Nonconvex Sparse Optimization and Algorithms

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Chinese Academy of Sciences, January 12, 2025

Joint work with Wanquan Liu (SYSU), Lingchen Kong (BJTU) and others

Outline

Introduction

First-Order Algorithms

Second-Order Algorithms

Future Work

Sparse Optimization

- Sparse optimization considers

$$\min_{x\in\mathbb{R}^n} \ f(x) + \lambda\|x\|_0$$

$$\Updownarrow$$

$$\min_{x\in\mathbb{R}^n} \ f(x) \quad \text{s.t.} \quad \|x\|_0 \leq s$$

  - x can be extended to matrices and tensors
  - $f(x)$ may be nonsmooth even nonconvex
  - $\|x\|_0$ counts the number of nonzeros
  - λ and s are parameters
- Also called compressed sensing and variable selection
- Broad applications in machine learning, pattern recognition and engineering
- `https://github.com/xianchaoxiu/Sparse-Optimization`

Algorithms

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$\ell_1 - \ell_p$ Minimization

- Xiu-Kong-Li-Qi, Computational Optimization and Applications, 2018

$$\min_{x \in \mathbb{R}^n} \quad \|Ax - b\|_1 + \lambda \|x\|_p^p \; (0 < p < 1) \tag{1}$$

- Consider the following ϵ-approximations

$$\min_{x \in \mathbb{R}^n} \; F_{\alpha,\epsilon}(x) = \|Ax - b\|_1 + \lambda \sum_{i=1}^{n} (|x_i|^\alpha + \epsilon_i)^{\frac{p}{\alpha}}$$

$$\Downarrow$$

$$\min_{x \in \mathbb{R}^n} \; F_\epsilon(x) = \|Ax - b\|_1 + \lambda \sum_{i=1}^{n} h_{u_\epsilon}(x_i) \tag{2}$$

where

$$h_{u_\epsilon}(x_i) = \min_{0 \le s \le u_\epsilon} p \left(|x_i| s - \frac{p-1}{p} s^{\frac{p}{p-1}} \right), \quad u_\epsilon = \left(\frac{\epsilon}{\lambda n} \right)^{\frac{p-1}{p}}$$

$\ell_1 - \ell_p$ Minimization

- (Definition) We say that $x^* \in \mathbb{R}^n$ is a generalized first-order stationary point of (1) if

$$0 \in (A^\top \mathrm{sgn}(Ax^* - b))_i x_i^* + \lambda p |x_i^*|^p, \quad i = 1, 2, \cdots, n$$

Furthermore, the following statement holds

$$|x_i^*| \; \geq \; (\frac{\lambda p}{\|A_i\|_1})^{\frac{1}{1-p}}, \quad \forall i \in T \tag{3}$$

- (Lower Bound) Let ϵ be a constant such that

$$0 < \epsilon < \lambda n \left(\frac{\|A_i\|_1}{\lambda p} \right)^{\frac{p}{p-1}} \tag{4}$$

Suppose that x^* is a generalized first-order stationary point of (2). Then, x^* is also a generalized first-order stationary point of (1). Moreover, the nonzero entries of x^* satisfy the lower bound property (3).

$\ell_1 - \ell_p$ Minimization

- (Convergent Theorem) Assume that ϵ satisfies (4) and set q as $\frac{1}{p} + \frac{1}{q} = 1$. Suppose that x^* is an accumulation point of $\{x^k\}$. Then x^* is a generalized first-order stationary point of (1). Moreover, the nonzero entries of x^* satisfy the lower bound (3).

Choose an arbitrary $x^0 \in \mathbb{R}^n$ and ϵ such that (4) holds. Set $k = 0$

1) Solve the weighted ℓ_1 minimization problem

$$x^{k+1} \in \operatorname{argmin}_x \left\{ \|Ax - b\|_1 + \lambda p \sum_{i=1}^n s_i^k |x_i| \right\}$$

where $s_i^k = \min\left\{ \left(\frac{\epsilon}{\lambda n}\right)^{\frac{1}{q}}, |x_i^k|^{\frac{1}{q-1}} \right\}$ for all i

2) Set $k \leftarrow k + 1$ and go to step 1)

End

$\ell_1 - \ell_p$ Minimization

- Comparison with FISTA

m	n	FISTA	Alg. 2	Alg. 3	Alg. 4	FISTA	Alg. 2	Alg. 3	Alg. 4
100	500	11.1587	0.0455	0.0303	0.0223	0.0008	0.4183	0.3087	0.2453
200	1000	8.6122	0.2097	0.1518	0.1279	0.0020	0.1413	0.0564	0.0484
300	1500	2.0159	0.1498	0.1195	0.1079	0.0067	0.2095	0.1293	0.1265
400	2000	2.3528	0.1057	0.0877	0.0799	0.1093	0.3648	0.2905	0.2791
500	2500	1.1584	0.1672	0.1491	0.1091	0.0310	0.4761	0.4799	0.4583
600	3000	0.9855	0.0972	0.0972	0.0972	0.0386	0.9324	0.7700	0.7684
700	3500	1.1239	0.0947	0.0940	0.0872	0.0756	1.7057	1.6983	1.5231
800	4000	0.8065	0.0958	0.0924	0.0861	0.1598	2.5905	2.4271	2.3562
900	4500	0.8734	0.0982	0.0981	0.0823	0.1546	3.3103	3.2272	3.2263
1000	5000	1.1301	0.0942	0.0912	0.0851	0.1937	4.0071	3.9719	4.1359

Fused Regression

- Xiu-Liu-Li-Kong, Computational Statistics & Data Analysis, 2019

$$\min_{\beta} \quad \frac{1}{2}\|y - X\beta\|^2 + \Phi_{\tau_1}(\beta) + \sum_{i=1}^{p} \Phi_{\tau_2}(\beta_{i+1} - \beta_i)$$

  - Φ_{τ_1} and Φ_{τ_2} can be the same or different
  - Nonconvex penalty functions: ℓ_p, SCAD, MCP, capped ℓ_1
- For notational simplicity, define

$$\min_{\beta} \quad \frac{1}{2}\|y - X\beta\|^2 + \Phi_{\tau_1}(\beta) + \Phi_{\tau_2}(D\beta)$$

with

$$D = \begin{pmatrix} -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -1 & 1 \end{pmatrix} \in \mathbb{R}^{(p-1)\times p}$$

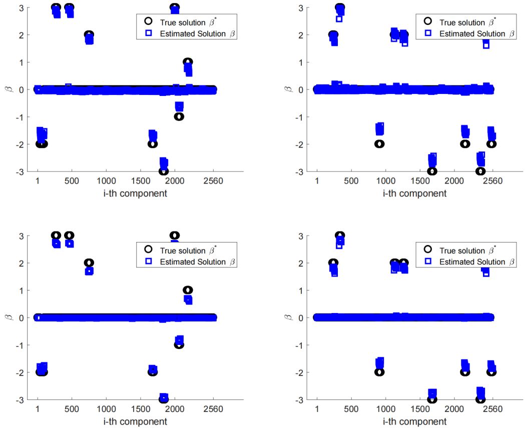
Fused Regression

- Alternating direction method of multipliers (ADMM)

$$\begin{aligned} \min_{\alpha,\gamma,\beta} \quad & \frac{1}{2}\|y - X\beta\|^2 + \Phi_{\tau_1}(\alpha) + \Phi_{\tau_2}(\gamma) \\ \text{s.t.} \quad & \alpha = \beta \\ & \gamma = D\beta \end{aligned}$$

- (Convergent Theorem) Suppose that $\{(\alpha^k, \gamma^k, \beta^k, w_1^k, w_2^k)\}$ is a generated sequence. Then the sequence converges to a stationary point.

- Recovery results



Sparse LDA

- Liu-Feng-Xiu-Liu, Pattern Recognition, 2024

$$\begin{aligned}\min_{Q}\ & \mathrm{Tr}\left(Q^\top S Q\right) + \lambda \|Q\|_{2,1} \\ \text{s.t.}\ & Q^\top Q = I\end{aligned}$$

$$\Downarrow$$

$$\begin{aligned}\min_{P,Q,E}\ & \mathrm{Tr}\left(Q^\top S Q\right) + \lambda_1 \|Q\|_{2,1} + \lambda_2 \|E\|_1 \\ \text{s.t.}\ & X = PQ^\top X + E,\ P^\top P = I\end{aligned}$$

$$\Downarrow$$

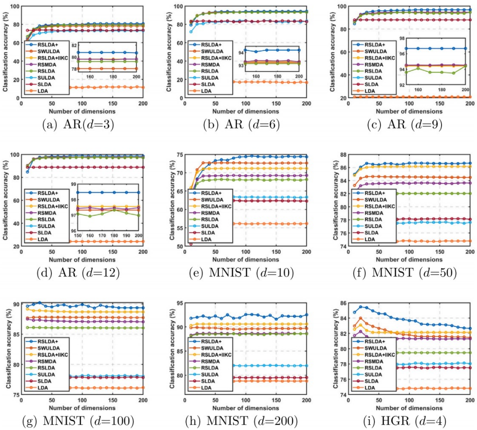
$$\begin{aligned}\min_{P,Q,E}\ & \mathrm{Tr}\left(Q^\top S Q\right) + \lambda_1 \|Q\|_{2,0} + \lambda_2 \|E\|_0 \\ \text{s.t.}\ & X = PQ^\top X + E,\ P^\top P = I\end{aligned}$$

$$\Downarrow$$

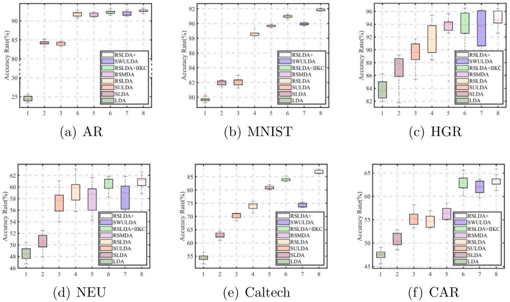
$$\begin{aligned}\min_{P,Q,E}\ & \mathrm{Tr}\left(Q^\top S Q\right) + \lambda_1 \|Q\|_{2,0} + \lambda_2 \|Q\|_0 + \lambda_3 \|E\|_0 \\ \text{s.t.}\ & X = PQ^\top X + E,\ P^\top P = I\end{aligned}$$

Sparse LDA

- Classification accuracy



- Model stability



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Sparse CCA

- Xiu-Yang-Kong-Liu, Applied Mathematics and Computation, 2020

$$\begin{aligned} \min_{\beta,\theta} \quad & -\beta^\top X^\top Y\theta + \lambda\|\beta\|_1 + \mu\|\theta\|_1 \\ \text{s.t.} \quad & \|X\beta\|^2 \le 1, \ \|Y\theta\|^2 \le 1 \end{aligned}$$

- Alternating minimization algorithm (AMA)
  - Update β by

$$\begin{aligned} \min_{\beta} \quad & -\beta^\top X^\top Y\theta + \lambda\|\beta\|_1 \\ \text{s.t.} \quad & \|X\beta\|^2 \le 1 \end{aligned} \tag{5}$$

  - Update θ by

$$\begin{aligned} \min_{\theta} \quad & -\beta^\top X^\top Y\theta + \mu\|\theta\|_1 \\ \text{s.t.} \quad & \|Y\theta\|^2 \le 1 \end{aligned}$$

Sparse CCA

- The dual optimization problem of (5) is

$$\begin{aligned} \min_{\alpha,\gamma} \quad & \frac{1}{2}\|\alpha - Y\theta\|^2 + \delta_{\lambda B_\infty}(\gamma) \\ \text{s.t.} \quad & X^\top \alpha - \gamma = 0 \end{aligned}$$

$$\Downarrow$$

$$\mathcal{L}_\delta(\alpha, \gamma; \beta) = \frac{1}{2}\|\alpha - Y\theta\|^2 + \delta_{\lambda B_\infty}(\gamma) - \beta^\top (X^\top \alpha - \gamma) + \frac{\delta}{2}\|X^\top \alpha - \gamma\|^2$$

- First apply a semi-smooth Newton method for solving

$$(\alpha^{k+1}, \gamma^{k+1}) = \arg\min_{\alpha,\gamma} \{\mathcal{L}_\delta(\alpha, \gamma; \beta^k)\}$$

  Then update the Lagrange multiplier by

$$\beta^{k+1} = \beta^k - \tau\delta_k (X^\top \alpha^{k+1} - \gamma^{k+1})$$

- (Convergent Theorem) The generated sequence $\{(\beta^k, \theta^k)\}$ converges to a stationary point.

Generalized CCA

- Li-Xiu-Liu-Miao, IEEE Signal Processing Letters, 2022

$$\min_{U,P_v} \sum_{v=1}^{M} \|U - X_v P_v\|_F^2$$
$$\text{s.t.} \quad U^\top U = I_d, \quad \|P_v\|_{2,0} \le s_v$$

- Alternating minimization algorithm (AMA)
  - Update U^{k+1} by

$$\min_{U} \sum_{v=1}^{M} \|U - X_v P_v^k\|_F^2$$
$$\text{s.t.} \quad U^\top U = I_d$$

  - Update $P_v^{k+1}(v = 1, \dots, M)$ by

$$\min_{P_v} \sum_{v=1}^{M} \|U^{k+1} - X_v P_v\|_F^2 \qquad (6)$$
$$\text{s.t.} \quad \|P_v\|_{2,0} \le s_v$$

Generalized CCA

- Denote $f(P_v) := \|U^{k+1} - X_v P_v\|_F^2$. Then

$$\nabla f(P_v) = 2X_v^\top (X_v P_v - U^{k+1}), \quad \nabla^2 f(P_v) = 2I_d \otimes X_v^\top X_v$$

- The α_v-stationary point of (6) can be given by

$$P_v = \Pi_{\mathcal{S}}(P_v - \alpha_v \nabla f(P_v))$$

$$\Downarrow$$

$$\begin{aligned} 0 &= P_v - \Pi_{\mathcal{S}}(P_v - \alpha_v \nabla f(P_v)) \\ &= \begin{pmatrix} (P_v)_{T_v} \\ (P_v)_{\overline{T}_v} \end{pmatrix} - \begin{pmatrix} (P_v)_{T_v} - \alpha_v \nabla_{T_v} f(P_v) \\ 0 \end{pmatrix} \\ &= \begin{pmatrix} \alpha_v \nabla_{T_v} f(P_v) \\ (P_v)_{\overline{T}_v} \end{pmatrix} \end{aligned}$$

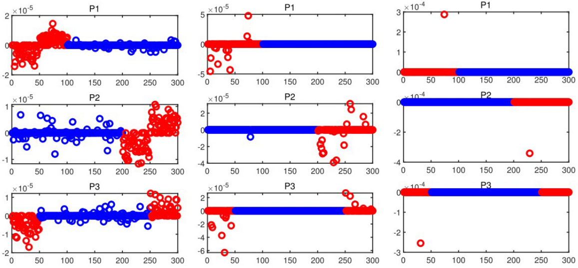
- Newton hard thresholding pursuit (NHTP)

Generalized CCA

- Runtime comparison

Problem Scale	GCCA	SGCCA	SCGCCA
(1,000;300;300;300)	0.04	0.04	**0.01**
(5,000;300;300;300)	0.23	0.28	**0.03**
(10,000;300;300;300)	0.40	0.41	**0.07**
(50,000;300;300;300)	2.32	2.27	**0.34**
(100,000;300;300;300)	4.58	4.35	**0.66**
(1,000;1,500;1,500;1,500)	0.42	0.40	**0.02**
(5,000;1,500;1,500;1,500)	1.35	1.16	**0.12**
(10,000;1,500;1,500;1,500)	2.63	2.24	**0.24**
(50,000;1,500;1,500;1,500)	13.21	10.56	**1.18**
(100,000;1,500;1,500;1,500)	26.60	22.53	**2.35**
(1,000;3,000;3,000;3,000)	1.53	1.58	**0.17**
(5,000;3,000;3,000;3,000)	3.92	3.49	**0.23**
(10,000;3,000;3,000;3,000)	6.87	5.65	**0.45**
(50,000;3,000;3,000;3,000)	32.02	23.18	**2.29**
(100,000;3,000;3,000;3,000)	667.69	629.54	**4.91**

- Extracted feature comparison



Distributed Optimization

- Qu-Chen-Xiu-Liu, Neurocomputing, 2024

$$\begin{aligned} \min_{Y \in \mathbb{R}^{n\times p}} \quad & \sum_{i=1}^{d} f_i(Y) \\ \text{s.t.} \quad & \|Y\|_{2,0} \leq s, \ \ Y^\top Y = I_p \end{aligned} \tag{7}$$

$$\Downarrow$$

$$\begin{aligned} \min_{Y \in \mathbb{R}^{n\times p}} \quad & \sum_{i=1}^{d} f_i(Y) + \frac{\mu}{4}\|Y^\top Y - I_p\|_F^2 \\ \text{s.t.} \quad & \|Y\|_{2,0} \leq s \end{aligned}$$

$$\Downarrow$$

$$\begin{aligned} \min_{Y, \{X_i\} \in \mathbb{R}^{n\times p}} \quad & \sum_{i=1}^{d} f_i(X_i) + \frac{\mu}{4}\|Y^\top Y - I_p\|_F^2 \\ \text{s.t.} \quad & X_i = Y, \ \forall i \in [d], \ \ \|Y\|_{2,0} \leq s \end{aligned} \tag{8}$$

Distributed Optimization

- (Lemma) Let $(\widetilde{Y}^*, \{\widetilde{X}_i^*\})$ be the (local) minimizer of (8). Then there exists $\mu_\epsilon > 0$ such that $\widetilde{Y}^*$ is an ϵ-(local) minimizer of (7) for any $\mu \geq \mu_\epsilon$.
- (Definition) We say $(Y^*, \{X_i^*\}, \{\Lambda_i^*\})$ is a KKT point of (8) if it satisfies

$$\begin{cases} 0 \in \nabla g(Y^*) + \sum_{i=1}^d \Lambda_i^* + \mathcal{N}_{\mathcal{S}}(Y^*) \\ 0 = \nabla f_i(X_i^*) - \Lambda_i^*, \ \forall i \in [d] \\ 0 = X_i^* - Y^*, \ \forall i \in [d] \end{cases}$$

- (Definition) We say $(Y^*, \{X_i^*\}, \{\Lambda_i^*\})$ is a stationary point of (8) if there exists $\alpha > 0$ such that

$$\begin{cases} Y^* = \mathcal{P}_{\mathcal{S}}(Y^* - \alpha(\nabla g(Y^*) + \sum_{i=1}^d \Lambda_i^*)) \\ 0 = \nabla f_i(X_i^*) - \Lambda_i^*, \ \forall i \in [d] \\ 0 = X_i^* - Y^*, \ \forall i \in [d] \end{cases}$$

- (Optimal Conditions) Suppose that $(Y^*, \{X_i^*\})$ is a local minimizer of (8). Then, there exists Λ_i^* $(i \in [d])$ such that $(Y^*, \{X_i^*\}, \{\Lambda_i^*\})$ is a KKT point of (8).

Distributed Optimization

- (Nonincreasing Lemma) Let $\{(Y^k, \{X_i^k\}, \{\Lambda_i^k\})\}$ be the generated sequence and $\beta \geq \sqrt{2}r$. Then the generated augmented Lagrangian sequence is nonincreasing, i.e.,

$$\mathcal{L}_{\boldsymbol{\beta}}(Y^{k+1}, \{X_i^{k+1}\}; \{\Lambda_i^{k+1}\}) \leq \mathcal{L}_{\boldsymbol{\beta}}(Y^k, \{X_i^k\}; \{\Lambda_i^k\})$$

- (Bounded Lemma) Suppose that $\beta \geq 2r$ holds. Then the sequence $\{(Y^k, \{X_i^k\}, \{\Lambda_i^k\})\}$ is bounded. Moreover, it satisfies

$$\begin{cases} \lim\limits_{k\to\infty} \|Y^{k+1} - Y^k\|_F = 0 \\ \lim\limits_{k\to\infty} \|X_i^{k+1} - X_i^k\|_F = 0, \ \forall i \in [d] \\ \lim\limits_{k\to\infty} \|\Lambda_i^{k+1} - \Lambda_i^k\|_F = 0, \ \forall i \in [d] \end{cases}$$

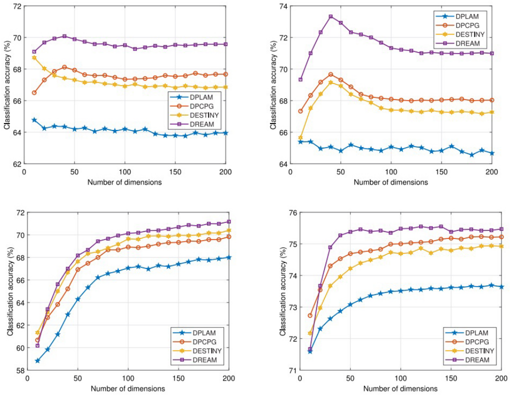
- (Convergent Theorem) Let $\{(Y^k, \{X_i^k\}, \{\Lambda_i^k\})\}$ be the generated sequence and $\beta \geq 2r$. Then, any accumulation point $(Y^*, \{X_i^*\}, \{\Lambda_i^*\})$ is a stationary point of (8).

Distributed Optimization

- Runtime comparison

Dataset	DPLAM	DPCPG	DESTINY	DREAM
YALE	0.13	0.09	0.04	**0.02**
ORL	1.19	0.593	0.57	**0.22**
CAR	2.10	1.64	1.53	**0.82**
AR	2.83	2.19	2.01	**1.71**
Vegetable	3.60	2.95	2.50	**2.29**
CIFAR-10	4.79	3.64	3.74	**2.94**

- Classification accuracy



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Future Work

Deep Unfolding Networks

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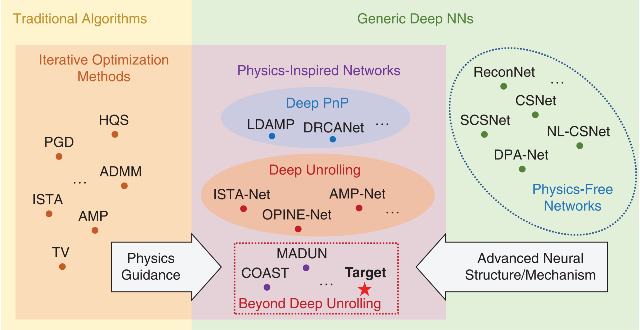

Large Language Models

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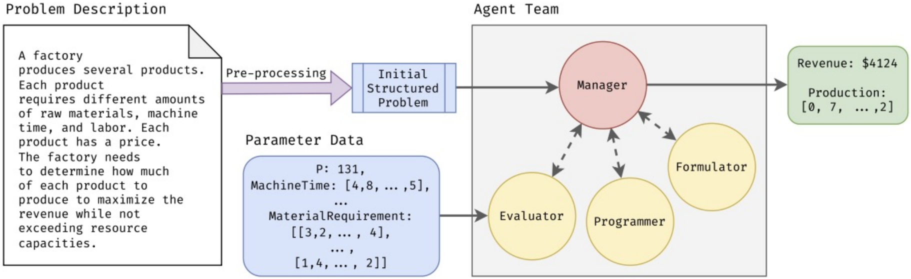

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