A Direct Multisearch Approach (DMS) for Many-Objective Derivative-Free Optimization

Everton José da Silva and Ana Luísa Custódio

UI/BD/151246/2021 UIDB/00297/2020 UIDP/00297/2020

Presentation Outline

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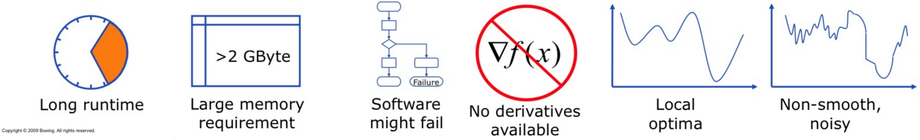
Multiobjective Derivative-free Optimization

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

$$F : \mathbb{R}^n \to \{\mathbb{R} \cup \{+\infty\}\}^m \text{ with } m \geq 2$$

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

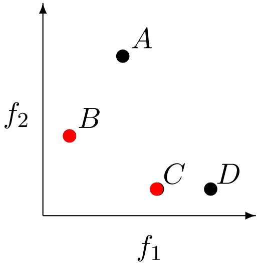


Direct MultiSearch (DMS) Main Lines

- 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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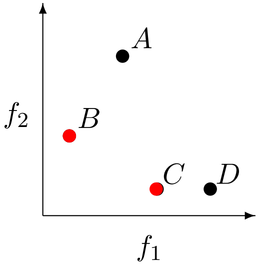

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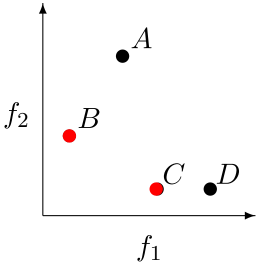

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- considers the search/poll paradigm with an optional search step

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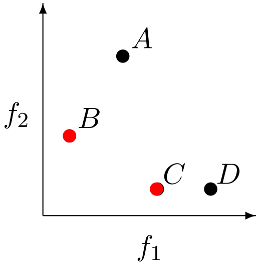

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$F(x) \leq F(y)$, with $F(x) \neq F(y)$

- generalizes directional direct search to MOO
- considers the search/poll paradigm with an optional search step
- computes approximations to the complete Pareto front

Direct MultiSearch (DMS) Main Lines

- constraints are addressed by an extreme barrier approach

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

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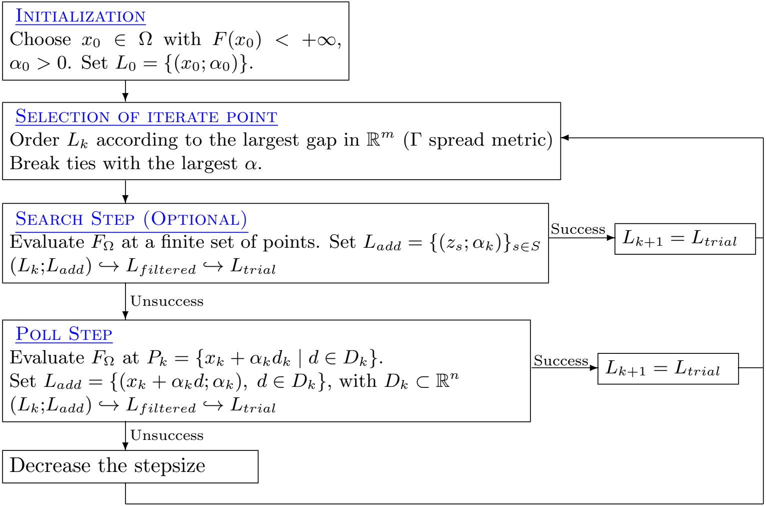
- keeps a list of feasible nondominated points
- poll centers are chosen from the list
- successful iterations correspond to list changes

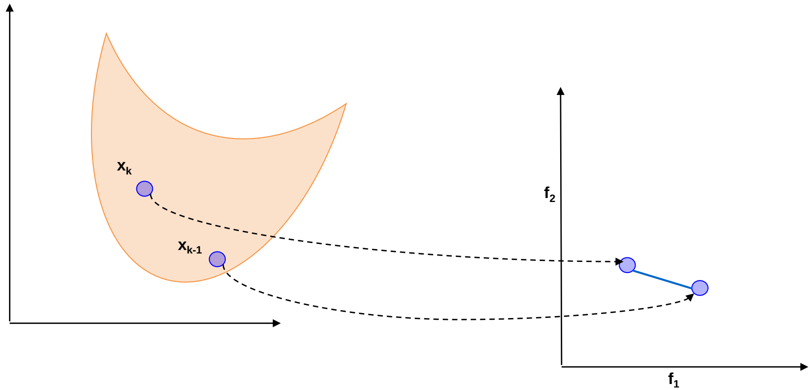
successful iteration $\Leftrightarrow$ new feasible nondominated point

Direct Multisearch - Algorithmic Structure



D_k **positive basis in** $\mathbb{R}^n$**;** $n + 1 \leq |D_k| \leq 2n$

Poll Step Example (Biobjective Problem)



L_k

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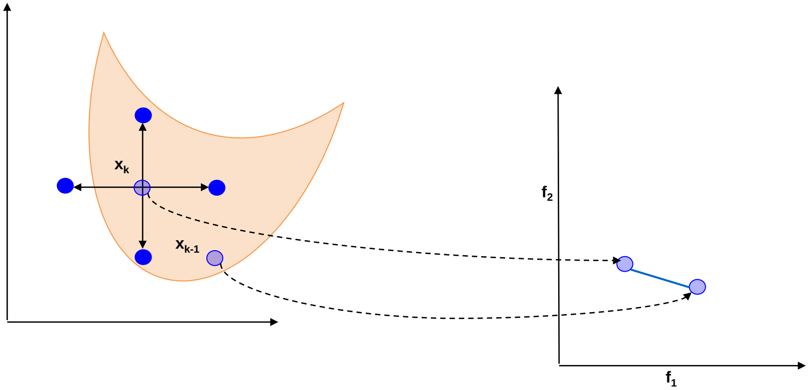

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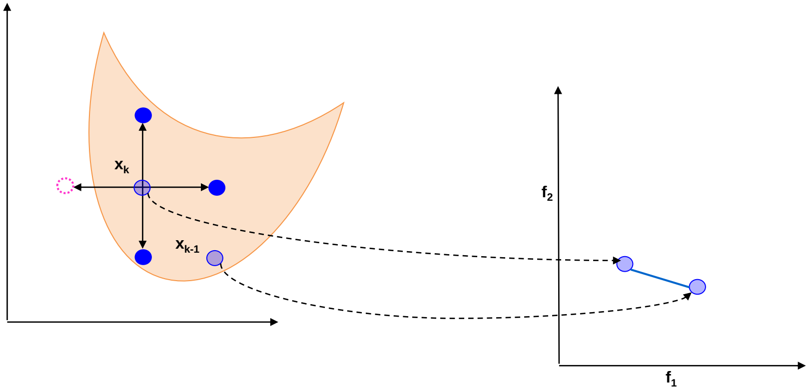

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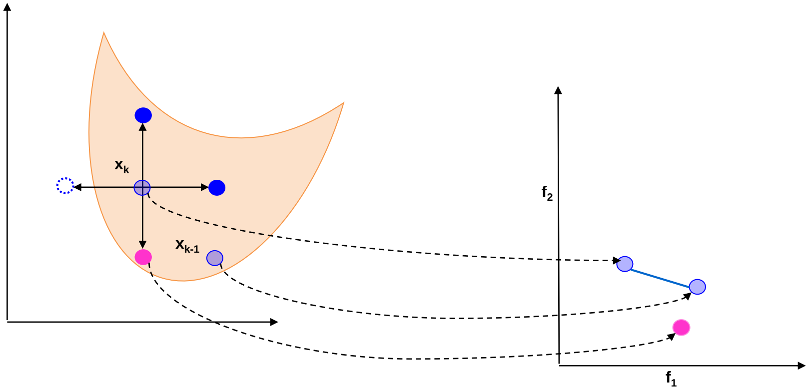

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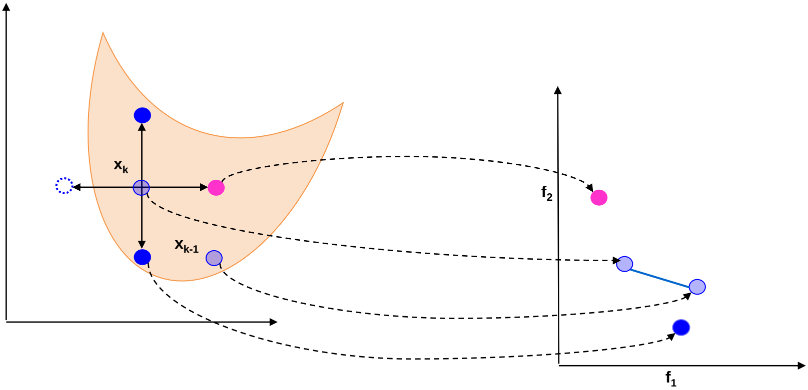

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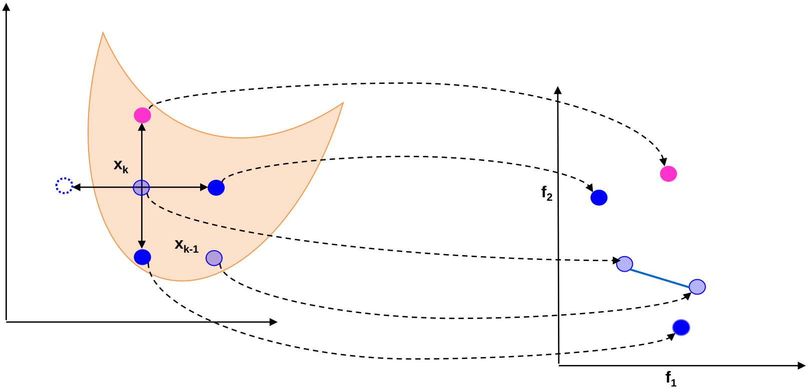

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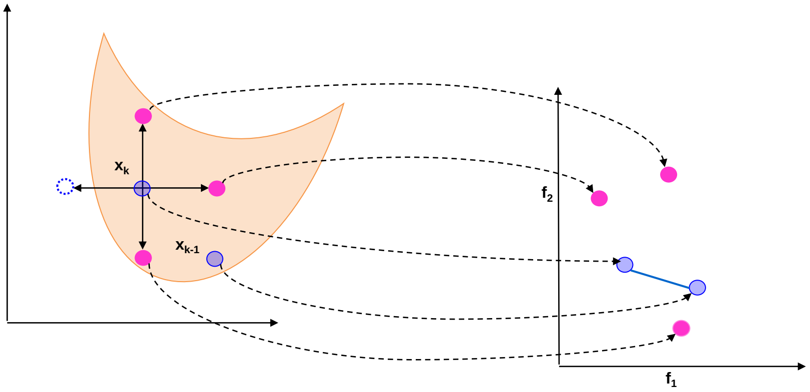

L_{add}

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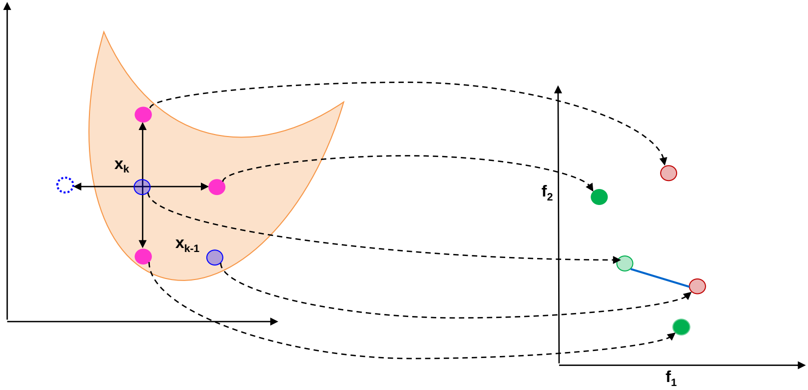

$L_{filtered}$

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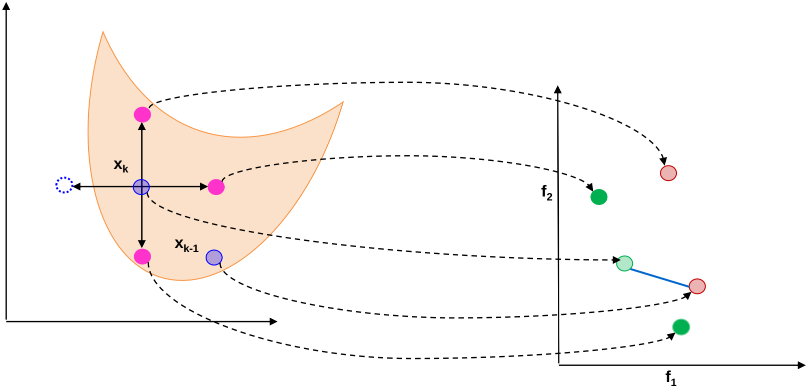

$L_{trial} = L_{filtered}$

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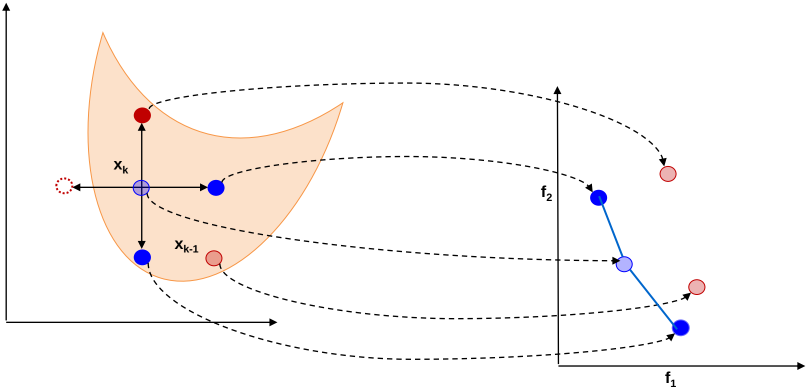

L_{k+1}

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What happens if the problem dimension is large? (n big)

- Increase in the dimension of the positive basis

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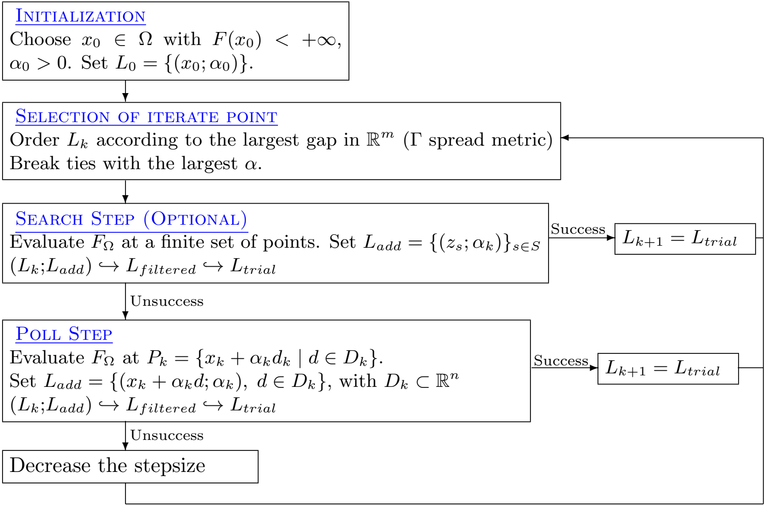
- Increase in the dimension of the positive basis
- Strategies to promote diversity required

Presentation Outline

1. Introduction
2. DMS-Reduction
3. Numerical Experiments
4. A Chemical Engineering Application
5. Conclusions and Future Work

DMS - Algorithmic Structure



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DMS-Reduction - Algorithmic Structure

Initialization

Choose $x_0 \in \Omega$, $\alpha_0 > 0$, and $r < n$.
Set $L_0 = \{(x_0; \alpha_0)\}$

Selection of iterate point

Choose $m_k \leq m$ and order L_k according to the largest gap in $\mathbb{R}^{m_k}$ (Γ spread metric in the reduced objective space). Break ties with the largest α.

Search Step (Optional)

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

Success → $L_{k+1} = L_{trial}$

Unsuccess ↓

Poll Step

Compute an adequate matrix $P_k \in \mathbb{R}^{r \times n}$.
Evaluate F_Ω at $P_k = \{x_k + \alpha_k P_k^\top d_k \mid d \in D_k\}$.
Set $L_{add} = \{(x_k + \alpha_k P_k^\top d; \alpha_k),\ d \in D_k\}$, with $D_k \subset \mathbb{R}^r$
$(L_k; L_{add}) \hookrightarrow L_{filtered} \hookrightarrow L_{trial}$

Success → $L_{k+1} = L_{trial}$

Unsuccess ↓

Decrease the stepsize

D_k positive basis in $\mathbb{R}^r$

Objective Subspace Building

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Anytime that dominance is checked, either at the search or poll steps, all the m objectives are taken into account

Variable Subspace Building

Correlation Approach

Select the subset of $r < n$ variables to keep, according to the correlation between objectives and variables. Consider $\mathcal{D}_k = [I_r \;\; -I_r]$. Compute $P_k \in \mathbb{R}^{r \times n}$ by adding $n - r$ columns of zeros to I_r, at columns corresponding to the indexes of the variables removed.

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Example: If $n = 4$, $r = 2$, and we want to remove the first and the third variables, we get:

$$\mathcal{D}_k = \begin{bmatrix} 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix} \quad \text{and} \quad P_k = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

then

$$P_k^\top D_k = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 \end{bmatrix}$$

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Sketching Approach

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- Hashing: P_k is a s-hashing matrix, where $s \in \mathbb{N}$ is the number of nonzero entries at randomly selected locations, each taking value $\pm 1/\sqrt{s}$
- Gaussian: P_k has entries which are independent and identically distributed in $\mathcal{N}(0, 1/r)$
- Orthogonal: $P_k = \sqrt{n/r} I_{r \times n} Q^\top$ where $I_{r \times n}$ denotes the first r rows of the $n \times n$ identity matrix I_n, and $Q \in \mathbb{R}^{n \times n}$ is the orthogonal factor in the QR decomposition $Z = QR \in \mathbb{R}^{n \times n}$ of a matrix Z with i.i.d. standard normal entries such that the diagonal entries of R are positive

L. Roberts and C. Royer
Direct Search Based on Probabilistic Descent in Reduced Spaces
SIAM J. Optim., 33 (4): 3057-3082, 2023.

Presentation Outline

Numerical Settings

- Testbed: DTLZ1-DTLZ6 and WFG1-WFG9
  - Number of components of the objective function (m) between 4 and 10
  - Number of decision variables (n) between 26 and 38
  - Final test set comprising 105 instances of bound-constrained problems
- DMS-Reduction
  - Deterministic:
    - Reduced space built using r equal to 10% of most correlated variables
    - $m = 2$ most conflicting
    - Correlation approach for variable subspace building
  - Stochastic:
    - Reduced space built using $r = 5$
    - $m = 2$ chosen randomly
    - Sketching approach for variable subspace building (1-hashing)
- Initialization DMS-Reduction*
- Stopping criterion all versions of DMS
  - $\alpha_k < 10^{-3}$ for all points in the list
  - Fixed budget of function evaluations

Initialization: Extreme Points & Middle Points

Extreme Points:

For each $\ell \in \{1, \ldots, m\}$ compute the extreme point given by

$$\overline{x}^{\ell} = \arg\min_{x \in \Omega} f_{\ell}(x)$$

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- Extreme points computed using the SID-PSM algorithm, initialized with the centroid of the box defined by bound constraints

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Incorporating minimum Frobenius norm models in direct search
Comput. Optim. Appl., 46: 265-278, 2010.

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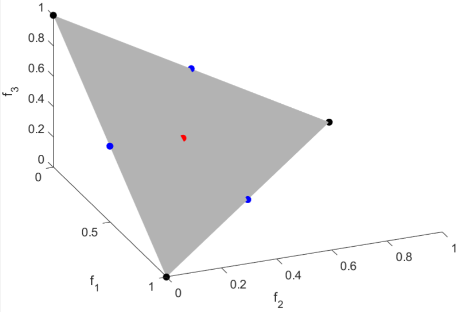
- Stopping criteria: Minimum stepsize 10^{-3} or a maximum of 500 function evaluations
- Budget Management: SID-PSM computes f_{ℓ}, not F, per iteration. Average budget for extreme points computation rounded up plus the final evaluation of F performed for each extreme point

Initialization: Extreme Points & Middle Points

Middle Points (Optional)

For each integer $\xi \in \{2, \ldots, m\}$, consider the set of combinations of ξ components of objective function (which has $\binom{m}{\xi}$ elements). Let J_ξ^ℓ be one of its elements. Compute the middle point as

$$\hat{x}^\ell = \frac{1}{\xi} \sum_{j \in J_\xi^\ell} \overline{x}^j, \quad \ell = 1, \ldots, \binom{m}{\xi}$$



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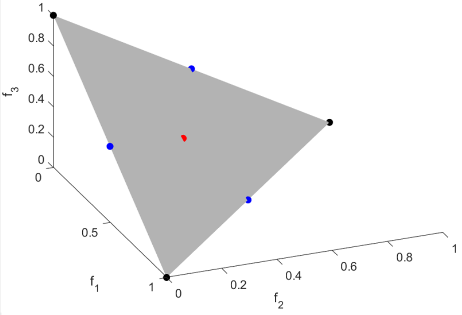


Final initialization list

$$L_0 := \left\{ (\overline{x}^\ell; \alpha_0), \ell = 1, \dots, m \right\} \cup \left\{ \bigcup_{\xi=2}^{m} \bigcup_{\ell=1}^{\binom{m}{\xi}} \{(\hat{x}^\ell; \alpha_0)\} \right\}$$

Other Solvers

- NSGA-III – Nondominated Sorting Genetic Algorithm

  K. Deb and H. Jain
  An evolutionary many-objective optimization algorithm using reference-point-based nondominated sorting approach, Part I: Solving problems with box constraints
  IEEE, 18: 577-601, 2014.

- KnEA – Knee point driven Evolutionary Algorithm

  X. Zhang, Y. Tian and Y. Jin
  A knee point-driven evolutionary algorithm for many-objective optimization
  IEEE, 19: 761–776, 2015.

- MOEA/DD – Many-objective evolutionary algorithm based on dominance and decomposition

  K. Li, K. Deb, Q. Zhang and S. Kwong
  An evolutionary many-objective optimization algorithm based on dominance and decomposition
  IEEE, 19: 694–716, 2015.

- MOMBI-II – Many-objective metaheuristic based on the R2 indicator II

  R. H. Gómez and C. A. Coello Coello
  Improved metaheuristic based on the R2 indicator for many-objective optimization
  GECCO, 7:679–686, 2015.

- GrEA – Grid-Based Evolutionary Algorithm

  S. Yang, M. Li, X. Liu and J. Zheng
  A grid-based evolutionary algorithm for many-objective optimization
  IEEE, 17: 721–736, 2013.

*Implementations in the MATLAB-based platform `PlatEMO`, freely available at `https://github.com/BIMK/PlatEMO`

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

- Purity

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

- Spreads Γ and Δ

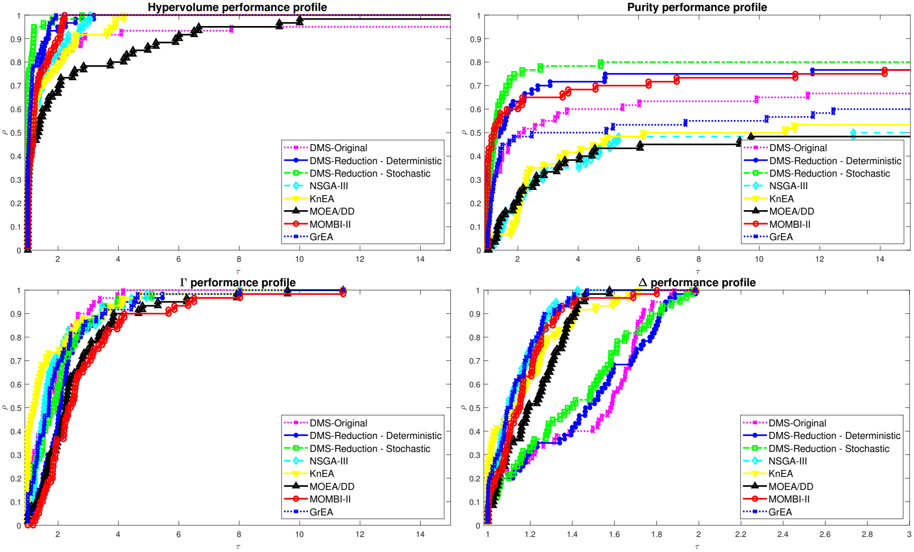
$$\Gamma_{p,s} = \max_{j \in \{1,\ldots,m\}} \left(\max_{i \in \{0,\ldots,N\}} \{d_i\} \right)$$

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

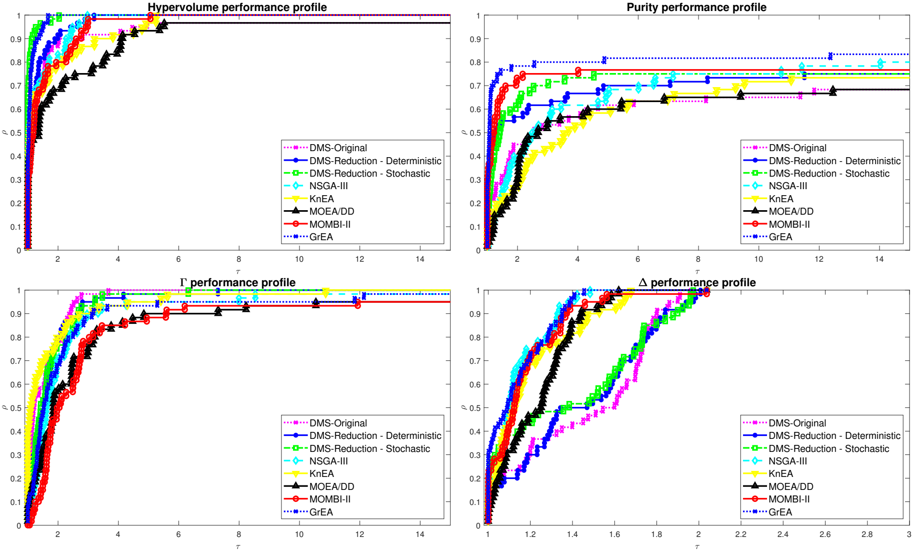
- Hypervolume

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

5k function evaluations

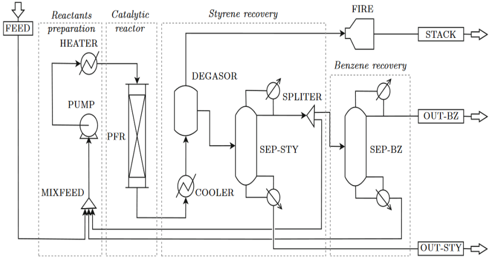


20k function evaluations



Presentation Outline

A Chemical Engineering Application - Styrene Production



- Triobjective problem
  - Net present value ($)
  - Purity of styrene
  - Overall ethylbenzene conversion into styrene

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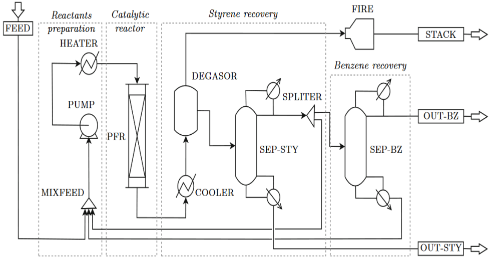

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- Blackbox simulation ($\simeq$ 1s/eval)

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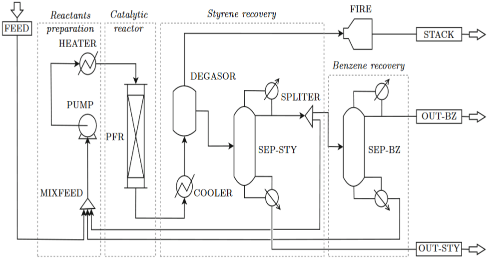

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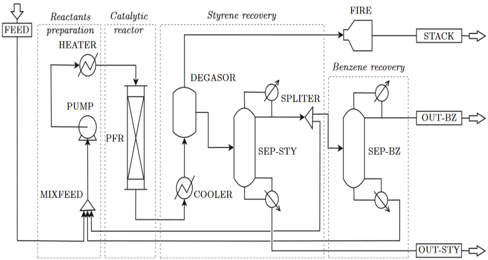
- Blackbox simulation ($\simeq$ 1s/eval)
- 8 variables subject to bounds - normalized to [0,100] intervals

A Chemical Engineering Application - Styrene Production



- Triobjective problem
  - Net present value ($)
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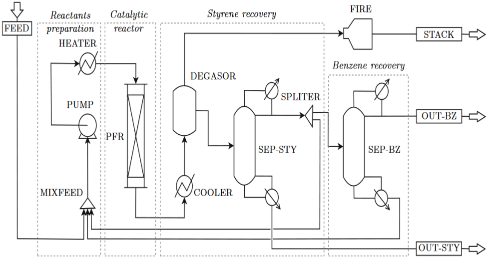

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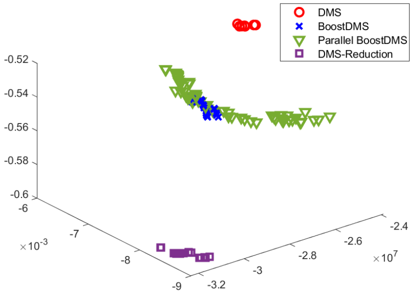
- 9 constraints related with industrial and environmental regulations, treated as hidden constraints
- Initialization at a single point provided in literature

C. Audet, V. Béchard, and S. Le Digabel
Nonsmooth optimization through mesh adaptive direct search and variable neighborhood search
J. Glob. Optim., 41: 299-318,2008.

Computed Pareto Fronts: All DMS versions



- **DMS** Pareto front is dominated by both **BoostDMS** and **Parallel BoostDMS**,which are dominated by **DMS-Reduction**

Solver	#Points
DMS	7
BoostDMS	26
Parallel BoostDMS	66
DMS-Reduction	16

Solver	Purity	Hypervolume	Gamma	Delta	# Function Evaluations
DMS	0%	0.0001	7.96e+6	1.0517	6741
BoostDMS	0%	0.0989	4.34e+6	1.1228	20000
Parallel BoostDMS	0%	0.1321	3.32e+6	1.2266	20000
DMS-Reduction	100%	0.9881	7.27e+6	1.1227	7995

Solvers Able to Handle Constraints

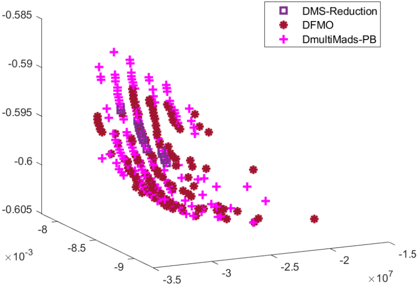
- DFMO

  G. Liuzzi, S. Lucidi and F. Rinaldi
  A derivative-free approach to constrained multiobjective nonsmooth optimization
  SIAM J. Optim., 26: 2744–2774, 2016.

- DMultiMADS-PB

  J. Bigeon, S. Le Digabel and L. Salomon
  Handling of constraints in multiobjective blackbox optimization
  Comput. Optim. Appl., 89: 69–113, 2024.

Computed Pareto Fronts



Solver	#Points
DFMO	122
DMultiMADS-PB	149
DMS-Reduction	16

Solver	Purity	Hypervolume	Gamma	Delta	# Function Evaluations
DMS-Reduction	87.5%	0.3675	13.8e+6	1.2073	7995
DFMO	46.7%	0.7033	5.11e+6	1.6886	20000
DMultiMADS-PB	58.4%	0.7149	5.20e+6	1.7989	20000

Presentation Outline

Conclusions and Future Work

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- DMS-Reduction introduces a novel approach that leverages search directions from variable subspaces
- It is tailored to effectively address challenges in many-objective scenarios
- The approach simultaneously reduces the number of objective function components and problem variables, thereby tackling large-scale challenges
- Extensive numerical experiments demonstrate the method's competitiveness and potential

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Future work

- Developing theoretical analysis for DMS-Reduction
- Implementation of a filter-inexact restoration approach to handle constraints

Thank you for your attention!