Randomized subspace methods for high-dimensional model-based derivative-free optimization

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AustMS 2025, Melbourne, Australia

December 10, 2025

Based on joint works with Warren Hare and Amy Wiebe

Outline

1. Introduction
2. Random subspace model-based trust-region algorithm
3. Constraints?
4. Summary

Derivative-free optimization (DFO)

Consider the optimization problem

$$\min_{x \in \mathbb{R}^n} f(x)$$

where f is given by a blackbox:

Derivative-free optimization is the mathematical study of optimization algorithms that do not use derivatives

Note: It does not mean that the derivatives do not exist

Model-based DFO

Model-based DFO methods:

- Use function values to build an approximation model of the objective
- Use the model to guide future iterations

Limitations:

- Number of function evals. is too high for large problems ($n \approx 1000$)

n	1	10	100	1000
$(n+1)(n+2)/2$	3	66	5151	501501

- Primarily designed for small- to medium-scale problems ($n \leq 100$)

Randomized subspace model-based DFO

Idea:

1. Select a low-dimensional affine subspace
2. Build and optimize a model to compute a step in this subspace
3. Change the affine subspace at the next iteration

Some existing papers:
[Zhang, 2012]; [Cartis, Roberts, 2023]; [Dzahini, Wild, 2024];
[Chen, Hare, Wiebe, 2024]; [Cartis, Roberts, 2024]
[Chen, Hare, Wiebe, 2025]

Outline

Model-based trust-region (MBTR) algorithm

for $k = 0, 1, \dots$ **do**

Construct a model m^k in $\mathbb{R}^n$:

$$m^k(s) = f(x^k) + (g^k)^\top s + \frac{1}{2} s^\top H^k s$$

Approximately solve the trust-region subproblem in $\mathbb{R}^n$:

$$s^k \approx \operatorname*{argmin}_{s \in \mathbb{R}^n} m^k(s), \quad s.t. \ \|s\| \leq \Delta^k$$

Evaluate $f(x^k + s^k)$ and apply descent ratio test

$$\rho^k = \frac{f(x^k) - f(x^k + s^k)}{m^k(\mathbb{0}) - m^k(s^k)} = \frac{true \ \ decrease}{predicted \ \ decrease}$$

Accept/reject step based on ρ^k and update trust region radius

Random subspace MBTR algorithm

for $k = 0, 1, \ldots$ **do**

Define an affine subspace $x^k + D^k\mathbb{R}^p$ by selecting $D^k \in \mathbb{R}^{n\times p}$
Construct a model $\widehat{m}^k$ in $\mathbb{R}^p$

Approximately solve the trust-region subproblem in $\mathbb{R}^p$:

$$\widehat{s}^k \approx \underset{\widehat{s}\in\mathbb{R}^p}{\operatorname{argmin}}\, \widehat{m}^k(\widehat{s}), \quad s.t. \ \|\widehat{s}\| \leq \Delta^k$$

and calculate the corresponding step $s^k \in \mathbb{R}^n$
Evaluate $f(x^k + s^k)$ and apply descent ratio test

$$\rho^k = \frac{f(x^k) - f(x^k + s^k)}{\widehat{m}^k(\mathbb{0}) - \widehat{m}^k(\widehat{s}^k)} = \frac{\textit{true decrease}}{\textit{predicted decrease}}$$

Accept/reject step based on ρ^k and update trust region radius

Model construction

Q-fully quadratic models

Definition. A model $m : \mathbb{R}^n \to \mathbb{R}$ is fully quadratic in $B(x, \Delta)$ if there exist $\kappa_f, \kappa_g, \kappa_h > 0$ s.t. for all $s \in \mathbb{R}^n$ with $\|s\| \leq \Delta$,

$$
\begin{aligned}
|f(x+s) - m(x+s)| &\leq \kappa_f \Delta^3 \\
\|\nabla f(x+s) - \nabla m(x+s)\| &\leq \kappa_g \Delta^2 \\
\left\|\nabla^2 f(x+s) - \nabla^2 m(x+s)\right\| &\leq \kappa_h \Delta
\end{aligned}
$$

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$$|f(x+s) - m(x+s)| \leq \kappa_f \Delta^3$$
$$\|\nabla f(x+s) - \nabla m(x+s)\| \leq \kappa_g \Delta^2$$
$$\left\|\nabla^2 f(x+s) - \nabla^2 m(x+s)\right\| \leq \kappa_h \Delta$$

Definition. [Chen, Hare, Wiebe, 2024]
Let $Q \in \mathbb{R}^{n \times p}$. A model $\widehat{m} : \mathbb{R}^p \to \mathbb{R}$ is Q-fully quadratic in $B(x, \Delta)$ if there exist $\kappa_f, \kappa_g, \kappa_h > 0$ s.t. for all $\widehat{s} \in \mathbb{R}^p$ with $\|\widehat{s}\| \leq \Delta$,

$$|f(x + Q\widehat{s}) - \widehat{m}(\widehat{s})| \leq \kappa_f \Delta^3$$
$$\left\|Q^\top \nabla f(x + Q\widehat{s}) - \nabla \widehat{m}(\widehat{s})\right\| \leq \kappa_g \Delta^2$$
$$\left\|Q^\top \nabla^2 f(x + Q\widehat{s}) Q - \nabla^2 \widehat{m}(\widehat{s})\right\| \leq \kappa_h \Delta$$

Constructing Q-fully quadratic models

Definition. [Custódio, Dennis Jr., Vicente, 2008] & [Hare, Jarry-Bolduc, Planiden, 2023]
Let $x^0 \in \mathbb{R}^n$ and $D = [d^1 \cdots d^p] \in \mathbb{R}^{n \times p}$
The generalized simplex gradient of f at x^0 over D is defined by

$$\nabla_s f(x^0; D) = \left(D^\top\right)^\dagger \delta_f(x^0; D)$$

where

$$\delta_f(x^0; D) = \begin{bmatrix} f(x^0 + d^1) - f(x^0) \\ f(x^0 + d^2) - f(x^0) \\ \vdots \\ f(x^0 + d^p) - f(x^0) \end{bmatrix}$$

The generalized simplex Hessian of f at x^0 over D is defined by

$$\nabla_s^2 f(x^0; D) = \left(D^\top\right)^\dagger \delta_{\nabla_s f}(x^0; D)$$

Constructing Q-fully quadratic models

Theorem. [Chen, Hare, Wiebe, 2024]
Let $x^0 \in \mathbb{R}^n$ and $D = QR$ have full col. rank, where $R = [r^1 \cdots r^p] \in \mathbb{R}^{p \times p}$
Let

$$m(x) = f(x^0) + \left(2\nabla_s f(x^0; D) - \nabla_s f(x^0; 2D)\right)^\top \left(x - x^0\right) + \frac{1}{2}\left(x - x^0\right)^\top \nabla_s^2 f(x^0; D; D)\left(x - x^0\right)$$

Then, the model $\widehat{m} : \mathbb{R}^p \to \mathbb{R}$ defined by $\widehat{m}(\widehat{s}) = m(x^0 + Q\widehat{s})$ is Q-fully quadratic in $B(x^0, \max_{1 \le i \le p} \|r^i\|)$

The $2\nabla_s f(x^0; D) - \nabla_s f(x^0; 2D)$ is a special case of the *Adapted Centred Simplex Gradient*, see Y. Chen and W. Hare. "Adapting the centred simplex gradient to compensate for misaligned sample points". In: *IMA J. Numer. Anal.* (2023)

Subspace selection

α-well-aligned matrices

Let $x + D\mathbb{R}^p$ be the affine subspace

Definition. [Cartis, Roberts, 2023]
Let $\alpha \in (0, 1)$. We say that $D \in \mathbb{R}^{n \times p}$ is α-well-aligned for f at x if

$$\left\| D^\top \nabla f(x) \right\| \geq \alpha \left\| \nabla f(x) \right\|$$

α-well-aligned matrices

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$$\left\| D^\top \nabla f(x) \right\| \geq \alpha \left\| \nabla f(x) \right\|$$

Theorem. [Dzahini, Wild, 2024] (Idea: Johnson–Lindenstrauss Lemma)
Let $\alpha, \delta \in (0, 1)$. Suppose $p \geq 4(1 - \alpha)^{-2} \ln(1/\delta)$ and let $D_{ij} \sim \mathcal{N}(0, 1/p)$
Then,

$$\mathbb{P}\left[D \text{ is } \alpha\text{-well-aligned for } f \text{ at x}\right] \geq 1 - \delta$$

Can we reuse past information to construct subspaces?

Suppose D has the form $D = [D^U \; D^R] \in \mathbb{R}^{n \times p}$, where

- $D^U \in \mathbb{R}^{n \times (p - p_{\text{rand}})}$ is picked from previous sample points
- $D^R \in \mathbb{R}^{n \times p_{\text{rand}}}$ is randomly generated

Theorem. [Chen, Hare, Wiebe, 2024]
Let $\alpha, \delta \in (0, 1)$
Suppose $p_{\text{rand}} \geq 4(1 - \alpha)^{-2} \ln(1/\delta)$ and let

$$D^R \sim \operatorname{proj}_{\operatorname{col}(D^U)^\perp} \left(\mathcal{MN} \left(\mathbb{0}, \frac{1}{p} I_n, I_{p_{\text{rand}}} \right) \right)$$

Then, there exists $\alpha_D > 0$ such that

$$\mathbb{P}\left[D \text{ is } \alpha_D\text{-well-aligned for } f \text{ at x}\right] \geq 1 - \delta$$

Outline

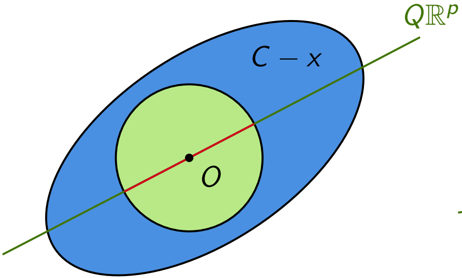
(C, Q)-fully linear models

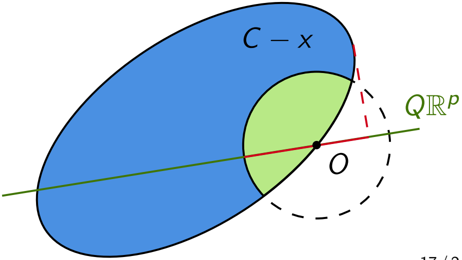
Let C be the constraint set (convex, closed, nonempty interior)

Definition. [Chen, Hare, Wiebe, 2025]
Let $Q \in \mathbb{R}^{n \times p}$. A model $\widehat{m} : \mathbb{R}^p \to \mathbb{R}$ is (C, Q)-fully linear in $B(x, \Delta)$ if there exist $\kappa_f, \kappa_g > 0$ s.t. for all $\widehat{s} \in Q^\top (C - x)$ with $\|\widehat{s}\| \leq \Delta$,

$$|f(x + Q\widehat{s}) - \widehat{m}(\widehat{s})| \leq \kappa_f \Delta^2$$

$$\max_{\substack{d \in Q^\top (C - x) \\ \|d\| \leq 1}} \left| \left(Q^\top \nabla f(x + Q\widehat{s}) - \nabla \widehat{m}(\widehat{s}) \right)^\top d \right| \leq \kappa_g \Delta$$





Constructing (C, Q)-fully linear models

Theorem. [Chen, Hare, Wiebe, 2025]
Let $x^0 \in \mathbb{R}^n$ and $D = QR$ have full col. rank, where $R = [r^1 \cdots r^p] \in \mathbb{R}^{p \times p}$
Let

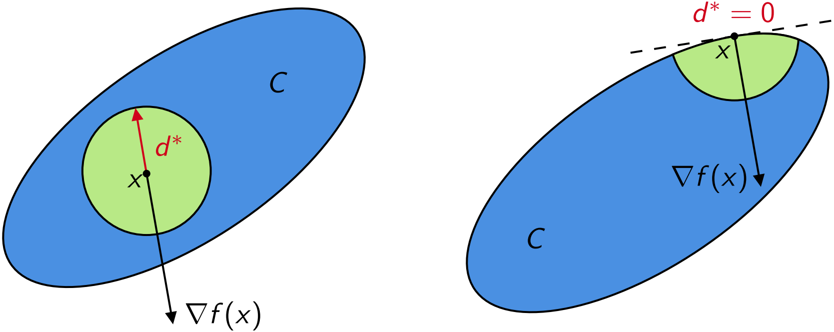
$$m(x) = f(x^0) + \nabla_s f(x^0; D)^\top \left(x - x^0\right)$$

Then, the model $\widehat{m} : \mathbb{R}^p \to \mathbb{R}$ defined by $\widehat{m}(\widehat{s}) = m(x^0 + Q\widehat{s})$ is (C, Q)-fully linear in $B(x^0, \max_{1 \le i \le p} \|r^i\|)$

First-order criticality measure

First-order criticality measure for convex-constrained optimization
[Conn, Gould, Toint, 2000]

$$\pi^f(x) = \left| \min_{\substack{x+d \in C \\ \|d\| \leq 1}} \nabla f(x)^\top d \right|$$



α-well-aligned matrices (convex-constrained version)

Let $x + D\mathbb{R}^p$ be the affine subspace and $D = QR$ be the QR factorization

Definition. [Chen, Hare, Wiebe, 2025]
Let $\alpha \in (0, 1)$. We say that $D \in \mathbb{R}^{n\times p}$ is α-well-aligned for f and C at x if

$$\left| \min_{\substack{d \in C - x \\ \|d\| \leq 1}} \nabla f(x)^\top Q Q^\top d \right| \geq \alpha \pi^f(x)$$

α-well-aligned matrices (convex-constrained version)

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Theorem. [Chen, Hare, Wiebe, 2025]
(Idea: Concentration on the Grassmannian)
Suppose $p \geq n\alpha$ and let $D_{ij} \sim \mathcal{N}(0, 1)$. Then,

$$\mathbb{P}\left[D \text{ is } \alpha\text{-well-aligned for } f \text{ and } C \text{ at x}\right]$$
$$\geq \text{complicated stuff that depends on } n,\ p,\ \alpha,\ \pi^f(x), \text{ and } \|\nabla f(x)\|$$

Convergence and complexity results

Let $\epsilon > 0$, (UC)=UnConstrained, and (CC)=Convex-Constrained

- (UC) $\mathbb{P}\left[\min_{k \leq K} \|\nabla f(x^k)\| < \epsilon\right] \geq 1 - e^{-C(K+1)}$

  (CC) $\mathbb{P}\left[\min_{k \leq K} \pi^f(x^k) < \epsilon\right] \geq 1 - e^{-C(\epsilon)(K+1)}$

- (UC) $\mathbb{P}\left[\inf_{k \geq 0} \|\nabla f(x^k)\| = 0\right] = 1$

  (CC) $\mathbb{P}\left[\inf_{k \geq 0} \pi^f(x^k) = 0\right] = 1$

- (UC) $\mathbb{E}\left[\min\left\{k \geq 0 : \left\|\nabla f(x^k)\right\| < \epsilon\right\}\right] = \mathcal{O}(\epsilon^{-2})$

  (CC) $\mathbb{E}\left[\min\left\{k \geq 0 : \pi^f(x^k) < \epsilon\right\}\right] = \mathcal{O}(\epsilon^{-4})$

(UC) from [Cartis, Roberts, 2023]; (CC) from [Chen, Hare, Wiebe, 2025]

Outline

Summary

In summary,

- High-dimensional DFO problems are hard
- Unconstrained problems can be effectively approached by randomized subspace methods
- Randomized subspace methods work for convex constrained problems, but the projection onto the feasible set is required

Future directions:

- Nonconvex constraints?
- Blackbox constraints?
- Random manifolds?

Thank you

- Y. Chen, W. Hare, and A. Wiebe. "Q-fully quadratic modeling and its application in a random subspace derivative-free method". In: *Computational Optimization and Applications* 89.2 (2024), pp. 317–360
- Y. Chen, W. Hare, and A. Wiebe. "CLARSTA: A random subspace trust-region algorithm for convex-constrained derivative-free optimization". In: *arXiv preprint arXiv:2506.20335* (2025)

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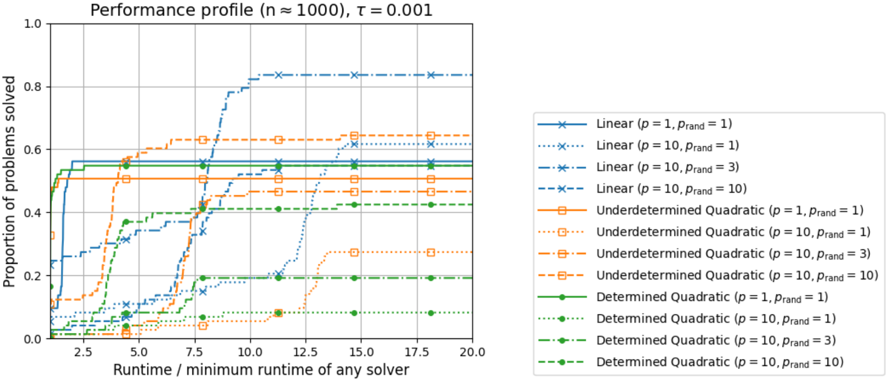
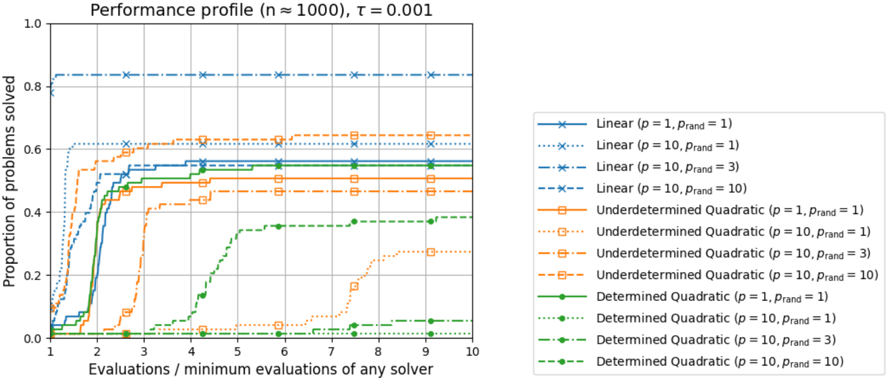
Comparing linear and quadratic models based on runtime



Success is defined as finding x^k such that
$f(x^k) \leq f(x^*) + \tau(f(x^0) - f(x^*))$ in less than $100(n+1)$ f-evals

Comparing linear and quadratic models based on fevals



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Comparison of runtime to reach f^*

Steps:

1. Run CLARSTA for $100(n+1)$ fevals and denote the result by f^*
2. Run COBYLA until f^* is reached or $100(n+1)$ fevals or 10^5 seconds are required

Results when $n = 1000$:

Problem		CLARSTA		COBYLA	
obj.	const.	nf	Total time (s)	nf	Total time (s)
C.R.	box	100100	6.451e+01	26716	6.196e+04
C.R.	ball	100100	6.913e+01	26337	2.048e+04
C.R.	halfspace	100100	7.349e+01	27054	2.113e+04
Trig.	box	100100	6.975e+03	N/A	1.000e+05*
Trig.	ball	100100	7.052e+03	100100*	8.678e+04
Trig.	halfspace	100100	6.901e+03	100100*	8.655e+04

*COBYLA does not reach f^*

Comparison of runtime to reach f^*

Results when $n = 10000$:

Problem		CLARSTA		COBYLA	
obj.	const.	nf	Total time (s)	nf	Total time (s)
C.R.	box	1000100	1.836e+03	N/A	1.000e+05*
C.R.	ball	1000100	1.960e+03	N/A	1.000e+05*
C.R.	halfspace	1000100	1.928e+03	N/A	1.000e+05*

*COBYLA does not reach f^*