Universität Konstanz

Reduced Basis Based Hierarchical Multiobjective Optimization

Michael Kartmann

University of Constance, 21th March, 2023

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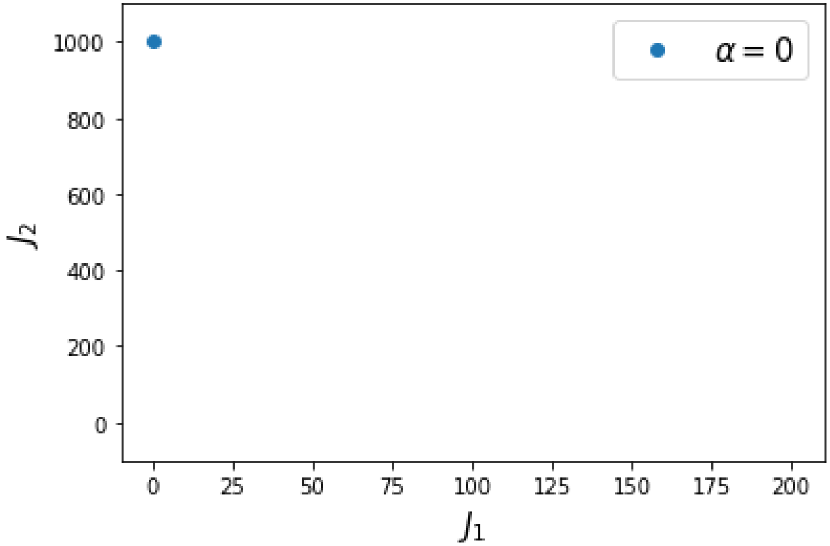

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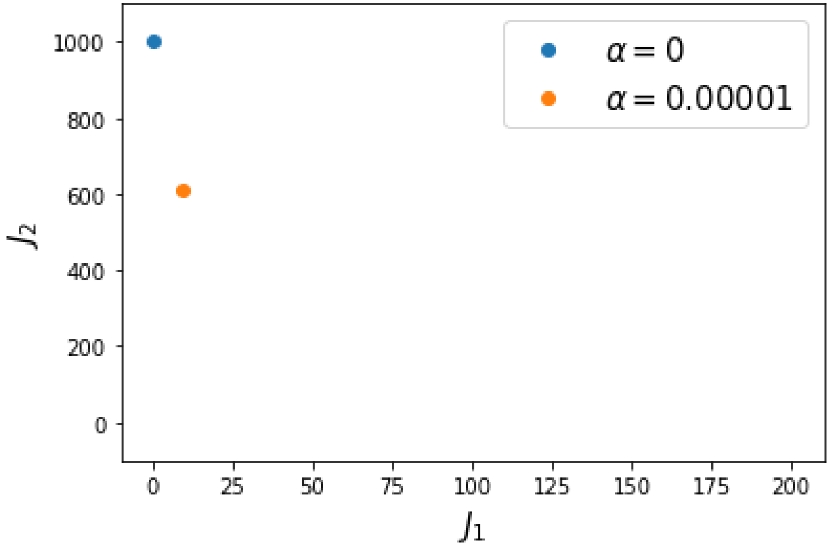

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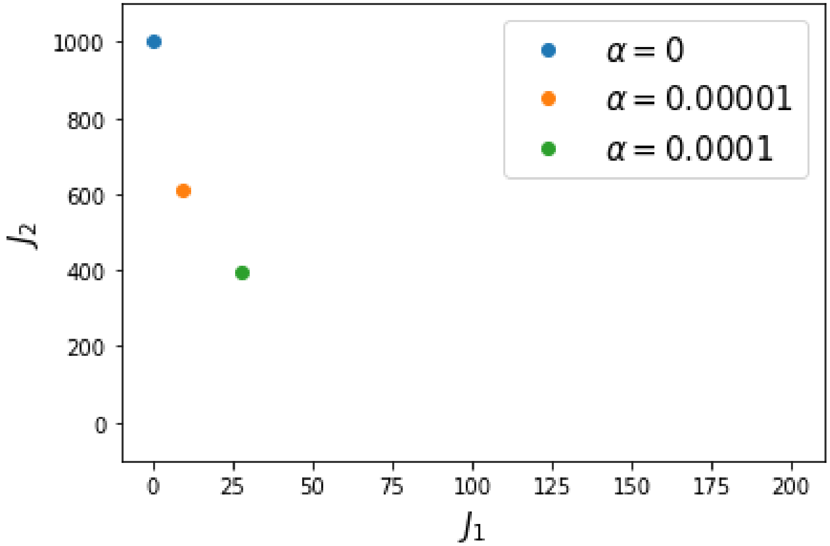

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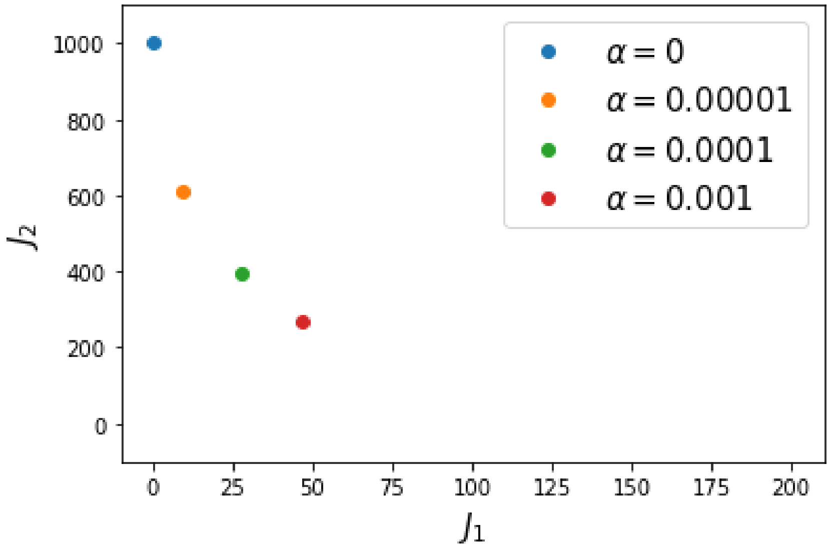

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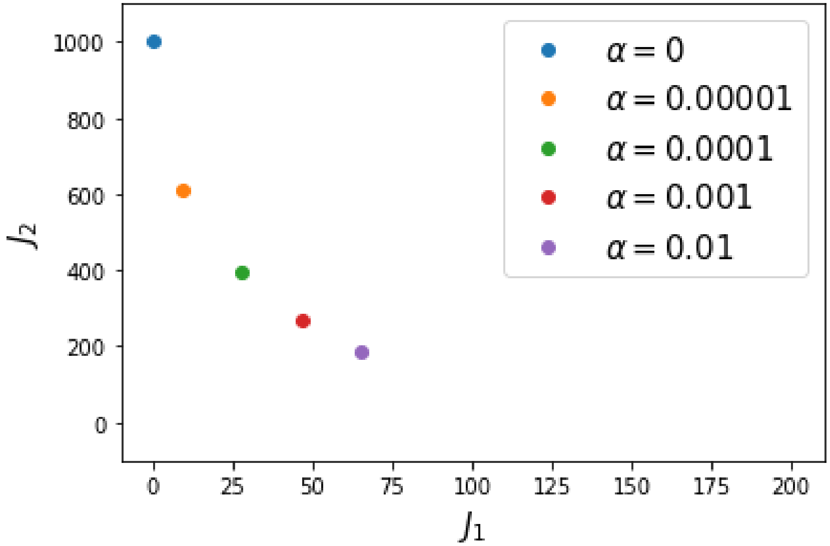

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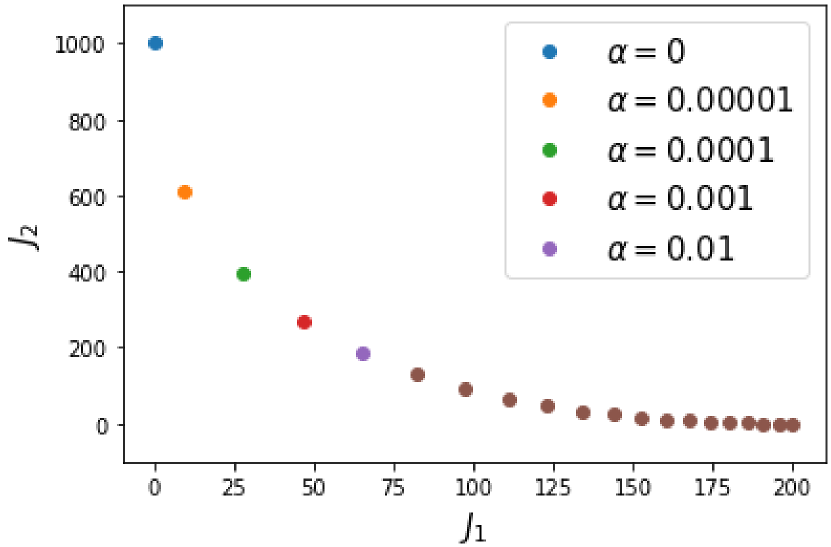
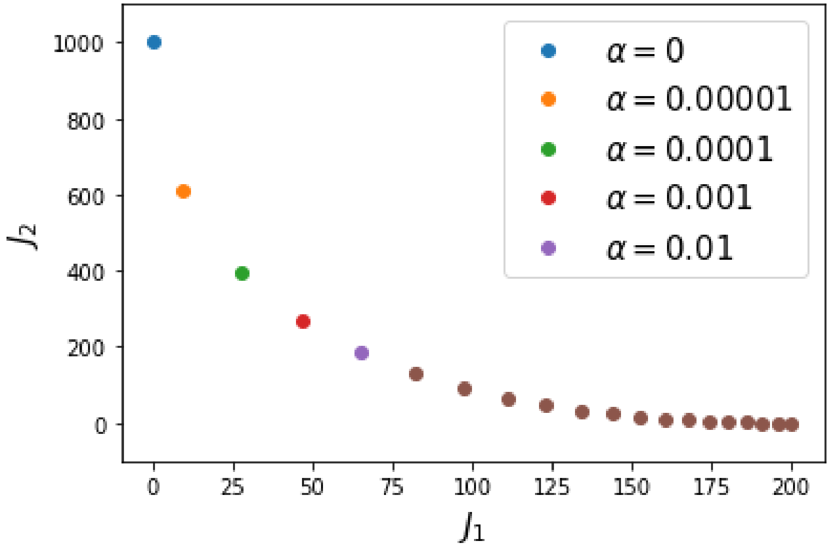


- this corresponds to applying the weighted-sum method (WSM) to the biobjective optimization problem

$$\min_{y,u} \begin{bmatrix} J_1(y) \\ J_2(u) \end{bmatrix}$$



Compute a homogeneous discretization of all optimal compromises (= Pareto set) fast!
$\Rightarrow$ Multiobjective Optimization

Two ingredients

Parametrized PDE	**Cost functions $J_1,\ldots,J_k$**

↓

Two computational challenges

Functions evaluation are expensive	**Uncountable set of optimal compromises**

↓

Two reduction techniques

Reduced Basis (RB) method	**Hierarchical Multiobjective Optimization**

Outline

Problem formulation

$$\min_{u \in U_{ad}} J(u) = \begin{bmatrix} J_1(u) \\ \vdots \\ J_k(u) \end{bmatrix} = \begin{bmatrix} \frac{\nu_1}{2}\|\mathcal{S}(u) - y_d^1\|_H^2 + \frac{\sigma_1}{2}\|u - u_d^1\|_U^2 \\ \vdots \\ \frac{\nu_k}{2}\|\mathcal{S}(u) - y_d^k\|_H^2 + \frac{\sigma_k}{2}\|u - u_d^k\|_U^2 \end{bmatrix} \qquad \text{(MOP)}$$

- Multiobjective cost function $J : U \to \mathbb{R}^k$ $(k \geq 2)$.
- Parameter space U, objective space $\mathbb{R}^k$.
- Convex and closed feasible set $U_{ad} \subset U$.
- $\mathcal{S} : U_{ad} \to H$ solution operator to a parametrized PDE.

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- no total order in $\mathbb{R}^k$ without a priori prioritizing components
- single-objective case: total odering $\Rightarrow$ isolated optima,
  multi-objective case: partial ordering $\Rightarrow$ uncountable set of optima.

1.1 Optimality Conditions

Theorem (First-order Optimality Condition [Kuhn, Tucker 1951])

Let $\bar{u} \in U_{ad}$ be an (unconstrained) Pareto optimal point.
Then there exists a weight vector $\bar{\alpha} \in \mathbb{R}^k_{\geq 0}$ with

$$\mathcal{F}(\bar{u}, \bar{\alpha}) := \begin{bmatrix} \sum_{i=1}^k \bar{\alpha}_i \nabla J_i(\bar{u}) \\ \sum\limits_{i=1}^k \bar{\alpha}_i - 1 \end{bmatrix} = 0. \tag{KKT}$$

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Definition (Pareto critical set)

$\bar{u}$ is called **Pareto critical**, if it satisfies (KKT) with the corresponding multipliers.
We define the **Pareto critical set** $\mathcal{P}$ as

$$\mathcal{P} := \{u \in U_{ad} \mid u \text{ is Pareto critical}\} \subset U_{ad}.$$

Two solution approaches based on the KKT conditions

1. Weighted-sum method (WSM) [Zadeh 1963]

- Idea: choose different $\alpha \in \mathbb{R}^k_{\geq 0}$ with $\sum_{i=1}^k \alpha_i = 1$ and solve the scalar optimization problem

$$\min_{u \in U_{ad}} \sum_{i=1}^{k} \alpha_i J_i(u). \qquad \text{(WSM}(\alpha)\text{)}$$

- Problems: only for convex problems, discretization is non-homogeneous.

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2. Continuation method (CM) [Hillermeier 2001]

- Idea: interpret the set of KKT points $z = (u, \alpha)$ as a solution manifold

$$\mathcal{M} := \mathcal{F}^{-1}(0) = \{z \mid \mathcal{F}(z) = 0\} \subset \mathbb{R}^{n+k}$$

and walk on it iteratively in an predictor/corrector manner.

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+ Hierarchical description of the Pareto (critical) set

1.2 Hierarchical Multiobjective Optimization

Definition (Subproblems for (MOP))

For subset $I \subset \{1, ..., k\}$, we set

$$J^I : U_{ad} \to \mathbb{R}^{|I|}, u \mapsto J^I(u) := (J_i(u))_{i \in I}$$

and define the corresponding subproblem by

$$\min_{u \in U_{ad}} J^I(u). \qquad (MOP^I)$$

Goal:

find the smallest collection of subsets $\mathcal{I} \subset \text{Pot}(\{1, ..., k\})$, such that for $I \in \mathcal{I}$ the Pareto critical sets $\mathcal{P}^I$ completely describe the Pareto critical set $\mathcal{P}$ of (MOP).

Example: Hierarchical Multiobjective Optimization of $k = 3$ Parabolas

$$\min_{x \in \mathbb{R}^2} J(x) = \begin{bmatrix} \frac{1}{2}\|x - x_d^1\|_2^2 \\ \frac{1}{2}\|x - x_d^2\|_2^2 \\ \frac{1}{2}\|x - x_d^3\|_2^2 \end{bmatrix} = \begin{bmatrix} \frac{1}{2}\|x - (1,1)\|_2^2 \\ \frac{1}{2}\|x - (1,-1)\|_2^2 \\ \frac{1}{2}\|x - (-1,-1)\|_2^2 \end{bmatrix}$$

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Lemma

The Pareto set is convex with $\mathcal{P} = \operatorname{conv}\{x_d^1, \ldots, x_d^2\}$, i.e. for every $x \in \mathcal{P}$ there exists $\alpha \in \Delta_k := \{\alpha \in \mathbb{R}^k_{\geq 0} \mid \sum_{i=1}^k \alpha_i = 1\}$ with

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Hierarchical approach:

1. Hierarchical Optimization: Minimize the components ($\mathcal{I} = \{\{1\}, \{2\}, \{3\}\}$).
2. Reconstruction: Build the convex hull of their minimizers.

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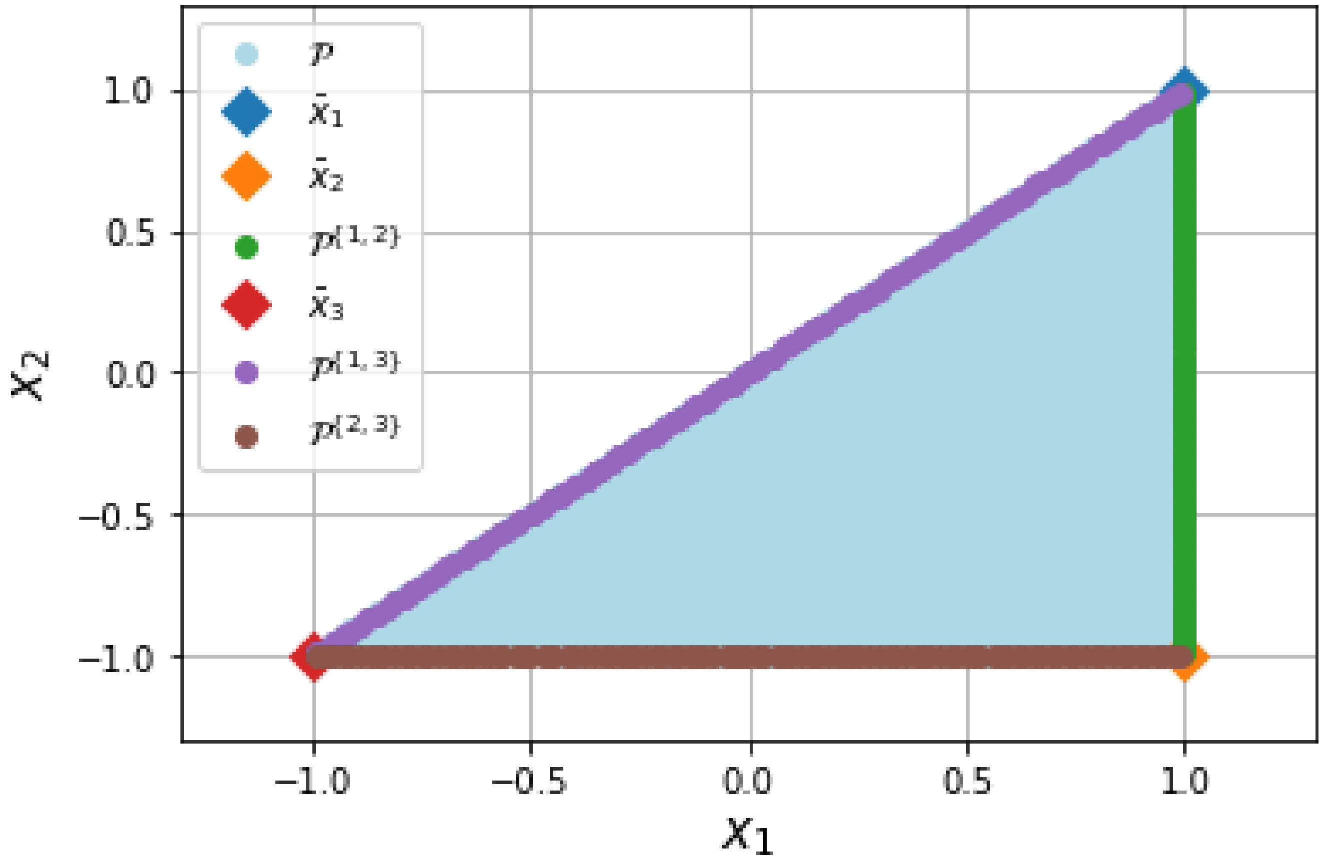
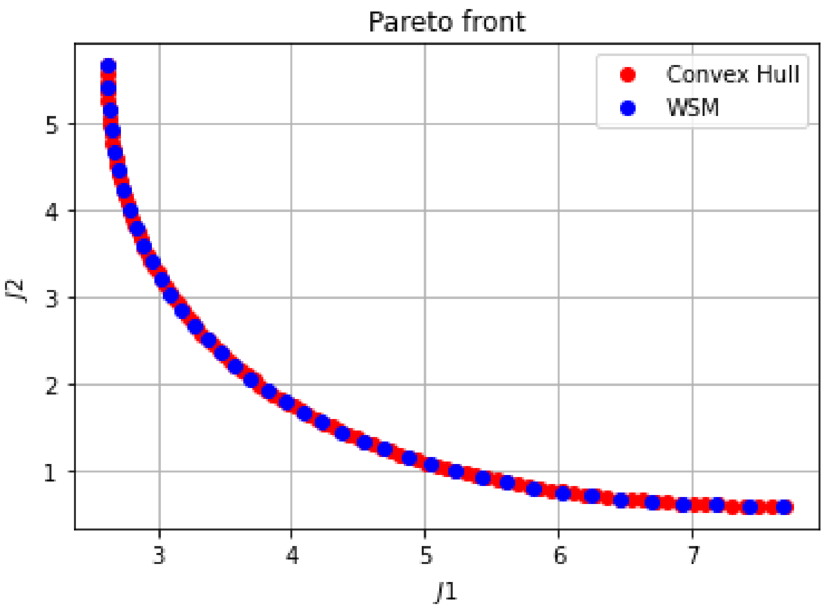


Extension to Linear-Quadratic Optimal Control Problems

$$\min_{u \in L^2(\Omega)} J(u) = \begin{bmatrix} \frac{1}{2}\|\mathcal{S}(u) - y_d^1\|_{L^2(\Omega)}^2 + \frac{\sigma}{2}\|u\|_{L^2(\Omega)}^2 \\ \frac{1}{2}\|\mathcal{S}(u) - y_d^2\|_{L^2(\Omega)}^2 + \frac{\sigma}{2}\|u\|_{L^2(\Omega)}^2 \end{bmatrix}, \tag{P1}$$

where $\mathcal{S}(u) = y$ solves

$$\begin{aligned} -\Delta y + y &= u \quad \text{in } \Omega, \\ \nabla y \cdot \eta &= 0 \quad \text{on } \partial\Omega. \end{aligned}$$



Algorithm	Time [s]
WSM (100 weights)	277
Convex Hull	5

2 Non-Convex Parameter Optimization

$$\min_{\boldsymbol{\mu}\in U_{ad}\subset\mathbb{R}^n} J(\boldsymbol{\mu}) = \begin{bmatrix} \frac{1}{2}\|\mathcal{S}(\boldsymbol{\mu}) - y_d^1\|^2_{L^2(\Omega)} \\ \vdots \\ \frac{1}{2}\|\mathcal{S}(\boldsymbol{\mu}) - y_d^{k-1}\|^2_{L^2(\Omega)} \\ \frac{1}{2}\|\boldsymbol{\mu}\|^2_{\mathbb{R}^n} \end{bmatrix}, \tag{MPOP}$$

where $\mathcal{S}(\boldsymbol{\mu}) = y \in H^1(\Omega)$ solves

$$\begin{aligned} -\nabla\cdot\left[\left(\sum_{i=1}^{n'} \boldsymbol{\mu}_i \chi_{\Omega_i}\right)\nabla \boldsymbol{y}\right] + \boldsymbol{\mu}_{n-1} b\cdot\nabla \boldsymbol{y} + \boldsymbol{\mu}_n \boldsymbol{y} &= f \quad \text{in } \Omega, \\ \nabla \boldsymbol{y}\cdot\eta &= 0 \quad \text{on } \partial\Omega. \end{aligned} \tag{PDE(μ)}$$

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⇒ for an unconstrained Pareto optima $\mu \in U_{ad}$ with weight vector $\alpha \in \mathbb{R}^k_{\geq 0}$ we have for $z = (\mu, \alpha)$

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$\Rightarrow$ for an unconstrained Pareto optima $\mu \in U_{ad}$ with weight vector $\alpha \in \mathbb{R}^k_{\geq 0}$ we have for $z = (\mu, \alpha)$

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- **Continuation method: Local search in the solution manifold of this underdetermined system!**

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Theorem (Foundation of Continuation methods [Hillermeier 2001])

If it holds $rk(\mathcal{F}'(z)) = n+1 \quad \forall z \in \mathcal{M}$. Then

$$\mathcal{M} := \mathcal{F}^{-1}(0) = \{z = (\mu, \alpha) \mid \mathcal{F}(z) = 0\} \subset \mathbb{R}^{n+k}$$

is a $(k-1)$-dimensional C^2- submanifold of the $\mathbb{R}^{n+k}$ and $T_z\mathcal{M} = \ker(\mathcal{F}'(z))$ for $z \in \mathcal{M}$.

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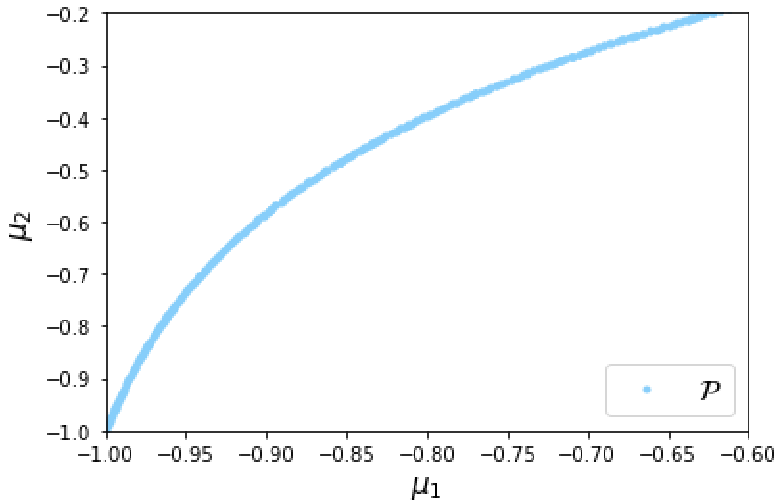

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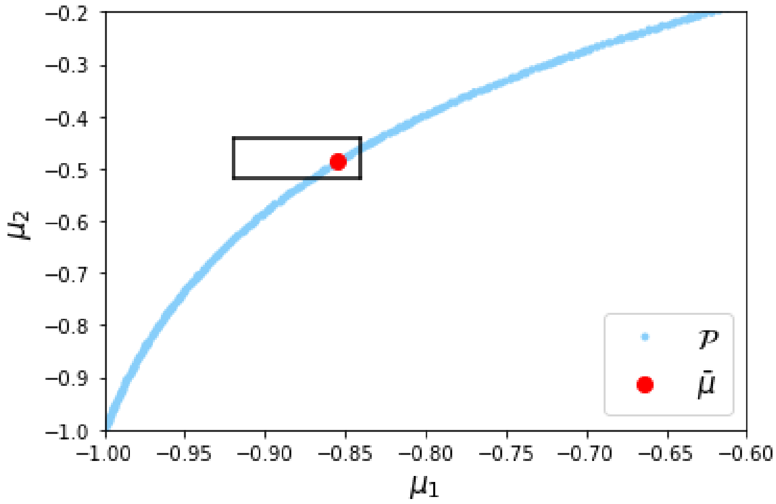

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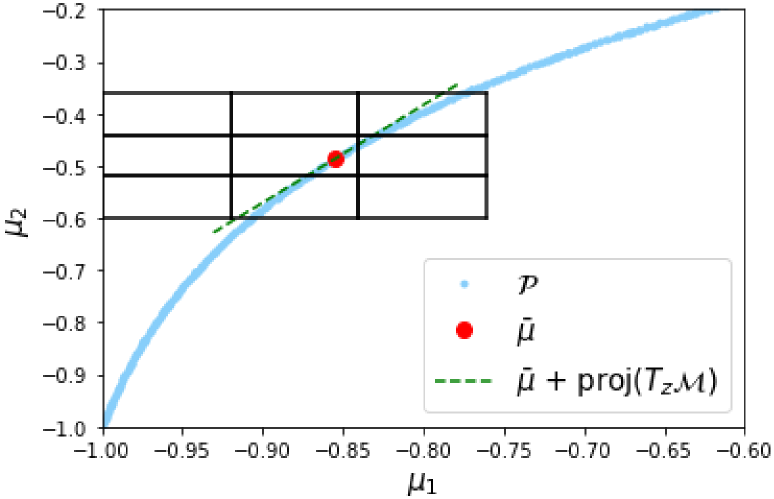
1. Initialize with $\bar{z} = (\bar{\mu}, \bar{\alpha}) \in \mathcal{M}$.
2. Predictorstep:
   a) compute $T_{\bar{z}}\mathcal{M} = \ker(\mathcal{F}'(\bar{z}))$.
   b) mark all neighbor boxes with non-empty intersection with $\bar{\mu}+ \text{proj}_n(T_{\bar{z}}\mathcal{M})$.



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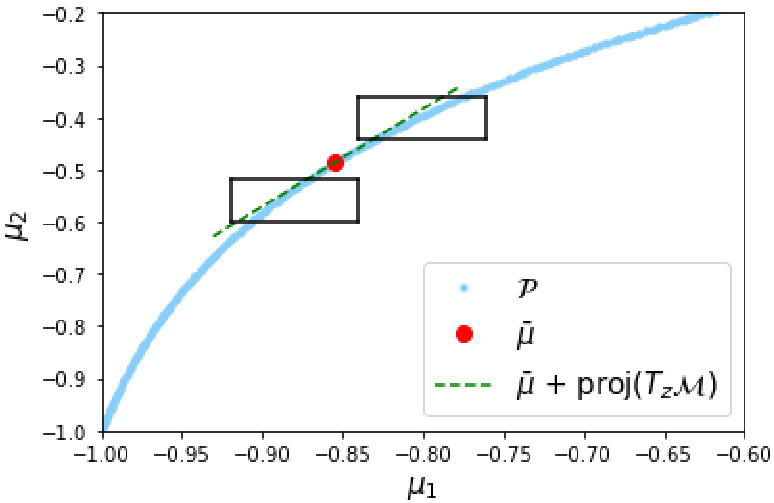

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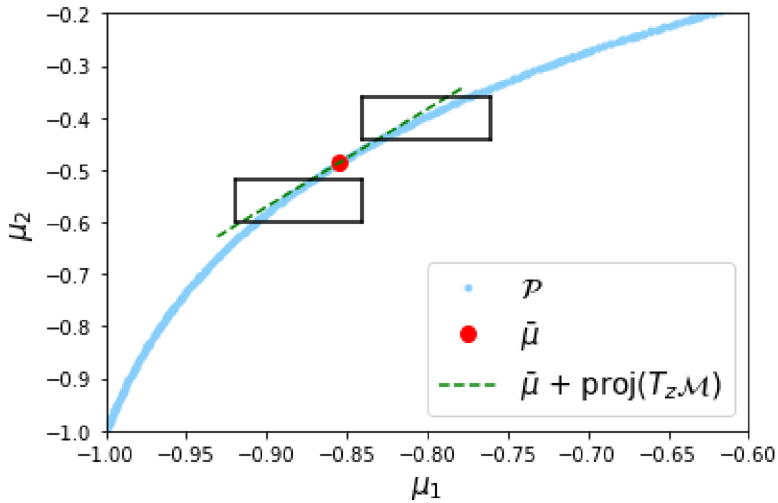
   b) mark all neighbor boxes with non-empty intersection with $\bar{\mu} +$ $\text{proj}_n(T_{\bar{z}}\mathcal{M})$.
3. Correctorstep: in every marked box B solve

$$\min_{\mu \in B,\ \alpha \in \Delta^k} \frac{1}{2} \left\| \sum_{i=1}^{k} \alpha_i \nabla J_i(\mu) \right\|_2^2. \qquad \text{(BoxProb(B))}$$



2.1 The Continuation Method (CM)

Theorem (Foundation of Continuation methods [Hillermeier 2001])

If it holds $rk(\mathcal{F}'(z)) = n+1 \quad \forall z \in \mathcal{M}$. Then

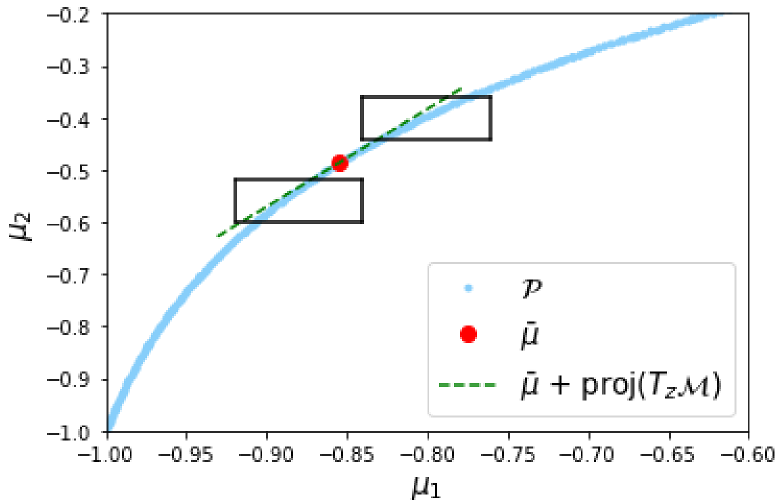
$$\mathcal{M} := \mathcal{F}^{-1}(0) = \{z = (\mu, \alpha) \mid \mathcal{F}(z) = 0\} \subset \mathbb{R}^{n+k}$$

is a $(k-1)$-dimensional C^2- submanifold of the $\mathbb{R}^{n+k}$ and $T_z\mathcal{M} = \ker(\mathcal{F}'(z))$ for $z \in \mathcal{M}$.

1. Initialize with $\bar{z} = (\bar{\mu}, \bar{\alpha}) \in \mathcal{M}$.
2. Predictorstep:
   a) compute $T_{\bar{z}}\mathcal{M} = \ker(\mathcal{F}'(\bar{z}))$.
   b) mark all neighbor boxes with non-empty intersection with $\bar{\mu}+ \text{proj}_n(T_{\bar{z}}\mathcal{M})$.
3. Correctorstep: in every marked box B solve

$$\min_{\mu \in B,\ \alpha \in \Delta^k} \frac{1}{2}\left\| \sum_{i=1}^{k} \alpha_i \nabla J_i(\mu) \right\|_2^2. \qquad \text{(BoxProb(B))}$$

4. Repeat!



2.2 The Hierarchical Inexact Continuation Method (HICM)

- obtain an RB approximation J^r of J satisfying

$$\sup_{\mu \in U_{ad}} \|\nabla J_i(\mu) - \nabla J_i^r(\mu)\|_2 \leq \varepsilon_i \quad \forall i \in \{1, \ldots, k\}.$$

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- inexact Pareto critical set

$$\mathcal{P} \subset \mathcal{P}_r := \left\{ \mu \in \mathbb{R}^n \,\middle|\, \exists \alpha \in \Delta_k : \left\| \sum_{i=1}^{k} \alpha_i \nabla J_i^r(\mu) \right\|_2^2 \leq (\alpha^T \varepsilon)^2 \right\}.$$

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- [Gebken, Peitz, Dellnitz 2019]: for $k > n$ we have

$$\partial \mathcal{P} \approx \mathcal{P}_E \subset \bigcup_{\substack{I \subset \{1,\dots,k\} \\ |I| = n}} \mathcal{P}^I \subset \bigcup_{\substack{I \subset \{1,\dots,k\} \\ |I| = n}} \mathcal{P}_r^I.$$

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- [Gebken, Peitz, Dellnitz 2019]: for $k > n$ we have

$$\partial \mathcal{P} \approx \mathcal{P}_E \subset \bigcup_{\substack{I \subset \{1,\dots,k\} \\ |I|=n}} \mathcal{P}^I \subset \bigcup_{\substack{I \subset \{1,\dots,k\} \\ |I|=n}} \mathcal{P}_r^I.$$

- modification of the boxproblem

$$\min_{\mu \in B \cap P_{ad},\ \alpha \in \Delta_n} \left\| \sum_{i \in I} \alpha_i \nabla J_i^r(\mu) \right\|_2^2 - (\alpha^T \varepsilon)^2. \qquad (\varepsilon\text{BoxProb(B)})$$

2.3 Numerical Results

$$\min_{\boldsymbol{\mu}\in[(0.5,-1),(3,1)]} J(\boldsymbol{\mu}) = \begin{bmatrix} \frac{1}{2}\|\mathcal{S}(\boldsymbol{\mu}) - \mathcal{S}(0.7, 0.8)\|^2_{L^2(\Omega)} \\ \frac{1}{2}\|\mathcal{S}(\boldsymbol{\mu}) - \mathcal{S}(2, 0.5)\|^2_{L^2(\Omega)} \\ \frac{1}{2}\|\mathcal{S}(\boldsymbol{\mu}) - \mathcal{S}(3, -0.5)\|^2_{L^2(\Omega)} \\ \frac{1}{2}\|\boldsymbol{\mu} - (0, 0)\|^2_{\mathbb{R}^2} \\ \frac{1}{2}\|\boldsymbol{\mu} - (1.5, -1)\|^2_{\mathbb{R}^2} \end{bmatrix} \qquad \text{(P2)}$$

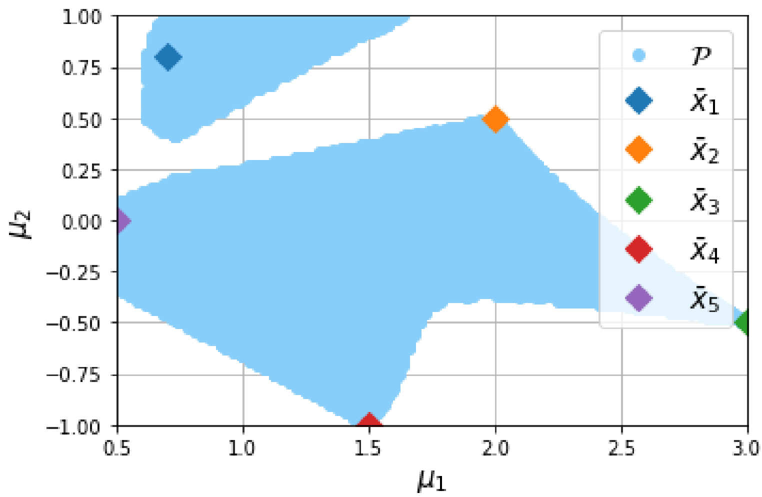
Discretization

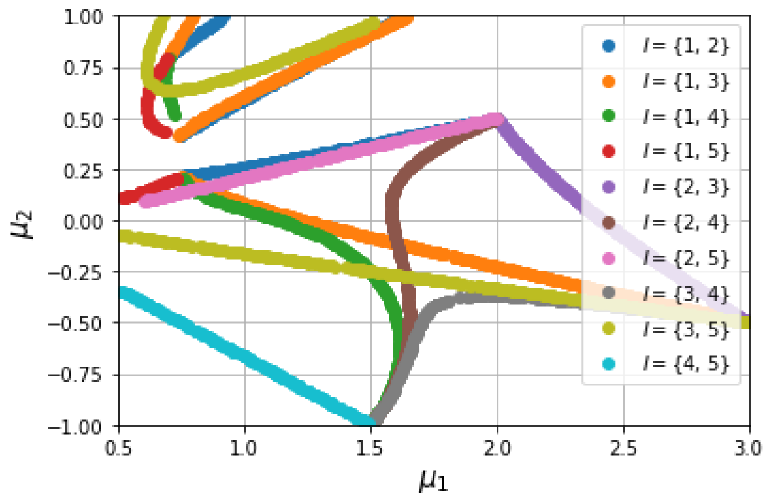
- **FOM:** P1 elements with 714 dofs.
- **ROM:** strong Greedy with $|P_{train}| = 100$ and $\|\varepsilon\|_\infty = 1e-2$ leading to a reduced basis with 14 elements.

Algorithms

- **Full Continuation** with radius $r = 0.0105$.
- **Hierarchical Continuation ($k = 5 > 2 = n$):** solve all 10 subproblems of size $n = 2$.

2.3 Numerical Results





Algorithm	Time [s]	# Boxes
FOM-CM	3847	4960
FOM-Hierarchical CM	623	1158
ROM-CM	419	5017
ROM-Hierarchical ICM	24	1120

3 Conclusion and Outlook

Conclusion:

- we applied two reduction techniques for PDE constrained MOPs.
- the hierarchical approach has the following advantages:
    1. We need less points in total to describe the Pareto (critical) set.
    2. Those points are cheaper available since only a subset of the objectives needs to be considered.
    3. The subproblems are independent of each other, which gives the possibility to exploit the special structure of the subproblem by using specialized solvers and parallelism.

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Outlook:

- Independency of k, neglect unnecesary subproblems.
- Adaptivity w.r.t the Reduced Basis.
- Sharp a posteriori error bounds for the gradients.
- Hierarchical structure for non-convex or non-smooth problems ($\partial\mathcal{P} \approx \mathcal{P}_E$?).

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