Power of Alternating Direction Method of Multipliers (ADMM) in Deep Learning

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Background Introduction

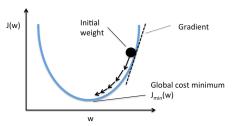
The dIADMM Algorithm

The pdADMM Algorithm

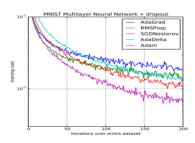
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SGD as a Deep Learning Optimizer

Stochastic gradient descent(SGD) and its variants are state-of-the-art optimizers in deep learning applications.



Stochastic Gradient Descent(SGD)

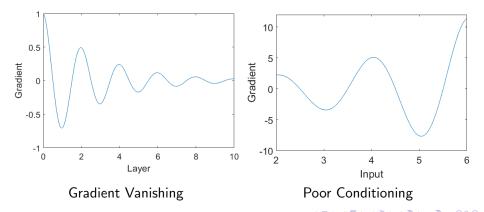


Outstanding Performance

Challenges of SGD

However, SGD suffers from several limitations including:

- Gradient vanishing: the error signal diminishes as the gradient is backpropagated.
- Poor conditioning: small input can change the gradient drastically.



The Motivations to Train Neural Networks via ADMM

The ADMM has the following advantages over SGD:

- Be immune to gradient vanishing and poor conditioning.
 The ADMM splits a neural network into layerwise components, and prevents the accumulative calculation of gradients.
- Have great potential of parallelism of deep neural network training.
 - The inherent nature of ADMM is to break an objective into multiple subproblems, each of which can be solved in parallel; while the parallel training of SGD is restricted by the backward locking (i.e. the calculation of gradient in one layer is dependent on its previous layers).

Existing Works on Training Neural Network using ADMM

Taylor et al. [1] deals with the following Multi-Layer Perceptron (MLP) model:

Problem (MLP Training Problem)

$$\min_{W_{l},b_{l},z_{l},a_{l}} R(z_{L};y) + \sum_{l=1}^{L} \Omega_{l}(W_{l})$$
s.t. $z_{l} = W_{l}a_{l-1} + b_{l}(l = 1, \dots, L), \ a_{l} = f_{l}(z_{l})(l = 1, \dots, L-1)$

where $W_I \in \mathbb{R}^{n_I \times n_{I-1}}$ and $b_I \in \mathbb{R}^{n_I}$ are a weight matrix and a bias for the I-th layer, respectively. n_I is the number of neurons for the I-th layer. z_I and a_I are the output of the linear mapping and the nonlinear mapping f_I for the I-th layer, respectively. $x = a_0$ and y are an input matrix and a predefined label vector, respectively. $R(z_L; y)$ and $\Omega_I(W_I)$ are a risk function and regularization terms, respectively. L is the number of layers.

Problem Relaxation

The MLP training problem contains multiple constraints, and hence is relaxed via imposing ℓ_2 penalties on the objective as follows:

Problem (Relaxed MLP training problem)

$$\min_{W_{l},b_{l},z_{l},a_{l}} F(W,b,z,a) = R(z_{L};y) + \sum_{l=1}^{L} \Omega_{l}(W_{l}) + (\nu/2) \sum_{l=1}^{L-1} (\|z_{l} - W_{l}a_{l-1} - b_{l}\|_{2}^{2} + \|a_{l} - f_{l}(z_{l})\|_{2}^{2})$$
s.t. $z_{L} = W_{L}a_{L-1} + b_{L}$

where $\mathbf{W} = \{W_l\}_{l=1}^L$, $\mathbf{b} = \{b_l\}_{l=1}^L$, $\mathbf{z} = \{z_l\}_{l=1}^L$, $\mathbf{a} = \{a_l\}_{l=1}^{L-1}$, $\nu > 0$ is a tuning parameter. As $\nu \to \infty$, the relaxed problem approaches the original problem. Then the augmented Lagrangian is formulated and subproblems are solved alternately.

Challenges of the Existing ADMM Work

- Slow convergence towards solutions.
 - The ADMM usually converges slowly to high accuracy, even for simple examples. It is often the case that ADMM becomes trapped in a modest solution.
- Cubic time complexity with regard to feature dimensions. The implementation of the ADMM is very time-consuming for real-world datasets. Previous experiments showed that ADMM required more than 7000 cores to train a neural network with just 300 neurons [1]. This computational bottleneck mainly originates from the matrix inversion, whose time complexity is approximately $O(n^3)$.
- The lack of convergence guarantees.
 - The convergence theory of the nonconvex ADMM cannot be directly applied to deep learning problem. This is because a typical deep learning problem consists of a combination of linear and nonlinear mappings, causing optimization problems to be highly nonconvex.

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dIADMM: Outline

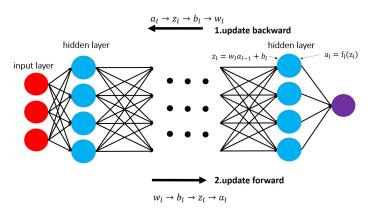
In order to deal with these challenges, we propose a deep learning Alternating Direction Method of Multipliers(dIADMM) [2]. Specifically,

| Challenge | Contribution |
|------------------------------------|--|
| Slow convergence | New update routine. |
| $O(n^3)$ time complexity | Reduce to $O(n^2)$ |
| | |
| | by quadratic approximation. |
| The lack of | by quadratic approximation. Proofs of convergence |
| The lack of convergence guarantees | |

Table: The improvement of the dIADMM algorithm.

dIADMM: Update Parameters Backward and then Forward

We propose a new update routine: the parameter information for all layers can be exchanged efficiently by updating parameters backward and then forward.



dIADMM: The Augmented Lagrangian

The Augmented Lagrangian is formulated mathematically as follows:

$$L_{\rho}(\mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{a}, u) = R(z_L; y) + \sum_{l=1}^{L} \Omega_l(W_l) + \phi(\mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{a}, u)$$

where $\phi(\mathbf{W},\mathbf{b},\mathbf{z},\mathbf{a},u)=(\nu/2)\sum_{l=1}^{L-1}(\|z_l-W_la_{l-1}-b_l\|_2^2+\|a_l-f_l(z_l)\|_2^2)+u^T(z_L-W_La_{L-1}-b_L)+(\rho/2)\|z_L-W_La_{L-1}-b_L\|_2^2, \ u \ \text{is a dual variable and} \ \rho>0 \ \text{is a hyperparameter.} \ \text{We denote} \ \overline{W}_l^{k+1}, \ \overline{b}_l^{k+1}, \ \overline{z}_l^{k+1} \ \text{and} \ \overline{a}_l^{k+1} \ \text{as the backward update of the dIADMM for the l-th layer in the $(k+1)$-th iteration , while $W_l^{k+1}, b_l^{k+1}, z_l^{k+1}$ and a_l^{k+1} are denoted as the forward update of the dIADMM for the l-th layer in the $(k+1)$-th iteration.$

dIADMM: Pseudocode

Algorithm 1 The dIADMM Algorithm

Require: $y, a_0 = x, \rho, \nu, k = 0.$

Ensure: W, b, z, a

1: while
$$\mathbf{W}^{k+1}$$
, \mathbf{b}^{k+1} , \mathbf{z}^{k+1} , \mathbf{a}^{k+1} not converged do

- 2: Update \overline{z}_L^{k+1} , \overline{b}_L^{k+1} and \overline{W}_L^{k+1} in order.
- 3: **for** I = L 1 to 1 **do**
 - Update \overline{a}_{l}^{k+1} , \overline{z}_{l}^{k+1} , \overline{b}_{l}^{k+1} , and \overline{W}_{l}^{k+1} in order.
- 5: end for
- 6: **for** l = 1 to L 1 **do**
- 7: Update W_{l}^{k+1} , b_{l}^{k+1} , z_{l}^{k+1} , a_{l}^{k+1} in order.
- 8: end for
- 9: Update W_L^{k+1} , b_L^{k+1} , and z_L^{k+1} in order.
- 10: $r^{k+1} \leftarrow z_L^{k+1} W_L^{k+1} a_{L-1}^{k+1} b_L^{k+1}$.#Compute Residual.
- 11: $u^{k+1} \leftarrow u^k + \rho r^{k+1}$.
- 12: $k \leftarrow k + 1$.
- 13: end while
- 14: Output **W**, **b**, **z**, **a**.

dIADMM: Quadratic Approximation(1)

In order to avoid matrix inversion, we apply the quadratic approximation techniques to subproblems. Take W_l^{k+1} as an example:

$$\begin{aligned} W_l^{k+1} \leftarrow \arg\min_{W_l} \phi(\{W_i^{k+1}\}_{i=1}^{l-1}, W_l, \{\overline{W}_i^{k+1}\}_{i=l+1}^{L}, \mathbf{b}_{l-1}^{k+1}, \mathbf{z}_{l-1}^{k+1}, \mathbf{a}_{l-1}^{k+1}, u^k) \\ &+ \Omega(W_l) \end{aligned}$$

We define $P_l(W_l; \theta_l^{k+1})$ as a quadratic approximation of ϕ , which is mathematically reformulated as follows:

$$P_{l}(W_{l}; \theta_{l}^{k+1}) = \phi(\mathbf{W}_{l-1}^{k+1}, \mathbf{b}_{l-1}^{k+1}, \mathbf{z}_{l-1}^{k+1}, \mathbf{a}_{l-1}^{k+1}, u^{k})$$

$$+ (\nabla_{\overline{W}_{l}^{k+1}} \phi)^{T} (\mathbf{W}_{l-1}^{k+1}, \mathbf{b}_{l-1}^{k+1}, \mathbf{z}_{l-1}^{k+1}, \mathbf{a}_{l-1}^{k+1}, u^{k}) (W_{l} - \overline{W}_{l}^{k+1})$$

$$+ \|\theta_{l}^{k+1} \circ (W_{l} - \overline{W}_{l}^{k+1})^{\circ 2}\|_{1}/2$$

where $\theta_l^{k+1} > 0$ is a parameter vector, which can be chosen by backtracking to satisfy the condition

 $\phi(\mathbf{W}_{l}^{k+1},\mathbf{b}_{l}^{k+1},\mathbf{z}_{l}^{k+1},\mathbf{a}_{l}^{k+1},u^{k}) \leq P_{l}(W_{l}^{k+1};\theta_{l}^{k+1}).$

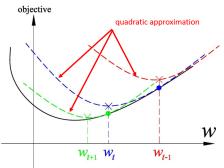
dIADMM: Quadratic Approximation(2)

We instead solve the following problem:

$$W_l^{k+1} \leftarrow \operatorname{arg\,min}_{W_l} P_l(W_l; \theta_l^{k+1}) + \Omega_l(W_l)$$

which is convex and may have a closed-form solution for ℓ_1 or ℓ_2 regularization.

The geometric interpretation of quadratic approximation is shown in the below figure:



dIADMM: Convergence Assumptions

Assumption (Closed-form Solution)

There exist activation functions $a_l = f_l(z_l)$ such that \overline{z}_l^{k+1} -subproblem and z_l^{k+1} -subproblem have closed form solutions $\overline{z}_l^{k+1} = \overline{h}(\overline{W}_{l+1}^{k+1}, \overline{b}_{l+1}^{k+1}, \overline{a}_l^{k+1})$ and $z_l^{k+1} = h(W_l^{k+1}, b_l^{k+1}, a_{l-1}^{k+1})$, respectively, where $\overline{h}(\bullet)$ and $h(\bullet)$ are continuous functions.

This assumption can be satisfied by common activation functions such as ReLU and leaky ReLU.

Assumption (Objective Function)

F(W,b,z,a) is coercive over the nonempty set $G=\{(W,b,z,a): z_L-W_La_{L-1}-b_L=0\}$. In other words, $F(W,b,z,a) \to \infty$ if $(W,b,z,a) \in G$ and $\|(W,b,z,a)\| \to \infty$. Moreover, $R(z_L;y)$ is Lipschitz differentiable with Lipschitz constant $H \ge 0$.

The cross-entropy loss and the least square loss are Lipschitz differentiable.

dIADMM: Convergence Properties(1)

If two assumptions hold, we can prove three convergence properties as follows:

Property (Boundness)

If $\rho > 2H$, then $\{W^k, b^k, z^k, a^k, u^k\}$ is bounded, and $L_{\rho}(W^k, b^k, z^k, a^k, u^k)$ is lower bounded.

Property (Sufficient Descent)

If $\rho > 2H$ so that $C_1 = \rho/2 - H/2 - H^2/\rho > 0$, then there exists C_2 such that

$$L_{\rho}(W^{k}, b^{k}, z^{k}, a^{k}, u^{k}) - L_{\rho}(W^{k+1}, b^{k+1}, z^{k+1}, a^{k+1}, u^{k+1})$$

$$\geq C_{2}(\sum_{l=1}^{L} (\|\overline{W}_{l}^{k+1} - W_{l}^{k}\|_{2}^{2} + \|W_{l}^{k+1} - \overline{W}_{l}^{k+1}\|_{2}^{2})$$

$$+ \|\overline{b}_{l}^{k+1} - b_{l}^{k}\|_{2}^{2} + \|b_{l}^{k+1} - \overline{b}_{l}^{k+1}\|_{2}^{2}) + \sum_{l=1}^{L-1} (\|\overline{a}_{l}^{k+1} - a_{l}^{k}\|_{2}^{2})$$

$$+ \|a_{l}^{k+1} - \overline{a}_{l}^{k+1}\|_{2}^{2}) + \|\overline{z}_{L}^{k+1} - z_{L}^{k}\|_{2}^{2} + \|z_{L}^{k+1} - \overline{z}_{L}^{k+1}\|_{2}^{2})$$

dIADMM: Convergence Properties(2)

The first two properties guarantee the convergence of the augmented Lagrangian, and the third one guarantees the boundness of subgradient:

Property (Subgradient Bound)

There exist a constant C>0 and $g\in\partial L_{\rho}(W^{k+1},b^{k+1},z^{k+1},a^{k+1})$ such that

$$||g|| \le C(||\mathbf{W}^{k+1} - \overline{\mathbf{W}}^{k+1}|| + ||\mathbf{b}^{k+1} - \overline{\mathbf{b}}^{k+1}|| + ||\mathbf{z}^{k+1} - \overline{\mathbf{z}}^{k+1}|| + ||\mathbf{a}^{k+1} - \overline{\mathbf{a}}^{k+1}|| + ||\mathbf{z}^{k+1} - \mathbf{z}^{k}||)$$

Based on three convergence properties, we can prove the convergence of the dIADMM algorithm to a critical point with a sublinear convergence rate o(1/k).

dIADMM: Convergence to a Critical Point Sublinearly

Theorem (Convergence to a Critical Point)

If $\rho > 2H$, then for the variables (W,b,z,a,u) in the relaxed MLP training problem, starting from any (W^0,b^0,z^0,a^0,u^0) , it has at least a limit point (W^*,b^*,z^*,a^*,u^*) , and any limit point (W^*,b^*,z^*,a^*,u^*) is a critical point. That is, $0 \in \partial L_\rho(W^*,b^*,z^*,a^*,u^*)$.

Theorem (Convergence Rate)

For a sequence $(W^k, b^k, z^k, a^k, u^k)$, define $c_k = \min_{0 \le i \le k} (\sum_{l=1}^L (\|\overline{W}_l^{i+1} - W_l^i\|_2^2 + \|W_l^{i+1} - \overline{W}_l^{i+1}\|_2^2 + \|\overline{b}_l^{i+1} - b_l^i\|_2^2 + \|b_l^{i+1} - \overline{b}_l^{i+1}\|_2^2) + \sum_{l=1}^{L-1} (\|\overline{a}_l^{i+1} - a_l^i\|_2^2 + \|a_l^{i+1} - \overline{a}_l^{i+1}\|_2^2) + \|\overline{z}_L^{i+1} - z_L^i\|_2^2 + \|z_L^{i+1} - \overline{z}_L^{i+1}\|_2^2)$, then the convergence rate of c_k is o(1/k).

Experimental Results: Convergence

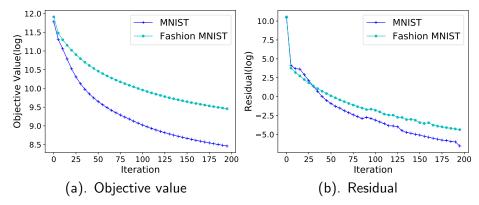


Figure: Convergence curves of dIADMM algorithm for MNIST and Fashion MNIST datasets when $\rho=1$: the dIADMM algorithm converged.

Experimental Results: Performance

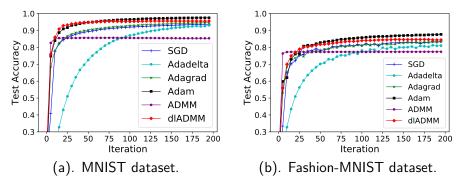


Figure: Test Performance of all methods for two datasets: the dIADMM algorithm outperformed most of the comparison methods.

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Backward Locking

The backward locking problem restrict the parallel training of SGD. For example, Module A can not finish Step 6 until Module B finishes Step 5.

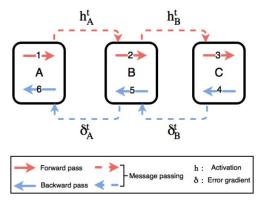
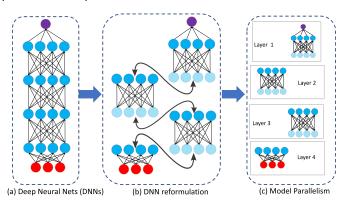


Figure: The mechanism of backpropagation.¹

¹This figure is borrowed from Huo et al. "Decoupled parallel backpropagation with convergence guarantee." ICML 2018.

pdADMM: Break the Backward Locking by Layer Splitting

The parallel deep learning Alternating Direction Method of Multipliers (pdADMM) can address the backward locking problem[3]. Specifically, by splitting the whole neural network into multiple layers, each of which can be optimized by an independent worker. Therefore, the layerwise training can be implemented in parallel.



pdADMM: Problem Formulation

Problem (MLP Training Problem Revisited)

$$\min_{W_l, b_l, z_l, a_l} R(z_L; y)$$

 $s.t.z_l = W_l a_{l-1} + b_l (l = 1, \dots, L), \ a_l = f_l(z_l) \ (l = 1, \dots, L - 1)$

Notice that a_l is both the input for the (l+1)-th layer and the output for the l-th layer. Let p_l and q_l be the input and output for the l-th layer, respectively. Then the MLP training problem can be relaxed to

Problem (Parallel MLP Training Problem)

$$\min_{\mathbf{p}, W, \mathbf{b}, \mathbf{z}, \mathbf{q}} F(\mathbf{p}, W, \mathbf{b}, \mathbf{z}, \mathbf{q}) = R(z_L; y)$$

$$+ (\nu/2) \left(\sum_{l=1}^{L} \|z_l - W_l \mathbf{p}_l - b_l\|_2^2 + \sum_{l=1}^{L-1} \|q_l - f_l(z_l)\|_2^2 \right)$$

$$s.t. \ p_{l+1} = q_l$$

where
$$\mathbf{p} = \{p_l\}_{l=1}^L$$
, $\mathbf{W} = \{W_l\}_{l=1}^L$, $\mathbf{b} = \{b_l\}_{l=1}^L$, $\mathbf{z} = \{z_l\}_{l=1}^L$, $\mathbf{q} = \{q_l\}_{l=1}^{L-1}$, and $\nu > 0$ is a tuning parameter.

The Augmented Lagrangian

The Augmented Lagrangian is formulated mathematically as follows:

$$L_{\rho}(\mathbf{p}, \mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{q}, \mathbf{u})$$

$$= F(\mathbf{p}, \mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{q}) + \sum_{l=1}^{L-1} (u_l^T (p_{l+1} - q_l) + (\rho/2) || p_{l+1} - q_l ||_2^2)$$

$$= R(z_L; y) + \phi(p_1, W_1, b_1, z_1) + \sum_{l=2}^{L} \phi(p_l, W_l, b_l, z_l, q_{l-1}, u_{l-1})$$

$$+ (\nu/2) \sum_{l=1}^{L-1} || q_l - f_l(z_l) ||_2^2$$

where $\phi(p_1, W_1, b_1, z_1) = (\nu/2)\|z_1 - W_1p_1 - b_1\|_2^2$, $\phi(p_l, W_l, b_l, z_l, q_{l-1}, u_{l-1}) = (\nu/2)\|z_l - W_lp_l - b_l\|_2^2 + u_{l-1}^T(p_l - q_{l-1}) + (\rho/2)\|p_l - q_{l-1}\|_2^2$, $u_l(l = 1, \cdots, L-1)$ are dual variables, $\rho > 0$ is a hyperparameter, and $\mathbf{u} = \{u_l\}_{l=1}^{L-1}$. Subproblems are solved by the quadratic approximation techniques and backtracking.

pdADMM: Pseudocode

Algorithm 2 the pdADMM Algorithm

Require: y, $p_1 = x$, ρ , ν .

Ensure: p, W, b, z, q.

- 1: Initialize k = 0.
- 2: **while** \mathbf{p}^k , \mathbf{W}^k , \mathbf{b}^k , \mathbf{z}^k , \mathbf{q}^k not converged **do**
- 3: Update p_l^{k+1} of different l in parallel.
- 4: Update W_l^{k+1} of different l in parallel.
- 5: Update b_l^{k+1} of different l in parallel.
- 6: Update z_I^{k+1} of different I in parallel.
- 7: Update q_I^{k+1} of different I in parallel.
- 8: $r_l^k \leftarrow p_{l+1}^{k+1} q_l^{k+1} (l = 1, \dots, L)$ in parallel # Compute residuals.
- 9: $u_I^{k+1} \leftarrow u_I^k + \rho r_I^k$ of different I in parallel.
- 10: $k \leftarrow k + 1$.
- 11: end while
- 12: Output $\mathbf{p}, \mathbf{W}, \mathbf{b}, \mathbf{z}, \mathbf{q}$.



pdADMM: Convergence Assumptions

Assumption

 $f_l(z_l)$ is Lipschitz continuous with coefficient S>0, and F(p,W,b,z,q) is coercive. Moreover, $\partial f_l(z_l)$ is bounded, i.e. there exists M>0 such that $\|\partial f_l(z_l)\| \leq M$.

The convergence conditions of the pdADMM algorithm are milder than those of the dlADMM algorithm.

| Algorithm | dIADMM | pdADMM | |
|-----------------------|--------------------------|------------------------------------|--|
| Objective | Coercive | Coercive | |
| Activation $f_l(z_l)$ | ReLU and leaky ReLU | ReLU, leaky ReLU, sigmoid and tanh | |
| Loss $R(z_L; y)$ | Lipschitz differentiable | No assumption | |

Table: Convergence Assumptions between dIADMM and pdADMM

pdADMM: Convergence Results

We can prove the convergence of the pdADMM to a critical point using the similar proofs as dIADMM, which is shown as follows:

Theorem (Convergence to a Critical Point)

If $\rho > \max(4\nu S^2, (\sqrt{17}+1)\nu/2)$, then for the variables (p,W,b,z,q,u) in the parallel MLP training problem, starting from any $(p^0,W^0,b^0,z^0,q^0,u^0)$, $(p^k,W^k,b^k,z^k,q^k,u^k)$ has at least a limit point $(p^*,W^*,b^*,z^*,q^*,u^*)$, and any limit point is a critical point of parallel MLP training problem. That is, $0 \in \partial L_\rho(p^*,W^*,b^*,z^*,q^*,u^*)$.

Theorem (Convergence Rate)

For a sequence $(p^k, W^k, b^k, z^k, q^k, u^k)$, define $c_k = \min_{0 \le i \le k} (\sum_{l=2}^L (\tau_i^{i+1}/2) \| p_l^{i+1} - p_l^i \|_2^2 + \sum_{l=1}^L (\theta_l^{i+1}/2) \| W_l^{i+1} - W_l^i \|_2^2 + \sum_{l=1}^L (\nu/2) \| b_l^{i+1} - b_l^i \|_2^2 + \sum_{l=1}^{L-1} C_1 \| z_l^{i+1} - z_l^i \|_2^2 + (\nu/2) \| z_L^{i+1} - z_L^i \|_2^2 + \sum_{l=1}^{L-1} C_2 \| q_l^{i+1} - q_l^i \|_2^2)$ where $C_1 = \nu/2 - 2\nu^2 S^2/\rho > 0$ and $C_2 = \rho/2 - 2\nu^2/\rho - \nu/2 > 0$, then the convergence rate of c_k is o(1/k).

Experimental Results: Convergence

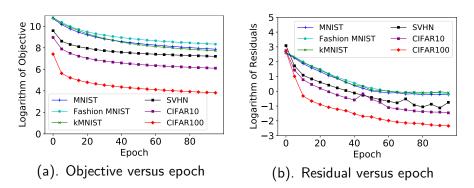


Figure: The convergence of the proposed pdADMM: the objective decreases monotonously, and the residual converges to 0.

Experimental Results: Speedup

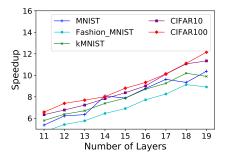


Figure: The relationship between speedup and the number of layers: the speedup increases linearly with the number of layers.

| Neurons# | Serial pdADMM | pdADMM(sec) | Speedup |
|----------|---------------|-------------|---------|
| | (sec) | | |
| 1500 | 237.66 | 26.78 | 8.87 |
| 1600 | 348.70 | 31.78 | 10.97 |
| 1700 | 390.51 | 35.79 | 10.91 |
| 1800 | 475.60 | 41.37 | 11.50 |
| 1900 | 465.57 | 45.87 | 10.15 |
| 2000 | 570.90 | 50.70 | 11.26 |
| 2000 | 570.9 | 50.7 | 11.26 |
| 2100 | 570 | 54.91 | 10.38 |
| 2200 | 678.83 | 63.59 | 10.68 |
| 2300 | 710.3 | 70.36 | 10.10 |
| 2400 | 766.82 | 62.5 | 12.27 |

Table: The relation between speedup and number of neurons on the MNIST dataset: the pdADMM runs 10 times faster than its serial version.

Experimental Results: Performance

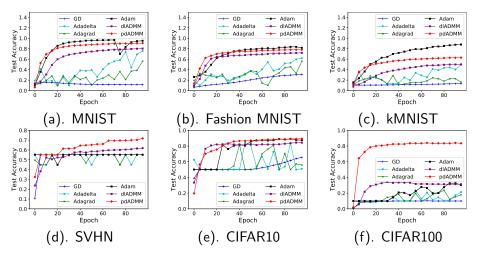


Figure: Test accuracy of all methods: pdADMM outperformed most comparison methods.

Code Release

dIADMM: https://github.com/xianggebenben/dlADMM pdADMM: https://github.com/xianggebenben/pdADMM

Thank you for your attention!

Reference



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