Notes on Neural Networks based on primal-dual splitting method

Rui, Zheng

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Contents

1 The Contribution

Ordered by priority from high to low

- We propose a Deep **** CNN for sparse image classification
- Overcome some problems of SGD

2 Introduction

Deep neural networks (DNNs) have have been used to solve a wide variety of applications such as image classification, object recognition, natural language processing, etc. For past decades, gradient descent-based methods such as backpropagation have mainly been widely used in various optimization techniques for training neural networks. However, it is clear that gradient descent-based learning methods are generally very slow due to improper learning steps or may easily converge to local minima.

3 Notation

For neural networks part, we denote: $\mathscr{D}(\mathbf{X},\mathbf{y})$ as dataset, which has N data samples (or equivalently to batch_size here, 'cause no online or stochastic opt is considered) and N_c classes; $\mathbf{y}$ as $N \times N_c$ label; $\mathbf{X}$ as $N \times W \times H \times C$ tensor input. where W, H, C represents width, height and channel respectively; For fully-connected layer, l represents l-th layer; L as last layer (softmax classifier); $\mathbf{W}_l, \mathbf{b}_l, \mathbf{a}_l, \mathbf{z}_l, h_l(\cdot)$ as

the weight, bias, activation output, summation output and activation function of l-th layer respectively; For the convolutional layer, $*$ denotes 2D conv operation; $\otimes$ as element-wise product; we use the same notation l as $l-th$ conv layer, but not to confuse with the FC. Lc as how many conv layers; $\mathbf{K}_{i,j}^l$ matrix as the l-th layer's conv kernel (for each conv layer, it has $i \times j$ number kernels); $\mathbf{T}_{i,j}^l$ as the unfolded "Toeplitz" (informally) matrix of corresponding $\mathbf{K}_{i,j}^l$; $\mathbf{c}_i^l$ as the input to l-th conv layer; $\mathbf{f}_j^l$ s the j-th feature map; b_j^l as layer's bias;

formally,

$$\mathbf{c}_j^l = h_l(\sum_{i=1}^{m}[\mathbf{c}_i^{l-1} * \mathbf{K}_{i,j}^l] + b_j^l) \tag{1}$$

$$= h_l(\mathbf{f}_j^l) \tag{2}$$

where inside the 2D-conv, u-th and v-th element of $\mathbf{c}_i^{l-1} * \mathbf{K}_{i,j}^l$ is :

$$\mathbf{c}_i^{l-1} * \mathbf{K}_{i,j}^l(u,v) = \sum_m \sum_n \mathbf{c}_i^{l-1}(u-m, v-n)\mathbf{K}_{i,j}^l(m,n) \tag{3}$$

which is just a element-wise product of kernel and corresponding patch on $\mathbf{c}$. This is very easy for backprop to obtain the gradient by chain rules, but however difficult for ADMM to solve (maybe Rui knows how to solve). Thus we rewrite the above matrix as operation of Toeplitz matrix:

$$\mathbf{c}_j^l = h_l(\sum_{i=1}^{m}[\mathbf{c}_i^{l-1}\mathbf{T}_{i,j}^l] + b_j^l) \tag{4}$$

Now it is just a simple matrix product inside, but it is extremely memory-consuming!. Notice that for equation (2), we could also use Fourier transform to solve that, and inverse Fourier. In case the Toeplitz doesn't work, we should also try this.

4 Problem formulation

Consider a dataset $\mathscr{D}(\mathbf{X},\mathbf{y})$ of n observations where $\mathbf{X}$ denotes an input matrix (covariates) of dimension $D_x \times n$ and $\mathbf{y}$ denotes the scalar output (or target) variable. Given this training dataset, we wish to make predictions for new inputs $\mathbf{x}^*$. A typical objective function to learn a DNNs with L layers has the form

$$J(\mathbf{w};\mathscr{D}) = L(\mathbf{w};\mathscr{D}) + \lambda\phi(\mathbf{w}) \tag{5}$$

. Here, the loss functions $L(\mathbf{w};\mathscr{D})$ are usually MSE or crossentropy: For 1) mean square error (MSE), the above equation generalizes to:

$$\begin{aligned} J(\mathbf{w};\mathbf{X},\mathbf{y}) &= \frac{1}{2N}\|\mathbf{y} - f(\mathbf{w},\mathbf{X})\|^2 + \lambda\phi(\mathbf{w}) \\ &= \frac{1}{2N}\|\mathbf{y} - f(\mathbf{w},\mathbf{X})\|^2 + \lambda\|\mathbf{w}\|_1 \end{aligned} \tag{6}$$

where f is the prediction function, $\mathbf{w}$ is the parameter we optimize, and λ is the constant.

For 2) crossentropy:

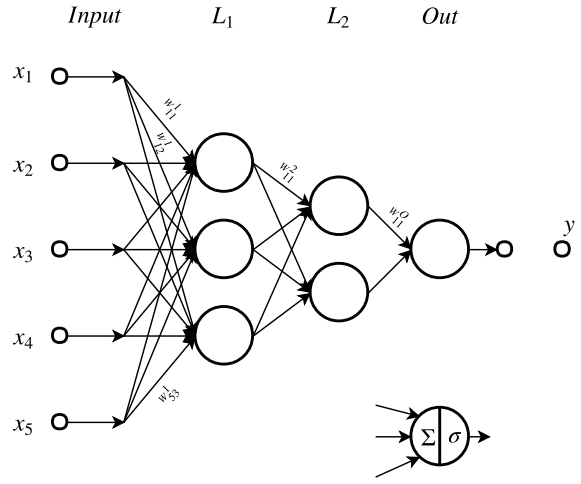
$$J(\mathbf{w};\mathbf{X},\mathbf{y}) = \sum_{i=1}^{N}(y_i \log f(\mathbf{w},\mathbf{x}) + (1-y_i)\log(1-f(\mathbf{w},\mathbf{x}))) + \lambda\phi(\mathbf{w}) \tag{7}$$

where $\lambda\phi(\mathbf{w})$ can be any regularizers (L1, L2 etc.), and $f(\cdot)$ is network function.

The aim here is to find the optimize values weights $\mathbf{w}$ of neural network to minimize the objective function.

4.1 One Example

For a simplest NN example. Here we will use the notation: $\mathbf{x} \in \mathbb{R}^5 : \mathbf{x} = \{x_1, x_2, ..., x_5\}$ and $y : y \in \mathbb{R}$ as the pair of data for training; w_{ij}^l denotes the weight that connects i-th neuron on $(l-1)$-th layer and j-th neuron on l-th layer; $\sigma_l(\cdot)$ is the activation function for l-th layer; o_i^l is the output from the i-th neuron of l-th layer; Out is the output of the neural network (last neuron):



The loss is:

$$J(\mathbf{W}; \mathbf{x}, y) = \frac{1}{2}(Out_{\mathbf{w},\mathbf{x}} - y)^2 + \text{regularizer on } \mathbf{w} \tag{8}$$

Let us show some forward example of it. Take output Out:

$$Out = \sigma_3(o_1^2 w_{11}^3 + o_2^2 w_{21}^3 + b^3) \tag{9}$$
$$= \sigma_3(\mathbf{o}^2 \mathbf{w}^3 + b_3) \tag{10}$$
$$= \sigma_3(\Sigma_1^3) \tag{11}$$

where $\mathbf{o}^2 = [o_1^2, o_2^2]$, $\mathbf{w}^3 = [w_{11}^3, w_{21}^3]^T$ and $\Sigma_1^3 = \mathbf{o}^2 \mathbf{w}^3 + b_3$. Let us continue for o_1^2 and o_2^2:

$$o_1^2 = \sigma_2(o_1^1 w_{11}^2 + o_2^1 w_{21}^2 + o_3^1 w_{31}^2 + b_1^2) \tag{12}$$
$$= \sigma_2(\Sigma_1^2) \tag{13}$$
$$o_2^2 = \sigma_2(o_1^1 w_{12}^2 + o_2^1 w_{22}^2 + o_3^1 w_{32}^2 + b_2^2) \tag{14}$$
$$= \sigma_2(\Sigma_2^2) \tag{15}$$
$$\mathbf{o}^2 = \sigma_2(\mathbf{o}^1 \mathbf{w}^2 + \mathbf{b}^2) \tag{16}$$

where $\mathbf{o}^1 = [o_1^1, o_2^1, o_3^1]$ and $\mathbf{w}^2 = \begin{bmatrix} w_{11}^2 & w_{21}^2 & w_{31}^2 \\ w_{12}^2 & w_{22}^2 & w_{32}^2 \end{bmatrix}^T$. and $\mathbf{o}^1 = \sigma_1(\mathbf{x}\mathbf{w}^1 + \mathbf{b}^1)$.

In traditional approach, we need to derive the gradient of the loss w.r.t each weight i.e.:

$$\frac{\partial J(\mathbf{W}; \mathbf{x}, y)}{\partial w_{ij}^l} \tag{17}$$

Those gradient can be efficiently obtained by backpropogation (BP). For simplicity, BP not discussed here.

If we use SGD, the update of weight is just: $w_{ij}^l(k+1) = w_{ij}^l(k) + \eta \frac{\partial J(\mathbf{W};\mathbf{x},y)}{\partial w_{ij}^l}$.

Based on SGD, we consider using ADMM to solve the objective function.

5 Spectro-temporal layer

Considering an LTI system:

$$\begin{aligned}\mathbf{x}_k &= \mathbf{A}\mathbf{x}_{k-1} + \mathbf{q}, \mathbf{q}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}) \\ y_k &= \mathbf{H}\mathbf{x}_k + r_k, r_k \sim \mathcal{N}(0, R)\end{aligned} \tag{18}$$

where $\mathbf{A}$, $\mathbf{Q}$ and $\mathbf{H}$ are defined as:

$$\mathbf{A} = \begin{bmatrix} 1 & & & \\ & \mathbf{A}_k^1 & & \\ & & \ddots & \\ & & & \mathbf{A}_k^M \end{bmatrix} \tag{19}$$

$$\mathbf{Q} = \begin{bmatrix} qb\Delta t & & & \\ & \mathbf{Q}_k^1 & & \\ & & \ddots & \\ & & & \mathbf{Q}_k^M \end{bmatrix} \tag{20}$$

$$\mathbf{H} = [1, \mathbf{H}^1, \ldots, \mathbf{H}^M] = [11010, \ldots, 10] \tag{21}$$

where $\mathbf{A}_k^j$ and $\mathbf{Q}_k^j$ are given in closed form:

$$\mathbf{A}_k^j = \exp\big(\mathbf{F}_j \Delta t\big) \tag{22}$$

$$= \begin{bmatrix} \cos\big(2\pi f_j \Delta t\big) & -\sin\big(2\pi f_j \Delta t\big) \\ \sin\big(2\pi f_j \Delta t\big) & \cos\big(2\pi f_j \Delta t\big) \end{bmatrix} \exp\big(-\Delta t \lambda_j\big) \tag{23}$$

$$\mathbf{Q}_k^j = \int_0^{\Delta t} \exp\big(\mathbf{F}_j(\Delta t - s)\big) \mathbf{L} \mathbf{Q}_k^j \mathbf{L}^\top \exp\big(\mathbf{F}_j(\Delta t - s)\big)^\top ds \tag{24}$$

$$= \frac{Q_k^j}{2\lambda^j}(1 - \exp\big(-2\Delta t \lambda_j\big))\mathbf{I} \tag{25}$$

We can use Kalman filter to easily estimate $\mathbf{x}_k$.

However, the point of spectro-temporal layer is that we set $\mathbf{A}$ and $\mathbf{Q}$ are paramiterized by **trainable** weight $\mathbf{w}$.

$$\begin{aligned}\mathbf{x}_k &= \mathbf{A}(\mathbf{w})\mathbf{x}_{k-1} + \mathbf{q}, \mathbf{q}_k \sim \mathcal{N}(\mathbf{0}, \mathbf{Q}(\mathbf{w})) \\ y_k &= \mathbf{H}\mathbf{x}_k + r_k, r_k \sim \mathcal{N}(0, R)\end{aligned} \tag{26}$$

We put a signal y as input of this layer. After Kalman estimation, it outputs a spectrogram (image) $\mathbf{X}$, we then feed that $\mathbf{X}$ into NN to classify. Because $\mathbf{A}$ and $\mathbf{Q}$ are trainable for NN, thus just optimize that NN loss function, but the computational cost is very expensive.

6 ADMM solver for MSE

We consider the original optimization problem (28). Firstly, we introduce an auxiliary variable $\mathbf{V}$, and have the following constrained problem

$$\begin{aligned}&\min_x \frac{1}{2}\|y - Hx\|_{R^{-1}}^2 + \frac{1}{2}\|\Psi x - m\|_{Q^{-1}}^2 + \lambda\|\Omega x\|_1 \\ &\text{s.t. } v = \Omega x.\end{aligned} \tag{27}$$

$$\begin{aligned} &\min_{W} \frac{1}{2} \sum_{n=1}^{N} \|\mathbf{y}_n - f(\mathbf{W}, \mathbf{x})\|^2 + \lambda \|\mathbf{V}\|_1 \\ &\text{s.t. } \mathbf{V} = \mathbf{W}. \end{aligned} \tag{28}$$

Then, Let $\mathscr{L}_\rho(x, v; \eta)$ be the augmented Lagrangian function of Eq. (28) which is defined as follows

$$\mathscr{L}_\rho(\mathbf{W}, \mathbf{V}; \boldsymbol{\eta}) \triangleq \frac{1}{2} \sum_{n=1}^{N} \|\mathbf{y}_n - f(\mathbf{W}, \mathbf{x})\|^2 + \lambda \|\mathbf{V}\|_1 + \langle \mathbf{V} - \mathbf{W}, \boldsymbol{\eta} \rangle + \frac{\rho}{2} \|\mathbf{V} - \mathbf{W}\|^2 \tag{29}$$

The solution of (29) can be obtained by the following steps [1]:

$$\begin{aligned} \mathbf{W}^{k+1} &:= \arg\min_{\mathbf{W}} \mathscr{L}_\rho(\mathbf{W}, \mathbf{V}^k; \boldsymbol{\eta}^k) \\ \mathbf{V}^{k+1} &:= \arg\min_{\mathbf{W}} \mathscr{L}_\rho(\mathbf{W}^{k+1}, \mathbf{V}; \boldsymbol{\eta}^k) \\ \boldsymbol{\eta}^{k+1} &:= \boldsymbol{\eta}^k + \rho(\mathbf{V}^{k+1} - \mathbf{W}^{k+1}) \end{aligned} \tag{30}$$

1. Input: $\mathbf{V}^0$, $\boldsymbol{\eta}^0$, ρ,
2. Loop: For $k = 1, 2, \cdots$ until termination criteria are met.
   - Calculate x^k by solving:

$$\begin{aligned} \mathbf{W}^{k+1} &= \arg\min_{\mathbf{W}} \ \mathscr{L}_\rho(\mathbf{W}, \mathbf{V}^k; \boldsymbol{\eta}^k) \\ &= \arg\min_{\mathbf{W}} \ \frac{1}{2} \sum_{n=1}^{N} \|\mathbf{y}_n - f(\mathbf{W}, \mathbf{x})\|^2 + + \frac{\rho}{2} \|\mathbf{V} - \mathbf{W} + \boldsymbol{\eta}\|^2 \end{aligned} \tag{31}$$

     Eq. 31 has the close-form expression. We could use RTS smoother to solve the problem (31)
   - Calculate $\mathbf{V}^k$ by solving:

$$\begin{aligned} \mathbf{V}^{k+1} &= \arg\min_{\mathbf{V}} \ \mathscr{L}_\rho(\mathbf{W}^{k+1}, \mathbf{V}; \boldsymbol{\eta}^k) \\ &= \lambda \|\mathbf{V}\|_1 + \frac{\rho}{2} \left\| \mathbf{V} - \mathbf{W}^{k+1} + \boldsymbol{\eta}^k \right\|^2 \\ &= \text{sign}(\mathbf{W}^{k+1} + \boldsymbol{\eta}^k/\rho) \circ \max(|\Omega x^{k+1} + \eta^k/\rho| - \lambda/\rho, 0) \end{aligned} \tag{32}$$

     where sign represents the signum function, and $\circ$ is the pointwise product.
   - Calculate η^k by solving:

$$\eta^{k+1} = \eta^k + \rho(\Omega x^{k+1} - v^{k+1}) \tag{33}$$

3. Output: x^{k+1}

7 Matlab example

References

[1] S. Boyd, N. Parikh, E. Chu, B. Peleato, and J. Eckstein. Distributed optimization and statistical learning via the alternating direction method of multipliers. *Foundations and Trends in Machine Learning.*, 3(1):1–122, 2011.