\ & & 2 \end{bmatrix}$$

- Usually we consider a convex loss function

$$\xi(z^{L+1,i}; y^i)$$

with respect to $z^{L+1,i}$

Hessian Matrix V

- Thus B^i is positive semi-definite
- The last term of $\nabla^2 f(\boldsymbol{\theta})$ may not be positive semi-definite
- Note that for a twice differentiable function $f(\boldsymbol{\theta})$

$$f(\boldsymbol{\theta}) \text{ is convex}$$

if and only if

$$\nabla^2 f(\boldsymbol{\theta}) \text{ is positive semi-definite}$$

Jacobian Matrix

- The Jacobian matrix of $z^{L+1,i}(\theta) \in R^{n_{L+1}}$ is

$$J^i = \begin{bmatrix} \frac{\partial z_1^{L+1,i}}{\partial \theta_1} & \cdots & \frac{\partial z_1^{L+1,i}}{\partial \theta_n} \\ \vdots & \vdots & \vdots \\ \frac{\partial z_{n_L}^{L+1,i}}{\partial \theta_1} & \cdots & \frac{\partial z_{n_L}^{L+1,i}}{\partial \theta_n} \end{bmatrix} \in R^{n_{L+1} \times n}, \ i = 1, \dots l.$$

- n_{L+1}: # of neurons in the output layer
- n: number of total variables
- $n_{L+1} \times n$ can be large

Gauss-Newton Matrix I

- The Hessian matrix $\nabla^2 f(\boldsymbol{\theta})$ is now not positive definite.
- We may need a positive definite approximation
- This is a deep research issue
- Many existing Newton methods for NN has considered the Gauss-Newton matrix (Schraudolph, 2002)

$$G = \frac{1}{C}\mathcal{I} + \frac{1}{l}\sum_{i=1}^{l}(J^i)^T B^i J^i$$

by removing the last term in $\nabla^2 f(\boldsymbol{\theta})$

Gauss-Newton Matrix II

- The Gauss-Newton matrix is positive definite if B^i is positive semi-definite
- This can be achieved if we use a convex loss function in terms of $\boldsymbol{z}^{L+1,i}(\boldsymbol{\theta})$
- We then solve

$$G\boldsymbol{d} = -\nabla f(\boldsymbol{\theta})$$

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