Generalized distances for practical optimization methods

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Part one - generalized distances

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$$= \mathbf{prox}_{\alpha g}(x_k - \alpha \nabla f(x_k))$$

Model based optimization

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- why use the Euclidean norm to define proximity?

Generalized distance functions

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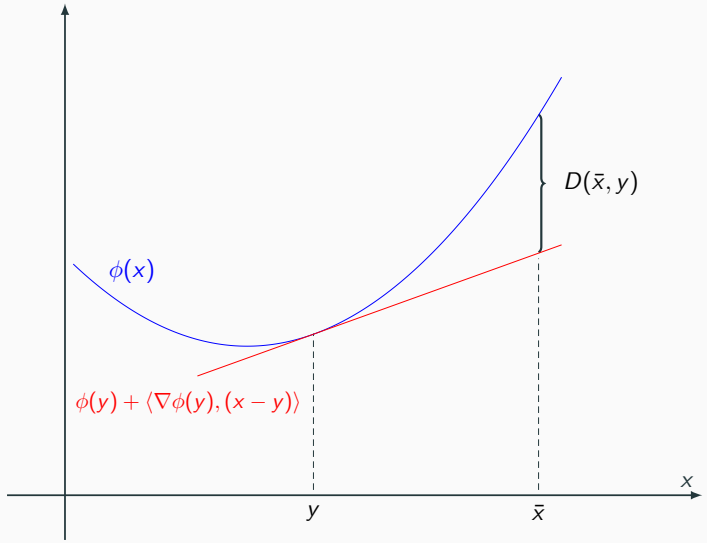
Why would we use a generalized distance?

1. Stronger convergence results for very specific problems.
2. Cheaper iterations (a proximal operator based on a Bregman divergence can be cheaper to evaluate than the standard prox).

Bregman divergences

$$D(x, y) = \phi(x) - \phi(y) - \langle \nabla\phi(y), x - y \rangle$$

- a Bregman divergence is defined through a *kernel* ϕ
- the kernel is convex and differentiable (other mathematical properties are required)



The most well-known textbook example

$$\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in \Delta \end{array}$$

- feasible set $\Delta = \{x \in \mathbf{R}^n \mid 1^T x = 1,\ x \geq 0\}$
- access to a subgradient oracle giving $g_k \in \partial f(x_k)$

The most well-known textbook example

- Choosing the *entropy* kernel $\phi(x) = \sum_{i=1}^{n} x_i \log x_i$ gives us *mirror descent*:

$$x_{k+1} = \operatorname*{argmin}_{x \in \Delta} \left(f(x_k) + \langle g_k, x - x_k \rangle + (1/\alpha) D_\phi(x, x_k) \right)$$

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- Projected subgradient method:

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- MD update can be worked out analytically, Euclidean projection can be done in $\mathcal{O}(n \log n)$ (requires a sort).

Why do theoretical optimizers love this example?

Assume known bounds on the size of subgradients: for all $x \in \Delta$,

$$\|g\|_\infty \leq G_\infty, \qquad \|g\|_2 \leq G_2, \qquad \forall g \in \partial f(x).$$

- MD with "optimal" constant step size:

$$f_{\text{best}}^k - f^\star \leq G_\infty \sqrt{\frac{2 \log n}{k}}$$

- PSM with "optimal" constant step size:

$$f_{\text{best}}^k - f^\star \leq G_2 \sqrt{\frac{1}{k}}$$

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- $\underbrace{f_{\text{best}}^k - f^\star \leq G_\infty \sqrt{\frac{2\log n}{k}}}_{\text{mirror descent}}, \qquad \underbrace{f_{\text{best}}^k - f^\star \leq G_2 \sqrt{\frac{1}{k}}}_{\text{projected subgradient method}}$

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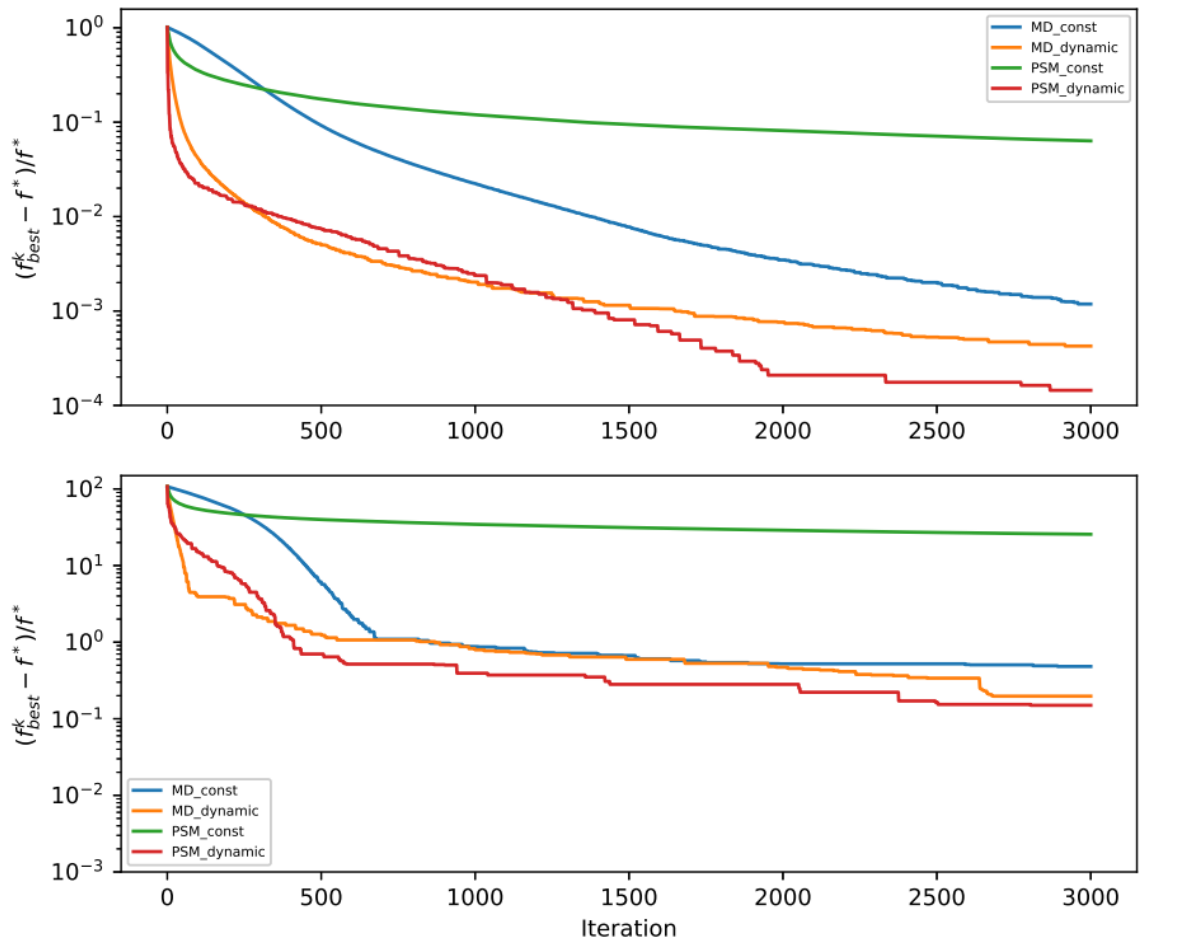
why they love MD!

Mirror descent in practice (example one)

$$\begin{array}{ll} \text{minimize} & f(x) = \|Ax - b\|_1 \\ \text{subject to} & x \in \Delta \end{array}$$

- called robust regression over the simplex

Mirror descent in practice (example one)



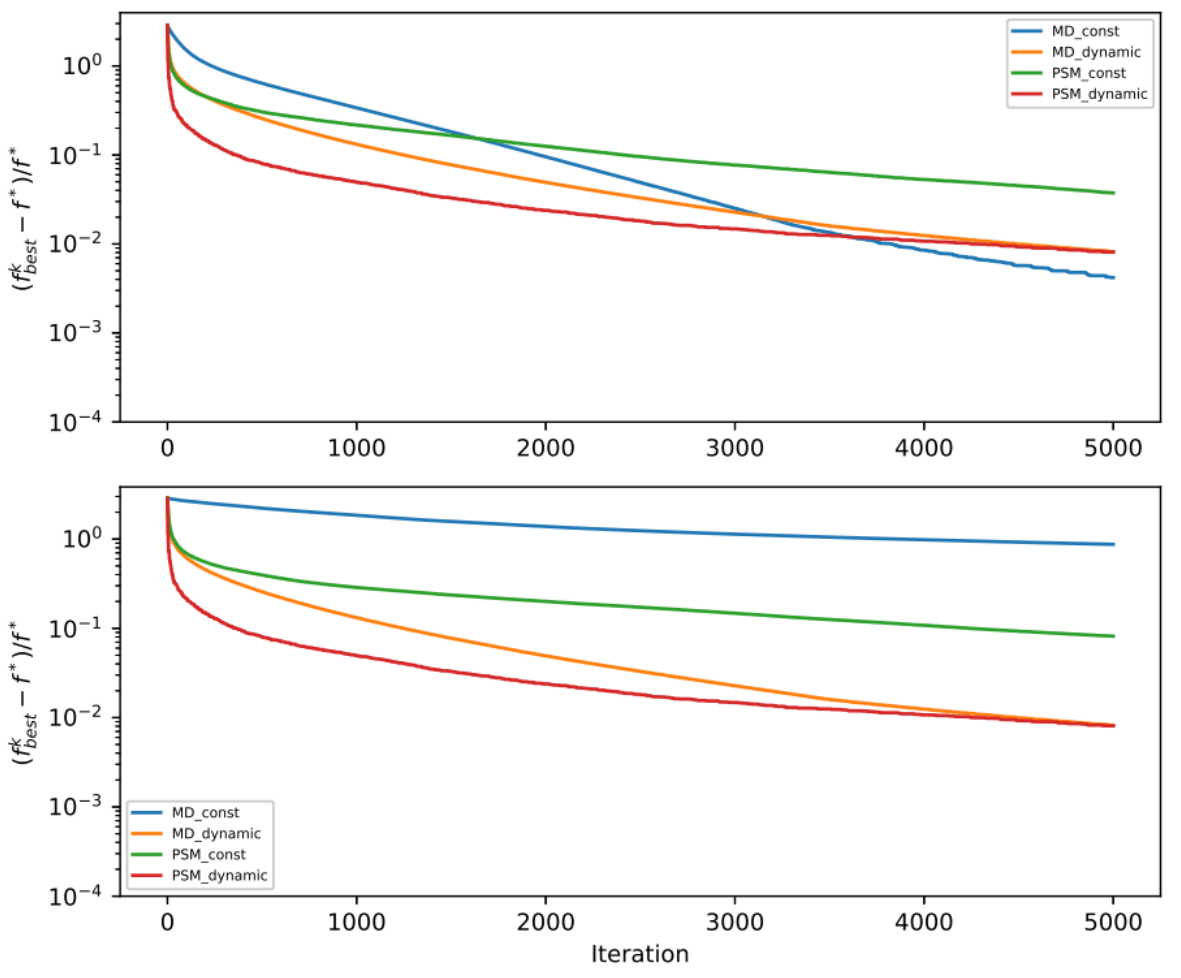
- data generated in two different ways

Mirror descent in practice (example two)

$$\begin{array}{ll} \text{minimize} & c^T x \\ \text{subject to} & Ax \leq b,\ x \geq 0 \end{array}$$

- entries of c, A and b are nonnegative
- called positive linear programming
- can be formulated as a minimization problem over the simplex

Mirror descent in practice (example two)



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- maybe not...
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- adaptive step sizes is what matters!
- disclaimer: I have only talked about *numerically* solving problems

Some important references on generalized distances

1. Three landmark papers: Bregman (1967), Nemirovski & Yudin (1983), Beck & Teboulle (2003)
2. A textbook dedicated to the topic: Censor & Zenios (1997)
3. More recent framework of relative smoothness: Bauschke, Bolte & Teboulle (2016) and Lu, Freund & Nesterov (2016)

Outline

1. Part one: generalized distances. ✓
2. Part two: trigonometric matrix polynomials and semidefinite programming.
3. Part three: new first-order methods

Part two - trigonometric matrix polynomials and semidefinite programming

Trigonometric matrix polynomials

- A *trigonometric matrix polynomial* of degree p is a function $F_{\mathcal{X}} : \mathbf{C} \to \mathbf{C}^{m\times m}$ of the form

$$F_{\mathcal{X}}(z) = X_0 + \sum_{k=1}^{p}(X_k z^k + X_k^T z^{-k})$$

- The matrices $X_0 \in \mathbf{S}^m$ and $X_k \in \mathbf{R}^{m\times m}$, $1 \leq k \leq p$ are called the *coefficients*
- $\mathcal{X} = (X_0, X_1, \ldots, X_p)$

Trigonometric matrix polynomials, crash course

- a zero-mean random *vector* $x \in \mathbf{R}^n$ has a *covariance matrix* $\Sigma = E[xx^T]$.
- a zero-mean random *time series* $\{x(t) \in \mathbf{R}^m,\ t \in \mathbf{Z}\}$ has a *spectral density matrix* $f : \mathbf{R} \to \mathbf{C}^{m\times m}$ given by

$$f(\omega) = \sum_{k=-\infty}^{\infty} R_k e^{-jk\omega},$$

where $j = \sqrt{-1}$. (Here $R_k = \mathrm{E}[x(t+k)x(t)^T]$, $k \geq 0$ are the *autocorrelation coefficients*.)

Trigonometric matrix polynomials, crash course

Roughly speaking, the power spectrum of a time series is analogous to the covariance matrix of a random vector:

- Nonnegativity:
  a) covariance matrix $\Sigma \succeq 0$
  b) spectral density matrix $f(\omega) \succeq 0$ for all $\omega \in \mathbf{R}$
- Graphical models:
  a) sparsity pattern of Σ^{-1} related to conditional independence
  b) sparsity pattern of $f(\omega)^{-1}$ related to conditional independence

SDP parameterization & complexity

$$X_0 + \sum_{k=1}^{p} (X_k z^k + X_k^T z^{-k}) \succeq 0, \qquad \forall z \in \mathbf{C} : |z| = 1.$$

The matrices $X_k,\ k = 0, \ldots, p$ have dimension $m \times m$.

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- **Example:**

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Solve time	1 sec	12 days

Outline

1. Part one - generalized distances ✓
2. Part two - trigonometric matrix polynomials and semidefinite programming ✓
3. Part three - Bregman first-order methods

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Cone of nonnegative trigonometric matrix polynomials

- constraint $F_{\mathcal{X}}(z) \succeq 0, \forall z \in \mathbf{C} : |z| = 1$ where

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- problems of the form

$$\begin{array}{ll} \text{minimize} & f(\mathcal{X}) \\ \text{subject to} & \mathcal{X} \in K \end{array}$$

A Bregman proximal operator

- For some $a > 0$, define g as

$$g(\mathcal{X}) = \begin{cases} 0 & \text{if } \mathcal{X} \in K,\ \mathbf{Tr}(X_0) = a \\ \infty & \text{otherwise.} \end{cases}$$

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- Bregman proximal operator

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- with a clever choice of the kernel the Bregman proximal operator can be evaluated efficiently

A Bregman proximal operator

- **Kernel** (entropy function):

$$\phi(\mathcal{X}) = -\frac{1}{2\pi}\int_0^{2\pi} \textbf{log det } F_{\mathcal{X}}(e^{j\omega})d\omega$$

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- **Kernel** (entropy function):

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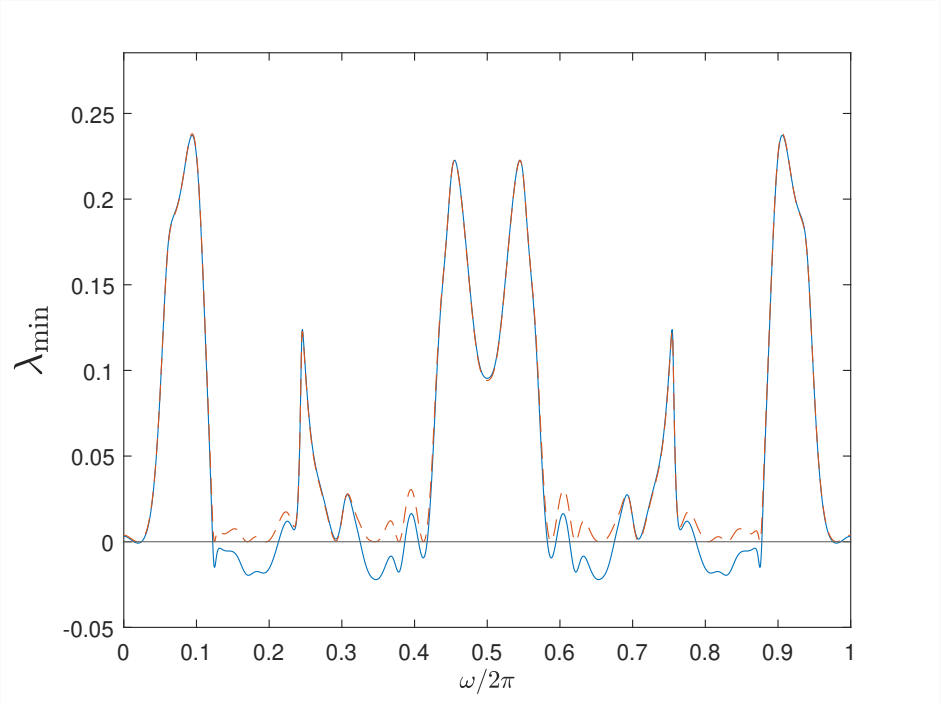
- we design an efficient method for evaluating $\textbf{prox}_g^{\phi}(\mathcal{V}, \mathcal{A})$:
  1. Main cost is solving positive definite block Toeplitz linear systems.
  2. Complexity is $\mathcal{O}(m^3p^2)$ per iteration.

Application one: nonnegative spectral estimation

$$\begin{array}{ll} \text{minimize} & \|\mathcal{X} - \hat{\mathcal{R}}^T\|^2 \\ \text{subject to} & \mathcal{X} \in K,\ \mathrm{Tr}(X_0) = \mathrm{Tr}(\hat{R}_0) \end{array}$$

- problem data $\hat{\mathcal{R}} = (\hat{R}_0, \ldots, \hat{R}_p)$ corresponds to a *power spectrum* that fails to be nonnegative



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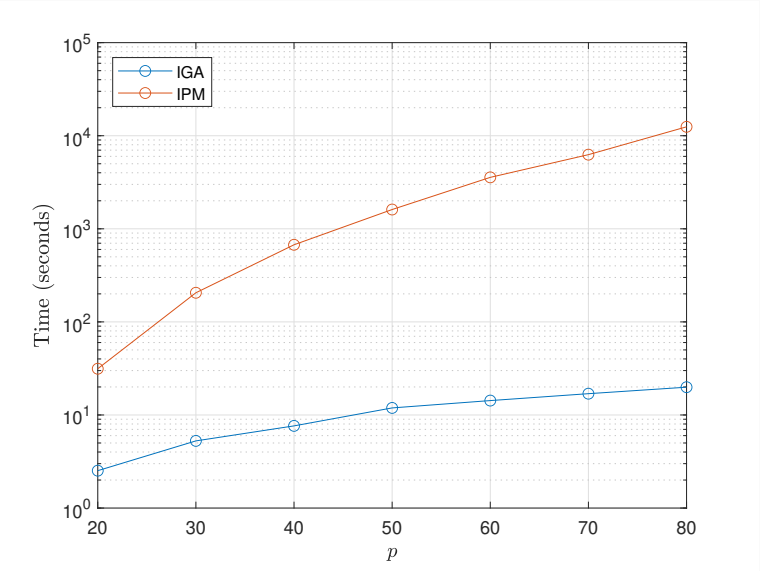
- Improved gradient algorithm:

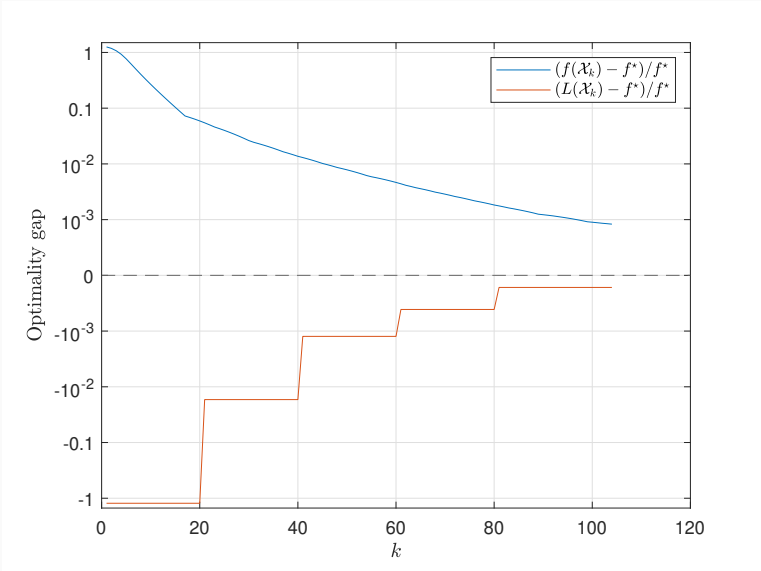
$$\begin{aligned}
\mathcal{Y}_{k+1} &= \mathcal{X}_k + \theta_k(\mathcal{V}_k - \mathcal{X}_k) \\
\mathcal{V}_{k+1} &= \mathbf{prox}^{\phi}_{\tau_k g}(\mathcal{V}_k, \tau_k \nabla f(\mathcal{Y}_{k+1})) \\
\mathcal{X}_{k+1} &= \mathcal{X}_k + \theta_k(\mathcal{V}_{k+1} - \mathcal{X}_k)
\end{aligned}$$

  a) an accelerated proximal gradient method that allows for a Bregman proximal operator
  b) main cost in each iteration is to evaluate the Bregman proximal operator

Numerical results



(a)



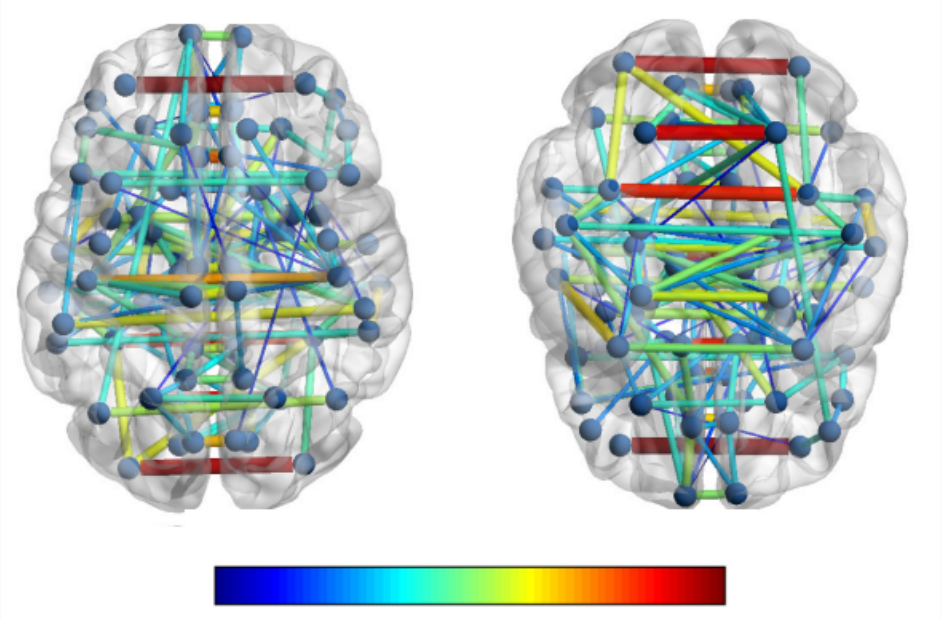
(b)

Application two: graphical models

- sparsity pattern of $f(\omega)^{-1}$ determines a *conditional independence graph*
- for Gaussian time series: $\{x_i(t), t \in \mathrm{Z}\}$ and $\{x_j(t), t \in \mathrm{Z}\}$ are conditionally independent, given $\{x_k(t), t \in \mathrm{Z}\}$ for $k \neq i, j, \iff (f(\omega)^{-1})_{ij} = 0.$
- encouraging sparsity when estimating $f(\omega)^{-1}$ makes sense

Example: functional connectivity analysis

A conditional independence graph visualized:



Problem formulation

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|\mathcal{X} - \hat{\mathcal{Y}}^T\|^2 + \gamma r(\mathcal{X}) \\ \text{subject to} & \mathcal{X} \in K,\ \mathbf{Tr}(X_0) = \mathbf{Tr}(\hat{Y}_0) \end{array}$$

- problem data $\hat{\mathcal{Y}} = (\hat{Y}_0, \ldots, \hat{Y}_p)$ corresponds to a *measured* inverse power spectrum
- the variable $\mathcal{X}$ represents a *sparsified* inverse power spectrum

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- the variable $\mathcal{X}$ represents a *sparsified* inverse power spectrum
- the regularizer r encourages a common sparsity pattern

Problem formulation

$$\begin{array}{ll} \text{minimize} & \frac{1}{2}\|\mathcal{X} - \hat{\mathcal{Y}}^T\|^2 + \gamma r(\mathcal{X}) \\ \text{subject to} & \mathcal{X} \in K,\ \mathbf{Tr}(X_0) = \mathbf{Tr}(\hat{Y}_0) \end{array}$$

- problem data $\hat{\mathcal{Y}} = (\hat{Y}_0, \ldots, \hat{Y}_p)$ corresponds to a *measured* inverse power spectrum
- the variable $\mathcal{X}$ represents a *sparsified* inverse power spectrum
- the regularizer r encourages a common sparsity pattern
- write as

$$\text{minimize } f(\mathcal{X}) + g(\mathcal{X})$$

where $g(\mathcal{X}) = \frac{1}{2}\|\mathcal{X} - \hat{\mathcal{R}}^T\|^2 + \gamma r(\mathcal{X})$ and

$$f(\mathcal{X}) = \begin{cases} 0 & \text{if } \mathcal{X} \in K,\ \mathbf{Tr}(X_0) = \mathbf{Tr}(R_0) \\ \infty & \text{otherwise,} \end{cases}.$$

Algorithm

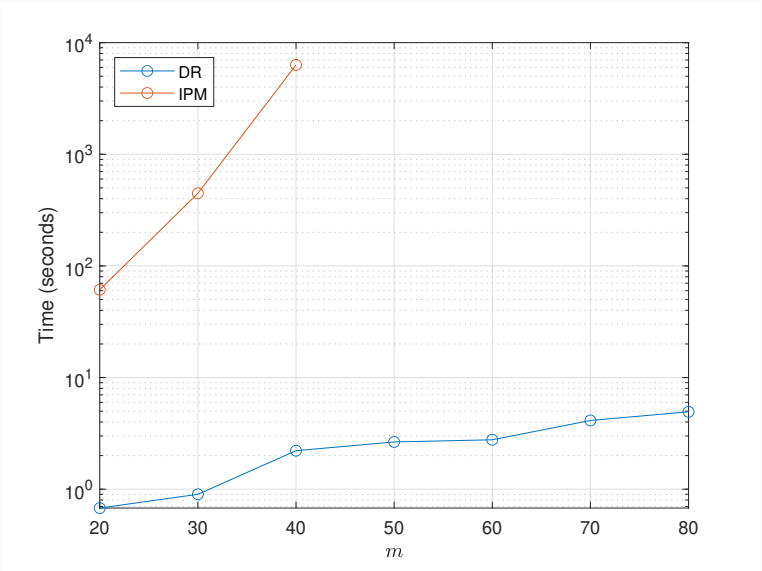
$$\text{minimize } f(\mathcal{X}) + g(\mathcal{X})$$

Bregman Douglas–Rachford:

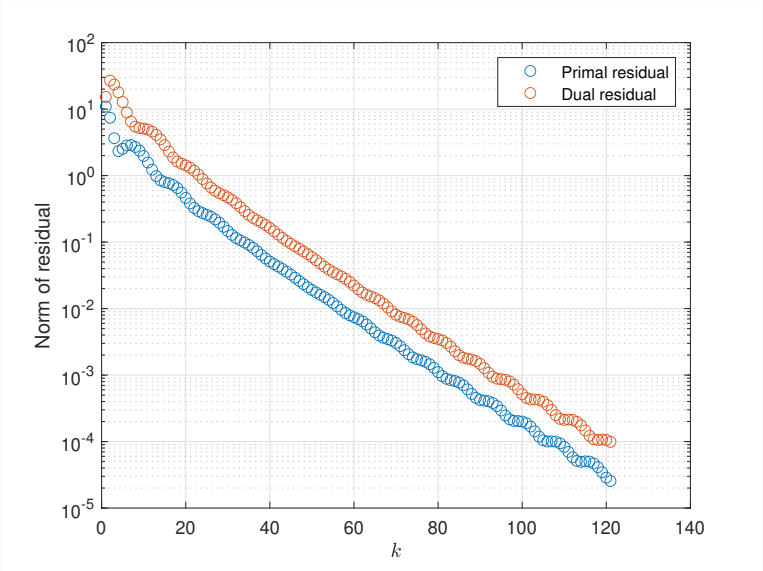
$$\mathcal{Y}_{k+1} = \mathbf{prox}_{\sigma g^*}(\mathcal{Y}_k + \sigma(2\mathcal{X}_k - \mathcal{X}_{k-1}))$$
$$\mathcal{X}_{k+1} = \mathbf{prox}^{\phi}_{\tau f}(\mathcal{X}_k, \tau\mathcal{Y}_{k+1})$$

Super simple algorithm!

Numerical results



(c)



(d)

Outline

1. Part one - generalized distances ✓
2. Part two - trigonometric matrix polynomials and semidefinite programming ✓
3. Part three - Bregman first-order methods ✓

Summary

- most work on generalized distances is theoretical
- useful in practice only for very specific problems
- when they apply they can be really fast

Thanks! Questions?