Newton Methods for Convolutional Neural Networks

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Abstract

Deep learning involves a difficult non-convex optimization problem, which is often solved by stochastic gradient (SG) methods. While SG is usually effective, it may not be robust in some situations. Recently, Newton methods have been investigated as an alternative optimization technique, but nearly all existing studies consider only fully-connected feedforward neural networks. They do not investigate other types of networks such as Convolutional Neural Networks (CNN), which are more commonly used in deep-learning applications. One reason is that Newton methods for CNN involve complicated operations, and so far no works have conducted a thorough investigation. In this work, we give details of all building blocks including function, gradient, and Jacobian evaluation, and Gauss-Newton matrix-vector products. These basic components are very important because with them further developments of Newton methods for CNN become possible. We show that an efficient *MATLAB* implementation can be done in just several hundred lines of code and demonstrate that the Newton method gives competitive test accuracy.

Keywords: Convolution Neural Networks, Newton methods, Large-scale classification, Subsampled Hessian.

1 Introduction

Deep learning is now widely used in many applications. To apply this technique, a difficult non-convex optimization problem must be solved. Currently, stochastic gradient (SG) methods and their variants are the major optimization technique used for deep learning (e.g., Krizhevsky et al., 2012; Simonyan and Zisserman, 2014). This situation is different from some application domains, where other types of optimization methods are more frequently used. One interesting research question is thus to study if other optimization methods can be extended to be viable alternatives for deep learning. In this work, we aim to address this issue by developing a practical Newton method for deep learning.

Some past works have studied Newton methods for training deep neural networks (e.g., Martens 2010; Vinyals and Povey 2012; Kiros 2013; Wang et al. 2015, 2018; He et al. 2016; Botev et al. 2017). Almost all of them consider fully-connected feedforward neural networks and some have shown the potential of Newton methods for being more robust than SG. Unfortunately, these works have not fully established Newton methods as a practical technique for deep learning because other types of networks such as Convolutional Neural Networks (CNN) are more commonly used in deep-learning applications. One important reason why CNN was not considered is because of the very complicated operations in implementing Newton methods. Up to now no works have shown details of all the building blocks such as function, gradient, and Jacobian evaluation, and Hessian-vector products. In particular, because interpreter-type languages such as *Python* or *MATLAB* have been popular for deep learning, how to easily implement efficient operations by these languages is an important research issue. In this work, we aim at a thorough investigation on the implementation of Newton methods for CNN. We focus on basic components because without them none of any recent improvement of Newton methods for fully-connected networks can be even tried. Our work will enable many further developments of Newton methods for CNN and maybe even other types of networks.

This paper is organized as follows. In Section 2, we introduce CNN. In Section 3, Newton methods for CNN are investigated and the detailed mathematical formulations of all operations are derived. In Section 4, we provide details for an efficient *MATLAB* implementation. The analysis of memory usage and computational complexity is in Section 5. Preliminary experiments to demonstrate the viability of Newton methods for CNN are in Section 6. Section 7 concludes this work. A list of symbols is in the appendix.

A simple and efficient *MATLAB* implementation in just a few hundred lines of code is available at

Programs used for experiments in this paper and supplementary materials can be found at the same page.

2 Optimization Problem of Convolutional Neural Networks

Consider a K-class problem, where the training data set consists of l input pairs $(Z^{1,i}, y^i)$, i = 1, ..., l. Here $Z^{1,i}$ is the *i*th input image with dimension $a^1 \times b^1 \times d^1$, where

 a^1 denotes the height of the input images, b^1 represents the width of the input images and d^1 is the number of color channels. If $Z^{1,i}$ belongs to the kth class, then the label vector is

$$\boldsymbol{y}^{i} = [\underbrace{0, \dots, 0}_{k-1}, 1, 0, \dots, 0]^{T} \in R^{K}.$$

A CNN (LeCun et al., 1989) utilizes a stack of convolutional layers followed by fully-connected layers to predict the target vector. Let L^c be the number of convolutional layers, and L^f be the number of fully-connected layers. The number of layers is

$$L = L^c + L^f.$$

Images

$$Z^{1,i}, i=1,\ldots,l$$

are input to the first layer, while the last (the Lth) layer outputs a predicted label vector

$$\hat{\boldsymbol{y}}^i, \ i=1,\ldots,l.$$

A hallmark of CNN is that both input and output of convolutional layers are explicitly assumed to be images.

2.1 Convolutional Layer

In a convolutional layer, besides the main convolutional operations, two optional steps are padding and pooling, each of which can also be considered as a layer with input/output images. To easily describe all these operations in a unified setting, for the *i*th instance, we assume the input image of the current layer is

$$Z^{\mathrm{in},i}$$

containing d^{in} channels of $a^{\text{in}} \times b^{\text{in}}$ images:

$$\begin{bmatrix} z_{1,1,1}^{i} & z_{1,b^{\text{in}},1}^{i} \\ & \ddots & \\ z_{a^{\text{in}},1,1}^{i} & z_{a^{\text{in}},b^{\text{in}},1}^{i} \end{bmatrix} \dots \begin{bmatrix} z_{1,1,d^{\text{in}}}^{i} & z_{1,b^{\text{in}},d^{\text{in}}}^{i} \\ & \ddots & \\ z_{a^{\text{in}},1,d^{\text{in}}}^{i} & z_{a^{\text{in}},b^{\text{in}},d^{\text{in}}}^{i} \end{bmatrix}.$$
 (1)

The goal is to generate an output image

$$Z^{\mathrm{out},i}$$

of d^{out} channels of $a^{\text{out}} \times b^{\text{out}}$ images.

Now we describe details of convolutional operations. To generate the output, we consider d^{out} filters, each of which is a 3-D weight matrix of size

$$h \times h \times d^{\text{in}}.$$

Specifically, the *j*th filter includes the following matrices

$$\begin{bmatrix} w_{1,1,1}^{j} & w_{1,h,1}^{j} \\ & \ddots & \\ & & \\ w_{h,1,1}^{j} & w_{h,h,1}^{j} \end{bmatrix}, \quad \dots \quad , \begin{bmatrix} w_{1,1,d^{\text{in}}}^{j} & w_{1,h,d^{\text{in}}}^{j} \\ & \ddots & \\ & \\ & &$$

and a bias term b_j .

The main idea of CNN is to extract local information by convolutional operations, each of which is the inner product between a small sub-image and a filter. For the *j*th filter, we scan the entire input image to obtain small regions of size (h, h) and calculate the inner product between each region and the filter. For example, if we start from the upper left corner of the input image, the first sub-image of channel *d* is

$$\begin{bmatrix} z_{1,1,d}^{i} & \dots & z_{1,h,d}^{i} \\ & \ddots & \\ z_{h,1,d}^{i} & \dots & z_{h,h,d}^{i} \end{bmatrix}.$$

We then calculate the following value.

$$\sum_{d=1}^{d^{\text{in}}} \left\langle \begin{bmatrix} z_{1,1,d}^{i} & \dots & z_{1,h,d}^{i} \\ & \ddots & \\ z_{h,1,d}^{i} & \dots & z_{h,h,d}^{i} \end{bmatrix}, \begin{bmatrix} w_{1,1,d}^{j} & \dots & w_{1,h,d}^{j} \\ & \ddots & \\ w_{h,1,d}^{j} & \dots & w_{h,h,d}^{j} \end{bmatrix} \right\rangle + b_{j},$$
(2)

where $\langle \cdot, \cdot \rangle$ means the sum of component-wise products between two matrices. This value becomes the (1, 1) position of the channel j of the output image.

Next, we must obtain other sub-images to produce values in other positions of the output image. We specify the stride s for sliding the filter. That is, we move s pixels vertically or horizontally to get sub-images. For the (2, 1) position of the output image, we move down s pixels vertically to obtain the following sub-image:

$$\begin{bmatrix} z_{1+s,1,d}^{i} & \dots & z_{1+s,h,d}^{i} \\ & \ddots & \\ z_{h+s,1,d}^{i} & \dots & z_{h+s,h,d}^{i} \end{bmatrix}.$$

Then the (2,1) position of the channel j of the output image is

$$\sum_{d=1}^{d^{\text{in}}} \left\langle \begin{bmatrix} z_{1+s,1,d}^{i} & \dots & z_{1+s,h,d}^{i} \\ & \ddots & \\ z_{h+s,1,d}^{i} & \dots & z_{h+s,h,d}^{i} \end{bmatrix}, \begin{bmatrix} w_{1,1,d}^{j} & \dots & w_{1,h,d}^{j} \\ & \ddots & \\ & &$$

Assume that vertically and horizontally we can move the filter a^{out} and b^{out} times, respectively. Therefore,

$$a^{\text{out}} = \lfloor \frac{a^{\text{in}} - h}{s} \rfloor + 1,$$

$$b^{\text{out}} = \lfloor \frac{b^{\text{in}} - h}{s} \rfloor + 1.$$
 (4)

For efficient implementations, we can conduct all operations including (2) and (3) by matrix operations. To begin, we concatenate the matrices of the different channels

in (1) to

$$Z^{\text{in},i} = \begin{bmatrix} z_{1,1,1}^{i} & \dots & z_{a^{\text{in}},1,1}^{i} & z_{1,2,1}^{i} & \dots & z_{a^{\text{in}},b^{\text{in}},1}^{i} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ z_{1,1,d^{\text{in}}}^{i} & \dots & z_{a^{\text{in}},1,d^{\text{in}}}^{i} & z_{1,2,d^{\text{in}}}^{i} & \dots & z_{a^{\text{in}},b^{\text{in}},d^{\text{in}}}^{i} \end{bmatrix}, \ i = 1,\dots,l.$$
(5)

We note that (2) is the inner product between the following two vectors

$$\begin{bmatrix} w_{1,1,1}^j & \dots & w_{h,1,1}^j & w_{1,2,1}^j & \dots & w_{h,h,1}^j & \dots & w_{h,h,d^{\text{in}}}^j & b_j \end{bmatrix}^T$$

and

$$\left[z_{1,1,1}^{i} \quad \dots \quad z_{h,1,1}^{i} \quad z_{1,2,1}^{i} \quad \dots \quad z_{h,h,1}^{i} \quad \dots \quad z_{h,h,d^{\mathrm{in}}}^{i} \quad 1\right]^{T} \cdot$$

Based on Vedaldi and Lenc (2015), we define the following two operators

$$\operatorname{vec}(M) = \begin{bmatrix} M_{:,1} \\ \vdots \\ M_{:,b} \end{bmatrix} \in R^{ab \times 1}, \text{ where } M \in R^{a \times b},$$

$$\operatorname{mat}(\boldsymbol{v})_{a \times b} = \begin{bmatrix} v_1 & v_{(b-1)a+1} \\ \vdots & \cdots & \vdots \\ v_a & v_{ba} \end{bmatrix} \in R^{a \times b}, \text{ where } \boldsymbol{v} \in R^{ab \times 1}.$$

$$(6)$$

There exists a 0/1 matrix

$$P_{\phi} \in R^{hhd^{\text{in}}a^{\text{out}}b^{\text{out}} \times d^{\text{in}}a^{\text{in}}b^{\text{in}}}$$

so that an operator

$$\phi: R^{d^{\mathrm{in}} \times a^{\mathrm{in}} b^{\mathrm{in}}} \to R^{hhd^{\mathrm{in}} \times a^{\mathrm{out}} b^{\mathrm{out}}}$$

defined as

$$\phi(Z^{\mathrm{in},i}) \equiv \mathrm{mat}\left(P_{\phi}\mathrm{vec}(Z^{\mathrm{in},i})\right)_{hhd^{\mathrm{in}} \times a^{\mathrm{out}}b^{\mathrm{out}}}, \ \forall i,$$
(8)

collects all sub-images in $Z^{\mathrm{in},i}.$ Specifically, $\phi(Z^{\mathrm{in},i})$ is

$$\begin{bmatrix} z_{1,1,1}^{i} & \cdots & z_{1+(a^{\text{out}}-1)\times s,1,1}^{i} & z_{1,1+s,1}^{i} & \cdots & z_{1+(a^{\text{out}}-1)\times s,1+(b^{\text{out}}-1)\times s,1}^{i} \\ z_{2,1,1}^{i} & \cdots & z_{2+(a^{\text{out}}-1)\times s,1,1}^{i} & z_{2,1+s,1}^{i} & \cdots & z_{2+(a^{\text{out}}-1)\times s,1+(b^{\text{out}}-1)\times s,1}^{i} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ z_{h,h,1}^{i} & \cdots & z_{h+(a^{\text{out}}-1)\times s,h,1}^{i} & z_{h,h+s,1}^{i} & \cdots & z_{h+(a^{\text{out}}-1)\times s,h+(b^{\text{out}}-1)\times s,1}^{i} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ z_{1,1,d^{\text{in}}}^{i} & \cdots & z_{1+(a^{\text{out}}-1)\times s,1,d^{\text{in}}}^{i} & z_{1,1+s,d^{\text{in}}}^{i} & \cdots & z_{1+(a^{\text{out}}-1)\times s,1+(b^{\text{out}}-1)\times s,d^{\text{in}}}^{i} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ z_{h,h,d^{\text{in}}}^{i} & \cdots & z_{h+(a^{\text{out}}-1)\times s,h,d^{\text{in}}}^{i} & z_{h,h+s,d^{\text{in}}}^{i} & \cdots & z_{h+(a^{\text{out}}-1)\times s,h+(b^{\text{out}}-1)\times s,d^{\text{in}}}^{i} \end{bmatrix}.$$

By considering

$$W = \begin{bmatrix} w_{1,1,1}^{1} & w_{2,1,1}^{1} & \dots & w_{h,h,d^{\text{in}}}^{1} \\ \vdots & \vdots & \ddots & \vdots \\ w_{1,1,1}^{d^{\text{out}}} & w_{2,1,1}^{d^{\text{out}}} & \dots & w_{h,h,d^{\text{in}}}^{d^{\text{out}}} \end{bmatrix} \in R^{d^{\text{out}} \times hhd^{\text{in}}} \text{ and } \boldsymbol{b} = \begin{bmatrix} b_{1} \\ \vdots \\ b_{d^{\text{out}}} \end{bmatrix} \in R^{d^{\text{out}} \times 1}, \quad (10)$$

all convolutional operations can be combined as

$$S^{\text{out},i} = W\phi(Z^{\text{in},i}) + \boldsymbol{b}\mathbb{1}_{a^{\text{out}}b^{\text{out}}}^T \in R^{d^{\text{out}} \times a^{\text{out}}b^{\text{out}}},$$
(11)

where

$$S^{\text{out},i} = \begin{bmatrix} s_{1,1,1}^{i} & \dots & s_{a^{\text{out}},1,1}^{i} & s_{1,2,1}^{i} & \dots & s_{a^{\text{out}},b^{\text{out}},1}^{i} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ s_{1,1,d^{\text{out}}}^{i} & \dots & s_{a^{\text{out}},1,d^{\text{out}}}^{i} & s_{1,2,d^{\text{out}}}^{i} & \dots & s_{a^{\text{out}},b^{\text{out}},d^{\text{out}}}^{i} \end{bmatrix}$$

and

$$\mathbb{1}_{a^{\text{out}b^{\text{out}}}} = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} \in R^{a^{\text{out}b^{\text{out}} \times 1}}.$$

Next, an activation function scales each element of $S^{\text{out},i}$ to obtain the output matrix $Z^{\text{out},i}$.

$$Z^{\operatorname{out},i} = \sigma(S^{\operatorname{out},i}) \in R^{d^{\operatorname{out}} \times a^{\operatorname{out}} b^{\operatorname{out}}}.$$
(12)

For CNN, commonly the following RELU activation function

$$\sigma(x) = \max(x, 0) \tag{13}$$

is used and we consider it in our implementation.¹

Note that by the matrix representation, the storage is increased from

$$d^{\rm in} \times a^{\rm in} b^{\rm in}$$

in (1) to

$$(hhd^{\rm in}) \times a^{\rm out}b^{\rm out}$$

in (9). From (4), roughly

$$\left(\frac{h}{s}\right)^2$$

folds increase of the memory occurs. However, we gain efficiency by using fast matrixmatrix multiplications in optimized BLAS (Dongarra et al., 1990).

2.1.1 Zero-padding

To better control the size of the output image, before the convolutional operation we may enlarge the input image to have zero values around the border. This technique is called zero-padding in CNN training. See an illustration in Figure 1.

¹To use Newton methods, $\sigma(x)$ should be twice differentiable, but the RELU function is not. For simplicity, we follow Krizhevsky et al. (2012) to assume $\sigma'(x) = 1$ if x > 0 and 0 otherwise. It is possible to use a differentiable approximation of the RELU function, though we leave this issue for future investigation.

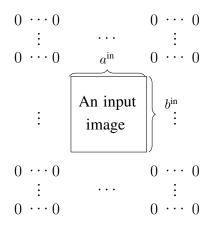


Figure 1: An illustration of the padding operation to have zeros around the border.

To specify the mathematical operation we can treat the padding operation as a layer of mapping an input $Z^{\text{in},i}$ to an output $Z^{\text{out},i}$. Let

$$d^{\rm out} = d^{\rm in}$$

There exists a 0/1 matrix

$$P_{\text{pad}} \in R^{d^{\text{out}}a^{\text{out}}b^{\text{out}} \times d^{\text{in}}a^{\text{in}}b^{\text{in}}}$$

so that the padding operation can be represented by

$$Z^{\text{out},i} \equiv \max(P_{\text{pad}} \text{vec}(Z^{\text{in},i}))_{d^{\text{out}} \times a^{\text{out}}b^{\text{out}}}.$$
(14)

2.1.2 Pooling Operations

For CNN, to reduce the computational cost, a dimension reduction is often applied by a pooling step after convolutional operations. Usually we consider an operation that can (approximately) extract rotational or translational invariance features. Among the various types of pooling methods such as average pooling, max pooling, and stochastic pooling, we consider max pooling as an illustration because it is the most used setting

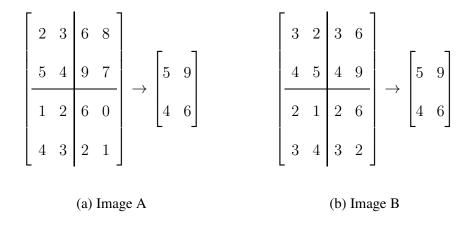


Figure 2: An illustration of max pooling to extract translational invariance features. The image B is derived from shifting A by 1 pixel in the horizontal direction.

for CNN. We show an example of max pooling by considering two 4×4 images, A and B, in Figure 2. The image B is derived by shifting A by 1 pixel in the horizontal direction. We split two images into four 2×2 sub-images and choose the max value from every sub-image. In each sub-image because only some elements are changed, the maximal value is likely the same or similar. This is called translational invariance and for our example the two output images from A and B are the same.

Now we derive the mathematical representation. Similar to Section 2.1.1, we consider the operation as a separate layer for the easy description though in our implementation pooling is just an operation at the end of the convolutional layer. Assume $Z^{\text{in},i}$ is an input image. We partition every channel of $Z^{\text{in},i}$ into non-overlapping sub-regions by $h \times h$ filters with the stride s = h.² This partition step is a special case of how we generate sub-images in convolutional operations. Therefore, by the same definition as

²Because of the disjoint sub-regions, the stride s for sliding the filters is equal to h.

(8) we can generate the matrix

$$\phi(Z^{\text{in},i}) = \max(P_{\phi} \operatorname{vec}(Z^{\text{in},i}))_{hh \times d^{\text{out}}a^{\text{out}}b^{\text{out}}},$$
(15)

where

$$a^{\text{out}} = \lfloor \frac{a^{\text{in}}}{h} \rfloor, \ b^{\text{out}} = \lfloor \frac{b^{\text{in}}}{h} \rfloor, \ d^{\text{out}} = d^{\text{in}}.$$
 (16)

To select the largest element of each sub-region, there exists a matrix

$$W^i \in R^{d^{\mathrm{out}}a^{\mathrm{out}}b^{\mathrm{out}} \times hhd^{\mathrm{out}}a^{\mathrm{out}}b^{\mathrm{out}}}$$

so that each row of W^i selects a single element from $vec(\phi(Z^{in,i}))$. Therefore,

$$Z^{\operatorname{out},i} = \operatorname{mat} \left(W^{i} \operatorname{vec}(\phi(Z^{\operatorname{in},i})) \right)_{d^{\operatorname{out}} \times a^{\operatorname{out}} b^{\operatorname{out}}}.$$
(17)

Note that different from (11) of the convolutional layer, W^i is a constant matrix rather than a weight matrix.

By combining (15) and (17), we have

$$Z^{\text{out},i} = \max\left(P^i_{\text{pool}} \text{vec}(Z^{\text{in},i})\right)_{d^{\text{out}} \times a^{\text{out}}b^{\text{out}}},$$
(18)

where

$$P_{\text{pool}}^{i} = W^{i} P_{\phi} \in R^{d^{\text{out}} a^{\text{out}} b^{\text{out}} \times d^{\text{in}} a^{\text{in}} b^{\text{in}}}.$$
(19)

2.1.3 Summary of a Convolutional Layer

For the practical implementation, we find it is more suitable to consider padding and pooling as part of the convolutional layers. Here we discuss details of considering all operations together. The whole convolutional layer involves the following procedure:

 $Z^{m,i} \rightarrow$ padding by (14) \rightarrow convolutional operations by (11), (12)

Table 1: Detailed information of operations at a convolutional layer.

Operation	$a^{\mathrm{in}},\ b^{\mathrm{in}},\ d^{\mathrm{in}}$	$a^{\text{out}}, b^{\text{out}}, d^{\text{out}}$	Input	Output
Padding: (14)	a^m, b^m, d^m	$a^m_{\mathrm{pad}},\ b^m_{\mathrm{pad}},\ d^m$	$Z^{m,i}$	$\operatorname{pad}(Z^{m,i})$
Convolution: (11)	$a^m_{\mathrm{pad}},\ b^m_{\mathrm{pad}},\ d^m$	$a^m_{\mathrm{conv}},\ b^m_{\mathrm{conv}},\ d^{m+1}$	$\operatorname{pad}(Z^{m,i})$	$S^{m,i}$
Convolution: (12)	$a^m_{\mathrm{conv}},\ b^m_{\mathrm{conv}},\ d^{m+1}$	$a^m_{\mathrm{conv}},\ b^m_{\mathrm{conv}},\ d^{m+1}$	$S^{m,i}$	$\sigma(S^{m,i})$
Pooling: (18)	$a^m_{\mathrm{conv}},\ b^m_{\mathrm{conv}},\ d^{m+1}$	$a^{m+1}, b^{m+1}, d^{m+1}$	$\sigma(S^{m,i})$	$Z^{m+1,i}$

$$\rightarrow$$
 pooling by (18) $\rightarrow Z^{m+1,i}$, (20)

where $Z^{m,i}$ and $Z^{m+1,i}$ are input and output of the *m*th layer, respectively.

We use the following symbols to denote image sizes at different stages of the convolutional layer.

$$a^m$$
, b^m : size in the beginning
 a^m_{pad} , b^m_{pad} : size after padding
 a^m_{conv} , b^m_{conv} : size after convolution.

Table 1 indicates how these values are a^{in} , b^{in} , d^{in} and a^{out} , b^{out} , d^{out} at different stages. We further denote the filter size, mapping matrices and weight matrices at the *m*th layer as

$$h^m$$
, P^m_{pad} , P^m_{ϕ} , $P^{m,i}_{\text{pool}}$, W^m , \boldsymbol{b}^m

Then from (14), (11), (12), (18), and Table 1, all operations can be summarized as

$$Z^{m+1,i} = \max(P^{m,i}_{\text{pool}} \text{vec}(\sigma(S^{m,i})))_{d^{m+1} \times a^{m+1}b^{m+1}},$$
(21)

where

$$S^{m,i} = W^m \operatorname{mat}(P^m_{\phi} P^m_{\operatorname{pad}} \operatorname{vec}(Z^{m,i}))_{h^m h^m d^m \times a^m_{\operatorname{conv}} b^m_{\operatorname{conv}}} + \boldsymbol{b}^m.$$

2.2 Fully-Connected Layer

After passing through the convolutional layers, we concatenate columns in the matrix in (21) to form the input vector of the first fully-connected layer.

$$z^{m,i} = \operatorname{vec}(Z^{m,i}), \ i = 1, \dots, l, \ m = L^c + 1.$$

In the fully-connected layers $(L^c < m \leq L)$, we consider the following weight matrix and bias vector between layers m and m + 1.

$$W^{m} = \begin{bmatrix} w_{11}^{m} & w_{21}^{m} & \cdots & w_{n_{m}1}^{m} \\ w_{12}^{m} & w_{22}^{m} & \cdots & w_{n_{m}2}^{m} \\ \vdots & \vdots & \vdots & \vdots \\ w_{1n_{m+1}}^{m} & w_{2n_{m+1}}^{m} & \cdots & w_{n_{m+1}n_{m}}^{m} \end{bmatrix}_{n_{m+1} \times n_{m}} \text{ and } \boldsymbol{b}^{m} = \begin{bmatrix} b_{1}^{m} \\ b_{2}^{m} \\ \vdots \\ b_{2}^{m} \\ \vdots \\ b_{n_{m+1}}^{m} \end{bmatrix}_{n_{m+1} \times 1}$$
(22)

where n_m and n_{m+1} are the numbers of neurons in layers m and m + 1, respectively.³ If $\boldsymbol{z}^{m,i} \in \mathbb{R}^{n_m}$ is the input vector, the following operations are applied to generate the output vector $\boldsymbol{z}^{m+1,i} \in \mathbb{R}^{n_{m+1}}$.

$$\boldsymbol{s}^{m,i} = W^m \boldsymbol{z}^{m,i} + \boldsymbol{b}^m, \tag{23}$$

$$z_j^{m+1,i} = \sigma(s_j^{m,i}), \ j = 1, \dots, n_{m+1}.$$
 (24)

For the activation function in fully-connected layers, except the last layer, we also consider the RELU function defined in (13). For the last layer, we use the following linear

 $³_{n_{L^c+1}} = d^{L^c+1}a^{L^c+1}b^{L^c+1}$ and $n_{L+1} = K$ is the number of classes.

function.

$$\sigma(x) = x. \tag{25}$$

2.3 The Overall Optimization Problem

At the last layer, the output $z^{L+1,i}$, $\forall i$ is obtained. We can apply a loss function to check how close $z^{L+1,i}$ is to the label vector y^i . In this work the following squared loss is considered.

$$\xi(\boldsymbol{z}^{L+1,i};\boldsymbol{y}^i) = ||\boldsymbol{z}^{L+1,i} - \boldsymbol{y}^i||^2.$$
(26)

We can collect all model parameters such as filters of convolutional layers in (10) and weights/biases in (22) for fully-connected layers into a long vector $\theta \in \mathbb{R}^n$, where n becomes the total number of variables from the discussion in this section.

$$n = \sum_{m=1}^{L^{c}} d^{m+1} \times (h^{m} \times h^{m} \times d^{m} + 1) + \sum_{m=L^{c}+1}^{L} n_{m+1} \times (n_{m} + 1).$$

The output $z^{L+1,i}$ of the last layer is a function of θ . The optimization problem to train a CNN is

$$\min_{\boldsymbol{\theta}} f(\boldsymbol{\theta}), \tag{27}$$

where

$$f(\boldsymbol{\theta}) = \frac{1}{2C} \boldsymbol{\theta}^T \boldsymbol{\theta} + \frac{1}{l} \sum_{i=1}^{l} \xi(\boldsymbol{z}^{L+1,i}; \boldsymbol{y}^i).$$
(28)

In (28), the second term is the average training loss, while a regularization term with the parameter C > 0 is used to avoid overfitting.

3 Hessian-free Newton Methods for Training CNN

To solve an unconstrained minimization problem such as (27), a Newton method iteratively finds a search direction d by solving the following second-order approximation.

$$\min_{\boldsymbol{d}} \nabla f(\boldsymbol{\theta})^T \boldsymbol{d} + \frac{1}{2} \boldsymbol{d}^T \nabla^2 f(\boldsymbol{\theta}) \boldsymbol{d},$$
(29)

where $\nabla f(\theta)$ and $\nabla^2 f(\theta)$ are the gradient vector and the Hessian matrix, respectively. In this section we present details of applying a Newton method to solve the CNN problem (27).

3.1 Procedure of the Newton Method

For CNN, the gradient of $f(\theta)$ is

$$\nabla f(\boldsymbol{\theta}) = \frac{1}{C}\boldsymbol{\theta} + \frac{1}{l} \sum_{i=1}^{l} (J^{i})^{T} \nabla_{\boldsymbol{z}^{L+1,i}} \xi(\boldsymbol{z}^{L+1,i}; \boldsymbol{y}^{i}),$$
(30)

where

$$J^{i} = \begin{bmatrix} \frac{\partial z_{1}^{L+1,i}}{\partial \theta_{1}} & \cdots & \frac{\partial z_{1}^{L+1,i}}{\partial \theta_{n}} \\ \vdots & \vdots & \vdots \\ \frac{\partial z_{nL+1}^{L+1,i}}{\partial \theta_{1}} & \cdots & \frac{\partial z_{nL+1}^{L+1,i}}{\partial \theta_{n}} \end{bmatrix}_{nL+1 \times n}, \quad (31)$$

is the Jacobian of $\boldsymbol{z}^{L+1,i}$. The Hessian matrix of $f(\boldsymbol{\theta})$ is

$$\nabla^{2} f(\boldsymbol{\theta}) = \frac{1}{C} \mathcal{I} + \frac{1}{l} \sum_{i=1}^{l} (J^{i})^{T} B^{i} J^{i} + \frac{1}{l} \sum_{i=1}^{l} \sum_{j=1}^{n_{L+1}} \frac{\partial \xi(\boldsymbol{z}^{L+1,i}; \boldsymbol{y}^{i})}{\partial z_{j}^{L+1,i}} \begin{bmatrix} \frac{\partial^{2} z_{j}^{L+1,i}}{\partial \theta_{1} \partial \theta_{1}} & \cdots & \frac{\partial^{2} z_{j}^{L+1,i}}{\partial \theta_{1} \partial \theta_{n}} \\ \vdots & \ddots & \vdots \\ \frac{\partial^{2} z_{j}^{L+1,i}}{\partial \theta_{n} \partial \theta_{1}} & \cdots & \frac{\partial^{2} z_{j}^{L+1,i}}{\partial \theta_{n} \partial \theta_{n}} \end{bmatrix}, \quad (32)$$

where \mathcal{I} is the identity matrix and

$$B_{ts}^{i} = \frac{\partial^{2} \xi(\boldsymbol{z}^{L+1,i}; \boldsymbol{y}^{i})}{\partial z_{t}^{L+1,i} \partial z_{s}^{L+1,i}}, \ t = 1, \dots, n_{L+1}, \ s = 1, \dots, n_{L+1}.$$
(33)

From now on for simplicity we let

$$\xi_i \equiv \xi_i(\boldsymbol{z}^{L+1,i}; \boldsymbol{y}^i).$$

In general (32) is not positive semi-definite, so $f(\theta)$ is non-convex for deep learning. The sub-problem (29) is difficult to solve and the resulting direction may not lead to the decrease of the function value. Following past works (Martens, 2010; Wang et al., 2015), we consider the following Gauss-Newton approximation (Schraudolph, 2002)

$$G = \frac{1}{C}\mathcal{I} + \frac{1}{l}\sum_{i=1}^{l} (J^i)^T B^i J^i \approx \nabla^2 f(\boldsymbol{\theta}).$$
(34)

In particular, if G is positive definite, then (29) becomes the same as solving the following linear system.

$$G\boldsymbol{d} = -\nabla f(\boldsymbol{\theta}). \tag{35}$$

After a Newton direction d is obtained, to ensure the convergence, we update θ by

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha \boldsymbol{d},$$

where α is the largest element in an exponentially decreased sequence like $\{1, \frac{1}{2}, \frac{1}{4}, \ldots\}$ satisfying

$$f(\boldsymbol{\theta} + \alpha \boldsymbol{d}) \le f(\boldsymbol{\theta}) + \eta \alpha \nabla f(\boldsymbol{\theta})^T \boldsymbol{d}.$$
(36)

In (36), $\eta \in (0, 1)$ is a pre-defined constant. The procedure to find α is called a back-tracking line search.

Past works (e.g., Martens, 2010; Wang et al., 2018) have shown that sometimes (35) is too aggressive, so a direction closer to the negative gradient is better. To this

end, in recent works of applying Newton methods on fully-connected networks, the Levenberg-Marquardt method (Levenberg, 1944; Marquardt, 1963) is used to solve the following linear system rather than (35).

$$(G + \lambda \mathcal{I})\boldsymbol{d} = -\nabla f(\boldsymbol{\theta}), \tag{37}$$

where λ is a parameter decided by how good the function reduction is. Specifically, if $\theta + d$ is the next iterate after line search, we define

$$\rho = \frac{f(\boldsymbol{\theta} + \boldsymbol{d}) - f(\boldsymbol{\theta})}{\nabla f(\boldsymbol{\theta})^T \boldsymbol{d} + \frac{1}{2}(\boldsymbol{d})^T G \boldsymbol{d}}$$

as the ratio between the actual function reduction and the predicted reduction. By using ρ , the parameter λ_{next} for the next iteration is decided by

$$\lambda_{\text{next}} = \begin{cases} \lambda \times \text{drop} & \rho > \rho_{\text{upper}}, \\ \lambda & \rho_{\text{lower}} \le \rho \le \rho_{\text{upper}}, \\ \lambda \times \text{boost} & \text{otherwise,} \end{cases}$$
(38)

where (drop,boost) are given constants. From (38) we can clearly see that if the functionvalue reduction is not satisfactory, then λ is enlarged and the resulting direction is closer to the negative gradient.

Next, we discuss how to solve the linear system (37). When the number of variables n is large, the matrix G is too large to be stored. For some optimization problems including neural networks, without explicitly storing G it is possible to calculate the product between G and any vector v (Martens, 2010; Le et al., 2011; Wang et al., 2018). For example, from (34),

$$(G + \lambda \mathcal{I})\boldsymbol{v} = (\frac{1}{C} + \lambda)\boldsymbol{v} + \frac{1}{l} \sum_{i=1}^{l} \left((J^{i})^{T} \left(B^{i} (J^{i} \boldsymbol{v}) \right) \right).$$
(39)

If the product between J^i and a vector can be easily calculated, then G does not need to be explicitly formed. Therefore, we can apply the conjugate gradient (CG) method to solve (35) by a sequence of matrix-vector products. This technique is called Hessianfree methods in optimization. Details of CG methods in a Hessian-free Newton framework can be found in, for example, Algorithm 2 of Lin et al. (2007).

Because the computational cost in (39) is proportional to the number of instances, subsampled Hessian Newton methods have been proposed (Byrd et al., 2011; Martens, 2010; Wang et al., 2015) to reduce the cost in solving the linear system (37). They observe that the second term in (34) is the average training loss. If the large number of data points are assumed to be from the same distribution, (34) can be reasonably approximated by selecting a subset $S \subset \{1, ..., l\}$ and having

$$G^{S} = \frac{1}{C}\mathcal{I} + \frac{1}{|S|}\sum_{i\in S} (J^{i})^{T}B^{i}J^{i} \approx G.$$

Then (39) becomes

$$(G^{S} + \lambda \mathcal{I})\boldsymbol{v} = (\frac{1}{C} + \lambda)\boldsymbol{v} + \frac{1}{|S|} \sum_{i \in S} \left((J^{i})^{T} \left(B^{i} (J^{i} \boldsymbol{v}) \right) \right) \approx (G + \lambda \mathcal{I})\boldsymbol{v}.$$
(40)

A summary of the Newton method is in Algorithm 1.

3.2 Gradient Evaluation

In order to solve (35), $\nabla f(\theta)$ is needed. It can be obtained by (30) if the Jacobian matrices J^i , i = 1, ..., l are available. From (39), it seems that $J^i, \forall i$ are also needed for the matrix-vector product in CG. However, as mentioned in Section 3.1, in practice a sub-sampled Hessian method is used, so from (40) only a subset of $J^i, \forall i$ are needed.

Algorithm 1 A standard subsampled Hessian Newton method for CNN.

1: (Compute $f(\theta^1)$.	
2: for $k = 1,, do$		
3:	Choose a set $S_k \subset \{1, \ldots, l\}$.	
4:	Compute $\nabla f(\boldsymbol{\theta}^k)$ and $J^i, \forall i \in S_k$.	
5:	Approximately solve the linear system in (37) by CG to obtain a direction d^k	
6:	$\alpha = 1.$	
7:	while true do	
8:	Update $\boldsymbol{\theta}^{k+1} = \boldsymbol{\theta}^k + \alpha \boldsymbol{d}^k$ and compute $f(\boldsymbol{\theta}^{k+1})$	
9:	if (36) is satisfied then	
10:	break	
11:	end if	
12:	$\alpha \leftarrow \alpha/2.$	
13:	end while	
14:	Calculate λ_{k+1} based on (38).	
15: end for		

Therefore we present a backward process to calculate the gradient without using Jacobian.

Consider two layers m and m + 1. The variables between them are W^m and b^m , so we aim to calculate the following gradient components.

$$\frac{\partial f}{\partial W^m} = \frac{1}{C}W^m + \frac{1}{l}\sum_{i=1}^l \frac{\partial \xi_i}{\partial W^m},\tag{41}$$

$$\frac{\partial f}{\partial \boldsymbol{b}^m} = \frac{1}{C} \boldsymbol{b}^m + \frac{1}{l} \sum_{i=1}^l \frac{\partial \xi_i}{\partial \boldsymbol{b}^m}.$$
(42)

Because (41) is in a matrix form, following past developments such as Vedaldi and Lenc (2015), it is easier to transform them to a vector form for the derivation. To begin, we list the following properties of the $vec(\cdot)$ function, in which \otimes is the Kronecker product.

$$\operatorname{vec}(AB) = (\mathcal{I} \otimes A)\operatorname{vec}(B),$$
 (43)

$$= (B^T \otimes \mathcal{I}) \mathbf{vec}(A), \tag{44}$$

$$\operatorname{vec}(AB)^T = \operatorname{vec}(B)^T (\mathcal{I} \otimes A^T),$$
 (45)

$$= \operatorname{vec}(A)^T (B \otimes \mathcal{I}). \tag{46}$$

We further define

$$rac{\partial oldsymbol{y}}{\partial {(oldsymbol{x})}^T} = egin{bmatrix} rac{\partial y_1}{\partial x_1} & \cdots & rac{\partial y_1}{\partial x_{|oldsymbol{x}|}} \\ dots & \ddots & dots \\ rac{\partial y_{|oldsymbol{y}|}}{\partial x_1} & \cdots & rac{\partial y_{|oldsymbol{y}|}}{\partial x_{|oldsymbol{x}|}} \end{bmatrix},$$

where \boldsymbol{x} and \boldsymbol{y} are column vectors.

For the convolutional layers, from (11) and Table 1, we have

$$\operatorname{vec}(S^{m,i}) = \operatorname{vec}(W^{m}\phi(\operatorname{pad}(Z^{m,i}))) + \operatorname{vec}(\boldsymbol{b}^{m}\mathbb{1}_{a^{m}_{\operatorname{conv}}\boldsymbol{b}^{m}_{\operatorname{conv}}}^{T})$$
$$= \left(\mathcal{I}_{a^{m}_{\operatorname{conv}}\boldsymbol{b}^{m}_{\operatorname{conv}}} \otimes W^{m}\right)\operatorname{vec}(\phi(\operatorname{pad}(Z^{m,i}))) + (\mathbb{1}_{a^{m}_{\operatorname{conv}}\boldsymbol{b}^{m}_{\operatorname{conv}}} \otimes \mathcal{I}_{d^{m+1}})\boldsymbol{b}^{m} \qquad (47)$$
$$= \left(\phi(\operatorname{pad}(Z^{m,i}))^{T} \otimes \mathcal{I}_{d^{m+1}}\right)\operatorname{vec}(W^{m}) + (\mathbb{1}_{a^{m}_{\operatorname{conv}}\boldsymbol{b}^{m}_{\operatorname{conv}}} \otimes \mathcal{I}_{d^{m+1}})\boldsymbol{b}^{m}, \qquad (48)$$

where (47) and (48) are from (43) and (44), respectively.

For the fully-connected layers, from (23), we have

$$\boldsymbol{s}^{m,i} = W^m \boldsymbol{z}^{m,i} + \boldsymbol{b}^m$$

$$= (\mathcal{I}_1 \otimes W^m) \, \boldsymbol{z}^{m,i} + (\mathbb{1}_1 \otimes \mathcal{I}_{n_{m+1}}) \boldsymbol{b}^m \qquad (49)$$

$$= ((\boldsymbol{z}^{m,i})^T \otimes \mathcal{I}_{m-1}) \operatorname{vec}(W^m) + (\mathbb{1}_1 \otimes \mathcal{I}_{m-1}) \boldsymbol{b}^m \qquad (50)$$

$$= \left((\boldsymbol{z}^{m,i})^T \otimes \mathcal{I}_{n_{m+1}} \right) \operatorname{vec}(W^m) + (\mathbb{1}_1 \otimes \mathcal{I}_{n_{m+1}}) \boldsymbol{b}^m,$$
(50)

where (49) and (50) are from (43) and (44), respectively.

An advantage of using (47) and (49) is that they are in the same form. Further, if for fully-connected layers we define

$$\phi(\operatorname{pad}(\boldsymbol{z}^{m,i})) = \mathcal{I}_{n_m} \boldsymbol{z}^{m,i}, \ L^c < m \le L+1,$$

then (48) and (50) are in the same form. Thus we can derive the gradient together. We begin with calculating the gradient for convolutional layers. From (48), we derive

$$\frac{\partial \xi_{i}}{\partial \operatorname{vec}(W^{m})^{T}} = \frac{\partial \xi_{i}}{\partial \operatorname{vec}(S^{m,i})^{T}} \frac{\partial \operatorname{vec}(S^{m,i})}{\partial \operatorname{vec}(W^{m})^{T}} \\
= \frac{\partial \xi_{i}}{\partial \operatorname{vec}(S^{m,i})^{T}} \left(\phi(\operatorname{pad}(Z^{m,i}))^{T} \otimes \mathcal{I}_{d^{m+1}} \right) \\
= \operatorname{vec} \left(\frac{\partial \xi_{i}}{\partial S^{m,i}} \phi(\operatorname{pad}(Z^{m,i}))^{T} \right)^{T}$$
(51)

and

$$\frac{\partial \xi_{i}}{\partial (\boldsymbol{b}^{m})^{T}} = \frac{\partial \xi_{i}}{\partial \operatorname{vec}(S^{m,i})^{T}} \frac{\partial \operatorname{vec}(S^{m,i})}{\partial (\boldsymbol{b}^{m})^{T}}
= \frac{\partial \xi_{i}}{\partial \operatorname{vec}(S^{m,i})^{T}} \left(\mathbb{1}_{a_{\operatorname{conv}}^{m}b_{\operatorname{conv}}^{m}} \otimes \mathcal{I}_{d^{m+1}} \right)
= \operatorname{vec} \left(\frac{\partial \xi_{i}}{\partial S^{m,i}} \mathbb{1}_{a_{\operatorname{conv}}^{m}b_{\operatorname{conv}}^{m}} \right)^{T},$$
(52)

where (51) and (52) are from (46). To calculate (51), $\phi(\text{pad}(Z^{m,i}))$ has been available from the forward process of calculating the function value. In (51) and (52), $\partial \xi_i / \partial S^{m,i}$ is also needed and can be obtained by a backward process. By assuming that $\partial \xi_i / \partial Z^{m+1,i}$ is available, we show details of calculating $\partial \xi_i / \partial S^{m,i}$ and $\partial \xi_i / \partial Z^{m,i}$ for layer *m*. From (20) we have the following workflow.

$$Z^{m,i} \leftarrow \text{padding} \leftarrow \text{convolution} \leftarrow \sigma(S^{m,i}) \leftarrow \text{pooling} \leftarrow Z^{m+1,i}.$$
 (53)

Because the RELU activation function is considered for the convolutional layers, we have

$$\frac{\partial \xi_i}{\partial \operatorname{vec}(S^{m,i})^T} = \frac{\partial \xi_i}{\partial \operatorname{vec}(Z^{m+1,i})^T} \frac{\partial \operatorname{vec}(Z^{m+1,i})}{\partial \operatorname{vec}(\sigma(S^{m,i}))^T} \frac{\partial \operatorname{vec}(\sigma(S^{m,i}))}{\partial \operatorname{vec}(S^{m,i})^T}$$
(54)

$$= \left(\frac{\partial \xi_i}{\partial \operatorname{vec}(Z^{m+1,i})^T} \frac{\partial \operatorname{vec}(Z^{m+1,i})}{\partial \operatorname{vec}(\sigma(S^{m,i}))^T}\right) \odot \operatorname{vec}(I[S^{m,i}])^T \quad (55)$$

$$= \left(\frac{\partial \xi_i}{\partial \operatorname{vec}(Z^{m+1,i})^T} P_{\operatorname{pool}}^{m,i}\right) \odot \operatorname{vec}(I[S^{m,i}])^T,$$
(56)

where (56) is from (21), \odot is Hadamard product (i.e., element-wise products),

$$I[S^{m,i}]_{(p,q)} = \begin{cases} 1 & \text{ if } s^{m,i}_{(p,q)} > 0, \\ 0 & \text{ otherwise,} \end{cases}$$

and because

$$\frac{\partial \text{vec}(\sigma(S^{m,i}))}{\partial \text{vec}(S^{m,i})^T}$$

is a diagonal matrix, (55) can be derived from (54).

Next, we must calculate $\partial \xi_i / \partial Z^{m,i}$ and pass it to the previous layer.

$$\frac{\partial \xi_{i}}{\partial \operatorname{vec}(Z^{m,i})^{T}} = \frac{\partial \xi_{i}}{\partial \operatorname{vec}(S^{m,i})^{T}} \frac{\partial \operatorname{vec}(S^{m,i})}{\partial \operatorname{vec}(\phi(\operatorname{pad}(Z^{m,i})))^{T}} \frac{\partial \operatorname{vec}(\phi(\operatorname{pad}(Z^{m,i})))}{\partial \operatorname{vec}(\operatorname{pad}(Z^{m,i}))^{T}} \frac{\partial \operatorname{vec}(\operatorname{pad}(Z^{m,i}))}{\partial \operatorname{vec}(Z^{m,i})^{T}} = \frac{\partial \xi_{i}}{\partial \operatorname{vec}(S^{m,i})^{T}} \left(\mathcal{I}_{a^{m}_{\operatorname{conv}}b^{m}_{\operatorname{conv}}} \otimes W^{m} \right) P_{\phi}^{m} P_{\operatorname{pad}}^{m}$$
(57)

$$= \operatorname{vec}\left((W^m)^T \frac{\partial \xi_i}{\partial S^{m,i}} \right)^T P^m_{\phi} P^m_{\text{pad}},$$
(58)

where (57) is from (8), (14) and (47), and (58) is from (45).

For fully-connected layers, by the same form in (49), (50), (47) and (48), we immediately get the following results from (51), (52), (56) and (58).

$$\frac{\partial \xi_i}{\partial \operatorname{vec}(W^m)^T} = \operatorname{vec}\left(\frac{\partial \xi_i}{\partial \boldsymbol{s}^{m,i}} (\boldsymbol{z}^{m,i})^T\right)^T$$
(59)

$$\frac{\partial \xi_i}{\partial (\boldsymbol{b}^m)^T} = \frac{\partial \xi_i}{\partial (\boldsymbol{s}^{m,i})^T}$$
(60)

$$\frac{\partial \xi_i}{\partial (\boldsymbol{z}^{m,i})^T} = \left((W^m)^T \frac{\partial \xi_i}{\partial (\boldsymbol{s}^{m,i})} \right)^T \mathcal{I}_{n_m} \\
= \frac{\partial \xi_i}{\partial (\boldsymbol{s}^{m,i})^T} W^m,$$
(61)

where

$$\frac{\partial \xi_i}{\partial (\boldsymbol{s}^{m,i})^T} = \frac{\partial \xi_i}{\partial (\boldsymbol{z}^{m+1,i})^T} \odot I[\boldsymbol{s}^{m,i}]^T.$$
(62)

Finally, we check the initial values of the backward process. From the square loss in (26) and the linear activation function in (25), we have

$$\frac{\partial \xi_i}{\partial \boldsymbol{z}^{L+1,i}} = 2(\boldsymbol{z}^{L+1,i} - \boldsymbol{y}^i),$$
$$\frac{\partial \xi_i}{\partial \boldsymbol{s}^{L,i}} = \frac{\partial \xi_i}{\partial \boldsymbol{z}^{L+1,i}}.$$

3.2.1 Some Notes on Practical Implementations

In practice, because we only store

$$Z^{m+1,i} = \max\left(P^{m,i}_{\text{pool}}\text{vec}(\sigma(S^{m,i}))\right)$$

rather than $\sigma(S^{m,i})$, instead of using (56), we conduct the following calculation.

$$\frac{\partial \xi_i}{\partial \operatorname{vec}(S^{m,i})^T} = \left(\frac{\partial \xi_i}{\partial \operatorname{vec}(Z^{m+1,i})^T} \odot \operatorname{vec}(I[Z^{m+1,i}])^T\right) P_{\operatorname{pool}}^{m,i}.$$
(63)

The reason is that, for (56),

$$\frac{\partial \xi_i}{\partial \text{vec}(Z^{m+1,i})^T} \times P_{\text{pool}}^{m,i}$$
(64)

generates a large zero vector and puts values of $\partial \xi_i / \partial \text{vec}(Z^{m+1,i})^T$ into positions selected earlier in the max pooling operation. Then, element-wise multiplications of (64) and $I[S^{m,i}]^T$ follow. Because positions not selected in the earlier max pooling procedure in (64) are zeros and they are still zeros after the Hadamard product between (64) and $I[S^{m,i}]^T$, (56) and (63) give the same results.

3.3 Jacobian Evaluation

For the matrix-vector product (34), the Jacobian matrix is needed. We note that it can be partitioned into L blocks.

$$J^{i} = \begin{bmatrix} J^{1,i} & J^{2,i} & \dots & J^{L,i} \end{bmatrix}, \ m = 1, \dots, L, \ i = 1, \dots, l,$$
(65)

where

$$J^{m,i} = \begin{bmatrix} \frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \text{vec}(W^m)^T} & \frac{\partial \boldsymbol{z}^{L+1,i}}{\partial (\boldsymbol{b}^m)^T} \end{bmatrix}.$$

The calculation is very similar to that for the gradient. For the convolutional layers, from (51) and (52), we have

$$\begin{bmatrix} \frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(W^m)^T} & \frac{\partial \boldsymbol{z}^{L+1,i}}{\partial (\boldsymbol{b}^m)^T} \end{bmatrix} = \begin{bmatrix} \frac{\partial \boldsymbol{z}_1^{L+1,i}}{\partial (\boldsymbol{b}^m)^T} & \frac{\partial \boldsymbol{z}_1^{L+1,i}}{\partial (\boldsymbol{b}^m)^T} \\ \vdots \\ \frac{\partial \boldsymbol{z}_{nL+1}^{L+1,i}}{\partial \operatorname{vec}(W^m)^T} & \frac{\partial \boldsymbol{z}_{nL+1}^{L+1,i}}{\partial (\boldsymbol{b}^m)^T} \end{bmatrix}$$
$$= \begin{bmatrix} \operatorname{vec}(\frac{\partial \boldsymbol{z}_1^{L+1,i}}{\partial S^{m,i}} \phi(\operatorname{pad}(Z^{m,i}))^T)^T & \operatorname{vec}(\frac{\partial \boldsymbol{z}_1^{L+1,i}}{\partial S^{m,i}} \mathbb{1}_{a_{\operatorname{conv}}^m} b_{\operatorname{conv}}^m)^T \\ \vdots \\ \operatorname{vec}(\frac{\partial \boldsymbol{z}_{nL+1}^{L+1,i}}{\partial S^{m,i}} \phi(\operatorname{pad}(Z^{m,i}))^T)^T & \operatorname{vec}(\frac{\partial \boldsymbol{z}_{nL+1}^{L+1,i}}{\partial S^{m,i}} \mathbb{1}_{a_{\operatorname{conv}}^m} b_{\operatorname{conv}}^m)^T \end{bmatrix}$$
$$= \begin{bmatrix} \operatorname{vec}\left(\frac{\partial \boldsymbol{z}_1^{L+1,i}}{\partial S^{m,i}} \left[\phi(\operatorname{pad}(Z^{m,i}))^T \ \mathbb{1}_{a_{\operatorname{conv}}^m} b_{\operatorname{conv}}^m\right]\right)^T \\ \vdots \\ \operatorname{vec}\left(\frac{\partial \boldsymbol{z}_{nL+1,i}^{L+1,i}}{\partial S^{m,i}} \left[\phi(\operatorname{pad}(Z^{m,i}))^T \ \mathbb{1}_{a_{\operatorname{conv}}^m} b_{\operatorname{conv}}^m\right]\right)^T \end{bmatrix}. \quad (66)$$

We use a backward process to calculate $\partial \boldsymbol{z}^{L+1,i}/\partial S^{m,i}$, $\forall i$. Assume that $\partial \boldsymbol{z}^{L+1,i}/\partial Z^{m+1,i}$ are available. From (63), we have

$$\frac{\partial z_j^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})^T} = \left(\frac{\partial z_j^{L+1,i}}{\partial \operatorname{vec}(Z^{m+1,i})^T} \odot \operatorname{vec}(I[Z^{m+1,i}])^T\right) P_{\text{pool}}^{m,i}, \ j = 1, \dots, n_{L+1}.$$

These vectors can be written together as

$$\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})^T} = \left(\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(Z^{m+1,i})^T} \odot \left(\mathbbm{1}_{n_{L+1}} \operatorname{vec}(I[Z^{m+1,i}])^T\right)\right) P_{\text{pool}}^{m,i}.$$
 (67)

We then generate $\partial z^{L+1,i} / \partial \text{vec}(Z^{m,i})^T$ and pass it to the previous layer. From (58),

we derive

$$\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(Z^{m,i})^{T}} = \begin{bmatrix} \frac{\partial z_{1}^{L+1,i}}{\partial \operatorname{vec}(Z^{m,i})^{T}} \\ \vdots \\ \frac{\partial z_{nL+1}^{L+1,i}}{\partial \operatorname{vec}(Z^{m,i})^{T}} \end{bmatrix}$$

$$= \begin{bmatrix} \operatorname{vec}\left((W^{m})^{T} \frac{\partial z_{1}^{L+1,i}}{\partial S^{m,i}}\right)^{T} P_{\phi}^{m} P_{\text{pad}}^{m} \\ \vdots \\ \operatorname{vec}\left((W^{m})^{T} \frac{\partial z_{nL+1}^{L+1,i}}{\partial S^{m,i}}\right)^{T} P_{\phi}^{m} P_{\text{pad}}^{m} \end{bmatrix}. \quad (68)$$

For the fully-connected layers, we follow the same derivation of gradient to have

$$\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(W^m)^T} = \left[\operatorname{vec}(\frac{\partial z_1^{L+1,i}}{\partial \boldsymbol{s}^{m,i}}(\boldsymbol{z}^{m,i})^T) \dots \operatorname{vec}(\frac{\partial z_{n_{L+1}}^{L+1,i}}{\partial \boldsymbol{s}^{m,i}}(\boldsymbol{z}^{m,i})^T)\right]^T, \quad (69)$$

$$\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial (\boldsymbol{b}^m)^T} = \frac{\partial \boldsymbol{z}^{L+1,i}}{\partial (\boldsymbol{s}^{m,i})^T},\tag{70}$$

$$\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial (\boldsymbol{z}^{m,i})^T} = \frac{\partial \boldsymbol{z}^{L+1,i}}{\partial (\boldsymbol{s}^{m,i})^T} W^m,\tag{71}$$

$$\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial (\boldsymbol{s}^{m-1,i})^T} = \frac{\partial \boldsymbol{z}^{L+1,i}}{\partial (\boldsymbol{z}^{m,i})^T} \odot \left(\mathbbm{1}_{n_{L+1}} I[\boldsymbol{z}^{m,i}]^T \right).$$
(72)

For layer L + 1, because of using (26) and the linear activation function, we have

$$rac{\partial oldsymbol{z}^{L+1,i}}{\partial (oldsymbol{s}^{L,i})^T} = \mathcal{I}_{n_{L+1}}.$$

3.4 Gauss-Newton Matrix-Vector Products

Conjugate gradient (CG) methods are used to solve (35). The main operation at each CG iteration is the Gauss-Newton matrix-vector product in (39) or (40) with the subsampled

setting.

From (65), we rearrange (34) to

$$G = \frac{1}{C}\mathcal{I} + \frac{1}{l}\sum_{i=1}^{l} \begin{bmatrix} (J^{1,i})^T \\ \vdots \\ (J^{L,i})^T \end{bmatrix} B^i \begin{bmatrix} J^{1,i} & \dots & J^{L,i} \end{bmatrix}$$
(73)

and the Gauss-Newton matrix vector product becomes

$$G\boldsymbol{v} = \frac{1}{C}\boldsymbol{v} + \frac{1}{l}\sum_{i=1}^{l} \begin{bmatrix} (J^{1,i})^{T} \\ \vdots \\ (J^{L,i})^{T} \end{bmatrix} B^{i} \begin{bmatrix} J^{1,i} & \dots & J^{L,i} \end{bmatrix} \begin{bmatrix} \boldsymbol{v}^{1} \\ \vdots \\ \boldsymbol{v}^{L} \end{bmatrix}$$
$$= \frac{1}{C}\boldsymbol{v} + \frac{1}{l}\sum_{i=1}^{l} \begin{bmatrix} (J^{1,i})^{T} \\ \vdots \\ (J^{L,i})^{T} \end{bmatrix} \begin{pmatrix} B^{i}\sum_{m=1}^{L} J^{m,i}\boldsymbol{v}^{m} \end{pmatrix},$$
(74)

where

$$oldsymbol{v} = egin{bmatrix} oldsymbol{v}^1 \ dots \ oldsymbol{v}^L \end{bmatrix}, \ oldsymbol{v} = egin{bmatrix} oldsymbol{v}^1 \ dots \ oldsymbol{v}^L \end{bmatrix}$$

and each $oldsymbol{v}^m, m=1,\ldots,L$ has the same length as the number of variables (including bias) at the *m*th layer.

For the convolutional layers, from (66) and (74), we have

$$J^{m,i}\boldsymbol{v}^{m} = \begin{bmatrix} \operatorname{vec}\left(\frac{\partial z_{1}^{L+1,i}}{\partial S^{m,i}} \left[\phi(\operatorname{pad}(Z^{m,i}))^{T} \mathbb{1}_{a_{\operatorname{conv}}^{m}b_{\operatorname{conv}}^{m}}\right]\right)^{T} \boldsymbol{v}^{m} \\ \vdots \\ \operatorname{vec}\left(\frac{\partial z_{n_{L+1}}^{L+1,i}}{\partial S^{m,i}} \left[\phi(\operatorname{pad}(Z^{m,i}))^{T} \mathbb{1}_{a_{\operatorname{conv}}^{m}b_{\operatorname{conv}}^{m}}\right]\right)^{T} \boldsymbol{v}^{m} \end{bmatrix}.$$
(75)

To simplify (75), we use the following property

_

$$\operatorname{vec}(AB)^T \operatorname{vec}(C) = \operatorname{vec}(A)^T \operatorname{vec}(CB^T)$$

to have that for example, the first element in (75) is

$$\operatorname{vec}\left(\frac{\partial z_{1}^{L+1,i}}{\partial S^{m,i}}\left[\phi(\operatorname{pad}(Z^{m,i}))^{T} \mathbb{1}_{a_{\operatorname{conv}}^{m}b_{\operatorname{conv}}^{m}}\right]\right)^{T} \boldsymbol{v}^{m}$$
$$=\frac{\partial z_{1}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})^{T}}\operatorname{vec}\left(\operatorname{mat}(\boldsymbol{v}^{m})_{d^{m+1}\times(h^{m}h^{m}d^{m}+1)}\left[\begin{array}{c}\phi(\operatorname{pad}(Z^{m,i}))\\\\\mathbb{1}_{a_{\operatorname{conv}}^{m}b_{\operatorname{conv}}^{m}}\end{array}\right]\right).$$

Therefore,

$$J^{m,i}\boldsymbol{v}^{m} = \frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})^{T}} \operatorname{vec}\left(\operatorname{mat}(\boldsymbol{v}^{m})_{d^{m+1} \times (h^{m}h^{m}d^{m}+1)} \begin{bmatrix} \phi(\operatorname{pad}(Z^{m,i})) \\ \mathbb{1}_{a_{\operatorname{conv}}^{m}b_{\operatorname{conv}}^{m}}^{T} \end{bmatrix} \right).$$
(76)

After deriving (76), from (74), we sum results of all layers

$$\sum_{m=1}^{L} J^{m,i} \boldsymbol{v}^m$$

and then calculate

$$\boldsymbol{q}^{i} = B^{i} (\sum_{m=1}^{L} J^{m,i} \boldsymbol{v}^{m}).$$
(77)

From (26) and (33),

$$B_{ts}^{i} = \frac{\partial^{2}\xi^{i}}{\partial z_{t}^{L+1,i}\partial z_{s}^{L+1,i}} = \frac{\partial^{2}(\sum_{j=1}^{n_{L+1}}(z_{j}^{L+1,i} - y_{j}^{i})^{2})}{\partial z_{t}^{L+1,i}\partial z_{s}^{L+1,i}} = \begin{cases} 2 & \text{if } t = s, \\ 0 & \text{otherwise,} \end{cases}$$
(78)

and we derive q^i by multiplying every element of $\sum_{m=1}^{L} J^{m,i} v^m$ by two.

After deriving (77), from (66) and (74), we calculate

$$\begin{split} &(J^{m,i})^{T}\boldsymbol{q}^{i} \\ &= \left[\operatorname{vec} \left(\frac{\partial z_{1}^{L+1,i}}{\partial S^{m,i}} \left[\phi(\operatorname{pad}(Z^{m,i}))^{T} \, \mathbb{1}_{a_{\operatorname{conv}}^{m} b_{\operatorname{conv}}^{m}} \right] \right) \quad \cdots \quad \operatorname{vec} \left(\frac{\partial z_{n_{L+1}}^{L+1,i}}{\partial S^{m,i}} \left[\phi(\operatorname{pad}(Z^{m,i}))^{T} \, \mathbb{1}_{a_{\operatorname{conv}}^{m} b_{\operatorname{conv}}^{m}} \right] \right) \right] \boldsymbol{q}^{i} \\ &= \sum_{j=1}^{n_{L+1}} q_{j}^{i} \operatorname{vec} \left(\frac{\partial z_{j}^{L+1,i}}{\partial S^{m,i}} \left[\phi(\operatorname{pad}(Z^{m,i}))^{T} \, \mathbb{1}_{a_{\operatorname{conv}}^{m} b_{\operatorname{conv}}^{m}} \right] \right) \\ &= \operatorname{vec} \left(\sum_{j=1}^{n_{L+1}} q_{j}^{i} \left(\frac{\partial z_{j}^{L+1,i}}{\partial S^{m,i}} \left[\phi(\operatorname{pad}(Z^{m,i}))^{T} \, \mathbb{1}_{a_{\operatorname{conv}}^{m} b_{\operatorname{conv}}^{m}} \right] \right) \right) \end{split}$$

$$= \operatorname{vec}\left(\left(\sum_{j=1}^{n_{L+1}} q_j^i \frac{\partial z_j^{L+1,i}}{\partial S^{m,i}}\right) \left[\phi(\operatorname{pad}(Z^{m,i}))^T \, \mathbb{1}_{a_{\operatorname{conv}}^m b_{\operatorname{conv}}^m}\right]\right)$$
$$= \operatorname{vec}\left(\operatorname{mat}\left(\left(\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})^T}\right)^T \boldsymbol{q}^i\right)_{d^{m+1} \times a_{\operatorname{conv}}^m b_{\operatorname{conv}}^m} \left[\phi(\operatorname{pad}(Z^{m,i}))^T \, \mathbb{1}_{a_{\operatorname{conv}}^m b_{\operatorname{conv}}^m}\right]\right). (79)$$

Similar to the results of the convolutional layers, for the fully-connected layers we

have

$$J^{m,i}\boldsymbol{v}^{m} = \frac{\partial \boldsymbol{z}^{L+1,i}}{\partial (\boldsymbol{s}^{m,i})^{T}} \operatorname{mat}(\boldsymbol{v}^{m})_{n_{m+1} \times (n_{m}+1)} \begin{bmatrix} \boldsymbol{z}^{m,i} \\ \mathbb{1}_{1} \end{bmatrix}.$$
(80)

$$(J^{m,i})^{T}\boldsymbol{q}^{i} = \operatorname{vec}\left(\left(\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial (\boldsymbol{s}^{m,i})^{T}}\right)^{T}\boldsymbol{q}^{i}\left[(\boldsymbol{z}^{m,i})^{T}\ \mathbb{1}_{1}\right]\right).$$
(81)

4 Implementation Details

We show that with a careful design, a Newton method for CNN can be implemented by a simple and short program. A *MATLAB* implementation is given as an illustration though modifications for other languages such as *Python* should be straightforward.

For the discussion in Section 3, we check each individual data. However, for practical implementations, all instances must be considered together for memory and computational efficiency. In our implementation, we store $Z^{m,i}$, $\forall i = 1, ..., l$ as the following matrix.

$$\begin{bmatrix} Z^{m,1} & Z^{m,2} & \dots & Z^{m,l} \end{bmatrix} \in R^{d^m \times a^m b^m l}.$$
(82)

Similarly, we store $\partial \xi_i / \partial \text{vec}(S^{m,i})^T$, $\forall i$ as

$$\begin{bmatrix} \frac{\partial \xi_1}{\partial S^{m,1}} & \dots & \frac{\partial \xi_l}{\partial S^{m,l}} \end{bmatrix} \in R^{d^{m+1} \times a^m_{\text{conv}} b^m_{\text{conv}} l}.$$
(83)

For $\partial \boldsymbol{z}^{L+1,i} / \partial \text{vec}(S^{m,i})^T$, $\forall i$, we consider

$$\begin{bmatrix} \frac{\partial z_1^{L+1,1}}{\partial S^{m,1}} & \dots & \frac{\partial z_{n_{L+1}}^{L+1,1}}{\partial S^{m,1}} & \dots & \frac{\partial z_{n_{L+1}}^{L+1,l}}{\partial S^{m,l}} \end{bmatrix} \in R^{d^{m+1} \times a_{\text{conv}}^m b_{\text{conv}}^m n_{L+1} l}$$
(84)

and will explain our decision. Note that (82)-(84) are only the main setting to store these matrices because for some operations they may need to be re-shaped.

For an easy description in some places we follow Section 2.1 to let

$$Z^{\mathrm{in},i}$$
 and $Z^{\mathrm{out},i}$

be the input and output images of a layer, respectively.

4.1 Generation of $\phi(\text{pad}(Z^{m,i}))$

MATLAB has a built-in function im2col that can generate $\phi(\text{pad}(Z^{m,i}))$ for s = 1and s = h. For general s, we notice that $\phi(\text{pad}(Z^{m,i}))$ is a sub-matrix of the output matrix of using MATLAB's im2col under s = 1. In supplementary materials we provide an efficient implementation to extract the sub-matrix. However, this approach is not ideal because first in other languages a subroutine like MATLAB's im2col may not be available, and second, generating a larger matrix under s = 1 causes extra time and memory.

Therefore, here we show an efficient implementation without relying on a subroutine like *MATLAB*'s im2col. For an easy description we follow Section 2.1 to consider

$$\operatorname{pad}(Z^{m,i}) = Z^{\operatorname{in},i} \to Z^{\operatorname{out},i} = \phi(Z^{\operatorname{in},i}).$$

Consider the following linear indices⁴ (i.e., counting elements in a column-oriented way) of $Z^{in,i}$:

$$\begin{bmatrix} 1 & d^{\text{in}} + 1 & \dots & (b^{\text{in}}a^{\text{in}} - 1)d^{\text{in}} + 1 \\ 2 & d^{\text{in}} + 2 & \dots & (b^{\text{in}}a^{\text{in}} - 1)d^{\text{in}} + 2 \\ \vdots & \vdots & \ddots & \vdots \\ d^{\text{in}} & 2d^{\text{in}} & \dots & (b^{\text{in}}a^{\text{in}})d^{\text{in}} \end{bmatrix} \in R^{d^{\text{in}} \times a^{\text{in}}b^{\text{in}}}.$$
(85)

Because every element in

$$\phi(Z^{\mathrm{in},i}) \in R^{hhd^{\mathrm{in}} \times a^{\mathrm{out}}b^{\mathrm{out}}},$$

is extracted from $Z^{\text{in},i}$, the task is to find the mapping between each element in $\phi(Z^{\text{in},i})$ and a linear index of $Z^{\text{in},i}$. Consider the following example.

$$a^{\text{in}} = 3, \ b^{\text{in}} = 2, \ d^{\text{in}} = 1, \ s = 1, \ h = 2.$$

Because $d^{in} = 1$, we omit the channel subscript. In addition, we omit the instance index *i*, so the image is

$$\begin{bmatrix} z_{11} & z_{12} \\ \\ z_{21} & z_{22} \\ \\ z_{31} & z_{32} \end{bmatrix}$$

By our representation in (5),

$$Z^{\rm in} = \begin{bmatrix} z_{11} & z_{21} & z_{31} & z_{12} & z_{22} & z_{32} \end{bmatrix}$$

and the linear indices from (85) are

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \end{bmatrix}$$

column-oriented setting.

⁴Linear indices refer to the sequence of how elements in a matrix are stored. Here we consider a

From (9),

$$\phi(Z^{\text{in}}) = \begin{bmatrix} z_{11} & z_{21} \\ z_{21} & z_{31} \\ z_{12} & z_{22} \\ z_{22} & z_{32} \end{bmatrix}.$$

Thus we store the following vector to indicate the mapping between linear indices of Z^{in} and elements in $\phi(Z^{in})$.

$$\begin{bmatrix} 1 & 2 & 4 & 5 & 2 & 3 & 5 & 6 \end{bmatrix}^T .$$
 (86)

It also corresponds to column indices of non-zero elements in P_{ϕ}^{m} .

To have a general setting we begin with checking how linear indices of $Z^{\text{in},i}$ can be mapped to the first column of $\phi(Z^{\text{in},i})$. For simplicity, we consider only channel j. From (9) and (85), we have

where the left column gives the linear indices in $Z^{in,i}$, while the right column shows the

corresponding values. We rewrite linear indices in (87) as

Clearly, every linear index in (88) can be represented as

$$(p+qa^{\rm in})d^{\rm in}+j,\tag{89}$$

where

$$p, q \in \{0, \dots, h-1\}$$

correspond to the pixel position in the convolutional filter.⁵

Next we consider other columns in $\phi(Z^{\text{in},i})$ by still fixing the channel to be j. From (9), similar to the right column in (87), each column contains the following elements from the *j*th channel of $Z^{\text{in},i}$.

$$z_{1+p+as,1+q+bs,j}^{\text{in},i}, \ a = 0, 1, \dots, a^{\text{out}} - 1,$$

 $b = 0, 1, \dots, b^{\text{out}} - 1,$ (90)

 $⁵_{More precisely, p+1 and q+1 are the pixel position.}$

where (1 + as, 1 + bs) denotes the top-left position of a sub-image in the channel j of $Z^{\text{in},i}$. From (85), the linear index of each element in (90) is

$$((1+p+as-1)+(1+q+bs-1)a^{in})d^{in}+j = (a+ba^{in})sd^{in}+\underbrace{(p+qa^{in})d^{in}+j}_{see (89)}.$$
(91)

Now we have known for each element of $\phi(Z^{\text{in},i})$ what the corresponding linear index in $Z^{\text{in},i}$ is. Next we discuss the implementation details, where the code is shown in Listing 1. First, we compute elements in (88) with j = 1 by applying *MATLAB*'s '+' operator, which has the implicit expansion behavior, to compute the outer sum of the following two arrays.

$$\begin{bmatrix} 1 \\ d^{\text{in}} + 1 \\ \vdots \\ (h-1)d^{\text{in}} + 1 \end{bmatrix} \text{ and } \begin{bmatrix} 0 & a^{\text{in}}d^{\text{in}} & \dots & (h-1)a^{\text{in}}d^{\text{in}} \end{bmatrix}.$$

The result is the following matrix

$$\begin{bmatrix} 1 & a^{in}d^{in} + 1 & \dots & (h-1)a^{in}d^{in} + 1 \\ d^{in} + 1 & (1+a^{in})d^{in} + 1 & \dots & (1+(h-1)a^{in})d^{in} + 1 \\ \vdots & \vdots & \dots & \vdots \\ (h-1)d^{in} + 1 & ((h-1)+a^{in})d^{in} + 1 & \dots & ((h-1)+(h-1)a^{in})d^{in} + 1 \end{bmatrix},$$
(92)

-

whose columns, if concatenated, lead to values in (88) with j = 1; see line 3 of the code. To get (89) for all channels $j = 1, ..., d^{in}$, we compute the outer sum of the vector form of (92) and

$$\begin{bmatrix} 0 & 1 & \dots & d^{\mathrm{in}} - 1 \end{bmatrix};$$

and then vectorize the resulting matrix; see line 4.

To obtain other columns in $\phi(Z^{\text{in},i})$, we first calculate a^{out} and b^{out} by (4) in lines 5-6. In the linear indices in (91), the second term corresponds to indices of the first column, while the first term is the following column offset

$$(a + ba^{in})sd^{in}, \ \forall a = 0, 1, \dots, a^{out} - 1,$$

 $b = 0, 1, \dots, b^{out} - 1.$

This is the outer sum of the following two arrays.

$$\begin{bmatrix} 0\\ \vdots\\ a^{\text{out}} - 1 \end{bmatrix} \times sd^{\text{in}} \quad \text{and} \quad \begin{bmatrix} 0 & \dots & b^{\text{out}} - 1 \end{bmatrix} \times a^{\text{in}}sd^{\text{in}};$$

see line 7 in the code. Finally, we compute the outer sum of the column offset and the linear indices in the first column of $\phi(Z^{\text{in},i})$; see line 8. In the end what we keep is the following vector

$$\begin{bmatrix} \text{Column index of non-zero} \\ \text{in each row of } P_{\phi}^{m} \end{bmatrix}_{hhd^{\text{in}a^{\text{out}b^{\text{out}}}}}.$$
(93)

Note that each row in the 0/1 matrix P_{ϕ}^m contains exactly only one non-zero element. We also see that (86) is an example of (93).

The obtained linear indices are independent of the values of $Z^{\text{in},i}$. Thus the above procedure only needs to be run once in the beginning. For any $Z^{\text{in},i}$, we apply the indices in (93) to extract $\phi(Z^{\text{in},i})$; see line 21-22 in Listing 1.

For the pooling operation $\phi(Z^{\text{in},i})$ is needed in (15). The same implementation can be used.

4.2 Construction of $P_{pool}^{m,i}$

Following (18), we use $Z^{in,i}$ and $Z^{out,i}$ to represent the input

$$\sigma(S^{m,i}) \in R^{d^{m+1} \times a^m_{\rm conv} b^m_{\rm conv}}$$

and the output

$$Z^{m+1,i} \in R^{d^{m+1} \times a^{m+1}b^{m+1}}$$

of the pooling operation, respectively. We need to store $P_{\text{pool}}^{m,i}$ because, besides function evaluations, it is used in gradient and Jacobian evaluations; see (56) and (67).⁶ From (19), we need both $P_{\phi}^{m,i}$ and $W^{m,i}$. Because $P_{\phi}^{m,i}$ is for partitioning each image to nonoverlapping sub-regions in (15) and (16), it is iteration independent. We obtain it in the beginning of the training procedure by the method in Section 4.1.

For $W^{m,i}$, it is iteration dependent because the maximal value of each sub-image is not a constant. Therefore, we construct

$$P_{\text{pool}}^{m,i} = W^{m,i} P_{\phi}^{m,i} \in R^{d^{m+1}a^{m+1}b^{m+1} \times d^{m+1}a^m_{\text{conv}}b^m_{\text{conv}}}$$

at the beginning of each Newton iteration, where a *MATLAB* implementation is given in Listing 2.

To begin, we get

$$Z^{\mathrm{in},i}, \ i = 1, \dots, l, \tag{94}$$

which are stored as a matrix in (82). Because (16) may not hold with a^{out} and b^{out} being integers, we consider a setting the same as (4). In line 11, we extract the linear indices

⁶Note that we do not really generate a sparse matrix $P_{\text{pool}}^{m,i}$ in (18). We only store column indices of non-zeros in $P_{\text{pool}}^{m,i}$.

of $Z^{\text{in},i}$ to appear in $\text{vec}(\phi(Z^{\text{in},i}))$, which as we mentioned has been generated in the beginning of the training procedure. The resulting vector P contains

$$hhd^{m+1}a^{m+1}b^{m+1}$$

elements and each element is in the range of

1, ...,
$$d^{m+1}a^m_{\text{conv}}b^m_{\text{conv}}$$

In line 12-13, we use P to generate

$$\left[\operatorname{vec}(\phi(Z^{\operatorname{in},1})) \cdots \operatorname{vec}(\phi(Z^{\operatorname{in},l}))\right] \in R^{hhd^{m+1}a^{m+1}b^{m+1} \times l}.$$
(95)

Next we rewrite the above matrix so that each column contains a sub-region:

$$\begin{bmatrix} z_{1,1,1}^{m,1} & z_{1,1,2}^{m,1} & \dots & z_{1+(a^{m+1}-1)\times s,1+(b^{m+1}-1)\times s,d^{m+1}} \\ \vdots & \vdots & \ddots & \vdots \\ z_{h,h,1}^{m,1} & z_{h,h,2}^{m,1} & \dots & z_{h+(a^{m+1}-1)\times s,h+(b^{m+1}-1)\times s,d^{m+1}}^{m,1} \end{bmatrix} \in R^{hh \times d^{m+1}a^{m+1}b^{m+1}l}.$$
 (96)

We apply a max function to get the largest value of each column and its index in the range of $1, \ldots, hh$. The resulting row vector has $d^{m+1}a^{m+1}b^{m+1}l$ elements; see line 14. In line 15, we reformulate it to be

$$d^{m+1} \times a^{m+1} b^{m+1} l$$

as the output $Z^{\text{out},i}, \forall i$.

Next we find linear indices that correspond to the largest elements obtained from (96). Because of operations discussed in Section III of supplementary materials, we decide to record linear indices in each $Z^{\text{in},i}$ corresponding to the selected elements, rather than linear indices in the whole matrix (82) of all $Z^{m,i}$, $\forall i$. We begin with

obtaining the following vector of linear indices of $Z^{in,i}$:

$$\begin{bmatrix} 1 \\ \vdots \\ d^{m+1}a^m_{\text{conv}}b^m_{\text{conv}} \end{bmatrix}.$$
(97)

Then we generate

$$\phi((97)),\tag{98}$$

which has $hhd^{m+1}a^{m+1}b^{m+1}$ elements; see line 22. Next, we mentioned that in line 14, not only the maximal value in each sub-region is obtained, but also the corresponding index in $\{1, \ldots, hh\}$ is derived. Therefore, for the selected max values of all instances, their positions in the range of

$$1, \ldots, hhd^{m+1}a^{m+1}b^{m+1}$$

are

$$\operatorname{mat}\left(\begin{bmatrix} \operatorname{row indices of} \\ \max \text{ values in (96)} \end{bmatrix} \right)_{d^{m+1}a^{m+1}b^{m+1} \times l} + hh\left(\begin{bmatrix} 0 \\ \vdots \\ d^{m+1}a^{m+1}b^{m+1} - 1 \end{bmatrix} \otimes \mathbb{1}_{l}^{T} \right);$$
(99)

see line 19. Next in line 23 we use (99) to extract values in (98) and obtain linear indices of the selected max values in each $Z^{in,i}$. To be more precise, the resulting matrix is

$$\begin{bmatrix} \text{Column index of non-zero} & \text{Column index of non-zero} \\ & \dots & \\ \text{in each row of } P_{\text{pool}}^{m,1} & \text{in each row of } P_{\text{pool}}^{m,l} \end{bmatrix} \in R^{d^{m+1}a^{m+1}b^{m+1} \times l}.$$
(100)

The reason is that because $P_{\text{pool}}^{m,i}$ is a 0/1 matrix and each row contains exactly only one value "1" to indicate the selected entry by max pooling, we collects the column index of the non-zero at each row to be a vector for future use.

4.3 Details of Padding Operation

To implement zero-padding, we first capture the linear indices of the input image in the padded image. For example, if the size of the input image is 3×3 and the output padded image is 5×5 , we have

0	0	0	0	0	
0	1	1	1	0	
0	1	1	1	0	,
0	1	1	1	0	
0	0	0	0	0	

where "1" values indicate positions of the input image. Based on the column-major order, we derive

 $pad_idx = \{7, 8, 9, 11, 12, 13, 16, 17, 18\}.$

This index set, obtained in the beginning of the training procedure, is used in the following situations. First, pad_idx contains row indices in P_{pad}^m of (14) that correspond to the input image. We can use it to conduct the padding operation in (14). Second, from (58) and (68) in gradient and Jacobian evaluations, we need

$$\boldsymbol{v}^T P_{\mathrm{pad}}^m$$
.

This can be considered as the inverse of the padding operation: we would like to remove zeros and get back the original image. We give details of finding pad_idx in Section II of supplementary materials.

4.4 Evaluation of $(v^i)^T P_{\phi}^m$ and $(v^i)^T P_{\text{pool}}^{m,i}$ in Gradient and Jacobian Evaluations

We show that several operations in gradient and Jacobian evaluations are either $(\boldsymbol{v}^i)^T P_{\phi}^m$ or $(\boldsymbol{v}^i)^T P_{\text{pool}}^{m,i}$, where \boldsymbol{v}^i is a vector. They can be calculated by a similar program. We give Listing 4 to conduct these operations with details explained below.

4.4.1 Evaluation of $(\boldsymbol{v}^i)^T P_{\phi}^m$

For (58) and (68), the following operation is applied.

$$(\boldsymbol{v}^i)^T P^m_\phi, \tag{101}$$

where

$$\boldsymbol{v}^{i} = \operatorname{vec}\left((W^{m})^{T} \frac{\partial \xi_{i}}{\partial S^{m,i}} \right)$$

for (58) and

$$\boldsymbol{v}_{u}^{i} = \operatorname{vec}\left((W^{m})^{T} \frac{\partial z_{u}^{L+1,i}}{\partial S^{m,i}} \right), \ u = 1, \dots, n_{L+1}$$
(102)

for (68).

Consider the same example in Section 4.1. We note that

$$(P_{\phi}^{m})^{T} \boldsymbol{v}^{i} = \left[v_{1} \ v_{2} + v_{5} \ v_{6} \ v_{3} \ v_{4} + v_{7} \ v_{8} \right]^{T},$$
(103)

which is a kind of "inverse" operation of $\phi(\text{pad}(Z^{m,i}))$: we accumulate elements in $\phi(\text{pad}(Z^{m,i}))$ back to their original positions in $\text{pad}(Z^{m,i})$. In *MATLAB*, given indices in (86), a function accumarray can directly generate the vector (103).

To calculate (58) over a batch of instances, we aim to have

$$\begin{bmatrix} (P_{\phi}^{m})^{T} \boldsymbol{v}^{1} \\ \vdots \\ (P_{\phi}^{m})^{T} \boldsymbol{v}^{l} \end{bmatrix}^{T} .$$
(104)

We can manage to apply MATLAB's accumarray on the vector

$$\begin{bmatrix} \boldsymbol{v}^{1} \\ \vdots \\ \boldsymbol{v}^{l} \end{bmatrix}, \qquad (105)$$

by giving the following indices as the input.

$$\begin{bmatrix} (93) \\ (93) + a_{pad}^{m} b_{pad}^{m} d^{m} \mathbb{1}_{h^{m}h^{m}d^{m}a_{conv}^{m}b_{conv}^{m}} \\ (93) + 2a_{pad}^{m} b_{pad}^{m} d^{m} \mathbb{1}_{h^{m}h^{m}d^{m}a_{conv}^{m}b_{conv}^{m}} \\ \vdots \\ (93) + (l-1)a_{pad}^{m} b_{pad}^{m} d^{m} \mathbb{1}_{h^{m}h^{m}d^{m}a_{conv}^{m}b_{conv}^{m}} \end{bmatrix},$$
(106)

where from Section 2.1.3,

$$a_{pad}^{m}b_{pad}^{m}d^{m}$$
 is the size of $pad(Z^{m,i})$, and
 $h^{m}h^{m}d^{m}a_{conv}^{m}b_{conv}^{m}$ is the size of $\phi(pad(Z^{m,i}))$ and \boldsymbol{v}_{i} .

That is, by using the offset $(i - 1)a_{pad}^m b_{pad}^m d^m$, accumarray accumulates v^i to the following positions:

$$(i-1)a_{\rm pad}^{m}b_{\rm pad}^{m}d^{m}+1, \ \dots, \ ia_{\rm pad}^{m}b_{\rm pad}^{m}d^{m}.$$
 (107)

To obtain (105), we can do a matrix-matrix multiplication as follows.

$$(105) = \operatorname{vec}\left((W^m)^T \begin{bmatrix} \frac{\partial \xi_1}{\partial S^{m,1}} & \dots & \frac{\partial \xi_l}{\partial S^{m,l}} \end{bmatrix} \right).$$
(108)

From (108), we can see why $\partial \xi_i / \partial \text{vec}(S^{m,i})^T$ over a batch of instances are stored in the form of (83). In line 26, the indices shown in (106) are generated and the variable V(:) in line 31 is the vector (105) calculated by (108).

To calculate (68) over a batch of instances, similar to (104) we conduct

$$\begin{bmatrix} (P_{\phi}^{m})^{T} \boldsymbol{v}_{1}^{1} \\ \vdots \\ (P_{\phi}^{m})^{T} \boldsymbol{v}_{n_{L+1}}^{1} \\ \vdots \\ (P_{\phi}^{m})^{T} \boldsymbol{v}_{n_{L+1}}^{l} \end{bmatrix}^{T}, \qquad (109)$$

where

$$\boldsymbol{v}_{u}^{i} = \operatorname{vec}\left((W^{m})^{T} \frac{\partial z_{u}^{L+1,i}}{\partial S^{m,i}}\right) \in R^{h^{m}h^{m}d^{m}a_{\operatorname{conv}}^{m}b_{\operatorname{conv}}^{m}\times 1}, \ u = 1, \dots, n_{L+1}$$

Similar to (108), we can calculate the vector

$$\begin{bmatrix} \boldsymbol{v}_{1}^{1} \\ \vdots \\ \boldsymbol{v}_{n_{L+1}}^{1} \\ \vdots \\ \boldsymbol{v}_{n_{L+1}}^{l} \end{bmatrix}$$
(110)

by

$$\operatorname{vec}\left((W^m)^T \begin{bmatrix} \frac{\partial z_1^{L+1,1}}{\partial S^{m,1}} & \cdots & \frac{\partial z_{n_{L+1}}^{L+1,1}}{\partial S^{m,1}} & \cdots & \frac{\partial z_{n_{L+1}}^{L+1,l}}{\partial S^{m,l}} \end{bmatrix} \right).$$
(111)

The formulation in (111) leads us to store

$$\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})}, \; \forall i$$

in the form of (84).

From (109), because each vector \boldsymbol{v}_u^i is accumulated to the following positions:

$$((i-1)n_{L+1} + (u-1))a_{\text{pad}}^m b_{\text{pad}}^m d^m + 1, \dots, ((i-1)n_{L+1} + u)a_{\text{pad}}^m b_{\text{pad}}^m d^m,$$

we can apply accumarray on the vector (110) with the following input indices.

$$\begin{bmatrix} (93) \\ \vdots \\ (93) + (n_{L+1} - 1)d^{m}a_{pad}^{m}b_{pad}^{m}\mathbb{1}_{h^{m}h^{m}d^{m}a_{conv}^{m}b_{conv}^{m}} \\ \vdots \\ (93) + (n_{L+1}l - 1)d^{m}a_{pad}^{m}b_{pad}^{m}\mathbb{1}_{h^{m}h^{m}d^{m}a_{conv}^{m}b_{conv}^{m}} \end{bmatrix}.$$
(112)

The implementation is the same as that for evaluating (58), except that (109) involves $n_{L+1}l$ vectors rather than l.

4.4.2 Evaluation of $(\boldsymbol{v}^i)^T P_{\text{pool}}^{m,i}$

We discuss details in supplementary materials.

4.5 Gauss-Newton Matrix-Vector Products

To derive (74), we first calculate

$$\begin{bmatrix} \sum_{m=1}^{L} J^{m,1} \boldsymbol{v}^{m} \\ \vdots \\ \sum_{m=1}^{L} J^{m,l} \boldsymbol{v}^{m} \end{bmatrix} \in R^{n_{L+1}l \times 1}.$$
 (113)

From (76), for a particular m, we have

$$\begin{bmatrix} J^{m,1}\boldsymbol{v}^{m} \\ \vdots \\ J^{m,l}\boldsymbol{v}^{m} \end{bmatrix} = \begin{bmatrix} \frac{\partial \boldsymbol{z}^{L+1,1}}{\partial \operatorname{vec}(S^{m,1})^{T}} \operatorname{vec} \left(\operatorname{mat}(\boldsymbol{v}^{m}) \begin{bmatrix} \phi(\operatorname{pad}(Z^{m,1})) \\ \mathbb{1}_{a_{\operatorname{conv}}b_{\operatorname{conv}}}^{T} \end{bmatrix} \right) \\ \vdots \\ \frac{\partial \boldsymbol{z}^{L+1,l}}{\partial \operatorname{vec}(S^{m,l})^{T}} \operatorname{vec} \left(\operatorname{mat}(\boldsymbol{v}^{m}) \begin{bmatrix} \phi(\operatorname{pad}(Z^{m,l})) \\ \mathbb{1}_{a_{\operatorname{conv}}b_{\operatorname{conv}}}^{T} \end{bmatrix} \right) \end{bmatrix}$$
$$= \begin{bmatrix} \frac{\partial \boldsymbol{z}^{L+1,l}}{\partial \operatorname{vec}(S^{m,1})^{T}} \boldsymbol{p}^{m,1} \\ \vdots \\ \frac{\partial \boldsymbol{z}^{L+1,l}}{\partial \operatorname{vec}(S^{m,l})^{T}} \boldsymbol{p}^{m,l} \end{bmatrix}, \qquad (114)$$

where

$$\operatorname{mat}(\boldsymbol{v}^m) \in R^{d^{m+1} \times (h^m h^m d^m + 1)}$$

and

$$\boldsymbol{p}^{m,i} = \operatorname{vec}\left(\operatorname{mat}(\boldsymbol{v}^{m}) \begin{bmatrix} \phi(\operatorname{pad}(Z^{m,i})) \\ \mathbb{1}_{a_{\operatorname{conv}}^{T} b_{\operatorname{conv}}^{m}} \end{bmatrix}\right).$$
(115)

A MATLAB implementation for (113) is shown in Listing 5. Given v^m , we calcu-

late

$$\operatorname{mat}(\boldsymbol{v}^{m}) \begin{bmatrix} \phi(\operatorname{pad}(Z^{m,1})) & \cdots & \phi(\operatorname{pad}(Z^{m,l})) \\ 1 & 1 \\ 1 \\ a_{\operatorname{conv}}^{T} b_{\operatorname{conv}}^{T} & \cdots & 1 \\ 1 \\ a_{\operatorname{conv}}^{T} b_{\operatorname{conv}}^{T} \end{bmatrix} \in R^{d^{m+1} \times a_{\operatorname{conv}}^{m} b_{\operatorname{conv}}^{m}l}; \quad (116)$$

see line 24. Next, we calculate

$$J^{m,i}\boldsymbol{v}^m = \frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})^T} \boldsymbol{p}^{m,i}, \ i = 1, \dots, l.$$
(117)

Because (117) involves l independent matrix-vector products, we consider the following trick to avoid a for loop in a *MATLAB* script. We note that (117) can be calculated by

summing up all rows of the following matrix

$$\left[\frac{\partial z_1^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})}\cdots \frac{\partial z_{n_{L+1}}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})}\right]_{d^{m+1}a_{\operatorname{conv}}^m b_{\operatorname{conv}}^m \times n_{L+1}} \odot \left[\boldsymbol{p}^{m,i}\cdots \boldsymbol{p}^{m,i}\right]_{d^{m+1}a_{\operatorname{conv}}^m b_{\operatorname{conv}}^m \times n_{L+1}}.$$
(118)

The result will be a row vector of $1 \times n_{L+1}$, which is the transpose of $J^{m,i} \boldsymbol{v}^m$. To do the above operation on all instances together, we reformulate (84) and (116) respectively to the following three-dimensional matrices:

$$d^{m+1}a^m_{\text{conv}}b^m_{\text{conv}} \times n_{L+1} \times l$$
 and $d^{m+1}a^m_{\text{conv}}b^m_{\text{conv}} \times 1 \times l$.

We then apply the . * operator in *MATLAB* and sum results along the first dimension; see line 25. The resulting matrix has the size

$$1 \times n_{L+1} \times l$$

and can be aggregated to the vector in (114); see line 26.

After deriving (113), from (77), we must calculate

$$\boldsymbol{q} = \begin{bmatrix} \boldsymbol{q}^{1} \\ \vdots \\ \boldsymbol{q}^{l} \end{bmatrix} = \begin{bmatrix} B^{1} \sum_{m=1}^{L} J^{m,1} \boldsymbol{v}^{m} \\ \vdots \\ B^{l} \sum_{m=1}^{L} J^{m,l} \boldsymbol{v}^{m} \end{bmatrix}.$$
 (119)

From (78), (119) can be derived by multiplying every element of (113) by two.

Next, for each layer m, from (74) and (79) we calculate

$$\sum_{i=1}^{l} J^{m,i} \boldsymbol{q}^{i}$$

$$= \sum_{i=1}^{l} \operatorname{vec} \left(\operatorname{mat} \left(\left(\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})^{T}} \right)^{T} \boldsymbol{q}^{i} \right)_{d^{m+1} \times a_{\operatorname{conv}}^{m} b_{\operatorname{conv}}^{m}} \left[\phi(\operatorname{pad}(Z^{m,i}))^{T} \mathbb{1}_{a_{\operatorname{conv}}^{m} b_{\operatorname{conv}}^{m}} \right] \right)$$
(120)

$$= \operatorname{vec} \left(\begin{bmatrix} \operatorname{mat}(\boldsymbol{u}^{m,1})_{d^{m+1} \times a^m_{\operatorname{conv}} b^m_{\operatorname{conv}}} & \dots & \operatorname{mat}(\boldsymbol{u}^{m,l})_{d^{m+1} \times a^m_{\operatorname{conv}} b^m_{\operatorname{conv}}} \end{bmatrix} \begin{bmatrix} \phi(\operatorname{pad}(Z^{m,1}))^T & \mathbb{1}_{a^m_{\operatorname{conv}} b^m_{\operatorname{conv}}} \\ \vdots & \vdots \\ \phi(\operatorname{pad}(Z^{m,l}))^T & \mathbb{1}_{a^m_{\operatorname{conv}} b^m_{\operatorname{conv}}} \end{bmatrix} \right)$$
(121)

where

$$\boldsymbol{u}^{m,i} = \left(\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})^T}\right)^T \boldsymbol{q}^i.$$

A *MATLAB* implementation for (121) is shown in Listing 6. To begin, we have the matrix (84) and the vector q in (119). We reshape (84) to

$$\begin{bmatrix} \frac{\partial z_1^{L+1,1}}{\partial \operatorname{vec}(S^{m,1})} & \dots & \frac{\partial z_{n_{L+1}}^{L+1,1}}{\partial \operatorname{vec}(S^{m,1})} & \dots & \frac{\partial z_{n_{L+1}}^{L+1,l}}{\partial \operatorname{vec}(S^{m,l})} \end{bmatrix} \in R^{d^{m+1}a_{\operatorname{conv}}^m b_{\operatorname{conv}}^m \times n_{L+1}l}.$$
 (122)

Then we calculate

$$egin{bmatrix} oldsymbol{u}^{m,1} & \dots & oldsymbol{u}^{m,l} \end{bmatrix}$$

together by reshaping

$$\left[(122) \right] \odot \left(\mathbb{1}_{d^{m+1} a_{\text{conv}}^m b_{\text{conv}}^m} \boldsymbol{q}^T \right) \in R^{d^{m+1} a_{\text{conv}}^m b_{\text{conv}}^m \times n_{L+1} l}$$
(123)

to

$$R^{d^{m+1}a^m_{\rm conv}b^m_{\rm conv}\times n_{L+1}\times l}$$

and summing along the second dimension; see line 26-27. Finally, we calculate (121) in line 28.

4.6 Mini-Batch Function and Gradient Evaluation

Later in Section 5.1 we discuss details of memory usage, where one important conclusion is that in several places of the Newton method, the memory consumption is proportional to the number of data. This fact causes difficulties in handling large data sets, so here we discuss some implementation techniques to reduce the memory usage.

In the subsampled Newton method discussed in Section 3.1, a subset S of the training data is used to derive the subsampled Gauss-Newton matrix for approximating the Hessian matrix. While a motivation of this technique is to trade a slightly less accurate direction for shorter running time per iteration, it also effectively reduces the memory consumption. For example, at the *m*th convolutional layer, we only need to store the following matrices

$$\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})^T}, \ \forall i \in S$$
(124)

for the Gauss-Newton matrix-vector products.

However, in function and gradient evaluations we still need the whole training data. Fortunately, both operations involve the summation of independent results over all instances, so we follow Wang et al. (2018) to have a mini-batch setting. By splitting the index set $\{1, \ldots, l\}$ of data to, for example, R equal-sized subsets S_1, \ldots, S_R , we sequentially calculate the result corresponding to each subset and accumulate them for the final output. Take the function evaluation as an example. For each subset, we must store only

$$Z^{m,i}, \forall m, \forall i \in S_r$$

so the memory usage can be dramatically reduced.

For the Gauss-Newton matrix-vector product, to calculate (124) under the subsampled scheme, we have a set S and use $Z^{m,i}$, $\forall i \in S$. However, under the mini-batch setting, the needed values may not be kept in the process of function evaluations. Our strategy is to let the last subset S_R be the same subset used for the sub-sampled Hessian. Then we can preserve the needed $Z^{m,i}$ for Gauss-Newton matrix-vector products.

5 Analysis of Newton Methods for CNN

In this section, based on the implementation details in Section 4, we analyze the memory and computational cost per iteration. We consider that all training instances are used. If the subsampled Hessian in Section 3 is considered, then in the Jacobian calculation and the Gauss-Newton matrix vector products, the number of instances l should be replaced by the subset size |S|. Furthermore, if mini-batch function and gradient evaluation in Section 4.6 is applied, the number of instance l in the function and gradient evaluation can also be replaced by |S|.⁷

In this discussion we exclude the padding and the pooling operations because first they are optional steps and second they are not the bottleneck. In addition, for simplicity, the bias term is not considered.

5.1 Memory Requirement

(1) Weight matrix: For every layer, we must store

$$W^m, m = 1, \ldots, L.$$

From (10) and (22), the memory usage is

$$\sum_{m=1}^{L^{c}} \left(d^{m+1} h^{m} h^{m} d^{m} \right) + \sum_{m=L^{c}+1}^{L} \left(n_{m+1} n_{m} \right) + \sum_{m=1}^{L^{c}} \left(n_{m+1} n_{m} n_{m} \right) + \sum_{m=1}^{L^{c}} \left(n_{m+1} n_{m} n_{m} \right) + \sum_{m=1}^{L^{c}} \left(n_{m+1} n_{m} n_{m} \right) + \sum_{m=1}^{L^{c}} \left(n_{m} n_{m} n_{m} n_{m} \right) + \sum_{m=1}^{L^{c}} \left(n_{m} n_{$$

⁷We mentioned in Section 4.6 that for simplicity, we set the mini-batch size be |S| in order to cooperate with the subsampled Hessian Newton methods.

(2) Gradient vector: For (41), the following matrix must be stored.

$$\frac{\partial f}{\partial \operatorname{vec}(W^m)^T}, \ m = 1, \dots, L.$$

Therefore, the memory usage is

$$\sum_{m=1}^{L^{c}} \left(d^{m+1} h^{m} h^{m} d^{m} \right) + \sum_{m=L^{c}+1}^{L} \left(n_{m+1} n_{m} \right).$$

(3) P_{ϕ}^{m} : In Section 4.1, we store each position's corresponding linear index in $Z^{m,i}$ in order to construct $\phi(Z^{m,i})$. The memory usage is

$$\sum_{m=1,\ldots,L^c} \left(h^m h^m d^m a^m_{\rm conv} b^m_{\rm conv} \right).$$

(4) Function evaluation: From Section 2, we store

$$Z^{m,i}, m = 1, \dots, L+1, \forall i.$$

Therefore, the memory usage is

$$l \times \left(\sum_{m=1}^{L^{c}} d^{m} a^{m} b^{m} + \sum_{m=L^{c}+1}^{L+1} n_{m}\right).$$
(125)

(5) $\phi(\operatorname{pad}(Z^{m,i}))$: From (11), (51), (76), and (79), $\phi(\operatorname{pad}(Z^{m,i}))$ is temporarily needed and its memory usage is

$$l \times \max_{m=1,\dots,L^c} \left(h^m h^m d^m a^m_{\text{conv}} b^m_{\text{conv}} \right).$$

Comparing to (125), the temporary memory for $\phi(pad(Z^{m,i}))$ is insignificant.

(6) Gradient evaluation: To obtain the gradient in each layer m, we also need to have the matrix

$$\frac{\partial \xi_i}{\partial \operatorname{vec}(S^{m,i})^T}$$

for calculating

$$\frac{\partial \xi_i}{\partial \text{vec}(S^{m-1,i})^T}$$

in the backward process. Note that there is no need to keep the matrices of all layers. All we have to store is the matrices for two adjacent layers. Thus, the memory usage is

$$l \times \max_{m=1,\dots,L^c} \left(d^m a^m_{\operatorname{conv}} b^m_{\operatorname{conv}} + d^{m+1} a^{m+1}_{\operatorname{conv}} b^{m+1}_{\operatorname{conv}} \right)$$

for the convolutional layers and

$$l \times \max_{m=L^c+1,...,L} (n_m + n_{m+1}).$$

for the fully-connected layers. This is much smaller than (125).

(7) Jacobian evaluation and Gauss-Newton matrix-vector products: Besides W^m and $Z^{m,i}$, from (76), (79), (80) and (81), we explicitly store

$$\frac{\partial \boldsymbol{z}^{L+1,i}}{\partial \operatorname{vec}(S^{m,i})^T}, \ m = 1, \dots, L, \ \forall i.$$

Thus, the memory usage is 8 .

$$l \times n_{L+1} \times \left(\sum_{m=1}^{L^c} d^{m+1} a^m_{\text{conv}} b^m_{\text{conv}} + \sum_{m=L^c+1}^L n_{m+1}\right).$$
 (126)

From the above discussion, (125) dominate the memory usage in the function and Gradient evaluation. On the other hand, (126) is the main cost for the Jacobian evaluation and Gauss-Newton matrix-vector products. The bottleneck is (126) because it is n_{L+1} times more than (125). To reduce the memory consumption, as mentioned, the sub-sampled Hessian technique in Section 3 reduces the usage in (126), while for (125) we use the mini-batch function and gradient evaluation in Section 4.6.

⁸Note that the dimension of $s^{m,i}$ is $R^{n_{m+1}}$.

5.2 Computational Cost

We show the computational cost for the *m*th convolutional/fully-connected layer.

- (1) Function evaluation:
 - Convolutional layers: From (8), (11), and (12), the computational cost is

$$\mathcal{O}(l \times h^m h^m d^m d^{m+1} a^m_{\text{conv}} b^m_{\text{conv}}).$$

• Fully-connected layers: From (23) and (24), the computational cost is

$$\mathcal{O}(l \times n_{m+1}n_m)$$

- (2) Gradient evaluation:
 - Convolutional layers: For (51), the computational cost is

$$\mathcal{O}(l \times h^m h^m d^m d^{m+1} a^m_{\text{conv}} b^m_{\text{conv}}).$$

For (56), the computational cost is

$$\mathcal{O}(l \times d^m a^m b^m).$$

For (58), the computational cost is

$$\mathcal{O}(l \times h^m h^m d^m d^{m+1} a^m_{\text{conv}} b^m_{\text{conv}}).$$

Therefore, the total computational cost for the gradient evaluation is

$$\mathcal{O}(l \times h^m h^m d^m d^{m+1} a^m_{\text{conv}} b^m_{\text{conv}}).$$

• Fully-connected layers: From (59) and (61), the computational cost is

$$\mathcal{O}(l \times n_{m+1}n_m).$$

For (62), the cost is smaller. Therefore, the total computational cost is

$$\mathcal{O}(l \times n_{m+1}n_m).$$

(3) Jacobian evaluation:

• Convolutional layers: The main computational cost is from (68):

$$\mathcal{O}\left(l \times n_{L+1} \times h^m h^m d^m d^{m+1} a^m_{\text{conv}} b^m_{\text{conv}}\right),$$

while others are less significant.

• Fully-connected layers: From (71), the computational cost is

$$\mathcal{O}(l \times n_{L+1} \times n_{m+1}n_m).$$

(4) CG: The computational cost is the number of CG iterations (#CG) times the cost of a Gauss-Newton matrix-vector product.

• Convolutional layers: The main computational cost is from (76) and (79):

$$\mathcal{O}\left(\#\mathbf{CG} \times l \times d^{m+1}h^m h^m d^m a^m_{\mathrm{conv}} b^m_{\mathrm{conv}}\right),$$

while the cost of (78) is insignificant.

• Fully-connected layers: Similarly, the main computational cost is from (80) and (81):

$$\mathcal{O}(\#\mathbf{CG} \times l \times n_{m+1}n_m).$$

- (5) line search: The computational cost is on multiple function evaluations.
 - Convolutional layers:

$$\mathcal{O}\left(\text{#line search} \times l \times d^{m+1}h^m h^m d^m a^m_{\text{conv}} b^m_{\text{conv}}\right).$$

• Fully-connected layers:

$$\mathcal{O}($$
#line search $\times l \times n_{m+1}n_m).$

We summarize the cost in a convolutional layer. Clearly, the cost is proportional to the number of instances, l. After omitting the term $\mathcal{O}(h^m h^m d^m d^{m+1} a_{\text{conv}}^m b_{\text{conv}}^m)$ in all operations, their cost can be compared in the following way.

$$\underbrace{l}_{\text{function/gradient}} \underbrace{l \times n_{L+1}}_{\text{Jacobian}} \underbrace{\#\text{CG} \times l}_{\text{CG}} \underbrace{\#\text{line search} \times l}_{\text{line search}}.$$

In general, the number of line search steps is small, so the CG procedure is often the bottleneck. However, if the sub-sampled Hessian Newton method is applied, l is replaced by the size of the subset, |S|, for the cost in the Jacobian evaluation and CG. Then the bottleneck may be shifted to function/gradient evaluations.

The discussion for the fully-connected layers is omitted because the result is similar to the convolutional layers.

6 Experiments

We choose the following image data sets for experiments. All the data sets are publicly available⁹ and the summary is in Table 2.

- MNIST: This data set, containing hand-written digits, is a widely used benchmark for data classification (LeCun et al., 1998).
- SVHN: This data set consists of the colored images of house numbers (Netzer et al., 2011).

 $⁹_{See \, \text{https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/datasets/.}}$

Table 2: Summary of the data sets, where $a^1 \times b^1 \times d^1$ represents the (height, width, channel) of the input image, l is the number of training data, l_t is the number of test data, and n_{L+1} is the number of classes.

Data set	$a^1 \times b^1 \times d^1$	l	l_t	n_{L+1}
MNIST	$28 \times 28 \times 1$	60,000	10,000	10
SVHN	$32 \times 32 \times 3$	73,257	26,032	10
CIFAR10	$32 \times 32 \times 3$	50,000	10,000	10
smallNORB	$32 \times 32 \times 2$	24,300	24,300	5

- CIFAR10: This data set, containing colored images, is a commonly used classification benchmark (Krizhevsky and Hinton, 2009).
- smallNORB: This data set is built for 3D object recognition (LeCun et al., 2004).
 The original dimension is 96 × 96 × 2 because every object is taken two 96 × 96 grayscale images from the different angles. These two images are then placed in two channels. To reduce the training time, we downsample each channel of every object with the max pooling (h = 3, s = 3) to the dimension 32 × 32.

All the data sets were pre-processed by the following procedure.

(1) Min-max normalization. That is, for each pixel of every image $Z^{1,i}$, we have

$$Z_{a,b,d}^{1,i} \leftarrow \frac{Z_{a,b,d}^{1,i} - \min}{\max - \min},$$

where max/min is the maximum/minimum value of all pixels in $Z^{1,i}$.

(2) Zero-centering. This is commonly applied before training CNN (Krizhevsky et al., 2012; Zeiler and Fergus, 2014). That is, for every pixel in image $Z^{1,i}$, we have

$$Z_{a,b,d}^{1,i} \leftarrow Z_{a,b,d}^{1,i} - \operatorname{mean}(Z_{a,b,d}^{1,:}),$$

where mean $(Z_{a,b,d}^{1,:})$ is the per-pixel mean value across all the training images.

We consider two simple CNN structures shown in Table 3. The parameters used in our algorithm are given as follows. For the initialization, we follow He et al. (2015) to set the weight values by multiplying random values from the $\mathcal{N}(0, 1)$ distribution and

$$\sqrt{\frac{2}{n_{\rm in}^m}},$$

where

$$n_{\rm in}^m = \begin{cases} d^m \times h^m \times h^m & \text{if } m \leq L^c, \\ \\ n_m & \text{otherwise.} \end{cases}$$

For a CG procedure, it is terminated if the following relative stopping condition holds or the number of CG iterations reaches a maximal number of iterations (denoted as CG_{max}).

$$||(G + \lambda \mathcal{I})\boldsymbol{d} + \nabla f(\boldsymbol{\theta})|| \le \sigma ||\nabla f(\boldsymbol{\theta})||, \qquad (127)$$

where $\sigma = 0.1$ and $CG_{max} = 250$. For the implementation of the Levenberg-Marquardt method, we set the initial $\lambda_1 = 1$ and (drop, boost, ρ_{upper} , ρ_{lower}) constants in (38) are (2/3, 3/2, 0.75, 0.25). In addition, the sampling rate for the Gauss-Newton matrix is set to 5%. The value of C in (28) is set to 0.01*l*. We terminate the Newton method after 100 iterations.

	3-layer CNN			5-lay	layer CNN		
	filter size	#filters	stride	filter size	#filters	stride	
conv 1	$5 \times 5 \times 3$	32	1	$5 \times 5 \times 3$	32	1	
pool 1	2×2	_	2	2×2	_	2	
conv 2	$3 \times 3 \times 32$	64	1	$3 \times 3 \times 32$	32	1	
pool 2	2×2	_	2	-	_	-	
conv 3	$3 \times 3 \times 32$	64	1	$3 \times 3 \times 32$	64	1	
pool 3	2×2	_	2	2×2	-	2	
conv 4	-	_	-	$3 \times 3 \times 64$	64	1	
pool 4	-	-	-	-	-	-	
conv 5	-	-	-	$3 \times 3 \times 64$	128	1	
pool 5	-	-	-	2×2	-	2	
full 1	-	-	-	-	-	-	

Table 3: Structure of convolutional neural networks. "conv" indicates a convolutional layer, "pool" indicates a pooling layer, and "full" indicates a fully-connected layer.

6.1 Preliminary Comparison Between Newton and Stochastic Gradient Methods

The goal is to compare SG methods with the proposed subsampled Newton method for CNN. For SG methods, we consider a mini-batch SG implementation with momentum in the Python deep learning library, *Keras* (Chollet et al., 2015). To have a fair comparison between SG and subsampled Newton methods, the following settings are the same for both approaches.

- Initial weights.
- Network structures.
- Objective function.
- Regularization parameter.

The mini-batch size is 128 for all SG experiments. The initial learning rate is selected from $\{0.003, 0.001, 0.0003, 0.0001\}$ by five-fold cross validation.¹⁰ The learning rate is decayed by using *Keras*' default factor 10^{-6} and the momentum coefficient is set to be 0.9. We terminate the training process after 1,000 epochs.

The results are shown in Table 4. For some sets, the performance of the SG method by using more layers is inferior to that by fewer layers. It seems overfitting occurs, so a tuning on SG's termination criterion may be needed. Overall, we see that under the same initial settings, the test accuracy of the subsampled Newton method (with the 5% sampling rate) is comparable to that of SG.

 $¹⁰_{We}$ use a stratified split of data in the cross validation procedure.

Table 4: Test accuracy by Newton and SG methods. We run 100 Newton iterations, while for SG, we run 1,000 epochs.

	3-layer CNN		5-laye	5-layer CNN		
	Newton	SG	Newton	SG		
MNIST	99.28%	99.22%	99.45%	99.40%		
SVHN	92.72%	93.00%	94.14%	94.46%		
CIFAR10	78.52%	80.17%	79.72%	79.65%		
smallNORB	95.01%	95.29%	95.55%	93.99%		

One question is how long the Newton method takes in comparison with SG. Our preliminary finding is that Newton is slower but not significant slower. However, in our settings, a single optimization problem is solved by the Newton method, while for SG, a cross validation procedure is conducted to select the initial learning rate. The selection procedure is known to be essential because of SG's high sensitivity on this parameter. If we take the cross-validation procedure into consideration, the overall cost of SG is higher. A thorough timing comparison is much needed and we leave it as a future research issue.

7 Conclusions

In this study, we establish all the building blocks of Newton methods for CNN. A simple and effective *MATLAB* implementation is developed for public use. Based on our

results, it is possible to further enhance Newton methods for CNN.

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A List of Symbols

Notation	Description
$oldsymbol{y}^i$	The label vector of the <i>i</i> th training instance.
$Z^{1,i}$	The input image of the <i>i</i> th training instance.
l	The number of training instances.
K	The number of classes.
θ	The model vector (weights and biases) of the neural network.
ξ	The loss function.
ξ_i	The training loss of the <i>i</i> th instance.
f	The objective function.
С	The regularization parameter.
L	The number of layers of the neural network.
L^c	The number of convolutional layers of the neural network.
L^f	The number of fully-connected layers of the neural network.
n_m	The number of neurons in the <i>m</i> th layer ($L^c < m \le L + 1$).
n	The total number of weights and biases.

Notation	Description
a^m	Height of the input image at the <i>m</i> th layer $(1 \le m \le L^c)$.
a^m_{pad}	Height of the image after padding at the <i>m</i> th layer $(1 \le m \le L^c)$.
$a^m_{ m conv}$	Height of the image after convolution at the <i>m</i> th layer $(1 \le m \le L^c)$.
b^m	Width of the input image at the <i>m</i> th layer $(1 \le m \le L^c)$.
b_{pad}^m	Width of the image after padding at the <i>m</i> th layer $(1 \le m \le L^c)$.
$b^m_{ m conv}$	Width of the image after convolution the <i>m</i> th layer $(1 \le m \le L^c)$.
d^m	the depth (or the number of channels) of the data at the mth layer (1 \leq
	$m \leq L^c$).
h^m	the height (width) of the filters at the m th layer.
W^m	The weight matrix in the <i>m</i> th layer.
$oldsymbol{b}^m$	The bias vector in the <i>m</i> th layer.
$S^{m,i}$	The result of $(W^m)^T \phi(\text{pad}(Z^{m,i})) + \boldsymbol{b}^m \mathbb{1}_{a^m b^m}^T$ in the <i>m</i> th layer for the <i>i</i> th
	instance $(1 \le m \le L^c)$.
$Z^{m+1,i}$	The output matrix (element-wise application of the activation function on
	$S^{m,i}$) in the <i>m</i> th layer for the <i>i</i> th instance $(1 \le m \le L^c)$.
$oldsymbol{s}^{m,i}$	The result of $(W^m)^T z^{m,i} + b^m$ in the <i>m</i> th layer for the <i>i</i> th instance $(L^c < $
	$m \leq L$).
$oldsymbol{z}^{m+1,i}$	The output vector (element-wise application of the activation function on
	$s^{m,i}$) in the <i>m</i> th layer for the <i>i</i> th instance ($L^c \le m \le L$).
σ	The activation function.
J^i	The Jacobian matrix of $\boldsymbol{z}^{L+1,i}$ with respect to $\boldsymbol{\theta}$.

Notation	Description
I	An identity matrix.
$lpha_k$	A step size at the k th iteration.
$ ho_k$	The ratio between the actual function reduction and the predicted reduction
	at the k th iteration.
λ_k	A parameter in the Levenberg-Marquardt method.

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Listing 1: MATLAB implementation for $\phi(Z^{\text{in},i})$

```
1
  function idx = find_index_phiZ(a,b,d,h,s)
2
3
  first_channel_idx = ([0:h-1]*d+1)' + [0:h-1]*a*d;
4 first_col_idx = first_channel_idx(:) + [0:d-1];
5 | out_a = floor((a - h)/s) + 1;
6 | out_b = floor((b - h)/s) + 1;
7
  column_offset = ([0:out_a-1]' + [0:out_b-1]*a)*s*d;
8 |idx = column_offset(:)' + first_col_idx(:);
9
  idx = idx(:);
10
11
12
   function phiZ = padding_and_phiZ(model, net, m)
13
14 | a = model.ht_input(m);
15 | b = model.wd_input(m);
16 num_data = size(net.Z{m},2)/a/b;
17
18
  phiZ = padding(model, net, m);
19
20 % Calculate phiZ
21
  phiZ = reshape(phiZ, [], num_data);
22
  phiZ = phiZ(net.idx_phiZ{m}, :);
23
24 | h = model.wd_filter(m);
25 d = model.ch_input(m);
26 phiZ = reshape(phiZ, h*h*d, []);
```

Listing 2: *MATLAB* implementation for $P_{\text{pool}}^{m,i}$

```
function [Zout, idx_pool] = maxpooling(model, net, m)
1
2
3
  a = model.ht_conv(m);
4
  b = model.wd_conv(m);
5 d = model.ch_input(m+1);
6 h = model.wd_subimage_pool(m);
7
8 % Z input: sigma(S_m)
9 | Z = net.Z\{m+1\};
10
11 P = net.idx_phiZ_pool{m};
12 | Z = reshape(Z, d*a*b, []);
13 Z = Z(P, :);
14
  [Z, max_id] = max(reshape(Z, h*h, []));
15 Zout = reshape(Z, d, []);
16
17
  outa = model.ht_input(m+1);
18 outb = model.wd_input(m+1);
19
  max_id = reshape(max_id, d*outa*outb, []) + h*h*[0:d*outa*outb
      -1]';
20
21
  idx_pool = [1:d*a*b];
22 |idx_pool = idx_pool(P);
23 |idx_pool = idx_pool(max_id);
```

Listing 3: MATLAB implementation for the index of zero-padding

```
1 function [idx_pad] = find_index_padding(model,m)
2
3 a = model.ht_input(m);
4 b = model.wd_input(m);
5 p = model.wd_p(m);
6
7 newa = 2*p + a;
8 idx_pad = reshape( (p+1:p+a)' + newa*(p:p+b-1), [], 1);
```

Listing 4: MATLAB implementation to evaluate $(\boldsymbol{v}^i)^T P_{\phi}^m$ and $(\boldsymbol{v}^i)^T P_{\text{pool}}^{m,i}$

```
function vTP = vTP(param, model, net, m, V, op)
1
2
   % output vTP: a row vector, where mat(vTP) is with dimension $
      d_prev a_prev b_prev \times num_v$.
3
4 |nL = param.nL;
   num_data = net.num_sampled_data;
5
6
7
   switch op
   case {'pool_gradient', 'pool_Jacobian'}
8
9
       a_prev = model.ht_conv(m);
10
       b_prev = model.wd_conv(m);
11
       d_prev = model.ch_input(m+1);
12
       if strcmp(op, 'pool_gradient')
13
           num_v = num_data;
14
           idx = net.idx_pool{m} + [0:num_data-1]*d_prev*a_prev*
              b_prev;
15
       else
16
           num_v = nL*num_data;
17
           idx = reshape(net.idx_pool{m}, [], 1, num_data) +
              reshape([0:nL*num_data-1]*d_prev*a_prev*b_prev, 1,
              nL, num_data);
18
       end
   case {'phi_gradient', 'phi_Jacobian'}
19
20
       a_prev = model.ht_pad(m);
21
       b_prev = model.wd_pad(m);
22
       d_prev = model.ch_input(m);
23
24
       if strcmp(op, 'phi_gradient'); num_v = num_data; else;
          num v = nL*num data; end
25
26
       idx = net.idx_phiZ{m}(:) + [0:num_v-1]*d_prev*a_prev*b_prev
          ;
27
   otherwise
28
       error('Unknown operation in function vTP.');
29
   end
30
31
   vTP = accumarray(idx(:), V(:), [d_prev*a_prev*b_prev*num_v 1])
                                   67
      ';
```

Listing 5: MATLAB implementation for Jv

```
1
          function Jv = Jv(param, model, net, v)
  2
  3
        nL = param.nL;
  4 \mid L = param.L;
  5 LC = param.LC;
  6 num_data = net.num_sampled_data;
  7
          var_ptr = model.var_ptr;
  8
          Jv = zeros(nL*num_data, 1);
  9
         for m = L : -1 : LC+1
10
11
                        var_range = var_ptr(m) : var_ptr(m+1) - 1;
12
                        n_m = model.full_neurons(m-LC);
13
14
                        p = reshape(v(var_range), n_m, []) * [net.Z{m}; ones(1,
                                   num_data)];
15
                         p = sum(reshape(net.dzdS{m}, n_m, nL, []) .* reshape(p, n_m
                                    , 1, []),1);
16
                         Jv = Jv + p(:);
17
          end
18
19
          for m = LC : -1 : 1
20
                         var_range = var_ptr(m) : var_ptr(m+1) - 1;
21
                         ab = model.ht_conv(m) *model.wd_conv(m);
22
                        d = model.ch_input(m+1);
23
24
                        p = reshape(v(var_range), d, []) * [padding_and_phi2(model,
                                       net, m); ones(1, ab*num_data)];
25
                         p = sum(reshape(net.dzdS{m}, d*ab, nL, []) .* reshape(p, d*ab, nL, []) .* reshape(p,
                                   ab, 1, []),1);
26
                         Jv = Jv + p(:);
27
          end
```

Listing 6: MATLAB implementation for $J^T q$

```
function u = JTq(param, model, net, q)
1
2
3
  nL = param.nL;
4 | L = param.L;
5 LC = param.LC;
  num_data = net.num_sampled_data;
6
7
  var_ptr = model.var_ptr;
8 | n = var_ptr(end) - 1;
9
  u = zeros(n, 1);
10
11
   for m = L : -1 : LC+1
12
       var_range = var_ptr(m) : var_ptr(m+1) - 1;
13
14
       u_m = net.dzdS\{m\} .* q';
15
       u_m = sum(reshape(u_m, [], nL, num_data), 2);
16
       u_m = reshape(u_m, [], num_data) * [net.Z{m}' ones(num_data
          , 1)];
17
       u(var_range) = u_m(:);
18
   end
19
20
   for m = LC : -1 : 1
21
       a = model.ht_conv(m);
22
       b = model.wd_conv(m);
23
       d = model.ch_input(m+1);
24
       var_range = var_ptr(m) : var_ptr(m+1) - 1;
25
26
       u_m = reshape(net.dzdS{m}, [], nL*num_data) .* q';
27
       u_m = sum(reshape(u_m, [], nL, num_data), 2);
28
       u_m = reshape(u_m, d, []) * [padding_and_phiZ(model, net, m
          ) ' ones(a*b*num_data, 1)];
29
       u(var_range) = u_m(:);
30
   end
```