Optimization without derivatives in larger dimensions and across networks

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What I intend to talk about...



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Optimization without derivatives, aka...

- Derivative-free optimization (DFO);
- Zeroth-order optimization;
- Black-box optimization;
- Simulation-based optimization;
- Hyperparameter tuning:
- Reinforcement learning?



Yann LeCun @ylecun · 9 févr.

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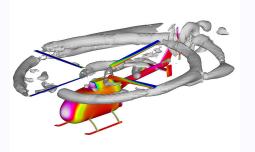
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What I really intend to talk about

- My line of work (1+2);
- Hopefully relevant to others.

Classical DFO problem: Rotor helicopter design (Booker et al. 1998)



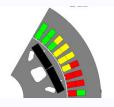
- About 30 parameters;
- 1 simulation: 2 weeks of computational fluid dynamics simulation;
- A simulation failed 60% of the time.

Ubiquitous in multidisciplinary optimization:

- Several codes interfaced;
- Numerical simulations;
- Large amount of calculation, possible failures.

Less classical example: Electrical engine design (D. Gaudrie, Stellantis)







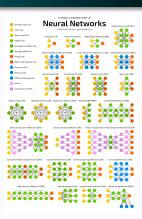


- About 50 continuous parameters;
- Multiobjective (3 functions), 6-dimensional constraint vector;
- Most points are infeasible!
- 1 simulation ≈ 5 minutes;
- Current practice: Run genetic algorithms for 3 weeks!

A modern challenge

Say you want to train a neural network...

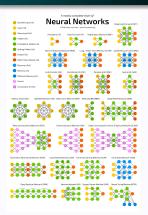
- What is your architecture? (Convolutional, Recurrent,etc)
- What is your training algorithm? (Adam, RMSProp, SG,etc)
- How do you choose your learning rate?



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Hyperparameter optimization

- Each change of hyperparameter involves another round of training (hours, days of CPU time + money!);
- Integer/Categorical/Continuous variables.

Goal: Reach automated ML!

Challenges for DFO

Scale up

- To millions of parameters? Maybe not...
- But a couple orders of magnitude may be helpful!
- ⇒ Dimensionality reduction.

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Be data-oriented

- Expensive calculations involving massive amounts of data...
- ...possibly distributed on several memory nodes.
- ⇒ Decentralized approaches.

Roadmap

- DFO and direct search
- 2 Direct search and reduced dimensions
- 3 Decentralizing direct search

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Outline

- DFO and direct search
 - Deterministic direct search
 - Direct search based on probabilistic descent
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Introductory assumptions and definitions

$$minimize_{\boldsymbol{x} \in \mathbb{R}^n} f(\boldsymbol{x}).$$

Assumptions

- f bounded below;
- *f* continuously differentiable (nonconvex).

Blackbox/Derivative-free setup

- Derivatives unavailable for algorithmic use.
- Only access to values of f or stochastic estimates.
- f depends on expensive simulations/procedures.

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Complexity in blackbox optimization

My goal as a derivative-free/blackbox optimizer

Develop algorithms with controlled

- Number of calls to f;
- Dependency on *n*.

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For this talk

Given $\epsilon \in (0,1)$ and, bound the number of function evaluations needed by a method to reach ${\it x}$ such that

$$\|\nabla f(\mathbf{x})\| \leq \epsilon$$

deterministically or in expectation/probability.

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Focus: dependency w.r.t. n.

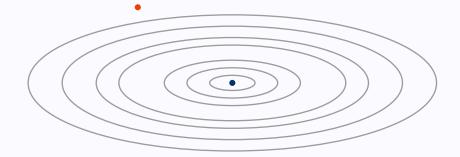
Two paradigms in derivative-free optimization

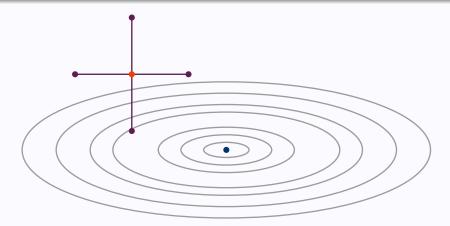
Model-based

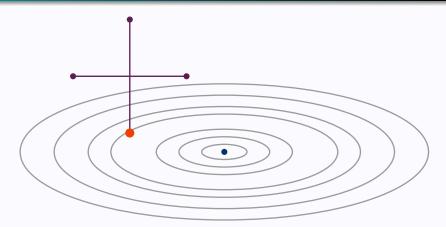
- Build a model of the objective;
- Response surface, surrogate modeling, etc.

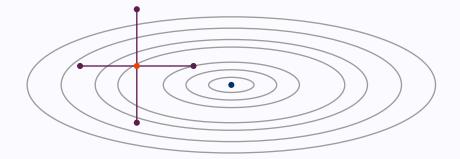
Direct search

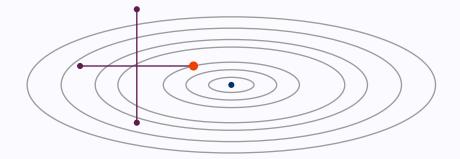
- Sample along appropriate directions;
- Zeroth-order, random search, etc.

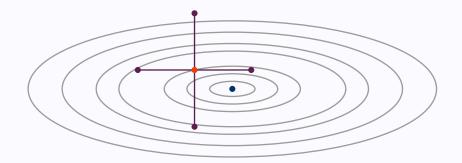


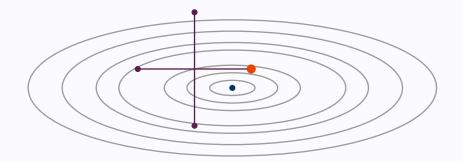


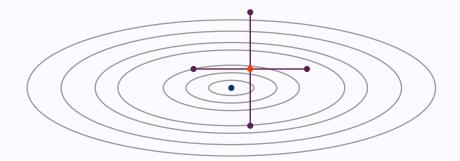


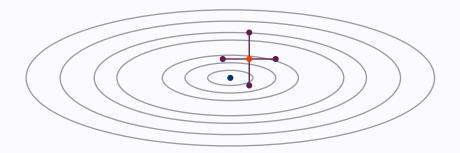


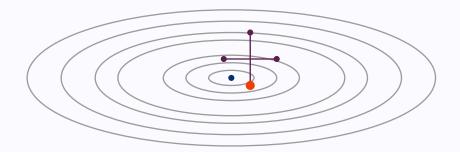












A simple direct-search framework

Inputs: $\mathbf{x}_0 \in \mathbb{R}^n \ 0 < \theta < 1 \le \gamma$, $\alpha_0 > 0$. Iteration k: Given (\mathbf{x}_k, α_k) ,

- Choose a set $\mathcal{D}_k \subset \mathbb{R}^n$ of m vectors.
- If $\exists \ \boldsymbol{d}_k \in \mathcal{D}_k$ such that

$$f(\mathbf{x}_k + \alpha_k \, \mathbf{d}_k) < f(\mathbf{x}_k) - \alpha_k^2 \|\mathbf{d}_k\|^2$$

set
$$\boldsymbol{x}_{k+1} := \boldsymbol{x}_k + \alpha_k \boldsymbol{d}_k$$
, $\alpha_{k+1} := \gamma \alpha_k$.

• Otherwise, set $\mathbf{x}_{k+1} := \mathbf{x}_k$, $\alpha_{k+1} := \theta \alpha_k$.

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Which vectors should we use?

Choosing \mathcal{D}_k

A measure of set quality

The set \mathcal{D}_k is called κ -descent for f at \mathbf{x}_k if

$$\max_{\boldsymbol{d} \in \mathcal{D}_k} \frac{-\boldsymbol{d}^{\mathrm{T}} \nabla f(\boldsymbol{x}_k)}{\|\boldsymbol{d}\| \|\nabla f(\boldsymbol{x}_k)\|} \ \geq \ \kappa \in (0,1].$$

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- Guaranteed when \mathcal{D}_k is a Positive Spanning Set (PSS);
- \mathcal{D}_k PSS $\Rightarrow |\mathcal{D}_k| \geq n+1$;
- Ex) $\mathcal{D}_{\oplus} := \{ \boldsymbol{e}_1, \dots, \boldsymbol{e}_n, -\boldsymbol{e}_1, \dots, -\boldsymbol{e}_n \}$ is always $\frac{1}{\sqrt{n}}$ -descent.

Key convergence arguments in direct search

Assumption: For every k, \mathcal{D}_k is κ -descent and contains m unit directions.

Small step size \Rightarrow Success

lf

$$\alpha_k < \mathcal{O}(\kappa \|\nabla f(\boldsymbol{x}_k)\|),$$

then $\mathbf{x}_{k+1} \neq \mathbf{x}_k$ and $\alpha_{k+1} \geq \alpha_k$.

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Step size goes to zero

Independently of the κ -descent property,

$$\exists \beta \in (0,\infty), \qquad \sum_{k=0}^{\infty} \alpha_k^2 < \beta < \infty \quad \left(\Rightarrow \lim_{k \to \infty} \alpha_k = 0 \right).$$

Worst-case complexity in deterministic direct search

Assumption: For every k, \mathcal{D}_k is κ -descent and contains m unit directions.

Theorem

Let $\epsilon \in (0,1)$ and N_{ϵ} be the number of function evaluations needed to reach \mathbf{x}_k such that $\|\nabla f(\mathbf{x}_k)\| \leq \epsilon$. Then,

$$N_{\epsilon} \leq \mathcal{O}\left(m \kappa^{-2} \epsilon^{-2}\right).$$

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- Unit norm can be replaced by bounded norm.
- Choosing $\mathcal{D}_k = \mathcal{D}_{\oplus}$, one has $\kappa = \frac{1}{\sqrt{n}}$, m = 2n, and the bound becomes

$$N_{\epsilon} \leq \mathcal{O}\left(n^2 \epsilon^{-2}\right).$$

• Optimal in the power of *n* for **deterministic** direct-search algorithms.

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A probabilistic property

Deterministic descent

The set \mathcal{D}_k is κ -descent for (f, \mathbf{x}_k) if

$$\max_{\boldsymbol{d} \in \mathcal{D}_k} \frac{-\nabla f(\boldsymbol{x}_k)^{\top} \boldsymbol{d}}{\|\nabla f(\boldsymbol{x}_k)\| \|\boldsymbol{d}\|} \ \geq \ \kappa \in (0,1].$$

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Probabilistic descent

The sequence $\{\mathcal{D}_k\}$ is said to be (p, κ) -descent if:

$$\mathbb{P}\left(\mathcal{D}_0 \; \kappa\text{-descent}\;\right) \; \geq \; p$$

$$\forall k \geq 1, \quad \mathbb{P}\left(\mathcal{D}_k \ \kappa\text{-descent} \ | \ \mathcal{D}_0, \dots, \mathcal{D}_{k-1}\right) \geq p,$$

Key arguments in probabilistic direct search (1/2)

Assumption: For every k, \mathcal{D}_k contains m unit directions.

Small step size \Rightarrow Success

If \mathcal{D}_k is κ -descent and

$$\alpha_{k} < \mathcal{O}(\kappa \|\nabla f(\mathbf{x}_{k})\|).$$

then $\mathbf{x}_{k+1} \neq \mathbf{x}_k$ and $\alpha_{k+1} \geq \alpha_k$.

Step size goes to zero

For all realizations of the method,

$$\sum_{k=0}^{\infty} \alpha_k^2 < \infty$$

Key arguments for probabilistic direct search (2/2)

A useful bound

Let $z_k = 1$ (\mathcal{D}_k κ -descent). For all realizations of the algorithm, one has

$$\sum_{\ell=0}^{k-1} z_{\ell} \leq \mathcal{O}\left(\frac{1}{\kappa^{2} \left(\min_{0 \leq \ell \leq k} \|\nabla f(\mathbf{x}_{\ell})\|\right)^{2}}\right) + \mathbf{p}_{0} k,$$

with $p_0 = \frac{1}{1+\mu}$, $\mu = \log_{\theta}(1/\gamma)$.

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with $p_0 = \frac{1}{1+\mu}$, $\mu = \log_{\theta}(1/\gamma)$.

- $\mathbb{P}(z_{\ell}=1|z_0,\ldots,z_{\ell-1})\geq p$ by assumption;
- $\{\sum_{\ell=0}^{k-1} z_{\ell}\}_{k}$ is a submartingale;
- As long as $p > p_0$, can relate the behavior of $\|\nabla f(\mathbf{x}_k)\|$ and that of $\sum_{\ell=0}^{k-1} z_{\ell}$.

Complexity results

Assumptions:

- $\{\mathcal{D}_k\}$ (p, κ) -descent, $p > p_0$.
- \mathcal{D}_k contains m unit vectors.

Probabilistic worst-case complexity (Gratton et al, '15)

Let $\epsilon \in (0,1)$ and N_{ϵ} the number of function evaluations needed to have $\|\nabla f(x_k)\| \leq \epsilon$. Then

$$\mathbb{P}\left(N_{\epsilon} \leq \mathcal{O}\left(\frac{m\,\kappa^{-2}\epsilon^{-2}}{p-p_0}\right)\right) \geq 1 - \exp\left(-\mathcal{O}\left(\frac{p-p_0}{p}(\kappa\,\epsilon)^{-2}\right)\right).$$

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Expected evaluation complexity

$$\mathbb{E}[N_{\epsilon}] \leq \mathcal{O}\left(\frac{m\kappa^{-2}\epsilon^{-2}}{p-p_0}\right) + \mathcal{O}(m).$$

A practical (p, κ) -descent sequence

Using 2 directions uniformly distributed over the unit sphere.

- Defines a $(p, \tau/\sqrt{n})$ -descent sequence, p > 1/2.
- Optimal (largest τ): Choose opposite directions!

A practical (p, κ) -descent sequence

Using 2 directions uniformly distributed over the unit sphere.

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Complexity bound

- Deterministic: $m = \mathcal{O}(n) \Rightarrow \mathcal{O}(n^2 \epsilon^{-2})$.
- Probabilistic $m = \mathcal{O}(1) \Rightarrow \mathcal{O}(n \epsilon^{-2})$.
- \Rightarrow Factor *n* improvement at the iteration level.

Not the only game in town

Gaussian smoothing approach: Draw $u_k \sim \mathcal{N}(0, I)$ and use

$$\frac{f(\mathbf{x} + \mu \mathbf{u}) - f(\mathbf{x})}{\mu} \mathbf{u}$$
 or $\frac{f(\mathbf{x} + \mu \mathbf{u}) - f(\mathbf{x} - \mu \mathbf{u})}{\mu} \mathbf{u}$.

Random gradient-free method (Nesterov and Spokoiny 2017), **Stochastic three-point method (Bergou et al, 2020)**.

 \Rightarrow Both achieve an $\mathcal{O}(n\epsilon^{-2})$ bound with predefined stepsizes.

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Random gradient-free method (Nesterov and Spokoiny 2017), Stochastic three-point method (Bergou et al, 2020).

- \Rightarrow Both achieve an $\mathcal{O}(n\epsilon^{-2})$ bound with predefined stepsizes.
 - Gaussian directions are not always bounded ⇒ Probabilistic analysis does not apply.
 - Same complexity but different directions ⇒ Can we provide a unified framework?

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Back to original direct search

Recall: Classical direct search

- Set $\mathcal{D}_k \subset \mathbb{R}^n$, $|\mathcal{D}_k| = m$, $cm(\mathcal{D}_k) \geq \kappa$;
- Complexity:

$$\mathcal{O}(m\kappa^{-2}\,\epsilon^{-2}).$$

- m may not depend on n (probabilistic)
- ...but κ depends on n (approximate $\nabla f(\mathbf{x}_k) \in \mathbb{R}^n$).

Meanwhile...

- Random embeddings (Cartis et al 2020, 2021);
- Random subspaces (Gratton et al, Kozak et al. 2021).

Reduce the dependency on n by working on low dimensions.

A new start (with Lindon Roberts)

Idea

- Consider a random subspace of dimension $r \leq n$;
- Use a PSS to approximate the projected gradient in the subspace;
- Guarantee sufficient gradient information in probability.

What it brings us

- Handle unbounded directions:
- Revisit the opposite uniform directions choice;
- Generalize the analysis to other settings, e.g. Gaussian.

Algorithm

Inputs: $\mathbf{x}_0 \in \mathbb{R}^n$, $\alpha_0 > 0$. Iteration k: Given (\mathbf{x}_k, α_k) ,

- Choose $P_k \in \mathbb{R}^{r \times n}$ at random.
- Choose $\mathcal{D}_k \subset \mathbb{R}^r$ having m vectors.
- If $\exists \ \boldsymbol{d}_k \in \mathcal{D}_k$ such that

$$f(\mathbf{x}_k + \alpha_k \mathbf{P}_k^{\mathrm{T}} \mathbf{d}_k) < f(\mathbf{x}_k) - \alpha_k^2 || \mathbf{P}_k^{\mathrm{T}} \mathbf{d}_k||^2,$$

set
$$\mathbf{x}_{k+1} := \mathbf{x}_k + \alpha_k \mathbf{P}_k^{\mathrm{T}} \mathbf{d}_k$$
, $\alpha_{k+1} := \gamma \alpha_k$.

• Otherwise, set $\mathbf{x}_{k+1} := \mathbf{x}_k$, $\alpha_{k+1} := \theta \alpha_k$.

Probabilistic properties

New polling sets

$$\left\{ oldsymbol{P}_{k}^{\mathrm{T}}oldsymbol{d}\midoldsymbol{d}\in\mathcal{D}_{k}
ight\} \subset\mathbb{R}^{n}.$$

- $P_k \in \mathbb{R}^{r \times n}$: Maps onto r-dimensional subspace;
- \mathcal{D}_k : Direction set in the subspace.

What do we want?

- Preserve information while applying $P_k/P_k^{\rm T}$.
- Approximate $-\boldsymbol{P}_k \nabla f(\boldsymbol{x}_k)$ using \mathcal{D}_k .

Probabilistic properties for P_k

$$m{P}_k$$
 is $(\eta, \sigma, P_{\sf max})$ -well aligned for $(f, m{x}_k)$ if
$$\left\{ egin{array}{ll} \| m{P}_k
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Probabilistic properties for P_k

$$\boldsymbol{P}_k$$
 is $(\eta, \sigma, P_{\mathsf{max}})$ -well aligned for (f, \boldsymbol{x}_k) if

$$\begin{cases}
\|\boldsymbol{P}_k \nabla f(\boldsymbol{x}_k)\| \geq \eta \|\nabla f(\boldsymbol{x}_k)\|, \\
\sigma_{\min}(\boldsymbol{P}_k) \geq \sigma, \\
\sigma_{\max}(\boldsymbol{P}_k) \leq P_{\max}.
\end{cases}$$

Ex)
$$P_k = I \in \mathbb{R}^{n \times n}$$
 is $(1, 1, 1)$ -well aligned.

Probabilistic properties for P_k

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Ex) $P_k = I \in \mathbb{R}^{n \times n}$ is (1, 1, 1)-well aligned.

Probabilistic version

$$\{P_k\}$$
 is $(q, \eta, \sigma, P_{\text{max}})$ -well aligned if:

$$\mathbb{P}\left(m{P}_0\left(m{q}, \eta, \sigma, P_{\mathsf{max}}
ight)\!\!$$
-well aligned) $\geq q$

$$orall k \geq 1, \quad \mathbb{P}\left((q, \eta, \sigma, P_{\mathsf{max}})\text{-well aligned } \mid oldsymbol{P}_0, \mathcal{D}_0, \dots, oldsymbol{P}_{k-1}, \mathcal{D}_{k-1}
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Probabilistic properties for \mathcal{D}_k

Deterministic descent

The set
$$\mathcal{D}_k$$
 is $(\kappa, d_{\mathsf{max}})$ -descent for (f, \boldsymbol{x}_k) if
$$\begin{cases} & \max_{\boldsymbol{d} \in \mathcal{D}_k} \frac{-\boldsymbol{d}^{\mathrm{T}} P_k \nabla f(\boldsymbol{x}_k)}{\|\boldsymbol{d}\| \|P_k \nabla f(\boldsymbol{x}_k)\|} \geq \kappa, \\ & \forall \boldsymbol{d} \in \mathcal{D}_k, \quad d_{\mathsf{max}}^{-1} \leq \|\boldsymbol{d}\| \leq d_{\mathsf{max}}. \end{cases}$$

Probabilistic properties for \mathcal{D}_k

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The set \mathcal{D}_k is (κ, d_{max}) -descent for (f, x_k) if

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Ex) D_{\oplus} is $(\frac{1}{\sqrt{n}}, 1)$ -descent.

Probabilistic properties for \mathcal{D}_{k}

Deterministic descent

The set \mathcal{D}_k is (κ, d_{max}) -descent for (f, \mathbf{x}_k) if

$$\left\{ \begin{array}{l} \max_{\boldsymbol{d} \in \mathcal{D}_k} \frac{-\boldsymbol{d}^{\mathrm{T}} \boldsymbol{P}_k \nabla f(\boldsymbol{x}_k)}{\|\boldsymbol{d}\| \|\boldsymbol{P}_k \nabla f(\boldsymbol{x}_k)\|} \geq \kappa, \\ \\ \forall \boldsymbol{d} \in \mathcal{D}_k, \quad d_{\mathsf{max}}^{-1} \leq \|\boldsymbol{d}\| \leq d_{\mathsf{max}}. \end{array} \right.$$

Ex) D_{\oplus} is $(\frac{1}{\sqrt{n}}, 1)$ -descent.

Probabilistic descent sets

 $\{\mathcal{D}_k\}$ is $(p, \kappa, d_{\text{max}})$ -descent if:

$$\mathbb{P}\left(\mathcal{D}_0\left(\kappa,d_{\mathsf{max}}
ight) ext{-descent}\mid extstyle{P}_0
ight)\ \geq\ \mu$$

Key arguments

Small step size + Good $P_k/\mathcal{D}_k \Rightarrow Success$

If P_k is $(\eta, \sigma, P_{\sf max})$ -well aligned, \mathcal{D}_k is $(\kappa, d_{\sf max})$ -descent, and

$$\alpha_k < \mathcal{O}\left(\frac{\kappa\eta}{P_{\mathsf{max}}^2 d_{\mathsf{max}}^3} \|\nabla f(\boldsymbol{x}_k)\|\right).$$

then $\mathbf{x}_{k+1} \neq \mathbf{x}_k$ and $\alpha_{k+1} \geq \alpha_k$.

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then $\mathbf{x}_{k+1} \neq \mathbf{x}_k$ and $\alpha_{k+1} \geq \alpha_k$.

A step size sequence goes to zero

For all realizations of the method,

$$\sum_{k \in \mathcal{K}} \alpha_k^2 < \mathcal{O}\left(\frac{d_{\max}^2}{\sigma^2}\right) < \infty,$$

where \mathcal{K} is the set of successful iterations for which \mathbf{P}_k is $(\eta, \sigma, P_{\text{max}})$ -well aligned and \mathcal{D}_k is (κ, d_{max}) -descent.

Martingale argument

Proposition

Define

$$z_k = 1 \left(\mathcal{D}_0 \left(\kappa, d_{\sf max} \right) \text{-descent and } \boldsymbol{P}_0 \left(q, \eta, \sigma, P_{\sf max} \right) \text{-well aligned} \right).$$

For all realizations of the algorithm, one has

$$\sum_{l=0}^{k} z_{\ell} \leq \mathcal{O}\left(\frac{1}{\left(\min_{0 \leq l \leq k} \|\nabla f(\mathbf{x}_{\ell})\|\right)^{2}}\right) + p_{0} k$$

with $p_0 = \max\left\{\frac{1}{1+\mu}, \frac{\mu}{1+\mu}\right\}$ and $\mu = \log_{\gamma}(1/\theta)$.

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- $\sum_{\ell} z_{\ell}$ satisfies a concentration bound;
- Best case: $\theta = \gamma^{-1} = 1/2$.

Complexity analysis

Theorem (Roberts and Royer, 2022)

Assume:

- $\{\mathcal{D}_k\}$ $(p, \kappa, d_{\text{max}})$ -descent, $|\mathcal{D}_k| = m$;
- $\{P_k\}$ $(q, \eta, \sigma, P_{\text{max}})$ -well aligned.

Let N_{ϵ} the number of function evaluations needed to have $\|\nabla f(\mathbf{x}_k)\| \leq \epsilon$.

$$\mathbb{P}\left(N_{\epsilon} \leq \mathcal{O}\left(\frac{m\phi\epsilon^{-2}}{pq - p_0}\right)\right) \geq 1 - \exp\left(-\mathcal{O}\left(\frac{pq - p_0}{pq}\phi\epsilon^{-2}\right)\right).$$

where $\phi = \eta^{-2} \sigma^{-2} P_{\text{max}}^4 d_{\text{max}}^8 \kappa^{-2}$.

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How does this bound depend on *n*?

Can we really improve the dimension dependence?

$$m\eta^{-2}\sigma^{-2}P_{\max}^4d_{\max}^8\kappa^{-2}\epsilon^{-2}$$
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A first simplification

•
$$\mathcal{D}_k = \{ \boldsymbol{e}_1, \dots, \boldsymbol{e}_r, -\boldsymbol{e}_1, \dots, -\boldsymbol{e}_r \}$$
 in \mathbb{R}^r ;

•
$$\kappa = \frac{1}{\sqrt{r}}$$
, $m = 2r$.

 \Rightarrow Bound becomes $2r^2\eta^{-2}\sigma^{-2}P_{\max}^4\epsilon^{-2}$.

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Using sketching techniques

\boldsymbol{P}_k	σ	$P_{\sf max}$
Identity	1	1
Gaussian	$\Theta(\sqrt{n/r})$	$\Theta(\sqrt{n/r})$
Hashing	$\Theta(\sqrt{n/r})$	\sqrt{n}
Orthogonal	$\sqrt{n/r}$	$\sqrt{n/r}$.

 \Rightarrow Get a bound in $\mathcal{O}(n\epsilon^{-2})$ even when $r = \mathcal{O}(1)$ and $\eta = \mathcal{O}(1)!$

Outline

- DFO and direct search
- Direct search and reduced dimensions
 - Algorithm and complexity
 - Numerical illustration
- 3 Decentralizing direct search

Experiments in larger dimensions

Benchmark:

- Medium-scale test set (90 CUTEst problems of dimension \approx 100);
- Large-scale test set (28 CUTEst problems of dimension \approx 1000).

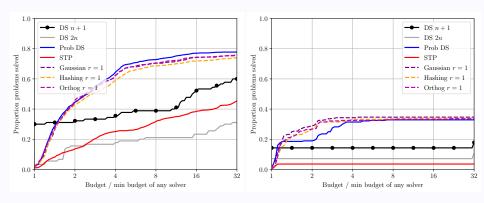
Budget: 200(n+1) evaluations.

Comparison:

- Deterministic methods with $\mathcal{D}_k = \mathcal{D}_{\oplus}$ or $\mathcal{D}_k = \{e_1, \dots, e_n, -\sum_{i=1}^n e_i\};$
- Probabilistic direct search with 2 directions;
- Stochastic Three Point;
- Reduced dimension methods with Gaussian/Hashing/Orthogonal P_k matrices + 2 directions in the subspace.

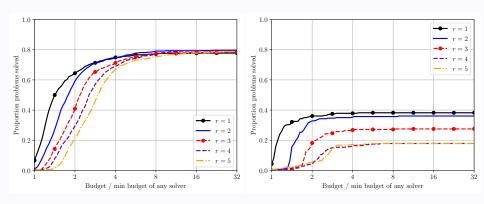
Goal: Satisfy $f(\mathbf{x}_k) - f_{best} \leq 0.1(f(\mathbf{x}_0) - f_{best})$.

Comparison of all methods



Left: Medium scale; Right: Large scale.

Gaussian matrices and the value of r



Left: Medium scale; Right: Large scale.

Summary of our findings

If you want to scale up...

- Can use less directions through sketching;
- But always a (hidden) dependency on n!

Numerically

- Sketches of dimension > 1 may improve things...
- ...but in general opposite Gaussian directions are quite good!

Outline

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Setup

$$\underset{\boldsymbol{x} \in \mathbb{R}^n}{\text{minimize}} f(\boldsymbol{x}) := \sum_{i=1}^N f_i(\boldsymbol{x}).$$

- All f_i s are $C^{1,1}$, $\sum_{i=1}^N f_i$ bounded below.
- Data for computing f_i is stored locally by an agent.
- N agents communicate through a network/graph.

Network structure

- Doubly stochastic matrix $\mathbf{W} = [w_{ij}] \in \mathbb{R}^{N \times N}$;
- \mathcal{N}_i : set of neighbors of agent i;
- $w_{ii} \neq 0$ iff i = j or $j \in \mathcal{N}_i$.

Popular approach: Consensus optimization

- Each agent i has a local vector $\mathbf{x}^{(i)}$;
- Agent i updates $x^{(i)}$ and communicates with its neighbors;
- Goal:

$$\underbrace{\sum_{i=1}^{N} \nabla f(\boldsymbol{x}^{(i)}) = 0}_{\text{optimality}}, \quad \underbrace{\boldsymbol{x}^{(i)} = \sum_{j=1}^{N} w_{ij} \boldsymbol{x}^{(j)}}_{\text{consensus}}.$$

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Penalized formulation $(\sigma > 0)$

$$\underset{\mathbf{x}^{(1)},...,\mathbf{x}^{(N)} \in \mathbb{R}^n}{\text{minimize}} \sum_{i=1}^{N} f_i(\mathbf{x}^{(i)}) + \sigma \left(\sum_{i=1}^{N} \|\mathbf{x}^{(i)}\|^2 - \sum_{i=1}^{N} \sum_{j=1}^{N} w_{ij} [\mathbf{x}^{(i)}]^{\mathrm{T}} \mathbf{x}^{(j)} \right).$$

Solving consensus problems

$$\underset{\mathbf{x}^{(1)},...,\mathbf{x}^{(N)} \in \mathbb{R}^n}{\text{minimize}} \sum_{i=1}^{N} f_i(\mathbf{x}^{(i)}) + \sigma \left(\sum_{i=1}^{N} \|\mathbf{x}^{(i)}\|^2 - \sum_{i=1}^{N} \sum_{j=1}^{N} w_{ij}[\mathbf{x}^{(i)}]^{\mathrm{T}} \mathbf{x}^{(j)} \right).$$

With derivatives

- Dual methods (ADMM, etc);
- Decentralized gradient descent:

$$\forall i = 1...N, \quad \boldsymbol{x}_{k+1}^{(i)} = \sum_{j=1}^{N} w_{ij} \boldsymbol{x}_{k}^{(j)} - \alpha_{k} \nabla f_{i}(\boldsymbol{x}_{k}^{(i)}).$$

Existing derivative-free techniques

- Approximate each gradient via finite differences.
- Randomized using STP-like approaches.

Bringing in direct search (with E. Bergou, Y. Diouane, V. Kungurtsev)

$$\underset{\boldsymbol{x^{(1)},...,\boldsymbol{x^{(N)}} \in \mathbb{R}^n}{\text{minimize}} \sum_{i=1}^{N} f_i(\boldsymbol{x^{(i)}}) + \sigma \left(\sum_{i=1}^{N} \|\boldsymbol{x^{(i)}}\|^2 - \sum_{i=1}^{N} \sum_{j=1}^{N} w_{ij} [\boldsymbol{x^{(i)}}]^{\mathrm{T}} \boldsymbol{x^{(j)}} \right).$$

Approach

Define

$$\mathcal{L}_i(\boldsymbol{x}^{(i)}) = f_i(\boldsymbol{x}^{(i)}) - \sum_{i=1}^{N} \sum_{i=1}^{N} w_{ij}[\boldsymbol{x}^{(i)}]^{\mathrm{T}} \boldsymbol{x}^{(j)}$$

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Define

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- Agent i runs a direct search method.
- \mathcal{L}_i changes over iterations \Rightarrow Forces decrease in the stepsize.

Algorithm

Inputs:
$$\mathbf{x}_0 \in \mathbb{R}^n$$
, $\mathbf{x}_0^{(i)} = \mathbf{x}_0 \ \forall i, \ \{\alpha_k\}_k \searrow 0, \ t > 0.$
Iteration k , Agent i : Given $\left(\mathbf{x}_k^{(i)}, \alpha_k\right)$,

- Choose a set $\mathcal{D}_k^{(i)} \subset \mathbb{R}^n$ of m unit vectors.
- If $\exists \ \boldsymbol{d}_k^{(i)} \in \mathcal{D}_k^{(i)}$ such that

$$f(\boldsymbol{x}_k^{(i)} + \alpha_k \, \boldsymbol{d}_k) < f(\boldsymbol{x}_k^{(i)}) - \alpha_k^{1+t},$$

set
$$\mathbf{x}_{k+1}^{(i)} := \mathbf{x}_k^{(i)} + \alpha_k \mathbf{d}_k^{(i)}$$
.

• Otherwise, set $\mathbf{x}_{k+1}^{(i)} := \mathbf{x}_k^{(i)}$.

First results: Convergence

minimize_{$$\mathbf{x}^{(1)},...,\mathbf{x}^{(N)} \in \mathbb{R}^n$$} $\sum_{i=1}^{N} f_i(\mathbf{x}^{(i)}) + \sigma \left(\sum_{i=1}^{N} \|\mathbf{x}^{(i)}\|^2 - \sum_{i=1}^{N} \sum_{j=1}^{N} w_{ij} [\mathbf{x}^{(i)}]^T \mathbf{x}^{(j)} \right)$

$$\forall i, \quad \mathcal{L}_i(\mathbf{x}^{(i)}) = f_i(\mathbf{x}^{(i)}) - \sum_{i=1}^N \sum_{j=1}^N w_{ij}[\mathbf{x}^{(i)}]^\mathrm{T} \mathbf{x}^{(j)}$$

Theorem (Bergou, Diouane, Kungurstev, R.)

Suppose that every agent runs direct-search iterations based on

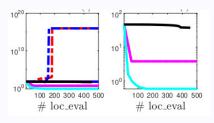
- $\mathcal{D}_{k}^{(i)}$ is κ -descent with unit vectors;
- $\alpha_k = \frac{\alpha_0}{(1+k)^u}$, $u \in (1/2,1)$;
- decrease in α_k^{1+t} with u(1+t) < 1.

Then,

$$\liminf_{k\to\infty}\sum_{i=1}^N\|\nabla\mathcal{L}_i(\boldsymbol{x}^{(i)})\|=0.$$

A toy example

$$\begin{split} & \text{minimize}_{\mathbf{x}(\mathbf{1})_{1},...,\mathbf{x}(N) \in \mathbb{R}} \sum_{i=\mathbf{1}}^{N} f_{i}(\mathbf{x}^{(i)}) + \sigma \left(\sum_{i=\mathbf{1}}^{N} \|\mathbf{x}^{(i)}\|^{2} - \sum_{i=\mathbf{1}}^{N} \sum_{j=\mathbf{1}}^{N} w_{ij} [\mathbf{x}^{(i)}]^{\mathrm{T}} \mathbf{x}^{(j)} \right) \\ \forall i, \quad & f_{i}(\mathbf{x}^{(i)}) = \frac{a_{i}}{\mathbf{1} + \exp(-\mathbf{x}_{i})} + b_{i} \log(1 + \mathbf{x}_{i}^{2}). \end{split}$$



Objective vs Number of calls to $f_i(\cdot)$.

- Blue/Red: Finite-difference techniques;
- Black: Standard direct-search for all nodes;
- Cyan: Separable minimization;
- Magenta: New method.

Summary

DFO and dimension dependence

- A revised probabilistic analysis that allows for dimensionality reduction;
- Complexity results suggest a fundamental limit $\mathcal{O}(n)$;
- One dimensional variants pretty interesting!

Direct search based on probabilistic descent in reduced spaces. L. Roberts and C. W. Royer (paper/Python toolbox coming soon!).

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Beyond centralized problems

- Typical zeroth-order approach: finite differences;
- Direct-search schemes may also be applicable.
- Challenge: Reason about a changing objective.

Decentralized direct search E. Bergou, Y. Diouane, V. Kungurtsev and C. W. Royer, in preparation.

What's next

Stochastic function values

- If sufficiently accurate in probability, things work out!
- Analysis of course (a lot) more technical.
- Challenge: Improve accuracy requirements.

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Thank you for your attention! clement.royer@dauphine.psl.eu