Kronecker-Factored Optimal Curvature

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Introduction

- Approximations of the **Fisher Information Matrix** (FIM) are crucial for deep neural networks.
- The **Kronecker-Factored Approximate Curvature** (K-FAC) approximates the FIM with a block-diagonal Kronecker-factored matrix using independence assumptions that are usually **not met in practice**.
- We propose the **Kronecker-Factored Optimal** Curvature (K-FOC) which is an **optimal** and **scalable** block-diagonal Kronecker-factored approximation of the FIM.

Background

Neural Networks

- $\mathbf{a}$: activation of layer $l-1$, $\mathbf{s}$: pre-activation of layer l
- Fully-connected layer:

$$\mathbf{s} = \mathbf{W}\begin{pmatrix}\mathbf{a}\\ 1\end{pmatrix} = \bar{\mathbf{a}}, \quad \mathbf{W} \in \mathbb{R}^{d_l \times (d_{l-1}+1)}$$

- Convolutional layer:

$$\mathbf{s}_{k,\mathbf{t}} = \mathbf{b}_k + \sum_{k'=1}^{c_{l-1}} \sum_{\delta \in \Delta} \mathbf{W}_{k,k',\delta} \mathbf{a}_{k',\zeta(\mathbf{t},\delta)}, \quad \mathbf{W} \in \mathbb{R}^{c_l \times c_{l-1} \times h_l^\Delta \times w_l^\Delta}$$

$$\hat{\mathbf{s}} = \hat{\mathbf{a}}(\hat{\mathbf{W}})^T, \quad \hat{\mathbf{W}} \in \mathbb{R}^{c_l \times (c_{l-1}|\Delta|+1)} =: \mathbb{R}^{c_l \times d_l} \quad \text{(extended vectorized form)}$$

Fisher Information Matrix

- Diagonal block for layer l:

$$\mathbf{F}_l = \mathbb{E}_{\mathbf{x}\sim Q_x} \mathbb{E}_{\mathbf{y}\sim p(\cdot|\mathbf{x},\theta)} \left[\frac{d \ln p(\mathbf{y}|\mathbf{x},\theta)}{d\theta_l} \frac{d \ln p(\mathbf{y}|\mathbf{x},\theta)}{d\theta_l}^T \right] =: \mathbb{E}\left[\mathcal{D}\theta_l (\mathcal{D}\theta_l)^T\right]$$

- Fully-connected layer:

$$\mathbf{F}_l = \mathbb{E}[\mathcal{D}\mathbf{s}(\mathcal{D}\mathbf{s})^T \otimes \bar{\mathbf{a}}(\bar{\mathbf{a}})^T] \approx \sum_{k=1}^{K_p} \mathcal{D}\mathbf{s}^k (\mathcal{D}\mathbf{s}^k)^T \otimes \frac{1}{K_p} \bar{\mathbf{a}}^k (\bar{\mathbf{a}}^k)^T \quad (K_p\text{: batch size})$$

- Convolutional layer:

$$\mathbf{F}_l = \mathbb{E}[\sum_{\mathbf{t}\in\mathcal{T}} \sum_{\mathbf{t}'\in\mathcal{T}} \mathcal{D}\mathbf{s}_{\mathbf{t}} (\mathcal{D}\mathbf{s})_{\mathbf{t}'}^T \otimes \hat{\mathbf{a}}_{\mathbf{t}} (\hat{\mathbf{a}}_{\mathbf{t}'})^T] \approx \sum_{k=1}^{K_p} \sum_{\mathbf{t}\in\mathcal{T}} \sum_{\mathbf{t}'\in\mathcal{T}} \mathcal{D}\mathbf{s}^k{}_{\mathbf{t}} (\mathcal{D}\mathbf{s}^k)_{\mathbf{t}'}^T \otimes \frac{1}{K_p} \hat{\mathbf{a}}_{\mathbf{t}}^k (\hat{\mathbf{a}}_{\mathbf{t}'}^k)^T$$

$\Rightarrow$ **For both layer types, a sum of Kronecker products needs to be computed.**

Our Method

Approximation of Sums of Kronecker Products

Problem.

$$\hat{\mathbf{L}}, \hat{\mathbf{R}} \in \underset{\mathbf{L}\in\mathbb{R}^{M\times M}, \mathbf{R}\in\mathbb{R}^{N\times N}}{\arg\min} \|\sum_{k=1}^{K} \mathbf{L}^k \otimes \mathbf{R}^k - \mathbf{L}\otimes\mathbf{R}\|_F. \tag{1}$$

Lemma 3.1. Let $M, N, K \in \mathbb{N}$, $\mathbf{L}^k \in \mathbb{R}^{M\times M}$ and $\mathbf{R}^k \in \mathbb{R}^{N\times N}$ for $k \in [K]$. Then

$$\|\sum_{k=1}^{K} \mathbf{L}^k \otimes \mathbf{R}^k - \mathbf{L}\otimes\mathbf{R}\|_F = \|\sum_{k=1}^{K} \operatorname{vec}(\mathbf{L}^k)\operatorname{vec}(\mathbf{R}^k)^T - \operatorname{vec}(\mathbf{L})\operatorname{vec}(\mathbf{R})^T\|_F.$$

Lemma 3.2. Let $\mathbf{A} = \sum_{k=1}^{K} \operatorname{vec}(\mathbf{L}^k)\operatorname{vec}(\mathbf{R}^k)^T$ and $\mathbf{A} = \sum_{i=1}^{r} \sigma_i \mathbf{u}_i \mathbf{v}_i^T$ be its singular value decomposition with $\sigma_1 \geq \dots \geq \sigma_r > 0$ and $\mathbf{u}_i^T\mathbf{u}_j = \mathbf{v}_i^T\mathbf{v}_j = \mathbb{1}[i=j]$. Then there is a solution of Equation 1 with

$$\operatorname{vec}(\hat{\mathbf{L}}) = \mathbf{u}_1, \operatorname{vec}(\hat{\mathbf{R}}) = \sigma_1\mathbf{v}_1.$$

If $\sigma_1 > \sigma_2$, the solution is unique up to changing the sign of both factors and Algorithm 1 converges almost surely to this solution.

Kronecker-Factored Optimal Curvature

As a consequence of Lemma 3.2, we can find optimal factors with the **power method**. However, computing $\mathbf{A}\mathbf{A}^T\operatorname{vec}(\hat{\mathbf{L}})$ has a complexity of $\mathcal{O}\left(n^{max}K(N^2+M^2)\right)$ with $\mathcal{O}\left(K(N^2+M^2)\right)$ memory. Therefore, we incorporate the structure of the matrix and its factors to **reduce the complexity**:

- **Algorithm 1**: Power method for sums of Kronecker products

  Main idea:
  - $\mathbf{A} = \sum_{k=1}^{K} \operatorname{vec}(\mathbf{L}^k)\operatorname{vec}(\mathbf{R}^k)^T$ is a **sum of outer products**.

  $$\Rightarrow \hat{\mathbf{R}} \leftarrow \sum_{k=1}^{K} \langle \mathbf{L}^k, \hat{\mathbf{L}}\rangle_F \mathbf{R}^k, \quad \hat{\mathbf{L}} \leftarrow \sum_{k=1}^{K} \langle \mathbf{R}^k, \hat{\mathbf{R}}\rangle_F \mathbf{L}^k$$

- **Algorithm 2**: Adaption for **convolutions** (and fully-connected layers viewed as convolutions with $\mathcal{T} = \{(1,1)\}$)

  Main idea:
  - $\mathbf{L}^{k,\mathbf{t},\mathbf{t}'} = \mathcal{D}\mathbf{s}^k{}_{\mathbf{t}} (\mathcal{D}\mathbf{s}^k)_{\mathbf{t}'}^T$ and $\mathbf{R}^{k,\mathbf{t},\mathbf{t}'} = \hat{\mathbf{a}}_{\mathbf{t}}^k (\hat{\mathbf{a}}_{\mathbf{t}'}^k)^T$ are **outer products** of vectors.
  - The summation is over **all combinations** of $\mathbf{t}, \mathbf{t}' \in \mathcal{T}$.

  $\Rightarrow$Pre-compute $\mathbf{X}^k = (\mathcal{D}\mathbf{s}^k)^T \hat{\mathbf{a}}^k$ for $k \in [K]$

  $$\hat{\mathbf{R}} \leftarrow \sum_{k=1}^{K_p} \mathbf{X}^k \hat{\mathbf{L}} (\mathbf{X}^k)^T, \quad \hat{\mathbf{L}} \leftarrow \sum_{k=1}^{K_p} (\mathbf{X}^k)^T \hat{\mathbf{R}} \mathbf{X}^k$$

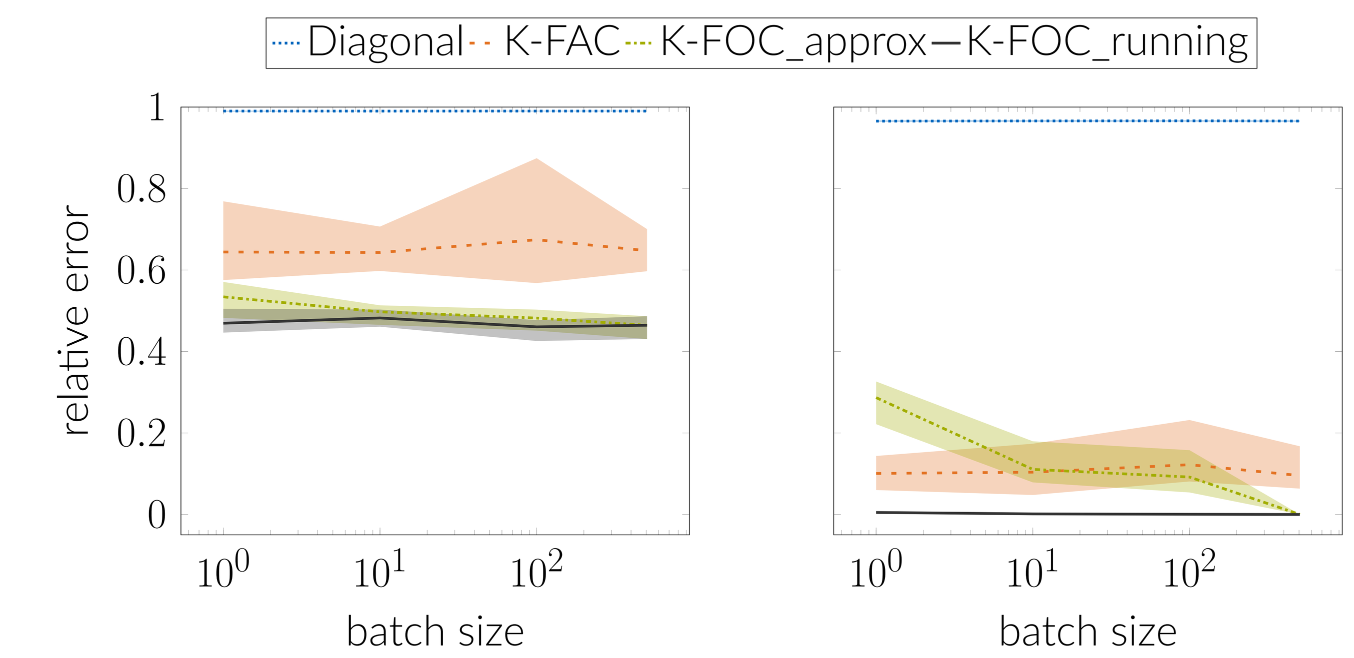
The algorithms have a **similar complexity as K-FAC** for practical applications.

Furthermore, we compare two methods to aggregate the batches in an online setting:

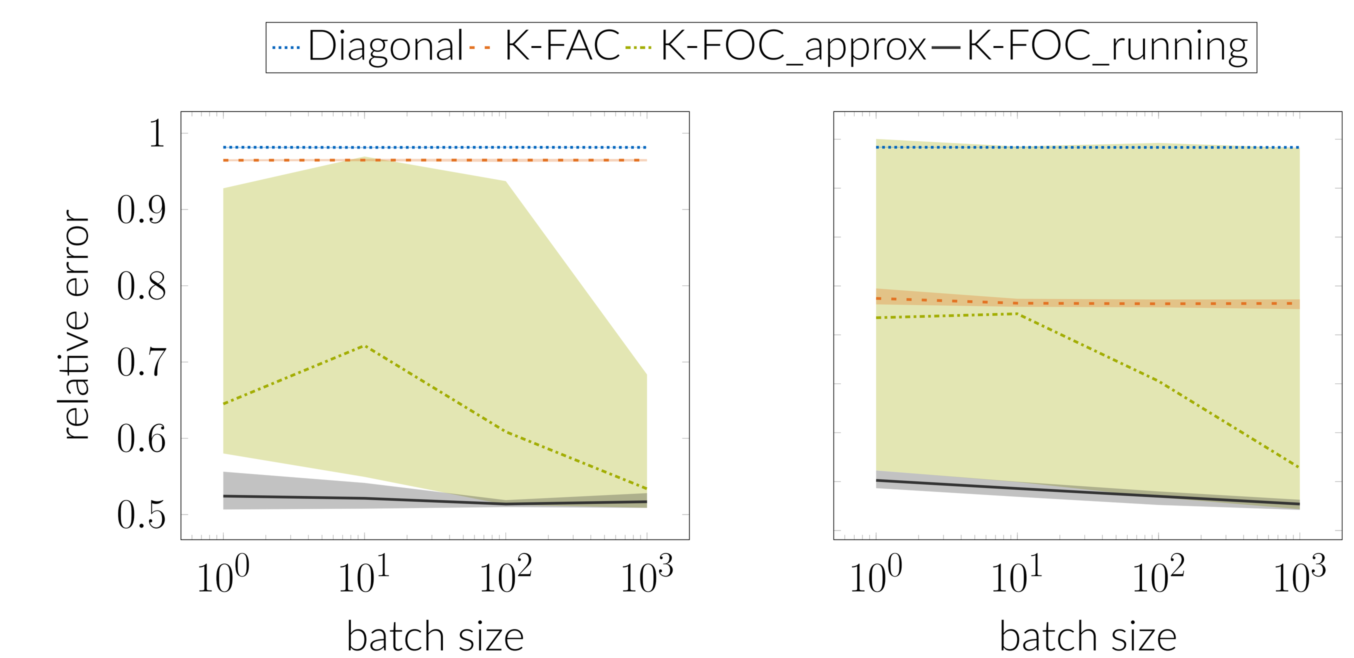
- **K-FOC_approx**: similar aggregation as K-FAC
- **K-FOC_running**: use Algorithm 1 to combine current estimate with a new batch

Results

Fully-connected layers



Convolutional layers



Conclusion

The **Kronecker-Factored Optimal Curvature**

- uses the **power iteration** to approximate the FIM,
- is **tractable** for convolutional and fully-connected layers and
- approximates the FIM **more accurately** than K-FAC.

References

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