Model-Based Derivative-Free Methods for Constrained Optimization

Joint work with Lindon Roberts (ANU)

Matthew Hough, University of Queensland $\Rightarrow$ University of Waterloo
mhough@uwaterloo.ca

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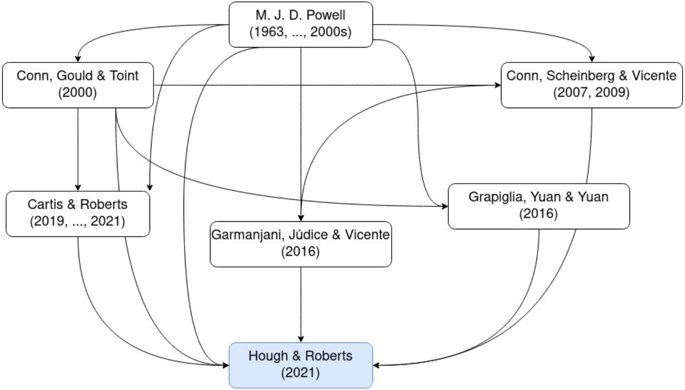
Background


M. J. D. Powell
(1963, ..., 2000s)
Conn, Gould & Toint
(2000)
Conn, Scheinberg & Vicente
(2007, 2009)
Cartis & Roberts
(2019, ..., 2021)
Grapiglia, Yuan & Yuan
(2016)
Garmanjani, Júdice & Vicente
(2016)
Hough & Roberts
(2021)

Outline

1. Introduction to DFO trust-region methods
2. Handling constraints
3. Application to composite minimization
4. Numerical results

The Problem

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

- $f : \mathbb{R}^n \to \mathbb{R}$ continuously differentiable and possibly nonconvex
- Assume we cannot evaluate $\nabla f(\boldsymbol{x})$
  - Black-box
  - Noisy
  - Computationally expensive
- Applications: climate modelling, experimental design, machine learning, etc
- Seeking a local minimizer (approx. stationary point: $\|\nabla f(\boldsymbol{x}^*)\| \leq \epsilon$)

Model-Based DFO

- Classic approach:

$$f(\boldsymbol{x}_k + \boldsymbol{s}) \approx m_k(\boldsymbol{s}) = f(\boldsymbol{x}_k) + \nabla f(\boldsymbol{x}_k)^T \boldsymbol{s} + \frac{1}{2}\boldsymbol{s}^T \nabla^2 f(\boldsymbol{x}_k)\boldsymbol{s}$$

- Instead, approximate:

$$f(\boldsymbol{x}_k + \boldsymbol{s}) \approx m_k(\boldsymbol{s}) = f(\boldsymbol{x}_k) + \boldsymbol{g}_k{}^T \boldsymbol{s} + \frac{1}{2}\boldsymbol{s}^T H_k \boldsymbol{s}$$

- Find $\boldsymbol{g}_k$ and H_k by interpolating f over a set of points

Model-Based DFO: Algorithm

(assuming our interpolation model is a good approx.)

1. Build local interpolation model:

$$f(\boldsymbol{x}_k + \boldsymbol{s}) \approx m_k(\boldsymbol{s})$$

2. Minimize the model within the trust-region Δ_k to get the step

$$\boldsymbol{s}_k = \arg\min_{s \in \mathbb{R}^d} m_k(\boldsymbol{s}) \quad \text{s.t. } \|\boldsymbol{s}\|_2 \leq \Delta_k$$

3. Evaluate $f(\boldsymbol{x}_k + \boldsymbol{s}_k)$, check sufficient decrease, select $\boldsymbol{x}_{k+1}$ and Δ_{k+1}
4. Update interpolation set with the new point $\boldsymbol{x}_k + \boldsymbol{s}_k$

Model-Based DFO: Interpolation Geometry

We may not get sufficient decrease if...

1. Δ_k is too large
2. m_k is not a good approximation to f (bad geometry)

Problems!

- How to ensure good geometry?
- How do we define good geometry?

Good geometry $\implies$ accurate model $\implies$ convergence

Model-Based DFO: Interpolation Geometry

- Need interpolation set $\{\boldsymbol{y}_0, \ldots, \boldsymbol{y}_n\}$ to be "well-poised" in $B(\boldsymbol{y}_0, \Delta)$
- **Λ-poised** if all $\boldsymbol{y}_t \in B(\boldsymbol{y}_0, \Delta)$ and exists $\Lambda \geq 1$ s.t.

$$\max |\ell_t(\boldsymbol{y})| \leq \Lambda, \quad \forall \boldsymbol{y} \in B(\boldsymbol{y}_0, \Delta)$$

  - $\ell_t(\boldsymbol{y}_s) = \delta_{s,t}$ for all s, t
  - Points are "well-spaced"

[Conn, Scheinberg & Vicente, 2009]

Model-based DFO: Interpolation Geometry

- Λ-poisedness $\implies$ fully linear model:
  - $|f(\boldsymbol{x}_k + \boldsymbol{s}) - m(\boldsymbol{s})| \leq \kappa_{ef} \Delta_k^2$
  - $\|\nabla f(\boldsymbol{x}_k + \boldsymbol{s}) - \nabla m(\boldsymbol{s})\| \leq \kappa_{eg} \Delta_k$

(κ_{ef}, κ_{eg} depend on Λ)

for all $\boldsymbol{y} \in B(\boldsymbol{y}_0, \Delta_k)$, $\|\boldsymbol{s}\| \leq \Delta_k$

- Fully linear model $\implies$ convergence
- Two important algorithms:
  1. Checks $\{\boldsymbol{y}_0, \ldots, \boldsymbol{y}_n\}$ is Λ-poised
  2. Makes $\{\boldsymbol{y}_0, \ldots, \boldsymbol{y}_n\}$ Λ-poised if it is not already

[Conn, Scheinberg & Vicente, 2009]

The Constrained Problem

$$\min_{\boldsymbol{x} \in \mathcal{C}} f(\boldsymbol{x})$$

- $f : \mathbb{R}^n \to \mathbb{R}$ continuously differentiable and possibly nonconvex
- Assume we cannot evaluate $\nabla f(\boldsymbol{x})$
- $\mathcal{C} \subseteq \mathbb{R}^d$ has nonempty interior, closed, and convex
  - Cannot evaluate f outside of $\mathcal{C}$
  - Only accessible via projection, $P_{\mathcal{C}} : \mathbb{R}^d \to \mathcal{C}$

Constrained DFO: Algorithm

1. Build local interpolation model from feasible points:

$$f(\boldsymbol{x}_k + \boldsymbol{s}) \approx m_k(\boldsymbol{s})$$

2. Minimize the model within $B(\boldsymbol{y}_0, \Delta_k) \cap \mathcal{C}$ to get the step

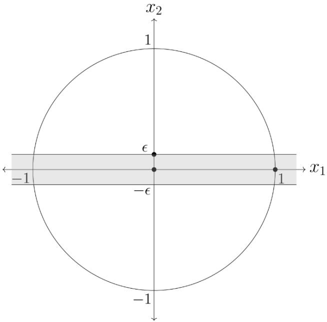
$$\boldsymbol{s}_k = \underset{\boldsymbol{s} \in B(\boldsymbol{y}_0, \Delta_k) \cap \mathcal{C}}{\arg\min} \; m_k(\boldsymbol{s})$$

3. Evaluate $f(\boldsymbol{x}_k + \boldsymbol{s}_k)$, check sufficient decrease, select $\boldsymbol{x}_{k+1}$ and Δ_{k+1}
4. Update interpolation set with the new point $\boldsymbol{x}_k + \boldsymbol{s}_k$

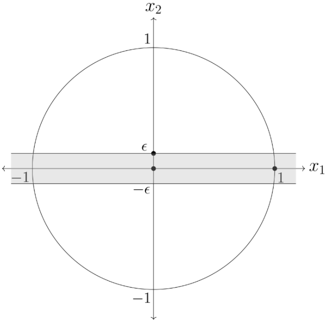
Constrained DFO: Geometry

- $\mathcal{C} = \{(x_1, x_2) \ : \ |x_2| \leq \epsilon\} \subseteq \mathbb{R}^2$
- $Y = \{(0,0), (1,0), (0,\epsilon)\} \subseteq B(\mathbf{0}, 1)$
- In $B(\mathbf{0}, 1)$, points are Λ-poised with $\Lambda \sim \epsilon^{-1}$

$\implies$ large κ_{ef}, κ_{eg}



Constrained DFO: Geometry



- $\mathcal{C} = \{(x_1, x_2) \; : \; |x_2| \leq \epsilon\} \subseteq \mathbb{R}^2$
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- In $B(\mathbf{0}, 1)$, points are Λ-poised with $\Lambda \sim \epsilon^{-1}$

$\implies$ large κ_{ef}, κ_{eg}

- **Λ-poised** if all $\boldsymbol{y}_t \in B(\boldsymbol{y}_0, \Delta) \cap \mathcal{C}$ and exists $\Lambda \geq 1$ s.t.

$$\max |\ell_t(\boldsymbol{y})| \leq \Lambda, \quad \forall \boldsymbol{y} \in B(\boldsymbol{y}_0, \Delta) \cap \mathcal{C}$$

- Now we have $\Lambda \leq 3$ independent of $\epsilon \implies$ improved error bounds

Constrained DFO: Geometry

- Λ-poisedness $\implies$ fully linear model in $B(\boldsymbol{x}_k, \Delta_k)$:

$$\max_{\substack{\boldsymbol{x}_k+\boldsymbol{s}\in\mathcal{C} \\ \|\boldsymbol{s}\|\leq\Delta_k}} |f(\boldsymbol{x}_k+\boldsymbol{s}) - m_k(\boldsymbol{s})| \leq \kappa_{ef}\Delta_k^2$$

$$\max_{\substack{\boldsymbol{x}_k+\boldsymbol{s}\in\mathcal{C} \\ \|\boldsymbol{s}\|\leq 1}} |(\nabla f(\boldsymbol{x}_k) - \boldsymbol{g}_k)^T \boldsymbol{s}| \leq \kappa_{eg}\Delta_k$$

- Slightly weaker:
  - $\nabla m(\boldsymbol{y}) \approx \nabla f(\boldsymbol{y})$ only at $\boldsymbol{y} = \boldsymbol{x}_k$
  - Only care about points in $\mathcal{C}$
- Still have important algorithms
  1. Check points are Λ-poised
  2. Make points Λ-poised if not

Constrained DFO: Measuring Progress

$$\pi^f(\boldsymbol{x}) := \left| \min_{\substack{x+s\in\mathcal{C} \\ \|s\|\leq 1}} \nabla f(\boldsymbol{x})^T \boldsymbol{s} \right| \quad \Longrightarrow \quad \pi^m(\boldsymbol{x}) := \left| \min_{\substack{x+s\in\mathcal{C} \\ \|s\|\leq 1}} \boldsymbol{g}_k{}^T \boldsymbol{s} \right|$$

- For $\mathcal{C} = \mathbb{R}^d$, $\pi^f(\boldsymbol{x}_k) = \|\nabla f(\boldsymbol{x}_k)\|$, and $\pi^g(\boldsymbol{x}_k) = \|\boldsymbol{g}_k\|$
- fully linear $\Longrightarrow$ $|\pi^f(\boldsymbol{x}_k) - \pi^m(\boldsymbol{x}_k)| \leq \kappa_{eg}\Delta_k$

[Conn, Gould & Toint, 2000]

Constrained DFO: Measuring Progress

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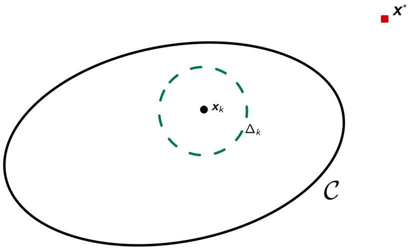
- For $\mathcal{C} = \mathbb{R}^d$, $\pi^f(\boldsymbol{x}_k) = \|\nabla f(\boldsymbol{x}_k)\|$, and $\pi^g(\boldsymbol{x}_k) = \|\boldsymbol{g}_k\|$
- fully linear $\implies |\pi^f(\boldsymbol{x}_k) - \pi^m(\boldsymbol{x}_k)| \le \kappa_{eg}\Delta_k$

Solution to $\pi^f(\boldsymbol{x})$ is given by $\boldsymbol{s}^\star := p(t, \boldsymbol{x}) - \boldsymbol{x}$

- where $p(t, \boldsymbol{x}) = P_{\mathcal{C}}(\boldsymbol{x} - t\nabla f(\boldsymbol{x}))$, $t \ge 0$,
- and $\|p(t, \boldsymbol{x}) - \boldsymbol{x}\| = 1$

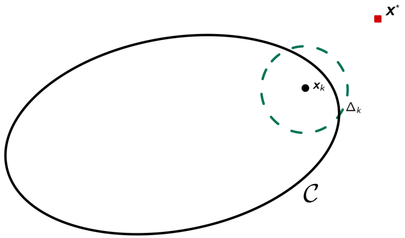
[Conn, Gould & Toint, 2000]

Constrained DFO: Measuring Progress



- $s^\star = P_{\mathcal{C}}(x - t\nabla f(x)) - x = -t\nabla f(x)$
- $1 = \|s^\star\| = t\|\nabla f(x)\| \implies t = \frac{1}{\|\nabla f(x)\|} \implies s^\star = \frac{-\nabla f(x)}{\|\nabla f(x)\|}$
- $\implies \pi^f(x) = \|\nabla f(x)\|$

Constrained DFO: Measuring Progress



- $P_C(\boldsymbol{x} - t\nabla f(\boldsymbol{x})) \neq \boldsymbol{x} - t\nabla f(\boldsymbol{x})$
- $\boldsymbol{s}^\star = p(t, \boldsymbol{x}) - \boldsymbol{x}$ gets smaller near the boundary
- $\implies \pi^f(\boldsymbol{x}) \to 0$ as approach constraints in direction of $x^\star$

Constrained DFO: Convergence Theory

1. Ensure we always have m_k fully linear (by ensuring good geometry)
2. Ensure $\pi_k^m \sim \Delta_k$
3. When $\pi^m(\boldsymbol{x}_k) \to 0$, we are also getting $\pi^f(\boldsymbol{x}_k) \to 0$
4. Standard convergence results follow

- Worst-case complexity: at most $\mathcal{O}(\epsilon^{-2})$ iterations to have $\pi_k^m \leq \epsilon$

Application to composite minimization

$$f(\boldsymbol{x}) = F(\boldsymbol{r}(\boldsymbol{x}))$$

- where $\boldsymbol{r} : \mathbb{R}^n \to \mathbb{R}^m$ is a black-box function
- Derivatives of $\boldsymbol{r}(\boldsymbol{x})$ are unavailable
- Classic example is $F(\boldsymbol{r}) = \frac{1}{2}\|\boldsymbol{r}\|^2$

Application to composite minimization

$$\min_{\boldsymbol{x}\in\mathbb{R}^d} f(\boldsymbol{x}) = \frac{1}{2}\|\boldsymbol{r}(\boldsymbol{x})\|_2^2, \qquad \boldsymbol{r}(\boldsymbol{x}) \in \mathbb{R}^n$$

- Typically linearize $\boldsymbol{r}$ at $\boldsymbol{x}_k$ using the Jacobian:

$$\boldsymbol{r}(\boldsymbol{x}_k+\boldsymbol{s}) \approx M(\boldsymbol{s}) = \boldsymbol{r}(\boldsymbol{x}_k)+J(\boldsymbol{x}_k)\boldsymbol{s}$$

- But in DFO, Jacobian is not available:

$$M(\boldsymbol{s}) = \boldsymbol{r}(\boldsymbol{x}_k) + J_k\boldsymbol{s}$$

- Find J_k by interpolation

End up with a local quadratic model

$$f(\boldsymbol{x}_k + \boldsymbol{s}) \approx m_k(\boldsymbol{s}) := \frac{1}{2}\|M_k(\boldsymbol{s})\|_2^2$$

Implementation

Open-source Python implementation: *DFO-LS*

- Github: `numericalalgorithmsgroup/dfols`

- Replace gradient-descent step with projected gradient-descent (PGD)
- Dykstra's algorithm for projecting onto $\mathcal{C}$
- New point becomes

$$\boldsymbol{x}_{k+1} = P_{\mathcal{Q}}(\boldsymbol{x}_k - t\boldsymbol{g}_k)$$

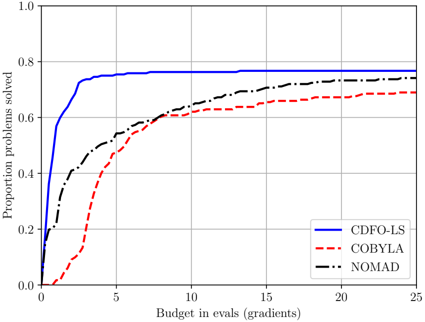
$\mathcal{Q} := \mathcal{C} \cap B(\boldsymbol{x}_k, \Delta_k)$

[Beck, 2017]

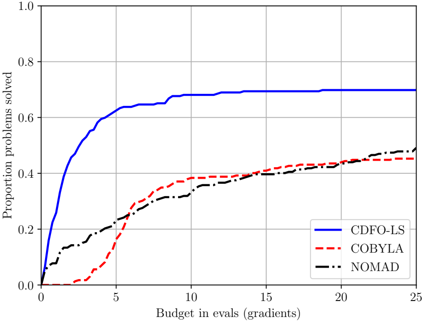
Numerical results

58 test problems with ball, box, halfspace, and no constraints

- [Moré & Wild, 2009], [Moré, Garbow, Hillstrom, 1981]



$\tau = 10^{-1}$



$\tau = 10^{-3}$

Constrained DFO: Summary

- Can ensure good geometry

  $\Longrightarrow$ fully linear model

  $\Longrightarrow$ error bound on approx. criticality measure

  $\Longrightarrow$ convergence

- Worst-case complexity same as in unconstrained case

Constrained DFO: Future Work

- Convergence and WCC theory for quadratic models
- Fully quadratic model, etc.

References

[1] Amir Beck. *First-Order Methods in Optimization*. Oct. 2017.

[2] Coralia Cartis and Lindon Roberts. "A derivative-free Gauss-Newton method". In: *Mathematical Programming Computation* 11.4 (2019), pp. 631–674.

[3] Andrew R. Conn, Nicholas I. M. Gould, and Philippe L. Toint. *Trust-Region Methods*. Vol. 1. MPS-SIAM Series on Optimization. Philadelphia: MPS/SIAM, 2000.

[4] Andrew R. Conn, Katya Scheinberg, and Luís N. Vicente. *Introduction to Derivative-Free Optimization*. Vol. 8. MPS-SIAM Series on Optimization. Philadelphia: MPS/SIAM, 2009.

[5] Jorge J. Moré, Burton S. Garbow, and Kenneth E. Hillstrom. "Testing Unconstrained Optimization Software". In: *ACM Transactions on Mathematical Software* 7.1 (Mar. 1981), pp. 17–41.

[6] Jorge J. Moré and Stefan M. Wild. "Benchmarking Derivative-Free Optimization Algorithms". In: *SIAM Journal on Optimization* 20.1 (Jan. 2009), pp. 172–191.