Applications of interior point methods for very large problems arising in imaging and optimal transport

Filippo Zanetti Jacek Gondzio
Samuli Siltanen Salla Latva-Aijo Matti Lassas

University of Edinburgh, School of Mathematics

Modern Techniques of Very Large Scale Optimization
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1. Interior point method introduction

2. Tomographic imaging applications

3. Optimal transport applications

Interior point method

Pair of primal-dual convex QPs

$$\min_{x}\ c^T x + \frac{1}{2} x^T Q x, \qquad \text{s.t. } Ax = b, \qquad x \geq 0,$$

$$\max_{y,\ s}\ b^T y - \frac{1}{2} x^T Q x, \qquad \text{s.t. } A^T y + s - Qx = c, \qquad s \geq 0,$$

$x, s, c \in \mathbb{R}^n$, $y, b \in \mathbb{R}^m$, $A \in \mathbb{R}^{m\times n}$, $Q \in \mathbb{R}^{n\times n}$ positive semidefinite.

An IPM enforces the non-negativity constraint using a **logarithmic barrier**.

At each iteration, a direction is computed that allows the approximation to get closer to **optimality** and **feasibility**.

Newton system

The search direction is found using the **Newton** method

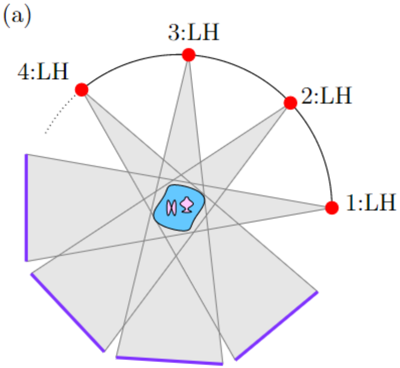
$$\begin{bmatrix} A & 0 & 0 \\ -Q & A^T & I \\ S & 0 & X \end{bmatrix} \begin{bmatrix} \Delta x \\ \Delta y \\ \Delta s \end{bmatrix} = \begin{bmatrix} r_P \\ r_D \\ r_\mu \end{bmatrix} = \begin{bmatrix} b - Ax \\ c + Qx - A^T y - s \\ \sigma\mu e - XSe \end{bmatrix}.$$

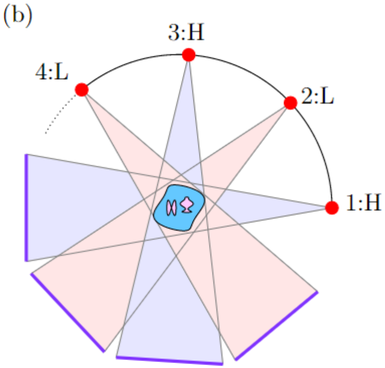
The system can be reduced to the **Normal equations**

$$A(Q+\Theta^{-1})^{-1}A^T\Delta y \;=\; r_P + A(Q+\Theta^{-1})^{-1}(r_D - X^{-1}r_\mu)$$

where $\Theta = XS^{-1}$, and solved using a factorization or the PCG.

Tomographic imaging





Tomographic imaging

Problem formulation

$$\min_{x\geq 0} \quad \underbrace{\|m - \mathcal{G}x\|^2}_{\substack{\text{Cost}\\ \text{function}}} \quad + \quad \underbrace{\alpha\|x\|^2}_{\substack{\text{Tikhonov}\\ \text{regularizer}}} \quad + \quad \underbrace{2\beta\, x_1^T x_2}_{\substack{\text{Inner product}\\ \text{regularizer}}}$$

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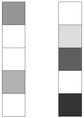

Tomographic imaging

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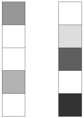


$$\Downarrow$$

QP formulation

$$\min_{x\geq 0} \ \frac{1}{2}x^T\mathcal{Q}x - m^T\mathcal{G}x, \tag{1}$$

where

$$\mathcal{Q} = \begin{bmatrix} c_{11}^2 + c_{21}^2 & c_{11}c_{12} + c_{21}c_{22} \\ c_{11}c_{12} + c_{21}c_{22} & c_{12}^2 + c_{22}^2 \end{bmatrix} \otimes R^TR + \begin{bmatrix} \alpha & \beta \\ \beta & \alpha \end{bmatrix} \otimes I,$$

$c_{11}, c_{12}, c_{21}, c_{22} > 0$, $\alpha > \beta > 0$.

R is accessed through matrix-vector products performed using the **Radon transform**.

IPM formulation

Lemma

If $\alpha \geq \beta$, problem (1) is convex.

Applying an IPM to this problem, we need to solve:

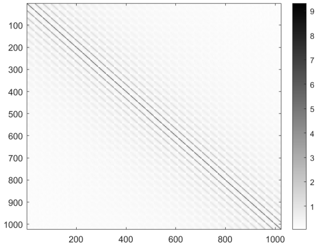
$$(\mathcal{Q} + X^{-1}S)\Delta\mathbf{x} = \mathbf{f}$$

This can be done using the Preconditioned Conjugate Gradient (PCG).

Gondzio, Lassas, Latva-Aijo, Siltanen, Z. *Material-separating regularizer for multi-energy X-ray tomography*. Inverse Problems, 38 (2022)

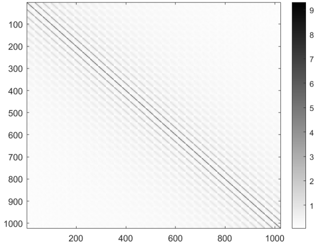
Preconditioner

$$\mathcal{Q} + X^{-1}S \quad = \quad \begin{bmatrix} c_{11}^2 + c_{21}^2 & c_{11}c_{12} + c_{21}c_{22} \\ c_{11}c_{12} + c_{21}c_{22} & c_{12}^2 + c_{22}^2 \end{bmatrix} \otimes \underbrace{R^T R} + \begin{bmatrix} \alpha & \beta \\ \beta & \alpha \end{bmatrix} \otimes I + X^{-1}S$$



Preconditioner

$$\mathcal{Q} + X^{-1}S = \begin{bmatrix} c_{11}^2 + c_{21}^2 & c_{11}c_{12} + c_{21}c_{22} \\ c_{11}c_{12} + c_{21}c_{22} & c_{12}^2 + c_{22}^2 \end{bmatrix} \otimes \underbrace{R^T R} + \begin{bmatrix} \alpha & \beta \\ \beta & \alpha \end{bmatrix} \otimes I + X^{-1}S$$



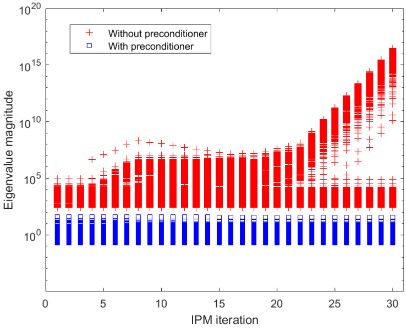
$$\mathcal{P} = \begin{bmatrix} c_{11}^2 + c_{21}^2 & c_{11}c_{12} + c_{21}c_{22} \\ c_{11}c_{12} + c_{21}c_{22} & c_{12}^2 + c_{22}^2 \end{bmatrix} \otimes \underbrace{\rho I} + \begin{bmatrix} \alpha & \beta \\ \beta & \alpha \end{bmatrix} \otimes I + X^{-1}S$$

Preconditioned matrix

Lemma

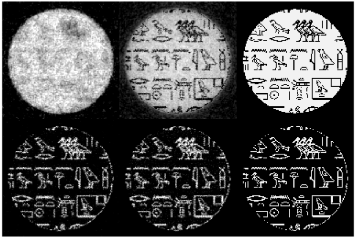
The eigenvalues of the preconditioned matrix $\mathcal{P}^{-1}(\mathcal{Q}+X^{-1}S)$ are independent of the IPM iteration and satisfy

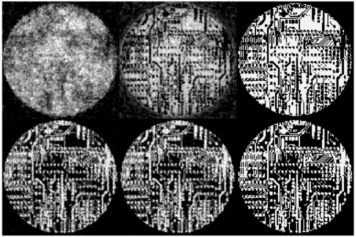
$$\lambda \in \left[\frac{\alpha-\beta}{\rho\Lambda_F+\alpha+\beta}, \frac{\sigma^2_{max}(R)\Lambda_F+\alpha+\beta}{\rho\lambda_F+\alpha-\beta}\right]$$



Results

JTV **IP** **Ground truth**





Discrete optimal transport

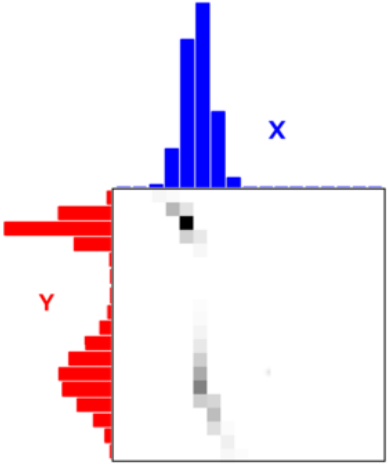


Image from en.wikipedia.org/wiki/Transportation_theory_(mathematics)

Problem formulation

Optimal transport formulation

$$\min_{\substack{\mathcal{P}\in\mathbb{R}_+^{m\times m}\\ \mathcal{P}\mathbf{e}_m=\mathbf{a},\ \mathcal{P}^T\mathbf{e}_m=\mathbf{b}}} \sum_{i,j} \mathcal{C}_{ij}\mathcal{P}_{ij}$$

Problem formulation

Optimal transport formulation

$$\min_{\substack{\mathcal{P}\in\mathbb{R}_+^{m\times m}\\ \mathcal{P}\mathbf{e}_m=\mathbf{a},\ \mathcal{P}^T\mathbf{e}_m=\mathbf{b}}} \quad \sum_{i,j} \mathcal{C}_{ij}\mathcal{P}_{ij}$$

$$\Downarrow$$

Kantorovich Linear Program

$$\begin{aligned} \min_{\mathbf{p}\in\mathbb{R}^{m^2}} \quad & \mathbf{c}^T\mathbf{p} \\ \text{s.t.} \quad & \begin{bmatrix} \mathbf{e}_m^T \otimes I_m \\ I_m \otimes \mathbf{e}_m^T \end{bmatrix} \mathbf{p} = \begin{bmatrix} \mathbf{a} \\ \mathbf{b} \end{bmatrix} = \mathbf{f} \\ & \mathbf{p} \geq 0 \end{aligned}$$

IPM formulation - 1

Highly structured constraint matrix

$$\begin{bmatrix}
1 & & & & & 1 & & & & & 1 & & & & & \\
 & 1 & & & & & 1 & & & & & 1 & & & & \dots \\
 & & 1 & & & & & 1 & & & & & 1 & & & \\
 & & & 1 & & & & & 1 & & & & & 1 & & \\
 & & & & \ddots & & & & & \ddots & & & & & \ddots & \\
1 & 1 & 1 & 1 & \dots & & & & & & & & & & & \\
 & & & & & 1 & 1 & 1 & 1 & \dots & & & & & & \dots \\
 & & & & & & & & & & 1 & 1 & 1 & 1 & \dots & \\
 & & & & & & & & \vdots & & & & & & &
\end{bmatrix}.$$

- $2m$ rows
- m^2 columns

IPM formulation - 2

Solved with a sparse mixed IPM-Column Generation approach:

- Keeps the iterates as **sparse** as possible
- Exploits **second order** method convergence

Linear system solved using the Schur complement of the normal equations:

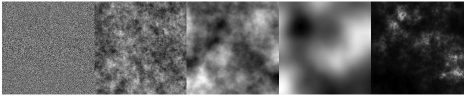
- PCG with **incompete Cholesky** factorization in the early stage
- Full LDL^T **factorization** in the late IPM iterations

Highly optimized **matrix-free sparse implementation**

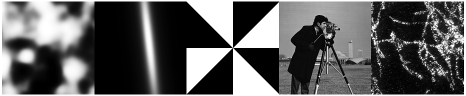
A full IPM would involve a **dense** Schur complement and very **large** and dense vectors

Test problems

DOTmark collection



Class 1 Class 2 Class 3 Class 4 Class 5



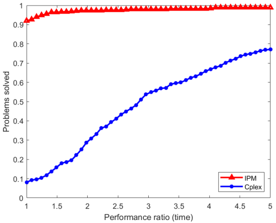
Class 6 Class 7 Class 8 Class 9 Class 10

res	Constraints	Variables ($\times 10^6$)
32	2,048	1.0
64	8,192	16.8
128	32,768	268.4
256	131,072	4,295.0

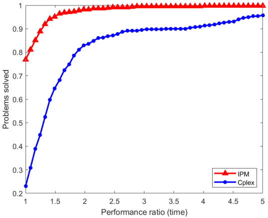
Cost functions: $1-$norm, $2-$norm, $\infty-$norm.

Results

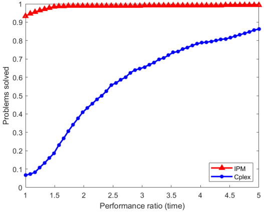
Comparison of **SparseIPM** and IBM ILOG Cplex **network simplex** solver



1−dist, 64 × 64



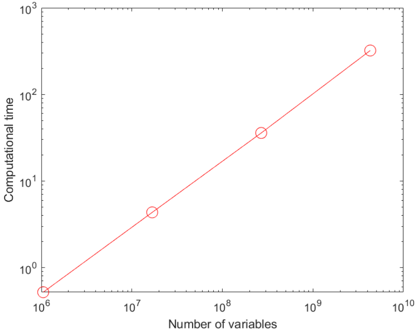
2−dist, 64 × 64



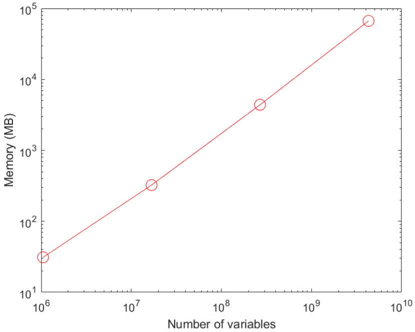
∞−dist, 64 × 64

Large instances results

Scalable results up to **4 Billion** variables (DOTmark class 1 problems)



Time



Memory

Thanks for the attention