Q-fully quadratic modeling and its application in a random subspace derivative-free method

Yiwen Chen

Department of Mathematics
University of British Columbia

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Joint work with Dr. Warren Hare and Dr. Amy Wiebe

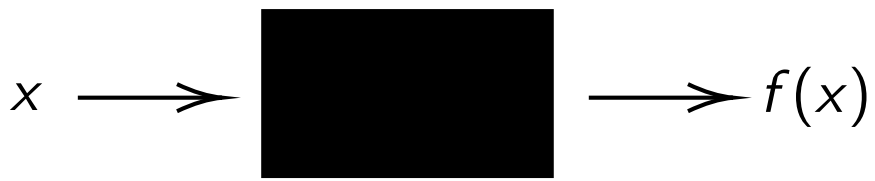
Outline

Optimization with blackbox objective function

Consider the optimization problem

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

where f is given by a blackbox:



Example

Consider a chemical process:

$$\left.\begin{array}{c}\text{Temperature}\\ \text{Humidity}\\ \text{Reaction time}\end{array}\right\} = x \longrightarrow \boxed{} \longrightarrow f(x) = \text{Product purity}$$

Goal:

$$\max\{f(x) : x_1 \in [273, 373], x_2 \in [30, 60], x_3 \in [1, 10]\}$$

Another example

Consider a computer simulation of earthquakes:

$$\left.\begin{array}{c}\text{Height}\\ \text{Material}\\ \text{Structure}\end{array}\right\} = x \longrightarrow \boxed{\phantom{\text{Simulation}}} \longrightarrow f(x) = \text{Stability of building}$$

Goal:

$$\max\{f(x) : x \text{ satisfies some constraints}\}$$

Derivative-free optimization (DFO)

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

Two categories of DFO methods

Direct search methods

- Maintain an incumbent solution and check a finite number of trial points for potential decrease
- E.g., Coordinate Search, MADS

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Model-based methods

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

Polynomial interpolation

Definition. For a given function $f(x)$ and set $Y = \{y^0, ..., y^s\}$, a polynomial $m(x)$ is a polynomial interpolation model of $f(x)$ if

$$m(y^i) = f(y^i), \quad i = 0, ..., s$$

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$$m(y^i) = f(y^i), \quad i = 0, ..., s$$

Note: In practice, $m(x)$ is determined by finding $\alpha_0, ..., \alpha_t$ such that

$$m(y^i) = \sum_{j=0}^{t} \alpha_j \phi_j(y^i) = f(y^i), \quad i = 0, ..., s$$

where the set of functions $\phi = \{\phi_0, ..., \phi_t\}$ is a polynomial basis

Linear interpolation model

Let $\phi = \{1, x_1, x_2, ..., x_d\}$ and $Y = \{y^0, ..., y^d\}$
Then a linear interpolation model $m(x)$ is determined by finding $\alpha_0, ..., \alpha_d$ such that

$$m(y^i) = \alpha_0 + \alpha_1 y_1^i + \cdots + \alpha_d y_d^i = f(y^i), \quad i = 0, ..., d$$

where y_j^i is the j-th element of y^i

Quadratic interpolation model

Let $\phi = \{1, x_1, x_2, ..., x_d, \frac{x_1^2}{2}, x_1x_2, ..., x_{d-1}x_d, \frac{x_d^2}{2}\}$ and $Y = \{y^0, ..., y^s\}$
Then a quadratic interpolation model $m(x)$ is determined by finding $\alpha_0, ..., \alpha_{\frac{(d+1)(d+2)}{2}-1}$ such that

$$m(y^i) = \alpha_0 + \alpha_1 y_1^i + \cdots + \alpha_d y_d^i + \alpha_{d+1}\frac{(y_1^i)^2}{2} + \cdots + \alpha_{\frac{(d+1)(d+2)}{2}-1}\frac{(y_d^i)^2}{2} = f(y^i), \quad i = 0, ..., s$$

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Note: If $s = \frac{(d+1)(d+2)}{2} - 1$ and the system has full rank, then $m(x)$ is called a determined quadratic interpolation model

If $s < \frac{(d+1)(d+2)}{2} - 1$ and the system has full rank, then $m(x)$ is called an underdetermined quadratic interpolation model

Model-based DFO: limitations

Limitations:

- Function evaluations are too expensive for large problems

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

- They are primarily designed for small- to medium-scale problems

Improving scalability by subspace decomposition

Idea:

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

Some existing papers:
[Zhang, 2012]; [Dzahini, Wild, 2022]; [Menickelly, 2023];
[Cartis, Roberts, 2023]

The inspirational question

Is it beneficial to use quadratic models instead of linear models?

Outline

Model-based trust-region (MBTR) algorithm

for $k = 0, 1, \ldots$ **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 $\mathbb{R}^n$:

$$s_k \approx \underset{s \in \mathbb{R}^n}{\operatorname{argmin}}\, m_k(s), \quad s.t. \;\; \|s\| \leq \Delta_k$$

Evaluate $f(x_k + s_k)$ and calculate ratio

$$\rho_k = \frac{f(x_k) - f(x_k + s_k)}{m_k(\mathbf{0}) - m_k(s_k)} = \frac{\textit{true decrease}}{\textit{predicted decrease}}$$

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 $\mathbb{R}^p$:

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

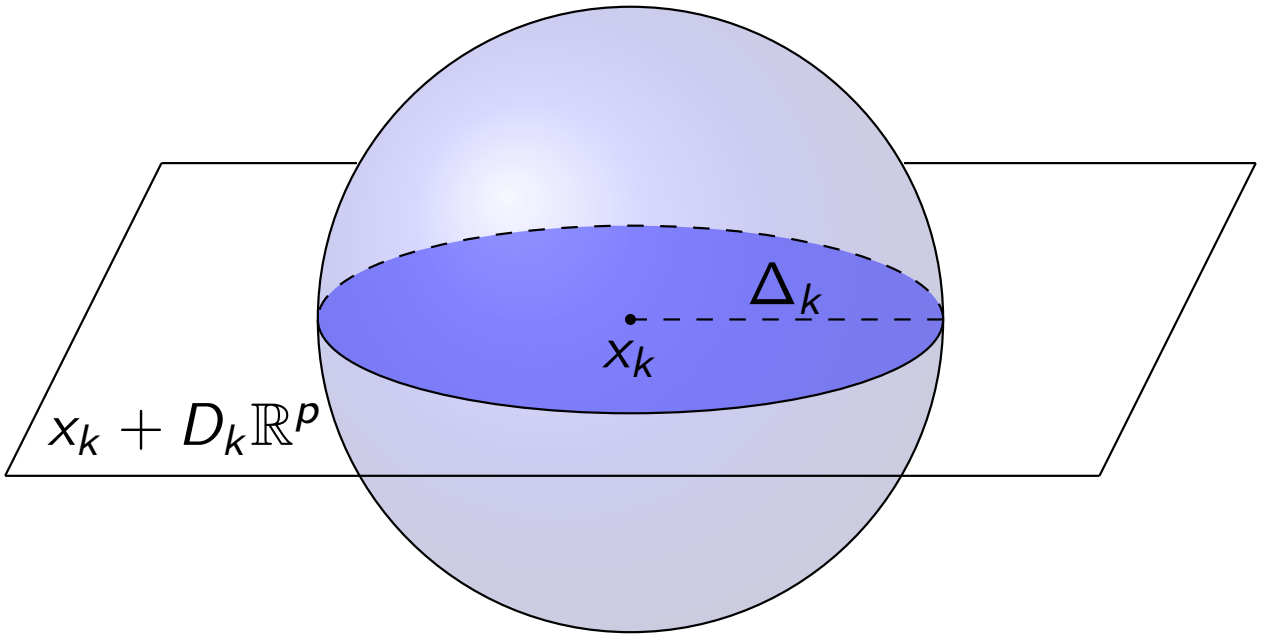
and calculate the corresponding step $s_k \in \mathbb{R}^n$

Evaluate $f(x_k + s_k)$ and calculate ratio

$$\rho_k = \frac{f(x_k) - f(x_k + s_k)}{\widehat{m}_k(\mathbf{0}) - \widehat{m}_k(\widehat{s}_k)} = \frac{\textit{true decrease}}{\textit{predicted decrease}}$$

Accept/reject step based on ρ_k and update trust region radius

Random subspace MBTR algorithm: visuals



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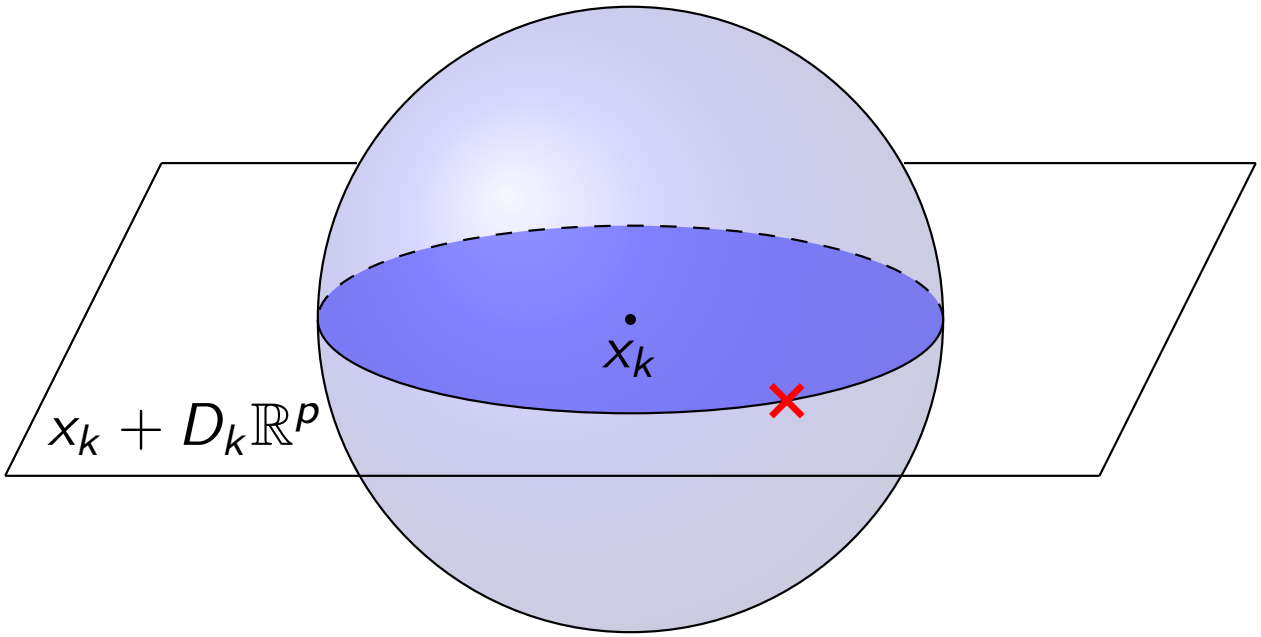

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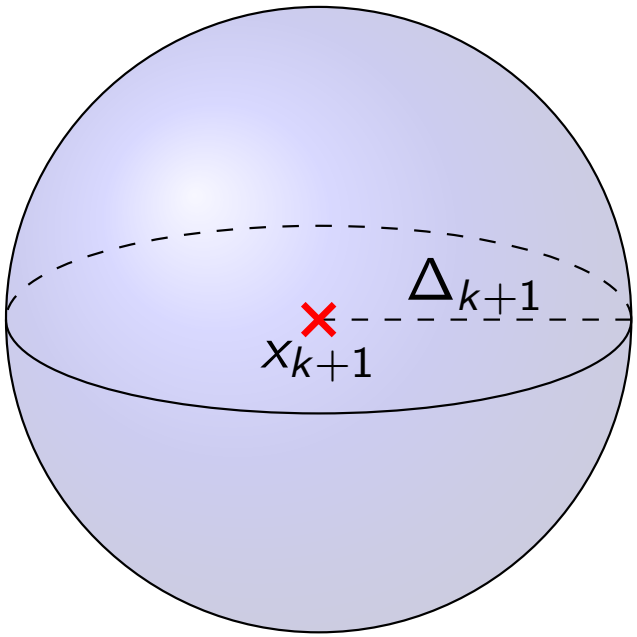

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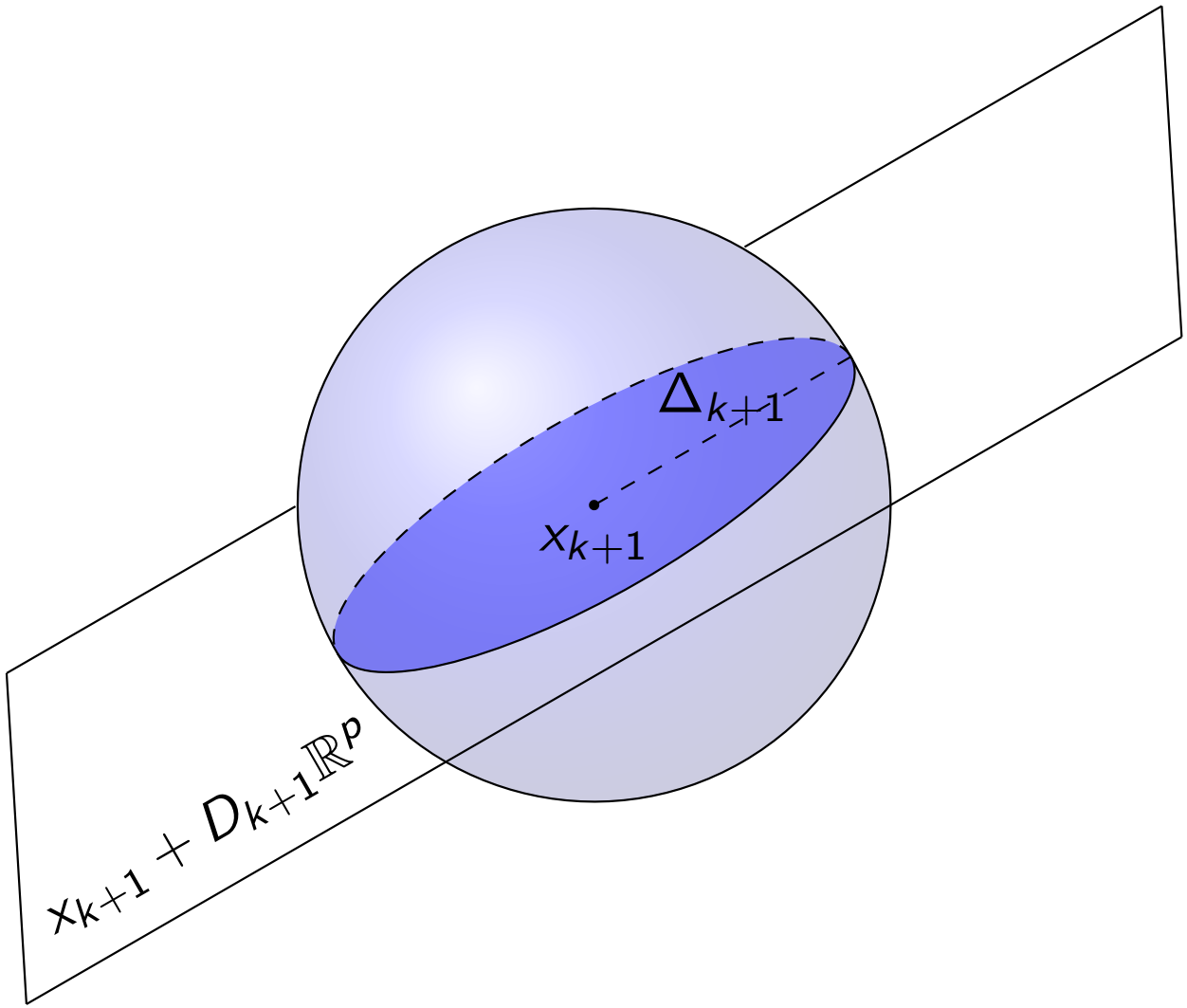

Model construction

Q-fully quadratic models

Definition. Let $f \in \mathcal{C}^2, x \in \mathbb{R}^n, \bar{\Delta} > 0$, and $Q \in \mathbb{R}^{n \times p}$
We say that $\{\widehat{m}_\Delta : \mathbb{R}^p \to \mathbb{R}\}_{\Delta \in (0, \bar{\Delta}]}$ is a class of Q-fully quadratic models of f at x if there exist $\kappa_{ef}(x), \kappa_{eg}(x), \kappa_{eh}(x) > 0$ such that for all $\Delta \in (0, \bar{\Delta}]$ and $\|\widehat{s}\| \leq \Delta$,

$$
\begin{aligned}
|f(x + Q\widehat{s}) - \widehat{m}_\Delta(\widehat{s})| &\leq \kappa_{ef}(x)\Delta^3, \\
\left\| Q^\top \nabla f(x + Q\widehat{s}) - \nabla \widehat{m}_\Delta(\widehat{s}) \right\| &\leq \kappa_{eg}(x)\Delta^2, \\
\left\| Q^\top \nabla^2 f(x + Q\widehat{s}) Q - \nabla^2 \widehat{m}_\Delta(\widehat{s}) \right\| &\leq \kappa_{eh}(x)\Delta
\end{aligned}
$$

Generalized simplex gradient

Definition. [Hare, Jarry-Bolduc, 2020]
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

$$\delta_f(x^0; D) = \begin{bmatrix} f(x^0 + d_1) - f(x^0) \\ f(x^0 + d_2) - f(x^0) \\ \vdots \\ f(x^0 + d_p) - f(x^0) \end{bmatrix}$$

Generalized simplex Hessian

Definition. [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 Hessian of f at x^0 over D is defined by

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

where

$$\delta_{\nabla_S f}(x^0; D) = \begin{bmatrix} \left(\nabla_S f(x^0 + d_1; D) - \nabla_S f(x^0; D)\right)^\top \\ \left(\nabla_S f(x^0 + d_2; D) - \nabla_S f(x^0; D)\right)^\top \\ \vdots \\ \left(\nabla_S f(x^0 + d_p; D) - \nabla_S f(x^0; D)\right)^\top \end{bmatrix}$$

Constructing Q-fully quadratic models

Definition. Suppose $D = QR$ has full column rank, where $Q \in \mathbb{R}^{n \times p}$ Let

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

The model $\widehat{m} : \mathbb{R}^p \to \mathbb{R}$ is defined by

$$\widehat{m}(\widehat{s}) = m(x^0 + Q\widehat{s})$$

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)

Constructing Q-fully quadratic models

Theorem. $\widehat{m}$ is a determined quadratic interpolation model of $f(x^0 + Q\widehat{s})$

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Theorem. If $f \in \mathcal{C}^{2+}$ and D has full-column rank, then $\widehat{m}$ belongs to a class of Q-fully quadratic models of f at x^0 with constants $\kappa_{ef}, \kappa_{eg}, \kappa_{eh}$ monotonically increasing w.r.t. $\|D^\dagger\|$

Subspace selection

α-well-aligned matrices

Definition. [Cartis, Roberts, 2023]
Let $f \in \mathcal{C}^1, x \in \mathbb{R}^n$, and $\alpha > 0$
We say that $A \in \mathbb{R}^{n \times z}$ is α-well-aligned for f at x if

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

Constructing α-well-aligned matrices

Theorem. [Dzahini, Wild, 2022]
Suppose $\alpha, \delta_S \in (0,1)$ and $z \geq 4(1-\alpha)^{-2} \ln(1/\delta_S)$
Let $A \in \mathbb{R}^{n \times z}$ such that $A_{ij} \sim \mathcal{N}(0, 1/z)$
Then for any $v \in \mathbb{R}^n$,

$$\mathbb{P}\left[\left\|A^\top v\right\| \geq \alpha \|v\|\right] \geq 1 - \delta_S$$

The $\mathbb{P}[\cdot]$ gives the probability of a random variable

Constructing α-well-aligned matrices

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Then for any $v \in \mathbb{R}^n$,

$$\mathbb{P}\left[\left\|A^\top v\right\| \geq \alpha \|v\|\right] \geq 1 - \delta_S$$

In particular, given $f \in \mathcal{C}^1$ and $x \in \mathbb{R}^n$, A is α-well-aligned for f at x with probability at least $1 - \delta_S$, i.e.,

$$\mathbb{P}\left[\left\|A^\top \nabla f(x)\right\| \geq \alpha \|\nabla f(x)\|\right] \geq 1 - \delta_S$$

The $\mathbb{P}[\cdot]$ gives the probability of a random variable

Can we reuse past information to construct subspaces?

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

- $D_k^U \in \mathbb{R}^{n \times (p - p_{\text{rand}})}$ is picked from D_{k-1}
- $D_k^R \in \mathbb{R}^{n \times p_{\text{rand}}}$ is randomly generated

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- $D_k^U \in \mathbb{R}^{n \times (p - p_{\text{rand}})}$ is picked from D_{k-1}
- $D_k^R \in \mathbb{R}^{n \times p_{\text{rand}}}$ is randomly generated
- D_k^U is picked such that $\sigma_{\min}(D_k^U)$ is as large as possible
- D_k^R consists of orthogonal columns and $\text{col}(D_k^R) \subseteq \text{col}(D_k^U)^{\perp}$

Constructing D_k

Recall: $\kappa_{ef}, \kappa_{eg}, \kappa_{eh}$ monotonically increasing w.r.t. $\|D_k^\dagger\|$

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Idea: Minimize $\|D_k^\dagger\| = 1/\sigma_{\min}(D_k) \Leftrightarrow$ Maximize $\sigma_{\min}(D_k)$

Constructing D_k

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Idea: Minimize $\|D_k^\dagger\| = 1/\sigma_{\min}(D_k) \Leftrightarrow$ Maximize $\sigma_{\min}(D_k)$

Theorem. Let $\widetilde{D} = [d_1 \cdots d_{q-1}] \in \mathbb{R}^{n\times(q-1)}$ where $2 \le q \le n$
Define $D(x) : \mathbb{R}^n \to \mathbb{R}^{n\times q}$ by $D(x) = [\widetilde{D}\ x]$
Then for all $x \in \mathbb{R}^n$ with $\|x\| = \Delta$, we have

$$\sigma_{\min}(D(x)) \le \min\left\{\sigma_{\min}(\widetilde{D}), \Delta\right\}.$$

In particular, if $x^* \in \mathbb{R}^n$ with $\|x^*\| = \Delta$ satisfies $d_i^\top x^* = 0$ for all $d_i \in \widetilde{D}$, then

$$\sigma_{\min}(D(x^*)) = \min\left\{\sigma_{\min}(\widetilde{D}), \Delta\right\}.$$

Constructing D_k^U

Idea: $\sigma_{\min}(D_k^U)$ should be as large as possible

Select p directions to previous sample points as the columns of D_k^U

for $\texttt{removed} = 1, ..., p_{\text{rand}}$ **do**

  Denote $D_k^U = [d_1^U \cdots d_m^U]$

  for $i = 1, ..., m$ **do**

    Define $M_i = \left[d_1^U \cdots d_{i-1}^U \; d_{i+1}^U \cdots d_m^U\right]$ and compute

$$\theta_i = \sigma_{\min}(M_i) \cdot \max\left(\frac{\left\|d_i^U\right\|^4}{\Delta_{k+1}^4}, 1\right)$$

  Remove the direction with the largest θ_i from D_k^U

Constructing D_k^R

Idea: D_k^R consists of orthogonal columns and $\mathrm{col}(D_k^R) \subseteq \mathrm{col}(D_k^U)^\perp$

Generate $A \in \mathbb{R}^{n \times p_{\mathrm{rand}}}$ with $A_{ij} \sim \mathcal{N}(0, 1/p_{\mathrm{rand}})$
Factorize $D_k^U = QR$ and calculate $\widetilde{A} = A - QQ^\top A$
Factorize $\widetilde{A} = \widetilde{Q}\widetilde{R}$
Return $\Delta_k \widetilde{Q}$

Algorithm modified from C. Cartis and L. Roberts. "Scalable subspace methods for derivative-free nonlinear least-squares optimization". In: *Math. Program.* 199.1-2 (2023), pp. 461–524

Subspace quality

Theorem. Suppose $f \in \mathcal{C}^1, \alpha, \delta_S \in (0,1)$ and $p_{\text{rand}} \geq 4(1-\alpha)^{-2} \ln(1/\delta_S)$ Then there exists $\alpha_D > 0$ such that D_k is α_D-well-aligned for f at x_k with probability at least $1 - \delta_S$

QARSTA

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

Define an affine subspace $x_k + D_k \mathbb{R}^p$ by selecting $D_k = [D_k^U \;\; D_k^R]$
Construct a Q_k-fully quadratic 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 calculate ratio

$$\rho_k = \frac{f(x_k) - f(x_k + s_k)}{\widehat{m}_k(\mathbf{0}) - \widehat{m}_k(\widehat{s}_k)} = \frac{\textit{true decrease}}{\textit{predicted decrease}}$$

Accept/reject step based on ρ_k and update trust region radius

Outline

Assumptions

- $f \in \mathcal{C}^{2+}$ and bounded below
- $\|\nabla^2 \widehat{m}_k\| \leq \kappa_H$ for all k
- Solution $\widehat{s}_k$ of the trust-region subproblem satisfy

$$\widehat{m}_k(\mathbf{0}) - \widehat{m}_k(\widehat{s}_k) \geq \frac{1}{2} \|\nabla \widehat{m}_k(\mathbf{0})\| \min\left(\Delta_k, \frac{\|\nabla \widehat{m}_k(\mathbf{0})\|}{\max\{\|\nabla^2 \widehat{m}_k\|, 1\}}\right)$$

- Each D_k is α_D-well-aligned for f at x_k with probability at least $1 - \delta_S$

Convergence results

Theorem. For all $\epsilon > 0$, there exist $C > 0$ and a sufficiently large K s.t.

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

The $\mathbb{P}[\cdot]$ and $\mathbb{E}[\cdot]$ give the probability and expected value of a random variable

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Theorem. If QARSTA is run with $\Delta_{\min} = 0$, then

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Theorem. $\mathbb{E}\left[\min\left\{k : \|\nabla f(x_k)\| \leq \epsilon\right\}\right] = \mathcal{O}(\epsilon^{-2})$

The $\mathbb{P}[\cdot]$ and $\mathbb{E}[\cdot]$ give the probability and expected value of a random variable

Outline

Questions

- Is it beneficial to use quadratic models instead of linear models?
- What is a good choice of p and p_{rand}?
- Advantages of exploiting the structure of objective functions?

Test problems

Two sets from the CUTEst collection [Gould, Orban, Toint, 2015] with dimension $n \approx 1000$:

- 73 unconstrained problems with various objective functions
- 32 unconstrained nonlinear least-squares problems, i.e.,

$$\min_{x \in \mathbb{R}^n} f(x) = \frac{1}{2} \sum_{i=1}^{m} g_i(x)^2$$

Solvers

Models:

- Linear model
- Underdetermined quadratic model
- Determined quadratic model
- Square-of-linear model (on the second problem set only)

Parameters:

- $p = 1, p_{\text{rand}} = 1$
- $p = 10, p_{\text{rand}} = 1$
- $p = 10, p_{\text{rand}} = 3$
- $p = 10, p_{\text{rand}} = 10$

Performance profiles

For each solver $S \in \mathcal{S}$ and problem $P \in \mathcal{P}$, define the performance ratio

$$r_{P,S} = \frac{t_{P,S}}{\min\{t_{P,S} : S \in \mathcal{S}\}},$$

where $t_{P,S} > 0$ is the performance measure

The performance profile of S is

$$\rho_S(\alpha) = \frac{1}{|\mathcal{P}|} |\{P \in \mathcal{P} : r_{P,S} \leq \alpha\}|$$

Stopping criteria and performance measure

For each solver S and problem P with dimension n_P
Stopping criteria:

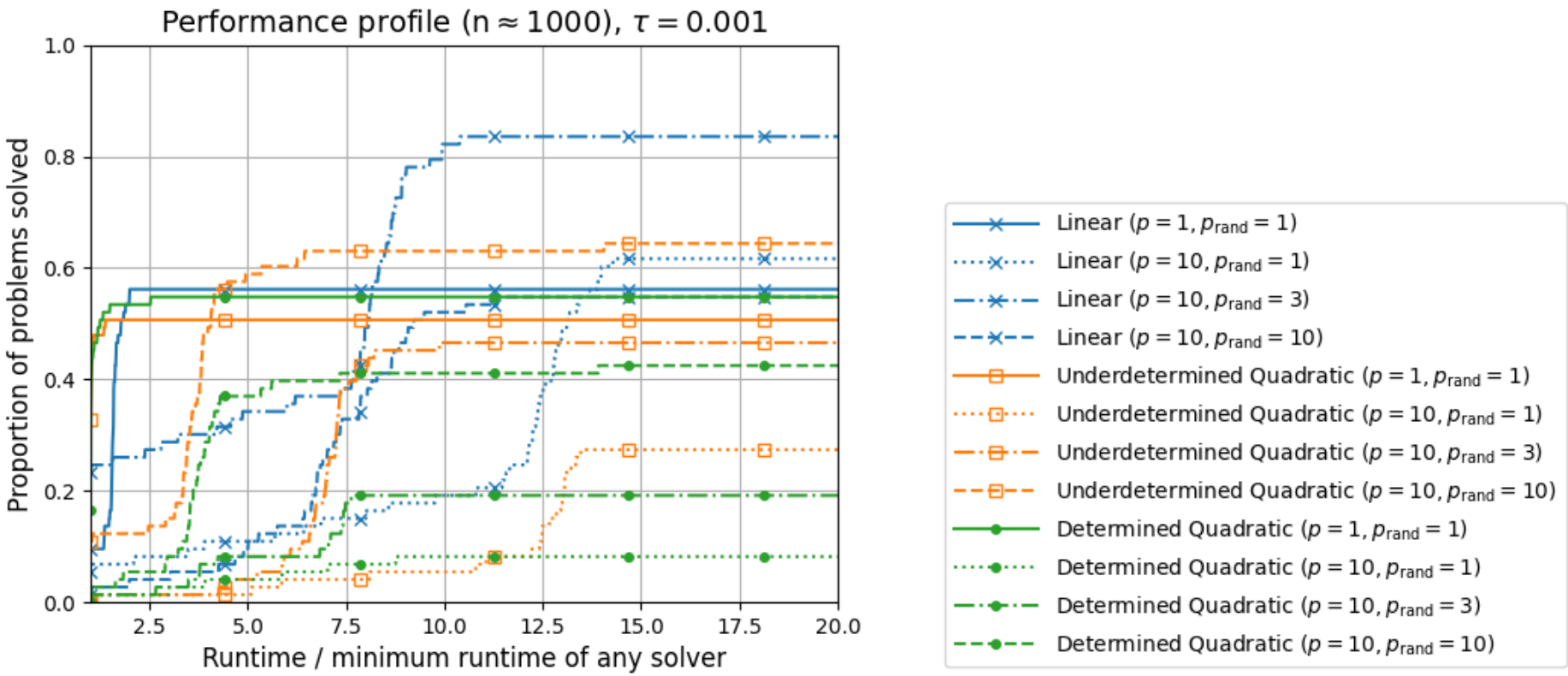
- $f(x_k) \leq f(x^*) + \tau\,(f(x_0) - f(x^*))$ (success)

or

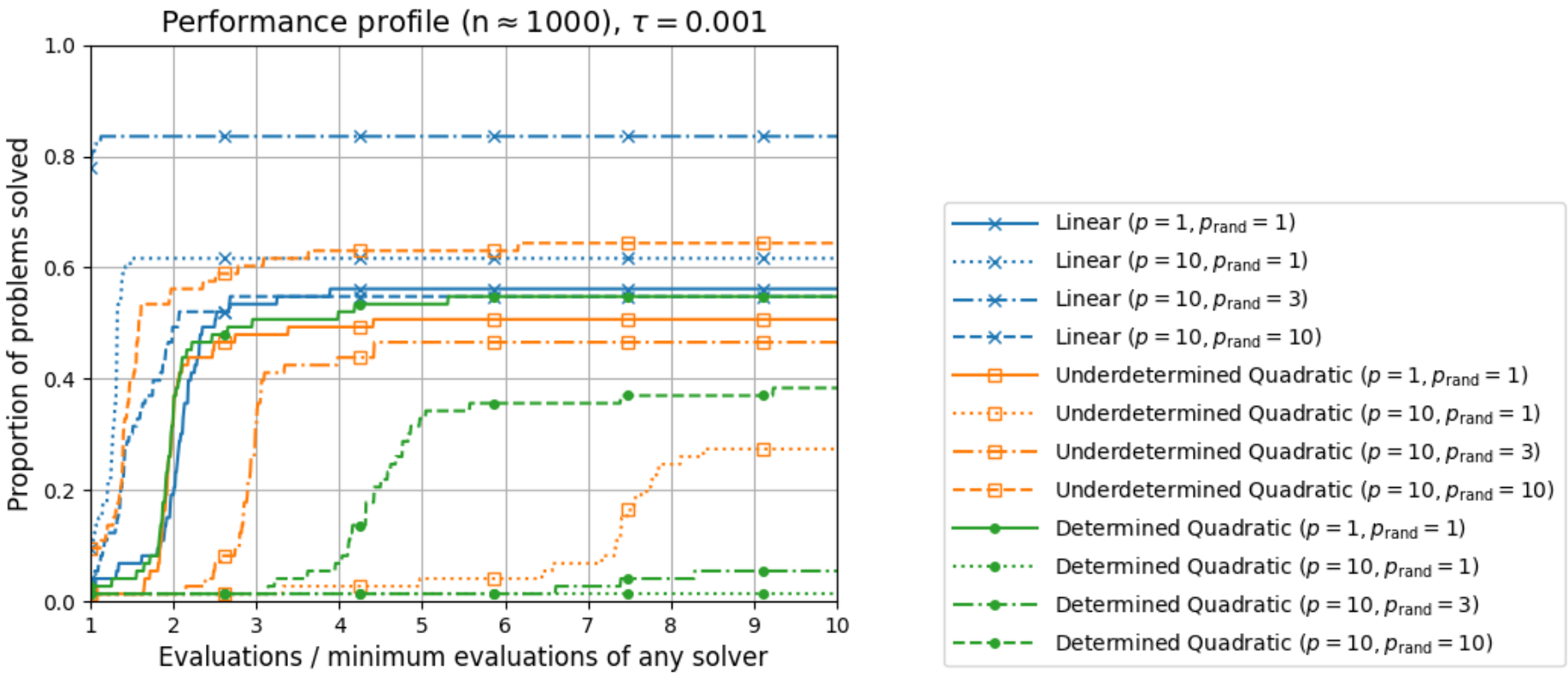
- more than $100(n_P + 1)$ function evaluations are needed (failure)

If success, then $t_{P,S}$ is the number of function evaluations or the runtime
If failure, then $t_{P,S} = \infty$

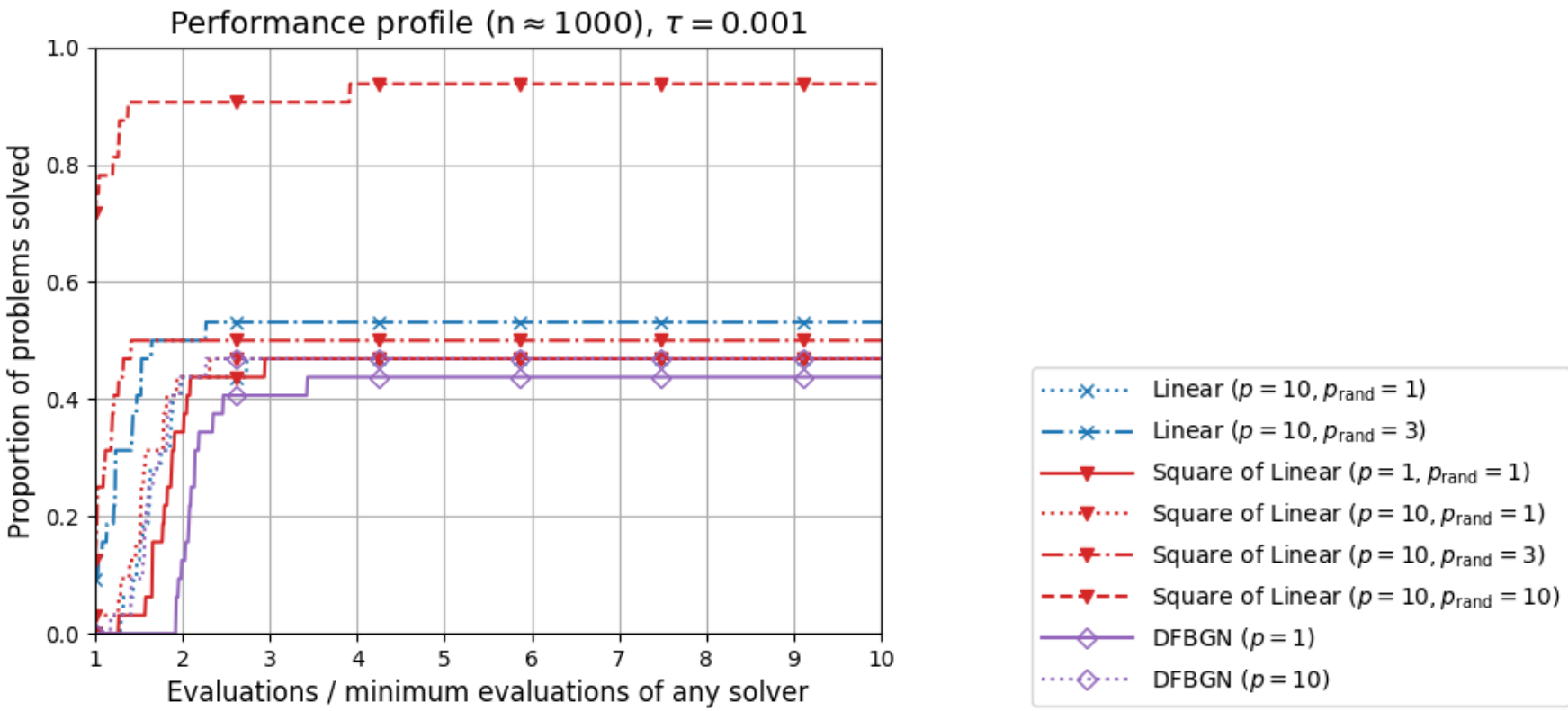
Comparing linear and quadratic models based on runtime



Comparing linear and quadratic models based on evals



Advantages of exploiting the structure of obj functions



Outline

Summary

In this research, we:

- Provided a Q-fully quadratic modeling technique that is easy to analyze and implement
- Proposed an algorithm with convergence analysis for general unconstrained DFO problems
- Demonstrated the efficiency of using quadratic models and exploiting the structure of objective functions

Future directions:

- Compare with other underdetermined quadratic models
- Design better strategies of selecting p and p_{rand}
- Handle constrained DFO problems

Thank you

- Yiwen Chen, Warren Hare, and Amy Wiebe. "Q-fully Quadratic Modeling and its Application in a Random Subspace Derivative-free Method". In: *arXiv preprint* (2023). URL: https://arxiv.org/abs/2312.03169