A derivative-free algorithm resilient to straggler function evaluations

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Based on joint works with W. Hare, G. Jarry-Bolduc, S. Kerleau

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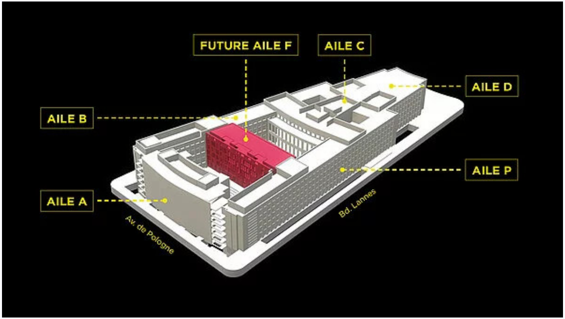
Motivation: Dauphine's *Nouveau Campus*



- New wing in construction ⇒ 2024.
- Others renovated in order: B, P, C+D, A.
- Expected year of completion: 2027.

Our task: Allocate office space during the renovation process.

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Our model for the Dauphine problem

- Huge integer LP, solved via Gurobi.
- ~ 20 hyperparameters defining the model.
- Parallel runs on the department server.

Sub-task: Optimize hyperparameters.

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- Cannot differentiate (easily) within Gurobi
  $\Rightarrow$ Derivative-free algorithms!
- Solving time depends on hyperparameters (3-48 hours for a feasible point!)
  $\Rightarrow$ Limited benefits of parallelism.

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Can we cook up an algorithm adapted to this setting?

Outline

1. Formal problem and algorithm
2. Building and using PkSS
3. Conclusion

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$$\text{minimize}_{x \in \mathbb{R}^n} f(x).$$

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- **Parallel evaluations of f allowed**.
- Evaluations can take unusually long⇒**Stragglers**.

A (simplified) direct-search framework

Inputs: $x_0 \in \mathbb{R}^n$, $\alpha_0 > 0$.

Iteration i**:** Given (x_i, α_i),

- Choose a set $\mathcal{D}_i \subset \mathbb{R}^n$ of m (nonzero) vectors.
- If $\exists\ d_i \in \mathcal{D}_i$ such that

$$f(x_i + \alpha_i\, d_i) < f(x_i) - \alpha_i^2 \|d_i\|^2$$

  set $x_{i+1} := x_i + \alpha_i d_i$, $\alpha_{i+1} := 2\alpha_i$.
- Otherwise, set $x_{i+1} := x_i$, $\alpha_{i+1} := \alpha_i/2$.

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- **Key**: Choice of $\mathcal{D}_i$.
- **Parallel version**: Works as long as all directions in $\mathcal{D}_i$ have been polled when $x_{i+1} = x_i$.

Classical direct-search theory

Usual tool: Positive spanning sets (PSS)

- $\mathcal{D} \subset \mathbb{R}^n$ PSS if it spans $\mathbb{R}^n$ by nonnegative linear combinations
  $\Rightarrow \; |\mathcal{D}| \geq n + 1$.

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  $\Rightarrow \ n+1 \leq |\mathcal{D}| \leq 2n$.

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Cosine measure

- For any $\mathcal{D} \subset \mathbb{R}^n$, the cosine measure of $\mathcal{D}$ is

$$\mathrm{cm}(\mathcal{D}) := \min_{v \neq 0} \max_{d \in \mathcal{D}} \frac{v^{\mathrm{T}} d}{\|v\| \|d\|}.$$

- $\mathcal{D}$ PSS $\Longleftrightarrow \mathrm{cm}(\mathcal{D}) > 0$.

Classical direct-search theory ('ed)

Theorem: Complexity of direct search

Apply direct search with $\mathcal{D}_i = \mathcal{D}\ \forall i$, $\mathcal{D}$ PSS. Then the method satisfies

$$\min_{0 \leq i \leq J} \|\nabla f(x_i)\| \leq \epsilon$$

in at most

$$J = \mathcal{O}\left(|\mathcal{D}|\, \mathrm{cm}(\mathcal{D})^{-2} \epsilon^{-2}\right)$$

function evaluations.

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Typical values

- $|\mathcal{D}| = \mathcal{O}(n)$.
- $\mathrm{cm}(\mathcal{D}) = \mathcal{O}(n^a)$, $a \in \{-0.5, -1\}$.

Direct search and stragglers

Inputs: $x_0 \in \mathbb{R}^n$, $\alpha_0 > 0$.
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- Choose a set $\mathcal{D}_i \subset \mathbb{R}^n$ of m (nonzero) vectors.
- If $\exists\ d_i \in \mathcal{D}_i \setminus \mathcal{S}_i$ such that

$$f(x_i + \alpha_i\, d_i) < f(x_i) - \alpha_i^2 \|d_i\|^2$$

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Straggler model: At every iteration i,

- $\exists \mathcal{S}_i \subset \mathcal{D}_i$ of **straggler directions** (f much longer to evaluate).
- $\mathcal{S}_i$ unknown before evaluations launched!
- Evaluations in $\mathcal{S}_i$ cannot be used in analyzing the method.

A new PSS property

Positive k-spanning sets (PkSS), $k \geq 1$

- $\mathcal{D} \subset \mathbb{R}^n$ PkSS if any $\mathcal{N} \subset \mathcal{D}$ with $|\mathcal{N}| = |\mathcal{D}| - k + 1$ is a PSS.

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- $\mathcal{D}$ positive k-basis if no proper subset of $\mathcal{D}$ is a PkSS.

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- Definition inherited from D. A. Marcus ('81, '84).
- $k = 1$: PSS/Positive basis.
- $\mathcal{D}$ PkSS $\Rightarrow$ $|\mathcal{D}| \geq \max\{k, n + 2k - 1\}$.

The k-cosine measure

- For any $\mathcal{D} \subset \mathbb{R}^n$, the k-cosine measure of $\mathcal{D}$ is

$$\mathrm{cm}_k(\mathcal{D}) := \min_{v \neq 0} \max_{\substack{\mathcal{N} \subset \mathcal{D} \\ |\mathcal{N}| = k}} \max_{d \in \mathcal{N}} \frac{v^\mathrm{T} d}{\|v\| \|d\|}.$$

- $\mathcal{D}$ PkSS $\Longleftrightarrow$ $\mathrm{cm}_k(\mathcal{D}) > 0$.

A new cosine measure (Hare, Jarry-Bolduc, Kerleau, R. '24)

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Properties

- Equivalent definition:

$$\mathrm{cm}_k(\mathcal{D}) = \min_{\substack{\mathcal{N} \subset \mathcal{D} \\ |\mathcal{N}|=|\mathcal{D}|-k+1}} \mathrm{cm}(\mathcal{N}).$$

- For any $\mathcal{D}$ (not necessarily PkSS !),

$$\mathrm{cm}(\mathcal{D}) \geq \cdots \geq \mathrm{cm}_{|\mathcal{D}|-1}(\mathcal{D}) \geq \mathrm{cm}_{|\mathcal{D}|}(\mathcal{D}).$$

Complexity of direct search

Theorem

- Apply direct search with $\mathcal{D}_i = \mathcal{D}\ \forall i$, $\mathcal{D}$ PkSS.
- Suppose less than k stragglers per iteration: $|\mathcal{S}_i| \le k-1\ \forall i$.

Then the method satisfies

$$\min_{0 \le i \le J} \|\nabla f(x_i)\| \le \epsilon$$

in at most

$$J = \mathcal{O}\left(|\mathcal{D}|\, \mathrm{cm}_k(\mathcal{D})^{-2} \epsilon^{-2}\right)$$

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Typical values?

- $|\mathcal{D}| \ge \mathcal{O}(n+k)$.
- $\mathrm{cm}_k(\mathcal{D}) = \mathcal{O}(?)$.

Outline

Produce PkSS in practice (1/2)

Our baseline: Maximal (coordinate) positive basis

- $\mathcal{D}_\oplus := \{e_1, \dots, e_n, -e_1, \dots, -e_n\}$, with $\{e_l\}_l$ coordinate basis vectors.
- $\beta\mathcal{D}_\oplus$: multiply all vectors by real β.

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First proposal: Duplicate vectors

Let $\beta_1, \dots, \beta_k$ be k distinct positive real numbers. The set

$$\mathcal{D}_{\oplus}^{\beta_{1:k}} := \bigcup_{j=1}^{k} \beta_j \mathcal{D}_{\oplus}$$

is a PkSS with $\mathrm{cm}_k(\mathcal{D}_{\oplus}^{\beta_{1:k}}) = \mathrm{cm}(\mathcal{D}_{\oplus}) = \frac{1}{\sqrt{n}}$.

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- Easy construction, even yields a positive k-basis!
- Lacks diversity, redundancy if coupled with line search.

Produce PkSS in practice (2/2)

Our baseline: Minimal (coordinate) positive basis

- $\mathcal{D}_{n+1} := \{e_1, \dots, e_n, -\sum_{l=1}^{n} e_l\}$, with $\{e_l\}$ coordinate basis vectors.
- $R\mathcal{D}_{n+1}$: Apply **Rotation matrix** $R \in \mathbb{R}^{n \times n}$ to all vectors.

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Second proposal: Rotate vectors

Let $R_1, \dots, R_k$ be k distinct positive real numbers. The set

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is a PkSS with $\mathrm{cm}_k(\mathcal{D}_{n+1}^{R_{1:k}}) \geq \mathrm{cm}(\mathcal{D}_{n+1}) = \frac{1}{\sqrt{n^2+2(n-1)\sqrt{n}}}$.

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Includes:

- Positive k-bases/PkSS with duplicates.
- PkSS with no duplicates but not positive k-bases.
- Positive k-basis with no duplicates!

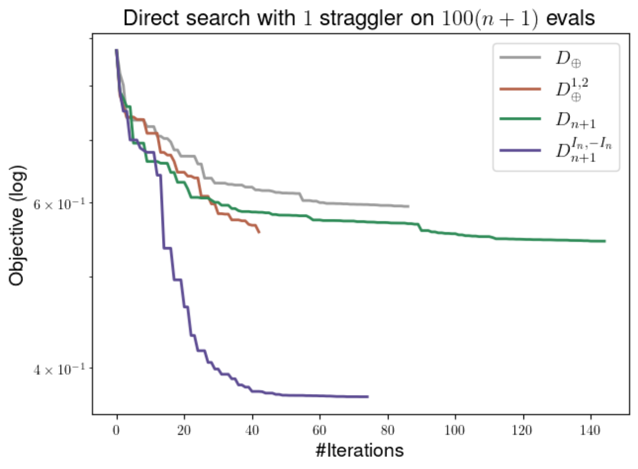
Robust linear regression (Carmon et al '17)

$$\underset{x\in\mathbb{R}^n}{\text{minimize}} \frac{1}{2n}\sum_{i=1}^{2n}\phi(a_i^{\mathrm{T}}x-b_i), \quad \phi(t)=\frac{t^2}{1+t^2}.$$

- a_i i.i.d Gaussian, $b_i = a_i^{\mathrm{T}}z + 3u_1 + u_2$, $\{z, u_1\}$ Gaussian, u_2 Bernoulli.

Comparison: Direct search with PSS/P2SS, one straggler/iteration.

$\mathcal{D}$	$\lvert\mathcal{D}\rvert$	$\text{cm}_?$
$\mathcal{D}_\oplus$	$2n$	$\text{cm} = \frac{1}{\sqrt{n}}$
$\mathcal{D}_\oplus^{1,2}$	$4n$	$\text{cm}_2 = \frac{1}{\sqrt{n}}$
$\mathcal{D}_{n+1}$	$n+1$	$\text{cm} = \frac{1}{\sqrt{n^2+2(n-1)\sqrt{n}}}$
$\mathcal{D}_{n+1}^{I_n,-I_n}$	$2n+2$	$\text{cm}_2 = \frac{1}{\sqrt{n^2+2(n-1)\sqrt{n}}}$.



- P2SSs can outperform PSSs with stragglers!
- On 100 runs, $\mathcal{D}_{n+1}^{I_n,-I_n}$ gives best results.

Summing up

DFO with stragglers

- Resilient notion of PSS.
- Convergent algorithm.
- Numerical proof of concept.

References

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  Working paper.

Opening for discussions

- About PkSS:
  - Upper bounds on the size of positive k-bases? (Nontrivial!)
  - Best PkSS in terms of ℓ-cosine measure?
  - Connections to strongly connected graphs and neighborly polytopes (!)

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Grazie mille!

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