AN ITERATIVE K-FAC ALGORITHM FOR DEEP LEARNING

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Yingshi Chen

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ABSTRACT

Kronecker-factored Approximate Curvature (K-FAC) method is a high efficiency second order optimizer for the deep learning. Its training time is less than SGD (or other first-order method) with same accuracy in many large-scale problems. The key of K-FAC is to approximates Fisher information matrix (FIM) as a block-diagonal matrix where each block is an inverse of tiny Kronecker factors. In this short note, we present CG-FAC—an new iterative K-FAC algorithm. It uses conjugate gradient method to approximate the nature gradient. This CG-FAC method is matrix-free, that is, no need to generate the FIM matrix, also no need to generate the Kronecker factors A and G. We prove that the time and memory complexity of iterative CG-FAC is much less than that of standard K-FAC algorithm.

1 Introduction

Optimizers[1][2] is the key component to reduce the training losses of deep learning[2]. Based on the order of derivative, optimization methods are mainly divided into two categories, first-order and second-order methods. First-order method uses gradient information to update parameters(weights) whereas second-order method would try to get fast convergence on the addition curvature information. Based on the search space, optimization methods can be divided into two categories: parameter space and distribution space. Nature gradient method[3][5] is a second order method in the distribution space, which is proposed by Shun-Ichi Amari in 1998 based on information geometry. Compare to the most widely used first-order method (SGD, ADAM,...[1][6][7]), Nature gradient contains more information in the distribution space, so it would find a better solution with faster speed. In actual application, it does face the same practical difficulties of second order methods. It does need high-performance methods to get the inverse of hessian matrix. The traditional matrix inversion algorithms (or other approximate algorithms) require too much computation and memory resource to be implemented in practical applications. Until recent years, some novel algorithms greatly reduce the memory usage and computational overhead. Especially the Kronecker-factored Approximate Curvature (K-FAC) method[8][10] by James Martens, etc. K-FAC is a method for efficiently approximating the natural gradient in real deep learning problems. It approximates the hessian matrix as Kronecker products of many smaller matrices, which are more efficiently to deal with (for example, LU decomposition, SVD decomposition, perform or other matrix operations).

In this short note, we present a new iterative K-FAC algorithm CG-FAC on the special structure of hessian matrix in deep networks. This method is matrix-free, that is, no need to generate the hessian matrix, also no need to generate all small Kronecker factors. So it requires much less calculation and memory usage than standard K-FAC algorithm.

2 Background and notation

In this section, we first give some concise definitions of optimization problems of deep learning. Given training data $D = (x_i, y_i), i = 1, 2, \ldots$, deep learning method tries to deduce the loss $\mathcal{L}$ between prediction $\hat{y} = f(\theta : x)$ and the target $y$. At each step of optimization process, the parameters $\theta$ would be updated along a direction $p$ and a step length $\eta$[1][12]:

$$\theta' = \theta + \eta p$$ (1)
An iterative K-FAC algorithm for Deep Learning

In the machine learning community, many methods have been proposed to find the proper search direction $p$.

**Stochastic gradient descent (SGD)**

A classical strategy is to choose $p$ along the steepest decent direction $\nabla_\theta \mathcal{L}$, which is most widely used technology in the deep learning method.

$$p = \arg \min_{\|p\| \leq \epsilon} \mathcal{L}(\theta + p) = \nabla_\theta \mathcal{L} \tag{2}$$

In the practical training process of deep learning, the data-sets would always be randomly shuffled and split into many batches. The optimization finds $p$ by back-propagation method in each mini-batch. This stochastic gradient descent (SGD) method has many variants [16], including AdaGrad [13], RMSprop [14], and Adam [7].

Adagrad adapts the learning rate specifically to individual features: that means that some of the weights in your data-set will have different learning rates than others. This works really well for sparse data-sets where a lot of input examples are missing. Adagrad has a major issue though: the adaptive learning rate tends to get really small over time.

RMSprop is a special version of Adagrad developed by Professor Geoffrey Hinton in his neural nets class. Instead of letting all of the gradients accumulate for momentum, it only accumulates gradients in a fixed window. RMSprop is similar to Adaprop, which is another optimizer that seeks to solve some of the issues that Adagrad leaves open.

Adam stands for adaptive moment estimation, and is another way of using past gradients to calculate current gradients. Adam also utilizes the concept of momentum by adding fractions of previous gradients to the current one. This optimizer has become pretty widespread, and is practically accepted for use in training neural nets.

**Quasi-Newton method**

Quasi-Newton methods [11] use list of successive gradients to approximate the inverse of Hessian matrix [15–17] makes some attempts to combine the Broyden-Fletcher-Golfgar-Shanno (BFGS) method and SGD method. Although Quasi-Newton method is widely used in scientific computing, it is really difficult to apply in deep learning. The number of parameters is very large. For example, AlexNet has 60 million parameters and BERT_large has 340 million parameters. The standard Quasi-Newton methods need much more computation resource than first-order method. And need much more time to converge.

**Natural gradient method**

[3–5] proposed a new search direction (Natural gradient) in the distribution space. That is, we are not only looking for suitable parameters, but also for the distributions that reflect the essence of the problem more deeply than parameters. The number and value of the parameters will vary greatly, but the distribution should be always the same. To measure the variance of distribution between steps, a common way is to use Kullback–Leibler divergence [18] as a metric of loss. As the loss gets smaller, the distribution changes smaller and smaller. Finally, we not only get a solution with minimal loss, but also a stable distribution corresponds to the problem. As the difference between formula (2) and formula (3) shows: the natural gradient method replaces the Euclidean metric with KL metric.

$$p = \arg \min_{\|p\| \leq \epsilon} \mathcal{L}(\theta + p) \tag{3}$$

Let the hessian of KL metric is $G$. Then the second-order search direction of formula (3) is:

$$\nabla_\theta \mathcal{L} = G^{-1} \nabla_\theta \mathcal{L} \tag{4}$$

This is just the definition of natural gradient. [19] pointed that the Fisher information matrix (FIM) is equal to the hessian matrix of the Kullback–Leibler distance. So we would update the parameters $\theta$ by $F$

$$\theta' = \theta + \eta F^{-1} \nabla_\theta \mathcal{L} \tag{5}$$

In the simplest case that $G$ is identity matrix, this is just the standard steepest decent method shown in formula (2). In practical case of deep learning, the dimension of $F$ is very large. For example, AlexNet has 60 million parameters and BERT_large has 340 million parameters. The standard second-order method would fail for such huge matrices or would be very slow compared to first-order method. A novel technique to get the inverse of $F$ is the following K-FAC method.
K-FAC method

K-FAC is the shortcut for Kronecker-factored Approximate Curvature (K-FAC). As the name suggests, this method approximates the FIM as Kronecker products of smaller matrices, which are more efficiently to deal with (LU decomposition, SVD decomposition...). Algorithm 1 gives the standard algorithm of this method. It would first generate diagonal block matrix for each layer. The dimension of each block is the number of parameters of corresponding layer. This decoupling technique brings great convenience for the parallel and distribute training.

Algorithm 1 Standard Kronecker-factored Approximate of FIM

**Input:**
A deep neural network with $N$ layers

**Output:** Approximate inverse of FIM

1: Call standard back propagation [20] for current batch.
2: Get matrix $A_i$ and $G_i$ for $i$th layer on the input $a_{i-1}$ and $g_i$(gradient of output):

\[
A_i = (a_{i-1} \cdot a_{i-1}^T) \quad G_i = (g_i \cdot g_i^T)
\]

3: Block diagonalization: $N$ diagonal block for $N$ layers:

\[
F \approx \hat{F} = \begin{bmatrix}
\hat{F}_1 \\
\hat{F}_2 \\
\vdots \\
\hat{F}_N
\end{bmatrix}
\]

4: Approximates each diagonal block with the Kronecker product of $A$ and $G$:

\[
\hat{F}_i = (a_{i-1} \cdot a_{i-1}^T) \otimes (g_i g_i^T) = A_{i-1} \otimes G_i
\]

5: Get the inverse of $\hat{F}_i$

\[
\hat{F}_i^{-1} = (A_{i-1} \otimes G_i)^{-1} = A_{i-1}^{-1} \otimes G_i^{-1}
\]

3 Iterative K-FAC algorithm

At each mini-batch $\mathcal{B}$, the classical SGD method would update the current weight $\theta$ by

\[
\theta' = \theta - \eta \frac{1}{|\mathcal{B}|} \sum_{j \in \mathcal{B}} \nabla_\theta L_j
\]  

(6)

where $\nabla_\theta L_j$ is the gradient of loss function $L$ at $j^{th}$ sample.

To use the second-order curvature information and more information from distribution space, we would update $\theta$ in the direction of nature gradient, that is

\[
\theta' = \theta - \eta \frac{1}{|\mathcal{B}|} F^{-1} \sum_{j \in \mathcal{B}} \nabla_\theta L_j
\]  

(7)

As algorithm 1 shows: for the $i^{th}$ layer of network, let its input is $a_{i-1}$(The activation of the $(i - 1)^{th}$ layer), the gradient of its output is $g_i$. K-FAC would update its weight by $\hat{F}_i$(a diagonal block of $F$) [3–5]

\[
\hat{F}_i = (a_{i-1} \cdot a_{i-1}^T) \otimes (g_i g_i^T) = A_{i-1} \otimes G_i
\]

(8)

This is a Kronecker-factorization of $\hat{F}_i$ and $A_{i-1}, G_i$ are the Kronecker factors.

In practical use, we usually use a dumped version to increase the robustness. That is, add $\gamma I$ to $\hat{F}_i$. Let $F_\gamma = \hat{F}_i + \gamma I, \nabla L = \frac{1}{|\mathcal{B}|} \sum_{j \in \mathcal{B}} \nabla_\theta L_j$, then the updating process is:

3
\[ \theta' = \theta - \eta F^{-1}_\gamma \nabla L \]  

(9)

So the main problem is to get the preconditioned gradient \( F^{-1}_\gamma \nabla L \). Let the unknown vector \( x = F^{-1}_\gamma \nabla L \), then

\[ F\gamma x = \nabla L \]  

(10)

There are mainly two ways to solve equation 10. Let \( n \) (CG) method [21, 22] to solve this equation. So this method is called CG-FAC. The following is the detail of this method.

Let the function \( FV \) shows, there is no need to generate the matrix \( F \) \( G \) steps to converge [21, 22]. In the real application of CG method, only need is matrix-free. Therefore, the memory complexity is CG-FAC is only BLAS vector operation). As the function \( FV \) of previous batch as the initial guess of CG method. Then only needs 10-20 internal steps. Therefore, CG-FAC needs the training process from batch to batch, the difference between gradients is small. We could use the nature gradient, which needs \( O(\gamma I) \) operations, which is much less than \( O(n_A^3 + n_G^3 + 2n(n_A + n_G)) \). Therefore, the algorithm complexity is \( O(n_A^3 + n_G^3 + 2n(n_A + n_G)) \).

Algorithm 2 CG-FAC method: approximate nature gradient with at most \( m \) iterations

Input: 
\( n \): The parameters size in \( i^{th} \) layer 
\( a_{i-1} \): The activation of the \((i-1)^{th}\) layer 
\( g_i \): The gradient of output in the \( i^{th} \) layer 
\( \mathbf{b} = \nabla L \): The gradient of parameters in \( i^{th} \) layer 
\( F_\gamma = F_{\gamma} + \gamma I \): The fisher information matrix (FIM) with dumping parameter 
\( \mathbf{x}_0 \): A guess of nature gradient (may use the value from previous batch)

1: \( \text{function } FV(v) \) 
2: \( \theta g_i^T a_{i-1} \) 
3: \( v_1 = g_i \theta a_{i-1}^T + \gamma v \) 
4: \( \text{return } v_1 \) 
5: \( p_0 = r_0 = b - F_\gamma \mathbf{x}_0 \) 
6: \( \rho_0 = \|r_0\|^2 \) 
7: \( \text{for } k = 0, 1, 2, \ldots, m \text{ do} \) 
8: \( u_k = FV(p_k) \) 
9: \( s_k = p_k : u_k \) 
10: \( \alpha_k = \rho_k / s_k \) 
11: \( x_{k+1} = x_k + \alpha p_k \) 
12: \( r_{k+1} = r_k - \alpha u_k \) 
13: \( \rho_{k+1} = \|r_{k+1}\|^2 \) 
14: \( \text{if } \rho_{k+1} \text{ is sufficiently small, then exit} \) 
15: \( \beta_k = \rho_{k+1} / \rho_k \) 
16: \( p_{k+1} = r_{k+1} + \beta_k p_k \) 
17: \( \text{return } x_{k+1} \): The approximation of nature gradient

At each internal step, CG method needs one matrix-vector operations \( F_\gamma p_k \) and 5 vector operations (in the sense of BLAS vector operation). As the function \( FV(v) \) shows, there are some fast methods on the special structure of \( A_{i-1} \) and \( G_i \). Each FV needs \( O(3n) \) operations. So the algorithm complexity of each step is \( O(8n) \). The CG needs at most \( n \) steps to converge [21, 22]. In the real application of CG method, only need \( m \ll n \) steps [21, 22]. For example, in the training process from batch to batch, the difference between gradients is small. We could use the nature gradient of previous batch as the initial guess of CG method. Then only needs 10-20 internal steps. Therefore, CG-FAC needs \( O(m(3n)) \) operations, which is much less than \( O(n_A^3 + n_G^3 + 2n(n_A + n_G)) \) operations in the direct methods. As the function FV shows, there is no need to generate the matrix \( F_\gamma, A_{i-1} \) and \( G_i \) in the iterative method. This method is matrix-free. Therefore, the memory complexity is CG-FAC is only \( O(n_A + n_G + n) \), which is also less than the \( O(n_A^3 + n_G^3 + n) \) of direct method. We would expect better data locality and higher cache hit ratio in the iterative method.
4 Conclusion

In this short note, we present an iterative K-FAC algorithm on the special structure of Fisher information matrix (FIM). This method is matrix-free, that is, no need to generate FIM, also no need to generate the Kronecker factors A and G. We will give more detailed experiments in later papers.

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