Simple Algorithms for Difficult Optimization Problems Illustrated

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Based on joint works with

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Outline

- Simple algorithms exploiting structures and data information
- Nonsmooth Convex – Nonconvex Smooth – Nonsmooth Nonconvex

3 ELEMENTARY PRINCIPLES

- **Approximation**
- **Regularization**
- **Decomposition**

Opening Remark and Credit

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About more than 386 years ago.....In 1629, Fermat suggested the following:

- Given f, solve for x:
- $\left[\dfrac{f(x+d)-f(x)}{d}\right]_{d=0} = 0$

...We can hardly expect to find a more general method to get the maximum or minimum points on a curve.....

Pierre de Fermat

Simple Minimization Methods

Practical Side

- Simple computational operations: inner products; No matrix inversion.
- Minimal storage of data; exploit smartly stored data.
- Easy access to function values, gradient/subgradients.
- Explicit iterative formula involving simple operations.

Theoretical Side

- Free of unknown/heuristic choices of parameters.
- Avoid nested optimization schemes/control-correction of accumulated errors.
- Versatile mathematical analytic tools broadly applicable..and with no pains!
- Complexity/Performance: mildly dependent on dimension/reasonable medium accuracy.

Natural Candidates: Schemes based on First Order Methods

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This simple problem captures the essence of many Ill-posed/underdetermined problems in applications.

Additional requirements/constraints have to be specified to make it a reasonable mathematical/computational task and often lead to interesting optimization models.

Linear Inverse Problems

Problem: Find $\mathbf{x} \in C \subset \mathbb{E}$ which "best" solves $\mathcal{A}(\mathbf{x}) \approx \mathbf{b}$, $\mathcal{A} : \mathbb{E} \to \mathbb{F}$,
where **b** (observable output), and $\mathcal{A}$ are known.

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Approach: via Regularization Models

- $g(\mathbf{x})$ is a "regularizer" (one – or sum of functions, convex or nonconvex)
- $d(\mathbf{b}, \mathcal{A}(\mathbf{x}))$ some "proximity" measure from $\mathbf{b}$ to $\mathcal{A}(\mathbf{x})$

$$\begin{aligned}
&\min \quad \{g(\mathbf{x}) : \ \mathcal{A}(\mathbf{x}) = \mathbf{b}, \ \mathbf{x} \in C\} \\
&\min \quad \{g(\mathbf{x}) : \ d(\mathbf{b}, \mathcal{A}(\mathbf{x})) \le \epsilon, \ \mathbf{x} \in C\} \\
&\min \quad \{d(\mathbf{b}, \mathcal{A}(\mathbf{x})) : \ g(\mathbf{x}) \le \delta, \ \mathbf{x} \in C\} \\
&\min \quad \{d(\mathbf{b}, \mathcal{A}(\mathbf{x})) + \lambda g(\mathbf{x}) : \ \mathbf{x} \in C\} \ (\lambda > 0)
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- Choices for $g(\cdot)$, $d(\cdot,\cdot)$ depends on the application at hand.
- **Nonsmooth and Nonconvex** regularizers g useful to describe desired features.

• Intensive research activities over the past 50 years...Now, much more...with emerging new applications and advances in computer power..

Example: Sparsity is a Common Desired Feature/Structure

Arises in Many Applications

- Sparse learning, feature selection, support vector machines, PCA,...
- Compressive sensing: recover a signal from few measurements
- Image processing: denoising, deblurring,....and much more....

Find the sparsest $\mathbf{x} \in \mathbb{R}^d$ subject to specific requirements S:

$$\min\{\|\mathbf{x}\|_0 : \quad \mathbf{x} \in S\}$$

where $\|\mathbf{x}\|_0$ denotes the number of nonzero component of $\mathbf{x}$.

Simplify design by zeroing values that are not needed: Trust topology design - bars that are not needed; Antenna Array beamforming - eliminate un-needed antenna ....etc..

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This is **Hard!**, (even is S is convex !).

Approaches

- Convex Relaxation Replace $\|\mathbf{x}\|_0$ by a relevant and more tractable objective. The l_1-norm $\|\mathbf{x}\|_1$ has been well known (since 70's) to promote sparsity.
- **Tackle directly the nonconvex problem "as is"?**. More on this soon...

Convex Nonsmooth Composite: Lagrangians Based Methods

Nonsmooth Convex with Separable Objective

$$(P) \qquad p_* = \inf\{\varphi(x) \equiv f(x) + g(Ax) : x \in \mathbb{R}^n\},$$

Here f, g are **both nonsmooth**, $A : \mathbb{R}^n \to \mathbb{R}^m$ a given linear map.

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Rockafellar ('76) has shown that the *Proximal Point Algorithm* can be applied to the dual and primal-dual formulation of (P) to produce:

- The Multipliers Method (augmented Lagrangian Method).
- **The Proximal Method of Multipliers (PMM).**
- Largely ignored over last 20 years.....Recent very strong revival in, image science, machine learning etc... within many algorithms **all being rooted in - and variants of – the PMM**.

The PMM–Proximal Method of Multipliers – Rockafellar (76)

PMM Generate (x^k, z^k) and dual multiplier y^k via

$$(x^{k+1}, z^{k+1}) \in \operatorname*{argmin}_{x,z}\{f(x) + g(z) + \langle y^k, Ax - z\rangle + \frac{c}{2}\|Ax - z\|^2 + q_k(x,z)\}$$

$$y^{k+1} = y^k + c(Ax^{k+1} - z^{k+1}), \quad (c > 0).$$

- The Augmented Lagrangian $=$ Penalized Lagrangian

$$L_c(x,z,y) := \overbrace{f(x) + g(z) + \langle y, Ax - z\rangle}^{\text{Lagrangian}} + \frac{c}{2}\|Ax - z\|^2, \ (c > 0).$$

- $q_k(x,z) := \frac{1}{2}\left(\|x - x^k\|^2_{M_1} + \|z - z^k\|^2_{M_2}\right)$ is the additional *primal proximal* term.
- The choice of $M_1 \in \mathbb{S}^n_+, M_2 \in \mathbb{S}^m_+$ is used to conveniently describe/analyze several variants of the PMM.
- $M_1 = M_2 \equiv 0$, recovers the Multiplier Methods (PPA on the dual).

Proximal Method of Multipliers–Key Difficulty

- Main computational step in PMM: to minimize w.r.t (x, z) the proximal Augmented Lagrangian:

$$f(x) + g(z) + \langle y^k, Ax - z\rangle + \frac{c}{2}\|Ax - z\|^2 + q_k(x, z).$$

- **The quadratic coupling term $\|Ax - z\|^2$, destroys the separability between x and z, preventing separate minimization in (x, z).**
- In many applications, separate minimization is often much easier.....

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Many Strategies available to overcome this difficulty:

- Approximate Minimization – linearized the quad term $\|Ax - z\|^2$ wrt (x, z).
- Alternating Minimization – à la "Gauss-Seidel" in (x, z).
- Mixture of the above – *Partial Linearization* with respect to one variable, combined with *Alternating Minimization* of the other variable.
- Result in various useful variants of the PMM.

Main Tool for Analysis: - Via a Unified PMM Scheme

Unified Scheme U

Start with (x^0, z^0, y^0) and for all $k \geq 0$, and generate the sequence $\{x^k, z^k, y^k\}$ as follows

$$x^{k+1} \in \operatorname{argmin}\left\{ f(x) + \frac{c}{2}\|Ax - z^k + c^{-1}y^k\|^2 + \frac{1}{2}\|x - x^k\|_{M_1}^2 \right\}, \tag{1}$$

$$z^{k+1} = \operatorname{argmin}\left\{ g(z) + \frac{c}{2}\|A\eta^k - z + c^{-1}y^k\|^2 + \frac{1}{2}\|z - z^k\|_{M_2}^2 \right\}, \tag{2}$$

$$y^{k+1} = y^k + c(Ax^{k+1} - z^{k+1}), \tag{3}$$

where we define:

$$\eta^k := \begin{cases} x^k, & \text{Parallel Steps,} \\ x^{k+1}, & \text{Alternating Steps.} \end{cases} \tag{4}$$

- Adequate choices of $M_1, M_2 \succeq 0$ allows to derive various algorithms along announced strategies.
- Allows to derive convergence and efficiency estimates via a simple unifying analysis for many – old and new – PMM based algorithms.

Examples I – Parallel Schemes $\eta^k \equiv x^k$

Well definiteness of scheme, convergence and complexity ensured with:

$$\clubsuit \quad M_1 - cA^T A \succeq 0, \text{ and } M_2 - cI_m \succeq 0.$$

- **Example 1:** $M_1 := \tau^{-1} I_n - cA^T A, \quad M_2 := (\sigma^{-1} - c) I_m$ for any $\tau, \sigma > 0$.
- Condition $\clubsuit \;\Rightarrow\; 2c \le \min\{\sigma^{-1}, \tau^{-1}\|A\|^2\}$.
- This recovers the PCPM algorithm [Chen-T. (94)]. Here we also establish its complexity.

- **Example 2:**
- Pick $M_1 := \tau^{-1} I_n - cA^T A, \quad M_2 := cI_m$.
- Condition $\clubsuit \;\Rightarrow\; \quad 2c\tau\|A\|^2 \le 1$.
- This appears to be a novel scheme.

Alernating Steps $\eta^k \equiv x^{k+1}$ - A Prototype : Alternating Direction of Proximal Method of Multipliers

Eliminate the coupling (x, z) via alternating minimization steps.

Glowinski-Marocco (75), Gabay-Mercier (76), Fortin-Glowinski (83), Ecsktein-Bertsekas (91) ...... the so-called *Alternating Direction of Mulipliers* (ADM),(based on the Multiplier Methods, i.e., $M_1 = M_2 \equiv 0$.)

(AD-PMM) Alternating Direction Proximal Method of Multipliers

1. Start with any $(x^0, z^0, y^0) \in \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R}^m$ and $c > 0$
2. For $k = 0, 1, \ldots$ generate the sequence $\{x^k, z^k, y^k\}$ as follows:

$$\begin{aligned} x^{k+1} &\in \operatorname{argmin}\left\{ f(x) + \frac{c}{2}\|Ax - z^k + c^{-1}y^k\|^2 + \frac{1}{2}\|x - x^k\|^2_{M_1} \right\}, \\ z^{k+1} &= \operatorname{argmin}\left\{ g(z) + \frac{c}{2}\|Ax^{k+1} - z + c^{-1}y^k\|^2 + \frac{1}{2}\|z - z^k\|^2_{M_2} \right\}, \\ y^{k+1} &= y^k + c(Ax^{k+1} - z^{k+1}). \end{aligned}$$

Nicely exploits separable f, g.
Useful when $(\mathbf{x}, \mathbf{z})$ steps are "easy" to implement *exactly* or *inexactly* (e.g., via strategies just mentioned).

Examples – Alternate Schemes $\eta^k \equiv x^{k+1}$

Well definiteness, convergence and complexity ensured with <u>any</u> $M_1, M_2 \succeq 0$.

(1) Classical ADM (Alternating Direction of Multipliers): $M_1 = M_2 = 0$ Glowinski-Marocco (75), Gabay-Mercier (76), Fortin-Glowinski (83), Ecsktein-Bertsekas (91) ...

- Alternates minimization of the standard Augmented Lagrangian L_c.
- Converges of the primal sequence $\{x^k\}$ is ensured with A has full column rank.

(2) AD-PMM with $M_1 = c^{-1}\mu_1 I_n$; $M_2 = c^{-1}\mu_2 I_m$ with $c, \mu_1, \mu_2 > 0$, [Eckstein (94)].

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(3) Partial Regularized ADMM: $M_1 \succ 0, M_2 \succeq 0$

- For example, one can use $M_1 := \tau^{-1} I_n$, and $M_2 = 0$.
- Allows to prove the convergence of the sequence $\{x^k\}$ without any assumption on the matrix A.

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(4) Mixed Srategy: Linearize and Alternating Minimization

- Linearization wrt x, combined with AM in z. This is achieved by choosing:
- $M_1 := \tau^{-1} I_n - cA^T A \succeq 0, \Leftrightarrow c\tau\|A\|^2 \leq 1; \qquad M_2 := 0.$
- This recovers the recent PD algorithm [Chambolle-Pock (2010)].

Global Rate of Convergence Results - [Shefi-T. (2014)]

The proposed unified simple framework covers/extends many schemes/results.

For all resulting schemes we have:

- $O(1/N)$ **Ergodic convergence rate** in primal-dual gap (bounded domains) and in function values (when g-Lipschitz continuous).
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PMM based schemes are not free of potential problems ..raising practical and theoretical issues:

- **The penalty parameter c is unknown:** trial/error runs, fine tuning, heuristics, ...
- Iteration complexity bounds **depend on c !**
- The (x, z) steps are not always "easy"..**Prox of composition with affine map**...Nested optimization
- Difficult to extend for sum of $m > 2$ convex composite functions with linear maps.

Any alternatives?..

For any sequence $\{\mathbf{w}^n\}$, any $N \geq 1$, the ergodic sequence $\mathbf{w}_N := \frac{1}{N}\sum_{n=1}^{N} \mathbf{w}^n$

A Convex-Concave Saddle-point Approach

$$\min_{u \in U} \max_{v \in V} \{K(u,v) := f(u) + \langle Au, v\rangle - g(v)\},\ U, V \text{ closed convex.}$$

f, g are convex functions, A is a linear map.

Obviously, recovers and extends the previous composite convex model.

Current methods which admit an $O(1/\varepsilon)$ efficiency estimate

- **PMM-Based:** Just discussed with its potential drawbacks.
- **Extragradient** [Korpelevitch, (1976), Nemirovsky (04), Auslender-T. (05)] (can also handle general variational inequalities).
  - Requires smooth data: f and g have Lipschitz-continuous gradients.
- **Smoothing/First Order Methods:** [Moreau (64)...Nesterov's (05), Beck-T. (12)]
  - Assume partial smoothness/compactness: $f \in C_L^{1,1}$, V compact.
  - Require a smoothing parameter in term of the accuracy fixed in advance.

Goal

An algorithm for a broader class of structured nonsmooth convex-concave saddle-point problem that achieves the nonasymptotic efficiency estimate $O(1/\varepsilon)$:

- Removes difficulties with current methods.
- Flexible enough to be applied to more general scenarios.
- Involves simple computational tasks.

A Class of Structured Convex-Concave Saddle-Point Model

$$\text{(M)} \qquad \min_{u \in \mathbb{R}^n} \max_{v \in \mathbb{R}^d} \left\{ K(u,v) := f(u) + \langle u, \mathcal{A}v \rangle - g(v) \right\},$$

Data Information

(i) $f : \mathbb{R}^n \to \mathbb{R}$ is convex $C^{1,1}_{L_f}$: $\|\nabla f(u_1) - \nabla f(u_2)\| \leq L_f \|u_1 - u_2\|$, $\forall u_1, u_2$.

(ii) $g_i : \mathbb{R}^{d_i} \to (-\infty, +\infty]$, $i = 1, 2, \ldots, m$, is a proper, (lsc) and convex function (possibly nonsmooth), and we let $g : \mathbb{R}^d \to (-\infty, +\infty]$

$$g(v) := \sum_{i=1}^{m} g_i(v); \; d := \sum_{i=1}^{m} d_i; \; v := (v_1, v_2, \ldots, v_m) \in \mathbb{R}^d.$$

(iii) $A_i : \mathbb{R}^{d_i} \to \mathbb{R}^n$, $i = 1, 2, \ldots, m$, is a linear map and we let $\mathcal{A} : \mathbb{R}^d \to \mathbb{R}^n$ be the linear map defined by $\mathcal{A}v = \sum_{i=1}^{m} A_i v_i$.

We assume that $K(\cdot, \cdot)$ has a saddle-point, i.e., there exists $(u^*, v^*) \in \mathbb{R}^n \times \mathbb{R}^d$ such that

$$K(u^*, v) \leq K(u^*, v^*) \leq K(u, v^*), \quad \forall \, u \in \mathbb{R}^n, \; v \in \mathbb{R}^d.$$

A Proximal Alternating Predictor Corrector (PAPC) for (M)
Drori -Sabach -T. (2015) – Advertising Time!

$$\text{(M)} \qquad \min_{u \in \mathbb{R}^n} \max_{v \in \mathbb{R}^d} \left\{ K(u, v) := f(u) + \langle u, \mathcal{A}v \rangle - g(v) \right\},$$

Algorithm based on fundamental and old ideas: **it blends duality, predictor-corrector steps, and proximal operation**.

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Features of PAPC - Fully exploits structures of a problem.

- PAPC **avoids the computational difficult task:** the prox of the composition with a linear map $(g \circ \mathcal{A})(\mathbf{x}) = g(\mathcal{A}\mathbf{x})$. **Only ask prox of $g(\cdot)$.**
- Can be easily applied to minimization problems **with sum of such composite terms in objective/constraints**.
- Constraints on the variable v, built-in thanks to g being extended valued.
- Constraints on the variable u can be easily handled via **The Dual Transportation Trick**, (see details in Paper).

The PAPC Method

PAPC

Initialization. $\left(u^0, v^0\right) \in \mathbb{R}^n \times \mathbb{R}^d$, $\tau > 0$, and $\{\sigma_i\}_{i=1}^m > 0$.
For $k = 1, 2, \ldots,$:

$$p^k = u^{k-1} - \tau\left(\mathcal{A}v^{k-1} + \nabla f\left(u^{k-1}\right)\right),$$

$$\clubsuit\ v_i^k = \mathrm{prox}_{\sigma_i}^{g_i}\left(v_i^{k-1} + \sigma_i A_i^T p^k\right), \quad i = 1, 2, \ldots, m,$$

$$u^k = u^{k-1} - \tau\left(\mathcal{A}v^k + \nabla f\left(u^{k-1}\right)\right).$$

Output: $\bar{u}^N = \frac{1}{N}\sum_{k=1}^N u^k$, $\bar{v}^N = \frac{1}{N}\sum_{k=1}^N v^k$.

$\clubsuit$ v step "decomposes" according to structure; **only** prox for each $g_i(\cdot)$, **not of** $g(A_i x)$.

The parameters (τ, σ_i) are defined in terms of problem's data L_f, A_i.

Each iteration requires *one* application of $\mathcal{A}$ and of $\mathcal{A}^T$ and one evaluation of ∇f.

The PAPC Method – Main Convergence Results -Drori-Sabach-T. (2015)

Shares the best theoretical rate $0(1/N)$ for convex-concave saddle point.

Let $\left\{\left(p^k, u^k, v^k\right)\right\}_{k\in\mathbb{N}}$ be a sequence generated by the PAPC algorithm with $\tau L_f \leq 1$ and $\sigma\tau\sum_{i=1}^m \|A_i\|^2 \leq 1$.

1. **Global Rate of Convergence -Ergodic**

$$K\left(\bar{u}^N, v\right) - K\left(u, \bar{v}^N\right) = O(1/N).$$

Bound constant in terms of Data (L_f, A_i)– Parameters free.

2. **Sequential Convergence:** The sequence $\{(u^k, v^k)\}_{k\in\mathbb{N}}$ converges to a saddle-point (u^*, v^*) of K.

PAPC Applies to Many Important Models

♣ Convex Problems with Sum of Composite Convex Functions with Linear Maps

1. $\min_{u\in\mathbb{R}^p}\left\{F(u)+\sum_{i=1}^m H_i(B_i u)\right\}.$
2. $\min_{x_i}\left\{\sum_{i=1}^m \psi(x_i) : \sum_{i=1}^m M_i x_i = b\right\}.$
3. $\min_{u\in\mathbb{R}^p}\left\{F(u) : \sum_{i=1}^m H_i(B_i u)\leq\alpha\right\}.$

For all these models, PAPC

- **Decomposes nicely according to given structure.**
- **Removes the difficult task of "computing prox of convex function composed with an affine map".**
- **Parameters are determined from problem's data info: L_f and A_i.**
- **Performs well in applications:** Image processing, Learning (Fused lasso)...

Non-Convex Smooth Models

Sparse PCA

Principal Component Analysis solves

$$\max\{x^T Ax : \|x\|_2 = 1,\ x \in \mathbf{R}^n\},\ (A \succeq 0)$$

while Sparse Principal Component Analysis solves

$$\max\{x^T Ax : \|x\|_2 = 1,\ \|\mathbf{x}\|_\mathbf{0} \leq \mathbf{k},\ x \in \mathbf{R}^n\},\ k \in (1, n] \text{ sparsity}$$

$\|x\|_0$ counts the number of nonzero entries of x

Issues:

1. Maximizing a Convex objective.
2. Hard Nonconvex Constraint $\|x\|_0 \leq k$.

Possible Approaches:

1. SDP Convex Relaxations
2. Approximation/Modified formulations: Many proposed approaches

Sparse PCA via Penalization/Relaxation/Approx.

♠ The problem of interest is the difficult sparse PCA problem **as is**

$$\max\{x^T Ax : \|x\|_2 = 1,\ \|x\|_0 \le k,\ x \in \mathbf{R}^n\}$$

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♠ Literature has focused on solving various modifications:

- l_0**-penalized PCA** $\max\{x^T Ax - s\|x\|_0 : \|x\|_2 = 1\},\ s > 0$
- **Relaxed** l_1**-constrained PCA** $\max\{x^T Ax : \|x\|_2 = 1,\ \|x\|_1 \leq \sqrt{k}\}$
- **Relaxed** l_1**-penalized PCA** $\max\{x^T Ax - s\|x\|_1 : \|x\|_2 = 1\}$
- **Approx-Penalized** $\max\{x^T Ax - sg_p(|x|) : \|x\|_2 = 1\}$ $g_p(x) \simeq \|x\|_0$
- **SDP-Convex Relaxations** $\max\{\mathrm{tr}(AX) :\ \mathrm{tr}\,(X) = 1, X \succeq 0, \|X\|_1 \leq k\}$

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- SDP-relaxations often too computationally expensive for large problems.
- No algorithm give bounds to the optimal solution of the **original problem**.
- Even when "Simple", these algorithms are for modifications:
  ♣ **do not solve the original problem of interest**
  ♣ **do require unknown penalty parameter s to be tuned**.

Quick Highlight of Simple Algorithms for "Modified Problems"

Type	Iteration	Per-Iteration Complexity	References
l_1-constrained	$x_i^{j+1} = \frac{\mathrm{sgn}(((A+\frac{\sigma}{2})x^j)_i)(\lvert((A+\frac{\sigma}{2})x^j)_i\rvert - \lambda^j)_+}{\sqrt{\sum_h (\lvert((A+\frac{\sigma}{2})x^j)_h\rvert - \lambda^j)_+^2}}$	$O(n^2)$, $O(mn)$	Witten et al. (2009)
l_1-constrained	$x_i^{j+1} = \frac{\mathrm{sgn}((Ax^j)_i)(\lvert(Ax^j)_i\rvert - s^j)_+}{\sqrt{\sum_h (\lvert(Ax^j)_h\rvert - s^j)_+^2}}$ where s^j is $(k+1)$-largest entry of vector $\lvert Ax^j\rvert$	$O(n^2)$, $O(mn)$	Sigg-Buhman (2008)
l_0-penalized	$z^{j+1} = \frac{\sum_i [\mathrm{sgn}((b_i^T z^j)^2 - s)]_+ (b_i^T z^j) b_i}{\lVert \sum_i [\mathrm{sgn}((b_i^T z^j)^2 - s)]_+ (b_i^T z^j) b_i \rVert_2}$	$O(mn)$	Shen-Huang (2008), Journee et al. (2010)
l_0-penalized	$x_i^{j+1} = \frac{\mathrm{sgn}(2(Ax^j)_i)(\lvert 2(Ax^j)_i\rvert - s\varphi_p'(\lvert x_i^j\rvert))_+}{\sqrt{\sum_h (\lvert 2(Ax^j)_h\rvert - s\varphi_p'(\lvert x_h^j\rvert))_+^2}}$	$O(n^2)$	Sriperumbudur et al. (2010)
l_1-penalized	$y^{j+1} = \operatorname{argmin}_y \{\sum_i \lVert b_i - x^j y^T b_i \rVert_2^2 + \lambda \lVert y \rVert_2^2 + s \lVert y \rVert_1\}$ $x^{j+1} = \frac{(\sum_i b_i b_i^T) y^{j+1}}{\lVert (\sum_i b_i b_i^T) y^{j+1} \rVert_2}$		Zou et al. (2006)
l_1-penalized	$z^{j+1} = \frac{\sum_i (\lvert b_i^T z^j\rvert - s)_+ \mathrm{sgn}(b_i^T z^j) b_i}{\lVert \sum_i (\lvert b_i^T z^j\rvert - s)_+ \mathrm{sgn}(b_i^T z^j) b_i \rVert_2}$	$O(mn)$	Shen-Huang (2008), Journee et al. (2010)

A Plethora of Models/Algorithms Revisited - [Luss-Teboulle (2013)]

All previous listed algorithms have been derived from various disparate approaches/motivations to solve **modifications** of SPCA: Expectation Maximization; Majorization-Mininimization techniques; DC programming; Alternating minimization etc...

1. **Are all these algorithms different? Any connection?**
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1. **Are all these algorithms different? Any connection?**
2. **Is it possible to tackle the difficult sparse PCA problem "as is"**

We have shown that:

- All the previously listed algorithms are a particular realization of a **"Father Algorithm": ConGradU** (based on the well-known Conditional Gradient Algorithm)
- **ConGradU CAN be applied directly to the original problem!**

Maximizing a Convex function over a Compact Nonconvex set

Classic Conditional Gradient Algorithm [Frank-Wolfe'56, Polyak'63, Dunn'79..]

$$\text{solves}: \max\{F(x) : x \in C\}, \quad \text{with} \quad F \text{ is } C^1;\ C \text{ convex compact}$$

$$\begin{aligned} x^0 \in C,\ p^j &= \operatorname{argmax}\{\langle x - x^j, \nabla F(x^j)\rangle : x \in C\} \\ x^{j+1} &= x^j + \alpha^j(p^j - x^j),\ \alpha^j \in (0,1] \text{ stepsize} \end{aligned}$$

♠ **Here : F is convex, possibly nonsmooth**; C is compact but **nonconvex**

Idea goes back to Mangasarian (96) developed for C a polyhedral set.

ConGradU – Conditional Gradient with Unit Step Size

$$x^0 \in C,\ x^{j+1} \in \operatorname{argmax}\{\langle x - x^j, F'(x^j)\rangle : x \in C\}$$

Notes:

1. F is not assumed to be differentiable and $F'(x)$ is a subgradient of F at x.
2. Useful when $\max\{\langle x - x^j, F'(x^j)\rangle : x \in C\}$ is *easy* to solve

Solving Original l_0-constrained PCA via ConGradU

Applying **ConGradU** directly to $\max\{x^T Ax : \|x\|_2 = 1,\ \|x\|_0 \leq k,\ x \in \mathbf{R}^n\}$ results in

$$\begin{aligned} x^{j+1} &= \operatorname{argmax}\{x^{jT} Ax : \|x\|_2 = 1,\ \|x\|_0 \leq k\} = \frac{T_k(Ax^j)}{\|T_k(Ax^j)\|_2} \\ T_k(a) &:= \operatorname*{argmin}_y\{\|x - a\|_2^2 : \|x\|_0 \leq k\} \end{aligned}$$

Despite the hard constraint, easy to compute: $(T_k(a))_i = a_i$ for the k largest entries (in absolute value) of a and $(T_k(x))_i = 0$ otherwise.

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Despite the hard constraint, easy to compute: $(T_k(a))_i = a_i$ for the k largest entries (in absolute value) of a and $(T_k(x))_i = 0$ otherwise.

- **Convergence:** Every limit point of $\{x^j\}$ converges to a stationary point.
- **Complexity:** $O(kn)$ or $O(mn)$

- **Thus, original problem can be solved using ConGradU with the same complexity as when applied to modifications!**
- Penalized/Modified problems require tuning **an unknown tradeoff penalty parameter** This can be very computationally expensive and not needed here.

ConGradU for a General Class of Problems

$$(G) \qquad \max_x \{f(x) + g(|x|) : x \in C\}$$

$$\begin{array}{ll} f : \mathbf{R}^n \to \mathbf{R} & \text{is convex, } C \subseteq \mathbf{R}^n \text{ is a compact set.} \\ g : \mathbf{R}^n_+ \to \mathbf{R} & \text{is convex differentiable and montonote decreasing} \end{array}$$

- Particularly useful for handling *approximate* l_0-penalized problems.

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- Particularly useful for handling *approximate* l_0-penalized problems.
- **CondGradU** applied to (G) produces the following simple:

Weighted l_1-norm maximization problem:

$$x^0 \in C, \ x^{j+1} = \text{argmax}\{\langle a^j, x\rangle - \sum_i w_i^j |x_i| : x \in C\}, \ j = 0, \dots,$$

where $w^j := -g'(|x^j|) > 0$ and $a^j := f'(x^j) \in \mathbf{R}^n$.

For *penalized/approximate penalized SPCA*, C is a unit ball, and above admits a **closed form solution**:

$$x^{j+1} = \frac{S_{w^j}(f'(x^j))}{\|S_{w^j}(f'(x^j))\|}, \ j = 0, \dots; \quad S_w(a) := (|a| - w)_+ \text{sgn}(a), \ \text{(Soft Threshold)}.$$

Non-Convex and NonSmooth

Goal and Results

Derive a simple self-contained convergence analysis framework for a broad class of nonconvex and nonsmooth minimization problems.

- A "Recipe" for proving global convergence to a critical point.
- An Example of a Simple/Useful Algorithm: PALM.
- Many Applications: phase retrieval for diffractive imaging, dictionary learning,... .... **Sparse nonnegative matrix factorization** ...and much more...

The Problem : An Abstract Formulation

Let $\Psi : \mathbb{R}^d \to (-\infty, +\infty]$ be a proper, lsc and bounded from below function.

$$(P) \qquad \inf \left\{ \Psi(z) : \; z \in \mathbb{R}^d \right\}.$$

Suppose $\mathcal{A}$ is a generic algorithm which generates a sequence $\left\{z^k\right\}_{k \in \mathbb{N}}$ via:

$$z^0 \in \mathbb{R}^d, z^{k+1} \in \mathcal{A}(z^k), \; k = 0, 1, \ldots.$$

Goal: Prove that the whole sequence $\left\{z^k\right\}_{k \in \mathbb{N}}$ converges to a critical point z^* of Ψ, i.e., $0 \in \partial\Psi(z^*)$.

Recall [Rockafellar-Wets (98)]

- (Limiting) Subdifferential $\partial\Psi(x)$:

$$\begin{aligned} x^* \in \partial\Psi(x) \quad &\text{iff} \quad (x_k, x^*) \to (x, x^*) \text{ s.t. } \Psi(x_k) \to \Psi(x) \text{ and} \\ \Psi(u) \quad &\geq \quad \Psi(x_k) + \langle x_k^*, u - x_k \rangle + o(\|u - x_k\|) \end{aligned}$$

- $x \in \mathbb{R}^d$ is a critical point of Ψ if $\partial\Psi(x) \ni 0$.

A General Recipe with 3 Main Steps

C1 **Sufficient decrease property:** Find a positive constant ρ_1 such that

$$\rho_1 \|z^{k+1} - z^k\|^2 \leq \Psi(z^k) - \Psi(z^{k+1}), \quad \forall k = 0, 1, \ldots.$$

C2 **A subgradient lower bound for the iterates gap:** Assume that $\left\{z^k\right\}_{k \in \mathbb{N}}$ is bounded. Find another positive constant ρ_2, such that

$$\left\|w^k\right\| \leq \rho_2 \|z^{k+1} - z^k\|, \quad w^k \in \partial\Psi(z^k), \quad \forall k = 0, 1, \ldots.$$

- These two steps are typical for *any descent* type algorithms but lead **ONLY to convergence of limit points.** [Ostrowski 1966].

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- These two steps are typical for *any descent* type algorithms but lead **ONLY to convergence of limit points.** [Ostrowski 1966].
- To get global convergence to a critical point ...We need more info on problem's data.
- To prove the result, we need an additional mathematical tool. **This is the third step of the recipe**.

The Third Main Step of the Recipe

C3. The Kurdyka-Łojasiewicz property: Assume that Ψ satisfies the KL property. Use this to prove that the generated sequence $\left\{z^k\right\}_{k\in\mathbb{N}}$ is a *Cauchy sequence*, and thus converges!

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This general recipe

- Singles out the 3 main ingredients at play to derive global convergence in the nonconvex and nonsmooth setting.
- In particular, thanks to a uniformization Lemma of the KL property, [Bolte, Sabach, T. (2014)] it is **applicable to any descent algorithm** without the need of going through the KL machinery for each particular algorithm.

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The remaining questions

- What is the KL property ?Łojasiewicz (68), Kurdyka (98), Bolte et al. (06,07,10)
- Are there many functions satisfying KL?

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Theorem 1 (Bolte-Daniilidis-Lewis (2006))

Let $\sigma : \mathbb{R}^d \to (-\infty, +\infty]$ be a proper and lsc function. If σ is semi-algebraic then it satisfies the KL property at any point of $\operatorname{dom}\sigma$.

Global Convergence to a Critical Point [Bolte-Sabach-T. 2014]

Global Convergence Result

Let $\Psi : \mathbb{R}^d \to (-\infty, +\infty]$ be a proper lsc and **semi-algebraic function** with $\inf \Psi > -\infty$. Assume that $\left\{\mathbf{z}^k\right\}_{k\in\mathbb{N}}$ is a sequence produced **by any algorithm** satisfying conditions C1 and C2. Let $\omega\left(\mathbf{z}^0\right)$ be the set of all limit points of the sequence $\left\{\mathbf{z}^k\right\}_{k\in\mathbb{N}}$.

If $\emptyset \neq \omega\left(\mathbf{z}^0\right) \subset \operatorname{crit}\Psi$, then the sequence $\left\{\mathbf{z}^k\right\}_{k\in\mathbb{N}}$ converges to a critical point $\mathbf{z}^*$ of Ψ.

Recall: Semi-algebraic sets and functions

(i) A semialgebraic subset of $\mathbb{R}^d$ is a finite union of sets

$$\{x \in \mathbb{R}^d : \ p_i(x) = 0, \ q_j(x) < 0, \ i \in I, \ j \in J\}$$

where $p_i, q_j : \mathbb{R}^d \to \mathbb{R}$ are real polynomial functions and I, J are finite.

(ii) A function σ is semi-algebraic if its graph

$$\left\{(u, t) \in \mathbb{R}^{n+1} : \ \sigma(u) = t\right\}$$

is a semi-algebraic subset of $\mathbb{R}^{n+1}$.

There is a Wealth of Semi-Algebraic Functions!

Some Semi-Algebraic Sets/Functions .."Starring" in Optimization/Applications

- Real polynomial functions.
- Indicator functions of semi-algebraic sets.
- In matrix theory: cone of PSD matrices, constant rank matrices, Stiefel manifolds...
- The function $x \to \operatorname{dist}(x, S)^2$ is semi-algebraic whenever S is a nonempty semi-algebraic subset of $\mathbb{R}^n$.
- $\|\cdot\|_0$ is semi-algebraic.
- $\|\cdot\|_p$ is semi-algebraic whenever $p > 0$ is rational.

Semi-Algebraic Property is Preserved under Many Operations

- Finite sums and product of semi-algebraic functions; Composition of semi-algebraic functions;
- Sup/Inf type function, *e.g.*, $\sup \{g(u, v) : \; v \in C\}$ is semi-algebraic when g is a semi-algebraic function and C a semi-algebraic set.

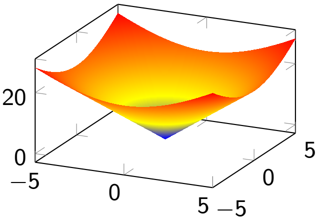
Sharpness: A Geometric Snapshot toward KL

Definition 2 (Sharpness)

A function $f : \mathbb{R}^n \to (-\infty, +\infty]$ is called sharp on the slice $[r_0 < f < r_1] := \left\{x \in \mathbb{R}^d : \ r_0 < f(x) < r_1\right\}$, if there exists $c > 0$ such that

$$\|\partial f(x)\|_{-} := \min\{\|\xi\| : \ \xi \in \partial f(x)\} \geq c > 0 \quad \forall x \in [r_0 < f < r_1].$$

Basic Example: $f(x) = \|x\|$.



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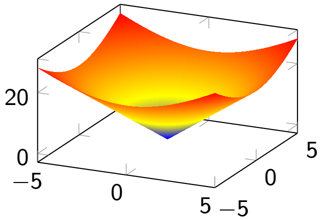

KL Property Informal: A KL function is a function whose values can be re-parametrized in the neighborhood of each of its critical point so that the resulting function becomes sharp.

KL Property [Łojasiewicz (68), Kurdyka (98), Bolte et al. (06,07,10)]

$$\Phi_\eta := \left\{\varphi \in C\left([0,\eta), \mathbb{R}_+\right) \text{concave}: \ \varphi \in C^1\left((0,\eta)\right), \varphi' > 0, \varphi(0) = 0\right\}, \eta \in (0,+\infty].$$

Definition 3 (Kurdyka-Łojasiewicz property)

Let $\sigma : \mathbb{R}^d \to (-\infty, +\infty]$ be proper and lsc.

(i) The function σ has the Kurdyka-Łojasiewicz (KL) property at $\overline{u}$ if there exist a neighborhood U of $\overline{u}$, and a function $\varphi \in \Phi_\eta$, such that the following inequality holds:

$$\varphi'\left(\sigma(u) - \sigma(\overline{u})\right) \operatorname{dist}\left(0, \partial\sigma(u)\right) \geq 1.$$

for all

$$u \in U \cap \left[\sigma(\overline{u}) < \sigma(u) < \sigma(\overline{u}) + \eta\right].$$

(ii) If σ satisfy the KL property at each point of $\operatorname{dom}\partial\sigma$ then σ is called a KL function.

The relevant aspect of this property is when $\overline{u}$ is critical, i.e., $0 \in \partial\sigma(\overline{u})$. In that case:

- it warrants that σ is *sharp* up to re-parametrization of its values.
- The re-parametrization function is called the *desingularizing function* of σ at $\overline{u}$.

Illustration on a Useful Optimization Model

$$(M) \qquad \text{minimize}_{x,y} \Psi(x,y) := f(x) + g(y) + H(x,y)$$

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Assumption 1

(i) $f : \mathbb{R}^n \to (-\infty, +\infty]$ *and* $g : \mathbb{R}^m \to (-\infty, +\infty]$ *proper and lsc functions.*

(ii) $H : \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$ *is a* C^1 *function.*

(iii) *Partial gradients of* H *are Lipshitz continuous:* $H(\cdot, y) \in C^{1,1}_{L(y)}$ *and* $H(x, \cdot) \in C^{1,1}_{L(x)}$.

- **NO convexity** is assumed in the objective and the constraints (built-in through f and g extended valued).

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- **NO convexity** is assumed in the objective and the constraints (built-in through f and g extended valued).
- The choice of two blocks of variables is only for the sake of simplicity of exposition. Same for the p-blocks case:

$$\text{minimize}_{x_1,\ldots,x_p} H(x_1, x_2, \ldots, x_p) + \sum_{i=1}^{p} f_i(x_i)$$

- This optimization model covers many applications: signal/image processing, machine learning, etc....Vast Literature..

The Algorithm: Proximal Alternating Linearization Minimization (PALM)

Cocktail Time! PALM simply "blends" old spices: AM and Prox-Gradient.

1. Initialization: start with any $\left(x^0, y^0\right) \in \mathbb{R}^n \times \mathbb{R}^m$.
2. For each $k = 0, 1, \ldots$ generate a sequence $\left\{\left(x^k, y^k\right)\right\}_{k \in \mathbb{N}}$:

2.1. Take $\gamma_1 > 1$, set $c_k = \gamma_1 L_1\left(y^k\right)$ and compute

$$x^{k+1} \in \mathrm{prox}_{c_k}^{f}\left(x^k - \frac{1}{c_k}\nabla_x H\left(x^k, y^k\right)\right).$$

2.2. Take $\gamma_2 > 1$, set $d_k = \gamma_2 L_2\left(x^{k+1}\right)$ and compute

$$y^{k+1} \in \mathrm{prox}_{d_k}^{g}\left(y^k - \frac{1}{d_k}\nabla_y H\left(x^{k+1}, y^k\right)\right).$$

Main computational step: prox of a "nonconvex" function.

Application to a Broad Class of Matrix Factorization Problems

Given $A \in \mathbb{R}^{m\times n}$ and $r \ll \min\{m, n\}$, find $X \in \mathbb{R}^{m\times r}$ and $Y \in \mathbb{R}^{r\times n}$ such that

$$\begin{cases} A \approx XY, \\ X \in \mathcal{K}_{m,r} \cap \mathcal{F}, \\ Y \in \mathcal{K}_{r,n} \cap \mathcal{G}. \end{cases}$$

Where

$$\begin{aligned} \mathcal{K}_{p,q} &= \left\{M \in \mathbb{R}^{p\times q} :\; M \geq 0\right\}, \\ \mathcal{F} &= \left\{X \in \mathbb{R}^{m\times r} :\; R_1(X) \leq \alpha\right\}, \\ \mathcal{G} &= \left\{Y \in \mathbb{R}^{r\times n} :\; R_2(Y) \leq \beta\right\}, \end{aligned}$$

Here R_1 and R_2 are lsc functions and $\alpha, \beta \in \mathbb{R}_+$ are given parameters. R_1 (R_2) are often used to describe some additional features of X (Y).

(MF) covers a very large number of problems in applications...

The Optimization Approach

We adopt the Constrained Nonconvex Nonsmooth Formulation

$$(MF) \qquad \min \left\{ d\left(A, XY\right) : \; X \in \mathcal{K}_{m,r} \cap \mathcal{F}, Y \in \mathcal{K}_{r,n} \cap \mathcal{G} \right\},$$

- $d : \mathbb{R}^{m \times n} \times \mathbb{R}^{m \times n} \to \mathbb{R}_+$ stands as a proximity function.
- Measures the quality of the approximation, satisfies $d\left(U, V\right) = 0$ if and only if $U = V$.

This formulation fits our general nonsmooth nonconvex model (M) with obvious identifications for H, f, g.

We now illustrate with semi-algebraic data on two important models.

Model I – Nonnegative Matrix Factorization Problems

Let the proximity measure be defined via the Frobenius norm

$$\begin{aligned} d(A, XY) &:= H(X, Y) = \frac{1}{2}\|A - XY\|_F^2, \text{ and} \\ \mathcal{F} &\equiv \mathbb{R}^{m\times r}; \quad \mathcal{G} \equiv \mathbb{R}^{r\times n}. \end{aligned}$$

The Problem (MF) reduces to the so called Nonnegative Matrix Factorization (NMF)

$$\min\left\{\frac{1}{2}\|A - XY\|_F^2 : X \geq 0, Y \geq 0\right\}.$$

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$$\min\left\{\frac{1}{2}\|A - XY\|_F^2 : X \geq 0, Y \geq 0\right\}.$$

- H is a real polynomial function hence semi-algebraic.
- $X \to H(X, Y)$ (for fixed Y) and $Y \to H(X, Y)$ (for fixed X), are $C^{1,1}$ with $L_1(Y) \equiv \left\|YY^T\right\|_F$, $L_2(X) \equiv \left\|X^TX\right\|_F$.
- H is C^2 on bounded subsets.

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Thus we can PALM it! The two computational steps reduce to projection onto the nonnegative cone of matrices–Trivial!..

$$
P_+(U) := \operatorname{argmin}\{\|U - V\|_F^2 : \ V \in \mathbb{R}^{m\times n}, V \geq 0\} = \max\{0, U\}.
$$

Model II - Sparse Constraints in Nonnegative Matrix Factorization

Consider in NMF the overall sparsity measure of a matrix defined by

$$R_1(X) = \|X\|_0 := \sum_i \|x_i\|_0 \,, \ (x_i \text{ column vector of } X) \quad ; R_2(Y) = \|Y\|_0 \,.$$

To apply PALM all we need is to compute the **prox of** $f := \delta_{X \geq 0} + \delta_{\|X\|_0 \leq s}$.
It turns out that this can be simply done!

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Proposition 1 (Proximal map formula for $f = \delta_{X \geq 0} + \delta_{\|X\|_0 \leq s}$)

Let $U \in \mathbb{R}^{m \times n}$. Then

$$\mathrm{prox}_1^f(U) = \mathit{argmin}\left\{\frac{1}{2}\|X - U\|_F^2 : X \geq 0, \|X\|_0 \leq s\right\} = T_s(P_+(U))$$

where

$$T_s(U) := \underset{V \in \mathbb{R}^{m \times n}}{\mathit{argmin}}\left\{\|U - V\|_F^2 : \ \|U\|_0 \leq s\right\}.$$

Computing T_s simply requires determining the s-th largest numbers of mn numbers. This can be done in $O(mn)$ time, and zeroing out the proper entries in one more pass of the mn numbers.

PALM for Sparse NMF

1. Initialization: Select random nonnegative $X^0 \in \mathbb{R}^{m \times r}$ and $Y^0 \in \mathbb{R}^{r \times n}$.
2. For each $k = 0, 1, \ldots$ generate a sequence $\left\{ \left(X^k, Y^k \right) \right\}_{k \in \mathbb{N}}$:

2.1. Take $\gamma_1 > 1$, set $c_k = \gamma_1 \left\| Y^k \left(Y^k \right)^T \right\|_F$ and compute

$$U^k = X^k - \frac{1}{c_k} \left(X^k Y^k - A \right) \left(Y^k \right)^T; \quad X^{k+1} \in \operatorname{prox}_{c_k}^{R_1} \left(U^k \right) = T_\alpha \left(P_+ \left(U^k \right) \right).$$

2.2. Take $\gamma_2 > 1$, set $d_k = \gamma_2 \left\| X^{k+1} \left(X^{k+1} \right)^T \right\|_F$ and compute

$$V^k = Y^k - \frac{1}{d_k} \left(X^{k+1} \right)^T \left(X^{k+1} Y^k - A \right); \quad Y^{k+1} \in \operatorname{prox}_{d_k}^{R_2} \left(V^k \right) = T_\beta \left(P_+ \left(V^k \right) \right).$$

- Applying our main Theorem, we get the global convergence result to a critical point.
- The algorithm is simple and appears to be efficient in practice.

For More Details, Results....

- R. Shefi and M. Teboulle. Rate of Convergence Analysis of Decomposition Methods Based on the Proximal Method of Multipliers for Convex Minimization. *SIAM J. Optimization*, **24**, 269–297, (2014).
- Y. Drori, S. Sabach and M. Teboulle. A simple algorithm for a class of nonsmooth convex-concave saddle-point problems. *Operations Research Letters*, **43**, 209–214, (2015).
- R. Luss and M. Teboulle. Conditional Gradient Algorithms for Rank One Matrix Approximations with a Sparsity Constraint. *SIAM Review*, **55**, 65-98, (2013).
- J. Bolte, S. Sabach, and M. Teboulle. Proximal alternating linearized minimization for nonconvex and nonsmooth problems. *Mathematical Programming, Series A*, **146**, 459–494, (2014).

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THANK YOU FOR YOUR ATTENTION!