

Addressing Constraints in Direct Multisearch

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UIDP/00297/2020

Presentation Outline

- ① Problem Definition
- ② DMS
- ③ DMS-FILTER-IR
- ④ LOG-DMS
- ⑤ Conclusions and Future Work

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Multiobjective Derivative-free Optimization

$$\min_{x \in \Upsilon \subseteq \mathbb{R}^n} F(x) \equiv (f_1(x), f_2(x), \dots, f_m(x))^{\top}$$

$$f_j : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}, \quad j = 1, \dots, m \geq 2$$

- several **objectives**, often **conflicting**
- **expensive** function evaluation
- **impossible** to use or approximate **derivatives**

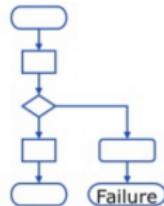
Blackboxes as illustrated by J. Simonis [ISMP 2009]



Long runtime



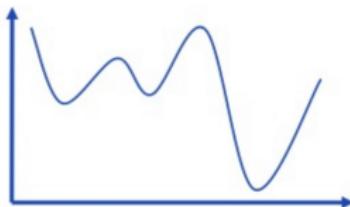
Large memory requirement



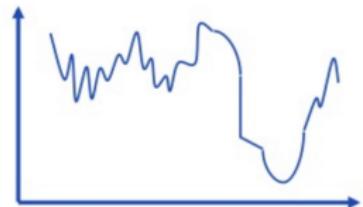
Software might fail



No derivatives available



Local optima



Non-smooth,
noisy

Numerical Optimization

Iterative Methods

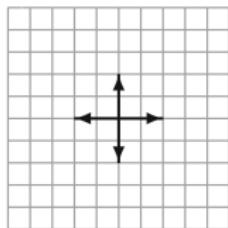
$$x_{k+1} = x_k + \alpha_k d_k$$

- Derivative-based methods: d_k should be a descent direction according to at least one of the objectives, i.e.

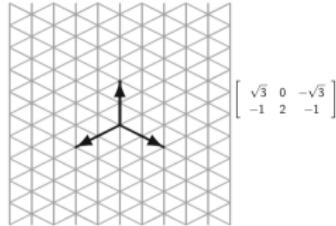
$$d_k^\top \nabla f_i(x_k) < 0, \quad \text{with } i \in \{1, \dots, m\}$$

- Derivative-free methods: when derivatives are not available and cannot be numerically approximated

- Directional Direct Search: Uses **positive spanning sets** for sampling in \mathbb{R}^2 :



$$\begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix}$$



$$\begin{bmatrix} \sqrt{3} & 0 & -\sqrt{3} \\ -1 & 2 & -1 \end{bmatrix}$$

$$pspan(D) = \mathbb{R}^2$$

Presentation Outline

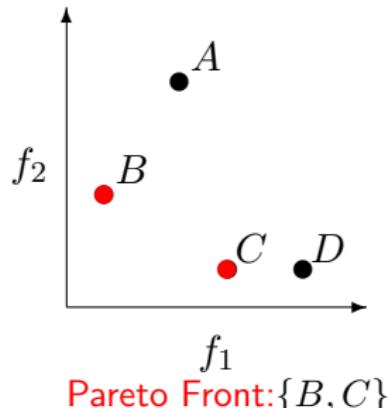
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Direct MultiSearch (DMS) Main Lines

- does **not aggregate** any of the objective function components
- makes use of Pareto dominance

Pareto Dominance (x dominates y)

$F(x) \leq F(y)$, with $F(x) \neq F(y)$



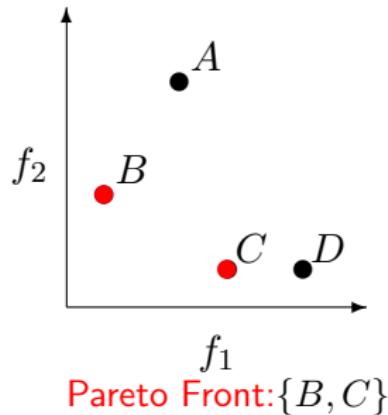
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- considers the **search/poll** paradigm with an optional search step
- computes **approximations to the complete Pareto front**

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Pareto Front: $\{B, C\}$

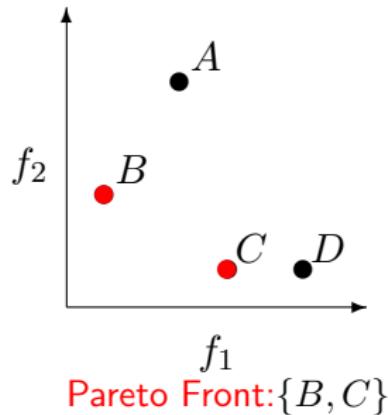
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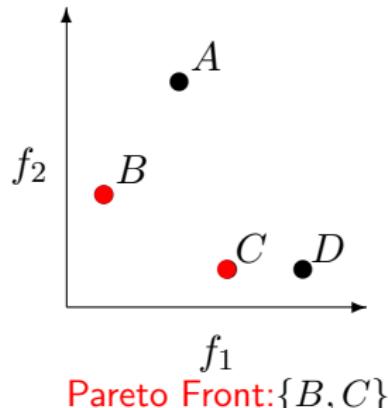
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Direct MultiSearch (DMS) Main Lines

- constraints are addressed by an **extreme barrier approach**

$$F_{\Upsilon}(x) = \begin{cases} F(x) & \text{if } x \in \Upsilon, \\ (+\infty, +\infty, \dots, +\infty)^{\top} & \text{otherwise} \end{cases}$$

- keeps a **list of feasible nondominated points**
- **poll centers** are chosen **from the list**
- **successful iterations** correspond to **list changes**
 - successful iteration \Leftrightarrow new feasible nondominated point

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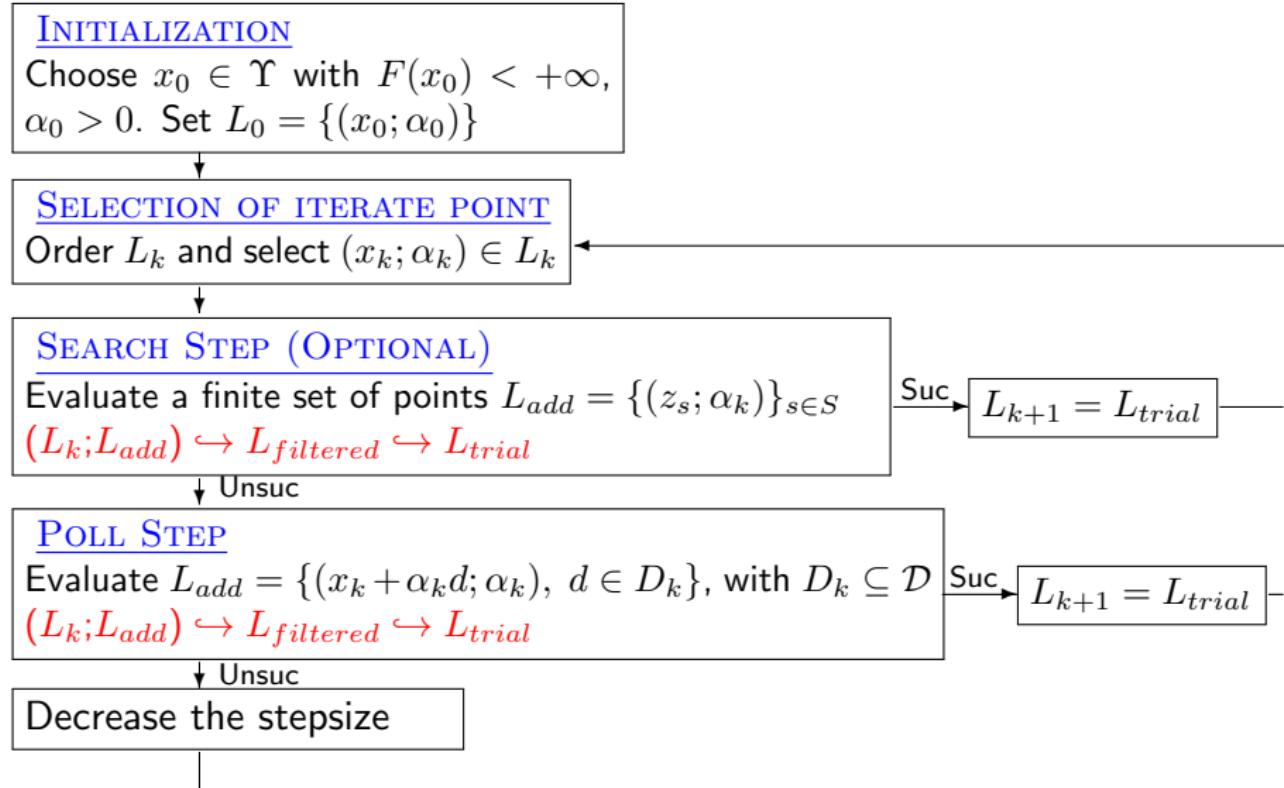
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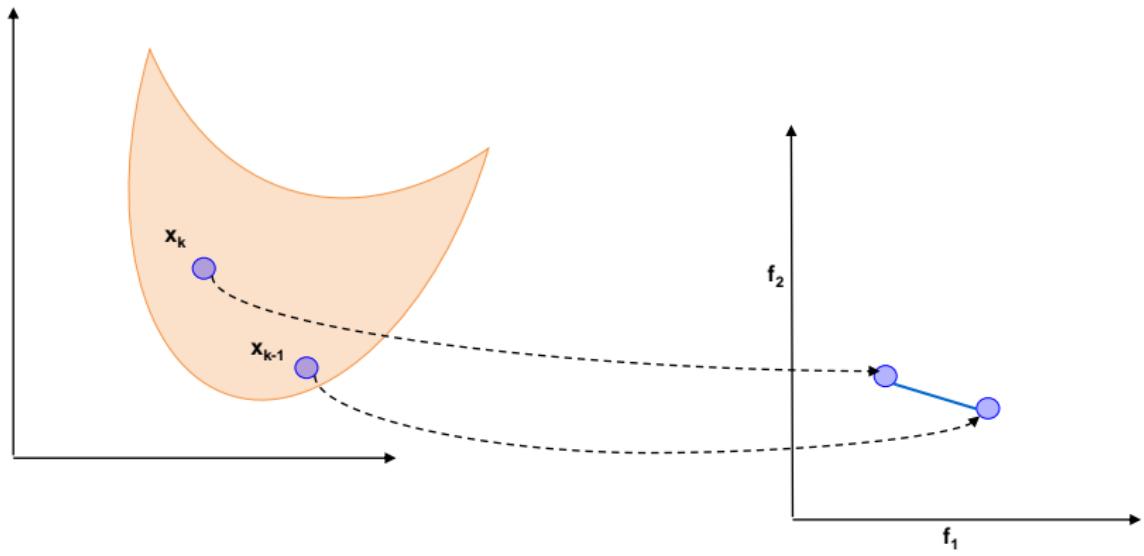
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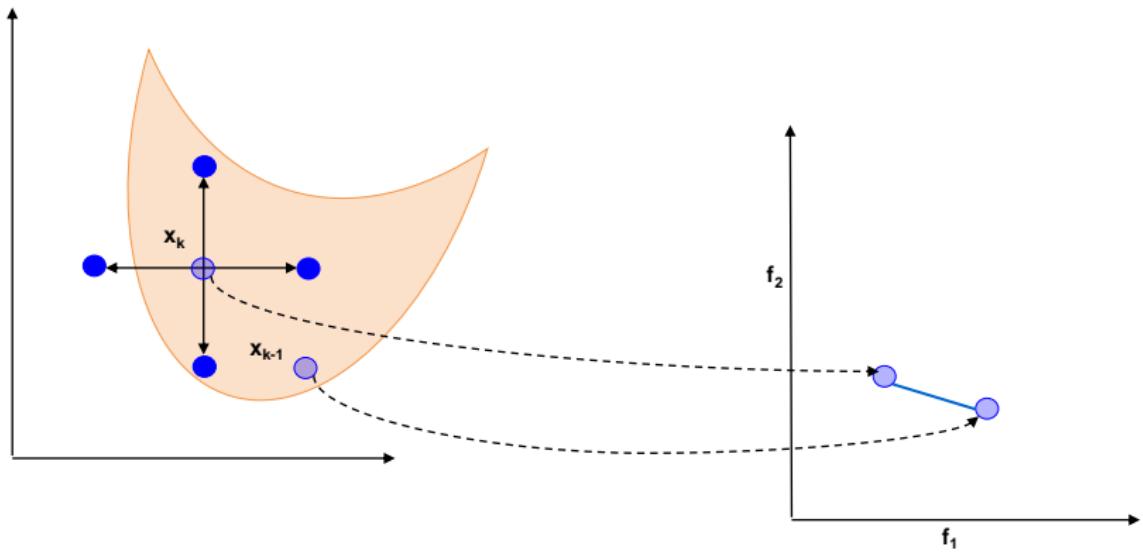
Direct Multisearch Structure



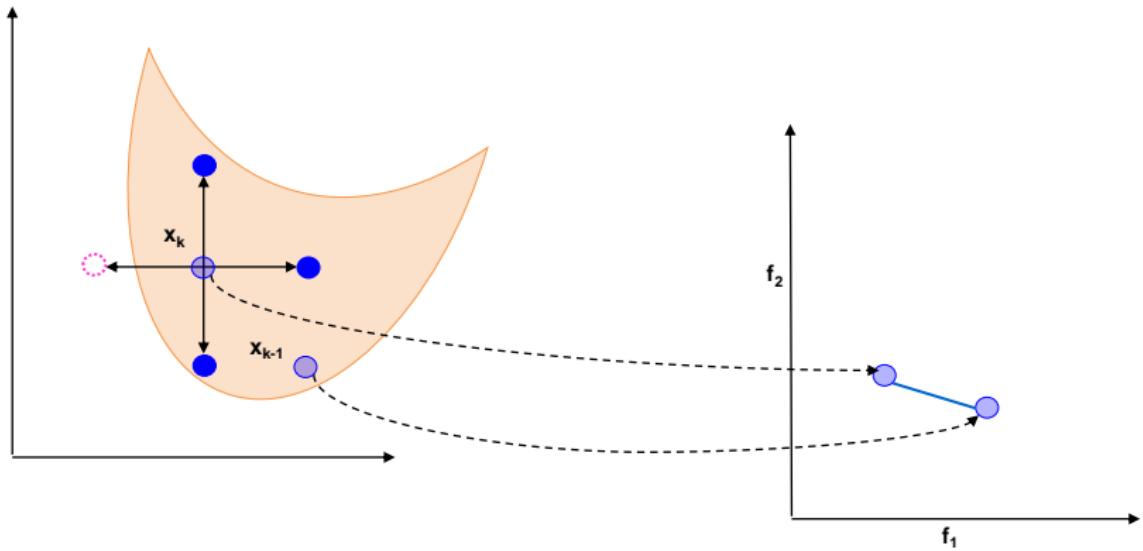
Poll Step Example (Biobjective Problem)



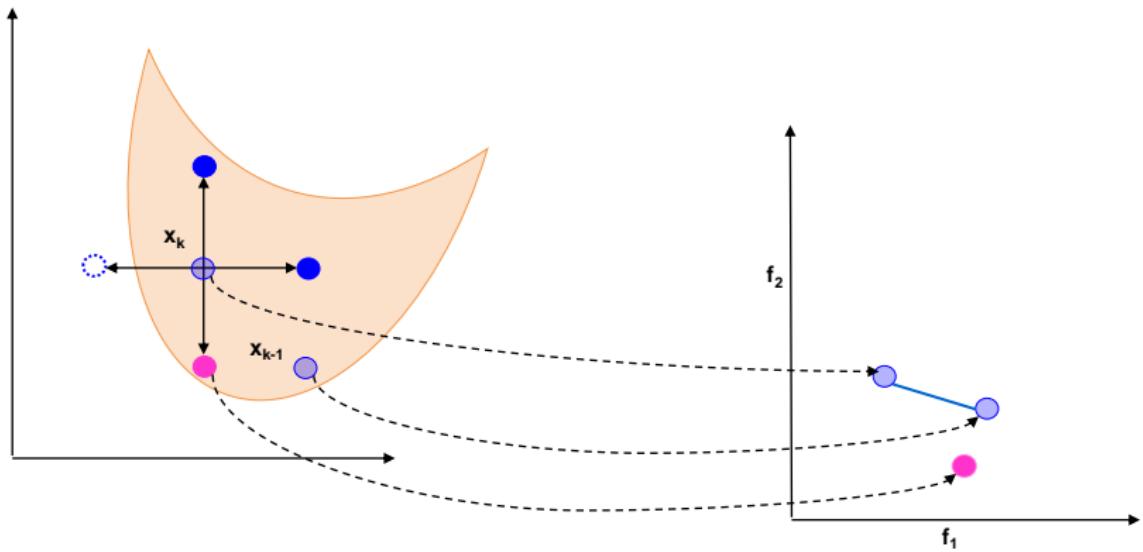
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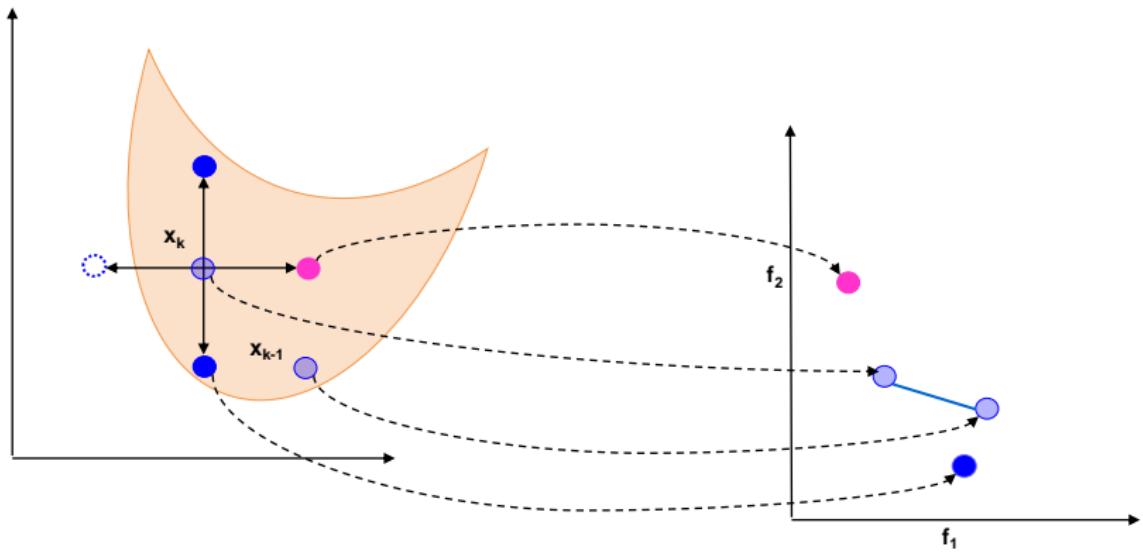
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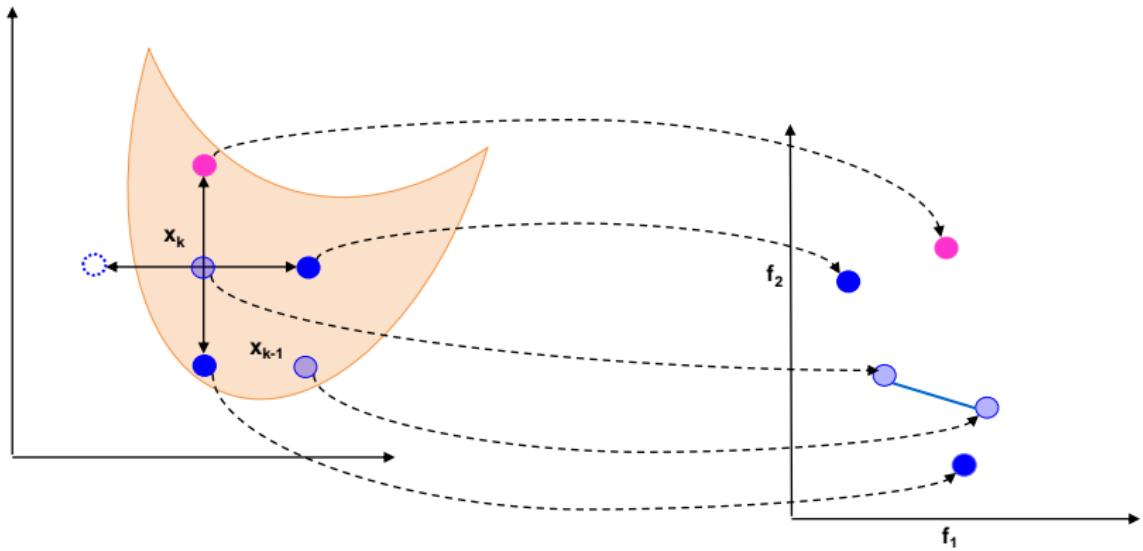
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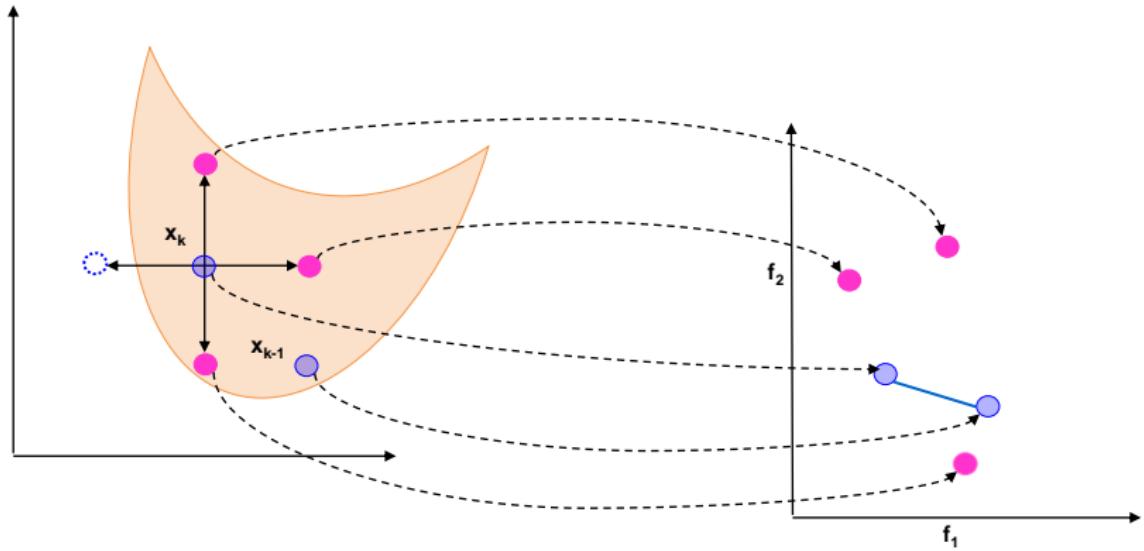
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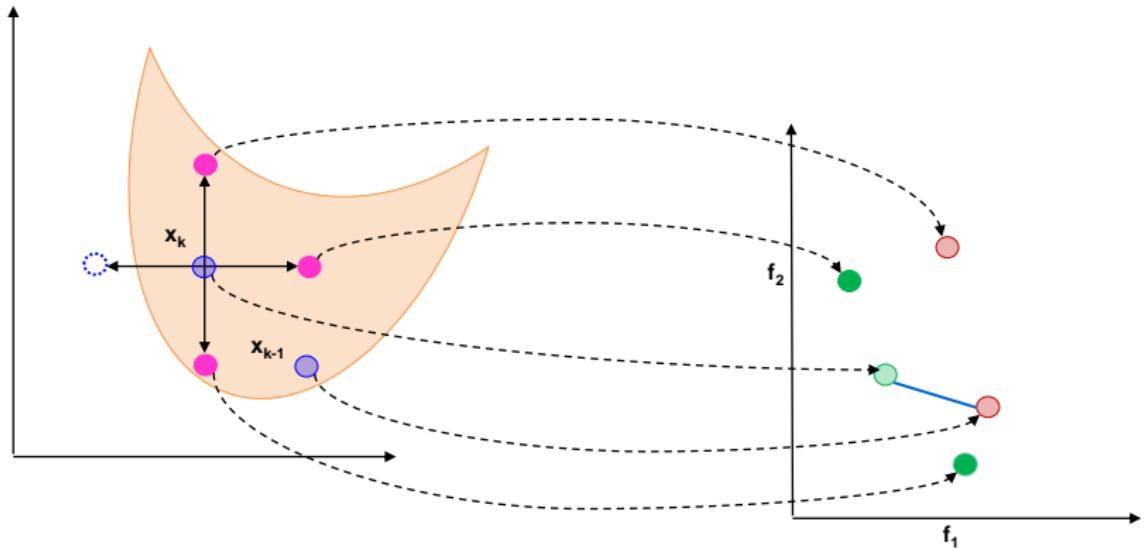


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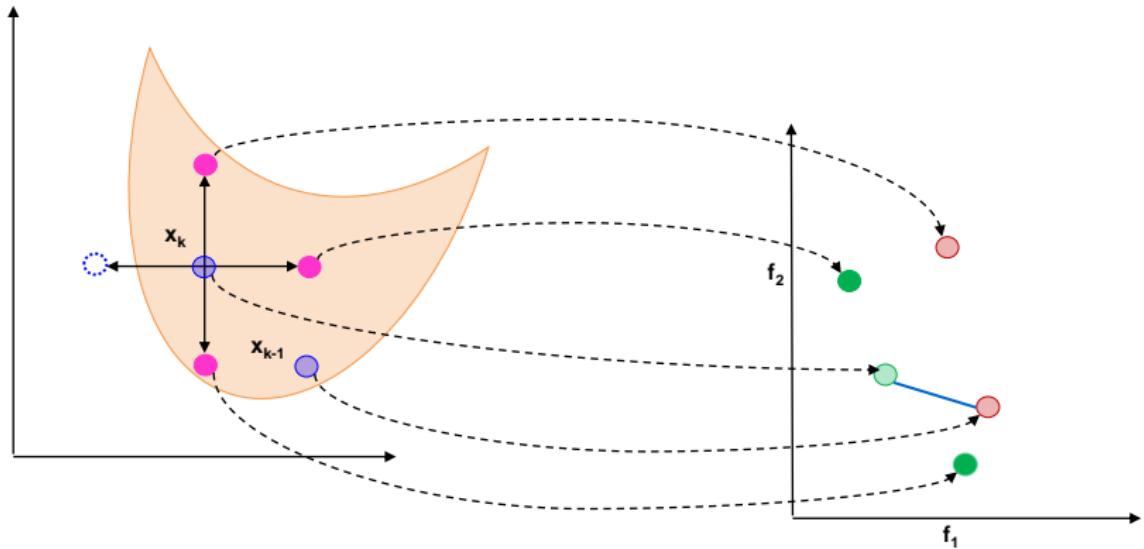
L_{add}

Poll Step Example (Biobjective Problem)



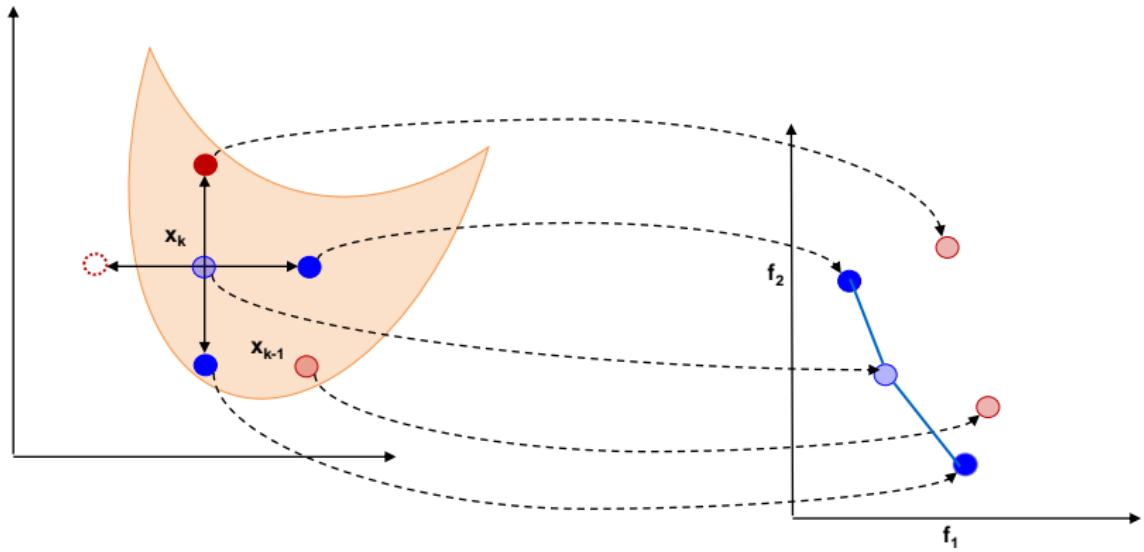
$L_{filtered}$

Poll Step Example (Biobjective Problem)



$$L_{trial} = L_{filtered}$$

Poll Step Example (Biobjective Problem)



Positive Spanning Sets and Constraints

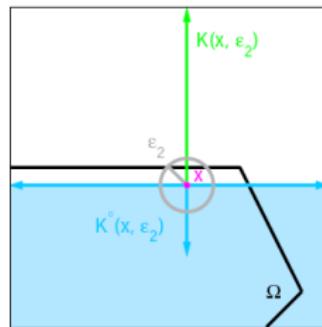
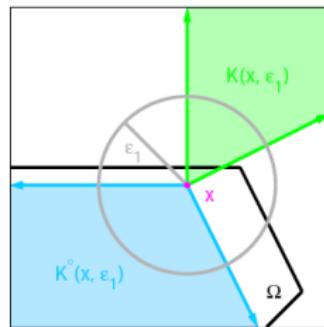
- Requires **asymptotical density** of the union of positive spanning sets **in the unit sphere**

In practice:

- Unconstrained or variable bounds: coordinate search

$$D = D_{\oplus} = [I \ - I]$$

- Linear constraints: directions must conform to geometry of nearby constraints



Abramson, Brezhneva, Dennis, and Pingel [2008]

Positive Spanning Sets and Constraints

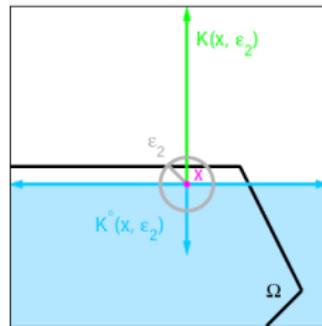
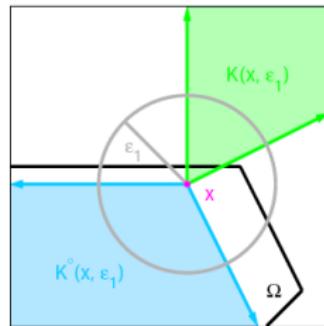
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Metrics for Performance Profiles (Dolan and Moré [2002])

- Purity

$$\frac{|F_{p,s} \cap F_p|}{|F_{p,s}|}$$

- Spreads Γ and Δ

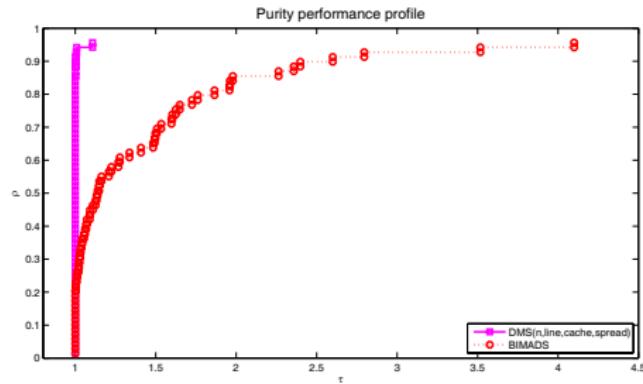
$$\Gamma_{p,s} = \max_{j \in \{1, \dots, m\}} \left(\max_{i \in \{0, \dots, N\}} \{d_i\} \right)$$

$$\Delta = \max_{j \in \{1, \dots, m\}} \left(\frac{d_0 + d_N + \sum_{i=1}^{N-1} |d_i - \bar{d}|}{d_0 + d_N + (N-1)\bar{d}} \right)$$

DMS Defaults

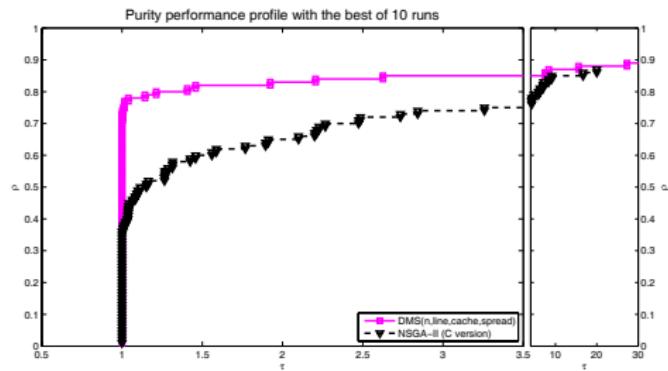
- List initialization: line sampling
- Search step: none
- Poll center selection: poll centers correspond to highest Γ metric value (ties broken by the largest step size)
- Polling strategy: complete coordinate search
- Stepsize update: halved at unsuccessful iterations
- Cache implementation: objective function values only computed for points that dist at least 10^{-3} from any previously evaluated point

Comparing DMS with Other Solvers (Purity)



Purity Metric

(percentage of points generated
in the reference Pareto front)

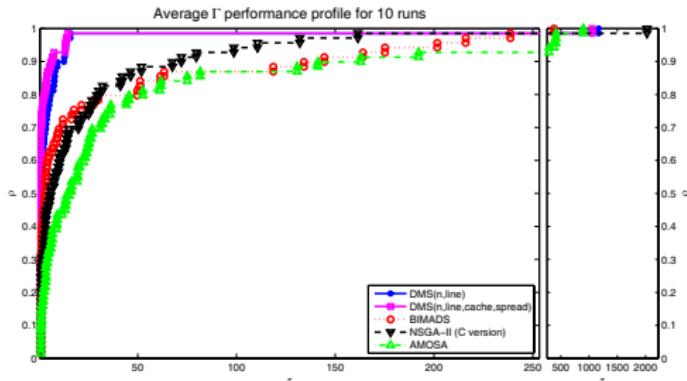


DMS
BIMADS
NSGA-II

Comparing DMS with Other Solvers (Spread)

Gamma Metric

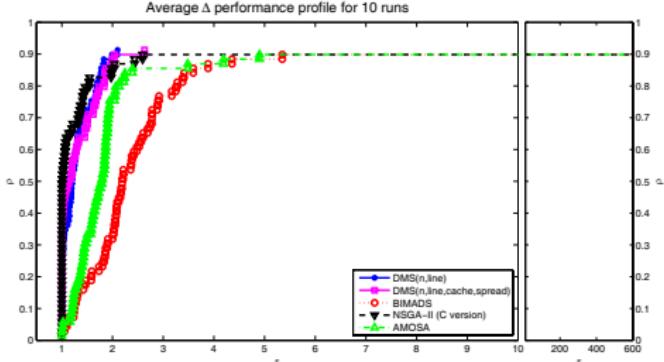
(largest gap in the Pareto front)



Delta Metric

(uniformity of gaps in the Pareto front)

DMS, **DMS**, **BIMADS**,
NSGA-II, **AMOSA**



Motivation

- DMS → A. L. Custódio, J. F. A. Madeira, A. I. F. Vaz, and L. N. Vicente, *Direct multisearch for multiobjective optimization*, SIAM J. Optim. (2011), 21, 1109–1140
- DFMO → G. Liuzzi, S. Lucidi, and F. Rinaldi, *A derivative-free approach to constrained multiobjective nonsmooth optimization*, SIAM J. Optim. (2016), 26, 2744–2774
- 93 biobjective problems with nonlinear constraints and variable bounds
 - number of variables between 3 and 30
 - number of nonlinear constraints between 1 and 29
 - maximum of 20000 function evaluations

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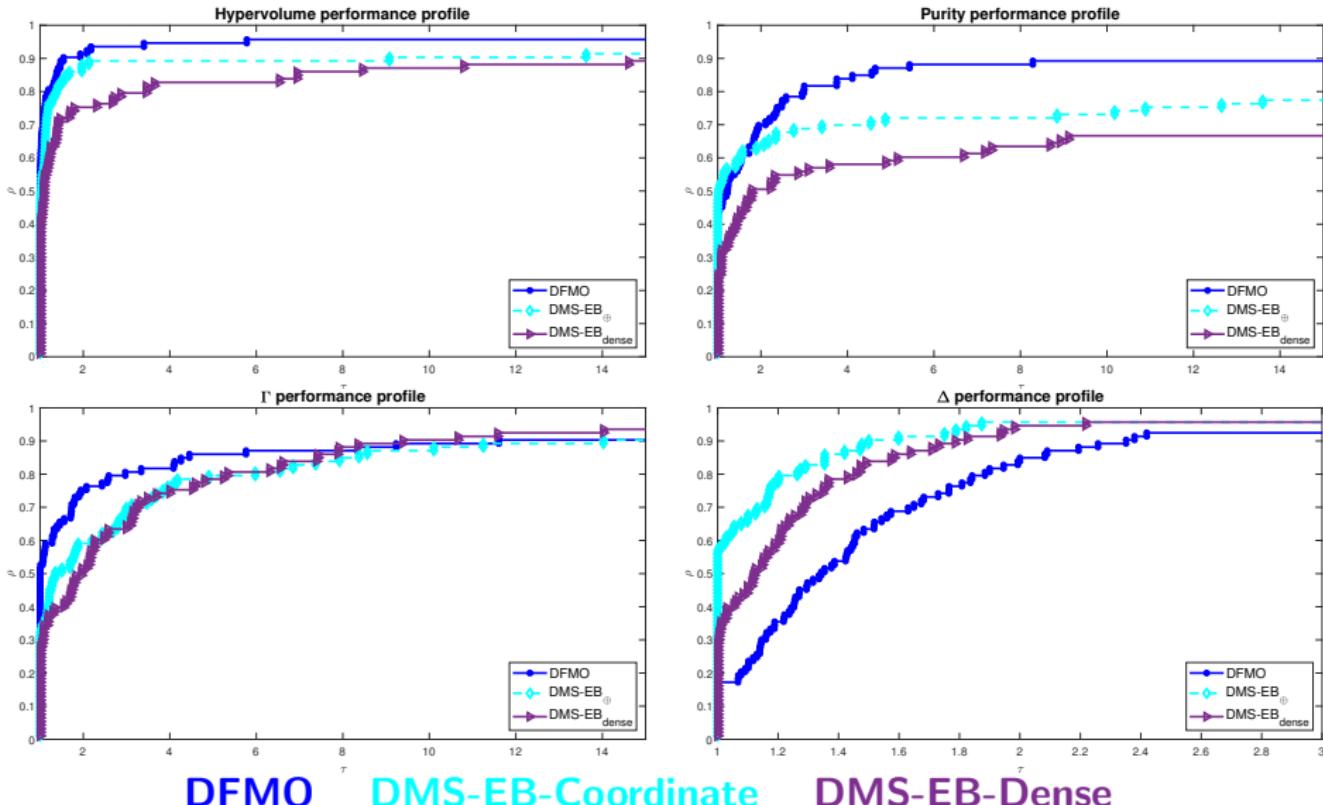
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- Hypervolume

$$HI_{p,s} = Vol\{b \in \mathbb{R}^m \mid b \leq U_p \wedge \exists a \in F_{p,s} : a \leq b\}$$

Nonlinear + Bound Constraints (Biobjective Problems)



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DMS Filter and Inexact Restoration Approach

Original Problem

$$\min_{x \in \Upsilon \subset \mathbb{R}^n} F(x) = (f_1(x), f_2(x), \dots, f_m(x))^\top$$

$$f_j : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}, \quad j = 1, 2, \dots, m \geq 2$$

with $\Upsilon = \Omega \cap X$ (where: Ω relaxable and X unrelaxable)

Reformulated Problem

$$\min_{x \in X} (f_1(x), f_2(x), \dots, f_m(x), h(x))^\top$$

Constraint Violation function

$$h(x) = \|C(x)_+\|_2^2 = \sum_{i=1}^p \max\{0, c_i(x)\}^2$$

Constraints in X continue to be addressed by an extreme barrier approach, and it is assumed $x_0 \in X$.

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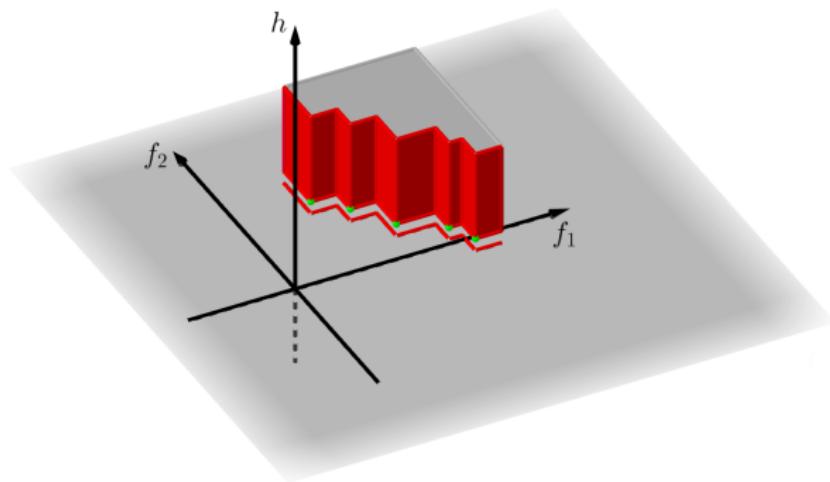
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List of Nondominated Points

A point x' is said to be filtered by the list L if any of the following properties hold:

- $h(x') > h_{\max}$ (for some fixed $h_{\max} > 0$)
- there is $x \in L$ such that $(F(x), h(x)) \leq (F(x'), h(x'))$ with $(F(x), h(x)) \neq (F(x'), h(x'))$



DMS Filter and Inexact Restoration Approach

- Relaxable feasibility is treated as an additional objective
- Priority given to feasible poll centers
- When all poll points associated with a poll center x_k are infeasible, switches to an infeasible poll center

Attempts to restore feasibility by solving:

$$\begin{aligned} \min_{y \in X} \quad & \frac{1}{2} \|y - x_k\|^2 \\ \text{s.t.} \quad & h(y) \leq \xi(\alpha_k)h(x_k), \end{aligned}$$

where $\xi : (0, +\infty) \rightarrow (0, 1)$, is continuous, and satisfies

$$\xi(t) \rightarrow 0 \text{ when } t \downarrow 0$$

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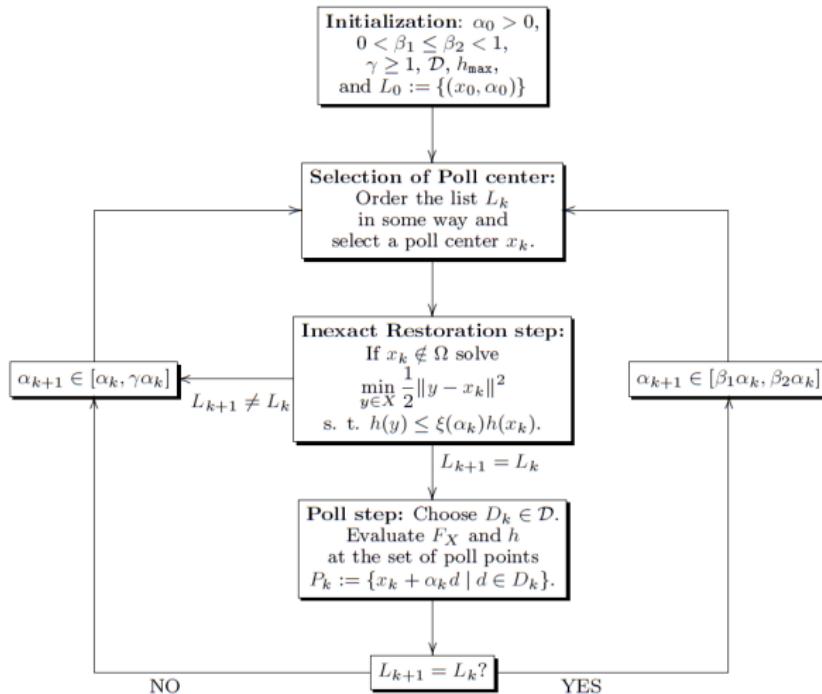
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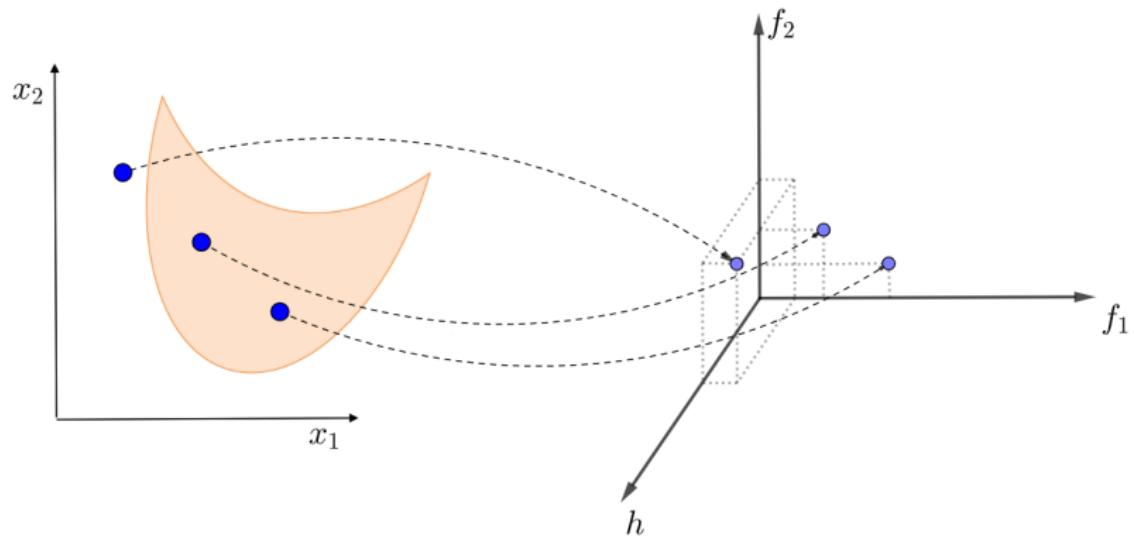
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DMS-FILTER-IR – Algorithmic Structure

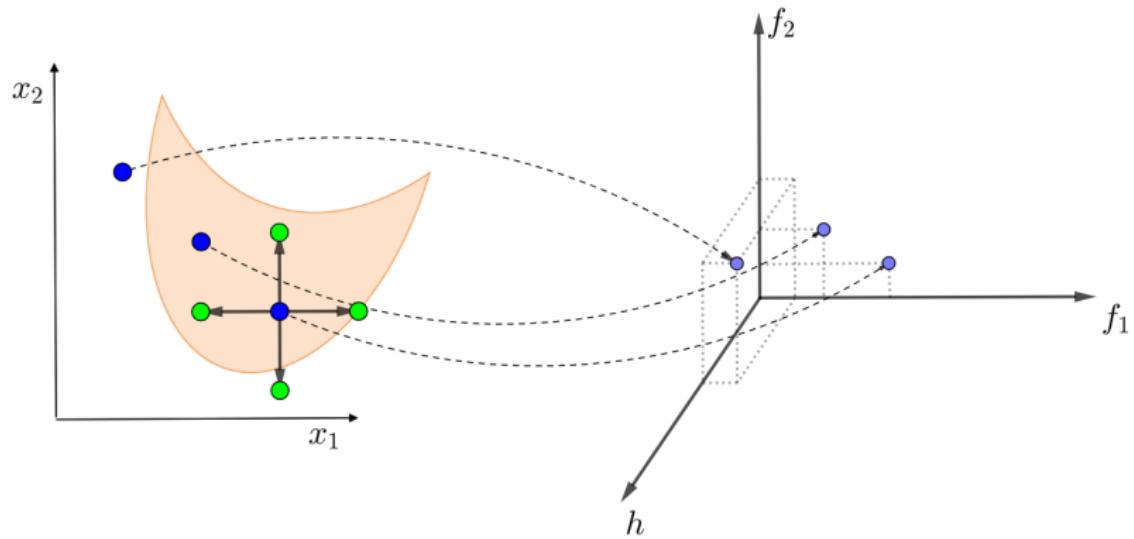


Solutions: $\{(x, \alpha) \in L \mid (F(x), h(x)) = (F(x), 0)\}$

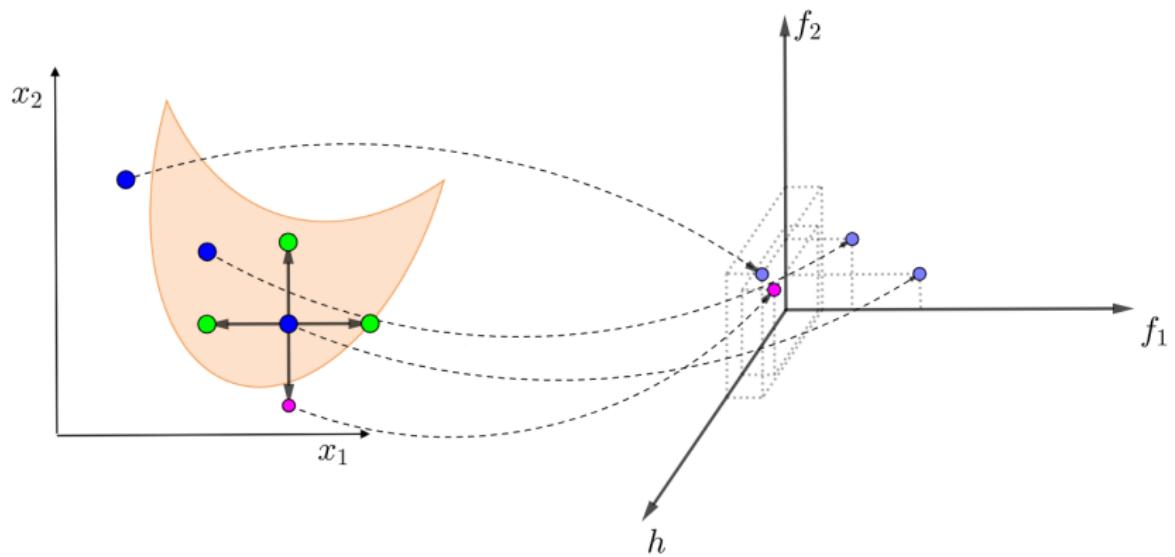
DMS-FILTER-IR – Poll Step



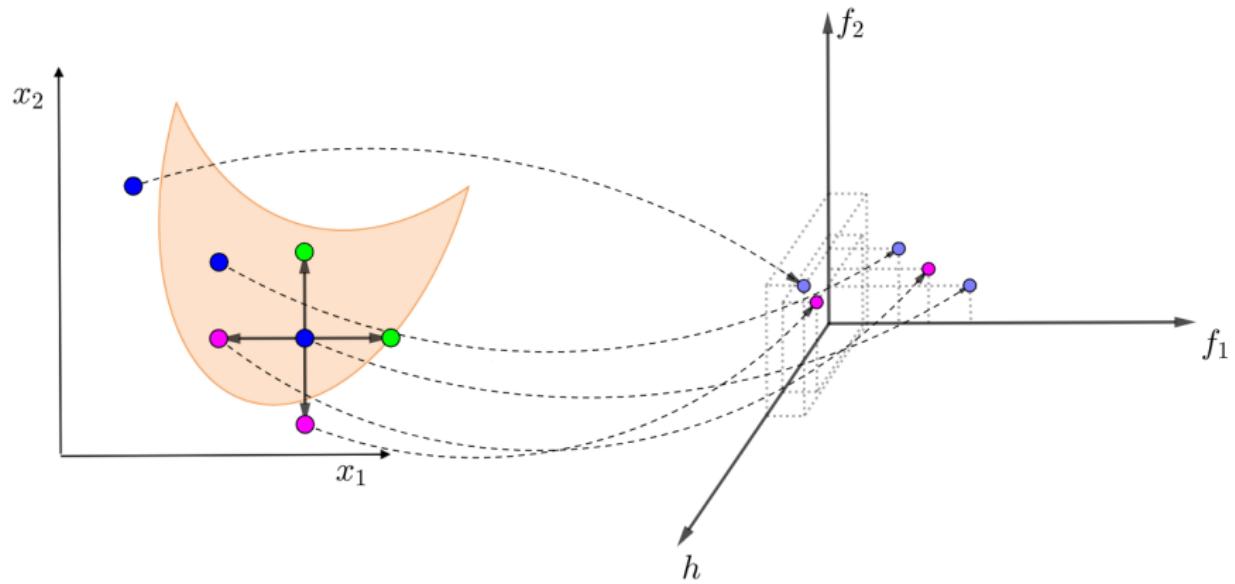
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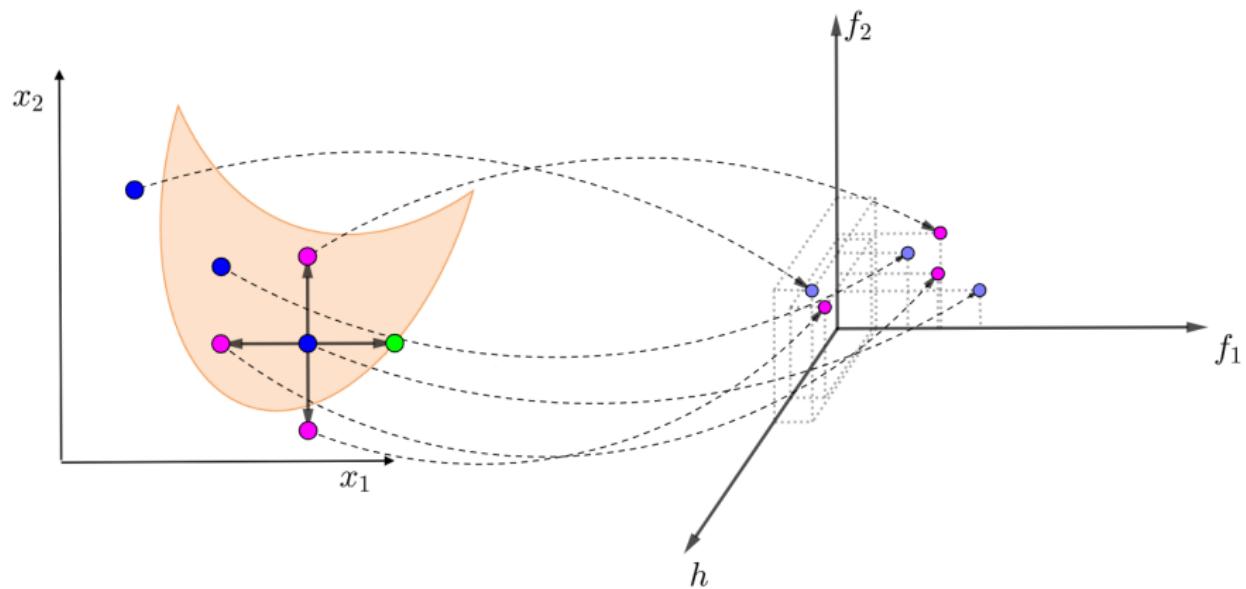
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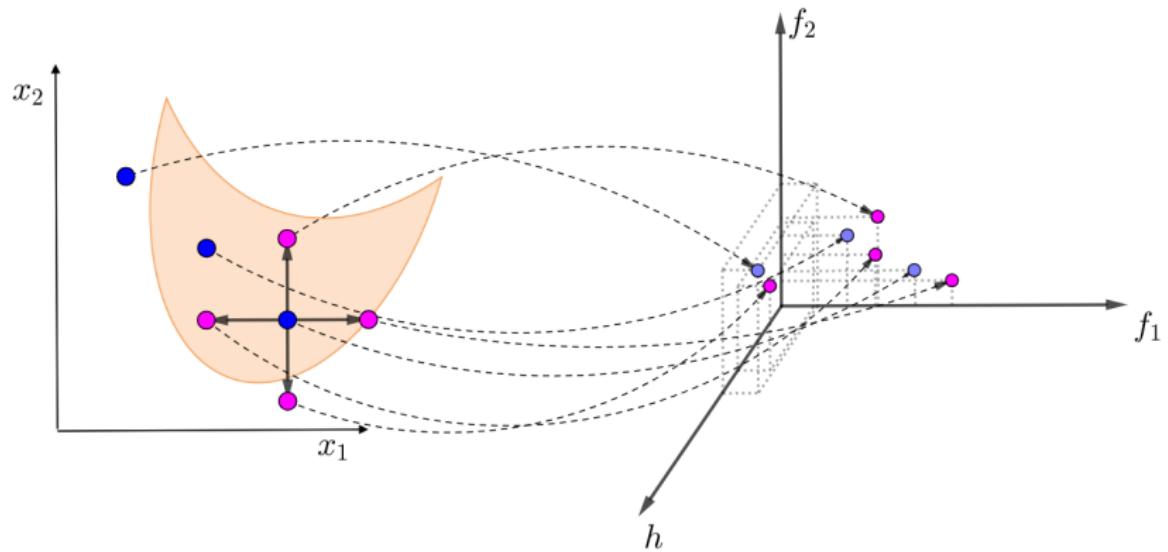
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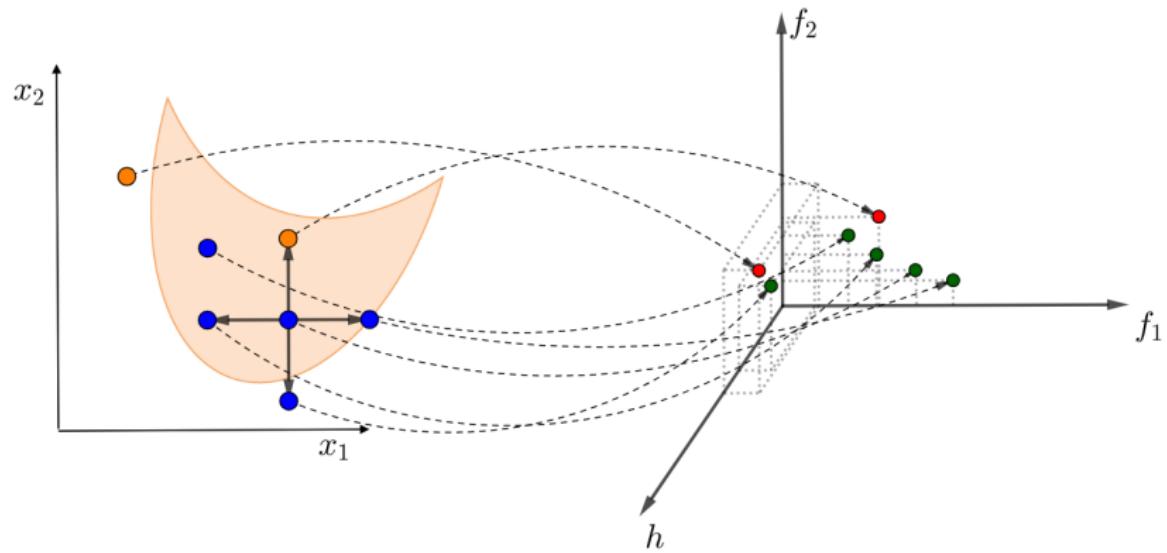
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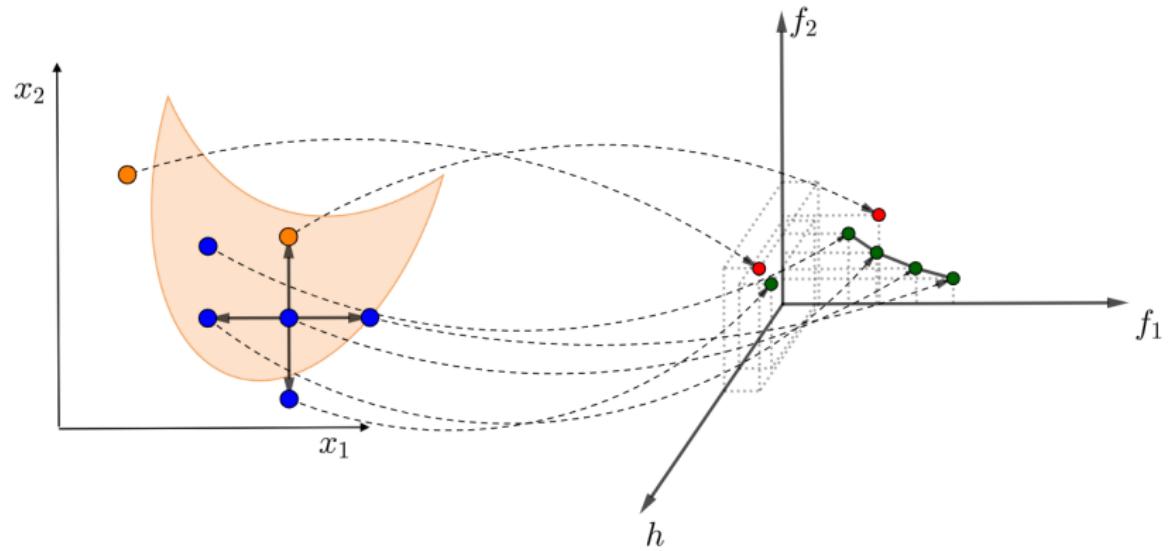
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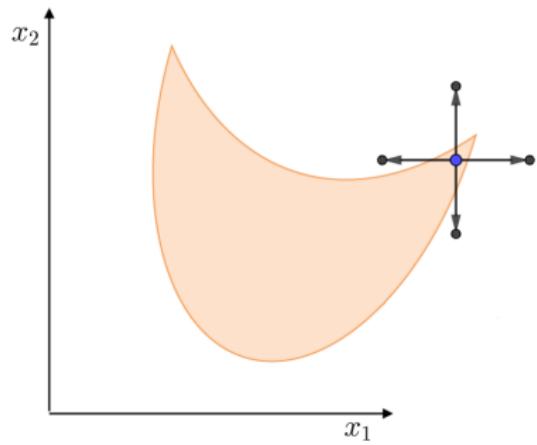
DMS-FILTER-IR – Poll Step



Poll Center Selection

Feasible to Infeasible

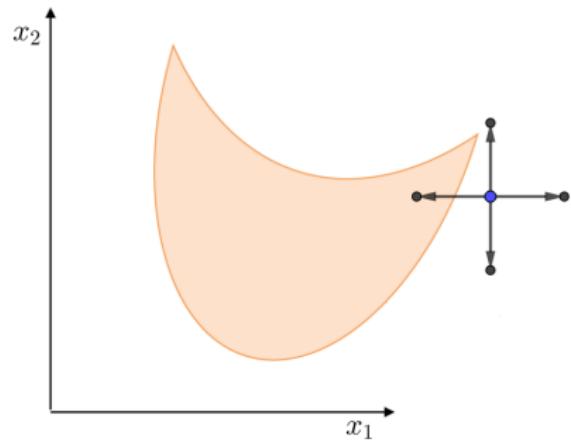
Polling only generates infeasible points



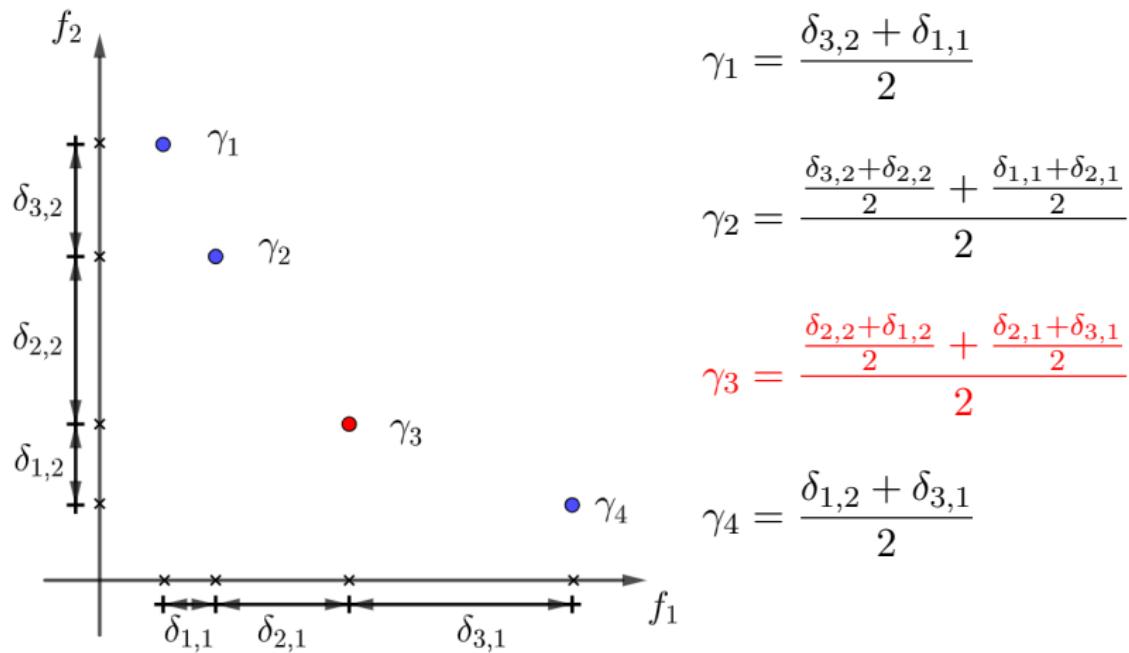
Infeasible to Feasible

Infeasible x_k generates feasible point by inexact restoration or polling

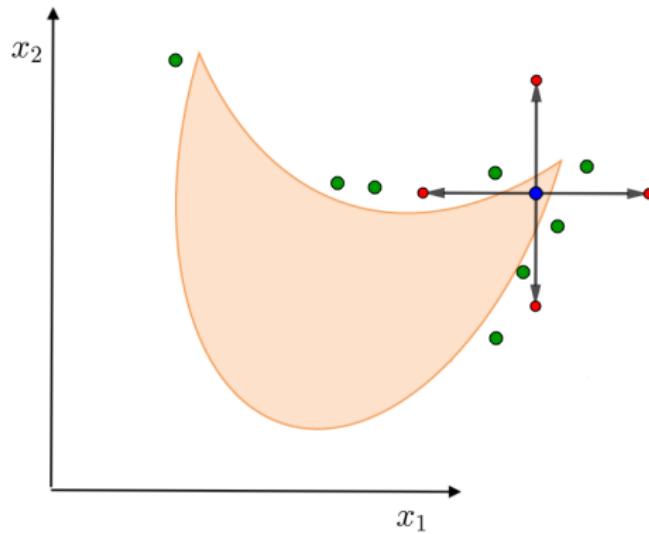
$$\begin{aligned} \min_{y \in X} \quad & \frac{1}{2} \|y - x_k\|^2 \\ \text{s.t.} \quad & h(y) \leq \xi(\alpha_k) h(x_k) \end{aligned}$$



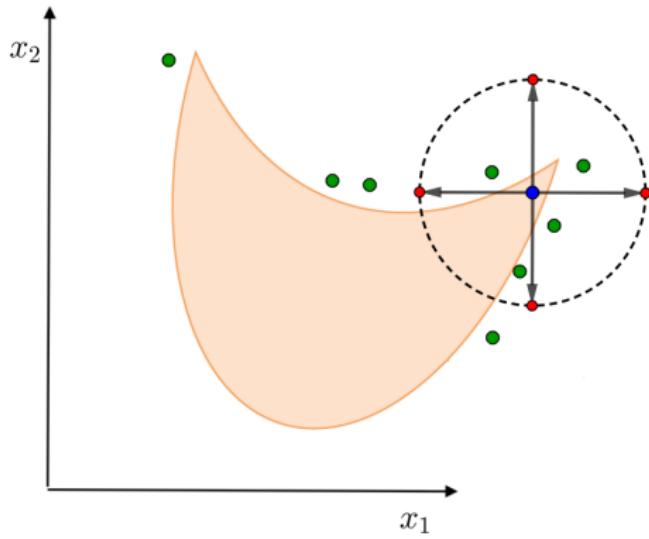
Feasible poll center - Most Isolated Point



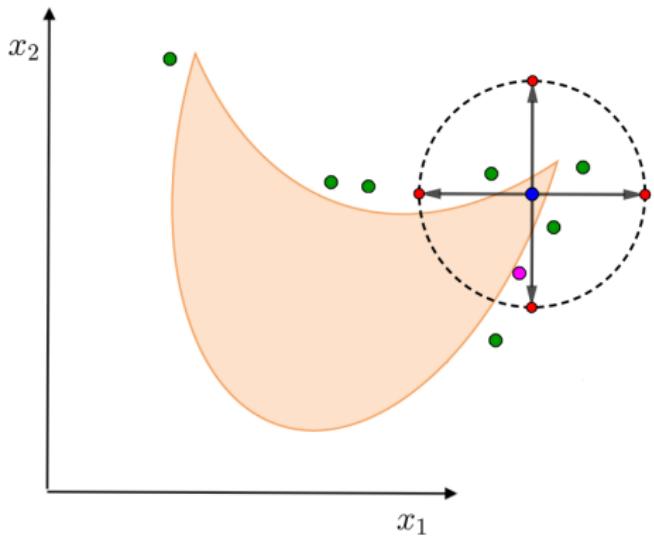
Infeasible Poll Center



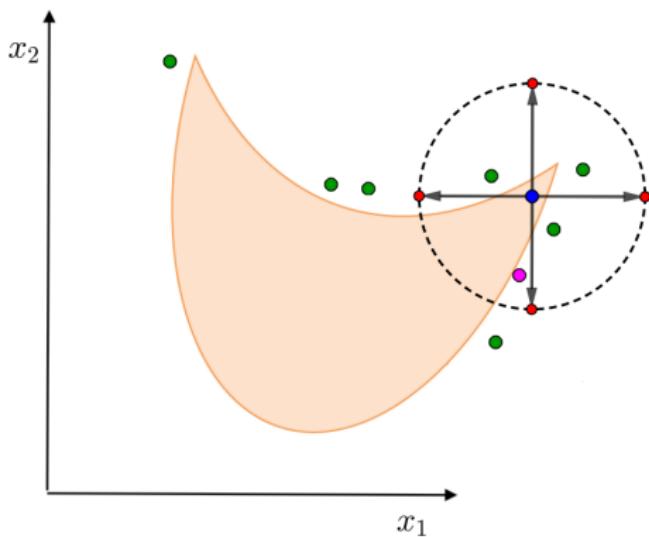
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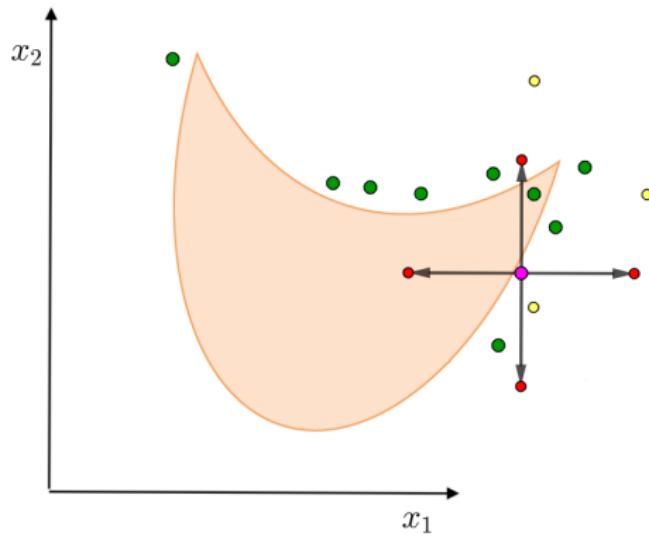


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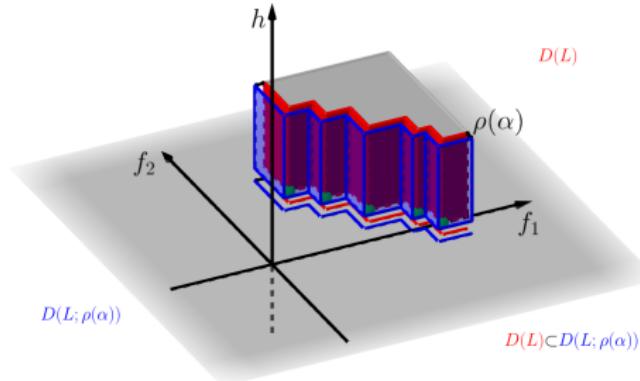
Convergence Analysis – Globalization Strategies

Using Integer Lattices (Torczon [1997], Audet and Dennis [2002])

- requires only simple decrease
- poll directions and step size must satisfy integer/rational requirements

Imposing Sufficient Decrease (Kolda, Lewis, and Torczon [2003])

- use of a forcing function
 $\rho : (0, +\infty) \rightarrow (0, +\infty)$, continuous, nondecreasing, and satisfying
 $\rho(t)/t \rightarrow 0$ when $t \downarrow 0$
- x is nondominated $\Leftrightarrow (F_X(x), h(x)) \notin D(L, \rho(\alpha))$



Convergence Results – Sequences

Refining sequence

A sequence $\{x_k\}_{k \in K}$, such that $k \in K$ is an unsuccessful iteration and $\lim_{k \in K} \alpha_k = 0$.

Theorem (Refining Subsequences)

There is at least a convergent refining subsequence of iterates $\{x_k\}_{k \in K}$, corresponding to unsuccessful poll steps, with $\lim_{k \in K} \alpha_k = 0$.

Let \bar{x} be the limit point of a convergent refining subsequence $\{x_k\}_{k \in K}$.

Definition (Refining Directions)

Refining directions for \bar{x} are limit points of $\{d_k/\|d_k\|\}_{k \in K}$, where $d_k \in D_k$ and $x_k + \alpha_k d_k \in \mathcal{S} := \{x \in X \mid h(x) \leq h_{\max}\}$.

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Convergence Results

Consider $\{x_k\}_{k \in K}$ a refining subsequence converging to $\bar{x} \in \mathcal{S} := \{x \in X \mid h(x) \leq h_{\max}\}$. Assume that F and h are Lipschitz continuous near \bar{x} . Under any globalization strategy:

Theorem

- If $d \in \text{int}(T_{\mathcal{S}}^{Cl}(\bar{x}))$ is a refining direction for \bar{x} then:
$$\exists j = j(d) \in \{1, \dots, m+1\} \text{ such that } f_j^{\circ}(\bar{x}; d) \geq 0$$
- If the set of refining directions for \bar{x} is dense in $\text{int}(T_{\mathcal{S}}^{Cl}(\bar{x})) \neq \emptyset$ then \bar{x} is a Pareto-Clarke critical point of \bar{F} in \mathcal{S} :
$$\forall d \in T_{\mathcal{S}}^{Cl}(\bar{x}), \exists j = j(d) \in \{1, \dots, m+1\} \text{ such that } f_j^{\circ}(\bar{x}; d) \geq 0$$

Convergence Results – Infeasible case

Theorem

Let h be continuous and consider $\{x_k\}_{k \in K}$ an **infeasible refining subsequence** such that for each $k \in K$, x_k is **used at a successful inexact restoration step**. Then DMS-FILTER-IR generates a **limit point** $\bar{y} \in \Upsilon$.

Convergence Results – Feasible case

Consider $\{x_k\}_{k \in K}$ a **feasible refining subsequence** converging to $\bar{x} \in \Upsilon$. Assuming a **globalization strategy based on integer lattices**, we have:

Corollary

- If $d \in \text{int}(T_{\Upsilon}^{Cl}(\bar{x}))$ is a refining direction for \bar{x} then:

$$\exists j = j(d) \in \{1, \dots, m\} \text{ such that } f_j^{\circ}(\bar{x}; d) \geq 0$$

- If the set of refining directions for \bar{x} is dense in $\text{int}(T_{\Upsilon}^{Cl}(\bar{x})) \neq \emptyset$ then \bar{x} is a Pareto-Clarke critical point of F in Υ :

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Numerical Results – Settings

- Comparison between:
 - **DMS-EB** versus **DMS-FILTER-IR**: best version of each one
- 93 biobjective problems with nonlinear constraints and bounds
 - number of variables between 3 and 30
 - number of nonlinear constraints between 1 and 29
- Initialization:
 - **DMS-EB**: Feasible point provided by Karmitsa [2007]
 - **DMS-FILTER-IR**: n -points equally spaced in the line segment, joining the variable upper and lower bounds
- Stopping criterion
 - $\alpha_k < 10^{-3}$ for all points in the list
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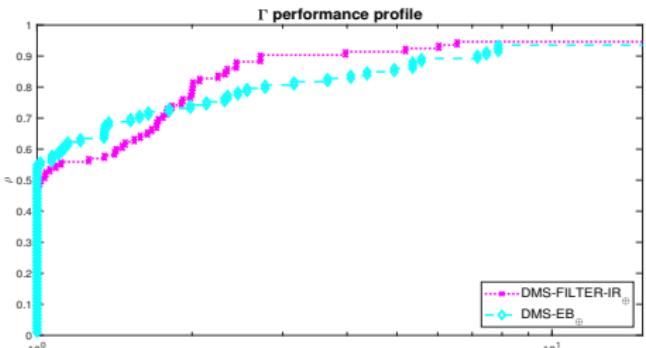
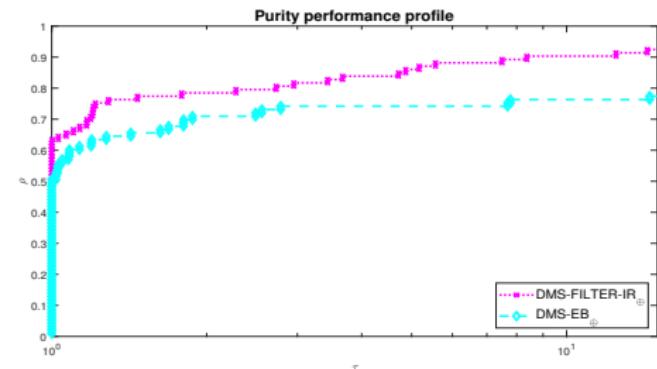
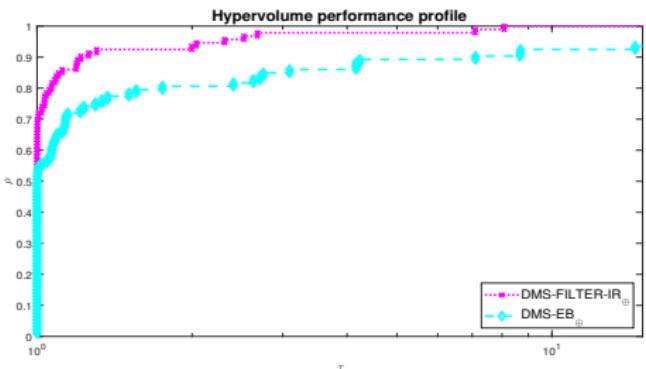
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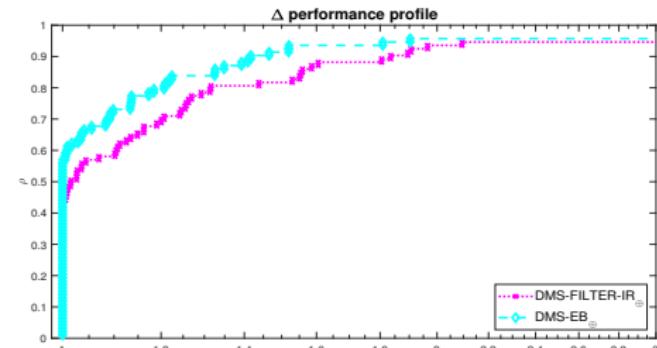
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Best version DMS vs DMS-FILTER-IR - 5k func. eval.



DMS-FILTER-IR - Coordinate



DMS-EB - Coordinate

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- Comparison among **DFMO**, **DMS-EB**, **DmultiMads-PB*** and **DMS-FILTER-IR**
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 - default values
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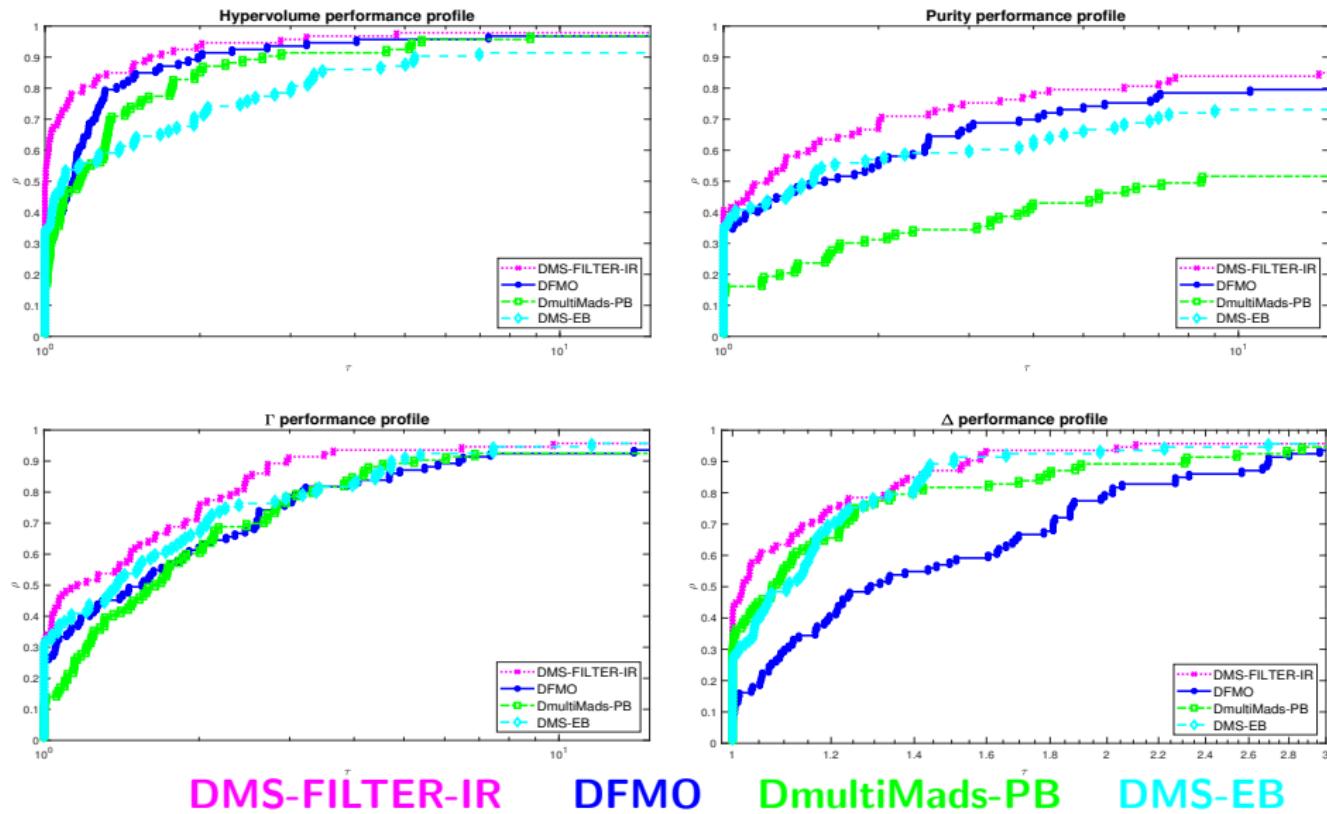
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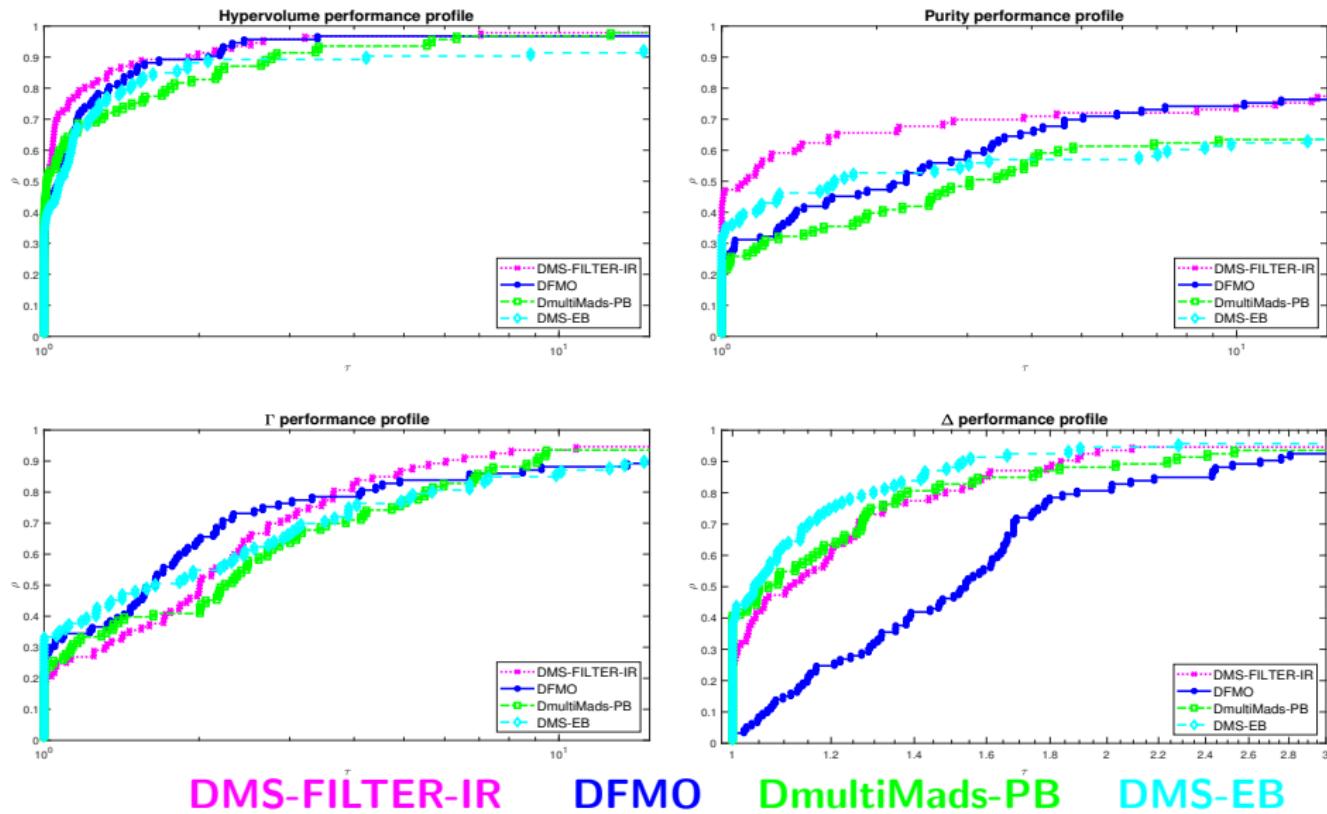
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Results - 500 function evaluations



Results - 5000 function evaluations



Presentation Outline

- ① Problem Definition
- ② DMS
- ③ DMS-FILTER-IR
- ④ LOG-DMS
- ⑤ Conclusions and Future Work

Logarithmic Barrier in Direct Multisearch

Original Problem

$$\begin{aligned} \min \quad & F(x) = (f_1(x), \dots, f_m(x))^\top \\ \text{s.t.} \quad & g(x) \leq 0 \\ & x \in X \end{aligned}$$

$$\begin{aligned} F : X &\subseteq \mathbb{R}^n \rightarrow \{\mathbb{R} \cup \{+\infty\}\}^m \\ g : X &\subseteq \mathbb{R}^n \rightarrow \{\mathbb{R} \cup \{+\infty\}\}^p \\ X &:= \{x \in \mathbb{R}^n \mid lb \leq x \leq ub\} \end{aligned}$$

Logarithmic Barrier function

$$Z_\ell(x; \rho) = \begin{cases} f_\ell(x) - \rho \sum_{i=1}^p \log(-g_i(x)) & \text{if } x \in X \text{ and } \max_{i=1, \dots, p} g_i(x) < 0, \\ +\infty & \text{otherwise.} \end{cases}$$

where $\ell = 1, \dots, m$ and $\rho > 0$.

- ρ must be driven to zero

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INITIALIZATION

Choose $x_0 \in X$ such that $g(x_0) < 0$, $\alpha_0 > 0$, \mathcal{D} , $\rho_0 > 0$, $\eta \geq 1$, $\theta \in (0, 1)$. Set $L_0 = \{(x_0; \alpha_0)\}$



SELECTION OF ITERATE POINT

Order L_k and select $(x_k; \alpha_k) \in L_k$



SEARCH STEP (OPTIONAL)

Evaluate a finite set of points $L_{add} = \{(z_s; \alpha_k)\}_{s \in S}$
 $(L_k; L_{add}) \hookrightarrow L_{filtered} \hookrightarrow L_{trial}$

Suc

$$L_{k+1} = L_{trial}$$



POLL STEP

Evaluate $L_{add} = \{(x_k + \alpha_k d; \alpha_k), d \in D_k\}$, with $D_k \subseteq \mathcal{D}$
 $(L_k; L_{add}) \hookrightarrow L_{filtered} \hookrightarrow L_{trial}$

Suc

$$L_{k+1} = L_{trial}$$



Decrease the stepsize

$$\alpha_{k+1} > \min\{\rho_k^\beta, (g_{\min})_k^2\}$$



$$\alpha_{k+1} \leq \min\{\rho_k^\eta, (g_{\min})_k^2\}$$

PENALTY UPDATE

$$\rho_{k+1} = \theta \rho_k$$

$$(g_{\min})_k = \min_{x \in L_k} \left\{ \min_{i=1, \dots, p} \{|g_i(x_k)|\} \right\}$$

Numerical Settings

- Comparison among **DMS**, **LOG-DMS**, and **DMS-FILTER-IR**
- Stopping criterion
 - **DMS**, **LOG-DMS**, and **DMS-FILTER-IR**:
 - $\alpha_k < 10^{-3}$ for all points in the list
 - All: maximum of 5000 function evaluations
- **LOG-DMS** maintains a cache
 - $P^{\text{cache}} \in \mathbb{R}^{n \times |\text{cache}|}$ - the points
 - $F^{\text{cache}} \in \mathbb{R}^{m \times |\text{cache}|}$ - values of the objective function
 - $G^{\text{cache}} \in \mathbb{R}^{p \times |\text{cache}|}$ - values of the constraints
- If the ρ_k is updated \rightarrow recompute $Z(\cdot; \rho_{k+1})$
- $\eta = 1$, $\theta = 10^{-2}$, and $\rho = 1$
 - in successful iterations we double the stepsize

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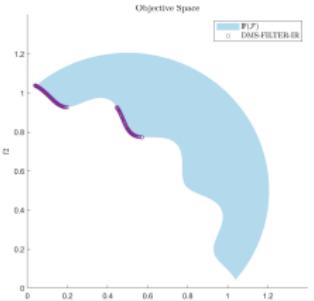
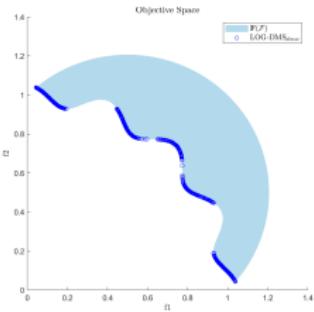
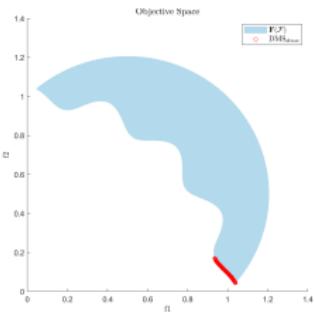
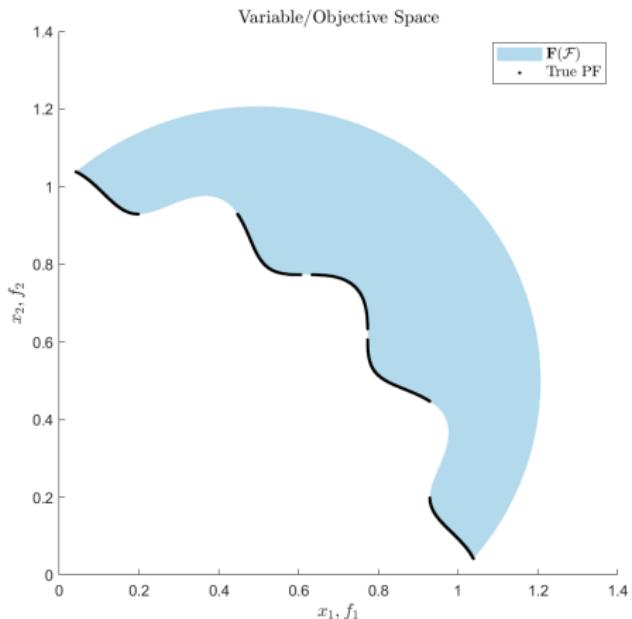
$$\min F(\mathbf{x}) = (x_1, x_2)^\top$$

$$s.t. \quad g_1(\mathbf{x}) = -x_1^2 - x_2^2 + 1 + 0.1 \cos\left(16 \arctan\left(\frac{x_1}{x_2}\right)\right) \leq 0$$

$$g_2(\mathbf{x}) = (x_1 - 0.5)^2 + (x_2 - 0.5)^2 - 0.5 \leq 0$$

$$\mathbf{x} \in X = [0, \pi] \times [0, \pi]$$

$$\mathbf{x}_0 = (1.1, 0.15)^\top$$



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Conclusions

- DMS-FILTER-IR extends filter methods, with an inexact restoration step, to the DMS framework
- DMS-FILTER-IR presents a well-supported convergence analysis
- DMS-FILTER-IR presents competitive numerical results for constrained biobjective derivative-free optimization problems
- LOG-DMS keeps the basic algorithmic features of DMS
- LOG-DMS provides a log-barrier approach to address nonlinear constraints in DMS

Future Work

- developing a competitive numerical implementation for problems with more than two objectives for DMS-FILTER-IR
- developing theoretical results and comprehensive numerical experiments for LOG-DMS

Paper: E. J. Silva and A. L. Custódio. “An inexact restoration direct multisearch filter approach to multiobjective constrained derivative-free optimization” In: Optim. Methods Softw. (2024), pp. 1–27.

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Thank you for your attention!

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