regularization for convolutional kernel tensors to avoid unstable gradient problem in convolutional neural networks

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Abstract
Convolutional neural networks are very popular nowadays. Training neural networks is not an easy task. Each convolution corresponds to a structured transformation matrix. In order to help avoid the exploding/vanishing gradient problem, it is desirable that the singular values of each transformation matrix are not large/small in the training process. We propose three new regularization terms for a convolutional kernel tensor to constrain the singular values of each transformation matrix. We show how to carry out the gradient type methods, which provides new insight about the training of convolutional neural networks.

Keywords: regularization, singular values, doubly block banded Toeplitz matrices, convolution, tensor.

1 Introduction
As we know, each convolution arithmetic corresponds to a linear structured transformation matrix. We use vec$(X)$ to denote the vectorization of $X$. If $X$ is a matrix, vec$(X)$ is the column vector got by stacking the columns of $X$ on top of one another. If $X$ is a tensor, vec$(X)$ is the column vector got by stacking the columns of the flattening of $X$ along the first index (see [5] for more on flattening of a tensor). We use $*$ to denote the convolution arithmetic in deep learning. Given a kernel $K$, the output $Y = K \ast X$ can be reshaped through
vec$(Y) = Mvec(X),$
where $M$ is the linear transformation matrix.

When training the deep neural networks, gradient exploding and vanishing are fundamental obstacles. It’s helpful to make the largest singular value of $M$ be smaller for controlling exploding gradients and it’s helpful to make the smallest singular value of $M$ be larger for controlling vanishing gradients. In this paper we will give three regularization terms about convolutional kernel $K$ to change the singular values of $M$ and show how to carry out gradient type methods for them.

When we refer to convolution in deep learning, there is no flip operation and only element-wise multiplication and addition are performed. Besides, in the field of deep learning, depending on different strides and padding patterns, there are many different forms of convolution arithmetic[4]. Without losing generality, in this paper we will adopt the same convolution with unit strides. We use $\lceil \cdot \rceil$ to round a number to the nearest integer greater than or equal to that number. If a convolutional kernel is a matrix $K \in \mathbb{R}^{k \times k}$ and the input is a matrix $X \in \mathbb{R}^{N \times N}$, each entry of the output $Y \in \mathbb{R}^{N \times N}$ is produced by
$$Y_{r,s} = (K \ast X)_{r,s} = \sum_{p=1}^{k} \sum_{q=1}^{k} X_{r-m+p\cdot s-m+q} K_{p,q},$$
where $m = \lceil k/2 \rceil$, , and $X_{i,j} = 0$ if $i \leq 0$ or $i > N$, or $j \leq 0$ or $j > N$.

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In convolutional neural networks, usually there are multi-channels and a convolutional kernel is represented by a 4 dimensional tensor. If a convolutional kernel is a 4 dimensional tensor $K \in \mathbb{R}^{k \times k \times g \times h}$ and the input is 3 dimensional tensor $X \in \mathbb{R}^{N \times N \times g}$, each entry of the output $Y \in \mathbb{R}^{N \times N \times h}$ is produced by

$$Y_{r,s,c} = (K * X)_{r,s,c} = \sum_{d \in \{1, \ldots, g\}} \sum_{p \in \{1, \ldots, k\}} \sum_{q \in \{1, \ldots, k\}} X_{r+m+p, s+m+q, d} K_{p, q, d, c},$$

where $m = r/k$ and $X_{r,s,d} = 0$ if $i \leq 0$ or $i > N$, or $j \leq 0$ or $j > N$.

In the community of deep learning, there have been papers devoted to enforcing the orthogonality or spectral norm regularization on the weights of a neural network [1, 3, 12, 19]. The difference between our paper and papers including [1, 3, 12, 19] and the references therein is about how to handle convolutions. They enforce the constraint directly on the $h \times (gkk)$ matrix reshaped from the kernel $K \in \mathbb{R}^{k \times k \times g \times h}$, while we enforce the the constraint on the transformation matrix $M$ corresponding to the convolution kernel $K$. In [13], the authors project a convolutional layer onto the set of layers obeying a bound on the operator norm of the layer and use numerical results to show this is an effective regularizer. A drawback of the method in [13] is that projection can prevent the singular values of the transformation matrix being large but can’t avoid the singular values to be too small.

In [7, 8, 17], regularization methods are proposed to let the corresponding transformation matrices be orthogonal, where the approach is to minimize the norm of $M^T M - I$. In this paper we propose new regularization methods for the convolutional kernel tensor $K$, which can reduce the largest singular value and increase the smallest singular value of $M$ independently or simultaneously depending on the need in the training process.

The rest of the paper is organized as follows. As we have mentioned, the input channels and the output channels maybe more than one so the kernel is usually represented by a tensor $K \in \mathbb{R}^{k \times k \times g \times h}$. In Section 3 we propose the penalty functions and calculate the partial derivatives for the case that the kernel $K$ is a $k \times k$ matrix. In Section 4 we propose the penalty functions and calculate the partial derivatives for the case that $K$ is a $k \times k \times g \times h$ tensor. In Section 4 we present numerical results to show the method is feasible and effective. In Section 5 we will give some conclusions and discuss some work that may be done in the future.

## 2 penalty function for one-channel convolution

When the numbers of input channels and the output channels are both 1, the convolutional kernel are a $k \times k$ matrix. Assuming the data matrix is $N \times N$, we use a $3 \times 3$ matrix as a convolution kernel to show the associated structured transformation matrix. Let $K$ be the convolutional kernel,

$$K = \begin{pmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{pmatrix}. $$

Then the transformation matrix $M$ such that $\text{vec}(Y) = M\text{vec}(X)$ for $Y = K * X$ is

$$M = \begin{pmatrix} A_0 & A_{-1} & 0 & 0 & \cdots & 0 \\ A_1 & A_0 & A_{-1} & \ddots & \ddots & \vdots \\ 0 & A_1 & A_0 & \ddots & \ddots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & A_{-1} & A_0 & 0 \\ 0 & \cdots & 0 & 0 & A_1 & A_0 \end{pmatrix} \quad (2.1)$$
Theorem 2.1. Assume \( M \in \mathbb{R}^{n \times n} \) is the doubly block banded Toeplitz matrix corresponding to the one channel convolution kernel \( K \in \mathbb{R}^{k \times k} \). If \( \Omega \) is the set of all indexes \((i, j)\) such that \( m_{ij} = K_{p, q} \), we have

\[
\frac{1}{2} \frac{\partial \|M\|^2_F}{\partial K_{p, q}} = \sum_{(i, j) \in \Omega} \frac{\partial \|M\|^2_F}{\partial m_{ij}} = \sum_{(i, j) \in \Omega} m_{ij}.
\]

where

\[
A_0 = \begin{pmatrix}
  k_{22} & k_{32} & 0 & 0 & \cdots & 0 \\
  k_{12} & k_{22} & k_{32} & \ddots & \ddots & \vdots \\
  0 & k_{12} & k_{22} & \ddots & \ddots & 0 \\
  0 & \ddots & \ddots & \ddots & \ddots & k_{32} \\
  \vdots & \ddots & \ddots & \ddots & \ddots & k_{12} \\
  0 & \cdots & 0 & k_{12} & k_{22}
\end{pmatrix}, \quad A_1 = \begin{pmatrix}
  k_{23} & k_{33} & 0 & 0 & \cdots & 0 \\
  k_{13} & k_{23} & k_{33} & \ddots & \ddots & \vdots \\
  0 & k_{13} & k_{23} & \ddots & \ddots & 0 \\
  0 & \ddots & \ddots & \ddots & \ddots & k_{33} \\
  \vdots & \ddots & \ddots & \ddots & \ddots & k_{13} \\
  0 & \cdots & 0 & k_{13} & k_{23}
\end{pmatrix},
\]

In this case, the transformation matrix \( M \) corresponding to the convolutional kernel \( K \) is a \( N^2 \times N^2 \) doubly block banded Toeplitz matrix, i.e., a block banded Toeplitz matrix with its blocks are banded Toeplitz matrices. For the details about Toeplitz matrices, please see references [2][10]. We will let \( n = N^2 \) and use \( \mathcal{T} \) to denote the set of all matrices like \( M \) in (2.1), i.e., doubly banded Toeplitz matrices with the fixed bandh.

For a matrix \( M \in \mathcal{T} \), The value of \( K_{p, q} \) will appear in different \((i, j)\) indexes. We use \( \Omega \) to denote this index set, to which each \((i, j)\) index corresponding to \( K_{p, q} \) belongs. That is to say, we have \( m_{ij} = K_{p, q} \) for each \((i, j) \in \Omega \) and \( m_{ij} \neq K_{p, q} \) for each \((i, j) \) that doesn’t satisfy \((i, j) \in \Omega \).

### 2.1 Regularization 1 to let the Frobenius norm of \( M \) be smaller

We will use \( \frac{1}{2} \|M\|^2_F \) as the penalty function to regularize the convolutional kernel \( K \), and calculate \( \partial \frac{1}{2} \|M\|^2_F / \partial K_{p, q} \).

The following lemma is easy but useful in the following derivation.

**Lemma 2.1.** The partial derivative of square of Frobenius norm of \( A \in \mathbb{R}^{n \times n} \) with respect to each entry \( a_{ij} \) is \( \partial \|A\|^2_F / \partial a_{ij} = 2a_{ij} \).

For a matrix \( M \in \mathcal{T} \), The value of \( K_{p, q} \) will appear in different \((i, j)\) indexes. We use \( \Omega \) to denote this index set, to which each \((i, j)\) index corresponding to \( K_{p, q} \) belongs. That is to say, we have \( m_{ij} = K_{p, q} \) for each \((i, j) \in \Omega \) and \( m_{ij} \neq K_{p, q} \) for each \((i, j) \) that doesn’t satisfy \((i, j) \in \Omega \). The chain rule formula about the derivative tells us that, if we want to calculate \( \partial \|M\|^2_F / \partial K_{p, q} \), we should calculate \( \partial \|M\|^2_F / \partial m_{ij} \) for all \((i, j) \in \Omega \) and take the sum, i.e.,

\[
\frac{1}{2} \frac{\partial \|M\|^2_F}{\partial K_{p, q}} = \frac{1}{2} \sum_{(i, j) \in \Omega} \frac{\partial \|M\|^2_F}{\partial m_{ij}} = \sum_{(i, j) \in \Omega} m_{ij}.
\]

We summarize the above results as the following theorem.

**Theorem 2.1.** Assume \( M \in \mathbb{R}^{n \times n} \) is the doubly block banded Toeplitz matrix corresponding to the one channel convolution kernel \( K \in \mathbb{R}^{k \times k} \). If \( \Omega \) is the set of all indexes \((i, j)\) such that \( m_{ij} = K_{p, q} \), we have

\[
\frac{1}{2} \frac{\partial \|M\|^2_F}{\partial K_{p, q}} = \sum_{(i, j) \in \Omega} m_{ij}.
\]
In this section we consider the case of multi-channel convolution. First we show the transformation matrix corresponding to multi-channel convolution. At each convolutional layer, we have convolution kernel $R$ and column $j$.

2.2 Regularization 2 to let the smallest singular value of $M$ be larger

To compute the gradient, we need the following classical result on the first order perturbation expansion about a simple singular value; see [14].

Lemma 2.2. Let $\sigma$ be a simple singular value of $A = [a_{ij}] \in \mathbb{R}^{m \times m}$ ($n \geq p$) with normalized left and right singular vectors $u$ and $v$. Then $\partial \sigma / \partial a_{ij}$ is $u(i)v(j)$, where $u(i)$ is the $i$-th entry of vector $u$ and $v(j)$ is the $j$-th entry of vector $v$.

We use the chain rule to get the following theorem.

Theorem 2.2. Assume the smallest singular value of $M$, which is denoted by $\sigma_{\min}(M)$, is simple and positive, where $M \in \mathbb{R}^{n \times n}$ is the doubly block banded Toeplitz matrix corresponding to the one channel convolution kernel $K \in \mathbb{R}^{k \times k}$. Assume $u$ and $v$ are normalized left and right singular vectors of $M$ associated with $\sigma_{\min}(M)$. If $\Omega$ is the set of all indexes $(i, j)$ such that $m_{ij} = K(c, d)$, we have

$$\partial \sigma_{\min}(M) / \partial K(c, d) = \sum_{(i,j) \in \Omega} u(i)v(j).$$

We can use the formula (2.3) to carry out the gradient type methods to let the smallest singular value of $M$ be larger.

2.3 Regularization 3 to let the singular values of $M$ be neither large nor small

We can combine Theorem 2.1 and Theorem 2.2 to let the singular values of $M$ be neither large nor small. As we know, $\|M\|^2_F$ is the squares sum of all singular values of $M$. If $M$ is $n \times n$, $\|M\|^2_F$ is the squares sum of $n$ singular values. We may choose $\neg n \sigma_{\min}(M) + \frac{1}{2} \|M\|^2_F$ as the regularization term to let the singular values of $M$ be neither large nor small. Thus we have the following theorem.

Theorem 2.3. Assume the smallest singular value of $M$, which is denoted by $\sigma_{\min}(M)$, is simple and positive, where $M \in \mathbb{R}^{n \times n}$ is the doubly block banded Toeplitz matrix corresponding to the one channel convolution kernel $K \in \mathbb{R}^{k \times k}$. Assume $u$ and $v$ are normalized left and right singular vectors of $M$ associated with $\sigma_{\min}(M)$. If $\Omega$ is the set of all indexes $(i, j)$ such that $m_{ij} = K(c, d)$, we have

$$\partial (\frac{1}{2} \|M\|^2_F - n \sigma_{\min}(M)) / \partial K(c, d) = \sum_{(i,j) \in \Omega} (m_{ij} - nu(i)v(j)).$$

3 The penalty function and the gradient for multi-channel convolution

In this section we consider the case of multi-channel convolution. First we show the transformation matrix corresponding to multi-channel convolution. At each convolutional layer, we have convolution kernel $K \in \mathbb{R}^{k \times k \times k \times h}$ and the input $X \in \mathbb{R}^{N \times N \times G}$; element $X_{r,s,d}$ is the value of the input unit within channel $d$ at row $i$ and column $j$. Each entry of the output $Y \in \mathbb{R}^{N \times N \times h}$ is produced by

$$Y_{r,s,e} = (K \ast X)_{r,s,e} = \sum_{d \in \{1, \ldots, G\}} \sum_{p \in \{1, \ldots, k\}} \sum_{q \in \{1, \ldots, k\}} X_{r-m+p,s-m+q,d}K_{p,q,d,e}$$
where $X_{i,j,d} = 0$ if $i \leq 0$ or $i > N$, or $j \leq 0$ or $j > N$. By inspection, $vec(Y) = Mvec(X)$, where $M$ is as follows

$$M = \begin{pmatrix}
M_{(1)(1)} & M_{(1)(2)} & \cdots & M_{(1)(g)} \\
M_{(2)(1)} & M_{(2)(2)} & \cdots & M_{(2)(g)} \\
\vdots & \vdots & \ddots & \vdots \\
M_{(b)(1)} & M_{(b)(2)} & \cdots & M_{(b)(g)}
\end{pmatrix},$$

(3.1)

and each $M_{c(d)} \in \mathcal{T}$, i.e., $M_{c(d)}$ is a $N^2 \times N^2$ doubly block banded Toeplitz matrix corresponding to the portion $K_{c:d,e}$ of $K$ that concerns the effect of the $d$-th input channel on the $c$-th output channel.

Similar as the proof in Section 2 we have the following theorem.

**Theorem 3.1.** Assume $M$ is the structured matrix corresponding to the multi-channel convolution kernel $K \in \mathbb{R}^{k \times k \times g \times h}$ as defined in (3.1). Given $(p,q,z,y)$, if $\Omega_{p,q,z,y}$ is the set of all indexes $(i,j)$ such that $m_{ij} = k_{p,q,z,y}$, we have

$$\frac{1}{2} \frac{\partial \|M\|^2_F}{\partial K_{p,q,z,y}} = \sum_{(i,j) \in \Omega_{p,q,z,y}} m_{ij}. \tag{3.2}$$

Then the gradient descent algorithm for the penalty function $\|M\|^2_F$ can be devised, where the number of channels maybe more than one.

**Theorem 3.2.** Assume $M$ is the structured matrix corresponding to the multi-channel convolution kernel $K \in \mathbb{R}^{k \times k \times g \times h}$ as defined in (3.1). Given $(p,q,z,y)$, if $\Omega_{p,q,z,y}$ is the set of all indexes $(i,j)$ such that $m_{ij} = k_{p,q,z,y}$, we have

$$\frac{\partial \sigma_{\min}(M)}{\partial K_{p,q,z,y}} = \sum_{(i,j) \in \Omega_{p,q,z,y}} u(i)v(j). \tag{3.3}$$

We present the detailed gradient descent algorithm for the three different penalty functions, where in Algorithm 3 min$(g,h)$ denotes the smaller one of $g$ and $h$.

**Algorithm 3.1.** Gradient Descent for $\mathcal{R}_{\alpha}(K) = \frac{1}{2} \|M\|^2_F$
1. Input: an initial kernel $K \in \mathbb{R}^{k \times k \times g \times h}$, input size $N \times N \times g$ and learning rate $\lambda$.
2. While not converged:
   3. Compute $G = \frac{1}{2} \frac{\|M\|^2}{\partial K_{p,q,z,y}} = \sum_{p,q,z,y=1}^{1} \sigma_{\min}(M)_{k,k,g,h}$, by (3.2);
4. Update $K = K - \lambda G$;
5. End

**Algorithm 3.2.** Gradient Descent for $\mathcal{R}_{\alpha}(K) = -\sigma_{\min}(M)$
1. Input: an initial kernel $K \in \mathbb{R}^{k \times k \times g \times h}$, input size $N \times N \times g$ and learning rate $\lambda$.
2. While not converged:
   3. Compute $G = \frac{\sigma_{\min}(M)}{\partial K_{p,q,z,y}} = \sum_{p,q,z,y=1}^{1} \sigma_{\min}(M)_{k,k,g,h}$, by (3.3);
4. Update $K = K - \lambda G$;
5. End

**Algorithm 3.3.** Gradient Descent for $\mathcal{R}_{\alpha}(K) = \frac{1}{2} \|M\|^2_F - \min(g,h)N^2\sigma_{\min}(M)$
1. Input: an initial kernel $K \in \mathbb{R}^{k \times k \times g \times h}$, input size $N \times N \times g$ and learning rate $\lambda$.
2. While not converged:
   3. Compute $G = \frac{1}{2} \frac{\|M\|^2}{\partial K_{p,q,z,y}} = \sum_{p,q,z,y=1}^{1} \sigma_{\min}(M)_{k,k,g,h}$, by (3.2) and (3.3);
4. Update $K = K - \lambda G$;
5. End
4 Numerical experiments

The numerical tests were performed on a laptop (3.0 Ghz and 16G Memory) with MATLAB R2016b. We use $M$ to denote the transformation matrix corresponding to the convolutional kernel. The largest singular value and smallest singular value of $M$ (denoted as $\sigma_{\text{max}}(M)$ and $\sigma_{\text{min}}(M)$), the iteration steps (denoted as “iter”) are demonstrated to show the effectiveness of our method. Numerical experiments are implemented on extensive test problems. In this paper we present the numerical results for some random generated multi-channel convolution kernels, where $K$ is generated by the following command

```matlab
rand('state',1);
K = rand(k,k,g,h);
```

We consider kernels of different sizes with $3 \times 3$ filters, namely $K \in \mathbb{R}^{3 \times 3 \times g \times h}$ for various values of $g,h$. For each kernel, we use $20 \times 20 \times g$ as the size of input data matrix. We then minimize the three different penalty functions using Algorithms 3.1, 3.2 and 3.3 respectively. We show the effects of changing the singular values of $M$. We present in Figures the results for $3 \times 3 \times 3 \times 1$ and $3 \times 3 \times 1 \times 3$ kernels. In the figures 4.1 and 4.3 we show the convergence of $\sigma_{\text{max}}(M)$ on the left axis scale and $\sigma_{\text{min}}(M)$ on the right axis scale.

![Figure 4.1: Changes of $\sigma_{\text{max}}(M)$ and $\sigma_{\text{min}}(M)$ for different kernel sizes](image)

Numerical experiments are done on other random generated examples, including random kernels with each entry uniformly distributed on $[0,1]$. The convergence figures of $\sigma_{\text{max}}(M)$ and $\sigma_{\text{min}}(M)$ are similar with the subfigures presented in the paper.

The efficiency of each method, i.e., the needed iteration steps to let $\sigma_{\text{max}}(M)$ and $\sigma_{\text{min}}(M)$ be bounded in a satisfying interval, is related with the step size $\lambda$. In our numerical experiments, for Algorithms 3.1 and 3.3 we use the step size $\lambda = 1e^{-5}$ while for Algorithms 3.2 we use the step size $\lambda = 1e^{-4}$. We can’t definitely tell how to choose the optimal step size currently.

5 Conclusions

In this paper, we provide a new regularization method to regularize the weights of convolutional layers in deep neural networks. We give new regularization terms about convolutional kernels to change the singular values of the corresponding structured transformation matrices. We propose gradient decent algorithms for the regularization terms. This method is shown to be effective.
In future, we will continue to devise other forms of penalty functions for convolutional kernels to constrain the singular values of corresponding transformation matrices.

6 Acknowledgements

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Figure 4.3: Changes of $\sigma_{\text{max}}(M)$ and $\sigma_{\text{min}}(M)$ for different kernel sizes

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