Linearly-constrained nonsmooth optimization for training autoencoders

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1. The optimization problem for training a deep neural network

The Model for The Neural Network

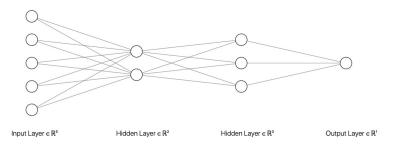
Given an input data $\{(x_n, y_n)\}_{n=1}^N$, where $x_n \in \mathbb{R}^{N_0}$, $y_n \in \mathbb{R}^{N_L}$:

Neural Networks (NN)- deep learning:

$$(1) \quad \min_{W_{\ell}, b_{\ell}, \ldots \atop \ell=1, 2, \ldots, L} \frac{1}{N} \sum_{n=1}^{N} \|\sigma_{L}(W_{L}\sigma_{L-1}(\cdots \sigma_{1}(W_{1}x_{n}+b_{1})+b_{2}\cdots)+b_{L})-y_{n}\|^{2}.$$

- N: the number of input data.
- L: the number of layers.
- N_{ℓ} : the number of neurons at the ℓ -th layer.
- σ_{ℓ} : the activation function. Here we use ReLU, i.e., $\sigma_{\ell}(z) = \max(z, 0)$.
- variables to be determined:
 - $W_{\ell} \in \mathbb{R}^{N_{\ell} \times N_{\ell-1}}$:
 - $b_{\ell} \in \mathbb{R}^{N_{\ell}}$.

An Example



Why we use ReLU?

- ReLU reduces the vanishing gradient problem by making the problem more sparse;
- ReLU becomes the most popular activation functions since 2012 ([Sun 2019]).

An Autoencoder is a special network with two layers.

Existing Approaches: SGD-based Methods

Properties

- calculating the gradient via the chain rule;
- in cases where nonsmooth activation functions are used, a subgradient in a neighborhood is often used.

Some SGD-based Methods

- Vanilla SGD ([Cramir 1946])
- Adagrad ([Duchi-Hazan-Singer 2011])
- AdagradDecay ([Duchi-Hazan-Singer 2011])
- Adadelata ([Zeiler 2012])
- Adam ([Kingma-Ba-Adam 2014])
- Adamax ([Kingma-Ba-Adam 2014])

Existing Approaches: SGD-based Methods (Cont'd)

Limitations

- neglecting the exactness in calculating the subgradient of the objective function;
- for solving a nonsmooth nonconvex problem, whether the SGD-based methods produce a convergent sequences is unknown;
- in practice, SGD-based approaches suffer from vanishing gradient phenomenon, poor conditioning, and saddle points that affect convergence.

An equivalent Model

Carreira Perpiñán-Wang 2014

(2)
$$\min_{\substack{W_{\ell}, u_{n,\ell}, b_{\ell}, \\ \ell=1, 2, \dots, L, \ n=1, 2, \dots, N}} \frac{1}{N} \sum_{n=1}^{N} \|u_{n,L} - y_{n}\|_{F}^{2}$$
s. t.
$$u_{n,\ell} = \sigma_{\ell}(W_{\ell}u_{n,\ell-1} + b_{\ell}),$$

$$n = 1, \dots, N, \ \ell = 1, \dots, L.$$

Here $u_{n,0} = x_n$, $u_{n,\ell}$: the output of the ℓ -th layer with respect to the n-th input data.

Solving (2) instead of (1) is able to alleviate the problems that SGD-based methods suffer.

Existing Approaches for Solving the Model (2)

- ℓ_2 penalty method: no exact penalty result.
 - Carreira-Perpinan-Wang 2014
 - Lau-Zeng-Wu-Yao 2018
 - Zeng-Lau-Lin-Yao 2019
- multi-block 'ADMM': hard to deal with the quadratic terms.
 - Taylor et. al. 2016
 - Zhang-Chen-Saligrama 2016
 - Evens-Latafat-Themelis 2020

The above methods have no convergence results!

 ℓ_1 penalty method: present the exact penalty result, and establish the subsequence convergence result ([Cui-He-Pang 2020]).

- limitation in theory: restrictive assumptions, which exclude ReLU;
- limitation in practice: cannot solve large-scale problems.

A New Penalty Approach

- using l₁ penalty terms;
- adding additional inequality constraints $u_{n,\ell} \ge 0$, $u_{n,\ell} \ge W_\ell u_{n,\ell-1} + b_\ell$.

$$\begin{split} \min_{\substack{W_{\ell}, u_{n,\ell}, b_{\ell}, \\ \ell=1, 2, \dots, L, \ n=1, 2, \dots, N}} & \frac{1}{N} \sum_{n=1}^{N} \| (W_{L} u_{n,L} + b_{L})_{+} - y_{n} \|_{2}^{2} \\ & + \beta \sum_{n=1}^{N} \sum_{\ell=1}^{L-1} e_{N_{\ell}}^{T} (u_{n,\ell} - (W_{\ell} u_{n,\ell-1} + b_{\ell})_{+}) \\ \text{s. t.} & u_{n,\ell} \geq 0, \ u_{n,\ell} \geq W_{\ell} u_{n,\ell-1} + b_{\ell}, \quad n = 1, \dots, N, \ \ell = 1, \dots, L. \end{split}$$

where $\beta > 0$, $e_{N_{\ell}} \in \mathbb{R}^{N_{\ell}}$ represent a vector whose elements are all 1.

- the subdifferential of the objective function enjoys an explicit expression;
- we first present the exact penalty results, regarding global solutions, local minimizers, Clarke stationary point and directional stationary point.

2. Autoencoders

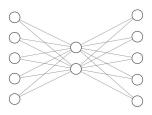
Autoencoders: Unsupervised Learning

Given data matrix $X = (x_1, x_2, ..., x_N)$ with $x_n \in \mathbb{R}^{N_0}$, $W \in \mathbb{R}^{N_1 \times N_0}$, $b = ((b_1)^T, (b_2)^T)^T$ with $b_1 \in \mathbb{R}^{N_1}$, $b_2 \in \mathbb{R}^{N_0}$.

Autoencoder: A special two-layer network

$$\min_{W,b} \frac{1}{N} \sum_{n=1}^{N} \|\sigma(W^T \sigma(W x_n + b_1) + b_2) - x_n\|_2^2.$$

- Encoder (representation): $\varphi_n(W, b) = \sigma(Wx_n + b_1)$.
- Decoder (prediction function): $\psi_n(W, b) = \sigma(W^T \varphi_n(W, b) + b_2).$



Input Layer $\in \mathbb{R}^5$ Hidden Layer $\in \mathbb{R}^2$ Output Layer $\in \mathbb{R}^5$

Features and Notations

Features:

- tied weight: $W = W_1 = W_2^{\mathrm{T}}$.
- \bullet $x_n = y_n$.

Notations:

- activation function $\sigma: \mathbb{R}^m \mapsto \mathbb{R}^m$ being ReLU, i.e., $\sigma(y) = \max\{y, 0\} = y_+.$
- variables to be determined: *W*, *b*.

Objective: to learn an encoder and an decoder for input X.

Limitation: training the basic model for autoencoders may lead to poor performance.

Limitations of The Existing Methods

SGD-based methods:

- neglecting the exactness in calculating the subgradient of the objective function;
- for solving a nonsmooth nonconvex problem, whether the SGD-based methods produce a convergent sequences is unknown;
- in practice, SGD-based approaches suffer from vanishing gradient phenomenon, poor conditioning, and saddle points that affect convergence.

methods for solving (2):

• due to the special structure $W_1 = W_2^{\rm T}$, this kind of methods cannot be used

Sparse Autoencoder

Sparse autoencoder:

$$\min_{W,b} \frac{1}{N} \sum_{n=1}^{N} \| (W^T (Wx_n + b_1)_+ + b_2)_+ - x_n \|_2^2 + \lambda_1 \sum_{n=1}^{N} e_{N_1}^T (Wx_n + b_1)_+ + \lambda_2 \| W \|_F^2.$$

- $\lambda_1, \lambda_2 > 0$, $\lambda_1 \sum_{n=1}^N e^T v_n + \lambda_2 ||W||_F^2$: regularization term.
- widely used in feature learning ([Goodfellow 2016]).

Regularization terms:

- for pursuing sparsity: $\sum_{n=1}^{N} \|\sigma(Wx_n + b_1)\|_1$ ([Ng et. al. 2011]);
- for avoiding overfitting phenomenon: $\mathcal{R}(W,b) = ||W||_F^2$, called weight decay ([Krogh-Hertz 1992]).

Equivalent Model with Additional Constraints

An equivalent model with auxiliary variables:

(R)
$$\min_{z} \frac{1}{N} \sum_{n=1}^{N} \left\| (W^{T} v_{n} + b_{2})_{+} - x_{n} \right\|_{2}^{2} + \lambda_{1} \sum_{n=1}^{N} e^{T} v_{n} + \lambda_{2} \|W\|_{F}^{2}$$
s. t. $v_{n} = (W x_{n} + b_{1})_{+}$,
for $n = 1, 2, ..., N$.

Notations:

- $e = (1, 1, ..., 1)^T \in \mathbb{R}^{N_1}$.
- $\bullet V = (v_1, v_2, \dots, v_N) \in \mathbb{R}^{N_1 \times N}.$
- $\bullet \ z = (W_{\cdot,1}^T, \dots, W_{\cdot,N_0}^T, b^T, v_1^T, \dots, v_N^T)^T.$
- reularization term $\mathcal{R}(z) = \lambda_1 \sum_{n=1}^N e^T v_n + \lambda_2 ||W||_F^2$.
- fidelity term $\mathcal{F}(z) := \frac{1}{N} \sum_{n=1}^{N} \left\| (W^T v_n + b_2)_+ x_n \right\|_2^2$.

A New Penalty Model

Let $\beta > 0$.

(RP)
$$\min_{z} O(z) := \mathcal{F}(z) + \mathcal{R}(z) + \beta \sum_{n=1}^{N} e^{T} (v_n - (Wx_n + b_1)_+)$$
s. t. $v_n \ge (Wx_n + b_1)_+$,
for $n = 1, 2, ..., N$.

Notes:

- $\sum_{n=1}^{N} \|v_n (Wx_n + b_1)_+\|_1$ equals $\sum_{n=1}^{N} e^T (v_n (Wx_n + b_1)_+)$.
- penalty term $\mathcal{P}(z) := \beta \sum_{n=1}^{N} e^{T} (v_n (Wx_n + b_1)_+).$
- Ω_2 : the feasible set of (RP).

Linear Constrained Regularized Autoencoder

Define

$$\Omega_3 := \{z : ||b||_{\infty} \le \alpha\},\$$

where
$$\alpha = \frac{\|X\|_F^2}{\lambda_1 N} + \sqrt{\frac{N_1 N_0}{\lambda_2 N}} \|X\|_F \|X\|_1.$$

We then reformulate (2) over Ω_3 as

$$(LRP) \qquad \qquad \min_{z \in \mathcal{Z}} O(z),$$

where
$$Z := \Omega_2 \cap \Omega_3 = \{z : Az \le c\}.$$

Here, $\nu = 2(NN_1 + N_0 + N_1)$,

$$A = \begin{bmatrix} X^{\mathrm{T}} \otimes I_{N_{1}} & e_{N_{1}} \otimes I_{N_{1}} & 0 & -I_{N_{1}N} \\ 0 & 0 & 0 & -I_{N_{1}N} \\ 0 & I_{N_{1}+N_{0}} & 0 \\ 0 & -I_{N_{1}+N_{0}} & 0 \end{bmatrix} \in \mathbb{R}^{\nu \times N_{2}}, \quad c = \begin{bmatrix} 0 \\ 0 \\ \alpha e_{N_{1}+N_{0}} \\ \alpha e_{N_{1}+N_{0}} \end{bmatrix} \in \mathbb{R}^{\nu},$$

where \otimes represents the Kronecker product.

3. Theoretical Analysis

Preliminaries

- The Clarke subdifferential [Clarke 1990] of a locally Lipschitz continuous function $f: \mathbb{R}^m \to \mathbb{R}$ at y^* is defined by $\partial f(y^*) = \operatorname{co}\left\{\lim_{y \to y^*} \nabla f(y): f \text{ is smooth at } y\right\}$.
- f'(y;d): the directional derivative of a directional differentiable function f at y along the direction d, i.e.,

$$f'(y;d) = \lim_{t \downarrow 0} \frac{f(y+td) - f(y)}{t}.$$

- $f^{\circ}(\overline{y};d) := \limsup_{\substack{y \to \overline{y} \\ t \downarrow 0}} \frac{f(y+td)-f(y)}{t}$ is the Clarke generalized directional derivative at \overline{y} along the direction d.
- A function f is said to be regular [Clarke 1990] at $\bar{y} \in \mathbb{R}^m$ provided that if for all d, the directional derivative $f'(\bar{y}; d)$ exists, and $f'(\bar{y}; d) = f^{\circ}(\bar{y}; d)$.
- The objective functions of (R), (RP) and (LRP) are then semismooth functions and directional differentiable [Mifflin 1977].

Preliminaries (Cont'd)

We call $\bar{z} \in \Omega_1$, $\bar{z} \in \Omega_2$, $\bar{z} \in \mathcal{Z}$ a d(irectional)-stationary point [Cui et al. 2020] of (R), (RP) and (LRP) respectively, if

$$\mathcal{F}'(\overline{z};d) + \nabla \mathcal{R}(\overline{z})^{\mathrm{T}} d \ge 0, \quad \forall d \in \mathcal{T}_{\Omega_1}(\overline{z}),$$
$$O'(\overline{z};d) \ge 0, \quad \forall d \in \mathcal{T}_{\Omega_2}(\overline{z}),$$
$$O'(\overline{z};d) \ge 0, \quad \forall d \in \mathcal{T}_{\mathcal{I}}(\overline{z}).$$

We call $\overline{z} \in \Omega_1$, $\overline{z} \in \Omega_2$, $\overline{z} \in \mathcal{Z}$ a generalized d(irectional)-stationary point of (R), (RP) and (LRP), respectively, if the above three inequalities hold with $\mathcal{F}^{\circ}(\overline{z};d)$ and $O^{\circ}(\overline{z};d)$ instead of $\mathcal{F}'(\overline{z};d)$ and $O'(\overline{z};d)$.

Main Contributions in theory

• The solution set of problem (LRP) is nonempty and bounded.

```
global minimizer
R:
                                    local minimizer
                                                             d-stationary point
                                                                                           generalized d-stationary point
                111
                                                                                                  \uparrow \mathcal{P} is regular at \bar{z}
RP ·
        global minimizer
                                    local minimizer
                                                             d-stationary point
                                                                                           generalized d-stationary point
       \bar{z} \in \Omega_3 \ \text{lift}
                                 \bar{z} \in \Omega_3 \ \text{lift}
                                                                 \bigcap O(\bar{z}) < \theta
                                                                                                 \uparrow \bar{z} \in int(\Omega_3), O(\bar{z}) < \theta
LRP: global minimizer
                                   local minimizer
                                                             d-stationary point
                                                                                           generalized d-stationary point
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4. A Smoothing Proximal Gradient Algorithm (SPG)

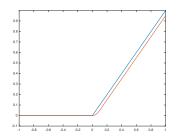
A Smoothing Function for ReLU

Definition 1

Let $\zeta:\mathbb{R}^m\mapsto R$ be continuous. We call $\widetilde{\zeta}:\mathbb{R}^m\times\mathbb{R}_+\mapsto R$ a smoothing function of ζ , if for all fixed $\mu>0$, $\widetilde{\zeta}(\cdot,\mu)$ is continuously differentiable, and $\lim_{y\to \overline{y},\mu\downarrow 0}\widetilde{\zeta}(y,\mu)=\zeta(\overline{y})$.

 μ -smoothing function $\widetilde{\sigma}(y,\mu): \mathbb{R}^m \times \mathbb{R}_+ \mapsto \mathbb{R}^m$ for $\sigma(y) = y_+: \mathbb{R}^m \mapsto \mathbb{R}^m$

$$\widetilde{\sigma}_i(y,\mu) = \begin{cases} 0 & \text{if } y_i < 0 \\ \frac{y_i^2}{2\mu} & \text{if } 0 \le y_i \le \mu \\ y_i - \frac{\mu}{2} & \text{if } y_i > \mu \end{cases}$$



 $\widetilde{\sigma}(y, \mu_1) > \widetilde{\sigma}(y, \mu_2)$ with $\mu_1 < \mu_2$.

A Smoothing Function for O(z)

A smoothing function for O(z) with $\mu > 0$:

$$\widetilde{O}(z,\mu):=\widetilde{\mathcal{H}}(z,\mu)+\mathcal{R}(z),$$

$$\widetilde{\mathcal{H}}(z,\mu):=\widetilde{\mathcal{F}}(z,\mu)+\widetilde{\mathcal{P}}(z,\mu),$$
 where

$$\widetilde{\mathcal{F}}(z,\mu) = \frac{1}{N} \sum_{n=1}^{N} \| (W^T v_n + b_2)_+ \|_2^2 + \frac{1}{N} \| X \|_F^2 - \frac{2}{N} \sum_{n=1}^{N} x_n^T \widetilde{\sigma}(W^T v_n + b_2, \mu),$$

$$\widetilde{\mathcal{P}}(z,\mu) = \beta \sum_{n=1}^{N} e^{T} (v_n - \widetilde{\sigma}(Wx_n + b_1, \mu))$$

are a smoothing function for $\mathcal{F}(z)$ and $\mathcal{P}(z)$, respectively.

- $\widetilde{O}(z, \mu_1) < \widetilde{O}(z, \mu_2)$ with $\mu_1 < \mu_2$.
- for $\mu > 0$, $z \in \mathcal{Z}$, $0 \le O(z) \le \widetilde{O}(z, \mu) \le O(z) + (||X||_1 + N_1 N\beta) \mu$.

Step 1: Initialization: choose $z^{(0)} \in \mathcal{Z}$, $0 < \mu^{(0)} < 1$, $0 < \tau_1 < 1$, $\tau_2 > 0$, $\tau_3 \ge 1$, and $L^{(0)} \ge 1$. Set k := 0.

Step 2: Set $z^{(k+1)}$ be the unique minimizer of the strongly convex quadratic program

$$\min_{z \in \mathcal{Z}} \left\langle \nabla_z \widetilde{\mathcal{H}}(z^{(k)}, \mu^{(k)}), z - z^{(k)} \right\rangle + \mathcal{R}(z) + \frac{L^{(k)}}{2} ||z - z^{(k)}||_2^2.$$

Step 3: Update the smoothing and proximal parameters $\mu^{(k+1)}$ and $L^{(k+1)}$ by

$$\begin{cases} (\mu^{(k+1)},\,L^{(k+1)}) := (\mu^{(k)},\,L^{(k)}), & \text{if } \widetilde{O}(z^{(k+1)},\mu^{(k)}) - \widetilde{O}(z^{(k)},\mu^{(k)}) < -\tau_2\frac{\mu^{(k)}}{L^{(k)}}, \\ (\mu^{(k+1)},\,L^{(k+1)}) := (\tau_1\mu^{(k)},\,\tau_3L^{(k)}), & \text{otherwise}. \end{cases}$$

Step 4: Increment k by one, return to step 2.

5. Numerical Performances of SPG

Implementation Details

- $\lambda_2 = 0.1$, $\lambda_1 = 0.0001$, $\beta = \frac{1}{N}$.
- \bullet $\tau_1 = 0.5, \tau_2 = 0.001, \mu^{(0)} = 0.001.$
- $\tau_3 = 1.1$, $L^{(0)} = L_* := \max\{1, \sqrt{N_0 N_1/N}, \beta, N_0/30\}$ ($L^{(0)}$ should not be too small).
- max iteration: 4000.
- initialization: $W^{(0)} = \text{randn}(N_1, N_0)/N$, $b^{(0)} = 0$ and $v_n^{(0)} = (W^{(0)}x_n)_+$ for all n = 1, 2, ..., N.
- stop criterion: $\mu^{(k)} \le 10^{-7}$.

Implementation Details (Cont'd)

• data type 1: under Gaussian distribution with some noises: we generate the data matrix $X_{\text{all}} = (x_1, x_2, \dots, x_{N+N_{\text{test}}})$ by setting

$$x_i \sim \mathcal{N}(\vartheta, \Sigma_0^{\mathrm{T}} \Sigma) + \epsilon_0 \mathcal{N}(0, 1)$$

for all $i=1,2,\ldots,N+N_{\text{test}}$, where $\vartheta=0.5+\text{randn}(N_0,1)$ and $\Sigma_0=\text{randn}(N_0,1)$. We then set all negative elements of X_{all} to be zero.

data type 2: distributed in [0, 1] with some noises:
 we generate the data matrix X_{all} by

$$X_{\text{all}} = \text{rand}(N + N_{\text{test}}, N_0) + \epsilon_0 \text{randn}(N + N_{\text{test}}, N_0).$$

We then set all negative elements of $X_{\rm all}$ to be zero.

- the first N and the last N_{test} columns of X_{all} are selected to be the training and test sets, respectively.
- noise: ϵ_0 (we set $\epsilon_0 = 0.05$).

Measurements

- FVal: the function value of (LRP), denoted by O(z).
- FeasVi: the average feasibility violation, denoted by $\frac{1}{NN_1}\sum_{n=1}^{N}\|v_n-(Wx_n+b_1)_+\|_1$.
- TrainErr: denoted by $\frac{1}{N} \sum_{n=1}^{N} ||(W^T(Wx_n + b_1)_+ + b_2)_+ x_n||_2^2$.
- TestErr: denoted by $\frac{1}{N_{\text{test}}} \sum_{n=N_{\text{test}}+1}^{N+N_{\text{test}}} \left\| (W^{\text{T}} v_n + b_2)_+ x_n \right\|_2^2$.
- Time: CPU time (s).

Algorithm performance of SPG

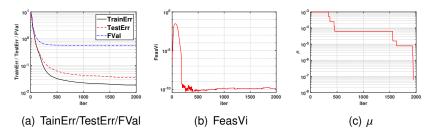
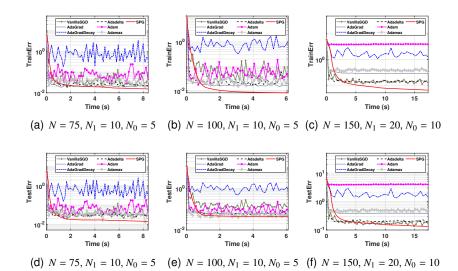


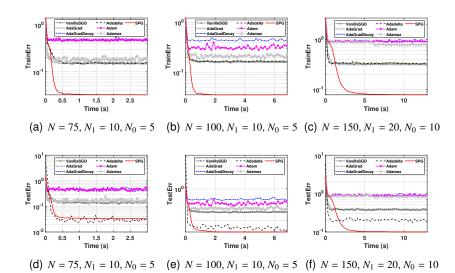
FIG 1: Algorithm performance of SPG

Here N = 100, $N_1 = 10$, $N_0 = 5$.

Comparisons on Random Data sets with data type 1



Comparisons on Random Data sets with data type 2



Comparisons on Random Data sets with N = 1000

We then consider to use Adadelta as a pre-process to accelerate SPG. More specifically, we first run Adadelta for 1000 epochs and then switch to SPG. We call the consequent hybrid algorithm SPG-ADA.

TAB 1: Comparisons between SPG-ADA and Adadelta with N = 1000.

		SPG-ADA				Adadelta		
N_0	N_1	TrainErr	TestErr	FeaErr	Time	TrainErr	TestErr	Time
5	20	3.297e-02	3.636e-02	1.234e-11	8.758	5.518e-02	5.847e-02	3.044
5	30	2.974e-02	3.103e-02	5.599e-12	10.592	5.470e-02	5.566e-02	3.623
5	40	2.960e-02	3.200e-02	7.238e-12	15.206	5.474e-02	5.632e-02	3.786
10	40	6.708e-02	7.727e-02	1.140e-11	19.184	1.257e-01	1.341e-01	5.590
10	60	6.867e-02	7.863e-02	5.138e-11	22.599	1.348e-01	1.436e-01	6.149
10	80	8.105e-02	9.057e-02	8.814e-11	25.701	1.364e-01	1.441e-01	7.169
20	80	1.824e-01	2.200e-01	3.020e-12	33.962	3.766e-01	4.265e-01	8.992
20	120	1.135e-01	2.611e-01	3.634e-12	38.191	4.051e-01	4.566e-01	12.275
20	160	1.946e-01	2.380e-01	2.181e-12	72.942	3.746e-01	4.240e-01	20.268

Results on Real datasets: Reconstruction on MNIST

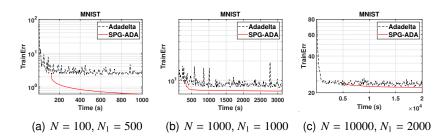
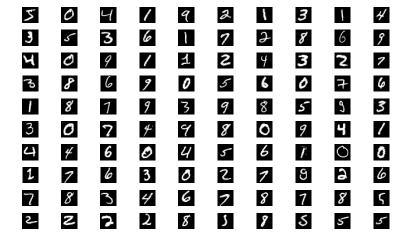


FIG 2: Comparisons between SPG-ADA and Adadelta on MNIST.

Results on Real datasets: Reconstruction on MNIST



(a) SPG

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Results on Real datasets: Reconstruction on MNIST



(a) Adam

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Conclusions

- the solution set is nonempty and bounded.
- first present the exact penalty results regarding global solutions, local minimizers, Clarke stationary point and directional stationary point.
- present an effective algorithm: global convergence √ to a Clarke stationary point √, which is stronger than a critical point.
- SPG can be used to solve large-scale problems, and a better TrainErr/TestErr is obtained (compared with that obtained by SGD-based algorithms).
- the Clarke stationary point always performs better than the critical point in the sense of TrainErr/TestErr.
- Wei Liu, Xin Liu, Xiaojun Chen. Linearly-constrained nonsmooth optimization for training autoencoders. Preprint, arXiv:2103.16232, 2021.

Thanks for your listening!

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