A Surrogate-model-based Algorithm for Multi-objective Optimization

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Presentation outline

1. Multi-objective optimization
2. Pareto optimality
3. A trust-region method for multi-objective optimization
4. Model computation
5. Performance profiles and metrics
6. Multi-objective model in conservation planning

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Multi-objective optimization problem

$$\min_{x \in X \subseteq \mathbb{R}^n} F(x) = (f_1(x), f_2(x), \ldots, f_q(x))^\top$$

$$f_i : \mathbb{R}^n \to \mathbb{R}, \; i = 1, \ldots, q \quad (q \geq 2)$$

$$X = \{x \in \mathbb{R}^n | \, lb \leq x \leq ub, \quad lb, ub \in \mathbb{R}^n\}$$

- Conflicting objectives

Derivative-free features:

- Expensive function evaluation
- Derivatives are not available and are impossible to estimate

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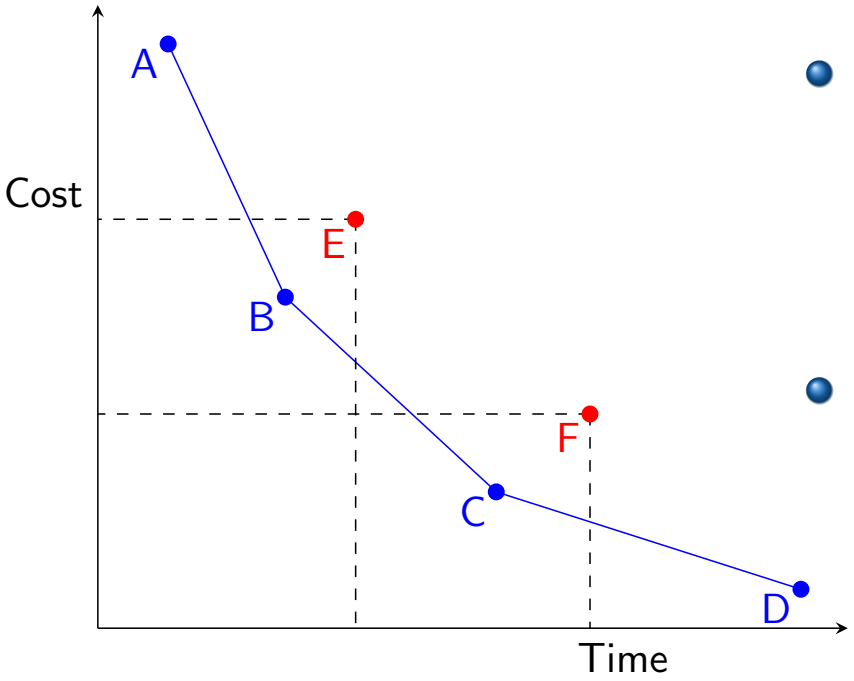
Goal

Develop an algorithm that computes an approximation to the complete Pareto front

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Dominated and nondominated points



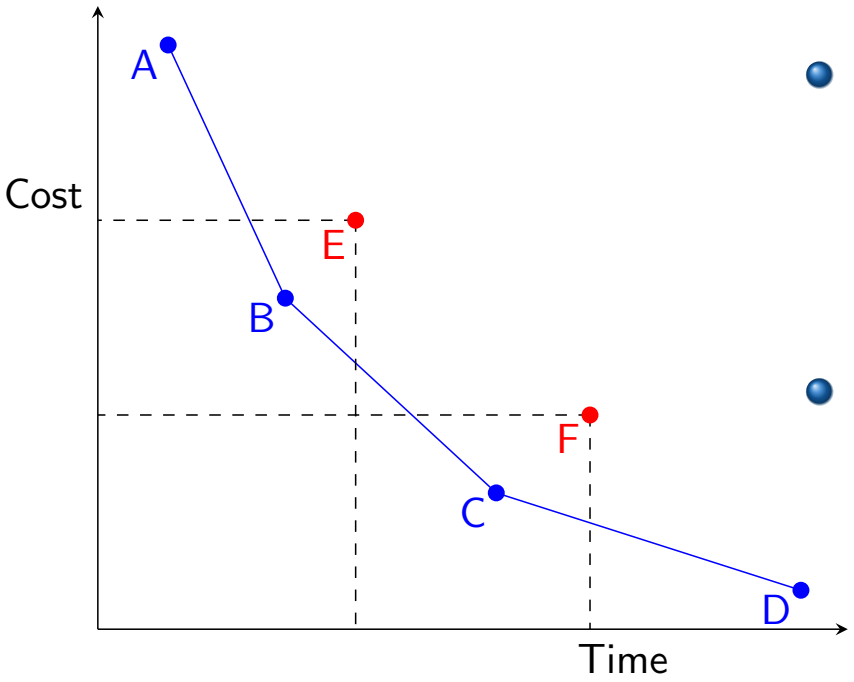
- Cost(B) $<$ Cost(E) & Time(B) $<$ Time(E)

  $\longrightarrow$ B dominates E (or E is dominated by B)

- Cost(C) $<$ Cost(F) & Time(C) $<$ Time(F)

  $\longrightarrow$ C dominates F

Dominated and nondominated points



- Cost(B) $<$ Cost(E) & Time(B) $<$ Time(E)

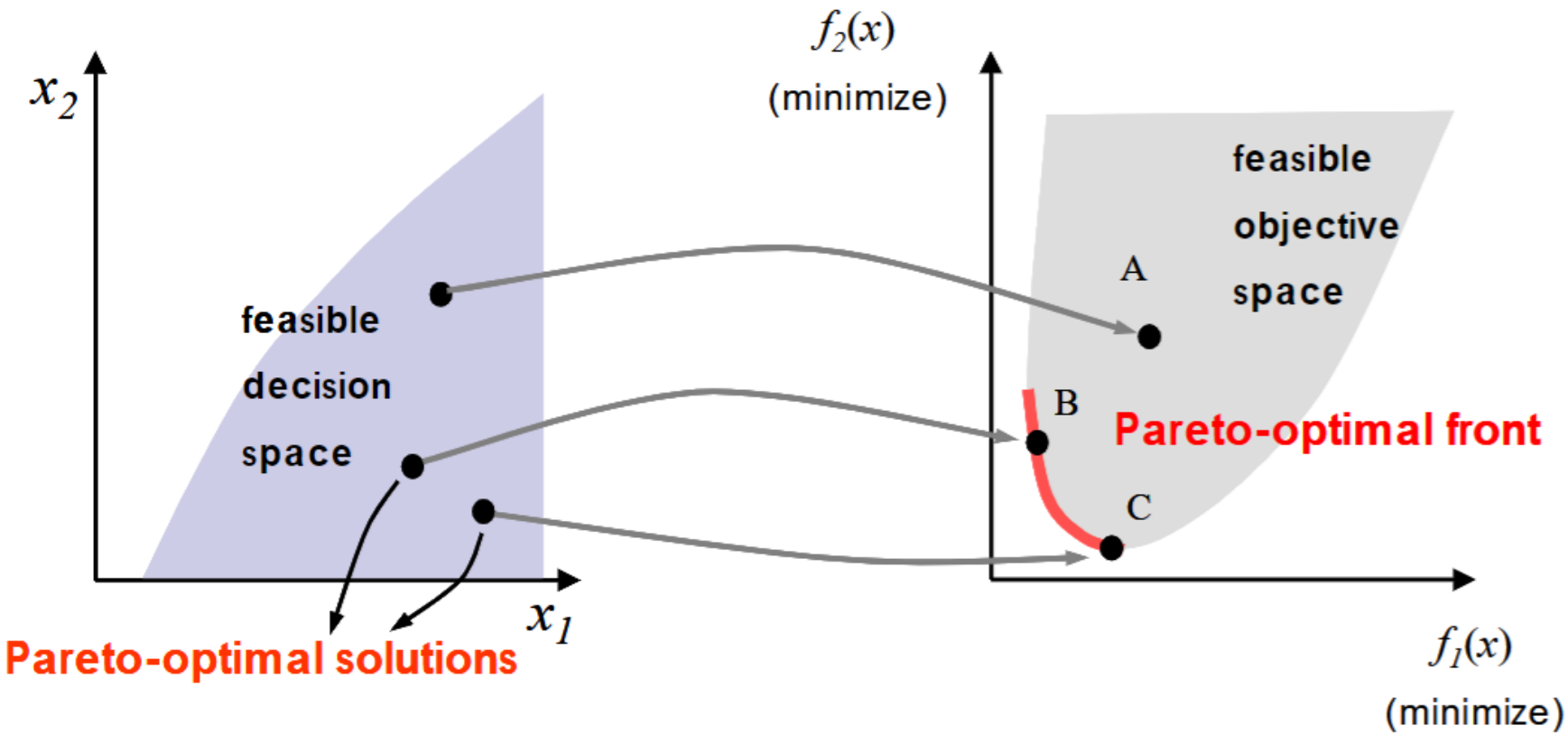
  $\longrightarrow$ B dominates E (or E is dominated by B)

- Cost(C) $<$ Cost(F) & Time(C) $<$ Time(F)

  $\longrightarrow$ C dominates F

- Nondominated points: A, B, C and D
- Dominated points: E and F
- Dominated points can not be solutions

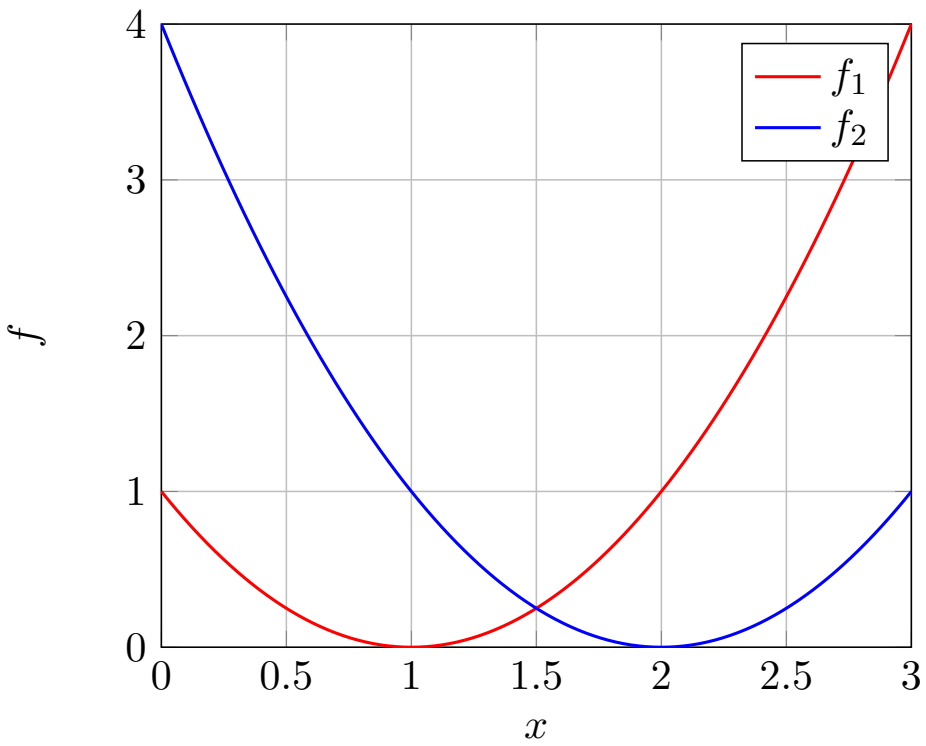
Pareto optimality

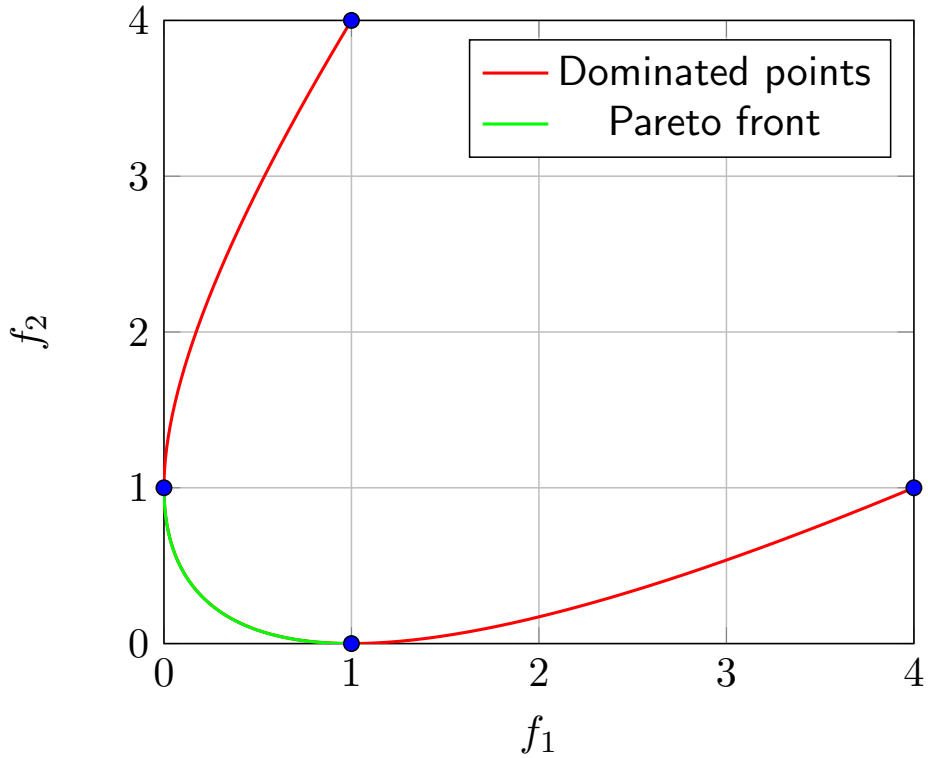


- Pareto front:
  - Set of nondominated points in feasible region

Pareto front example

$$\min f_1(x) = (x-1)^2$$
$$\min f_2(x) = (x-2)^2$$
$$\text{s.t. } 0 \leq x \leq 3$$



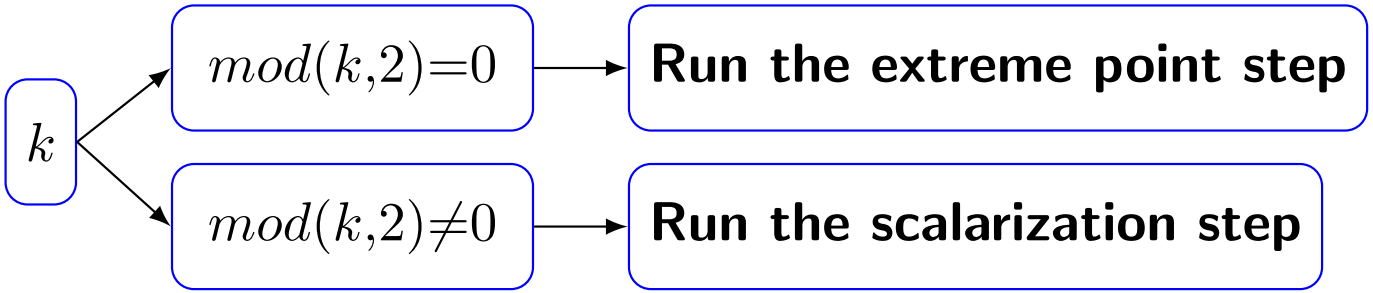


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Main algorithmic structure

For $k = 0, 1, ...$



Check the stopping criteria

Extreme point step

For $i = 1, ..., q$

Do a single-objective

trust-region iteration on f_i

Extreme point step

For $i = 1, ..., q$

Do a single-objective

trust-region iteration on f_i

Example

$$\min F(x) = (f_1(x), f_2(x))^\top$$

$$f_1(x) = (x_1 - 1)^2 + (x_1 - x_2)^2$$

$$f_2(x) = (x_2 - 3)^2 + (x_1 - x_2)^2$$

$$-1 \leq x_1 \leq 5$$

$$-1 \leq x_2 \leq 5$$

Extreme point step

For $i = 1, ..., q$

Do a single-objective

trust-region iteration on f_i

Example

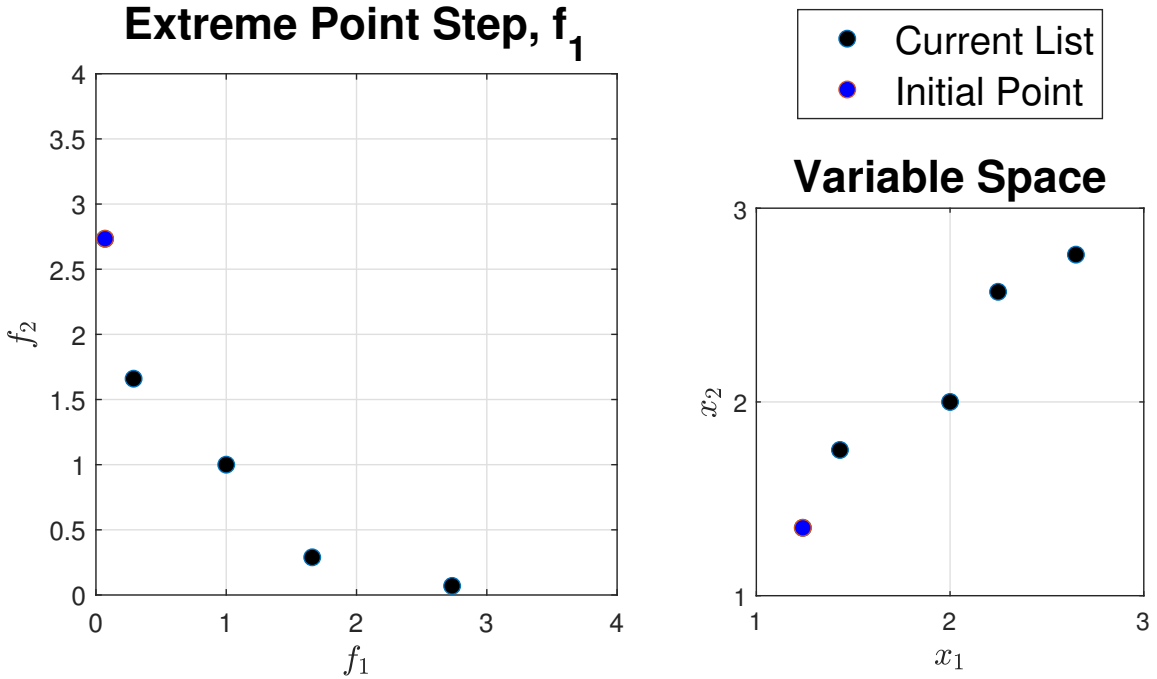
$$\min F(x) = (f_1(x), f_2(x))^\top$$

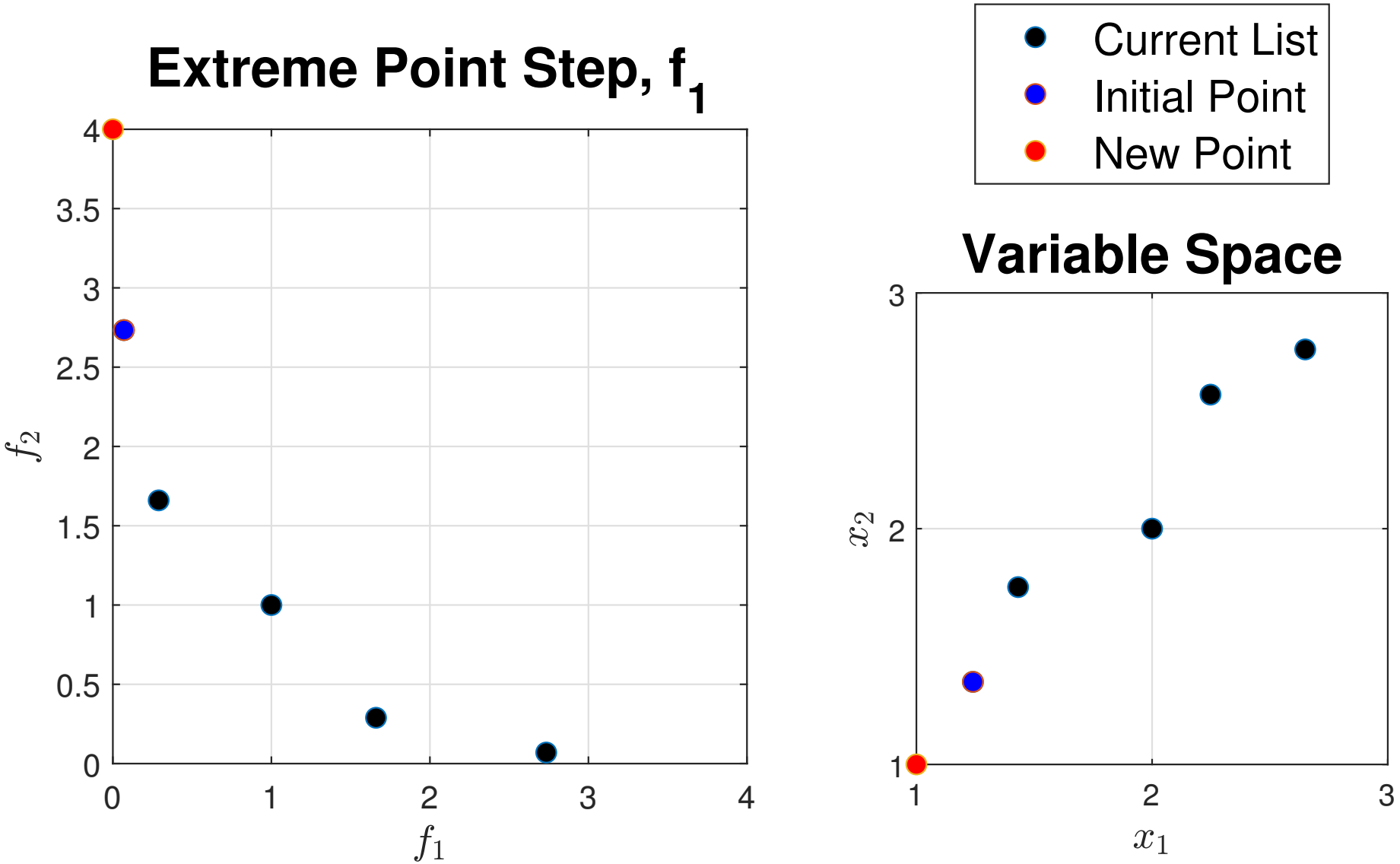
$$f_1(x) = (x_1 - 1)^2 + (x_1 - x_2)^2$$

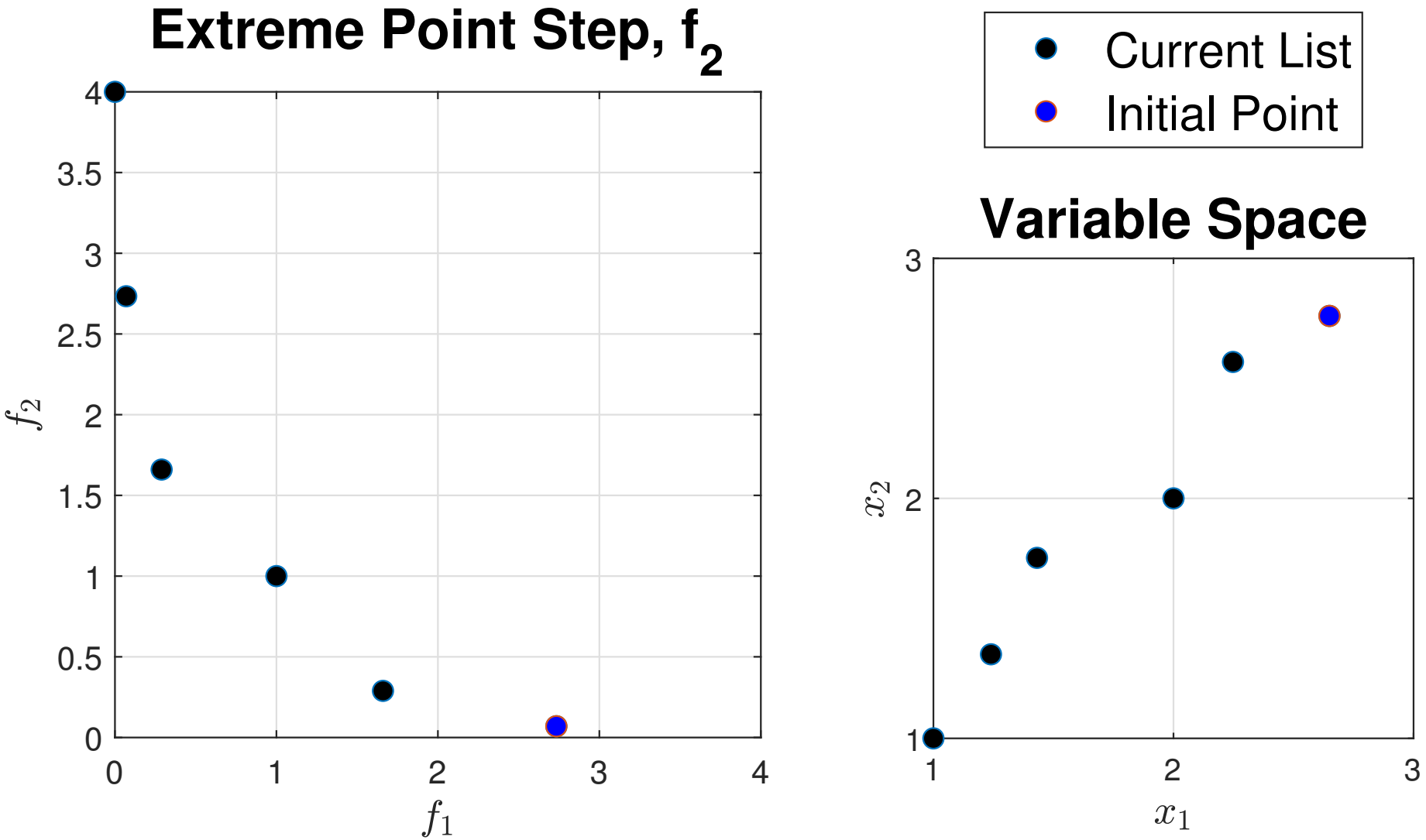
$$f_2(x) = (x_2 - 3)^2 + (x_1 - x_2)^2$$

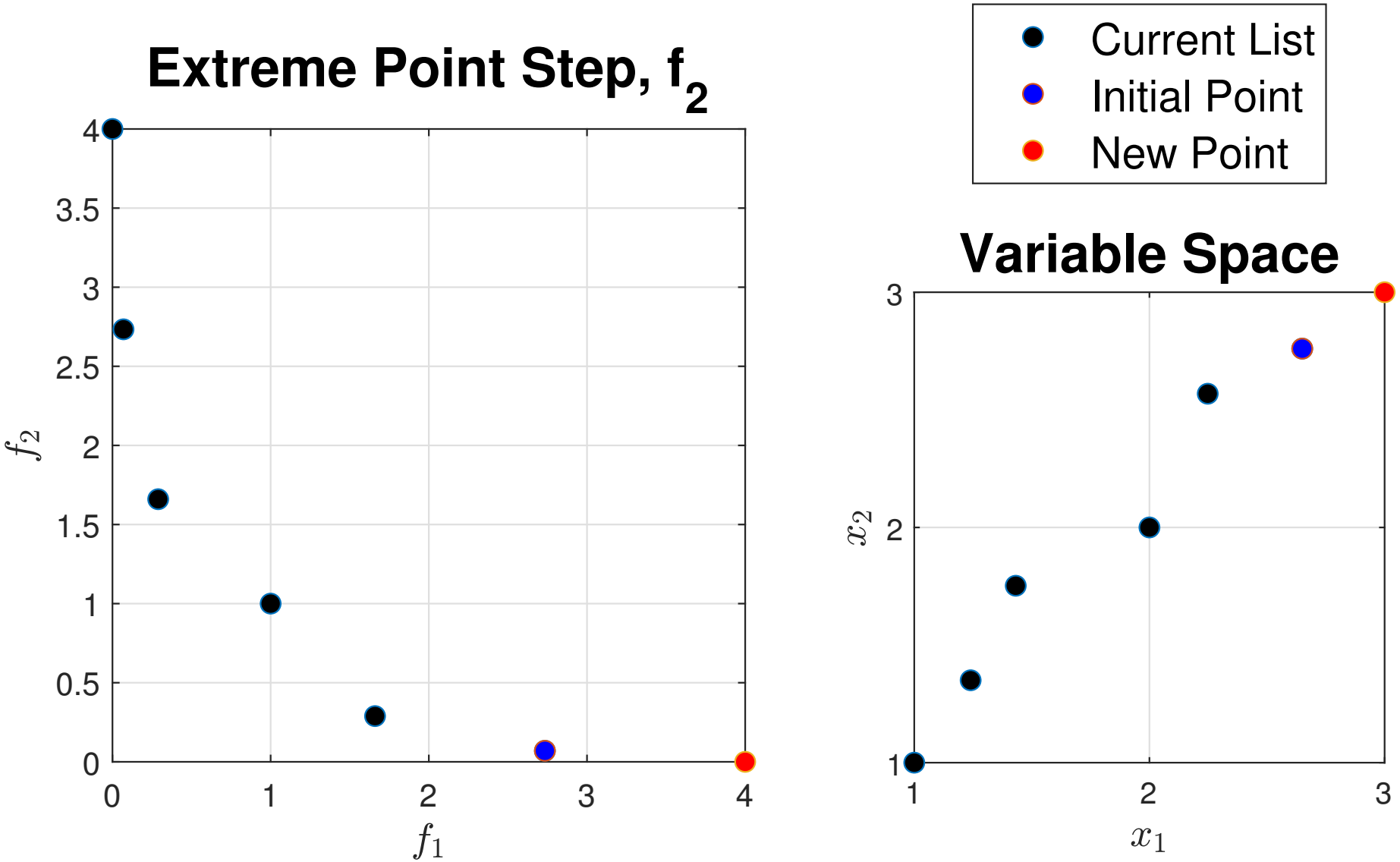
$$-1 \leq x_1 \leq 5$$

$$-1 \leq x_2 \leq 5$$




Extreme Point Step, f1
Current List
Initial Point
New Point
Variable Space
f_1
f_2
x_1
x_2

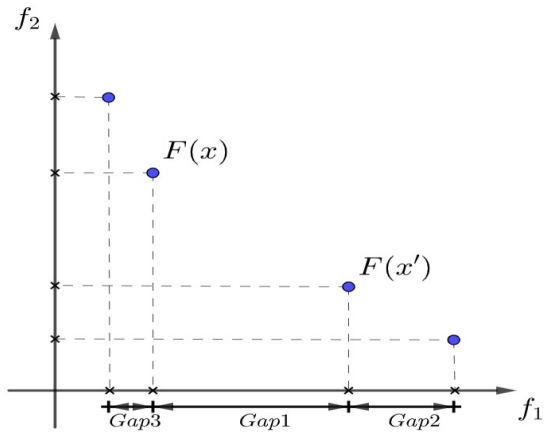

Extreme Point Step, f2
Current List
Initial Point
Variable Space
f2
f1
x2
x1
0
0.5
1
1.5
2
2.5
3
3.5
4


Extreme Point Step, f2
Current List
Initial Point
New Point
Variable Space
f_1
f_2
x_1
x_2
0
0.5
1
1.5
2
2.5
3
3.5
4

Scalarization step: initial point

For $i = 1, ..., q$

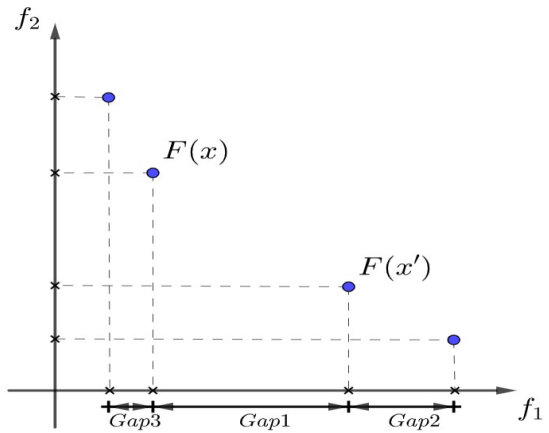
- Sort $\{f_i(x) | x \in L\}$
- Compute and sort the gaps
- Select the largest gap

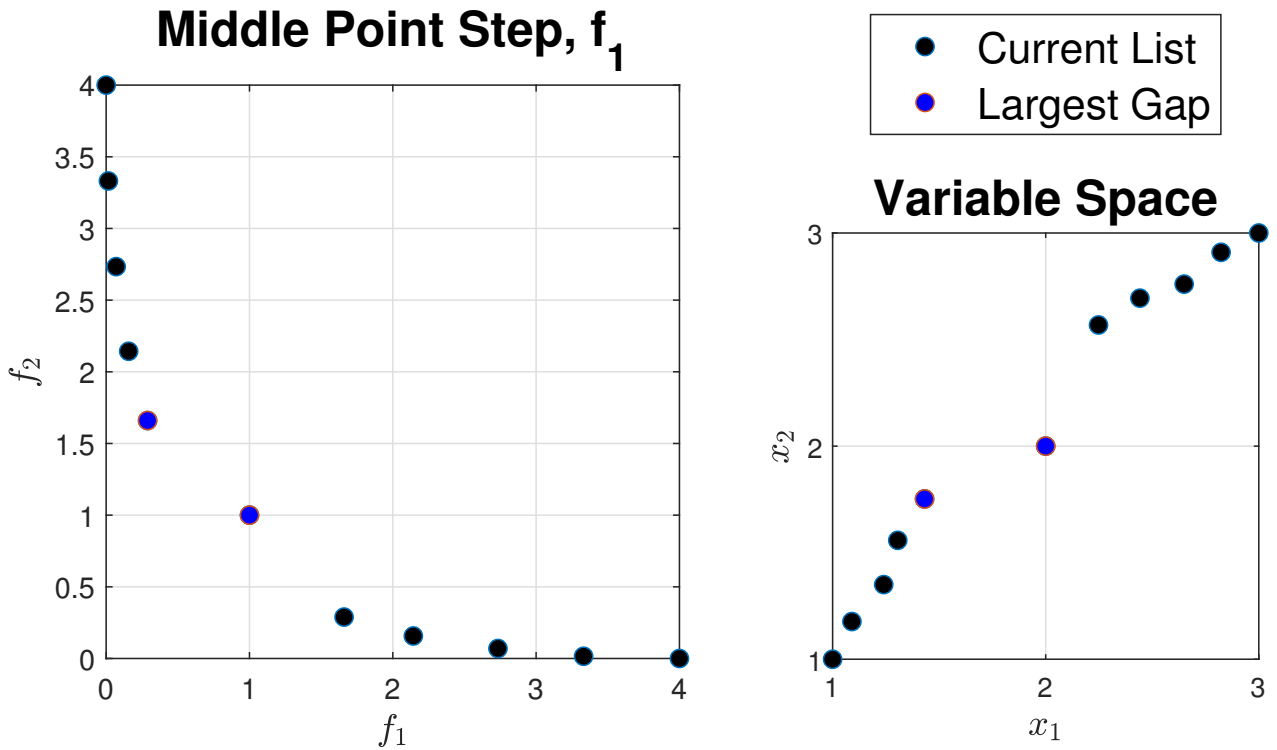


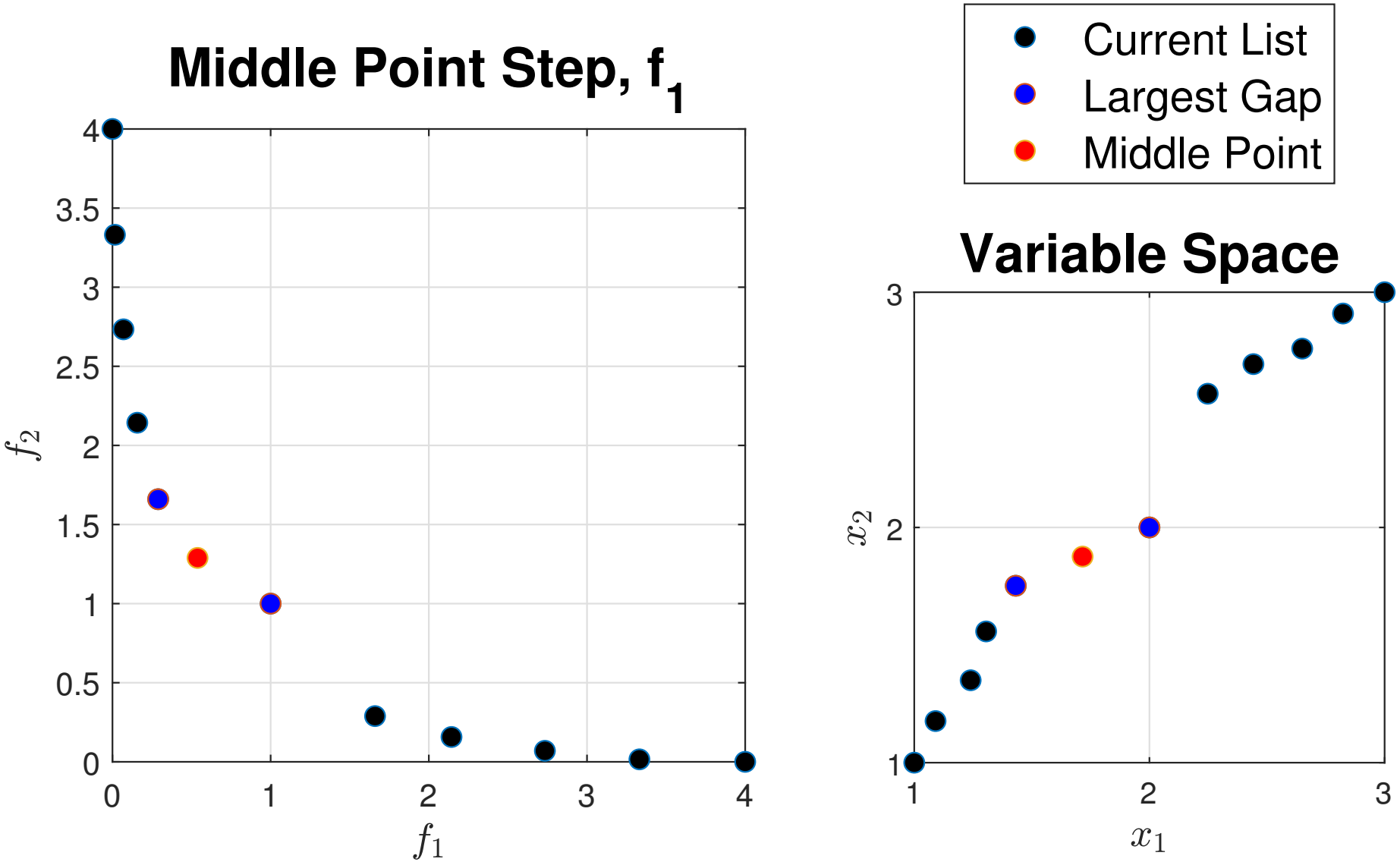
Scalarization step: initial point

For $i = 1, ..., q$

- Sort $\{f_i(x) | x \in L\}$
- Compute and sort the gaps
- Select the largest gap






Middle Point Step, f1
Current List
Largest Gap
Middle Point
Variable Space
f2
f1
x2
x1
0
0.5
1
1.5
2
2.5
3
3.5
4

Scalarization step: model minimization

Compute models m_l, $l = 1, ..., q$, centered at x^i_{sc}

Compute x^{i*}_{sc} by solving

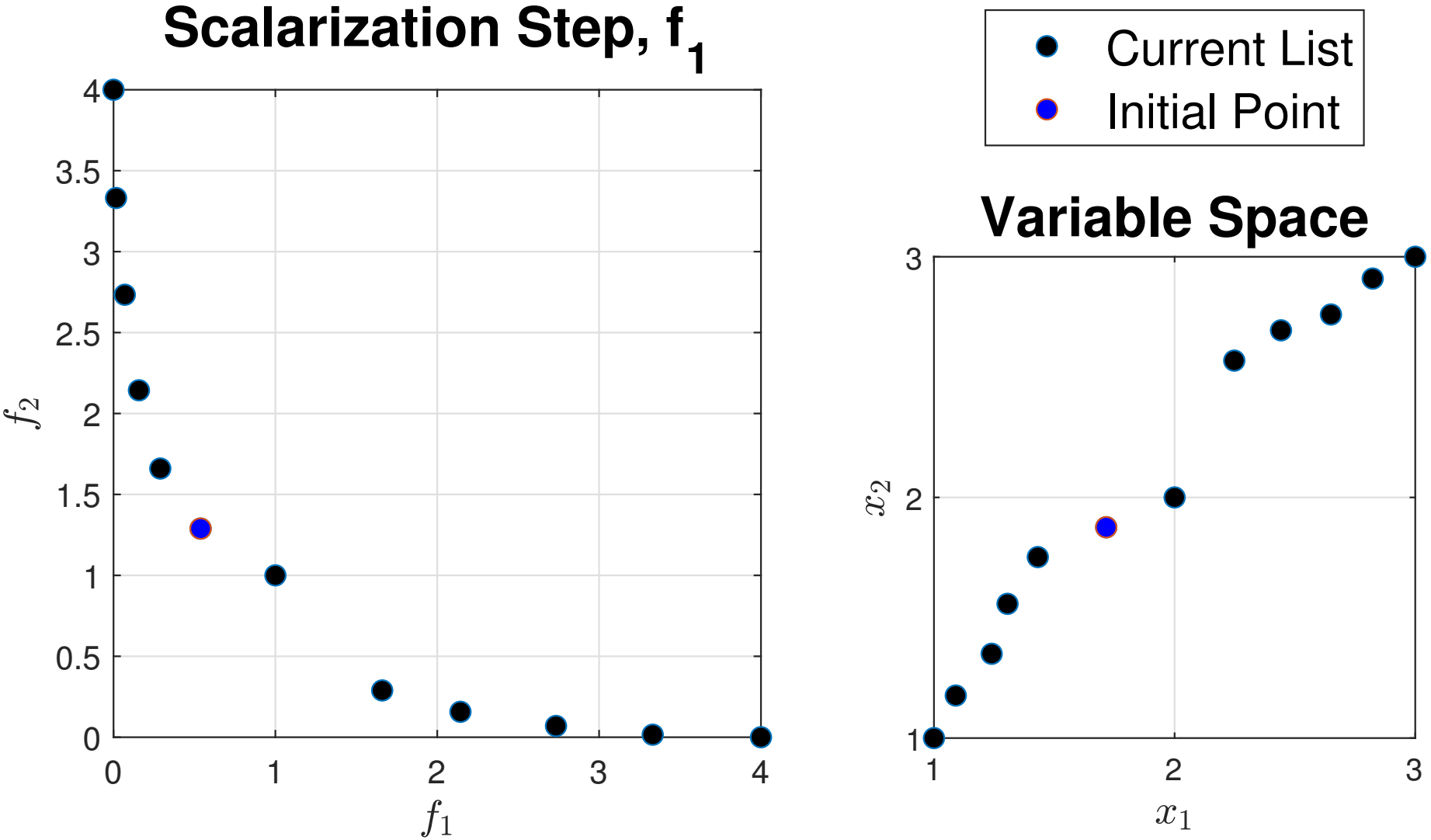
$$\min t$$

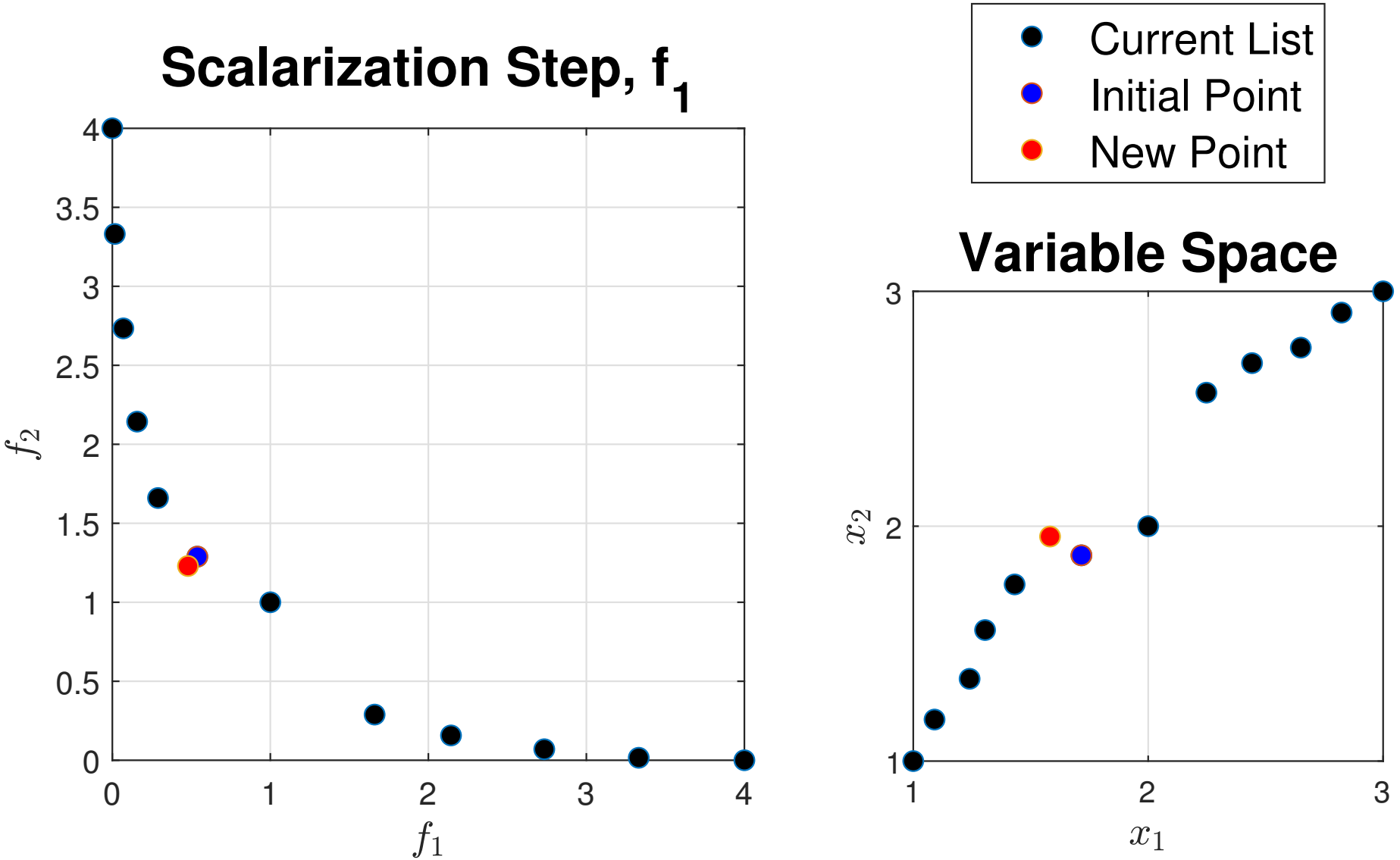
$$\text{s.t.} \quad m_l(x) - m_l(x^i_{sc}) \leq t, \ l = 1, ..., q$$

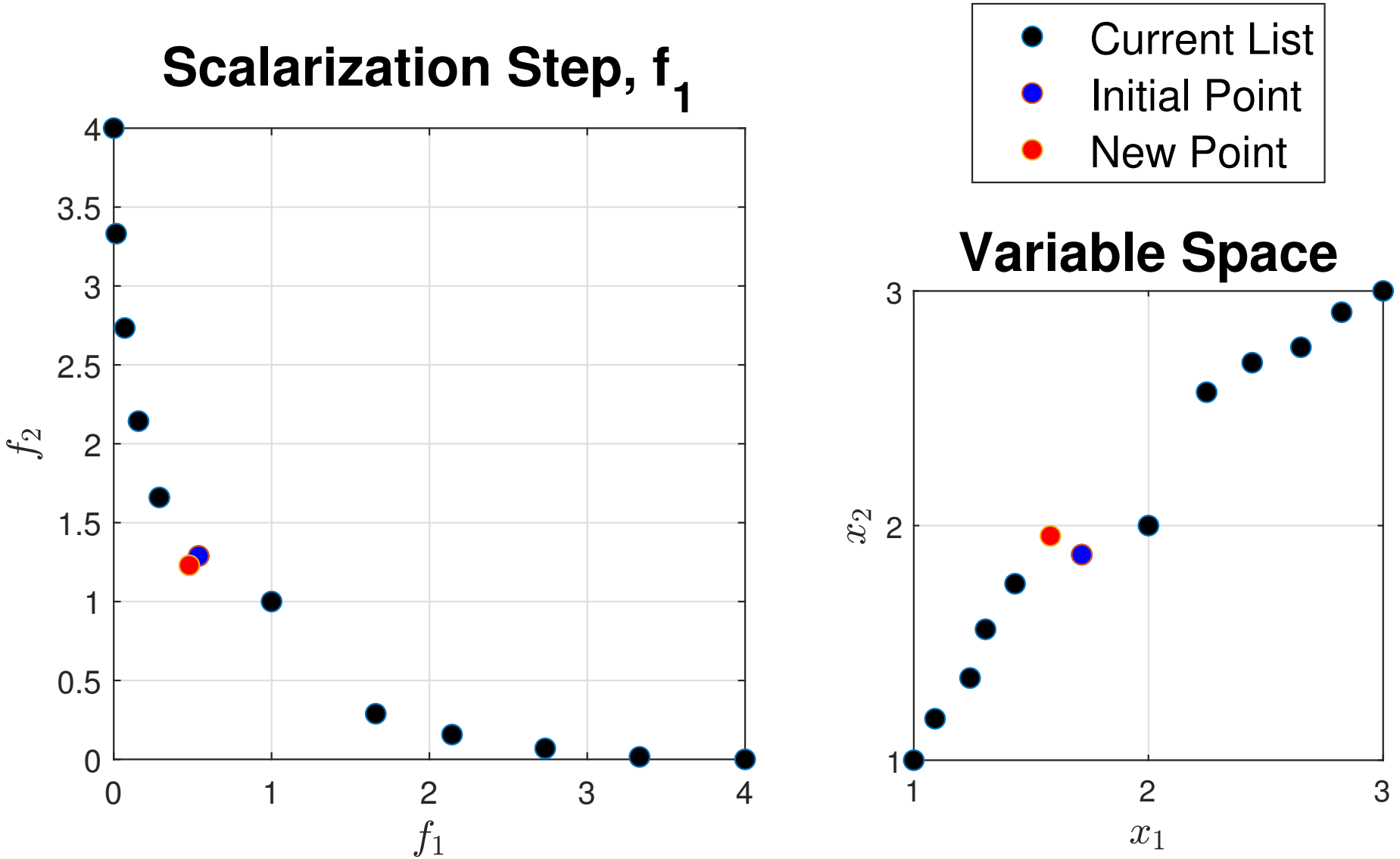
$$x \in B(x^i_{sc}, \Delta^i_{sc})$$

$$lb \leq x \leq ub$$

$$t \in \mathbb{R}$$


Scalarization Step, f1
Current List
Initial Point
Variable Space
f2
f1
x2
x1
0
0.5
1
1.5
2
2.5
3
3.5
4

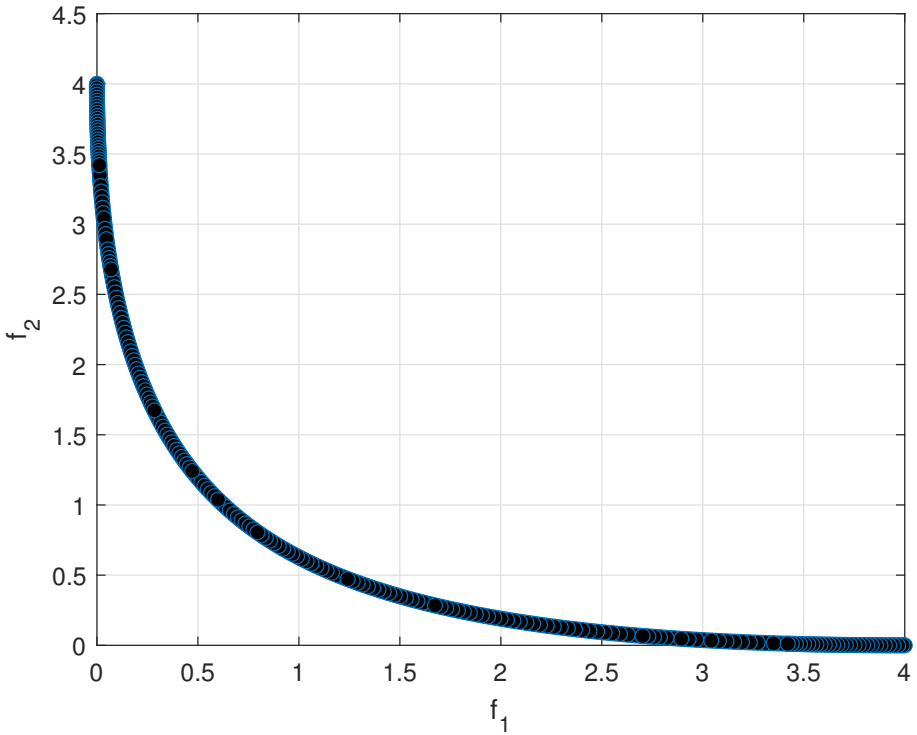

Scalarization Step, f1
Current List
Initial Point
New Point
Variable Space
f2
f1
x2
x1
0
0.5
1
1.5
2
2.5
3
3.5
4

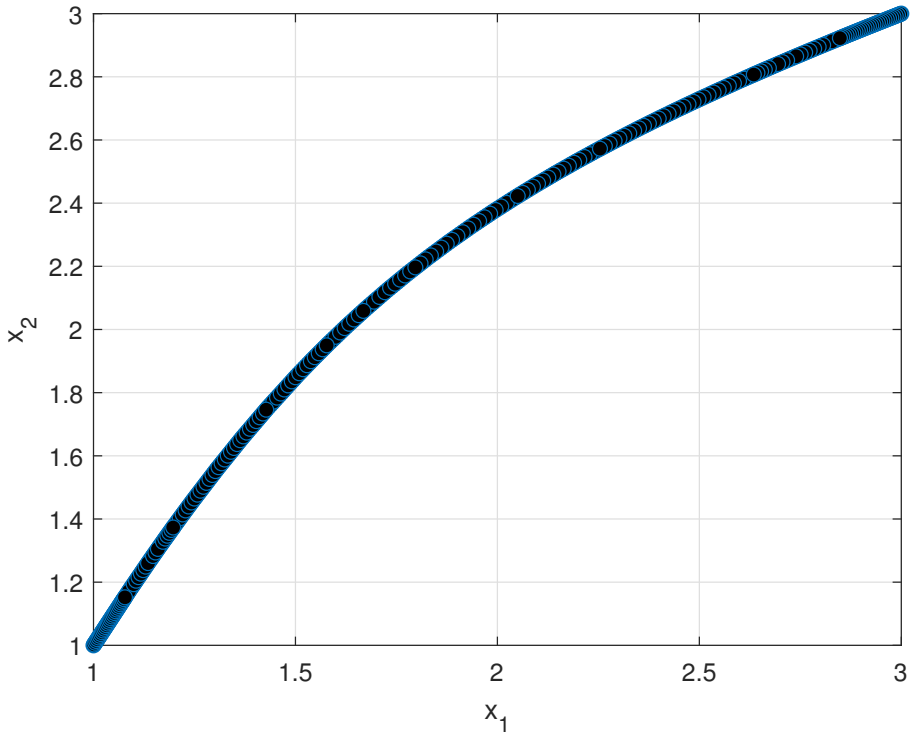


Then, we proceed with the same procedure by considering f_2

Obtained Pareto front by 500 function evaluations

$$\begin{aligned}
\min\ & f_1(x) = (x_1 - 1)^2 + (x_1 - x_2)^2 \\
\min\ & f_2(x) = (x_2 - 3)^2 + (x_1 - x_2)^2 \\
\text{s.t.}\ & -1 \leq x_1 \leq 5 \\
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\end{aligned}$$





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Derivative-based optimization: Taylor models

$$m_i(x) = f_i(x_c) + \nabla f_i(x_c)^\top (x - x_c) + \frac{1}{2}(x - x_c)^\top \nabla^2 f_i(x_c)(x - x_c)$$

Derivative-based optimization: Taylor models

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Derivative-free optimization:

$$m_i(x) = f_i(x_c) + g_i^\top (x - x_c) + \frac{1}{2}(x - x_c)^\top H_i (x - x_c), \quad i = 1, \ldots, q$$

Sample set $Y = \{y^0, y^1, \ldots, y^p\}$ → Interpolation conditions $m_i(y^j) = f_i(y^j), \quad j = 0, \ldots, p$

Numerical interpolation techniques

- $p + 1 = \frac{(n+1)\times(n+2)}{2} \longrightarrow$ Determined interpolation models
- $n + 2 \leq p + 1 < \frac{(n+1)\times(n+2)}{2} \longrightarrow$ Minimum Frobenius norm models

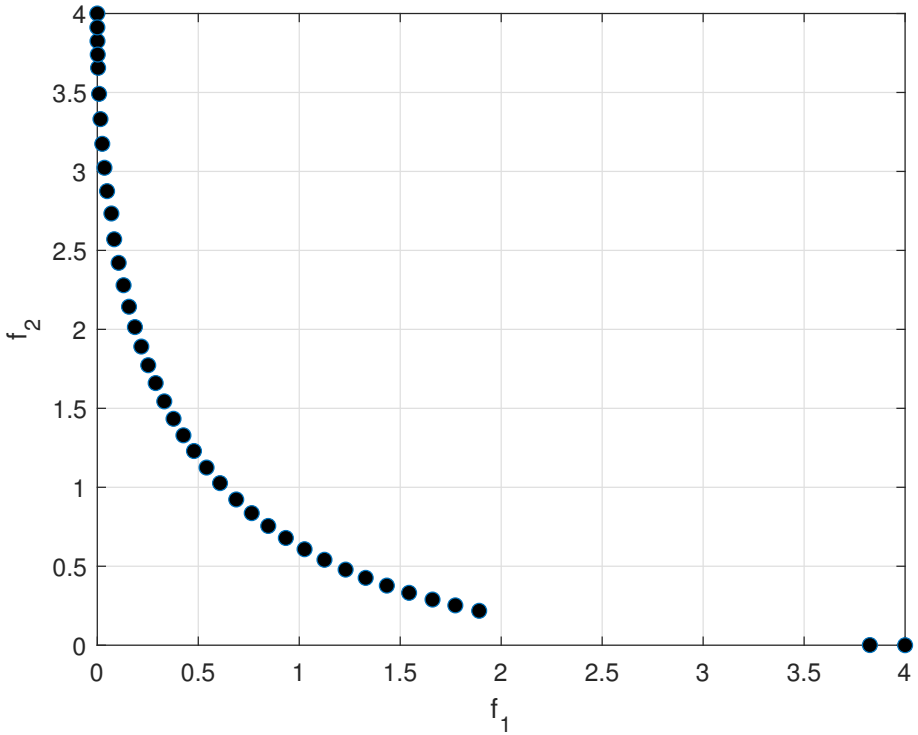
$$\min \|H_i\|^2$$

$$\text{s.t.} \quad m_i(x_j) = f_i(x_j), \quad j = 0, ..., p$$

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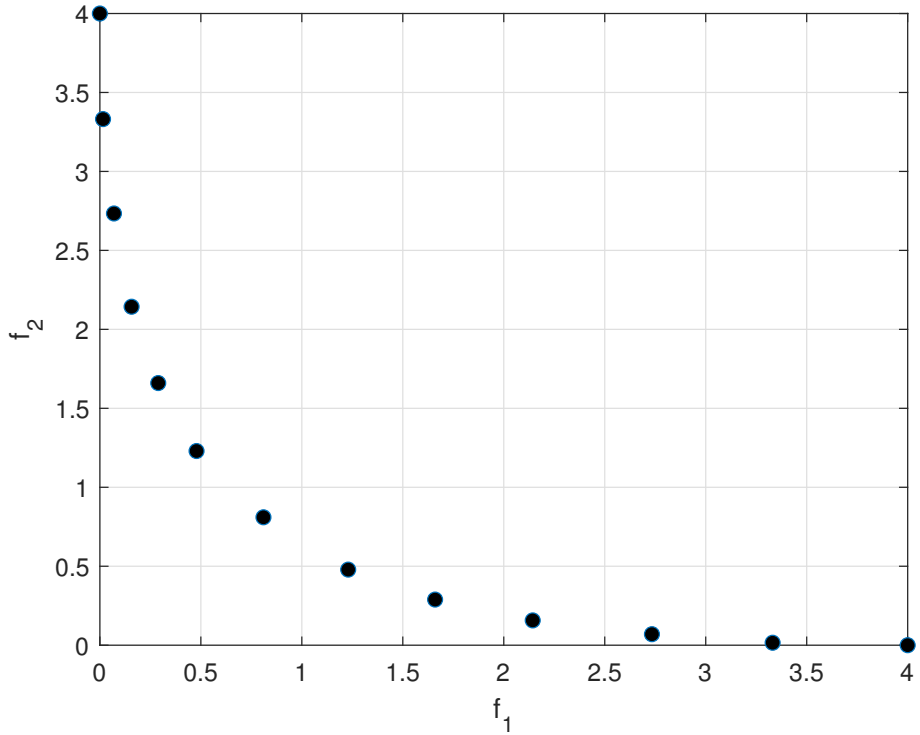
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$$-1 \leq x_2 \leq 5$$



Quantity ✓

Spread ×



Quantity ×

Spread ✓

Performance profiles and metrics

P: set of problems S: set of solvers

$t_{p,s}$: metric value for problem p when solved by solver s

$$r_{p,s} = \frac{t_{p,s}}{\min\{t_{p,\bar{s}} : \bar{s} \in S\}}$$

$$\rho_s(\tau) = \frac{1}{|P|} \text{ size}\{p \in P : r_{p,s} \leq \tau\}$$

E. D. Dolan, J .J. Moré, Benchmarking optimization software with performance profiles. Math. Prog., 91, 201-213 (2002)

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Metrics:

- Purity – Percentage of points generated in the reference Pareto front
- Hypervolume – Volume of the dominated region
- Spread – Largest gap (Γ) and gap uniformity (Δ) in the Pareto front

Problem collection and numerical settings

Test problems:

- 54 bound constrained MOO problems

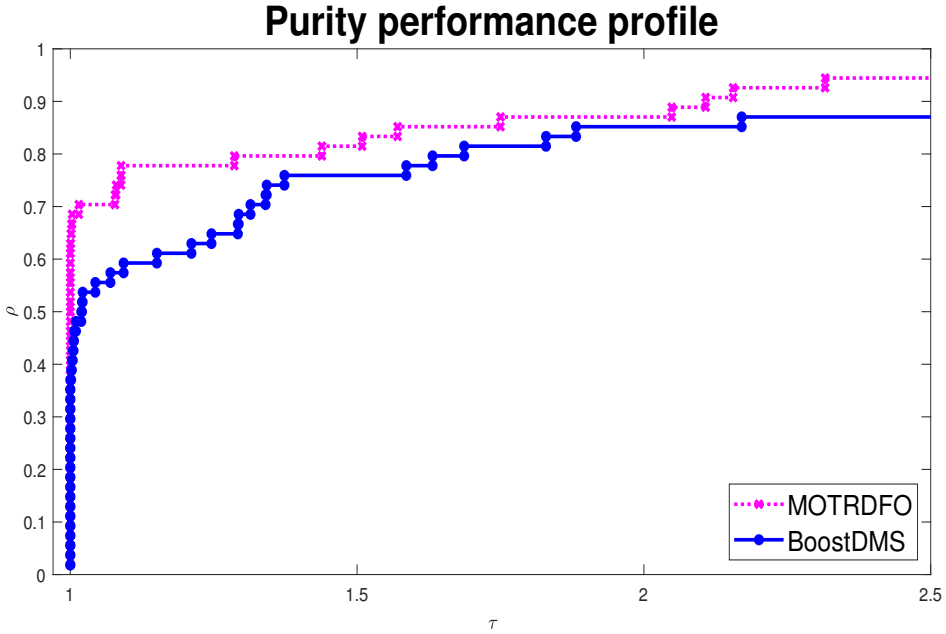
MOTRDFO

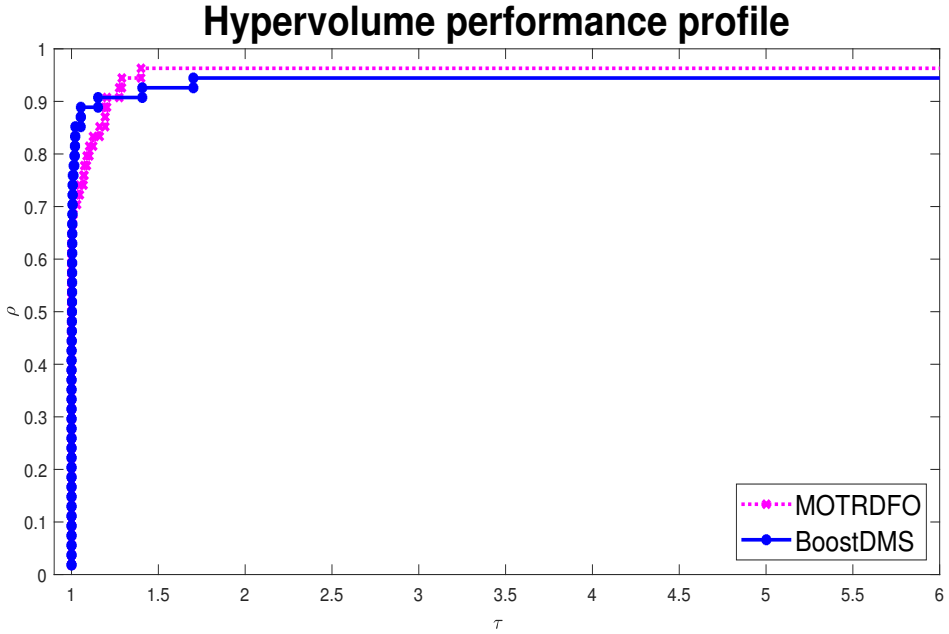
- Multi-objective trust-region derivative-free optimization algorithm
- All default settings

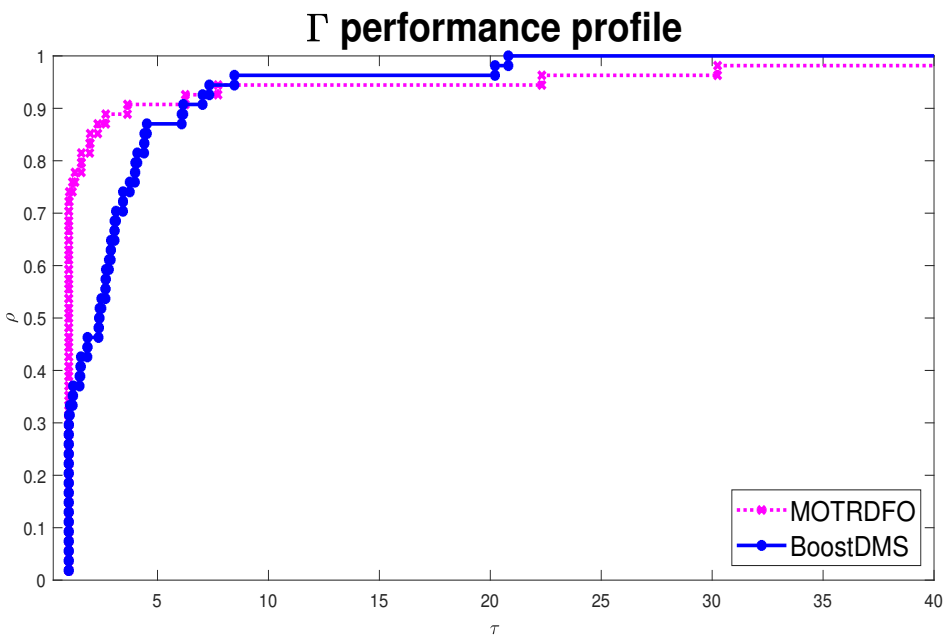
BOOSTDMS

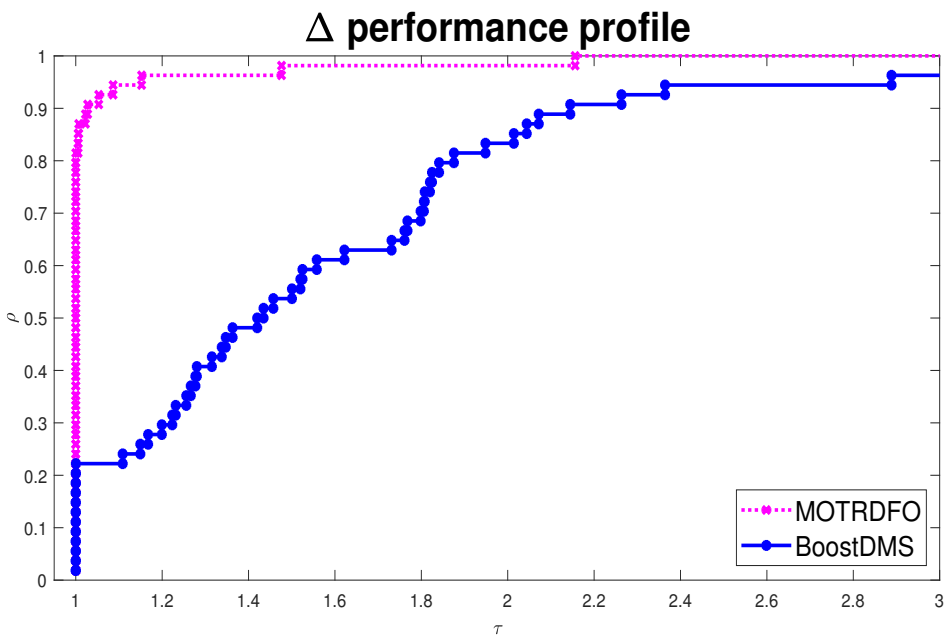
- C.P. Brás and A.L. Custódio, On the use of polynomial models in multiobjective directional direct search, Computational Optimization and Applications, 77, 897-918 (2020)
- All default settings

MOTRDFO VS BOOSTDMS









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Multi-objective model in conservation planning

I: Set of planning units (indexed by i)
J: Set of species (indexed by j)
Parameters:

c_i: Cost of planning unit i

D_{ij}: Genetic diversity of planning unit i for species j

L_{ijk}: Presence/absence of lineage k for species j in planning unit i

n_j: Number of lineages for species j

A_j: Target level of genetic diversity for species j

B_{jk}: Target level of occurrences for lineage k of species j

B_c: Total cost-budget constraint

Decision Variables:

x_i: Binary decision variable indicating whether planning unit $i \in I$ is selected

y: The percentage of target shortfalls for genetic diversity (Continuous variable)

w: The percentage of target shortfalls for lineage occurrence (Continuous variable)

Multi-objective model in conservation planning

Objective Functions:

$$\text{Minimize: } y$$

$$\text{Minimize: } w$$

Constraints:

$$\sum_{i \in I} D_{ij}\, x_i + A_j\, y \geq A_j, \quad \forall j \in J$$

$$\sum_{i \in I} L_{ijk}\, x_i + B_{jk}\, w \geq B_{jk}, \quad \forall j \in J,\ \forall k \in \{1, \ldots, n_j\}$$

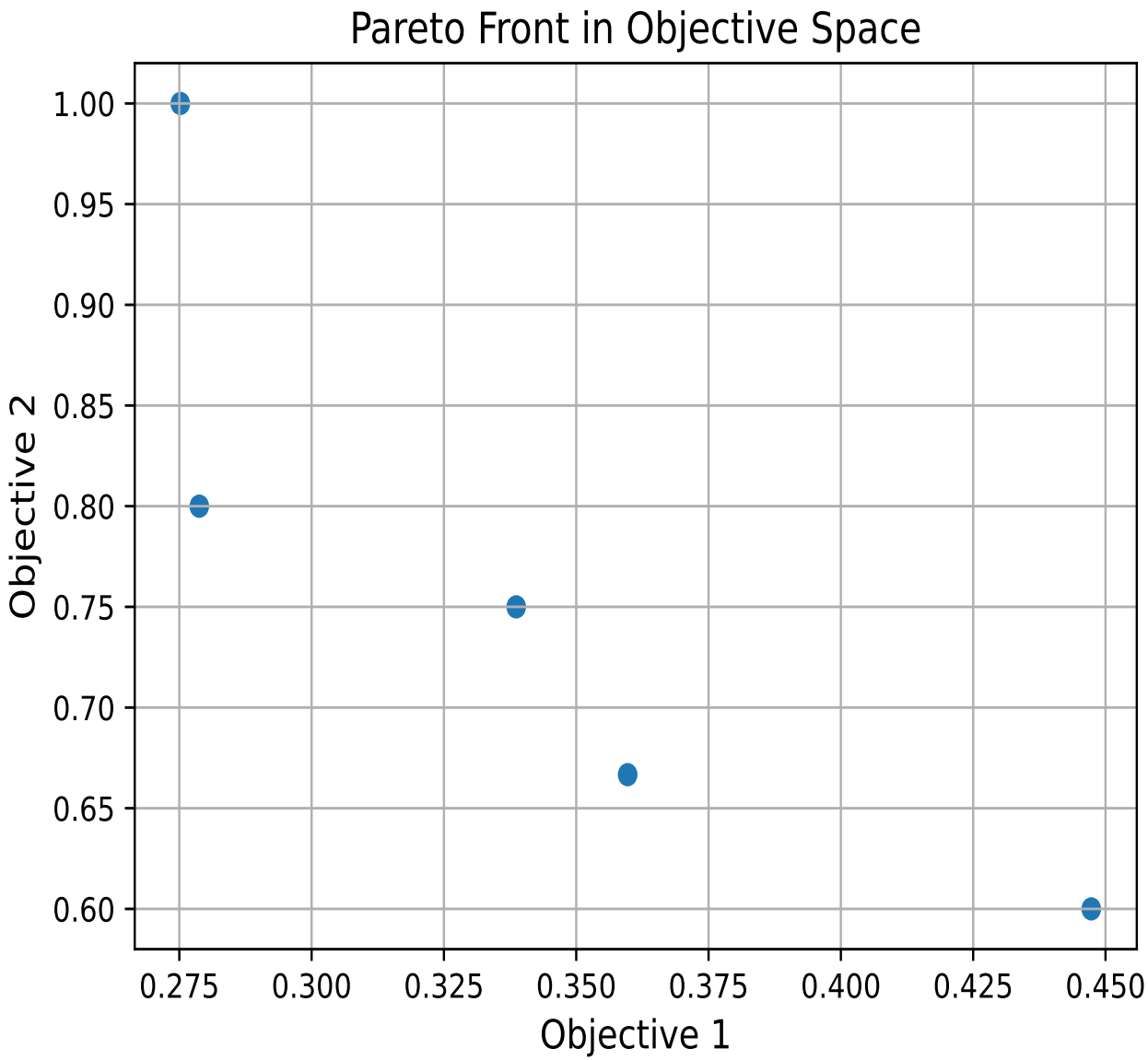
$$\sum_{i \in I} c_i\, x_i \leq B_c$$

$$0 \leq y \leq 1$$

$$0 \leq w \leq 1$$

$$x_i \in \{0, 1\} \quad \forall i \in I$$

The approximation to the complete Pareto front



Thank you for your attention!



PLACES

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