Structured second-order methods via natural-gradient descent

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Abstract
We propose new structured second-order methods and structured adaptive-gradient methods obtained by performing natural-gradient descent on structured parameter spaces. Natural-gradient descent is an attractive approach to design new algorithms in many settings such as gradient-free, adaptive-gradient, and second-order methods. Our structured methods not only enjoy a structural invariance but also admit a simple expression. Finally, we test the efficiency of our proposed methods on both deterministic non-convex problems and deep learning problems.

1. Introduction
Newton’s method is a powerful optimization method and is invariant to any invertible linear transformation. Unfortunately, it is computationally intensive due to the inverse of the Hessian computation. Moreover, it could perform poorly in non-convex settings since the Hessian matrix can be neither positive-definite nor invertible. To address these issues, structural extensions are proposed such as BFGS. However, these extensions often lose the linear invariance. Moreover, existing extensions are often limited to one kind of structures and may not perform well in stochastic settings.

In this paper, we introduce new efficient and structured 2nd-order updates that incorporate flexible structures and preserve a structural invariance. Unlike existing second-order methods, our methods can be readily used in non-convex and stochastic settings. Moreover, structured and efficient adaptive-gradient methods are easily obtained for deep leaning by using the Gauss-Newton approximation of the Hessian. This work is an extension and application of the structured natural-gradient method (Lin et al., 2021).

Many machine learning applications can be expressed as the following unconstrained optimization problem.

$$\min_{\mu \in \mathbb{R}^p} \ell(\mu)$$  (1)

where function $\ell$ is a loss function. Instead of directly solving (1), we consider to solve the following optimization problem over a probabilistic distribution $q$.

$$\min_{\tau \in \Omega_r} \mathbb{E}_{q(w|\tau)}[\ell(w)] - \gamma \mathcal{H}(q(w|\tau)),$$  (2)

where $q(w|\tau)$ is a parametric distribution with parameters $\tau$ in the parameter space $\Omega_r$, $\mathcal{H}(q(w))$ is Shannon’s entropy, and $\gamma \geq 0$ is a constant. Problem (2) arises in many settings such as gradient-free problems (Baba, 1981; Beyer, 2001; Spall, 2005), reinforcement learning (Sutton et al., 1998; Williams & Peng, 1991; Teboulle, 1992; Mnih et al., 2016), Bayesian inference (Zellner, 1986), and robust or global optimization (Mobahi & Fisher III, 2015; Leordeanu & Hebert, 2008; Hazan et al., 2016).

Natural-gradient descent (NGD) is an attractive method to solve (2). A standard NGD update with step-size $\beta > 0$ is

$$\tau_{t+1} ← \tau_t - \beta \hat{g}_\tau,$$  (3)

where natural gradients $\hat{g}_\tau$ are computed as below.

$$\hat{g}_\tau := F_\tau^{-1}(\tau) \nabla \tau \left[ \mathbb{E}_{q(w|\tau)} [\ell(w)] - \gamma \mathcal{H}(q(w|\tau)) \right]$$

and

$$F_\tau := \mathbb{E}_q[ \nabla \log q(w|\tau)(\nabla^2 \log q(w|\tau)) ]$$

is the Fisher information matrix (FIM).

Khan et al. (2017; 2018) show a connection between the standard NGD for (2) and Newton’s method for (1), when $q(w|\tau)$ is a Gaussian distribution $\mathcal{N}(w|\mu, S^{-1})$ with $\tau = \{\mu, S\}$, where $\mu$ is the mean and $S$ is the precision.

$$\mu_{t+1} ← \mu_t - \beta S_t^{-1} \mathbb{E}_{q(w|\tau)}[\nabla w \ell(w)],$$

$$S_{t+1} ← (1 - \beta \gamma) S_t + \beta \mathbb{E}_{q(w|\tau)}[\nabla^2 w \ell(w)],$$  (4)

The standard Newton’s update for problem (1) is recovered by approximating the expectations at the mean $\mu$ and using step-size $\beta = 1$ when $\gamma = 1$ (Khan & Rue, 2020).

Since the precision $S$ lies in a positive-definite matrix space, the update (4) may violate the constraint (Khan et al., 2018). Lin et al. (2020) propose an extension by introducing a correction term. With this modification, we obtain a Newton-like update in (5) for stochastic and non-convex problems.

$$\mu_{t+1} ← \mu_t - \beta S_t^{-1} \mathbb{E}_{q_t}[\nabla w \ell(w)],$$

$$S_{t+1} ← (1 - \beta \gamma) S_t + \beta \mathbb{E}_{q_t}[\nabla^2 w \ell(w)] + \frac{\beta^2}{2} G_t S_t^{-1} G_t,$$  (5)

where $G_t := \mathbb{E}_{q_t}[\nabla^2 w \ell(w)] - \gamma S_t$ and $q_t(w) := \mathcal{N}(w|\mu_t, S_t)$. By setting $0 < \beta < 1$ and $\gamma = 1$, we obtain...
We consider a second-order update with a moving average on $S$, where the correction colored in red is added to handle the positive-definite constraint. Lin et al. (2020) study (5) in doubly stochastic settings (e.g., stochastic variational inference using (2)), where noise comes from the mini-batch sampling and the Monte Carlo approximation to the expectations.

The structured natural-gradient method generalizes several NGD methods including gradient-free methods (Glasmachers et al., 2010) and these second-order methods (Lin et al., 2020; Khan et al., 2018). We could obtain adaptive-gradient methods from a second-order update by using the Gauss-Newton approximation or randomized linear algebra to approximate the Hessian. In this paper, we show that new structured second-order methods for problem (1) with a structural invariance can be easily derived from these NGD updates. We further show that these structured methods preserve a structural invariance. Finally, we test these structured methods on problems of numerical optimization and deep learning.

2. Tractable NGD for structured Gaussians

The structured natural-gradient method (Lin et al., 2021) is a systematic approach to incorporate flexible structured covariances with simple updates. We will show that structured second-order methods for problem (1) with a structural invariance can be easily derived from these NGD updates.

We use $S_{++}^{p×p}$, $S^{p×p}$, and $GL^{p×p}$ to denote the set of symmetric positive definite matrices, symmetric matrices, and invertible matrices, respectively. We define map $h$ on matrix $M$ as $h(M) := I + M + \frac{1}{2}M^2$.

2.1. Full covariance

We consider a $p$-dimensional Gaussian distribution $q(w) = \mathcal{N}(w|\mu, S^{−1})$, where $S \in S_{++}^{p×p}$ is the precision matrix and $\Sigma = S^{−1}$ is the covariance matrix. We consider the following covariance structure $S = BB^T$, where $B \in GL^{p×p}$ is an invertible matrix. Using the structured NGD method, the update for (2) is expressed as:

$$
\begin{align*}
\mu_{t+1} &\leftarrow \mu_t - \beta S_t^{-1}g_{\mu_t}, \\
B_{t+1} &\leftarrow B_t h\left(\frac{\beta}{2} B_t^{-1} g_{\Sigma_t} B_t^{-T}\right),
\end{align*}
$$

where $g_{\mu}$ and $g_{\Sigma}$ are vanilla gradients for $\mu$ and $\Sigma$. We can show in (6), $B_{t+1} \in GL^{p×p}$ whenever $B_t \in GL^{p×p}$. Thus, $B_{t+1}$ is invertible if initial $B_0$ is invertible.

By Stein’s identity (Opper & Archambeau, 2009), we have

$$
g_{\mu} = \mathbb{E}_q[\nabla_w \ell(w)], \quad g_{\Sigma} = \frac{1}{2} \mathbb{E}_q \left[\nabla_w^2 \ell(w)\right] - \frac{\gamma}{2} S
$$

Using $S = BB^T$ and (7), the update in (6) can be expressed as a second-order update as in (5) in terms of $\mu$ and $S$:

$$
\begin{align}
\mu_{t+1} &\leftarrow \mu_t - \beta S_t^{-1} \mathbb{E}_q[\nabla_w \ell(w)] \\
S_{t+1} &\leftarrow (1 - \beta \gamma) S_t + \beta \mathbb{E}_q \left[\nabla_w^2 \ell(w)\right] + \frac{\beta^2}{2} G_t S_t^{-1} G_t + O(\beta^3)
\end{align}
$$

where $O(\beta^3)$ contains higher order terms.

Using (7) and approximating the expectations in (6) at the mean $\mu$, we obtain an update for (1), where $S = BB^T$.

A Newton-like update for (1)

$$
\begin{align}
\mu_{t+1} &\leftarrow \mu_t - \beta S_t^{-1} \nabla_{\mu} \ell(\mu_t) \\
B_{t+1} &\leftarrow B_t h\left(\frac{\beta}{2} B_t^{-1} \left(\nabla_{\mu} \ell(\mu_t) - \gamma S_t B_t^{-T}\right)\right)
\end{align}
$$

Since (1) only contains $\mu$, we can view $B$ in (8) as an axillary variable induced by the (hidden) geometry of Gaussian distribution. Compared to the classical geometric interpretation for Newton’s method, this new view allows us to handle the positive-definite constraint and exploit structures in $B$. Moreover, update (8) is invariant to any invertible linear transformation like Newton’s method for (1). Consider a linear transformation $\mu = Ky$ of the variable $\mu$ in the original problem (1), where $K \in GL^{p×p}$ is an known invertible matrix. Let $f(y) := \ell(Ky)$ be a new loss function. The update for a new problem $\min_{y \in \mathbb{R}^p} f(y)$ is

$$
\begin{align}
y_{t+1} &\leftarrow y_t - \beta C_t^{-T} C_t^{-1} \nabla_y f(y_t) \\
C_{t+1} &\leftarrow C_t h\left(\frac{\beta}{2} C_t^{-1} \nabla_y^2 f(y_t) C_t^{-T} - \gamma I\right).
\end{align}
$$

By the construction, we have $\mu_0 = Ky_0$. Since $K$ is known, we can initialize $C_0$ and $B_0$ so that $C_0 = K^T B_0 \in GL^{p×p}$. By induction, the following relationships hold. $C_{t+1} = K^T B_{t+1}$ and $\mu_{t+1} = Ky_{t+1}$ for any $t \geq 0$.

Since $\mu_{t+1} = Ky_{t+1}$, we have $f(y_{t+1}) = \ell(Ky_{t+1}) = \ell(\mu_{t+1})$. This expression shows that the update on $f$ is also the same as that on $\ell$ at each iteration. Thus, this update is invariant to any invertible linear transformation $K \in GL^{p×p}$.
2.2. Structured covariances

To construct structured covariances, we will use structured restrictions of $GL^{p \times p}$. Note that $GL^{p \times p}$ is a general linear group (GL group) (Belk, 2013). Structured restrictions give us subgroups of $GL^{p \times p}$. We will first discuss a block triangular group. More structures are illustrated in Fig. 1.

$B_{\text{up}}(k)$ denotes the block upper-triangular $p$-by-$p$ matrix space, where $k$ is the block size with $0 \leq k \leq p$, $d_0 = p-k$, and $D_{++}^{d_0 \times d_0}$ is a diagonal and invertible matrix space.

$B_{\text{up}}(k) = \left\{ \begin{vmatrix} B_A & B_B \\ 0 & B_D \end{vmatrix} : B_A \in GL^{k \times k}, B_D \in D_{++}^{d_0 \times d_0} \right\}$

$B_{\text{up}}(k)$ is indeed a matrix (Lie) group closed under matrix multiplication. Its members are all invertible matrices.

By the structured NGD method, we define another set for $B_{\text{up}}(k)$, where $D_{++}^{d_0 \times d_0}$ is the diagonal matrix space.

$M_{\text{up}}(k) = \left\{ \begin{vmatrix} M_A & M_B \\ 0 & M_D \end{vmatrix} : M_A \in S^{k \times k}, M_D \in D_{++}^{d_0 \times d_0} \right\}$

Set $M_{\text{up}}(k)$, which is indeed a Lie sub-algebra, is designed for $B_{\text{up}}(k)$ so that $h(M) \in B_{\text{up}}(k)$ whenever $M \in M_{\text{up}}(k)$.

Now, consider a $p$-dimensional Gaussian distribution $q(w) = \mathcal{N}(w; \mu, S^{-1})$, where $S \in S^{p \times p}$ is the precision. We consider the following covariance structure $S = BB^T$, where $B \in B_{\text{up}}(k)$ is a member of the group. Using the structured NGD method, the update for (2) is expressed as:

$\mu_{t+1} \leftarrow \mu_t - \beta S_t^{-1} g_{\mu_t}$

$B_{t+1} \leftarrow B_t h\left( \beta C_{\text{up}} \odot \kappa_{\text{up}}(2B_t^{-1}g_{\mu_t}B_t^{-T}) \right)$ (9)

where $\odot$ is the element-wise product, $\kappa_{\text{up}}(X)$ extracts non-zero entries of $M_{\text{up}}(k)$ from $X$ so that $\kappa_{\text{up}}(X) \in M_{\text{up}}(k)$ and $C_{\text{up}}$ is a constant matrix defined below.

$C_{\text{up}} = \begin{bmatrix} \frac{1}{2}I & J_B \\ 0 & \frac{1}{2}I_d \end{bmatrix} \in M_{\text{up}}(k)$

where $J$ is a matrix of ones and factor $\frac{1}{2}$ appears in the symmetric part of $C_{\text{up}}$.

Update (9) preserves the group structure: $B_{t+1} \in B_{\text{up}}(k)$ if $B_t \in B_{\text{up}}(k)$. When $k = p$, $B_{\text{up}}(k)$ becomes the invertible matrix space $GL^{p \times p}$. Therefore, the update in (9) recovers the update in (6) with a complete covariance structure when $k = p$. Similarly, the update in (9) becomes a NGD update with a diagonal covariance when $k = 0$. When $0 < k < p$, (9) becomes a NGD update with a structured covariance.

We obtain an update for problem (1) by approximating the expectations in (9) at $\mu$ and using (7), where $S = BB^T$.

A structured second-order update for (1)

$\mu_{t+1} \leftarrow \mu_t - \beta S_t^{-1} \nabla_\mu f(\mu_t)$

$B_{t+1} \leftarrow B_t h\left( \beta C_{\text{up}} \odot \kappa_{\text{up}}(B_t^{-1}\nabla_\mu^2 f(\mu_t)B_t^{-T} - I) \right)$ (10)
We can similarly show that this update (10) is invariant to any transformation \( K^T \in \mathcal{B}_p(k) \). Therefore, the update enjoys a group structural invariance since \( \mathcal{B}_p(k) \) is a group.

Thanks to the sparsity of group \( \mathcal{B}_p(k) \) (Lin et al., 2021), the update in (10) has low time complexity \( O(k^2 p) \). We compute \( S^{-1} \nabla_\mu \ell(\mu) \) and \( B h(M) \) in \( O(k^2 p) \) since \( B \) and \( h(M) \) are in \( \mathcal{B}_p(k) \). We compute/approximate diagonal entries of Hessian \( \nabla_\mu^2 \ell(\mu) \) and use \( k \) Hessian-vector-products for non-zero entries of \( \kappa_{up}(B^{-1} \nabla_\mu^2 \ell(\mu) B^{-T}) \) (see Eq. (54) in Appx. J.1.7 of Lin et al. (2021)). We store non-zero entries of \( B \) with space complexity \( O((k + 1)p) \).

Lin et al. (2021) show that there is a block arrowhead structure (O’leary & Stewart, 1990) over \( S_{up} = BB^T \):

\[
S_{up} = \begin{bmatrix}
B_A & B_B^T + B_B B_D^T & B_B B_D \\
B_B B_D & B_D^T \\
B_D & B_D^T
\end{bmatrix}
\]

and over \( \Sigma_{up} = S_{up}^{-1} \), which has a low-rank structure:

\[
\Sigma_{up} = U_k U_k^T + \begin{bmatrix} 0 & 0 \\ 0 & B_D^2 \\ \end{bmatrix}, \quad U_k = \begin{bmatrix} -B_A^{-T} \\ -B_D^{-1} B_B B_A^{-T} \\
\end{bmatrix}
\]

where \( U_k \) is a rank-\( k \)-matrix since \( B_A^T \) is invertible.

Similarly, we define a lower-triangular group \( B_{low}(k) \):

\[
B_{low}(k) = \left\{ \begin{bmatrix} B_A & 0 & \cdot & \cdot \\ B_C & B_D \end{bmatrix} : B_A \in \text{GL}^{k \times k}, B_D \in D_{++}^{d_A \times d_D} \right\}
\]

We consider a CNN model with 9 hidden layers. We employ \( L_2 \) regularization with weight \( 10^{-2} \). We test our structured second-order updates for (1) with a structural invariance when we approximate the expectations at the mean.

A more flexible structure is to construct a hierarchical structure inspired by the Heisenberg group (Schulz & Seesana, 2018) by replacing a diagonal group\(^1\) in \( B_D \) with a block triangular group, where \( 0 \leq k_1 + k_2 \leq p \) and \( d_0 = p - k_1 - k_2 \)

\[
B_{up}(k_1, k_2) = \left\{ \begin{bmatrix} B_A & B_B \\ B_C & B_D \end{bmatrix} : B_D \in \begin{bmatrix} D_{++}^{d_1 \times d_1} & B_D \end{bmatrix}, B_D \in \text{GL}^{k_2 \times k_2} \right\}
\]

where \( B_A \in \text{GL}^{k_1 \times k_1}, B_D, B_D \in D_{++}^{d_A \times d_D}, B_D \in \text{GL}^{k_2 \times k_2} \).

If the Hessian \( \nabla_\mu^2 \ell(\mu) \) has a model-specific structure, we could use a customized group to capture such a structure in the precision. For example, the Hessian of layer-wise matrix weights of a NN admits a Kronecker form. We can use a Kronecker product group to capture such a structure. This group can reduce the time complexity from the quadratic complexity to a linear one in \( k \) (see Appx. I.1 of Lin et al. (2021) and Fig. 2). By approximating the expectations at the mean and the Hessian by the Gauss-Newton, the structured NGD method gives us a structured adaptive update for NNs. This update also enjoys a group structural invariance. Existing structured adaptive methods such as KFAC (Martens & Grosse, 2015) and Shampoo (Gupta et al., 2018) do not have the invariance. Moreover, our update is different from existing NG methods for NN. These existing NG methods use the empirical Fisher defined by \( \ell \) while ours uses the exact Fisher of the Gaussian \( q \). Our method does not have the issue studied by Kunstner et al. (2019).

We could obtain more structured second-order updates by using many subgroups (e.g., invertible circulant matrix groups, invertible triangular-Toeplitz matrix groups) of the GL\(^p\times_p\) group and groups obtained from existing groups via the group conjugation by an element of the orthogonal group.

3. Numerical Results

3.1. Structured Second-order Optimization

We consider 200-dimensional \( (p = 200) \), non-separable, valley-shaped test functions for optimization: Rosenbrock:

\[
\ell_{\text{up}}(w) = \frac{1}{p} \sum_{i=1}^p \left[ 100(w_i + w_i^2) + (w_i - 1)^2 \right]
\]

and Dixon-Price:

\[
\ell_{\text{dp}}(w) = \frac{1}{p} \left[ (w_i - 1)^2 + \sum_{i=2}^p i(2w_i^2 - w_i - 1)^2 \right]
\]

We test our structured second-order updates for (1), where we set \( \gamma = 1 \) in our updates. We consider these structures in the precision \( S \): the upper triangular structure (denoted by “Tri-up”), the lower triangular structure (denoted by “Tri-low”), the upper Heisenberg structure (denoted by “Hs-up”), and the lower Heisenberg structure (denoted by “Hs-low”), where second-order information is used. For our updates, we compute Hessian-vector products and diagonal entries of the Hessian without computing the whole Hessian. We consider baseline methods: the BFGS method from SciPy and the Adam optimizer, where the step-size is tuned for Adam. Figure 2a-2b show the performances of all methods\(^2\), where our updates with a lower Heisenberg structure converge faster than BFGS and Adam.

3.2. Optimization for Deep Learning

We consider a CNN model with 9 hidden layers. For a smooth objective, we use average pooling and GELU (Hendrycks & Gimpel, 2016) as activation functions. We employ \( L_2 \) regularization with weight \( 10^{-2} \). We set \( \gamma = 1 \) in our updates. We train the model with our structured adaptive updates (see Appx. I of Lin et al. (2021)) for matrix weights at each layer of NN on datasets “STL-10”, “CIFAR-10”, “CIFAR-100”. We use a Kronecker product group structure of two lower-triangular groups (referred to as “Tri-low”) for computational complexity reduction. We train the model with mini-batches. We compare our

\(^1D_{++}^{d_A \times d_D} \) is indeed a diagonal matrix group.

\(^2\)Empirically, we find out that a lower structure in the precision performs better than an upper structure for optimization tasks including optimization for neural networks. For variational inference, the trend is opposite.
updates to Adam, where the step-size for each method is tuned by grid search. We use the same initialization and hyper-parameters in all methods. We report results in terms of test accuracy, where we average the results over 5 runs with distinct random seeds. From Figures 2-3, we can see our structured updates have a linear iteration cost like Adam while achieve higher test accuracy.

4. Conclusion

We propose structured second-order updates for unconstrained optimization and structured adaptive updates for NNs. These updates seem to be promising. An interesting direction is to evaluate these updates in large-scale settings.

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