Optimization on Product Submanifolds of Convolution Kernels

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Abstract—We address a problem of optimization on product of embedded submanifolds of convolution kernels (PEMs) in convolutional neural networks (CNNs). First, we explore metric and curvature properties of PEMs in terms of component manifolds. Next, we propose a SGD method, called C-SGD, by generalizing the SGD methods employed on kernel submanifolds for optimization on product of different collections of kernel submanifolds. Then, we analyze convergence properties of the C-SGD considering sectional curvature properties of PEMs. In the theoretical results, we expound the constraints that can be used to compute adaptive step sizes of the C-SGD in order to assure the asymptotic convergence.

1 INTRODUCTION

Product manifolds have been used to solve various optimization problems in machine learning, pattern recognition, and computer vision. In the recent works, stochastic gradient descent (SGD) methods have been employed on embedded kernel submanifolds [5] and Grassmann manifolds [4] of convolution kernels (weights) of convolutional neural networks (CNNs) [1], [2]. Ozay and Okatani [5] proposed a SGD method to train CNNs using embedded kernel submanifolds of convolution kernels with convergence properties. Products of the Stiefel manifolds are used for action recognition by employing CNNs in [3].

In this paper, we address a problem of optimization on products of embedded kernel submanifolds (PEMs) using a SGD method to train CNNs considering its convergence properties. Our contribution can be summarized as follows:

1) We first explore the effect of geometric properties of product manifolds, such as sectional curvature and geodesic distance, on convergence properties of PEMs compared to that of the SGD employed on component manifolds.

2) Next, we generalize the SGD methods employed on kernel submanifolds [2], [3], [5] for optimization on product of different collections of kernel submanifolds using a SGD algorithm, called C-SGD.

3) In the theoretical results, we first explore the effect of geometric properties of component manifolds on the convergence of a SGD employed on PEMs. Then, we employ the results for adaptive step size estimation of the SGD. Moreover, we provide an example for employment of the theoretical results for optimization on PEMs of the sphere.

2 OPTIMIZATION ON PRODUCT MANIFOLDS FOR TRAINING OF CNNS

We address the problem of optimization on products of kernel submanifolds to train CNNs using an SGD method. Suppose that we are given a set of training samples $S = \{s_i = (I_i, y_i)\}_{i=1}^N$ of a random variable $s$ drawn from a distribution $\mathcal{P}$ on a measurable space $\mathcal{S}$, where $y_i$ is a class label of the $i$th image $I_i$. An $L$-layer CNN consists of a set of tensors $W = \{W_l\}_{l=1}^L$, where $W_l = (W_{d,l} \in \mathbb{R}^{A_l \times B_l \times C_l})_{d=1}^D$ and $W_{d,l} = [W_{c,d,l} \in \mathbb{R}^{A_l \times B_l \times C_l}]_{c=1}^C$ is a tensor composed of kernels (weight matrices) $W_{c,d,l}$ constructed at each layer $l = 1, 2, \ldots, L$, for each $c^{th}$ channel $c = 1, 2, \ldots, C_l$ and each $d^{th}$ kernel $d = 1, 2, \ldots, D_l$.

At each $l^{th}$ convolution layer, we compute a feature representation $f_l(X_l; W_l)$ by compositionally employing non-linear functions, and convolving an image $I$ with kernels by

$$f_l(X_l; W_l) = f_1(\cdots f_1(X_1; W_1)),$$

where $X_1 := I$ is an image for $l = 1$, and $X_{l} = [X_{c,l}]_{c=1}^{C_l}$. The $c^{th}$ channel of the data matrix $X_{c,l}$ is convolved with the kernel $W_{c,d,l}$ to obtain the $d^{th}$ feature map $X_{c,l} := X_{d,l}$ by

$$X_{d,l} = W_{c,d,l} \ast X_{c,l}, \forall c, d, l \in \mathbb{L}.$$ Given a batch of samples $s \in S$, we denote a value of a classification loss function for a kernel $\omega := W_{c,d,l}$ by $L(\omega, s)$, and the loss function of kernels $W$ utilized in the CNN by $L(W, s)$. If we assume that $s$ contains a single sample, then, an expected loss or cost function of the CNN is computed by

$$L(W) = \mathbb{E}_{\mathcal{P}} \{L(W, s)\} = \int L(W, s) d\mathcal{P}.$$ (2)

The expected loss $L(\omega)$ for $\omega$ is computed by

$$L(\omega) = \mathbb{E}_{\mathcal{P}} \{L(\omega, s)\} = \int L(\omega, s) d\mathcal{P}.$$ (3)

For a finite set of samples $S$, $L(W)$ is approximated by an empirical loss $\frac{1}{|S|} \sum_{s=1}^{S} L(W, s)$, where $|S|$ is the size of $S$ (similarly, $L(\omega)$ is approximated by the empirical loss for $\omega$). Then, feature representations are learned using SGD by solving

$$\min_{W} L(W).$$ (4)

In the SGD algorithms [5], [2], [3], each kernel is assumed to reside on an embedded kernel submanifold $\mathcal{M}_{c,d,l}$ at the $l^{th}$ layer.

1. We use shorthand notation for matrix concatenation such that $[W_{c,d,l}^{(1)}, \ldots, W_{c,d,l}^{(C_l)}] = [W_{c,d,l}^{(1)}, \ldots, W_{c,d,l}^{(C_l)}]$.

2. We ignore the bias terms in the notation for the sake of simplicity.
of a CNN, such that $\omega \in \mathcal{M}_{c,d,t}, \forall c,d$. In this work, we propose a SGD algorithm called C-SGD by generalizing the SGD algorithms employed on kernel submanifolds \cite{5, 2, 3} for optimization on product of different collections of the submanifolds, which are defined next.

**Definition 2.1** (Product of embedded kernel submanifolds of convolution kernels). Suppose that $\mathcal{G}_l = \{ \mathcal{M}_l : l \in \mathbb{Z}_l \}$ is a collection of kernel submanifolds $\mathcal{M}_l$ of dimension $d_l$, which is identified by a set of indices $\mathbb{Z}_l$, $\forall l = 1, 2, \ldots, L$. Moreover, suppose that $G_l \subseteq G_l$ is a subset of manifolds identified by $\mathbb{T}_{G_l} \subseteq G_l$.

A $G_l$ product manifold of convolution kernels ($G_l$-PEM) constructed at the $l^{th}$ layer of an $L$ layer CNN is a product of embedded kernel manifolds belonging to $G_l$ which is computed by

$$
\mathcal{M}_G = \prod_{l \in \mathbb{T}_{G_l}} \mathcal{M}_l,
$$

where $\times$ is the topological Cartesian product. Given any kernel $\omega_l \in \mathcal{M}_l$, the product map

$$
\phi_l : U_l \rightarrow \mathbb{R}^{d_l},
$$

where $d_l = \sum_{i \in \mathbb{T}_{G_l}} d_i$, $(U_l, \phi_l)$ is a coordinate chart for $\mathcal{M}_l$ with $\omega_l \in U_l$, $\phi_l(\omega_l) = \phi_1 \times \phi_2$, and $U_l = \phi_1 \times U_i$. A kernel $\omega_l \in \mathcal{M}_G$ is then obtained by concatenating kernels belonging to $\mathcal{M}_l \in G_l, \forall l \in G_l$, using $\omega_l = (\omega_{l_1}, \omega_{l_2}, \ldots, \omega_{l_{|G_l|}})$, where $|G_l|$ is the cardinality of $G_l$. The product smooth manifold structure is defined by the smooth map

$$
\phi_l \circ \psi_l^{-1} = \times_{i \in \mathbb{T}_{G_l}} \phi_i \times \psi_i^{-1},
$$

where $\psi_l = \times_{i \in \mathbb{T}_{G_l}} \psi_i$. A $G_l$-PEM is simply called a product of embedded kernel submanifolds of convolution kernels (PEM).

When we employ a C-SGD on a $G_l$-PEM $\mathcal{M}_G$, each kernel $\omega$ is moved on the $G_l$-PEM in the descent direction of gradient of loss at each $t^{th}$ step of the C-SGD. More precisely, direction and amount of movement of a kernel $\omega_l$ is determined at the $t^{th}$ step and the $l^{th}$ layer by

1) projection of the gradient $\nabla E_L(\omega_l)$, which is obtained using back-propagation from the upper layer, onto the tangent space $\mathcal{T}_{\omega_l} \mathcal{M}_G$ at $\nabla E_L(\omega_l)$ (line 6 of Algorithm 1),

2) movement of $\omega_l^t$ on $\mathcal{T}_{\omega_l} \mathcal{M}_G$ according to a function of the learning rate to $v_l$ (line 7 of Algorithm 1), and

3) projection of the moved kernel at $v_l$ onto the manifold $\mathcal{M}_G$ to compute $\omega_l^{t+1}$ (line 8 of Algorithm 1).

Convergence properties of the C-SGD are affected first by the smooth manifold structure of $\mathcal{M}_G$, as defined in Definition 2.1. In addition, convergence rate is affected by metric and curvature properties of $\mathcal{M}_G$ which are analyzed in the next theorem.

**Lemma 2.2** (Metric and curvature properties of PEMS). If each kernel submanifold $\mathcal{M}_l$ is a Riemannian manifold endowed with a metric $g_l$, then a $G_l$-PEM is endowed with the metric $g_G = \bigoplus_{i \in \mathbb{T}_{G_l}} g_i$ defined by

$$
g_G(l) = \sum_{i \in \mathbb{T}_{G_l}} (u_i, v_i) = \sum_{i \in \mathbb{T}_{G_l}} g_i(u_i, v_i),
$$

where $u_i \in \mathcal{T}_{\omega} \mathcal{M}_i$ and $v_i \in \mathcal{T}_{\omega} \mathcal{M}_i$ are tangent vectors belonging to the tangent space $\mathcal{T}_{\omega} \mathcal{M}_i$ computed at $\omega_i \in \mathcal{M}_i$. In addition, if $C_i$ is the Riemannian curvature tensor of $\mathcal{M}_i$ and $x_i, y_i \in \mathcal{T}_\omega \mathcal{M}_i$, then the Riemannian curvature tensor $C_G$ on $\mathcal{M}_G$ is computed by

$$
C_G(l) = \sum_{i \in \mathbb{T}_{G_l}} C_i(\sum_{j \in \mathbb{T}_{G_l}} u_j, \sum_{j \in \mathbb{T}_{G_l}} v_j, \sum_{j \in \mathbb{T}_{G_l}} x_j, \sum_{j \in \mathbb{T}_{G_l}} y_j) = \hat{C},
$$

where $\hat{C} = \sum_{i \in \mathbb{T}_{G_l}} C_i(u_i, v_i, x_i, y_i)$. It follows that the $\mathcal{M}_G$ has never strictly positive sectional curvature $\varepsilon_C$ in the metric $\hat{C}$. In addition, no compact $\mathcal{M}_G$ admits a metric with negative sectional curvature $\varepsilon_C$.

We compute the metric of a $G_l$-PEM $\mathcal{M}_G$ using metrics identified on the component manifolds $\mathcal{M}_l$ employing $\hat{C}$ given in Lemma 2.2. In addition, we use the sectional curvature of the $\mathcal{M}_G$, given in Lemma 2.2 to analyze convergence of the C-SGD, and to compute adaptive step size. Note that some sectional curvatures vanish on the $\mathcal{M}_G$ by the lemma. For instance, suppose that each $\mathcal{M}_l$ is a unit two-sphere $S^2$, $\forall l \in \mathbb{T}_{G_l}$. Then, $\mathcal{M}_G$ computed by \cite{5} has unit curvature along two-dimensional subspaces of its tangent spaces, called two-planes. On the other hand, $\mathcal{M}_G$ has zero curvature along all two-planes spanning exactly two distinct spheres. Therefore, learning rates need to be computed adaptively according to sectional curvatures at each layer of the CNN and at each epoch of the C-SGD for each kernel $\omega$ on each manifold $\mathcal{M}_G$. In order to explore this property more precisely, we introduce the following theorem.

**Theorem 2.3**. Suppose that there exists a local minimum $\omega_{G_l} \in \mathcal{M}_G, \forall G_l \subseteq G_l, \forall l$, and $\exists \phi > 0$ such that

$$
\inf_{\rho_{G_l}, \phi} \left(\phi_{G_l}^{-1}(\omega_{G_l}), \nabla E_L(\omega_{G_l})\right) < 0, \quad \text{where } \phi \text{ is an exponential map or a twice continuously differentiable retraction, } \langle \cdot, \cdot \rangle \text{ is the inner product and } \rho_{G_l} \equiv \rho(\omega_{G_l}, \omega_{G_l}) \text{ is the geodesic distance between } \omega_{G_l} \text{ and } \hat{\omega}_{G_l} \text{ on } \mathcal{M}_G.
$$

In addition, suppose that the following conditions are satisfied for each $\mathcal{M}_G$:

(i) **Condition on learning rate** $g(t, \Theta)$:

$$
\sum_{t=0}^{\infty} g(t, \Theta) = +\infty \quad \text{and} \quad \sum_{t=0}^{\infty} g(t, \Theta)^2 < \infty.
$$

(ii) **Condition on step size and direction** $h(\nabla E_L(\omega_{G_l}), g(t, \Theta))$:

$$
h(\nabla E_L(\omega_{G_l}), g(t, \Theta)) = \frac{g(t, \Theta)}{g(\omega_{G_l})} \nabla E_L(\omega_{G_l}),
$$

where $g(\omega_{G_l}) = \max \{1, \Gamma_1^t\}$, $\Gamma_2 = (R_{G_l}^t)^2 \Gamma_2$, $\Gamma_2 = \max \{2, \Gamma_2^t\}$, $\Gamma_2^t = \frac{1}{1 + \varepsilon_C(\rho_{G_l}, \rho_{G_l})}$, $\varepsilon_C$ is the sectional curvature of $\mathcal{M}_G$, $R_{G_l}^t \equiv \|\nabla E_L(\omega_{G_l})\|$, and

$$
||\nabla E_L(\omega_{G_l})||_2^2 \leq \sum_{\omega_{G_l}} \|\nabla E_L(\omega_{G_l})\|^2.
$$

Then, the loss function and the gradient converges almost surely (a.s.) by $E_L(\omega_{G_l}) \overset{a.s.}{\rightarrow} E(\omega_{G_l})$, and $\nabla E_L(\omega_{G_l}) \overset{a.s.}{\rightarrow} 0$, for each $\mathcal{M}_G, \forall l$.

Conditions (i) and (ii) given in Theorem 2.3 can be used to compute adaptive learning rates and step sizes to train CNNs by optimization using the C-SGD algorithm (Algorithm 1) assuring convergence to minima. As an example, we use the results obtained from Lemma 2.2 in Theorem 2.3 to compute adaptive step sizes for the sphere in the following theorem.
Algorithm 1 C-SGD on products of kernel submanifolds.

1: **Input:** \( T \) (number of iterations), \( S \) (training set),
\( \Theta \) (set of hyperparameters), \( L \) (a loss function), \( \mathcal{L}_{G_l}, \forall l \) (sets of indices).

2: **Initialization:** Construct a collection of products of kernel submanifolds \( G_l, \forall l = 1, 2, \ldots, L \), and initialize kernels \( \omega^l_{G_l} \in M_{G_l}, \forall G_l \subseteq G_l, \forall l \).

3: **for** each iteration \( t = 1, 2, \ldots, T \) **do**
4: **for** each layer \( l = 1, 2, \ldots, L \) **do**
5: Compute the Euclidean gradient \( \nabla L(\omega^l_{G_l}) \).
6: \( \text{grad} L(\omega^l_{G_l}) := \Pi_{G_l}(\text{grad}_E L(\omega^l_{G_l}), \Theta) \).
7: \( v_t := h(\text{grad} L(\omega^l_{G_l}), g(t, \Theta)) \).
8: \( \omega_{G_l}^{t+1} := \phi_{\omega_{G_l}^t} (v_t), \forall \omega_{G_l}^t \).
9: \( t := t + 1 \).
10: **end for**
11: **end for**
12: **Output:** A set of estimated kernels \( \{\omega^l_{G_l}\}_{l=1}^L \).

**Corollary 2.4.** Suppose that \( M_l \) are identified by \( d_r \geq 2 \) dimensional unit sphere \( S^d_r \), and \( \rho_{G_l} \leq \tilde{c}^{-1}, \) where \( \tilde{c} \) is an upper bound on the sectional curvatures of \( M_{G_l}, \forall l \) at \( \omega^l_{G_l} \in M_{G_l}, \forall l \). If condition (i) given in Theorem 2.3 is satisfied, and step size is computed using (11) with \( g(\omega^l_{G_l}) = \max \{1, (R^l_{G_l})^2 (2 + R^l_{G_l})^2\} \), then \( L(\omega^l_{G_l}) \xrightarrow{\text{n.s.}} L(\hat{\omega}_{G_l}) \), and \( \nabla L(\omega_{G_l}^t) \xrightarrow{\text{n.s.}} 0 \), for each \( M_{G_l}, \forall l \).

3 Conclusion

We address a problem of optimization on product of embedded submanifolds of convolution kernels (PEMs) in convolutional neural networks (CNNs). In our theoretical results, we first explore metric and curvature properties of PEMs and show that PEMs have strictly positive sectional curvature. Next, we propose a SGD method, called C-SGD, by generalizing the SGD methods employed on kernel submanifolds for optimization on product of different collections of kernel submanifolds. Then, we analyze convergence properties of C-SGD employed on PEMs considering their sectional curvature properties. In the theoretical results, we expound the constraints that can be used to compute adaptive step size of C-SGD in order to assure its asymptotic convergence. Moreover, we employ the proposed methods for computation of adaptive step size of C-SGD for optimization on PEMs of the sphere. Our proposed C-SGD and the theoretical results can be used to train CNNs using products of different kernels at different layers by estimating adaptive step size of C-SGD with assurance of convergence.

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