Eigenvalue-corrected Natural Gradient Based on a New Approximation

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Abstract

Using second-order optimization methods for training deep neural networks (DNNs) has attracted many researchers. A recently proposed method, Eigenvaluecorrected Kronecker Factorization (EKFAC) (George et al., 2018), proposes an interpretation of viewing natural gradient update as a diagonal method, and corrects the inaccurate re-scaling factor in the Kronecker-factored eigenbasis. Gao et al. (2020) considers a new approximation to the natural gradient, which approximates the Fisher information matrix (FIM) to a constant multiplied by the Kronecker product of two matrices and keeps the trace equal before and after the approximation. In this work, we combine the ideas of these two methods and propose Trace-restricted Eigenvalue-corrected Kronecker Factorization (TEKFAC). The proposed method not only corrects the inexact re-scaling factor under the Kronecker-factored eigenbasis, but also considers the new approximation method and the effective damping technique proposed in Gao et al. (2020). We also discuss the differences and relationships among the Kronecker-factored approximations. Empirically, our method outperforms SGD with momentum, Adam, EKFAC and TKFAC on several DNNs.

1 Introduction

Deep learning has made significant progress in various natural language and computer vision applications. But as models becoming more and more complex, deep neural networks (DNNs) usually have huge parameters (for example, VGG16 has over 1.5 million

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parameters) to be trained, which takes a long time. Therefore, the research of more efficient optimization algorithms has attracted many researchers.

Among the algorithms for training DNNs, the most popular and widely used method is Stochastic Gradient Descent (SGD) (Robbins and Monro, 1951). During training, the goal of SGD is to find the optimal parameters ω to minimize the objective function $h(\omega)$. The parameters ω are updated by: $\omega \leftarrow \omega - \eta \nabla_{\omega} h$, where η is the learning rate. To achieve better training performance, many variants of SGD also have been proposed, such as momentum (Qian, 1999), Nesterov's acceleration (Nesterov, 1983) and etc. However, SGD only considers first-order gradient information, which leads to some deficiencies, including relatively-slow convergence and sensitivity to hyper-parameter settings.

To avoid these problems, the second-order optimization algorithm may be a good choice. More importantly, second-order optimization algorithms can greatly accelerate convergence by using curvature matrix to correct gradient through training. The parameters update rule is: $\omega \leftarrow \omega - \eta F^{-1} \nabla_{\omega} h$, where F^{-1} is the inverse of curvature matrix. The curvature matrix F is defined differently in second-order optimization algorithms. For Newton's method, F is the Hessian matrix which represents second-order derivatives. For natural gradient method (Amari, 1998), F is the Fisher information matrix (FIM) which represents covariance of second-order gradient statistics. However, the curvature matrix and its inverse dramatically increase computing and storage costs. It is impractical to compute and invert an exact curvature matrix directly. Therefore, many approximate methods have been proposed.

A simple but crude method is diagonal approximation, such as AdaGrad (Duchi et al., 2011), RMSprop (Tieleman and Hinton, 2012), Adam (Kingma and Ba, 2014) and etc. These algorithms are computationally tractable but lose much curvature matrix information. More elaborate algorithms are no longer limited to diagonal approximation. For Newton's methods, quasi-Newton method (Dennis and Moré, 1977; Le et al., 2011; Berahas et al., 2019; Goldfarb et al., 2020) can be used to approximate the Hessian matrix and its advantages over Newton's method is that the Hessian matrix does not need to be inverted directly. Hessian-Free optimization approach (Martens, 2010; Kiros, 2013; Pan et al., 2017) provides a matrix-free conjugate-gradient algorithm for approximating the Hessian matrix. For natural gradient methods, Kronecker-factored Approximate Curvature (KFAC) (Martens and Grosse, 2015) presents efficient block diagonal approximation and block tri-diagonal approximation of the FIM in fully-connected neural networks. This method has been further extended to convolutional neural networks (Grosse and Martens, 2016), recurrent neural networks (Martens et al., 2018) and variational Bayesian neural networks (Bae et al., 2018; Zhang et al., 2018). KFAC has also been used in large-scale distributed computing for deep neural networks (Ba et al., 2017; Osawa et al., 2019; Pauloski et al., 2020; Yang et al., 2020).

In particular, George et al. (2018) proposes a new explanation for the natural gradient update, in which the natural gradient update is viewed as diagonal method in Kronecker-factored eigenbasis. And under this interpretation, the re-scaling factor under the KFAC eigenbasis is not exact. So Eigenvalue-corrected Kronecker Factorization (EKFAC) is proposed to correct the inaccurate re-scaling factor. Recently, Gao et al. (2020) adopts a new model to approximate the FIM called Trace-restricted Kronecker Factorization (TKFAC). TKFAC approximates the FIM as a constant multiple of the Kronecker product of two matrices. In experiments, TKFAC has better performance than KFAC. Therefore, it is natural for us to consider the TKFAC's model under the interpretation proposed in EKFAC.

In this work, we combine the ideas of EKFAC and TKFAC, then present Tracerestricted Eigenvalue-corrected Kronecker Factorization (TEKFAC). Our contribution can be summarized as follows:

- Instead of approximating FIM to the Kronecker product of two smaller matrices, we consider EKFAC based on the approximation model adopted by TKFAC. So, we change the Kronecker-factored eigenbasis in EKFAC and propose TEKFAC, which not only corrects the inexact re-scaling factor but also takes the advantages of TKFAC.
- We discuss the relationships and differences among the several methods, including KFAC, EKFAC, TKFAC and TEKFAC. Empirically, we compare TEKFAC with SGD with momentum (SGDM), Adam, EKFAC and TKFAC using the SVHN, CIFAR-10 and CIFAR-100 datasets on VGG16 and ResNet20. Our method has more excellent performance than these baselines.

2 Methods to Approximate the Natural Gradient

2.1 Natural Gradient

During the training process of DNNs, the purpose is to minimize a loss function $h(\omega)$. Throughout this paper, we use $\mathbb{E}[\cdot]$ to represent the mean of the samples (x, y) and the cross-entropy loss function is computed as

$$h(\omega) = \mathbb{E}[-\log p(y|x,\omega)],$$

where ω is a vector of parameters, x is the input, y is the label, and $p(y|x,\omega)$ represents the density function of the neural network's predictive distribution $P_{y|x}(\omega)$.

Natural gradient was first proposed by Amari (1998). It gives the steepest descent direction in the distribution space rather than the space of parameters. In distribution space, the distance between two distributions $P(\omega)$ and $P(\omega + \Delta \omega)$ is measured by the K-L divergence: $D_{\text{KL}}(P(\omega) || P(\omega + \Delta \omega)) \approx \frac{1}{2} \omega^{\top} F \omega$, where F is the FIM, and is defined as

$$F = \mathbb{E}[\nabla_{\omega} \log p(y|x,\omega)\nabla_{\omega} \log p(y|x,\omega)^{\top}].$$
(2.1)

The natural gradient is usually defined as $F^{-1}\nabla_{\omega}h$, and it provides the update direction for natural gradient descent. So, the parameters are updated by

$$\omega \leftarrow \omega - \eta F^{-1} \nabla_{\omega} h, \qquad (2.2)$$

where η is the learning rate.

2.2 KFAC

For DNNs which have millions or even billions of parameters, it is impractical to compute the exact FIM and its inverse matrix. KFAC provides an useful approximation. Consider a DNN with L layers and denote the inputs a_{l-1} which are the activations of the previous layer, outputs s_l , and weight W_l for the *l*-th layer. Then, we have $s_l = W_l a_{l-1}$. For simplicity, we will use the following notation:

$$\mathcal{D}t := \nabla_t \log p(y|x,\omega), u_l := \mathcal{D}s_l,$$

where t is an arbitrary parameter. Therefore, the gradient of weight is $\mathcal{D}W_l = a_{l-1}u_l$, and the Eq. (2.1) can be written as $F = \mathbb{E}[\mathcal{D}\omega\mathcal{D}\omega^{\top}]$.

Firstly, KFAC approximates the FIM F as a block diagonal matrix

$$F \approx diag(F_1, F_2, \cdots, F_L) = diag(\mathbb{E}[\mathcal{D}\omega_1 \mathcal{D}\omega_1^\top], \mathbb{E}[\mathcal{D}\omega_2 \mathcal{D}\omega_2^\top], \cdots, \mathbb{E}[\mathcal{D}\omega_L \mathcal{D}\omega_L^\top]), \quad (2.3)$$

where $\omega_l = \operatorname{vec}(W_l)$ for any $l \in \{1, 2, \cdots, L\}$.

Then, each block matrix of the FIM can be written as

$$F_{l} = \mathbb{E}[\mathcal{D}\omega_{l}\mathcal{D}\omega_{l}^{\top}] = \mathbb{E}[(a_{l-1}\otimes u_{l})(a_{l-1}\otimes u_{l})^{\top}] \approx \mathbb{E}[a_{l-1}^{\top}a_{l-1}] \otimes \mathbb{E}[u_{l}^{\top}u_{l}] = A_{l-1}\otimes U_{l}, \quad (2.4)$$

where \otimes represents the Kronecker product, $A_{l-1} = \mathbb{E}[a_{l-1}a_{l-1}^{\top}]$ and $U_l = \mathbb{E}[u_l u_l^{\top}]$. Due to the properties of Kronecker product $(A_{l-1} \otimes U_l)^{-1} = A_{l-1}^{-1} \otimes U_l^{-1}$ and $(A_{l-1} \otimes U_l) \operatorname{vec}(X) = \operatorname{vec}(U_l X A_{l-1}^{\top})$ for any matrix X, decomposing F_l into A_{l-1} and U_l not only saves the cost of storing and inverting the exact FIM, but also enables tractable methods to compute the approximate natural gradient

$$(A_{l-1} \otimes U_l)^{-1} \nabla_{\omega_l} h = (A_{l-1} \otimes U_l)^{-1} \operatorname{vec}(\nabla_{W_l} \phi) = \operatorname{vec}(U_l^{-1}(\nabla_{W_l} \phi) A_{l-1}^{-1}).$$

2.3 EKFAC

George et al. (2018) proposes an other interpretation of the natural gradient update $F^{-1}\nabla_{\omega}h$. Let $F = Q_F \Lambda_F Q_F^{\top}$ be the eigendecomposition of the FIM, where Λ is a diagonal matrix with eigenvalues and Q is an orthogonal matrix whose columns correspond to eigenvectors. Then, the natural gradient update will be

$$F^{-1}\nabla_{\omega}h = Q_F \overbrace{\Lambda_F^{-1} Q_F^{\top} \nabla_{\omega}h}^{(b)}.$$
(2.5)

The Eq. (2.5) can be explained by three steps: (a) multiplying $\nabla_{\omega} h$ by Q_F^{\top} , which projects the gradient vector $\nabla_{\omega} h$ to the eigenbasis Q_F ; (b) multiplying by the diagonal matrix Λ_F , which re-scales the coordinates in that eigenbasis by the diagonal inverse

matrix Λ_F^{-1} ; (c) multiplying by Q_F , which projects the re-scaled coordinates back to the initial basis. The re-scaling factor can be computed by $(\Lambda_F)_{ii} = \mathbb{E}[(Q_F^{\top} \nabla_{\omega} h)_i^2]$, whose entries are the second moment of the vector $Q_F^{\top} \nabla_{\omega} h$ (the gradient vector in the eigenbasis). Under this interpretation, for a diagonal approximation of the FIM, the re-scaling factor is $(\Lambda_F)_{ii} = \mathbb{E}[(\nabla_{\omega} h)_i^2]$ and the eigenbasis can be chosen as the identity matrix I. Although the re-scaling factor is efficient, obtaining an exact eigenbasis is difficult, the eigenbasis I is too crude which leads to great approximation error.

KFAC decomposes the FIM F into two Kronecker factors A_{l-1} and U_l . Because A_{l-1} and U_l are real symmetric positive semi-define matrices, they can be expressed as $A_{l-1} = Q_{A_{l-1}} \Lambda_{A_{l-1}} Q_{A_{l-1}}^{\top}$ and $U_l = Q_{U_l} \Lambda_{U_l} Q_{U_l}^{\top}$ by eigendecomposition. By the property of Kronecker product, Eq. (2.4) can be written as

$$F_{l} \approx A_{l-1} \otimes U_{l} = (Q_{A_{l-1}} \Lambda_{A_{l-1}} Q_{A_{l-1}}^{\top}) \otimes (Q_{U_{l}} \Lambda_{U_{l}} Q_{U_{l}}^{\top})$$

= $(Q_{A_{l-1}} \otimes Q_{U_{l}})(\Lambda_{A_{l-1}} \otimes \Lambda_{U_{l}})(Q_{A_{l-1}} \otimes Q_{U_{l}})^{\top}.$ (2.6)

According to this interpretation, $Q_{A_{l-1}} \otimes Q_{U_l}$ gives the eigenbasis of the Kronecker product $A_{l-1} \otimes U_l$. Compared with diagonal approximations, KFAC provides a more exact eigenbasis approximation of the full FIM eigenbasis. However, the re-scaling factor is not accurate under the KFAC eigenbasis, that is $(\Lambda_{A_{l-1}} \otimes \Lambda_{U_l})_{ii} \neq \mathbb{E}[((Q_{A_{l-1}} \otimes Q_{U_l})^\top \nabla_{\omega_l} h)_i^2]$. EKFAC corrects this inexact re-scaling factor by defining

$$(\Lambda_l^*)_{ii} = \mathbb{E}[((Q_{A_{l-1}} \otimes Q_{U_l})^\top \nabla_{\omega_l} h)_i^2].$$

Then, F_l can be approximated as

$$F_l \approx (Q_{A_{l-1}} \otimes Q_{U_l}) \Lambda_l^* (Q_{A_{l-1}} \otimes Q_{U_l})^\top.$$
(2.7)

2.4 **TKFAC**

Recently, Gao et al. (2020) proposed a new approximation of F_l , which approximates F_l as a Kronecker product scaled by a coefficient σ_l , i.e.,

$$F_l \approx \sigma_l \Phi_l \otimes \Psi_l, \tag{2.8}$$

where $0 < \sigma_l < \infty$ is an unknown parameter, Φ_l and Ψ_l are two unknown matrices with known traces. Denote $\Lambda_{l-1} = a_{l-1}a_{l-1}^{\top}$ and $\Gamma_l = u_l u_l^{\top}$. Then, the factors in Eq. (2.8) can be computed by

$$\sigma_{l} = \frac{\mathbb{E}[\operatorname{tr}(\Lambda_{l-1})\operatorname{tr}(\Gamma_{l})]}{\operatorname{tr}(\Phi_{l})\operatorname{tr}(\Psi_{l})}, \Phi_{l} = \frac{\operatorname{tr}(\Phi_{l})\mathbb{E}[\operatorname{tr}(\Gamma_{l})\Lambda_{l-1}]}{\mathbb{E}[\operatorname{tr}(\Lambda_{l-1})\operatorname{tr}(\Gamma_{l})]}, \Psi_{l} = \frac{\operatorname{tr}(\Psi_{l})\mathbb{E}[\operatorname{tr}(\Lambda_{l-1})\Gamma_{l}]}{\mathbb{E}[\operatorname{tr}(\Lambda_{l-1})\operatorname{tr}(\Gamma_{l})]}.$$
 (2.9)

An important property of TKFAC is to keep the traces equal, i.e., $\operatorname{tr}(F_l) = \operatorname{tr}(\sigma_l \Phi_l \otimes \Psi_l) = \sigma_l \operatorname{tr}(\Phi_l) \operatorname{tr}(\Psi_l)$. Theoretically, the upper bound of TKFAC's approximation error is smaller than KFAC in general cases. What's more, experimental results show that

TKFAC can keep smaller approximation error than KFAC during training. In practice, to reduce computing costs, we can assume that $tr(\Phi_l) = tr(\Psi_l) = 1$. So, Eq. (2.9) can be simplified as

$$\sigma_{l} = \mathbb{E}[\operatorname{tr}(\Lambda_{l-1})\operatorname{tr}(\Gamma_{l})], \ \Phi_{l} = \frac{\mathbb{E}[\operatorname{tr}(\Gamma_{l})\Lambda_{l-1}]}{\mathbb{E}[\operatorname{tr}(\Lambda_{l-1})\operatorname{tr}(\Gamma_{l})]}, \ \Psi_{l} = \frac{\mathbb{E}[\operatorname{tr}(\Lambda_{l-1})\Gamma_{l}]}{\mathbb{E}[\operatorname{tr}(\Lambda_{l-1})\operatorname{tr}(\Gamma_{l})]}.$$
(2.10)

3 Methods

3.1 TEKFAC

EKFAC corrects the inexact re-scaling factor in KFAC based on the model that F_l is approximated the Kronecker product of two smaller matrices. If we think of TKFAC in terms of the interpretation adopted by EKFAC, the re-scaling factor in TKFAC is also inexact. So, in this section, we combine the ideas of these two methods and propose a new method called TEKFAC, which can keep track of the diagonal variance in TKFAC eigenbasis.

TKFAC approximates F_l as a Kronecker product of two factors Φ_l, Ψ_l and scaled by the coefficient σ_l . It is easy to know that Φ_l and Ψ_l are symmetric positive semi-define matrices, according to eigendecomposition, we can obtain

$$F_l \approx \sigma_l \Phi_l \otimes \Psi_l = \sigma_l (Q_{\Phi_l} \Lambda_{\Phi_l} Q_{\Phi_l}^{\top}) \otimes (Q_{\Psi_l} \Lambda_{\Psi_l} Q_{\Psi_l}^{\top}) = \sigma_l (Q_{\Phi_l} \otimes Q_{\Psi_l}) (\Lambda_{\Phi_l} \otimes \Lambda_{\Psi_l}) (Q_{\Phi_l} \otimes Q_{\Psi_l})^{\top},$$
(3.1)

where $\Lambda_{\Phi_l}, \Lambda_{\Psi_l}$ are two diagonal matrices with eigenvalues of Φ_l, Ψ_l and $Q_{\Phi_l}, \Lambda_{\Phi_l}$ are two orthogonal matrices whose columns are eigenvectors of Φ_l, Ψ_l , respectively. As the interpretation in subsection 3.2, $Q_{\Phi_l} \otimes Q_{\Psi_l}$ gives the TKFAC eigenbasis, and the rescaling factor can be selected as $\sigma_l(\Lambda_{\Phi_l} \otimes \Lambda_{\Psi_l})$. However, this re-scaling factor is also not guaranteed to match the second moment of the gradient vector in TKFAC eigenbasis, that is $(\Lambda_{\Phi_l} \otimes \Lambda_{\Psi_l})_{ii} \neq \mathbb{E}[((Q_{\Phi_l} \otimes Q_{\Psi_l})^\top \nabla_{\omega_l} h)_i^2]$. Therefore, combined with the idea of EKFAC, we redefine the re-scaling factor by

$$(\Theta_l)_{ii} = \mathbb{E}[((Q_{\Phi_l} \otimes Q_{\Psi_l})^\top \nabla_{\omega_l} h)_i^2], \qquad (3.2)$$

where Θ_l is a diagonal matrix. Eq. (3.2) defines a more accurate re-scaling factor. Then, we can obtain the new approximation defined as follows

$$F_l \approx (Q_{\Phi_l} \otimes Q_{\Psi_l}) \Theta_l (Q_{\Phi_l} \otimes Q_{\Psi_l})^\top.$$
(3.3)

Similar to the analysis process of EKFAC, we can proof that Θ_l is the optimal diagonal scaling factor under the TKFAC eigenbasis. That is Θ_l is the optimal solution to the following problem.

$$\min_{\Lambda_l} \quad \|F_l - (Q_{\Phi_l} \otimes Q_{\Psi_l}) \Lambda_l (Q_{\Phi_l} \otimes Q_{\Psi_l})^\top\|_F$$

s.t. Λ_l is a diagonal matrix

According to this conclusion, we can easily prove the following theorem. For simplicity, we omit the subscript in the following theorem.

Theorem 3.1. Let F_{TKFAC} and F_{TEKFAC} are the approximate matrices of the FIM F, *i.e.*,

$$F_{\text{TKFAC}} = (Q_{\Phi} \otimes Q_{\Psi})(\sigma \Lambda_{\Phi} \otimes \Lambda_{\Psi})(Q_{\Phi} \otimes Q_{\Psi})^{\top},$$

$$F_{\text{TEKFAC}} = (Q_{\Phi} \otimes Q_{\Psi})\Theta(Q_{\Phi} \otimes Q_{\Psi})^{\top},$$

then, we have $||F - F_{\text{TEKFAC}}||_F \le ||F - F_{\text{TKFAC}}||_F$.

Proof. Because

$$\Theta = \arg\min_{\Lambda} \|F - (Q_{\Phi} \otimes Q_{\Psi}) \Lambda (Q_{\Phi} \otimes Q_{\Psi})^{\top}\|_{F}$$

and for the diagonal matrices $\Lambda_{\Phi} \otimes \Lambda_{\Psi}$, Θ_l

$$(\Lambda_{\Phi} \otimes \Lambda_{\Psi})_{ii} \neq \mathbb{E}[((Q_{\Phi} \otimes Q_{\Psi})^{\top} \nabla_{\omega} h)_{i}^{2}] = \Theta_{ii}$$

Therefore, we have

$$\|F - (Q_{\Phi} \otimes Q_{\Psi})\Theta(Q_{\Phi} \otimes Q_{\Psi})^{\top}\|_{F} \le \|F - (Q_{\Phi} \otimes Q_{\Psi})(\sigma\Lambda_{\Phi} \otimes \Lambda_{\Psi})(Q_{\Phi} \otimes Q_{\Psi})^{\top}\|_{F}$$

that is

$$\|F - F_{\text{TEKFAC}}\|_F \le \|F - F_{\text{TKFAC}}\|_F.$$

The proof is complete.

So, TEKFAC provides a more accurate approximation for the FIM than TKFAC in theory. To use the second-order optimization methods effectively in practice, a suitable damping technique is also necessary. Crucially, powerful second-order optimizers like KFAC and EKFAC usually require more complicated damping techniques, otherwise, they will tend to fail completely. KFAC introduces an effective damping technique by adding $\sqrt{\lambda I}$ to the Kronecker factors A_{l-1} and U_l . In EKFAC, since the re-scaling factor has been revised and redefined, it is no longer useful to add damping to the Kronecker factors, and the damping should be added to the re-scaling factor. TKFAC adopts the same damping technique as KFAC for FNNs and proposes a new automatic tuning damping for CNNs. For TEKFAC, we also use the same damping technique as EKFAC for FNNs and the new damping technique adopted in TKFAC for CNNs, i.e.,

$$F_l \approx (Q_{\Phi_l} \otimes Q_{\Psi_l})(\Theta_l + \lambda I)(Q_{\Phi_l} \otimes Q_{\Psi_l})^{\top}$$
(3.4)

where λ is a reasonably large positive scalar for FNNs and

$$\lambda = \frac{\max\{\operatorname{tr}(\Theta_l), \vartheta\}}{\dim(\Theta_l)}$$
(3.5)

for CNNs. In Eq. (3.5), ϑ is a reasonably large positive scalar and dim denotes the number of the rows (or columns) of Θ_l . What's more, in order to keep pace with convolution layers, we expanded the FIM of the fully connected layer in CNNs by a factor of β as described in Gao et al. (2020), where $\beta = \max_{l \in \{\text{convolutional layers}\}} \{\max\{\text{tr}(\Theta_l), \vartheta\}/\dim(\Theta_l)\}$. This damping technique for CNNs was first used in Gao et al. (2020). The purpose is to dynamically adjust the damping based on the FIM's trace during training, so the damping can be adapted to the FIM's elements to avoid the problem that the damping is large enough to transform the second-order optimizer into the first-order one during training.

Algorithm 1 TEKFAC algorithm

Require: η : learning rate **Require:** λ : damping parameter **Require:** β_1 : exponential moving average parameter of the re-scaling factor Θ_l **Require:** β_2 : exponential moving average parameter of factors Φ_l and Ψ_l **Require:** $T_{\text{FIM}}, T_{\text{EIG}}, T_{\text{RE}}$: FIM, eigendecomposition and re-scaling update intervals $k \leftarrow 0$ Initialize $\{\delta_l\}_{l=1}^L, \{\Phi_l\}_{l=1}^L, \{\Psi_l\}_{l=1}^L$ and $\{\Theta_l\}_{l=1}^L$ while convergence is not reached do if $k \equiv 0 \pmod{T_{\text{FIM}}}$ then Update the factors $\{\delta_l\}_{l=1}^L$, $\{\Phi_l\}_{l=1}^L$ and $\{\Psi_l\}_{l=1}^L$ using Eq. (2.10) end if if $k \equiv 0 \pmod{T_{\text{EIG}}}$ then Compute the eigenbasis Q_{Φ_l} and Q_{Ψ_l} using Eq. (3.1), (3.7) and (3.9) end if if $k \equiv 0 \pmod{T_{\text{RE}}}$ then Update the re-scaling factor $\{\Theta_l\}_{l=1}^L$ using Eq. (3.2), (3.4) and (3.6) end if $\nabla_{l}^{(k)} \leftarrow (Q_{\Phi_{l}}^{\top} \otimes Q_{\Psi_{l}}^{\top})^{(k)} \nabla_{\omega_{l}} h^{(k)}$ $\nabla_{l}^{(k)} \leftarrow \nabla_{l}^{(k)} / (\operatorname{vec}(\Theta_{l}^{(k)} + \lambda I)) \text{ (element-wise scaling)}$
$$\begin{split} \nabla_l^{(k)} &\leftarrow (Q_{\Phi_l} \otimes Q_{\Psi_l})^{(k)} \nabla_l^{(k)} \\ \omega_l^{(k)} &\leftarrow \omega_l^{(k-1)} - \eta \nabla_l^{(k)} \end{split}$$
 $k \leftarrow k+1$ end while

For each layer, EKFAC estimates the Kronecker factors A_{l-1} , U_l and the re-scaling factor $(\Lambda_l^*)_{ii}$ using exponential moving average. Similarly, we can obtain the exponential moving average updates for TEKFAC in Eq. (3.3).

$$(\Theta_l)_{ii}^{(k+1)} \leftarrow \beta_1(\Theta_l)_{ii}^{(k+1)} + (1 - \beta_1)(\Theta_l)_{ii}^{(k)}, \tag{3.6}$$

$$\Phi_l^{(k+1)} \leftarrow \beta_2 \Phi_l^{(k+1)} + (1 - \beta_2) \Phi_l^{(k)}, \tag{3.7}$$

$$\Psi_l^{(k+1)} \leftarrow \beta_2 \Psi_l^{(k+1)} + (1 - \beta_2) \Psi_l^{(k)}, \tag{3.8}$$

where β_1 and β_2 are two exponential moving average parameters of the re-scaling factor and Kronecker factors. Finally, TEKFAC updates the parameters by

$$\omega_l^{(k+1)} \leftarrow \omega_l^{(k)} - \eta (Q_{\Phi_l} \otimes Q_{\Psi_l})^{(k+1)} [(\Theta_l + \lambda I)^{(k+1)}]^{-1} (Q_{\Phi_l}^\top \otimes Q_{\Psi_l}^\top)^{(k+1)} \nabla_{\omega_l} h^{(k+1)}.$$
(3.9)

Drawing inspiration of EKFAC and TKFAC, we present TEKFAC. Using TEKFAC for training DNNs mainly involves: a) computing the TEKFAC eigenbasis by eigendecomposition; b) estimating the re-scaling factor Θ_l as defined in Eq. (3.2); c) computing the gradient and updating model's parameters. The full algorithm of TEKFAC is given in Algorithm 1, in which the Kronecker product can be computed efficiently by the following identity: $(A \otimes U) \operatorname{vec}(X) = \operatorname{vec}(U^{\top}XA)$.

3.2 Discussion of different methods

Because the scale of the curvature matrix for DNNs is too large, it is impractical to compute the exact curvature matrix and its inverse matrix for DNNs. In order to effectively use natural gradient descent in training DNNs, KFAC was firstly proposed in (Martens and Grosse, 2015), then EKFAC (George et al., 2018) and TKFAC (Gao et al., 2020) were presented gradually. In the last subsection, we propose TEKFAC. In this subsection, we will discuss the relationships and differences of these methods.

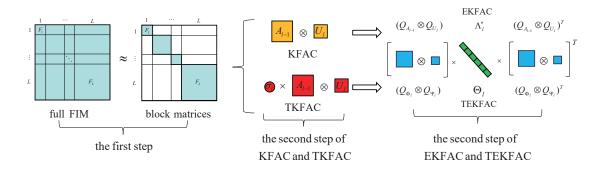


Figure 1: Illustration of the approximation process of KFAC, EKFAC, TKFAC and TEKFAC.

The approximation process of these methods can be divided into two steps. In the first step, they all decompose the FIM into block matrices according to layers of DNNs. By assuming that parameters of different layers are independent, the inverse of the full FIM is simplified as the inverse of these small block matrices. This step doesn't make any difference for all these methods. In the second step, KFAC approximates different block matrices as the Kronecker product of two much smaller matrices, EKFAC reinterprets the KFAC by eigenvalue decomposition and corrects the inaccurate re-scaling factor under the KFAC eigenbasis, TKFAC approximates different block matrices as a Kronecker

product scaled by a coefficient, TEKFAC corrects the inaccurate re-scaling factor under the TKFAC eigenbasis based on the ideas of EKFAC. The two approximate processes of these methods are illustrated in Figure 1. We also summarize the different approximate models and re-scaling factors of these methods in Table 1.

optimizer	F_l	re-scaling factor
KFAC(Martens and Grosse, 2015)	$A_{l-1} \otimes U_l$	$\Lambda_{A_{l-1}}\otimes\Lambda_{U_l}$
EKFAC(George et al., 2018)	$A_{l-1} \otimes U_l$	$\operatorname{diag}(\mathbb{E}[((Q_{A_{l-1}} \otimes Q_{U_l})^\top \nabla_{\omega_l} h)^2])$
TKFAC(Gao et al., 2020)	$\sigma_l \Phi_l \otimes \Psi_l$	$\sigma_l(\Lambda_{\Phi_l}\otimes\Lambda_{\Psi_l})$
TEKFAC	$\sigma_l \Phi_l \otimes \Psi_l$	$\operatorname{diag}(\mathbb{E}[((Q_{\Phi_l} \otimes Q_{\Psi_l})^\top \nabla_{\omega_l} h)^2])$

Table 1: Summary of some optimizers

In TKFAC, an important property is to keep the traces equal before and after the approximation. For TEKFAC, this property can be still kept because

$$\operatorname{tr}(F_l^{(\mathrm{TEKFAC})}) = \operatorname{tr}((Q_{\Phi_l} \otimes Q_{\Psi_l}) \Theta_l (Q_{\Phi_l} \otimes Q_{\Psi_l})^{\top}) = \operatorname{tr}(\Theta_l)$$
$$= \sum_i (\Theta_l)_{ii} = \sum_i \mathbb{E}[((Q_{\Phi_l} \otimes Q_{\Psi_l})^{\top} \nabla_{\omega_l} h)_i^2]$$
$$= \operatorname{tr}(\mathbb{E}[(Q_A \otimes Q_U)^{\top} \nabla_{\omega} h (\nabla_{\omega} h)^{\top} (Q_A \otimes Q_U)])$$
$$= \operatorname{tr}(\mathbb{E}[\nabla_{\omega} h (\nabla_{\omega} h)^{\top}]) = \operatorname{tr}(F_l),$$

where $F_l^{(\text{TEKFAC})}$ represents the approximation defined by Eq. (3.3) and F_l is the exact FIM. Similar to this conclusion, EKFAC can also keep the traces equal. However, we should note that EKFAC is based on the KFAC (Eq. (2.4)) and correcting the re-scaling factor, then the traces can be kept equal. TKFAC proposes a different approximation (Eq. (2.8)) and uses a trace operator to get the calculation formula under the condition that the trace is equal. The motivations for EKFAC and TKFAC are different. Finally, the relationships among these methods are summarized in Figure 4.

4 Experiments

To show the effectiveness of TEKFAC, we empirically demonstrate its performance on several standard benchmark datasets for some deep CNNs. Experimental results are given in the following subsection.

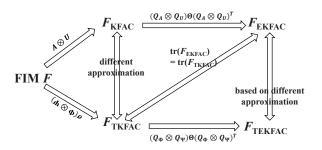


Figure 2: Illustration of the relationships of KFAC, EKFAC, TKFAC and TEKFAC.

4.1 Setup

Datasets and models: In this paper, we employ three commonly used image classification datasets: CIFAR-10, CIFAR-100 (Krizhevsky et al., 2009) and SVHN (Netzer et al., 2011). These datasets all consist of colored images with 32×32 pixels. More details of these datasets are described in Table 2. We adopt a standard data augmentation scheme including random crop and horizontal flip for CIFAR-10/100, and we do not use data augmentation for SVHN. We consider the performance of different methods on two widely used deep CNNs: VGG16 (Simonyan and Zisserman, 2014) and ResNet20 (He et al., 2016).

Dataset	#classes	#training set	#testing set
CIFAR-10	10	50000	10000
CIFAR-100	100	50000	10000
SVHN	10	73257	26032

Table 2: Statistics of the datasets used in experiments.

Baselines and hyper-parameters selection: Our method mainly modify the EK-FAC eigenbasis according to the model adopted in TKFAC, so we mainly focus on the performance of TEKFAC compared with EKFAC and TKFAC. Therefore, we choose SGDM, Adam, EKFAC and TKFAC as baselines. We mainly refer to the parameters setting $^{1-2}$ in recent related articles (Bae et al., 2018; Gao et al., 2020; Zhang et al., 2019). For all experiments, the hyper-parameters are tuned as follows:

- learning rate η : {1e-4, 3e-4, 1e-3, 3e-3, 1e-2, 3e-2, 1e-1, 3e-1, 1, 3}. The initial learning rate is multiplied by 0.1 every 20 epochs for SVHN and every 40 epochs for CIFAR10/100.
- damping λ : {1e-8, 1e-6, 1e-4, 3e-4, 1e-3, 3e-3, 1e-2, 3e-2, 1e-1, 3e-1}.
- the parameter to restrict trace ϑ : {1e-4, 1e-3, 1e-2, 1e-1, 1, 10, 100}.
- moving average parameter $\beta_1, \beta_2 : \beta_1 = \beta_2 = 0.95$.
- momentum: 0.9.
- $T_{\rm FIM} = T_{\rm EIG} = 50, T_{\rm INV} = 200.$
- batch size: 128 for SVHN, CIFAR-10/100.

For all methods, we use batch normalization and don't use weight decay. All experiments are run on a single RTX 2080Ti GPU using TensorFlow and repeated three times.

¹https://github.com/pomonam/NoisyNaturalGradient

²https://github.com/gd-zhang/Weight-Decay

4.2 **Results of experiments**

Results of CIFAR-10, CIFAR-100 and SVHN: We perform extensive experiments on three standard datasets to investigate the effectiveness of TEKFAC. The main results on SVHN and CIFAR10/100 are shown in Figure 3 and Table 3. Figure 3 shows the results of SGDM, Adam, EKFAC, TKFAC and TEKFAC on these three datasets in terms of testing accuracy. In Figure 3, we can see that all the second order optimizers (EKFAC, TKFAC and TEKFAC and TEKFAC) converge faster than SGDM and Adam. On SVHN and CIFAR-10, TEKFAC achieves same or faster convergence as TKFAC (faster than EKFAC clearly on all datasets) while achieving better accuracy. On CIFAR-100, although TEKFAC converges slower in the first few epochs, it can achieve same convergence as TKFAC after about 30 epochs with better accuracy. The final testing accuracies are summarized in Table 3.

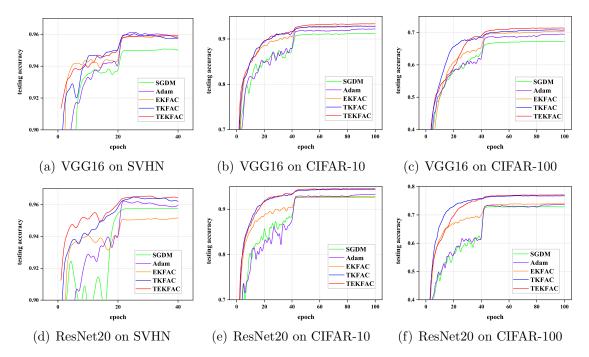


Figure 3: The curves of testing accuracy with epochs for SGDM, Adam, EKFAC, TKFAC and TEKFAC on SVHN, CIFAR-10 and CIFAR-100. The models we used here are VGG16 and ResNet20. All results are repeated three runs and the curves show the average results.

Table 3 illustrates the testing accuracies of various methods (SGDM, Adam, EKFAC, TKFAC and TEKFAC) with different models (VGG16 and ResNet20) on the SVHN, CIFAR-10 and CIFAR-100 datasets. These experiments are repeated for three times and the results are reported in mean \pm standard deviation. As shown in Table 3, TEK-FAC can achieve higher average accuracy than other baselines in all cases. Compared with EKFAC, TEKFAC greatly improves the testing accuracies of all datasets. For ex-

ample, TEKFAC improves 0.96% and 3.06% than EKFAC on the CIFAR-100 dataset. Compared with TKFAC, TEKFAC is also able to improve the testing accuracies. For TEKFAC, on the one hand, the idea of EKFAC is combined to correct the inexact re-scaling factor; on the other hand, the new approximation method and the effective damping technique proposed in TKFAC are considered, so a more effective algorithm is obtained. These results also illustrate this point.

Table 3: Results of the SVHN, CIFAR-10 and CIFAR-100 datasets on VGG16 and ResNet20 for SGDM, Adam, EKFAC, TKFAC and TEKFAC. We give the final testing accuracies (mean \pm standard deviation over three runs) after 40 epochs for SVHN and 100 epochs for CIFAR.

Dataset	Model	SGDM	Adam	EKFAC	TKFAC	TEKFAC
SVHN	VGG16	94.98 ± 0.09	$95.80{\pm}~0.11$	$95.87 \pm \ 0.13$	95.75 ± 0.21	$\textbf{95.93}{\pm~0.16}$
SVHN	$\operatorname{ResNet20}$	95.78 ± 0.15	$95.93{\pm}~0.12$	$95.16 \pm\ 0.07$	$96.20{\pm}~0.39$	$\textbf{96.45}{\pm}~\textbf{0.14}$
CIFAR-10	VGG16	$91.19 \pm\ 0.15$	$92.21{\pm}~0.14$	$92.67{\pm}~0.22$	$92.83 \pm\ 0.13$	$\textbf{93.35}{\pm~0.17}$
CIFAR-10	$\operatorname{ResNet20}$	92.79 ± 0.14	$93.22 \pm\ 0.18$	$92.66 \pm\ 0.17$	$94.38 \pm \ 0.04$	$94.56{\pm}~0.12$
CIFAR-100	VGG16	$67.29 \pm \ 0.28$	$69.47 \pm\ 0.25$	$70.41{\pm}~0.26$	$70.82{\pm}~0.12$	$71.37{\pm}~0.18$
CIFAR-100	$\operatorname{ResNet20}$	72.94 ± 0.11	$73.70{\pm}~0.18$	$73.98{\pm}~0.21$	$76.73{\pm}~0.18$	$\textbf{77.04}{\pm}~\textbf{0.15}$

Sensitivity to hyper-parameters: We also consider the performance of TEKFAC with different hyper-parameters. For TEKFAC, a parameter ϑ is added to avoid the traces becoming too small during training as TKFAC, so the parameter ϑ needs to be tuned during traing. Therefore, we mainly consider the effect of the learning rate η and the parameter ϑ . We present the results of TEKFAC with different settings on CIFAR-100 with ResNet20.

Table 4: Testing accuracies of different parameter ϑ on CIFAR-100 with ResNet20 for TEKFAC.

Parameter ϑ	0.0001	0.001	0.01	0.1
Testing accuracy	76.81 ± 0.28	$76.65 {\pm}~0.12$	$77.04{\pm}~0.15$	76.71 ± 0.17
Parameter ϑ	1	10	100	
Testing accuracy	76.03 ± 0.26	74.74 ± 0.11	73.68 ± 0.09	

Table 4 shows the testing accuracies with different settings of ϑ , where ϑ is set to 0.0001, 0.001, 0.01, 0.1, 1, 10 and 100, respectively. The learning rate set to 0.001. Figure 4 shows the curves of the testing accuracies with epochs for different ϑ . It is clear that the final testing accuracy is similar when $\vartheta \in \{0.0001, 0.001, 0.01, 0.1\}$. However, the testing accuracy decreases rapidly when $\vartheta \ge 1$. On the other hand, we can see that ϑ also affects the speed of training from Figure 4. When $\vartheta \in \{0.0001, 0.001, 0.001, 0.01, 0.01, 0.1, 1\}$,

TEKFAC converges slower but may have higher accuracy if ϑ is smaller. When $\vartheta \in \{10, 100\}$, TEKFAC converges slowly and has lower accuracy. Therefore, we need to select ϑ carefully to achieve good performance with the balance of training speed and final accuracy. For example, we choose $\vartheta = 0.01$ on ResNet20 in this paper. Of course, 0.01 is not suitable for all networks, and ϑ should be changed for different DNNs.

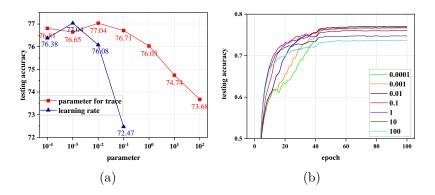


Figure 4: Results of different parameters. (a) The final testing accuracies of different parameter ϑ and learning rate η with epochs for TEKFAC; (b) The curves of testing accuracies of different ϑ with epochs for TEKFAC. The ϑ is set to 0.0001, 0.001, 0.01, 0.1, 1, 10, 100 and η is set to 0.0001, 0.001, 0.01, 0.1, 0.1.

Table 4 shows the testing accuracies with different settings of the learning rate η , where η is set to 0.0001, 0.001, 0.01, and 0.1, respectively. The parameter ϑ is set to 0.01. We can see that the learning rate also has a great influence on the results of TEKFAC. For CIFAR-100 on ResNet20, 0.001 is a good selection.

Table 5: Testing accuracies of different learning rate η on CIFAR-100 with ResNet20 for TEKFAC.

Learning tate η	0.0001	0.001	0.01	0.1
Testing accuracy	76.38 ± 0.15	$77.04{\pm}~0.15$	76.08 ± 0.14	72.47 ± 0.23

5 Conclusions

Inspired by the idea of EKFAC and the new approximation of natural gradient adopted by TKFAC, we proposed TEKFAC algorithm in this work. It not only corrected the inexact re-scaling factor under the TKFAC eigenbasis but also changed the EKFAC eigenbasis based on the new approximation. The relationships of recent methods have also been discussed. Experimental results showed that our method outperformed SGDM, Adam, EKFAC and TKFAC. Of course, the performance of our method on other DNNs or more complex large-scale training tasks needs to be further studied.

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