Mathematics of Data: From Theory to Computation

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Lecture 13: Primal-dual optimization III

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EE-556 (Fall 2020)



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Recall - Swiss army knife of convex formulations

A primal problem prototype

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{A}\mathbf{x} - \mathbf{b} \in \mathcal{K}, \ \mathbf{x} \in \mathcal{X} \right\},$$

- ▶ f is proper, closed and convex
- \triangleright \mathcal{X} and \mathcal{K} are nonempty, closed convex sets
- $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \mathbb{R}^n$ are known
- An optimal solution \mathbf{x}^* to (3) satisfies $f(\mathbf{x}^*) = f^*$, $\mathbf{A}\mathbf{x}^* \mathbf{b} \in \mathcal{K}$ and $\mathbf{x}^* \in \mathcal{X}$

Broad context for (3):

- Many real-world applications (e.g., linear inverse problems, matrix completion) can be directly formulated as (3).
- Often times, computational limitations require the translation of existing unconstrained problems (e.g., composite convex minimization, consensus optimization, and convex splitting) into constrained ones (3).
- Many standard convex optimization formulations naturally fall under (3), such as linear programming, convex quadratic programming, second order cone programming, semidefinite programming and geometric programming.

Recall - Swiss army knife of convex formulations

A primal problem prototype

$$f^{\star} := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{A}\mathbf{x} - \mathbf{b} \in \mathcal{K}, \ \mathbf{x} \in \mathcal{X} \right\},$$

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- An optimal solution \mathbf{x}^* to (3) satisfies $f(\mathbf{x}^*) = f^*$, $\mathbf{A}\mathbf{x}^* \mathbf{b} \in \mathcal{K}$ and $\mathbf{x}^* \in \mathcal{X}$

A simplified template

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{A}\mathbf{x} = \mathbf{b}, \right\},$$
 (1)

- ▶ f is proper, closed and convex
- $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \mathbb{R}^n$ are known
- An optimal solution \mathbf{x}^* to (1) satisfies $f(\mathbf{x}^*) = f^*$, $\mathbf{A}\mathbf{x}^* = \mathbf{b}$.

Recall - Finding the solutions of (1)

A performance metric: Time-to-reach ϵ

time-to-reach ϵ = number of iterations to reach ϵ × per iteration time

A key issue: Number of iterations to reach ϵ

The notion of ϵ -accuracy is elusive in constrained optimization!

Our definition of ϵ -accurate solutions [32]

Given a numerical tolerance $\epsilon \geq 0$, a point $\mathbf{x}^{\star}_{\epsilon} \in \mathbb{R}^p$ is called an ϵ -solution of (1) if

$$\begin{cases} f(\mathbf{x}_{\epsilon}^{\star}) - f^{\star} & \leq \epsilon \text{ (objective residual),} \\ \|\mathbf{A}\mathbf{x}_{\epsilon}^{\star} - \mathbf{b}\| & \leq \epsilon \text{ (feasibility gap),} \end{cases}$$

▶ When \mathbf{x}^{\star} is unique, we can also obtain $\|\mathbf{x}_{\epsilon}^{\star} - \mathbf{x}^{\star}\| \leq \epsilon$ (iterate residual).

Remark: $\circ \epsilon$ can be different for the objective, feasibility gap, or the iterate residual.

Plenty of primal-dual methods for solving (1):

- Penalty and augmented Lagrangian methods:
 - Exact penalty method [2].
 - Quadratic penalty method [3].
 - ► Augmented Lagrangian method [21, 26].
- Variants of the Arrow-Hurwitz's method:
 - Proximal-based decomposition (Chen-Teboulle's algorithm) [7].
 - Primal-dual Hybrid Gradient (PDHG) method and its variants [13, 16].
 - ► Chambolle-Pock's algorithm [6], and its variants, e.g., He-Yuan's variant [18].
- Osplitting techniques from monotone inclusions:
 - ▶ Primal-dual splitting algorithms [1, 8, 33, 9, 10].
 - Three-operator splitting [11].
- o Dual splitting techniques:
 - Alternating minimization algorithms (AMA) [14, 33].
 - ► Alternating direction methods of multipliers (ADMM) [12, 20].
 - ▶ Accelerated variants of AMA and ADMM [10, 17].
 - Preconditioned ADMM, Linearized ADMM and inexact Uzawa algorithms [6, 24].
- o Second-order decomposition methods:
 - ▶ Dual (quasi) Newton methods [35].
 - ▶ Smoothing decomposition methods via barriers functions [23, 30].

See Lecture 12

See Lecture 12

See Lecture 12

This lecture

Recall - Quadratic penalty & Lagrangian formulations

$$\circ$$
 The problem: $f^\star := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{A}\mathbf{x} = \mathbf{b}
ight\}$

o Reformulations:

Quadratic Penalty	The Lagrangian
$f^* = f(\mathbf{x}^*) + \frac{\beta}{2} \mathbf{A}\mathbf{x}^* - \mathbf{b} ^2, \forall \beta > 0.$	$f^* = f(\mathbf{x}^*) + \max_{\mathbf{\lambda} \in \mathbb{R}^n} \langle \mathbf{\lambda}, \mathbf{A} \mathbf{x}^* - \mathbf{b} \rangle.$
$F_{\beta}(\mathbf{x}) = f(\mathbf{x}) + \frac{\beta}{2} \ \mathbf{A}\mathbf{x} - \mathbf{b}\ ^2.$	$F_{\boldsymbol{\lambda}}(\mathbf{x}) = f(\mathbf{x}) + \max_{\boldsymbol{\lambda} \in \mathbb{R}^n} \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle$
	$= f(\mathbf{x}) + \begin{cases} 0, & \text{if } \mathbf{A}\mathbf{x} = \mathbf{b}, \\ +\infty, & \text{if } \mathbf{A}\mathbf{x} \neq \mathbf{b}. \end{cases}$
$\min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) \colon \mathbf{A}\mathbf{x} = \mathbf{b} \right\} \equiv \lim_{\beta \to \infty} \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) + \frac{\beta}{2} \ \mathbf{A}\mathbf{x} - \mathbf{b}\ ^2 \right\}$	$\left \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) \colon \mathbf{A}\mathbf{x} = \mathbf{b} \right\} \equiv \min_{\mathbf{x} \in \mathbb{R}^p} \max_{\mathbf{\lambda} \in \mathbb{R}^n} \left\{ f(\mathbf{x}) + \langle \mathbf{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle \right\} \right $

Recall - Quadratic penalty & Lagrangian methods

$$\circ$$
 The problem: $f^\star := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{A}\mathbf{x} = \mathbf{b}
ight\}$

o The methods:

Quadratic penalty method (QP)

- **1.** Choose $\mathbf{x}^0 \in \mathbb{R}^p$ and $\beta_0 > 0$.
- 2. For $k=0,1,\cdots$ perform:

2.a.
$$\mathbf{x}^k := \arg\min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) + \frac{\beta_k}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 \right\}.$$

2.b. Update $\beta_{k+1} > \beta_k$.

o Drawbacks:

$$\mathbf{x}^{k} := \arg\min_{\mathbf{x} \in \mathbb{R}^{p}} \left\{ f(\mathbf{x}) + \frac{\beta_{k}}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^{2} \right\}$$
 becomes ill-conditioned as $\beta_{k} \to \infty$.

Dual subgradient method (DSGM)

- **1.** Choose $\lambda^0 \in \mathbb{R}^n$.
- **2.** For $k = 0, 1, \dots$, perform:
 - $\mathbf{2.a.}\ \mathbf{x}^*(\boldsymbol{\lambda}^k) := \arg\min_{\mathbf{x} \in \mathbb{R}^p} \Big\{ \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}^k) := f(\mathbf{x}) + \langle \boldsymbol{\lambda}^k, \mathbf{A}\mathbf{x} \mathbf{b} \rangle \Big\}.$
 - **2.b.** Compute the subgradient $\nabla d(\boldsymbol{\lambda}^k) := \mathbf{A}\mathbf{x}^*(\boldsymbol{\lambda}^k) \mathbf{b}$.
 - 2.c. Update $oldsymbol{\lambda}^{k+1} := oldsymbol{\lambda}^k + rac{R}{\sqrt{k+1}}
 abla d(oldsymbol{\lambda}^k)$

where R is a given constant.

Drawbacks:

- $\blacktriangleright d(\lambda)$ is not necessarily smooth \implies slower rates.
- $\mathbf{x}^*(\hat{\boldsymbol{\lambda}}^k)$ is not necessarily well-defined for all $\boldsymbol{\lambda}$.
- Finding R is not always straightforward.

Idea - Combine Lagrangian and penalty approaches

Quadratic penalty:
$$F_{eta}(\mathbf{x}) = f(\mathbf{x}) + rac{eta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2$$

+

The Lagrangian: $\mathcal{L}(\mathbf{x}, \pmb{\lambda}) = f(\mathbf{x}) + \langle \pmb{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b}
angle$



Augmented Lagrangian (AL): $\mathcal{L}_{\beta}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2$

Properties of AL

 \circ The dual function is concave and $\frac{1}{\beta}$ -smooth:

$$d_{\beta}(\boldsymbol{\lambda}) = \min_{\mathbf{x} \in \mathbb{R}^p} \bigg\{ f(\mathbf{x}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 \bigg\}.$$

Can apply gradient or accelerated gradient methods in the dual!

 \circ β does not need to increase until infinity.

No more ill-conditioned subproblems!

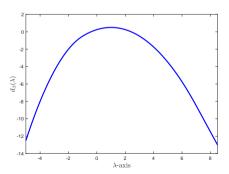
Example: Behavior of the AL dual function

Consider a constrained convex problem:

$$\begin{aligned} & \min_{\mathbf{x} \in \mathbb{R}^3} & \left\{ f(\mathbf{x}) := x_1^2 + x_2^2 \right\}, \\ & \text{s.t.} & \frac{2x_3 - x_1 - x_2 = 1}{\mathbf{x} \in \mathcal{X}} := [-2, 2] \times [-2, 2] \times [0, 2]. \end{aligned}$$

The AL dual function is concave, smooth and defined as

$$d_{\beta}(\boldsymbol{\lambda}) := \min_{\mathbf{x} \in \mathcal{X}} \left\{ x_1^2 + x_2^2 + \boldsymbol{\lambda} (2x_3 - x_1 - x_2 - 1) + (\beta/2) \|2x_3 - x_1 - x_2 - 1\|_2^2 \right\}$$



Example: Behavior of the AL dual function

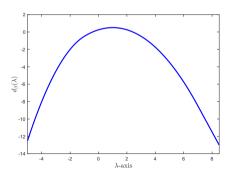
Consider a constrained convex problem:

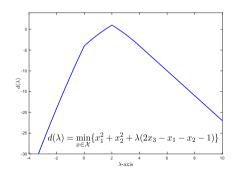
$$\label{eq:min_problem} \begin{split} \min_{\mathbf{x} \in \mathbb{R}^3} & \quad \left\{ f(\mathbf{x}) := x_1^2 + x_2^2 \right\}, \\ \text{s.t.} & \quad 2x_3 - x_1 - x_2 = 1, \\ & \quad \mathbf{x} \in \mathcal{X} := [-2, 2] \times [-2, 2] \times [0, 2]. \end{split}$$

The AL dual function is concave, smooth and defined as

$$d_{\beta}(\boldsymbol{\lambda}) := \min_{\mathbf{x} \in \mathcal{X}} \left\{ x_1^2 + x_2^2 + \boldsymbol{\lambda} (2x_3 - x_1 - x_2 - 1) + (\beta/2) \|2x_3 - x_1 - x_2 - 1\|_2^2 \right\}$$

VS





Augmented dual problem

Dual problem:

$$d^* := \max_{\mathbf{\lambda} \in \mathbb{R}^n} \left\{ d(\mathbf{\lambda}) = \min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x}) + \langle \mathbf{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle \right\}. \tag{2}$$

Augmented dual problem:

$$d_{\beta}^* := \max_{\boldsymbol{\lambda} \in \mathbb{R}^n} \left\{ d_{\beta}(\boldsymbol{\lambda}) = \min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 \right\}, \quad \beta > 0.$$
 (3)

Augmented dual problem

Dual problem:

$$d^* := \max_{\boldsymbol{\lambda} \in \mathbb{R}^n} \left\{ d(\boldsymbol{\lambda}) = \min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle \right\}.$$
 (2)

Augmented dual problem:

$$d_{\beta}^* := \max_{\boldsymbol{\lambda} \in \mathbb{R}^n} \left\{ d_{\beta}(\boldsymbol{\lambda}) = \min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 \right\}, \quad \beta > 0.$$
 (3)

Relation between augmented dual problem and dual problem

If a primal solution exists and Slater's condition holds, we have

- ► The dual solution set of (3) coincides with the one of the dual problem (2).
- $f^{\star} = d^{\star} = d^{*}_{\beta}$ for any $\beta > 0$.
- o Recall: The augmented dual problem (3) is smooth and concave
 - ⇒ Gradient and accelerated gradient methods can be applied to solve it.

Augmented Lagrangian method: The ideal algorithm

$$d_{\beta}(\lambda) = \min_{\mathbf{x} \in \mathbb{R}^{p}} \left\{ f(\mathbf{x}) + \langle \lambda, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^{2} \right\}$$

$$\mathbf{x}_{\beta}^{*}(\lambda) \in \arg \min_{\mathbf{x} \in \mathbb{R}^{p}} \left\{ f(\mathbf{x}) + \langle \lambda, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^{2} \right\}$$
(4)

Augmented Lagrangian method (ALM)

- **1**. Choose $\lambda^0 \in \mathbb{R}^n$ and $\beta > 0$.
- **2**. For $k = 0, 1, \cdots$:
 - 2.a. Solve (4).
 - **2.b**. Compute $\nabla d_{\beta}(\boldsymbol{\lambda}^k) := \mathbf{A}\mathbf{x}^*_{\beta}(\boldsymbol{\lambda}^k) \mathbf{b}$.
 - **2.c**. Update $\boldsymbol{\lambda}^{k+1} := \boldsymbol{\lambda}^k + \beta \nabla d_{\beta}(\boldsymbol{\lambda}^k)$.

Augmented Lagrangian method: The ideal algorithm

$$d_{\beta}(\lambda) = \min_{\mathbf{x} \in \mathbb{R}^{p}} \left\{ f(\mathbf{x}) + \langle \lambda, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^{2} \right\}$$

$$\mathbf{x}_{\beta}^{*}(\lambda) \in \arg \min_{\mathbf{x} \in \mathbb{R}^{p}} \left\{ f(\mathbf{x}) + \langle \lambda, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^{2} \right\}$$
(4)

Augmented Lagrangian method (ALM)

- **1**. Choose $\lambda^0 \in \mathbb{R}^n$ and $\beta > 0$.
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 - **2.c.** Update $\boldsymbol{\lambda}^{k+1} := \boldsymbol{\lambda}^k + \beta \nabla d_{\beta}(\boldsymbol{\lambda}^k)$.

Accelerated ALM (AALM)

- **1.** Choose $\lambda^0 \in \mathbb{R}^n$ and $\beta > 0$. Set $\tilde{\lambda}^0 := \lambda^0$ and $t_0 := 1$
- **2.** For $k = 0, 1, \cdots$, perform:
 - 2.a. Solve (4).
 - **2.b.** Compute $\nabla d_{\beta}(\tilde{\boldsymbol{\lambda}}^k) := \mathbf{A}\mathbf{x}^*_{\beta}(\tilde{\boldsymbol{\lambda}}^k) \mathbf{b}$.
 - **2.c.** Update $\boldsymbol{\lambda}^{k+1} := \tilde{\boldsymbol{\lambda}}_k + \beta \nabla d_{eta}(\tilde{\boldsymbol{\lambda}}^k),$

$$\tilde{\boldsymbol{\lambda}}^{k+1} := \boldsymbol{\lambda}^{k+1} + ((t_k - 1)/t_{k+1})(\boldsymbol{\lambda}^{k+1} - \boldsymbol{\lambda}^k),$$

$$t_{k+1} := (1 + \sqrt{1 + 4t_k^2})/2.$$

Convergence of ALM and AALM

Theorem (Convergence [19])

 \circ Let $\{oldsymbol{\lambda}^k\}$ be the sequence generated by ALM. Then

$$d^\star - d_eta(oldsymbol{\lambda}^k) \leq rac{\|oldsymbol{\lambda}^0 - oldsymbol{\lambda}^\star\|_2^2}{2eta(k+1)}.$$

 \circ Let $\{\lambda^k\}$ be the sequence generated by AALM. Then

$$d^{\star} - d_{\beta}(\boldsymbol{\lambda}^{k}) \leq \frac{2\|\boldsymbol{\lambda}^{0} - \boldsymbol{\lambda}^{\star}\|_{2}^{2}}{\beta(k+1)^{2}}.$$

Remarks:

- o Guarantees are given for the dual problem and not for the primal!
- \circ Approximate solution for primal via averaging: $\mathbf{x}^{\epsilon} = \frac{1}{k} \sum_{i=0}^{k-1} \mathbf{x}^*_{\beta}(\boldsymbol{\lambda}^i)$ [40]

Drawbacks and enhancements

At each step, ALM solves

$$\mathbf{x}_{\beta}^{*}(\boldsymbol{\lambda}) := \arg \min_{\mathbf{x} \in \mathbb{R}^{p}} \left\{ \mathcal{L}_{\beta}(\mathbf{x}, \boldsymbol{\lambda}) := f(\mathbf{x}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^{2} \right\}.$$
 (5)

Drawbacks

- 1. Drawback 1: The quadratic term $\|\mathbf{A}\mathbf{x} \mathbf{b}\|^2$ in (5) destroys the separability as well as the tractable proximity of f.
- 2. Drawback 2: Solving (5) exactly is impractical.

Drawbacks and enhancements

At each step, ALM solves

$$\mathbf{x}_{\beta}^{*}(\boldsymbol{\lambda}) := \arg \min_{\mathbf{x} \in \mathbb{R}^{p}} \left\{ \mathcal{L}_{\beta}(\mathbf{x}, \boldsymbol{\lambda}) := f(\mathbf{x}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^{2} \right\}.$$
 (5)

Drawbacks

- 1. Drawback 1: The quadratic term $\|\mathbf{A}\mathbf{x} \mathbf{b}\|^2$ in (5) destroys the separability as well as the tractable proximity of f.
- 2. Drawback 2: Solving (5) exactly is impractical.

Enhancements

- 1. Allow inexactness of solving (5), while guaranteeing the same convergence rate.
- 2. Linearize the term $\|\mathbf{A}\mathbf{x} \mathbf{b}\|^2$ in the same way we did for Quadratic Penalty formulations.

An inexact approach for subproblems of ALM

o Primal subproblem as a composite optimization problem:

$$\mathbf{x}_{\beta}^{*}(\lambda) := \arg \min_{\mathbf{x} \in \mathbb{R}^{p}} \left\{ \mathcal{L}_{\beta}(\mathbf{x}, \lambda) := \underbrace{f(\mathbf{x}) + \langle \lambda, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle}_{=:h(\mathbf{x})} + \underbrace{\frac{\beta}{2} \underbrace{\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^{2}}_{\text{proximally tractable}}}_{\text{tractable}} \right\}.$$
(6)

⇒ can use accelerated proximal methods (e.g. FISTA) to solve this up to some accuracy.

Conceptual inexact augmented Lagrangian method:

- **1**. Choose $\lambda^0 \in \mathbb{R}^n$, $\beta > 0$ and a decreasing sequence $\epsilon_k \geq 0$, $\forall k$.
- **2**. For $k = 0, 1, \dots$, perform:
 - **2.a.** Solve (6) with FISTA until $\mathcal{L}_{\beta}(\mathbf{x}_{\beta}^{\epsilon_k}(\boldsymbol{\lambda}^k), \boldsymbol{\lambda}^k) \leq \mathcal{L}_{\beta}(\mathbf{x}_{\beta}^*(\boldsymbol{\lambda}^k), \boldsymbol{\lambda}^k) + \epsilon_k$.
 - **2.b.** Update $\lambda^{k+1} := \lambda^k + \beta(\mathbf{A}\mathbf{x}_{\beta}^{\epsilon_k}(\lambda^k) \mathbf{b})$.

Remarks:

- \circ Conceptual since $\mathbf{x}^*_{\beta}(\pmb{\lambda}^k)$ is unknown.
- \circ Solve (6) for increasing (explicit) number of iterations $m_k > 0$.
- See advanced material at the end of the lecture for DL-ASGARD method.

Linearized Augmented Lagrangian method

1. Majorize the augmented Lagrangian:

$$\mathbf{x}^{k+1} := \arg\min_{\mathbf{x} \in \mathcal{X}} \left\{ f(\mathbf{x}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 + \frac{1}{2} \|\mathbf{x} - \mathbf{x}^k\|_{\mathbf{Q}_k}^2 \right\}.$$

2. Using the same calculation as in Lecture 12, when $\mathbf{Q}_k = \alpha_k \mathbf{I} - \beta \mathbf{A}^{\top} \mathbf{A} \succeq 0$ and $\alpha_k \geq \beta \|\mathbf{A}\|^2$, we get:

$$\mathbf{x}^{k+1} = \operatorname{prox}_{\frac{1}{\alpha_k} f} \left(\mathbf{x}^k - \frac{1}{\alpha_k} \mathbf{A}^\top \left(\boldsymbol{\lambda}^k + \beta \left(\mathbf{A} \mathbf{x}^k - \mathbf{b} \right) \right) \right)$$

3. Picking $\alpha_k = \beta ||\mathbf{A}||^2$, we obtain the following method:

Linearized augmented Lagrangian method (LALM)

- 1. Choose $\mathbf{x}^0 \in \mathbb{R}^p$, $\boldsymbol{\lambda}^0 \in \mathbb{R}^n$ and $\beta > 0$.
- **2.** For $k = 0, 1, \ldots$:

$$\mathbf{x}^{k+1} := \operatorname{prox}_{\frac{1}{\beta \|A\|^2} f} \left(\mathbf{x}^k - \frac{1}{\beta \|A\|^2} \mathbf{A}^\top \left(\boldsymbol{\lambda}^k + \beta \left(\mathbf{A} \mathbf{x}^k - \mathbf{b} \right) \right) \right),$$
$$\boldsymbol{\lambda}^{k+1} := \boldsymbol{\lambda}^k + \beta \left(\mathbf{A} \mathbf{x}^{k+1} - \mathbf{b} \right).$$

Convergence of Linearized ALM

Theorem (Convergence [36])

Let $\beta > 0$ and define $\bar{\mathbf{x}}_k = \frac{1}{k} \sum_{i=1}^k \mathbf{x}_i$. Then, the iterates of LALM satisfy:

$$\left\|\mathbf{A}\bar{\mathbf{x}}^k - \mathbf{b}\right\| \le \frac{1}{k} \left(\frac{\beta}{2} \|\mathbf{x}^0 - \mathbf{x}^*\|^2 + \frac{\max\left\{(1 + \|\boldsymbol{\lambda}^*\|)^2, 4\|\boldsymbol{\lambda}^*\|^2\right\}}{\beta}\right)$$

$$|f(\bar{\mathbf{x}}^k) - f(\mathbf{x}^\star)| \le \frac{1}{k} \left(\frac{\beta}{2} ||\mathbf{x}^0 - \mathbf{x}^\star||^2 + \frac{\max\left\{ (1 + ||\boldsymbol{\lambda}^\star||)^2, 4||\boldsymbol{\lambda}^\star||^2 \right\}}{\beta} \right)$$

Remarks:

- o Guarantees are for the primal and in fact optimal [25].
- o No need to solve difficult subproblems at each iteration.
- \circ Guarantees are for $\bar{\mathbf{x}}^k$, and not \mathbf{x}^k .

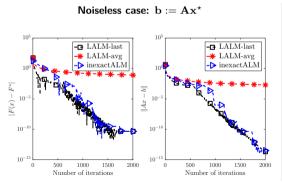
Example: Basis pursuit

Problem: Basis pursuit

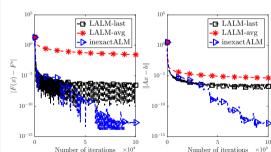
Given $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \mathbb{R}^n$, solve

$$F^{\star} := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \|\mathbf{x}\|_1 : \mathbf{A}\mathbf{x} = \mathbf{b} \right\}.$$

- Applications in de-noising, data compression.
- ightharpoonup Experiment: ${f A}$ is a row-normalized standard Gaussian matrix, ${f x}^\star$ is a k-sparse randomly generated vector.



Noisy case: $b := Ax^* + \mathcal{N}(0, 10^{-3})$



Nonconvex optimization problems with nonlinear constraints

Problem template

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) + g(\mathbf{A}(\mathbf{x})) \right\},\tag{7}$$

- $f: \mathbb{R}^p \to \mathbb{R}$ is a proper continuously-differentiable & nonconvex
- $g:\mathbb{R}^n \to \mathbb{R}$ is proper, lower-semicontinuous
- $\mathbf{A}: \mathbb{R}^p o \mathbb{R}^n$ is a nonlinear operator and $\mathbf{b} \in \mathbb{R}^n$
- An optimal solution \mathbf{x}^* to (7) satisfies $f(\mathbf{x}^*) = f^*$, $\mathbf{A}(\mathbf{x}^*) = \mathbf{b}$.

Example: Blind Image Deconvolution

- o One of the most challenging problems in imaging sciences
 - Fig. Goal: Recover an image ${f X}$ and an unknown blurring transformation ${f T}$ from a blurred image ${f B} \in \mathbb{R}^{p imes q}$.
 - Formally:

$$\min_{\mathbf{T} \in \mathbb{R}^{r \times s} \left\{ h(\mathbf{X}, \mathbf{T}) + \frac{1}{2} ||\mathbf{T} * \mathbf{X} - \mathbf{B}||^2 \right\},\,$$

where $h: \mathbb{R}^{p \times q} \times \mathbb{R}^{r \times s} \mathbb{R} \to (-\infty, +\infty]$ is a non-convex & possibly non-smooth regularizer.

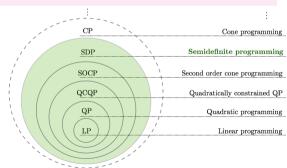
Remark: o Advanced material at the end of the lecture covers inexact Augmented Lagrangian for (7).

Recall the prototype problem

A primal problem prototype

$$f^* := \min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) : \mathbf{A}\mathbf{x} = \mathbf{b}, \ \mathbf{x} \in \mathcal{X} \right\},\tag{8}$$

- f is a proper, closed and convex function.
- $\mathbf{A} \in \mathbb{R}^{n \times p}$ and $\mathbf{b} \in \mathbb{R}^n$ are known.
- $ightharpoonup \mathcal{X}$ is nonempty, closed and convex.
- We further assume \mathcal{X} is a bounded set! This assumption is motivated by practical applications.
- Standard convex optimization formulations in (8):
 - ► linear programming
 - quadratic programming
 - convex quadratic programming
 - second order cone programming
 - semidefinite programming



The SDP formulation

The standard form of an SDP

$$egin{array}{ll} \min & \langle \mathbf{C}, \mathbf{X}
angle \ \mathbf{x} \in \mathcal{X} \end{array}$$
 s.t. $\langle \mathbf{A}_i, \mathbf{X}
angle = b_i, ext{ for } i = 1, \dots m$

- $\mathcal{X} = \{\mathbf{X} \in \mathbb{R}^{p \times p} : \mathbf{X} \succeq 0\}$ the positive semidefinite cone.
- $\mathbf{C} \in \mathbb{R}^{p \times p}$, $\mathbf{A}_i \in \mathbb{R}^{p \times p}$ are symmetric and $b_i \in \mathbb{R}$, and are given. By definition, $\langle \mathbf{A}_i, \mathbf{X} \rangle = \mathrm{Tr}(\mathbf{A}_i^T \mathbf{X})$.
- ▶ Any SDP can be written in standard form.

Trace-constrained SDPs

Consider the following SDP formulation:

$$\begin{array}{ll} \min & \langle \mathbf{C}, \mathbf{X} \rangle \\ \text{s.t.} & \langle \mathbf{A}_i, \mathbf{X} \rangle = b_i, \text{ for } i = 1, \dots m \\ & \langle \mathbf{I}, \mathbf{X} \rangle \coloneqq \mathrm{Tr}(\mathbf{X}) = \alpha \in \mathbb{R}_+ \longleftarrow \text{ the trace constraint} \end{array}$$

- ▶ Observe that (9) belongs to the template (8).
- This formulation is of broad interest [41]. In the sequel, SDP relaxations for non-convex problems.
- ▶ Problem (9) can be large in practice, making Interior Point Methods inefficient.

(9)

Example: Finding maximum-weight cut of a graph

 \circ Goal: Given an undirected graph G=(V,E) with a set of weights $c:E\to\mathbb{R}_+$

$$\min_{x \in \mathbb{Z}^p} \left\{ \frac{1}{2} \sum_{\{i,j\} \in E} c_{ij} (1 - x_i x_j) : x_i \in \{-1, +1\} \right\}$$

 $({\sf Weighted\ max-cut})$

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 (Weighted max-cut)

- o The SDP approach: Lift & relax
 - lift as a matrix optimization problem $X = xx^*$:

$$\min_{x \in \mathbb{R}^{p \times p}} \left\{ \frac{1}{2} \sum_{\{i,j\} \in E} c_{ij} (1 - \mathbf{X}_{ij}) : \operatorname{diag}(\mathbf{X}) = 1, \ \mathbf{X} \succeq 0, \ \mathbf{X}^* = \mathbf{X}, \ \operatorname{rank}(x) = \mathbf{1} \right\}$$

relax the non-convex rank constraint

$$\min_{\mathbf{X} \in \mathbb{R}^{p \times p}} \left\{ \underbrace{\frac{1}{2} \sum_{\{i,j\} \in E} c_{ij} (1 - \mathbf{X}_{ij})}_{\text{tr}(\mathbf{C}\mathbf{X})} : \underbrace{\operatorname{diag}(\mathbf{X}) = 1}_{\mathbf{A}(\mathbf{X}) = \mathbf{b}}, \ \mathbf{X} \succeq 0, \ \mathbf{X}^* = \mathbf{X} \right\}$$
 (Max-cut SDP)

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 (Max-cut SDP)

o Always delivers solutions 0.87856 times the optimal value after randomized rounding

Example: Clustering with minimal sum-of-squares

- o **Goal:** Given data points $s_1, s_2, \dots, s_p \in \mathbb{R}^q$, assign them into k disjoint clusters.
 - ▶ ▷ Minimize the sum of squared distances of all points to their cluster centers

$$\min_{z} \left\{ \sum_{i=1}^{k} \sum_{i=1}^{p} z_{ij} \|s_{i} - w_{j}(z)\|^{2} : \sum_{i=1}^{k} z_{ij} = 1, \sum_{i=1}^{p} z_{ij} \ge 1, z_{ij} \in \{0, 1\} \right\}$$
 (MinSumClu.)

where $z\!\in\!\{0,1\}^{p\times k}$ is the assignment matrix with $z_{ij}=\begin{cases}1 & \text{if } s_i\!\in\!j\text{th cluster}\\0 & \text{otherwise}\end{cases}$

where w_1,\dots,w_k are cluster centers with $w_j(z)=\left(\sum_{i=1}^p z_{ij}s_i\right)\left(\sum_{i=1}^p z_{ij}\right)^{-1}$

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The SDP approach: Lift & relax (details omitted)

$$\min_{\boldsymbol{x} \in \mathbb{R}^{p \times p}} \left\{ \operatorname{tr}(\mathbf{C}\mathbf{X}) : \mathbf{X} \geq 0, \ \mathbf{X}\mathbf{1} = \mathbf{1}, \ \mathbf{X} \succeq 0, \ \mathbf{X}^* = \mathbf{X}, \ \operatorname{tr}(\mathbf{X}) = k \right\}$$
 (Clustering SDP)

• where $\mathbf{X} = z(z^*z)^{-1}z^*$ and $c_{i,i} = ||s_i - s_i||^2$

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 (Clustering SDP)

- where $\mathbf{X} = z(z^*z)^{-1}z^*$ and $c_{ij} = \|s_i s_j\|^2$
- o Improved guarantees over LP relaxations

J.Peng and Y.Wei, Approximating K-means-type clustering via semidefinite programming, 2005

Example: Neural networks

 \circ Goal: Approximate the ℓ_{∞} -Lipschitz constant L_f of 1-layer ReLU network

$$h_{\mathbf{x}}(\mathbf{a}) := \mathbf{x}_2^T \sigma(\mathbf{X}_1 \mathbf{a} + \mathbf{x}_1)$$

▶ applications to verification, robustness against adversarial examples, generalization...

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- ▶ applications to verification, robustness against adversarial examples, generalization...
- o The SDP approach: Lift & relax (details omitted)

$$L_f \leq \bar{L}_f := -\frac{1}{4} \min_{\mathbf{X} \in \mathbb{RP}^{\times p}} \left\{ \operatorname{tr}(\mathbf{CX}) : \mathbf{X} \succeq 0, \operatorname{diag}(\mathbf{X}) = \mathbf{1}, \mathbf{X} = \mathbf{X}^* \right\}$$

$$\mathbf{C} := -\begin{bmatrix} \mathbf{0} & \mathbf{0} & \mathbf{1}^T \mathbf{X}_2^T \mathsf{Diag}(\mathbf{x}_2) \\ \mathbf{0} & \mathbf{0} & \mathbf{X}_1^T \mathsf{Diag}(\mathbf{x}_2) \\ \mathsf{Diag}(\mathbf{x}_2)^T \mathbf{X}_1 \mathbf{1} & \mathsf{Diag}(\mathbf{x}_2)^T \mathbf{X}_1 & \mathbf{0} \end{bmatrix}$$

Example: Neural networks

 \circ Goal: Approximate the ℓ_{∞} -Lipschitz constant L_f of 1-layer ReLU network

$$h_{\mathbf{x}}(\mathbf{a}) := \mathbf{x}_2^T \sigma(\mathbf{X}_1 \mathbf{a} + \mathbf{x}_1)$$

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Slide 24/56

o An open research area

Ragunathan et al. SDP relaxations for certifying robustness agains adversarial examples. ICLR2017

F. Latorre, P. Rolland, and V. Cevher. Lipschitz constant estimation of neural networks via sparse polynomial optimization. ICLR 2020.

CGM with quadratic penalty

Classical CGM does not apply to (3)

- ▶ lmo of the intersection of $\{x : Ax = b\}$ and \mathcal{X} is difficult to compute.
- ▶ Idea: Combine the CGM framework with the quadratic penalty approach.

Quadratic penalty strategy

A quadratic penalty formulation:

$$\min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \overbrace{f(\mathbf{x}) + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2}^{f_{\boldsymbol{\beta}}(\mathbf{x})} : \mathbf{x} \in \mathcal{X} \right\}$$

- $\beta > 0$ is the penalty parameter and $f_{\beta}(\mathbf{x})$ is the penalized objective function.
- Note that $f_{\beta}(\mathbf{x})$ is convex and smooth with parameter $L + \beta \|\mathbf{A}\|^2$.

A simple strategy [39] \Rightarrow Take a CGM step on f_{β} and increase β progressively

Homotopy conditional gradient method (HCGM)

- 1. Choose $\mathbf{x}^0 \in \mathcal{X}$, and $\beta_0 > 0$.
- **2.** For $k = 0, 1, \ldots$

$$\hat{\mathbf{x}}^k := \text{Imo}_{\mathcal{X}}(\nabla f(\mathbf{x}^k) + \beta_k \mathbf{A}^T (\mathbf{A}\mathbf{x}^k - \mathbf{b})).$$

$$\mathbf{x}^{k+1} := (1 - \gamma_k)\mathbf{x}^k + \gamma_k \hat{\mathbf{x}}^k,$$

 $\mathbf{x}^{k+1} := (1 - \gamma_k)\mathbf{x}^k + \gamma_k \hat{\mathbf{x}}^k,$ where $\gamma_k := \frac{2}{k+2}$ and $\beta_k := \beta_0 \sqrt{k+2}$.

Convergence guarantees of HCGM

Recall Lagrange duality

$$\mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) := f(\mathbf{x}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle$$

$$\max_{\boldsymbol{\lambda}} \min_{\mathbf{x} \in \mathcal{X}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda}) \leq \min_{\mathbf{x} \in \mathcal{X}} \max_{\boldsymbol{\lambda}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda})$$

$$\min_{\mathbf{x} \in \mathcal{X}} \max_{\boldsymbol{\lambda}} \mathcal{L}(\mathbf{x}, \boldsymbol{\lambda})$$

$$\text{(Duality)}$$

- λ is called the Lagrange multiplier.
- ▶ The function $d(\lambda)$ is called the dual function, and it is concave!
- ▶ The optimal dual objective value is $d^* = d(\lambda^*)$.

(Duality) holds with equality under weak assumptions \Rightarrow (Strong duality).

Theorem (Simplified[39])

Assume that strong duality holds. Then, the iterates of HCGM satisfy

$$\begin{cases} |f(\mathbf{x}^k) - f^*| & \in \mathcal{O}(k^{-1/2}) \\ \|\mathbf{A}\mathbf{x}^k - \mathbf{b}\| & \in \mathcal{O}(k^{-1/2}). \end{cases}$$

^{*} For an extension of HCGM to the case $\mathbf{A}\mathbf{x} - \mathbf{b} \in \mathcal{K}$, please see Appendix A_1 .

^{**}There exist stochastic variants of HCGM, which are not covered in this lecture. Those interested may refer to [22, 34].

Augmented Lagrangian CGM: CGAL

Augmented Lagrangian approach

Augmented problem formulation:

$$\min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 : \mathbf{A}\mathbf{x} = \mathbf{b}, \ \mathbf{x} \in \mathcal{X} \right\}$$

Write down the Lagrangian:

$$\mathcal{L}_{\beta}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{x} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2$$

▶ Note that $\mathcal{L}_{\beta}(\cdot \boldsymbol{\lambda})$ is smooth with parameter $L + \beta \|\mathbf{A}\|^2$.

- Our strategy [37] \Rightarrow $\begin{cases} 1. \text{ Take a CGM step wrt } \mathcal{L}_{\beta}(\cdot, \lambda) \text{ (primal)} \\ 2. \text{ Take a gradient step wrt } \mathcal{L}_{\beta}(\mathbf{x}, \cdot) \text{(dual)} \\ 3. \text{ Increase } \beta \text{ progressively} \end{cases}$

Challenge: Step size in the dual domain (step 2.)

Convergence guarantees of CGAL

Conditional gradient augmented Lagrangian method (CGAL)

- **1.** Choose $\mathbf{x}^0 \in \mathcal{X}$. $\boldsymbol{\lambda}^0 \in \mathbb{R}^n$. and $\beta_0 > 0$.
- **2.** For $k = 0, 1, \ldots$:

$$\hat{\mathbf{x}}^k := \text{Imo}_{\mathcal{X}}(\nabla f(\mathbf{x}^k) + \mathbf{A}^T \boldsymbol{\lambda}^k + \beta_k \mathbf{A}^T (\mathbf{A} \mathbf{x}^k - \mathbf{b}))$$

$$\mathbf{x}^{k+1} := (1 - \gamma_k)\mathbf{x}^k + \gamma_k \hat{\mathbf{x}}^k$$

$$\mathbf{A}^{k+1} := \mathbf{\lambda}_{0}^{k} + \omega_{k}(\mathbf{A}\mathbf{x}^{k+1} - \mathbf{b})$$

 $\mathbf{\lambda}^{k+1} := \mathbf{\lambda}^k + \omega_k (\mathbf{A}\mathbf{x}^{k+1} - \mathbf{b})$ where $\gamma_k := \frac{2}{k+2}$, and $\beta_k := \beta_0 \sqrt{k+2}$.

Theorem (Simplified)

Assume that strong duality holds. Let us choose dual step size ω_k by the following rule

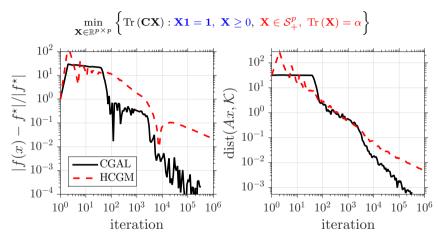
$$\omega_k = \alpha_k := \min \left\{ \frac{1}{\beta_0}, \ \frac{\eta_k^2 (L_f + \boldsymbol{\lambda}_{k+1}) D_{\mathcal{X}}^2}{2 \|\mathbf{A} \mathbf{x}^{k+1} - \mathbf{b}\|^2} \right\} \quad \text{if} \quad \|\boldsymbol{\lambda}^k + \alpha_k (\mathbf{A} \mathbf{x}^{k+1} - \mathbf{b})\| \leq D_{\mathcal{Y}}$$

and $\omega_k = 0$ otherwise, for some $D_{\mathcal{V}} \geq 0$. Then, the iterates of CGAL satisfy

$$\begin{cases} |f(\mathbf{x}^k) - f^{\star}| & \in \mathcal{O}(\frac{1}{\sqrt{k}}) \\ \|\mathbf{A}\mathbf{x}^k - \mathbf{b}\| & \in \mathcal{O}(\frac{1}{\sqrt{k}}) \end{cases}$$

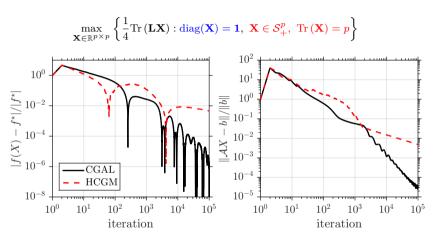
^{*} For an extension of CGAL to the case $Ax - b \in \mathcal{K}$, please see Appendix A_2 .

Example: k-means clustering



- ► Test setup with preprocessed MNIST dataset [39]
- p=1000 & $\alpha=10$ is the number of clusters
- Note: the worst-case guarantee is the same for HCGM and CGAL, but CGAL performs better in practice.

Example: Max-cut SDP



- UF Sparse graphs: GSet collection, G40 dataset p=2000
- ▶ L is graph Laplacian matrix.
- Note: the worst-case guarantee is the same for HCGM and CGAL, but CGAL performs better in practice.

Towards scalable semidefinite programming

Structures in SDP relaxations

$$\min_{\mathbf{X} \in \mathbb{R}^{p \times p}} \left\{ \mathsf{Tr}(\mathbf{CX}) : \mathcal{A}\mathbf{X} = b, \mathbf{X} \succeq 0, \mathsf{Tr}(\mathbf{X}) = \alpha \right\}$$
 (10)

- \circ **X** has $\mathcal{O}(p^2)$ -degrees of freedom \implies needs $\Theta(p^2)$ storage
- \circ Optimal solutions \mathbf{X}^{\star} typically or approximately have $\mathcal{O}(rp)$ -degrees of freedom
 - $r = \text{rank } \& r \ll p \text{ (low-rank)}$
 - ightharpoonup need $\Theta(rp)$ storage for a rank-r approximate solution
- \circ Example SDP's typically have $n = \tilde{\mathcal{O}}(p)$ affine constraints
 - During optimization we need to keep track of quantities such as

$$A(uv^*)$$
 $u^*(A^*z)$ $(A^*z)v$, $u \in \mathbb{R}^p$, $v \in \mathbb{R}^p$, $z \in \mathbb{R}^n$

 \implies need $\Omega(n+p)$ storage for computations

Towards scalable semidefinite programming

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$$\min_{\mathbf{X} \in \mathbb{R}^{p \times p}} \left\{ \mathsf{Tr}(\mathbf{CX}) : \mathcal{A}\mathbf{X} = b, \mathbf{X} \succeq 0, \mathsf{Tr}(\mathbf{X}) = \alpha \right\}$$
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- \circ **X** has $\mathcal{O}(p^2)$ -degrees of freedom \implies needs $\Theta(p^2)$ storage
 - \longleftarrow this becomes a major problem
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 - During optimization we need to keep track of quantities such as

$$A(uv^*) \quad u^*(A^*z) \quad (A^*z)v, \qquad u \in \mathbb{R}^p, \ v \in \mathbb{R}^p, \ z \in \mathbb{R}^n$$

 \implies need $\Omega(n+p)$ storage for computations

 $\Theta(n+rp)$ storage

Towards scalable semidefinite programming

Structures in SDP relaxations

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 \implies need $\Omega(n+p)$ storage for computations

- ▶ Relevant SDPs are often large \implies HCGM, CGAL have a storage bottleneck (e.g., MaxCut for graph of $2e^6$ nodes $\rightarrow \sim 2e^{12}$ variables!!)
- ► Can we leverage the problem structure for better storage performance? See advanced material.

Wrap up!

Last lecture! HW and mock exam...

*An explicit inexact ALM: ASGARD-DL

Inexact ALM (Double Loop ASGARD [31])

- **1.** $\mathbf{x}^0 = \hat{x}^{0,0} = \bar{x}^{0,0} = \hat{x}^{0,0} \in \mathbb{R}^p$. $\lambda_0 \in \mathbb{R}^n$, $\beta_k > 0$, $\tau_0 = 1$, $m_0 > 2$, $\omega > 1$.
- 2. For $k = 0, 1, \dots$ perform:

2.a For
$$i=0,1,\cdots,m_k-1$$
: // accelerated proximal method $\hat{\mathbf{x}}^{k,i}=(1-\tau_k)\bar{\mathbf{x}}^{k,i}+\tau_k\tilde{\mathbf{x}}^{k,i}$

$$\tilde{\mathbf{x}}^{k,i+1}=\operatorname{prox}_{\frac{f}{\beta_k\|A\|^2}}\left(\tilde{\mathbf{x}}^{k,i}-\frac{1}{\beta_k\|\mathbf{A}\|^2}A^\top(\mathbf{\lambda}^k+\beta_k(A\hat{\mathbf{x}}^{k,i}-\mathbf{b}))\right)$$

$$\bar{\mathbf{x}}^{k,i+1}=\hat{\mathbf{x}}^{k,i}+\tau_k(\tilde{\mathbf{x}}^{k,i+1}-\tilde{\mathbf{x}}^{k,i})$$

$$\tau_{k+1}=\frac{2}{k+2}$$
2.b Update primal and dual variables:

2.b Update primal and dual variables:

Remarks:

- o Corresponds to inexact ALM with explicit inner termination rule.
- \circ Attains optimal $\mathcal{O}(1/k)$ on the last iterate, with good empirical performance (see slide 17).

*AL schemes for non-convex problems - challenges

Challenges

- o More complicated requirements to prove global convergence of generic schemes for (7) (e.g., [27]):
 - ► ∃ superset of the feasible-set, where feasibility is 'good-enough' (information zone IZ)
 - ▶ Objective & constraints need to be 'sufficiently-regular' within the IZ
 - ► The iterates of the AL algorithm need to
 - ► Enter the IZ in a finite number of steps.
 - Stay inside the IZ thereafter.
- o Literature studying this setting is scarce, and global convergence is not well-understood.

Set-up

Assume the following template:

$$\min_{\mathbf{x} \in \mathbb{R}^p} f(\mathbf{x}) + g(\mathbf{x}) \text{ s.t. } \mathbf{A}(\mathbf{x}) = \mathbf{b}$$
 (11)

- $f:\mathbb{R}^p \to \mathbb{R}$ is a continuously-differentiable non-convex function that is L_f -smooth.
- $g: \mathbb{R}^p \to \mathbb{R}$ is a proximal-friendly convex function.
- ► $\mathbf{A} : \mathbb{R}^p \to \mathbb{R}^n$ is a smooth nonlinear operator i.e., $\exists L_{\mathbf{A}} > 0$ s.t.: $\|\mathbf{J}_{\mathbf{A}}(\mathbf{x}) \mathbf{J}_{\mathbf{A}}(\mathbf{x})\| \le L_{\mathbf{A}} \|\mathbf{x} \mathbf{y}\|$, where \mathbf{J} is the Jacobian of \mathbf{A} .

San

*AL schemes for non-convex problems - optimality conditions

Reformulating (11) in terms of AL

 \circ Solving (11) is equivalent to solving the following reformulation:

$$\min_{\mathbf{x}} \max_{\lambda} \mathcal{L}_{\beta}(\mathbf{x}, \boldsymbol{\lambda}) + g(\mathbf{x})$$

where for a given $\beta > 0$, $\mathcal{L}_{\beta}(\mathbf{x}, \boldsymbol{\lambda}) = f(\mathbf{x}) + \langle \mathbf{A}(\mathbf{x}) - \mathbf{b}, \boldsymbol{\lambda} \rangle + \frac{\beta}{2} ||\mathbf{A}(\mathbf{x}) - \mathbf{b}||^2$ - the Augmented Lagrangian.

Optimality conditions of (11)

 $\circ \mathbf{x} \in \mathbb{R}^p$ is a first order stationary point (FOS) of (11) if $\exists \pmb{\lambda} \in \mathbb{R}^n$ s.t.

$$-\nabla \mathcal{L}_{\beta}(\mathbf{x}, \boldsymbol{\lambda}) \in \partial g(\mathbf{x})$$
 and $\mathbf{A}(\mathbf{x}) = b$.

 \circ When g=0 and \mathbf{x} is a FOS, \mathbf{x} is also a second-order stationary point (SOS) if:

$$\lambda_{\min}\left(\nabla_{\mathbf{x}\mathbf{x}}\mathcal{L}_{\beta}(\mathbf{x},\boldsymbol{\lambda})\right) \geq 0$$

- o Approximate stationarity is then defined for a given $\epsilon > 0$ as:
 - FOS: $\operatorname{dist}\left(-\nabla\mathcal{L}_{\beta}(\mathbf{x},\boldsymbol{\lambda}),\partial g(\mathbf{x})\right)\leq\epsilon\quad\text{ and }\quad\|\mathbf{A}(\mathbf{x})-b\|\leq\epsilon$
 - SOS: $\lambda_{\min} \left(\nabla_{\mathbf{x}\mathbf{x}} \mathcal{L}_{\beta}(\mathbf{x}, \boldsymbol{\lambda}) \right) > -\epsilon$

*An Inexact AL scheme for non-convex problems

o Main idea of [28]: solve primal problems with increasing accuracy ϵ_k and carefully choose the dual stepsize σ_k .

ALM - conceptual (reference)

Inexact ALM - nonconvex (IALM)

- **1**. Choose $\lambda_0 \in \mathbb{R}^n$ and $\beta > 0$.
- **2**. For $k = 0, 1, \ldots$
 - **2.a**. Solve (4) to get \mathbf{x}^{k+1} .

2.b. Update $oldsymbol{\lambda}^{k+1} := oldsymbol{\lambda}^k + eta \left(\mathbf{A} \mathbf{x}^*_eta(oldsymbol{\lambda}^k) - \mathbf{b}
ight)$.

- **1.** Choose b>1, $\boldsymbol{\lambda}^0\in\mathbb{R}^n$, $\sigma_0>0$, τ_f , $\tau_s>0$.
- **2.** For $k = 0, 1, \dots$, perform:
 - **2.aa**. Set $\epsilon_{k+1} = 1/\beta_k$
 - **2.a.** Get \mathbf{x}^{k+1} with a solver of choice, s.t.:

$$\operatorname{dist}(-\nabla_x \mathcal{L}_{\beta_k}(\mathbf{x}^{k+1}, \boldsymbol{\lambda}_k), \partial g(\mathbf{x}^{k+1})) \leq \epsilon_{k+1}, \quad \text{[FOS]}$$

$$\lambda_{\min}(\nabla_{\mathbf{x}\mathbf{x}}\mathcal{L}_{\beta_k}(\mathbf{x}^{k+1}, \boldsymbol{\lambda}^k)) \ge -\epsilon_{k+1}$$
 [SOS]

2.b. Update

$$\beta_{k+1} = b^{k+1}$$

$$\sigma_{k+1} = \sigma_0 \min \left(1, \frac{\|\mathbf{A}(\mathbf{x}^1) - \mathbf{b}\| \log^2(2)}{\|\mathbf{A}(\mathbf{x}^{k+1}) - \mathbf{b}\| (k+1) \log^2(k+2)} \right)$$

$$\boldsymbol{\lambda}^{k+1} = \boldsymbol{\lambda}^k + \sigma_{k+1} \left(\mathbf{A}(\mathbf{x}^{k+1}) - b \right)$$

2.c. Stop if $\operatorname{dist}(-\nabla_x \mathcal{L}_{\beta_k}(\mathbf{x}^{k+1}, \pmb{\lambda}_k), \partial g(\mathbf{x}^{k+1}))$

$$+ \|\mathbf{A}(\mathbf{x}^{k+1}) - b\| \le \tau_f \quad [FOS]$$

and if also $\lambda_{\min}(\nabla_{\mathbf{x}\mathbf{x}}\mathcal{L}_{\beta_k}(\mathbf{x}^{k+1},\boldsymbol{\lambda}^k)) \geq -\epsilon_{k+1}$ [SOS]

*Convergence of the Inexact AL for non-convex problems

A key assumption

- o For convex AL schemes we rely on Slater's condition to prove convergence.
- \circ We need a similar kind of assumption for our non-convex problem, called regularity condition 1 : for some $\nu>0$, assume

$$\nu \|\mathbf{A}(\mathbf{x}^k) - \mathbf{b}\| \le \operatorname{dist}\left(-\mathbf{J}_{\mathbf{A}}(\mathbf{x}^k)^{\top}(\mathbf{A}(\mathbf{x}^k) - \mathbf{b}), \frac{\partial g(\mathbf{x}^k)}{\beta_{k-1}}\right), \quad \forall k$$
(12)

 \circ Informally, condition (12) ensures that step 2.a of IALM improves feasibility as β_k grows.

Theorem [28] (Simplified)

Under the framework (11) and assumption (12), IALM reaches

- FOS with $\tilde{\mathcal{O}}(\epsilon^3)$ complexity and
- SOS with $\tilde{\mathcal{O}}(\epsilon^5)$ complexity,

where $\tilde{\mathcal{O}}$ hides logarithmic factors².

²To simplify this statement we left out the fact that these complexities are attained under a specific choice of solver in step 2.a for each of the cases. Specifically, the Accelerated Proximal Gradient Method (APGM) was used to reach FOS points, and the Trust Region Method was used to reach SOS points. These, however, are out of the scope of this course.



¹Regularity conditions can take many forms, this is just one of them.

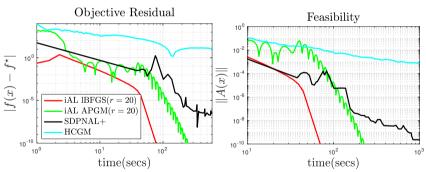
*Example: k-means clustering

o Model free k-means clustering SDP:

$$\min_{\mathbf{X} \in \mathbb{R}^{p \times p}} \left\{ \mathsf{Tr}(\mathbf{CX}): \ \mathbf{X1} = \mathbf{1}, \ \mathbf{X} \geq 0, \ \mathbf{X} \in \mathcal{S}^p_+, \ \mathsf{Tr}\left(\mathbf{X}\right) = \alpha \right\}$$

Nonconvex formulation:

$$\min_{\mathbf{u} \in \mathbb{R}^p} \bigg\{ \mathsf{Tr}(\mathbf{C}\mathbf{u}\mathbf{u}^*): \ \mathbf{u}\mathbf{u}^*\mathbf{1} = \mathbf{1}, \ \mathbf{u} \geq 0, \ \|\mathbf{u}\|_F \leq \sqrt{\alpha} \bigg\},$$

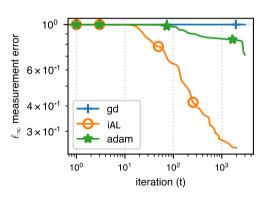


In the plot legends, IBFGS and APGM[15] refer to solvers used in Step 2.a. of IALM. SDPNAL+[29] is a state-of-the-art SDP solver and HCGM

*Example: DARN with GANs (MNIST)

o De-adversarial-noise with generative adversarial networks:

$$\min_{\boldsymbol{w}, \mathbf{z}} \{ \| \boldsymbol{w} - (\boldsymbol{w}_0 + \eta) \|_{\star} : \ \boldsymbol{w} = \mathbf{G}(\mathbf{z}) \}$$



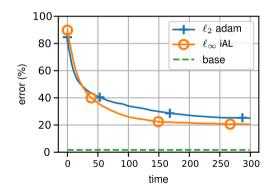




Figure: ℓ_∞ error per iteration

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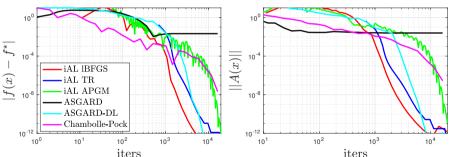
*Example: Basis Pursuit

o Convex formulation:

$$\min_{\mathbf{x} \in \mathbb{R}^p} \left\{ \|\mathbf{x}\|_1: \ \mathbf{A}\mathbf{x} = \mathbf{b}
ight\}$$

o Non-convex formulation:

$$\text{change of variables} \begin{cases} \mathbf{x} & := \mathbf{x}^+ - \mathbf{x}^- \\ \mathbf{x}^+ & := \mathbf{u}_1^{\circ 2}, \ \mathbf{x}^- := \mathbf{u}_2^{\circ 2} \text{ and } \mathbf{u} := [\mathbf{u}_1^\top, \mathbf{u}_2^\top]^\top & \longrightarrow & \min_{\mathbf{u} \in \mathbb{R}^p} \left\{ \|\mathbf{u}\|_2^2 : \ \bar{\mathbf{A}} \mathbf{u}^{\circ 2} = \mathbf{b} \right\} \\ \bar{\mathbf{A}} & := [\mathbf{A}, -\mathbf{A}]$$



In the plot legends, TR [5] refers to the solver used in Step 2.a. of IALM. ASGARD-DL is the IAL you saw earlier for the convex formulation and Chambolle-Pock is the algorithm presented in Lecture 12.

*Towards scalable semidefinite programming

The road to storage optimality

- ► SDPs often have a low rank solutions \implies instead of storing $\mathbf{X}_{k \in \{1...T\}}$ at every iteration, use a compressed representation S_k given by a matrix sketching technique.
- Formally Consider a PSD matrix $\mathbf{X} \in \mathbb{R}^{p \times p}$ and let R > 0 be a parameter that controls the storage cost of a sketch (and its accuracy). Construct a so-called Nyström sketch by drawing a fixed standard normal matrix $\mathbf{\Omega} \in \mathbb{R}^{p \times R}$, and produce a sketch \mathbf{S} of \mathbf{X} as follows:

$$\mathbf{S} = \mathbf{X}\mathbf{\Omega} \in \mathbb{R}^{p \times R}$$

Reconstruction - Given Ω and S, we recover a rank-R approximation \hat{X} of X by

$$\hat{\mathbf{X}} := \mathbf{S}(\mathbf{\Omega}^T \mathbf{S})^{\dagger} \mathbf{S}^T \quad \text{ with } \quad \mathbb{E}_{\mathbf{\Omega}} \left[\|\mathbf{X} - \hat{\mathbf{X}}\|_* \right] \le \left(1 + \frac{r}{R + r + 1} \right) \|\mathbf{X} - [\mathbf{X}]_r\|_* \quad \forall r < R$$
 (13)

where $\|\cdot\|_*$ denotes the nuclear norm and $[\cdot]_r$ is an r-truncated singular-value decomposition of the matrix, which is a best rank-r approximation with respect to every unitarily-invariant norm.

 \blacktriangleright \Longrightarrow We can reduce the storage from $\Theta(p^2)$ to $\Theta(rp)!$

*The algorithm - SketchyCGAL

▶ The Augmented Lagrangian of (10) is

$$\mathcal{L}_{\beta}(\mathbf{X}, \boldsymbol{\lambda}) = \text{Tr}(\mathbf{C}\mathbf{X}) + \langle \boldsymbol{\lambda}, \mathbf{A}\mathbf{X} - \mathbf{b} \rangle + \frac{\beta}{2} \|\mathbf{A}\mathbf{X} - \mathbf{b}\|^{2}, \qquad \nabla_{\mathbf{X}} \mathcal{L}_{\beta}(\mathbf{X}, \boldsymbol{\lambda}) = C + \mathbf{A}^{T} (\boldsymbol{\lambda}^{k} + \beta_{k} (\mathbf{A}\mathbf{X}^{k} - \mathbf{b}))$$

- ► The constraint set of (10) is $\mathcal{X} = \{\mathbf{X} \in \mathbb{R}^{p \times p} : \mathbf{X} \succeq 0, \operatorname{Tr}(\mathbf{X}) = \alpha\}$ and $\operatorname{Imo}_{\mathcal{X}}(\mathbf{Y}) = \alpha vv^T$ where v is the eigenvector corresponding to the minimum eigenvalue of \mathbf{Y} .
- ullet The algorithm performs linear updates directly on $\mathbf{z}_k := \mathbf{A}\mathbf{X}_k \in \mathbb{R}^n \implies$ the iterates \mathbf{X}_k become implicit!

SketchvCGAL (simplified)³ CGAL **1.** Choose $\mathbf{X}^0 = \mathbf{0}_{n \times n} \in \mathcal{X}$, $\boldsymbol{\lambda}^0 = \mathbf{0}_n$, $\beta_0 > 0$, T > 0. 1. Choose $\lambda^0 = \mathbf{0}_n$, $\mathbf{z}_0 = \mathbf{0}_n$, $\mathbf{S} = \mathbf{0}_{n \times R}$. $\beta_0 > 0, T > 0, R > 0, \Omega = \text{randn}(p, R).$ 2. For $k = 0, 1, \dots, T$: **2.** For $k = 0, 1, \dots T$: $(\mathcal{E}, v_k) := \mathsf{ApproxMinEvec}(\mathbf{C} + \mathbf{A}^T (\boldsymbol{\lambda}^k + \beta_k (\mathbf{A} \mathbf{X}^k - \mathbf{b})))$ $(\mathcal{E}, v_k) := \mathsf{ApproxMinEvec}(\mathbf{C} + \mathbf{A}^T(\boldsymbol{\lambda}^k + \beta_k(\mathbf{z}^k - \mathbf{b})))$ $\mathbf{z}^{k+1} := (1 - \gamma_k)\mathbf{z}^k + \gamma_k \mathbf{A}(\alpha v_k v_k^T)$ $\mathbf{X}^{k+1} := (1 - \gamma_k)\mathbf{X}^k + \gamma_k(\alpha v_k v_k^T)$ $\lambda^{k+1} := \lambda^k + \omega_k (\mathbf{A}^{\mathbf{X}^{k+1}} - \mathbf{b})$ $\boldsymbol{\lambda}^{k+1} := \boldsymbol{\lambda}^k + w_k(\mathbf{z}^{k+1} - \mathbf{b})$ $\mathbf{S}^{k+1} := (1 - \gamma_k)\mathbf{S}^k + \gamma_k v_k (v_k^T \Omega) \leftarrow \text{update the sketch}$ where $\gamma_k := \frac{2}{k+1}$, and $\beta_k := \frac{\sqrt{k+1}}{\beta_k}$. where $\gamma_k := \frac{2}{k+2}$, and $\beta_k := \frac{\sqrt{k+2}}{\beta}$. 3. Recover $\hat{\mathbf{X}}_T$ from \mathbf{S}_T using (13)

³Certain implementation details have been omitted for clarity. Those interested can refer to [41].

*SketchyCGAL: Convergence

- o Observations:
 - ightharpoonup The iterate update procedure of SketchyCGAL is the same as that of CGAL, though \mathbf{X}^k are implicit:

$$egin{align*} \mathbf{z}^{k+1} &= (1-\gamma_k)\mathbf{z}^k + \gamma_k\mathbf{A}(lpha vv^T) \ ext{by def. of } \mathbf{z}^k &
ightarrow &= \mathbf{A}\left((1-\gamma_k)\mathbf{X}^k + \gamma_klpha vv^T
ight) \ &= \mathbf{A}\mathbf{X}^{k+1} \end{aligned}$$

- The same computation holds for the sketch updates, where $\mathbf{S}^{k+1} = (1 \gamma_k)\mathbf{S}^k + \gamma_k \mathbf{v} \mathbf{v}^T \Omega = \mathbf{X}^{k+1} \mathbf{\Omega}$.
- the variables in SketchyCGAL track the variables of some invocation of CGAL and inherit their behavior.

Theorem [41]

Assume problem (10) satisfies strong duality, and let Ψ^* be its solution set. Then

- 1. The **implicit** iterates converge to the solution set Ψ^* at the same rate as CGAL.
- 2. For each r < R, the iterates $\hat{\mathbf{X}}_k$ computed by SketchyCGAL satisfy

$$\lim \sup_{k \to \infty} \mathbb{E}_{\Omega} \mathrm{dist}_*(\hat{\mathbf{X}}_k, \boldsymbol{\Psi}^*) \leq (1 + \frac{r}{R - r - 1}) \max_{\mathbf{Y} \in \boldsymbol{\Psi}^*} \|\mathbf{Y} - [\mathbf{Y}]_r\|_*$$

Here, $dist_*$ is the nuclear-norm distance between a matrix and a set of matrices.

*Example: Convex phase retrieval

Problem formulation

$$f^* := \min_{\mathbf{X} \in \mathbb{C}^{p \times p}} \left\{ \text{Tr}(\mathbf{X}) : \quad \mathcal{A}(\mathbf{X}) = \mathbf{b}, \quad \|\mathbf{X}\|_* \le \kappa, \quad \mathbf{X} \succeq 0 \right\}. \tag{14}$$

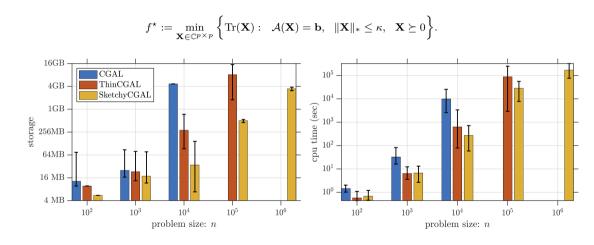
*This formulation is a convex and semidefinite relaxation of the original, much more difficult Phase Retrieval problem of recovering $\mathbf{x}^{\natural} \in \mathbb{C}^p$ from the measurements

$$\mathbf{b} \in \mathbb{R}^n, \ b_i = \left| \langle \mathbf{a}_i, \mathbf{x}^{\dagger} \rangle \right|^2 + \omega_i,$$

where $\mathbf{a}_i \in \mathbb{C}^p$ are known measurement vectors, ω_i models noise. Details can be found in [4, 38].

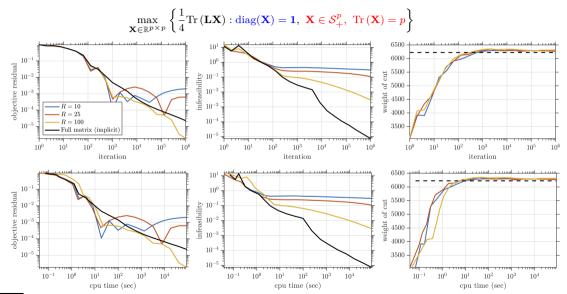
- ► This type of problem arises, for example, in X-ray crystallography and astronomical imaging.
- ▶ Note that the problem is constrained to $\mathcal{X} := \{\mathbf{X} \in \mathbb{R}^{p \times p} : \mathbf{X} \succeq 0, \|\mathbf{X}\|_* \le \kappa\}$, which is convex and compact.
- $ightharpoonup \mathcal{X}$ has an expensive prox operator, but an efficient lmo.

*Example: Convex Phase Retrieval memory usage



ThinCGAL is a memory-efficient variant of CGAL not addressed in this lecture.

*Example: Max-Cut SDP



Appendix A₁: Generalization of HCGM for $Ax - b \in \mathcal{K}$ (self-study)

Quadratic penalty strategy for $\min\{f(\mathbf{x}) : \mathbf{A}\mathbf{x} - \mathbf{b} \in \mathcal{K}, \mathbf{x} \in \mathcal{X}\}$

Define the distance function

$$\operatorname{dist}(\mathbf{y}, \mathcal{K}) := \min_{\mathbf{z} \in \mathcal{K}} \|\mathbf{y} - \mathbf{z}\|.$$

Quadratic penalty takes the form

$$\min_{\mathbf{x} \in \mathbb{R}^p} \left\{ f(\mathbf{x}) + \frac{\beta}{2} \operatorname{dist}^2(\mathbf{A}\mathbf{x} - \mathbf{b}, \mathcal{K}) : \mathbf{x} \in \mathcal{X} \right\}$$

Gradient of $dist^2(\mathbf{z}, \mathcal{K})$ is

$$\nabla dist^{2}(\mathbf{y}, \mathcal{K}) = 2(\mathbf{y} - proj_{\mathcal{K}}(\mathbf{y})).$$

Hence, HCGM can be generalized by changing lmo step as

$$\hat{\mathbf{x}}^k := \text{Imo}_{\mathcal{X}}(\nabla f(\mathbf{x}^k) + \beta_k \mathbf{A}^T (\mathbf{A}\mathbf{x}^k - \mathbf{b} - \text{proj}_{\mathcal{K}}(\mathbf{A}\mathbf{x}^k - \mathbf{b}))).$$

Same guarantees hold, by replacing $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|$ by $\operatorname{dist}(\mathbf{A}\mathbf{x} - \mathbf{b}, \mathcal{K})$.

Appendix A₂: Generalization of CGAL for $Ax - b \in \mathcal{K}$ (self-study)

Augmented Lagrangian for $\min\{f(\mathbf{x}) : \mathbf{A}\mathbf{x} - \mathbf{b} \in \mathcal{K}, \mathbf{x} \in \mathcal{X}\}$

Similarly, CGAL can be extended for $\mathbf{A}\mathbf{x} - \mathbf{b} \in \mathcal{K}$ constraint, by replacing

▶ lmo step as

$$\hat{\mathbf{x}}^k := \text{lmo}_{\mathcal{X}} \left(\nabla f(\mathbf{x}^k) + \mathbf{A}^T \lambda^k + \beta_k \mathbf{A}^T \left(\mathbf{A} \mathbf{x}^k - \mathbf{b} - \text{proj}_{\mathcal{K}} (\mathbf{A} \mathbf{x}^k - \mathbf{b} + \beta_k^{-1} \lambda^k) \right) \right)$$

and dual update step as

$$\lambda^{k+1} := \lambda^k + \omega_k \left(\mathbf{A} \mathbf{x}^{k+1} - \mathbf{b} + \mathrm{proj}_{\mathcal{K}} (\mathbf{A} \mathbf{x}^{k+1} - \mathbf{b} + \beta_{k+1}^{-1} \lambda^k) \right)$$

Same guarantees hold, by replacing $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|$ by $\operatorname{dist}(\mathbf{A}\mathbf{x} - \mathbf{b}, \mathcal{K})$.

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