Stochastic Gradient Methods for Neural Networks

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Outline

1. Gradient descent
2. Mini-batch SG
3. Adaptive learning rate
4. Discussion
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1. Gradient descent
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NN Optimization Problem I

- Recall that the NN optimization problem is

\[
\min_{\theta} f(\theta)
\]

where

\[
f(\theta) = \frac{1}{2C} \theta^T \theta + \frac{1}{l} \sum_{i=1}^l \xi(z^{L+1,i}(\theta); y^i, Z^{1,i})
\]

- Let’s simplify the loss part a bit

\[
f(\theta) = \frac{1}{2C} \theta^T \theta + \frac{1}{l} \sum_{i=1}^l \xi(\theta; y^i, Z^{1,i})
\]

- The issue now is how to do the minimization
Gradient Descent I

- This is one of the most used optimization method
- First-order approximation

\[ f(\theta + \Delta \theta) \approx f(\theta) + \nabla f(\theta)^T \Delta \theta \]

- Solve

\[ \min_{\Delta \theta} \nabla f(\theta)^T \Delta \theta \]
subject to \[ \|\Delta \theta\| = 1 \]  \hspace{1cm} (1)

- If no constraint, the above sub-problem goes to \(-\infty\)
The solution of (1) is

$$\Delta \theta = - \frac{\nabla f(\theta)}{\|\nabla f(\theta)\|}$$

This is called steepest descent method

In general all we need is a descent direction

$$\nabla f(\theta)^T \Delta \theta < 0$$
Gradient Descent III

From

\[ f(\theta + \alpha \Delta \theta) = f(\theta) + \alpha \nabla f(\theta)^T \Delta \theta + \frac{1}{2} \alpha^2 \Delta \theta^T \nabla^2 f(\theta) \Delta \theta + \cdots, \]

if

\[ \nabla f(\theta)^T \Delta \theta < 0, \]

then with a small enough \( \alpha \),

\[ f(\theta + \alpha \Delta \theta) < f(\theta) \]
Because we only consider an approximation

\[ f(\theta + \Delta \theta) \approx f(\theta) + \nabla f(\theta)^T \Delta \theta \]

we may not have the strict decrease of the function value

That is,

\[ f(\theta) < f(\theta + \Delta \theta) \]

may occur

In optimization we then need a step selection procedure
Line Search II

- Exact line search

\[
\min_{\alpha} f(\theta + \alpha \Delta \theta)
\]

This is a one-dimensional optimization problem

- In practice, people use backtracking line search

- We check

\[
\alpha = 1, \beta, \beta^2, \ldots
\]

with \(\beta \in (0, 1)\) until

\[
f(\theta + \alpha \Delta \theta) < f(\theta) + \nu \nabla f(\theta)^T (\alpha \Delta \theta)
\]
Here

\[ \nu \in (0, \frac{1}{2}) \]

The convergence is well established.

For example, under some conditions, Theorem 3.2 of Nocedal and Wright (1999) has that

\[ \lim_{k \to \infty} \nabla f(\theta^k) = 0, \]

where \( k \) is the iteration index

This means we can reach a stationary point of a non-convex problem
The standard back-tracking line search is simple and useful.

However, the convergence is slow for difficult problems.

Thus in many optimization applications, methods of using second-order information (e.g., quasi Newton or Newton) are preferred.

$$f(\theta + \Delta \theta) \approx f(\theta) + \nabla f(\theta)^T \Delta \theta + \frac{1}{2} \Delta \theta^T \nabla^2 f(\theta) \Delta \theta$$

These methods have fast final convergence.
An illustration (modified from Tsai et al. (2014))

Slow final convergence  Fast final convergence
But fast final convergence may not be needed in machine learning

The reason is that an optimal solution $\theta^*$ may not lead to the best model

We will discuss such issues again later
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Estimation of the Gradient I

- Recall the function is
  \[ f(\theta) = \frac{1}{2C} \theta^T \theta + \frac{1}{l} \sum_{i=1}^{l} \xi(\theta; y^i, Z^{1,i}) \]

- The gradient is
  \[ \frac{\theta}{C} + \frac{1}{l} \nabla \theta \sum_{i=1}^{l} \xi(\theta; y^i, Z^{1,i}) \]

- Going over all data is time consuming
Estimation of the Gradient II

What if we use a subset of data

\[ E(\nabla_\theta \xi(\theta; y, Z^1)) = \frac{1}{l} \nabla_\theta \sum_{i=1}^{l} \xi(\theta; y^i, Z^{1,i}) \]

We may just use a subset \( S \)

\[ \frac{\theta}{C} + \frac{1}{|S|} \nabla_\theta \sum_{i: i \in S} \xi(\theta; y^i, Z^{1,i}) \]
Algorithm 1

1. Given an initial learning rate $\eta$.
2. while do
3. Choose $S \subset \{1, \ldots, l\}$.
4. Calculate
   
   $$\theta \leftarrow \theta - \eta \left(\frac{\theta}{C} + \frac{1}{|S|} \nabla \theta \sum_{i:i \in S} \xi(\theta; y^i, Z^{1;i})\right)$$

5. May adjust the learning rate $\eta$
6. end while

- It’s known that deciding a suitable learning rate is difficult
Algorithm II

- Too small learning rate: very slow convergence
- Too large learning rate: the procedure may diverge
In comparison with gradient descent you see that we don’t do line search
Indeed we cannot. Without the full gradient, the sufficient decrease condition may never hold.

\[ f(\theta + \alpha \Delta \theta) < f(\theta) + \nu \nabla f(\theta)^T (\alpha \Delta \theta) \]

Therefore, we don’t have a “descent” algorithm here
It’s possible that

\[ f(\theta^{\text{next}}) > f(\theta) \]

Though people frequently use “SGD,” it’s unclear if “D” is suitable in the name of this method
Momentum I

- This is a method to improve the convergence speed
- A new vector $\bm{v}$ and a parameter $\alpha \in [0, 1)$ are introduced

$$
\begin{align*}
\bm{v} & \leftarrow \alpha \bm{v} - \eta \left( \frac{\theta}{C} + \frac{1}{|S|} \nabla_{\theta} \sum_{i : i \in S} \xi(\theta; y_i, Z^{1, i}) \right) \\
\theta & \leftarrow \theta + \bm{v}
\end{align*}
$$
Essentially what we do is

\[ \theta \leftarrow \theta - \eta \text{(current sub-gradient)} \]
\[ -\alpha \eta \text{(prev. sub-gradient)} \]
\[ -\alpha^2 \eta \text{(prev. prev. sub-gradient)} - \cdots \]

There are some reasons why doing so can improve the convergence speed, though details are not discussed here.
Adaptive learning rate

AdaGrad I

- Scaling learning rates inversely proportional to the square root of sum of past gradient squares (Duchi et al., 2011)

- Update rule:

\[
g \leftarrow \frac{\theta}{C} + \frac{1}{|S|} \nabla_{\theta} \sum_{i:i \in S} \xi(\theta; y^i, Z^{1,i})
\]

\[
r \leftarrow r + g \odot g
\]

\[
\theta \leftarrow \theta - \frac{\epsilon}{\sqrt{r + \delta}} \odot g
\]

- \( r \): sum of past gradient squares
AdaGrad II

- $\epsilon$ and $\delta$ are given constants
- $\odot$: Hadamard product (element-wise product of two vectors/matrices)
- A large $g$ component
  $\Rightarrow$ a larger $r$ component
  $\Rightarrow$ fast decrease of the learning rate
- Conceptual explanation from Duchi et al. (2011):
  - frequently occurring features $\Rightarrow$ low learning rates
  - infrequent features $\Rightarrow$ high learning rates
AdaGrad III

“the intuition is that each time an infrequent feature is seen, the learner should take notice.”

- But how is this explanation related to $g$ components?
- Let’s consider linear classification. Recall our optimization problem is

$$\frac{\mathbf{w}^T \mathbf{w}}{2} + C \sum_{i=1}^{l} \xi(\mathbf{w}; y_i, \mathbf{x}_i)$$
AdaGrad IV

- For methods such as SVM or logistic regression, the loss function can be written as a function of $\mathbf{w}^T \mathbf{x}$

$$\xi(\mathbf{w}; y, \mathbf{x}) = \hat{\epsilon}(\mathbf{w}^T \mathbf{x})$$

Then the gradient is

$$\mathbf{w} + C \sum_{i=1}^{l} \hat{\epsilon}'(\mathbf{w}^T \mathbf{x}_i) \mathbf{x}_i$$

- Thus the gradient is related to the density of features
AdaGrad V

- The above analysis is for linear classification
- But now we have a non-convex neural network!
- Empirically, people find that the sum of squared gradient since the beginning causes too fast decrease of the learning rate
The original reference seems to be the lecture slides at https://www.cs.toronto.edu/~tijmen/csc321/slides/lecture_slides_lec6.pdf

Idea: they think AdaGrad’s learning rate may be too small before reaching a locally convex region

That is, OK to sum all past gradient squares in convex, but not non-convex

Thus they do “exponentially weighted moving average”
RMSProp II

- Update rule

\[
\begin{align*}
    r &\leftarrow \rho r + (1 - \rho)g \odot g \\
    \theta &\leftarrow \theta - \frac{\epsilon}{\sqrt{\delta + r}} \odot g
\end{align*}
\]

- AdaGrad:

\[
\begin{align*}
    r &\leftarrow r + g \odot g \\
    \theta &\leftarrow \theta - \frac{\epsilon}{\sqrt{r + \delta}} \odot g
\end{align*}
\]
Somehow the setting is a bit heuristic and the reason behind the change (from AdaGrad to RMSProp) is not really that strong.
ADAM (Adaptive Moments) I

- The update rule (Kingma and Ba, 2015)

\[
g \leftarrow \frac{\theta}{C} + \frac{1}{|S|} \nabla \theta \sum_{i : i \in S} \xi(\theta; y^i, Z^{1,i})
\]

\[
s \leftarrow \rho_1 s + (1 - \rho_1) g
\]

\[
r \leftarrow \rho_2 r + (1 - \rho_2) g \odot g
\]

\[
\hat{s} \leftarrow \frac{s}{1 - \rho_1^t}
\]

\[
\hat{r} \leftarrow \frac{r}{1 - \rho_2^t}
\]

\[
\theta \leftarrow \theta - \frac{\epsilon}{\sqrt{\hat{r}} + \delta} \odot \hat{s}
\]
t is the current iteration index

Roughly speaking, ADAM is the combination of

- Momentum
- RMSprop

From Goodfellow et al. (2016),

\[
\frac{\epsilon}{\sqrt{\hat{r}} + \delta} \odot \hat{s}
\]

(i.e., the use of momentum combined with rescaling) “does not have a clear theoretical motivation”
The two steps

\[ \hat{s} \leftarrow \frac{s}{1 - \rho_1^t} \]

\[ \hat{r} \leftarrow \frac{r}{1 - \rho_2^t} \]

are called “bias correction”

Why “bias correction”? 
They hope that

\[ E[s_t] = E[g_t] \]

and

\[ E[r_t] = E[g_t \odot g_t], \]

where \( t \) is the iteration index.
For $s_t$, we have

\[
\begin{align*}
    s_t &= \rho_1 s_{t-1} + (1 - \rho_1) g_t \\
    &= \rho_1 (\rho_1 s_{t-2} + (1 - \rho_1) g_{t-1}) + (1 - \rho_1) g_t \\
    &= (1 - \rho_1) \sum_{i=1}^{t} \rho_1^{t-i} g_i
\end{align*}
\]

We assume that $s$ is initialized as $0$.
Then

\[
E[s_t] = E[(1 - \rho_1) \sum_{i=1}^{t} \rho_1^{t-i} g_i]
\]

\[
= E[g_t](1 - \rho_1) \sum_{i=1}^{t} \rho_1^{t-i}
\]

Note that we assume

\[E[g_i], \forall i \geq 1\]

are the same
Next,

\[(1 - \rho_1) \sum_{i=1}^{t} \rho_1^{t-i} = (1 - \rho_1)(1 + \cdots + \rho_1^{t-1}) = 1 - \rho_1^t\]

Thus

\[E[s_t] = E[g_t](1 - \rho_1^t)\]

and they do

\[\hat{s} \leftarrow \frac{s}{1 - \rho_1^t}\]

The situation for $E[g_t \odot g_t]$ is similar.

How about ADAM’s practical performance?

From Goodfellow et al. (2016), “generally regarded as being fairly robust to the choice of hyperparameter, though the learning rate may need to be changed from the default”
However, from the web page we referred to for deriving the bias correction, “The original paper ... showing huge performance gains in terms of speed of training. However, after a while people started noticing, that in some cases Adam actually finds worse solution than stochastic gradient”

One example of showing the above is Wilson et al. (2017)

We may do some experiments later
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Discussion

Choosing Stochastic Gradient Algorithms

- From Goodfellow et al. (2016), “there is currently no consensus”
- Further, “the choice ... seemed to depend on the user’s familiarity with the algorithm”
- This isn’t very good. Can we have some systematic investigation?
Why Stochastic Gradient Widely Used? I

The special property of data classification is essential

\[ E(\nabla_{\theta} \xi(\theta; y, Z^1)) = \frac{1}{\ell} \nabla_{\theta} \sum_{i=1}^{\ell} \xi(\theta; y^i, Z^{1,i}) \]

Indeed stochastic gradient is less used outside machine learning

- Easy implementation. It’s simpler than methods using, for example, second derivative
- Non-convexity plays a role
Why Stochastic Gradient Widely Used? II

- For convex, other methods are efficient to find the global minimum
- But for non-convex, efficiency to reach a stationary point is less useful
- A global minimum usually gives a good model (loss minimized), but for a stationary point we are less sure

All these explain why SG is popular for deep learning

What are your opinions? Any other reasons you can think of
Issues of Stochastic Gradient I

- We have shown several variants
- Don’t you think some settings are a bit ad hoc?
- There are reasons behind each change. But some are just heuristic
- Can we try a paradigm completely different?
- But before that we need some first-hand experiences and know implementation details.
References I


