NATIONAL TECHNICAL UNIVERSITY OF ATHENS (NTUA)
SCHOOL OF MECHANICAL ENGINEERING
PARALLEL CFD & OPTIMIZATION UNIT (PCOpt/NTUA)

Adjoint-Assisted Pareto Front Tracing

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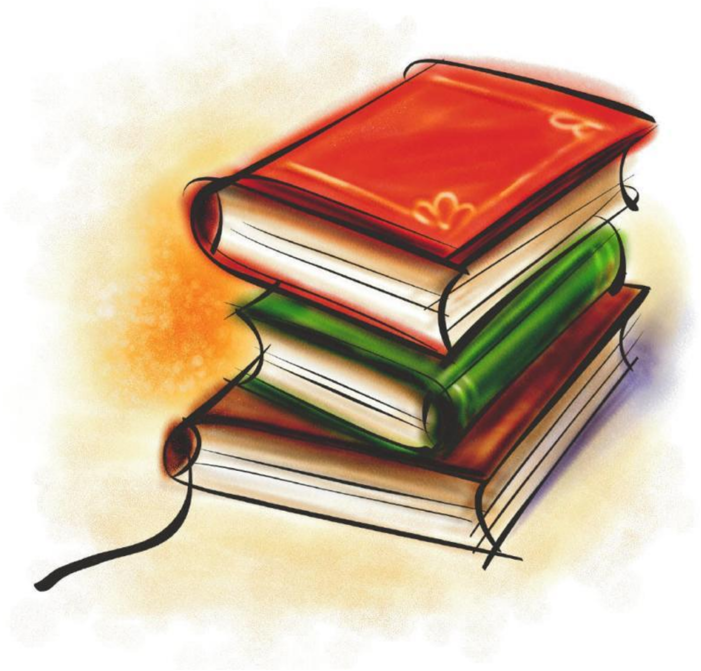


The Prediction – Correction Method

MOO Problem Definition

MOO problem with M_o (or, just, M) objectives:

$$\begin{aligned} \min\ \boldsymbol{f}(\boldsymbol{b}) &= \min\{f_1(\boldsymbol{b}), \ldots, f_M(\boldsymbol{b})\} \\ \text{s.t. } \boldsymbol{c}(\boldsymbol{b}) &= 0 \\ \boldsymbol{g}(\boldsymbol{b}) &\leq 0 \end{aligned}$$

Standard handling with a GBM:
Minimise the weighted sum of the M objectives

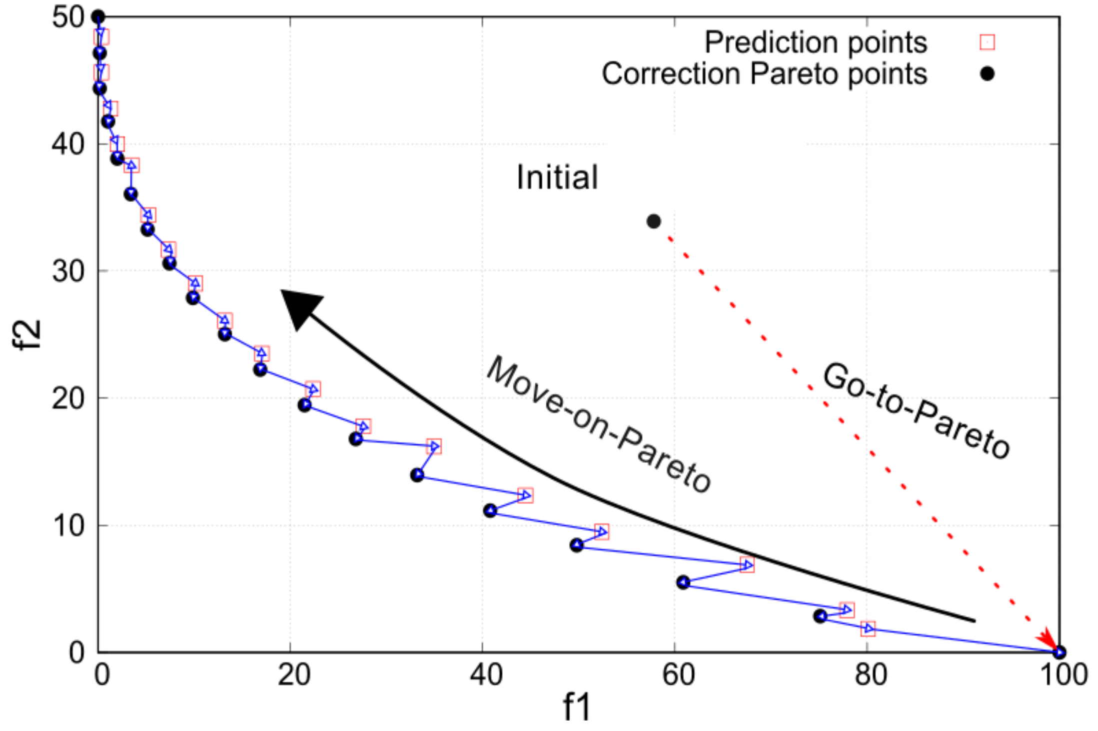
$$\min F_w(\boldsymbol{b}) = \sum_{j=1}^{M} w_j f_j(\boldsymbol{b})$$

Adjoint–assisted Pareto Front Tracing – Concept:

A two-phase method:

Phase 1: Go-to-Pareto: Compute a point that belongs to the Pareto front.

Phase 2: Move-on-Pareto: Move from one Pareto point to the next by considering the local curvature of the front (without restarting from the same initial point).

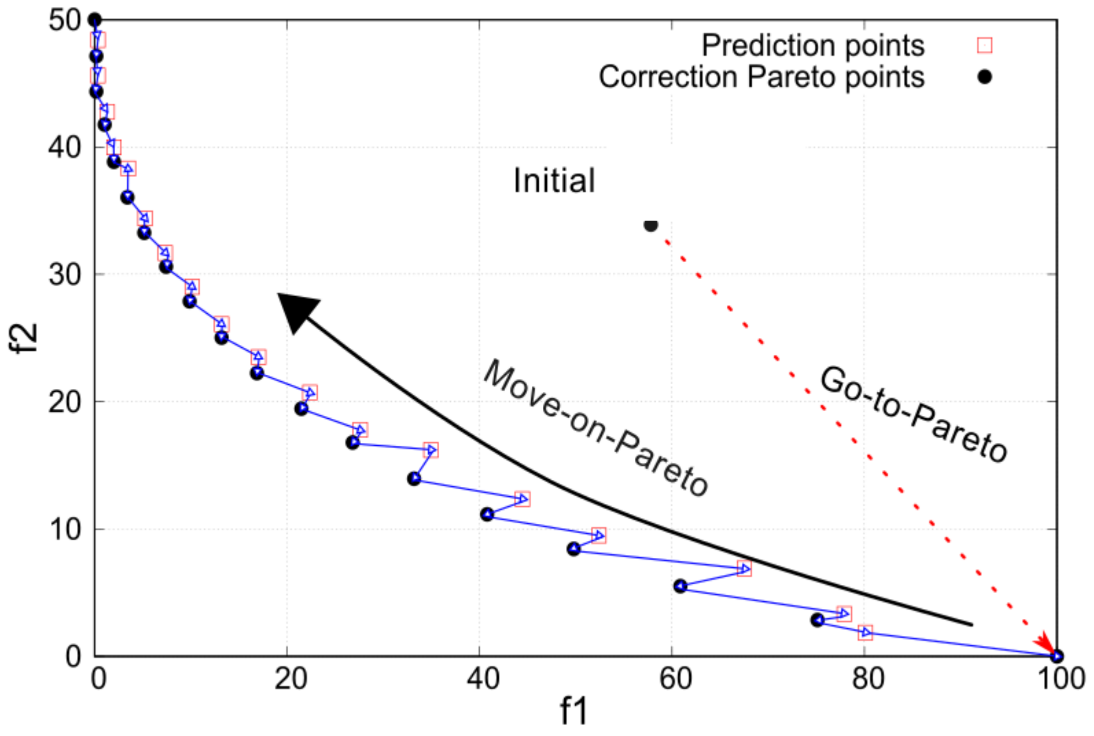


Phase 1: Go-to-Pareto

Solve a SOO problem for min. f_1 or min f_2?

Standard GBM by setting all but one weight equal to 0

$$\min F_w(\boldsymbol{b}) = \sum_{j=1}^{M} w_j f_j(\boldsymbol{b})$$



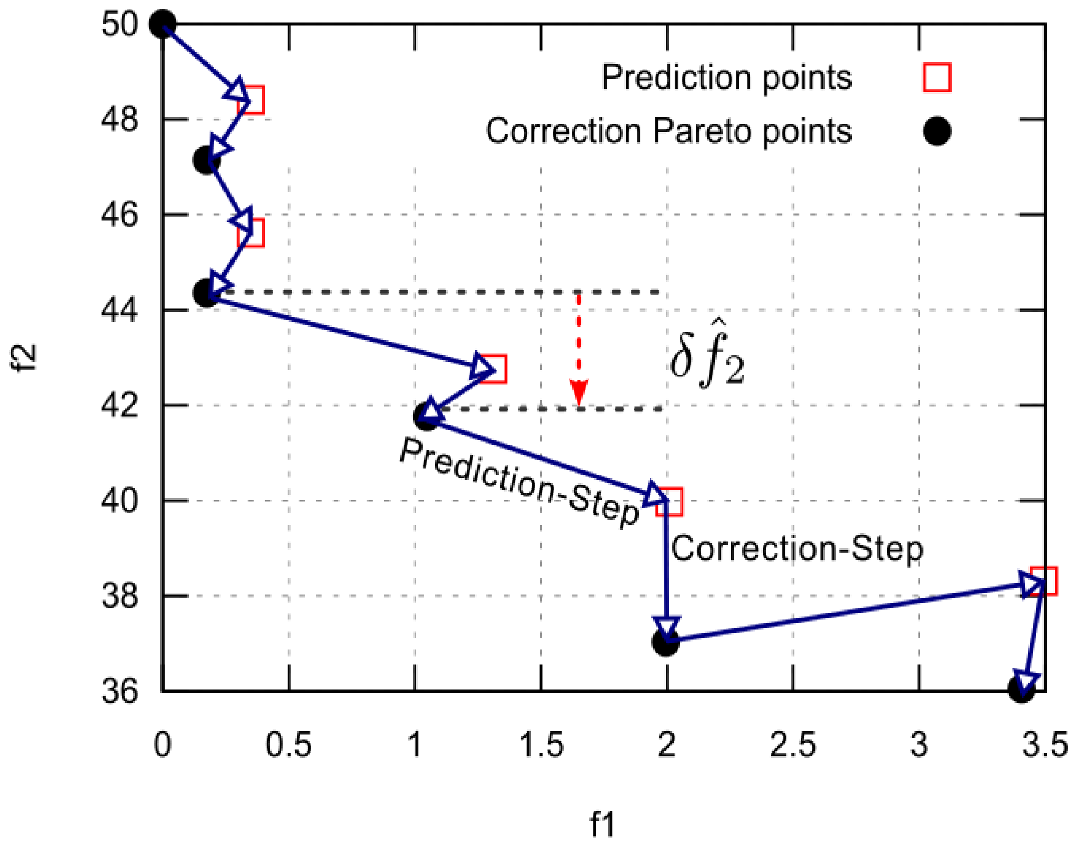
Phase 2: Move-on-Pareto

How can we define the new target Pareto point?

Two-step method

Step 1: Prediction: Formulate the Karush-Kuhn-Tucker (KKT) conditions and satisfy the requirements of the implicit function theorem.

Step 2: Correction: bring the predicted point onto the Pareto front (using ALM or SQP).



Prediction Step – An Example (1/3)

Assume the two-objective unconstrained problem: $\min\{f_1(\boldsymbol{b}), f_2(\boldsymbol{b})\}, \quad \boldsymbol{b} \epsilon R^3$

Re-formulate it as:

$$\min f_1(\boldsymbol{b})$$
$$s.t.\, f_2(\boldsymbol{b}) - \hat{f}_2 = 0$$

Lagrangian: $L(\boldsymbol{b}, \hat{\lambda}_2) = f_1(\boldsymbol{b}) - \hat{\lambda}_2 \left(f_2(\boldsymbol{b}) - \hat{f}_2\right)$

KKT conditions:

$$\left.\begin{aligned} \frac{\vartheta f_1}{\vartheta b_1} - \hat{\lambda}_2 \frac{\vartheta f_2}{\vartheta b_1} &= 0 \\ \frac{\vartheta f_1}{\vartheta b_2} - \hat{\lambda}_2 \frac{\vartheta f_2}{\vartheta b_2} &= 0 \\ \frac{\vartheta f_1}{\vartheta b_3} - \hat{\lambda}_2 \frac{\vartheta f_2}{\vartheta b_3} &= 0 \\ f_2(\boldsymbol{b}) - \hat{f}_2 &= 0 \end{aligned}\right\} \quad \boldsymbol{H}(\boldsymbol{b}, \hat{\lambda}_2, \hat{f}_2) = 0$$

4 equations

Prediction Step – An Example (2/3)

The new system of 4 equations: $\boldsymbol{H}(\boldsymbol{b}, \hat{\lambda}_2, \hat{f}_2) = 0$

Set: $\boldsymbol{z}(\boldsymbol{b}, \hat{\lambda}_2)$

$$\boldsymbol{z} = \boldsymbol{h}(\hat{f}_2)$$

or

$$z_1 = b_1 = h_1(\hat{f}_2)$$
$$z_2 = b_2 = h_2(\hat{f}_2)$$
$$z_3 = b_3 = h_3(\hat{f}_2)$$
$$z_4 = \hat{\lambda}_2 = h_4(\hat{f}_2)$$

$$\frac{\vartheta \boldsymbol{H}}{\vartheta \hat{f}_2} + \frac{\vartheta \boldsymbol{H}}{\vartheta \boldsymbol{z}} \frac{\vartheta \boldsymbol{h}}{\vartheta \hat{f}_2} = \boldsymbol{0} \Rightarrow \frac{\vartheta \boldsymbol{h}}{\vartheta \hat{f}_2} = -\left[\frac{\vartheta \boldsymbol{H}}{\vartheta \boldsymbol{z}}\right]^{-1} \frac{\vartheta \boldsymbol{H}}{\vartheta \hat{f}_2}$$

First-order Taylor expansion:

$$\Rightarrow \boldsymbol{z}^{new} = \boldsymbol{z}^{old} + \frac{\vartheta \boldsymbol{h}}{\vartheta \hat{f}_2} (\hat{f}_2^{new} - \hat{f}_2^{old})$$

Prediction Step – An Example (3/3)

$$\underbrace{\frac{\vartheta \boldsymbol{H}}{\vartheta \hat{f}_2}}_{4\text{x}1} + \underbrace{\frac{\vartheta \boldsymbol{H}}{\vartheta \boldsymbol{z}}}_{4\text{x}4} \underbrace{\frac{\vartheta \boldsymbol{h}}{\vartheta \hat{f}_2}}_{4\text{x}1} = \underbrace{\boldsymbol{0}}_{4\text{x}1}$$

$$\frac{\vartheta \boldsymbol{H}}{\vartheta \hat{f}_2} = \begin{bmatrix} \vartheta H_1/\vartheta \hat{f}_2 \\ \vartheta H_2/\vartheta \hat{f}_2 \\ \vartheta H_3/\vartheta \hat{f}_2 \\ \vartheta H_4/\vartheta \hat{f}_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \end{bmatrix}$$

$\nabla_b^2 L$

$$\frac{\vartheta \boldsymbol{H}}{\vartheta \boldsymbol{z}} = \begin{bmatrix} \vartheta H_1/\vartheta b_1 & \cdots & \vartheta H_1/\vartheta \hat{\lambda}_2 \\ \vdots & \ddots & \vdots \\ \vartheta H_4/\vartheta b_1 & \cdots & \vartheta H_4/\vartheta \hat{\lambda}_2 \end{bmatrix} = \begin{bmatrix} \frac{\vartheta^2 f_1}{\vartheta b_1^2} - \hat{\lambda}_2 \frac{\vartheta^2 f_2}{\vartheta b_1^2} & \frac{\vartheta^2 f_1}{\vartheta b_1 \vartheta b_2} - \hat{\lambda}_2 \frac{\vartheta^2 f_2}{\vartheta b_1 \vartheta b_2} & \frac{\vartheta^2 f_1}{\vartheta b_1 \vartheta b_3} - \hat{\lambda}_2 \frac{\vartheta^2 f_2}{\vartheta b_1 \vartheta b_3} & -\frac{\vartheta f_2}{\vartheta b_1} \\ \frac{\vartheta^2 f_1}{\vartheta b_1 \vartheta b_2} - \hat{\lambda}_2 \frac{\vartheta^2 f_2}{\vartheta b_1 \vartheta b_2} & \frac{\vartheta^2 f_1}{\vartheta b_2^2} - \hat{\lambda}_2 \frac{\vartheta^2 f_2}{\vartheta b_2^2} & \frac{\vartheta^2 f_1}{\vartheta b_2 \vartheta b_3} - \hat{\lambda}_2 \frac{\vartheta^2 f_2}{\vartheta b_2 \vartheta b_3} & -\frac{\vartheta f_2}{\vartheta b_2} \\ \frac{\vartheta^2 f_1}{\vartheta b_1 \vartheta b_3} - \hat{\lambda}_2 \frac{\vartheta^2 f_2}{\vartheta b_1 \vartheta b_3} & \frac{\vartheta^2 f_1}{\vartheta b_2 \vartheta b_3} - \hat{\lambda}_2 \frac{\vartheta^2 f_2}{\vartheta b_2 \vartheta b_3} & \frac{\vartheta^2 f_1}{\vartheta b_3^2} - \hat{\lambda}_2 \frac{\vartheta^2 f_2}{\vartheta b_3^2} & -\frac{\vartheta f_2}{\vartheta b_3} \\ \frac{\vartheta f_2}{\vartheta b_1} & \frac{\vartheta f_2}{\vartheta b_2} & \frac{\vartheta f_2}{\vartheta b_3} & 0 \end{bmatrix}$$

Prediction – Correction Scheme – Generalisation (1/5)

Re-formulate the MOO problem as:

$$\min f_1(\boldsymbol{b})$$
$$\text{s.t. } f_k(\boldsymbol{b}) = \hat{f}_k$$
$$\boldsymbol{c}(\boldsymbol{b}) = 0$$
$$\boldsymbol{g}(\boldsymbol{b}) \leq 0$$

M-1 additional constraints

User-defined values

Lagrangian:

$$\min \mathcal{L}(\boldsymbol{b}, \hat{\boldsymbol{\lambda}}, \boldsymbol{\lambda}, \boldsymbol{\mu}) = f_1(\boldsymbol{b}) - \sum_{k=2}^{M} \hat{\lambda}_k (f_k(\boldsymbol{b}) - \hat{f}_k) - \sum_{i=1}^{M_e} \lambda_i c_i(\boldsymbol{b}) - \sum_{j=1}^{M_{ie}} \mu_j g_j(\boldsymbol{b})$$

M_e equality constraints
M_{ie} inequality constraints

Prediction – Correction Scheme – Generalisation (2/5)

KKT conditions:

$$\nabla_{\boldsymbol{b}}\mathcal{L}(\boldsymbol{b},\hat{\boldsymbol{\lambda}},\boldsymbol{\lambda},\boldsymbol{\mu}) = \nabla_{\boldsymbol{b}} f_l(\boldsymbol{b}) - \sum_{k=2}^{M}\hat{\lambda}_k \nabla_{\boldsymbol{b}} f_k(\boldsymbol{b}) - \sum_{i=1}^{M_e}\lambda_i \nabla_{\boldsymbol{b}} c_i(\boldsymbol{b}) - \sum_{j=1}^{M_{ie}}\mu_j \nabla_{\boldsymbol{b}} g_j(\boldsymbol{b}) = 0$$

$$f_k(\boldsymbol{b}) - \hat{f}_k = 0\ ,\ \forall k \in [2, M]$$

$$c_i(\boldsymbol{b}) = 0\ ,\ \forall i \in [1, M_e]$$

$$g_j(\boldsymbol{b}) \leq 0\ ,\ \forall j \in [1, M_{ie}]$$

$$\mu_j g_j(\boldsymbol{b}) = 0\ ,\ \forall j \in [1, M_{ie}]$$

$$\mu_j \leq 0\ ,\ \forall j \in [1, M_{ie}]$$

Prediction – Correction Scheme – Generalisation (3/5)

$$\left.\begin{aligned}
f_k(\boldsymbol{b}) - \hat{f}_k &= 0\ ,\ \forall k \in [2, M] \\
c_i(\boldsymbol{b}) &= 0\ ,\ \forall i \in [1, M_e] \\
g_j(\boldsymbol{b}) &\leq 0\ ,\ \forall j \in [1, M_{ie}] \\
\mu_j g_j(\boldsymbol{b}) &= 0\ ,\ \forall j \in [1, M_{ie}]
\end{aligned}\right\} \quad \boldsymbol{H}(b, \hat{\boldsymbol{\lambda}}, \boldsymbol{\lambda}, \boldsymbol{\mu}, \hat{\boldsymbol{f}}) = \boldsymbol{0}$$

$$\mu_j \leq 0\ ,\ \forall j \in [1, M_{ie}]$$

or

$$\boldsymbol{H}(\boldsymbol{z}, \hat{\boldsymbol{f}}) = \boldsymbol{0} \Leftrightarrow \boldsymbol{z} = \boldsymbol{h}(\hat{\boldsymbol{f}})$$ **with** $$\boldsymbol{z} = [b, \hat{\boldsymbol{\lambda}}, \boldsymbol{\lambda}, \boldsymbol{\mu}]^T$$

Prediction – Correction Scheme – Generalisation (4/5)

Total derivative of *H*:

$$\frac{\partial \boldsymbol{H}}{\partial \hat{\boldsymbol{f}}} + \frac{\partial \boldsymbol{H}}{\partial \boldsymbol{z}} \frac{\partial \boldsymbol{h}}{\partial \hat{\boldsymbol{f}}} = \boldsymbol{0}$$

or

$$\frac{\partial \boldsymbol{h}}{\partial \hat{\boldsymbol{f}}} = -\left[\frac{\partial \boldsymbol{H}}{\partial \boldsymbol{z}}\right]^{-1} \frac{\partial \boldsymbol{H}}{\partial \hat{\boldsymbol{f}}}$$

with

$$\frac{\partial \boldsymbol{H}}{\partial \boldsymbol{z}} = \begin{bmatrix} \nabla^2_{\boldsymbol{bb}}\mathcal{L} & -(\nabla_{\boldsymbol{b}} f_k)^T & -(\nabla_{\boldsymbol{b}} c_k)^T & -(\nabla_{\boldsymbol{b}} g_k)^T \\ -\nabla_{\boldsymbol{b}} f_k & 0 & 0 & 0 \\ -\nabla_{\boldsymbol{b}} c_k & 0 & 0 & 0 \\ -\nabla_{\boldsymbol{b}} g_k & 0 & 0 & 0 \end{bmatrix}$$

and

$$\frac{\partial \boldsymbol{H}}{\partial \hat{\boldsymbol{f}}} = \begin{bmatrix} \boldsymbol{0} \\ -I \\ \boldsymbol{0} \\ \boldsymbol{0} \end{bmatrix}$$

Prediction step:

$$\boldsymbol{z}^{pred} = \boldsymbol{z} + \frac{\partial \boldsymbol{z}}{\partial \hat{\boldsymbol{f}}} \Delta \hat{\boldsymbol{f}}$$

The user-defined steps of the M-1 objective functions set as constraints

Prediction – Correction Scheme – Generalisation (5/5)

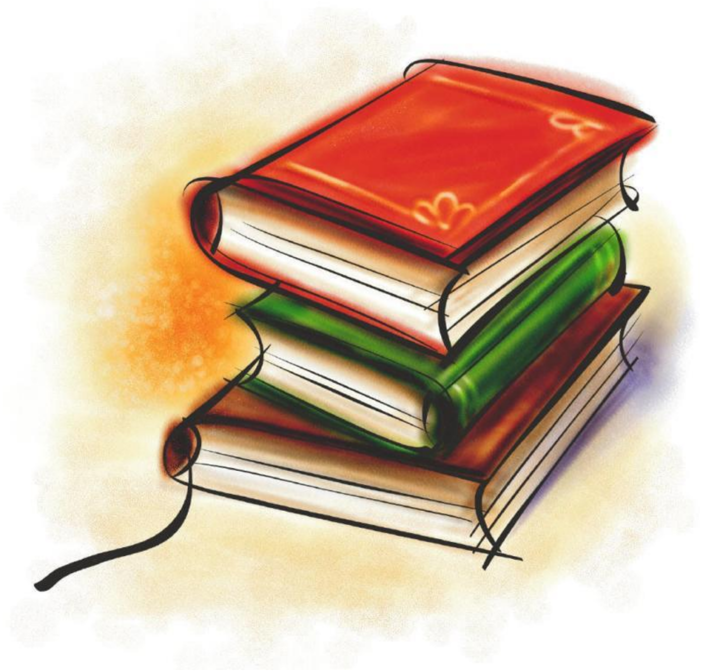
The corresponding b^{pred} included in z^{pred} may not belong to the Pareto.

A <u>Correction step</u> is necessary

Solve:

$$\min f_1(b)$$
$$\text{s.t. } f_k(b) - \hat{f}_k = 0\ ,\ \forall k \in [2, M]$$

using any constraint optimisation method such as ALM, SQP, etc.



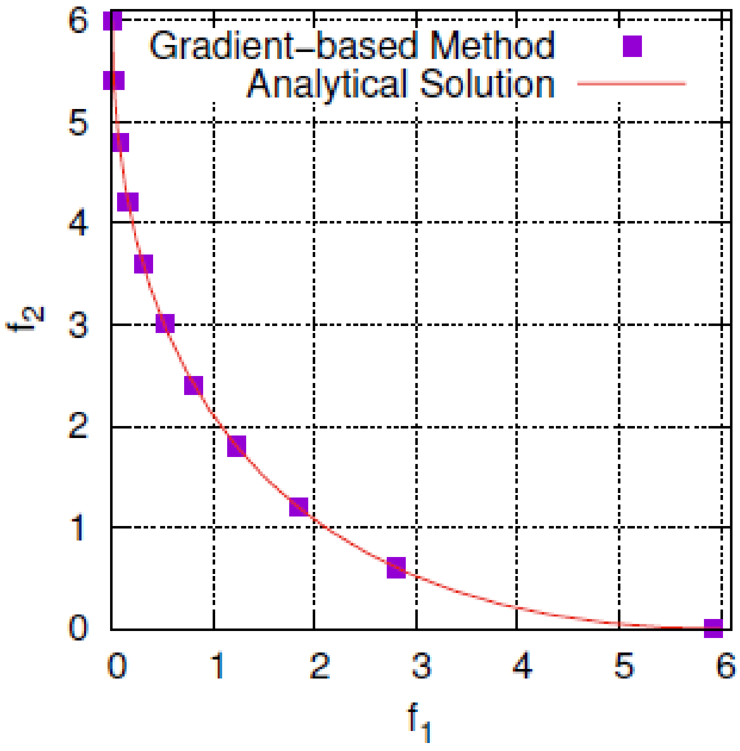
Examples – Applications

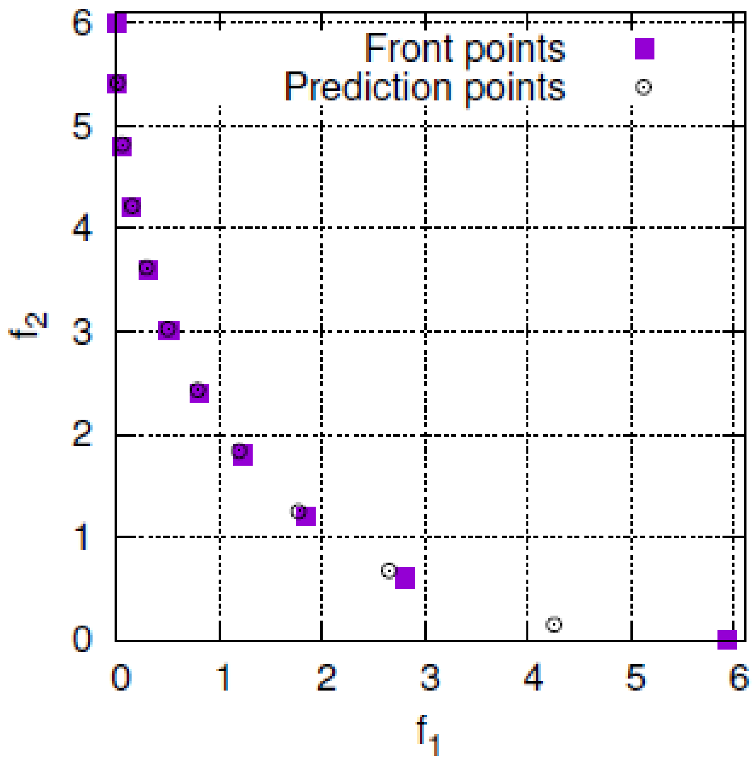
Simple Mathematical Example

Convex two objective problem:

Min.
$$\begin{cases} f_1(\boldsymbol{b}) = \sum_{i=1}^{N=6} (b_i - 3)^2 \\ f_2(\boldsymbol{b}) = \sum_{i=1}^{N=6} (b_i - 4)^2 \end{cases}$$

$b_i \in [1,6]$





— Analytical Pareto front
■ GBM computed front
o Points after the prediction step

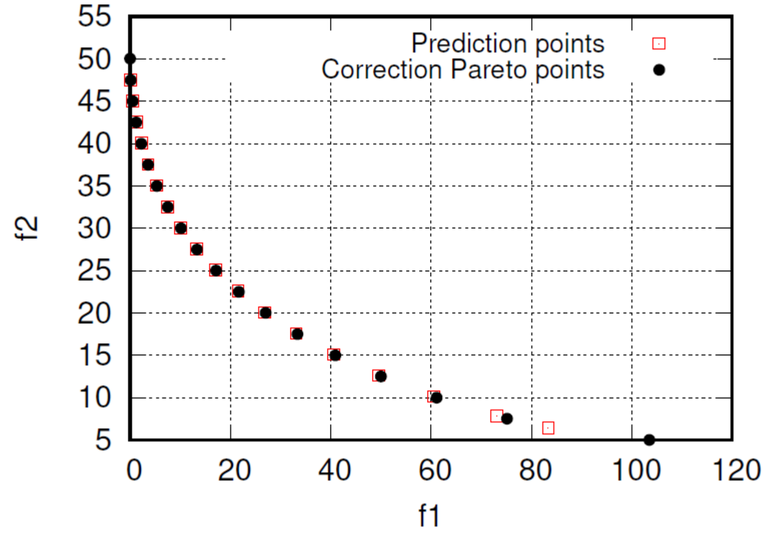
Bihn and Korn Benchmark Problem

Minimise
$$\begin{cases} f_1(b_1,b_2) = 4b_1^2 + 4b_2^2 \\ f_2(b_1,b_2) = (b_1-5)^2+(b_2-5)^2 \end{cases} \qquad b_1 \in [0,5]\,,\, b_2 \in [0,3]$$

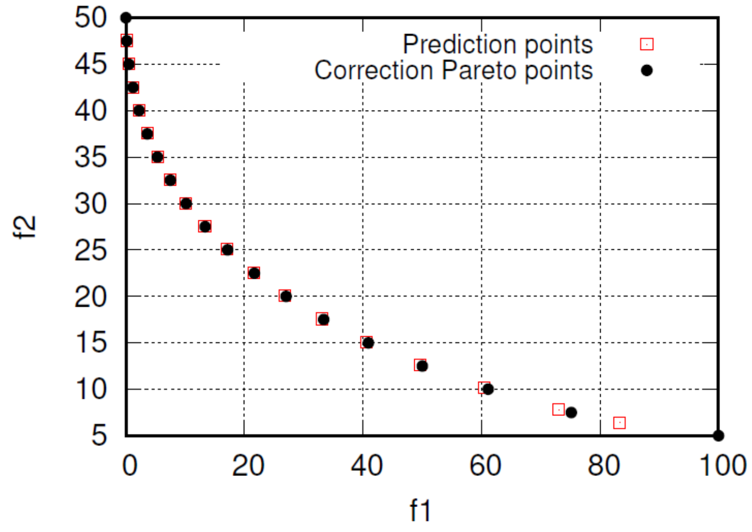
s.t.
$$(b_1-5)^2+b_2^2 \leq 25$$
$$(b_1-8)^2+(b_2+3)^2 \geq 7.7$$

The effect of approximating the Hessian

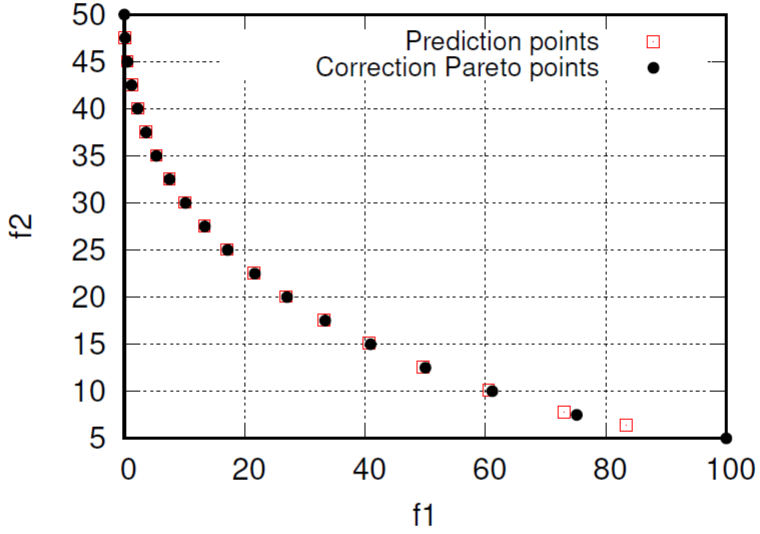
ALM: Cost 288 cycles



SQP (SR1): Cost 79 cycles



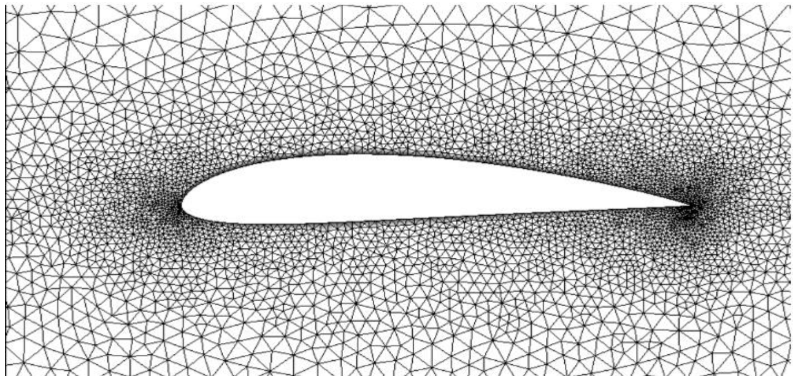
SQP (Analytic): Cost 52 cycles



Aerodynamic ShpO – Case 1 –Benefits of the Prediction-Correction Scheme (1/2)

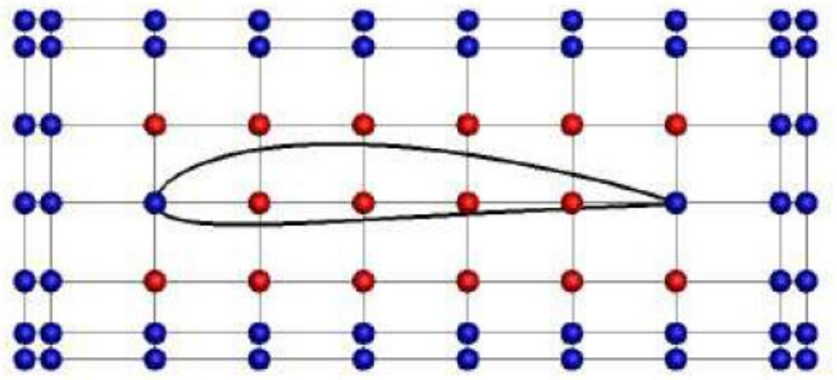
- **NACA 4415 airfoil, inviscid flow: M_∞=0.7, AoA =2°.**

- **Parametrisation with a 10x7 NURBS lattice; red control points can be displaced in the normal-to-the-chord direction → N=16 design variables.**



- **Objectives:**
  1. **Min. drag coefficient**
  2. **Max. lift coefficient**

$$\min \begin{cases} f_1(\boldsymbol{b}) = \quad c_D(\boldsymbol{b}) \\ f_2(\boldsymbol{b}) = -\, c_L(\boldsymbol{b}) \end{cases}$$



- **Consider two optimisation scenarios:**

  GBM-1: Repetitive solution of SOO constrained problems with user defined c_L values; use the previously computed point on the Pareto front as initialisation (only the correction step).

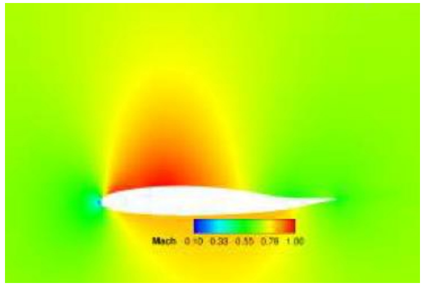
  GBM-2: Use the prediction-correction Pareto tracing method.

Aerodynamic ShpO – Case 1 –Benefits of the Prediction-Correction Scheme (2/2)

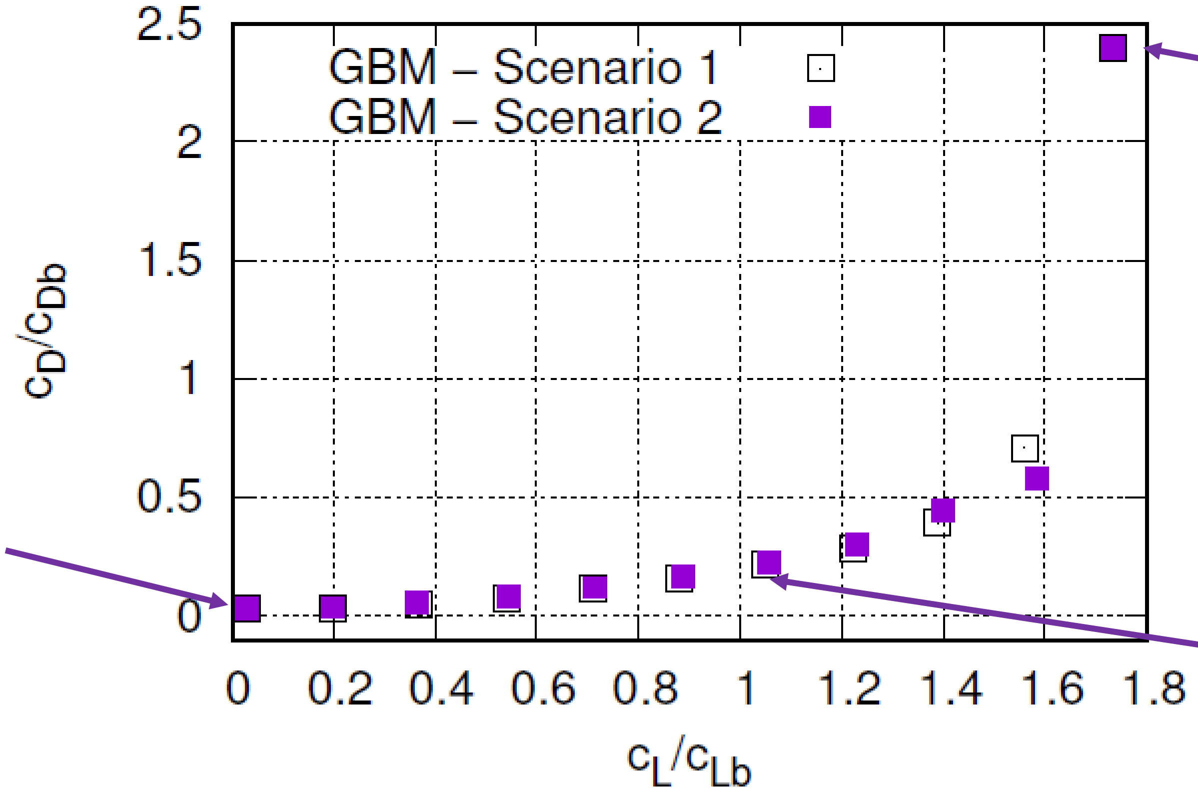
Go-to-Pareto: **44TUs**.

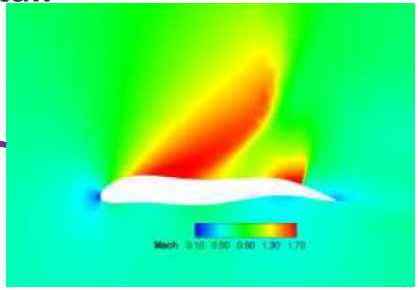
GBM – 1: Repetitive solution of SOO constrained problems. ~21 TUs per Pareto point → 255 TUs in total.

GBM – 2: Prediction – Correction method. ~12 TUs per point →165 TUs in total.

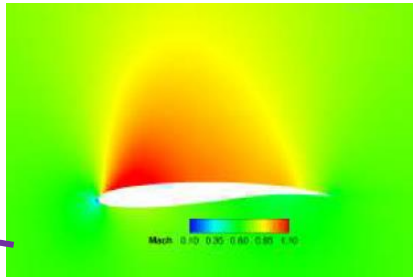


min c_L, min c_D





max c_L, max c_D



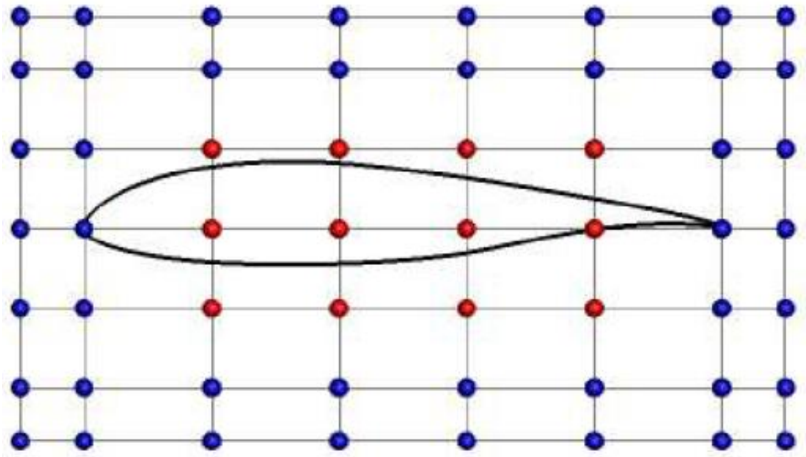
The Prediction – Correction method divided the cost by ~2.

Aerodynamic ShpO – Case 2 (1/2)

- NLF(01)-04122 airfoil at transonic flow: Re=4 10^6, M_∞=0.7, AoA =2.03°, Tu=0.15%.
- Parametrisation with a 8x7 NURBS lattice; red control points can be displaced in the normal-to-the-chord direction → N=12 design variables.
- Objectives:
  1. Min. drag coefficient
  2. Max. lift coefficient

$$\min \begin{cases} f_1(b) = c_D(b) \\ f_2(b) = -\,c_L(b) \end{cases}$$

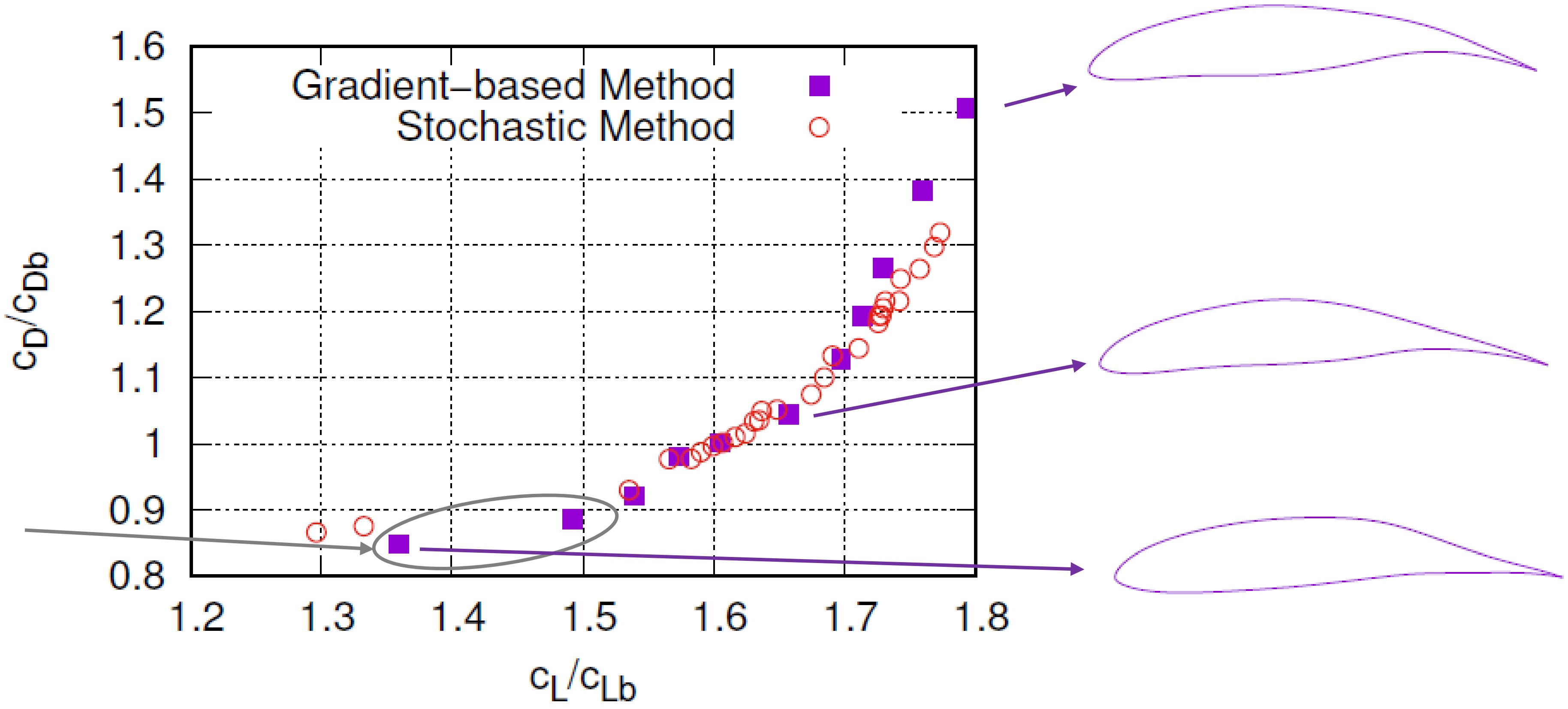
- Compare the Prediction-Correction GBM with a GFM (Stochastic algorithm; MAEA of EASY).



Aerodynamic ShpO – Case 2 (2/2)

GBM (Prediction – Correction method). Go-to-Pareto: 15TUs; Move-on-Pareto: ~15TUs per Pareto point→165 TUs in total.
GFM (Stochastic method) → 255 TUs in total.

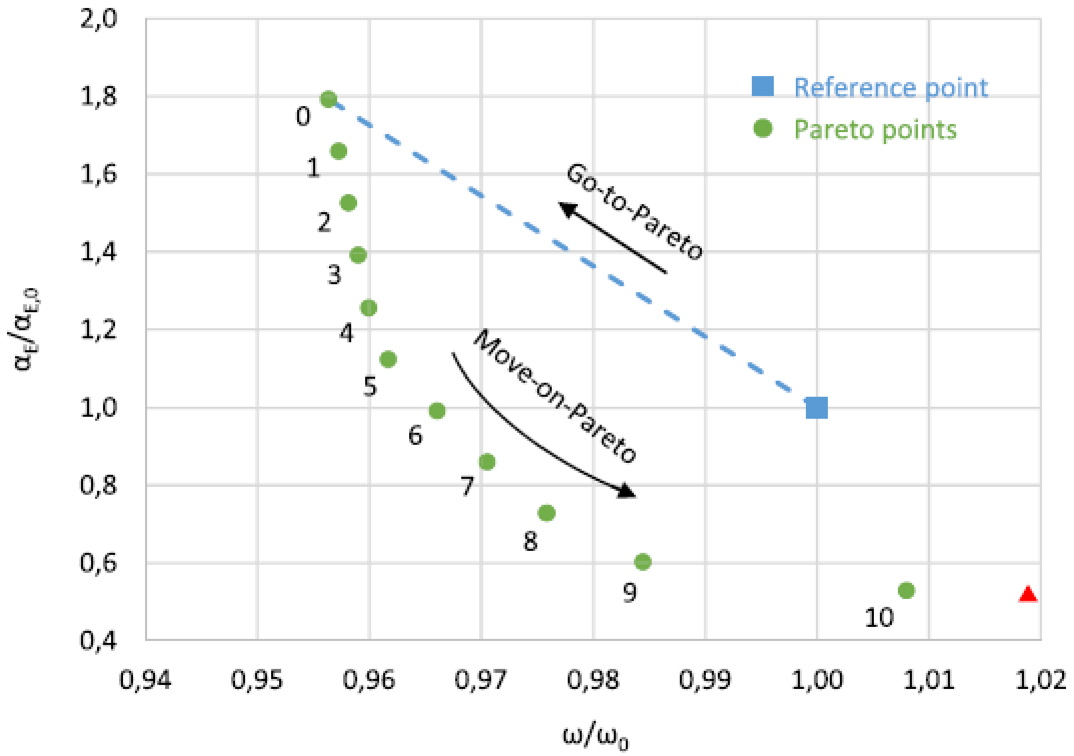
GBM may compute points in areas not well explored from the GFM and/or dominate those of the GFM



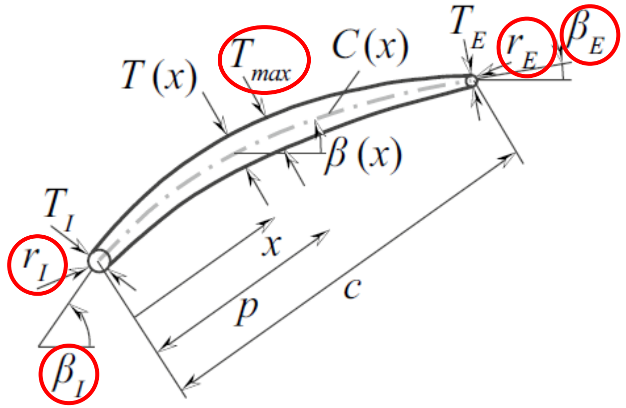
The Prediction – Correction method required ~50 less function calls than a well-performing MAEA.

ShpO of a Compressor Stator (1/2)

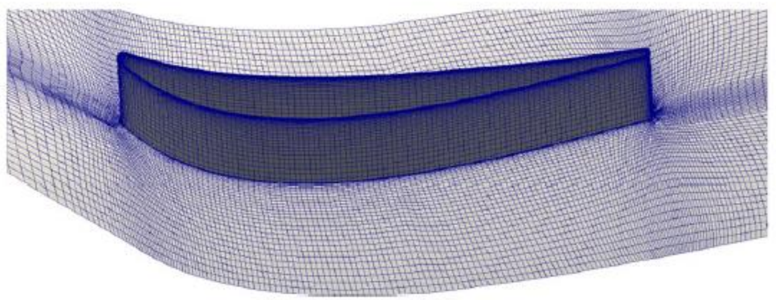
- **Compressor stator at turbulent flow; N=45 design variables.**
- **Objectives:**
  1. **Min. total pressure losses (ω) between the inlet and exit.**
  2. **Min. flow angle deviation from the axial direction at the stator exit (α_E).**



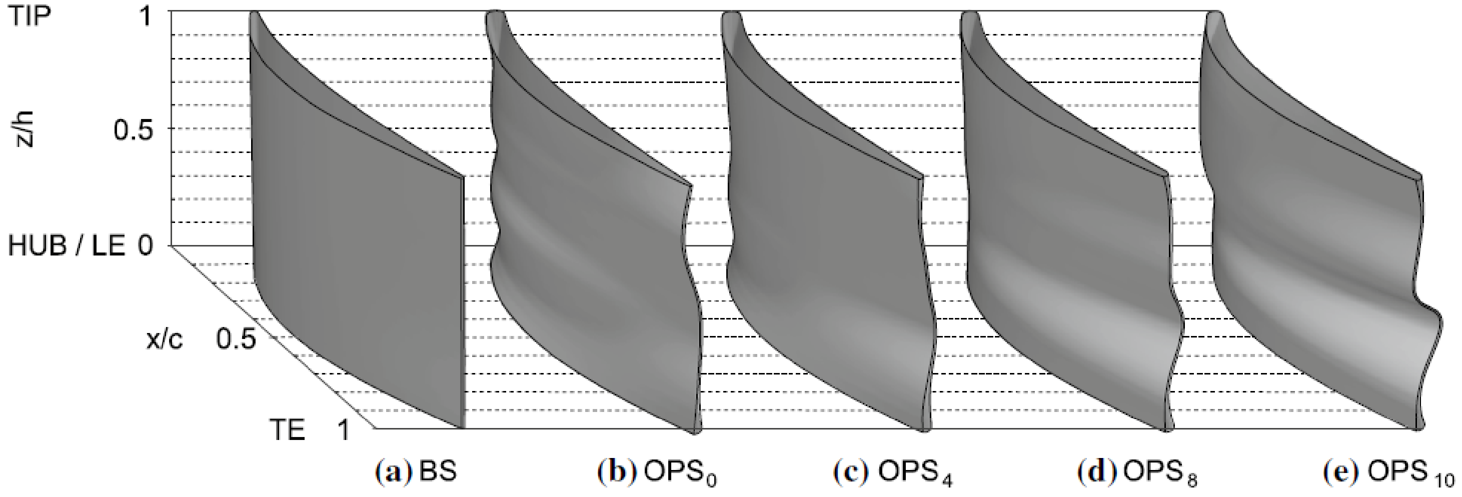
Go-to-Pareto: 36TUs
Move-on-Pareto: 159TUs

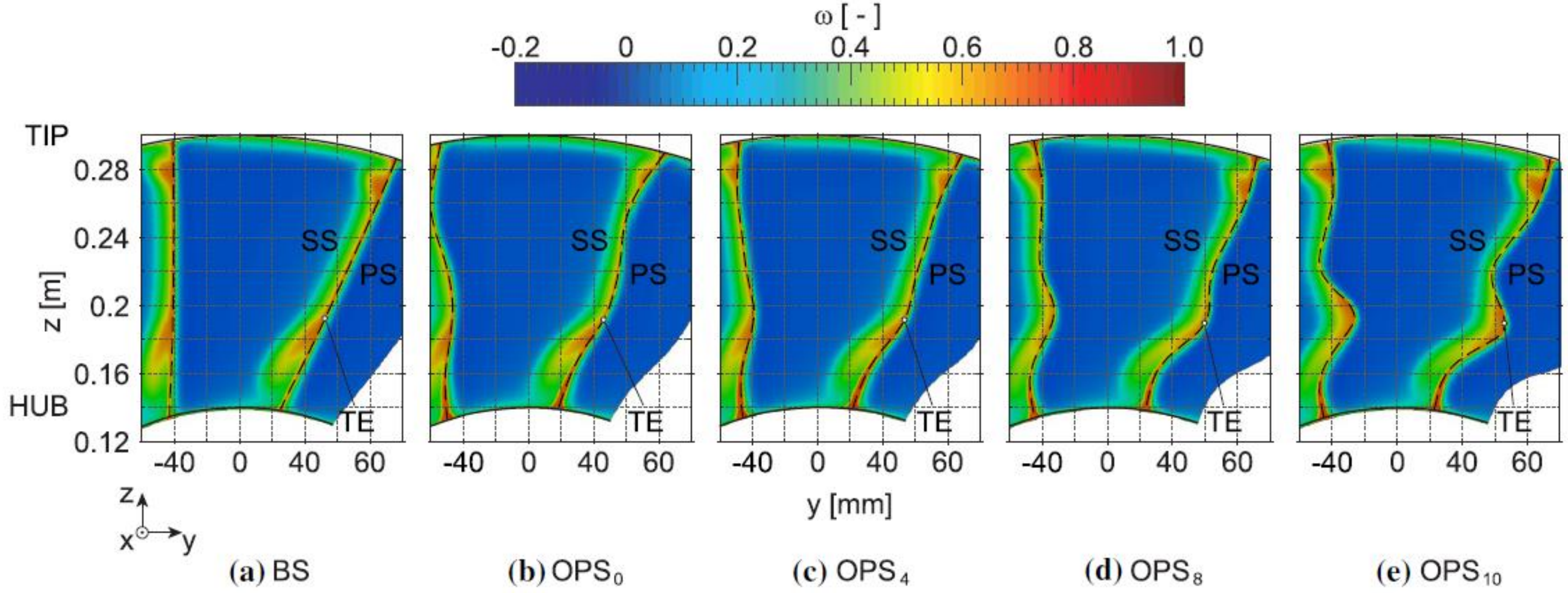


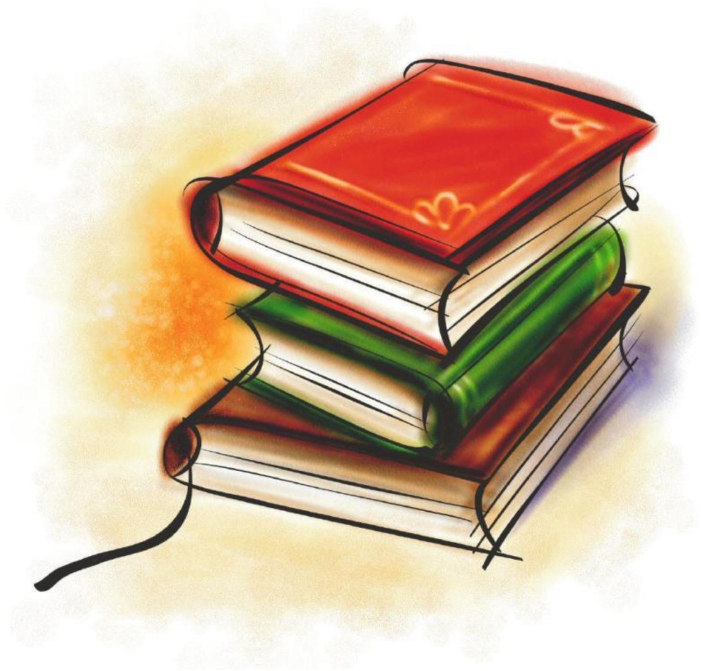
Parametrisation of the blade section



ShpO of a Compressor Stator (2/2)



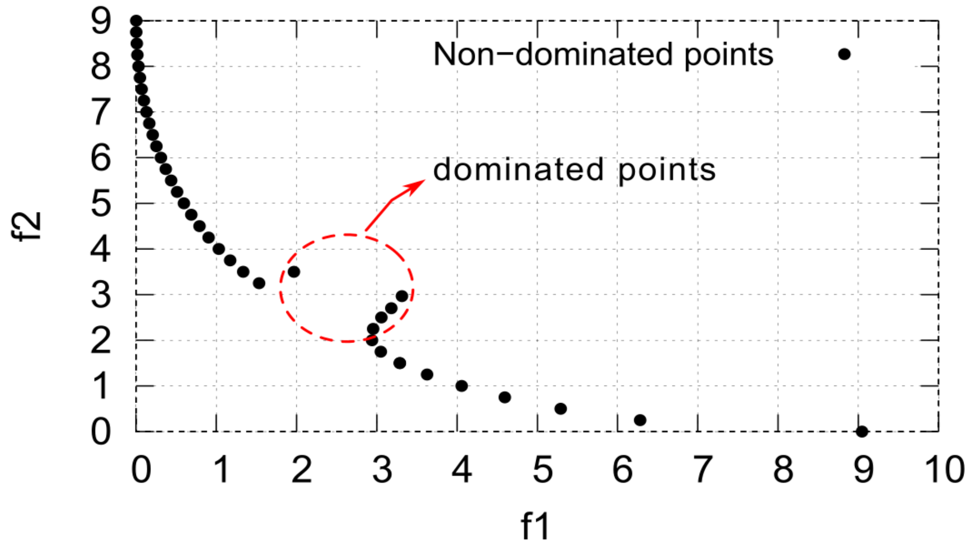




Handling Discontinuous Pareto Fronts

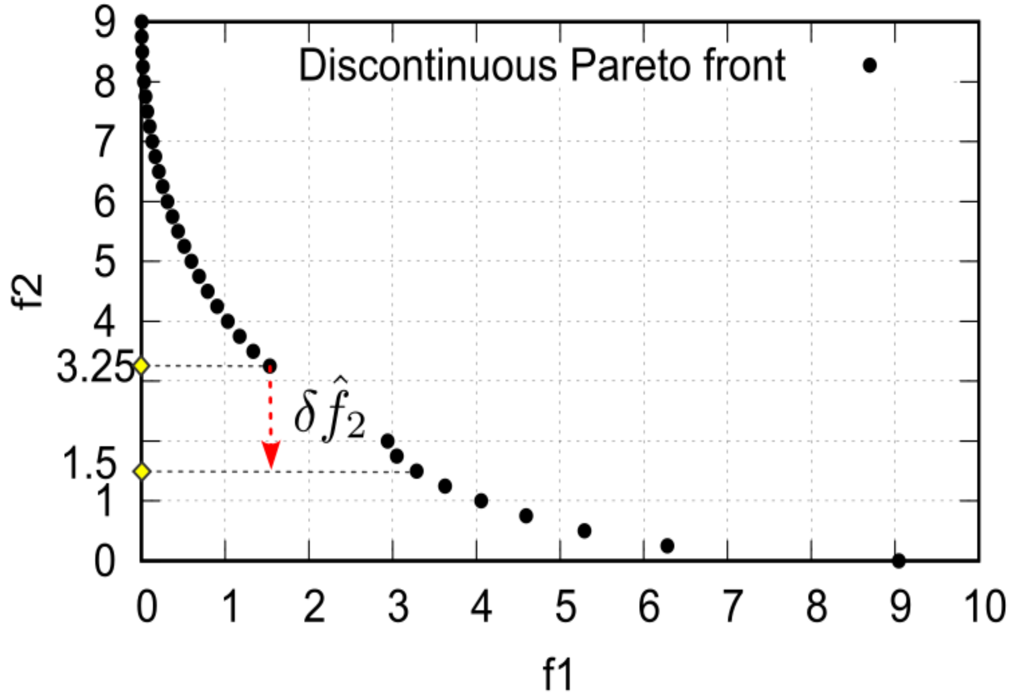
Discontinuous Fronts

- Possible discontinuity in the design space (due to constraints?) is not known a priori.
- Need for an enhanced algorithm:
  - Detect the discontinuities. Dominance check for each new point.
  - Skip “gaps” and continue the Move-on-Pareto.



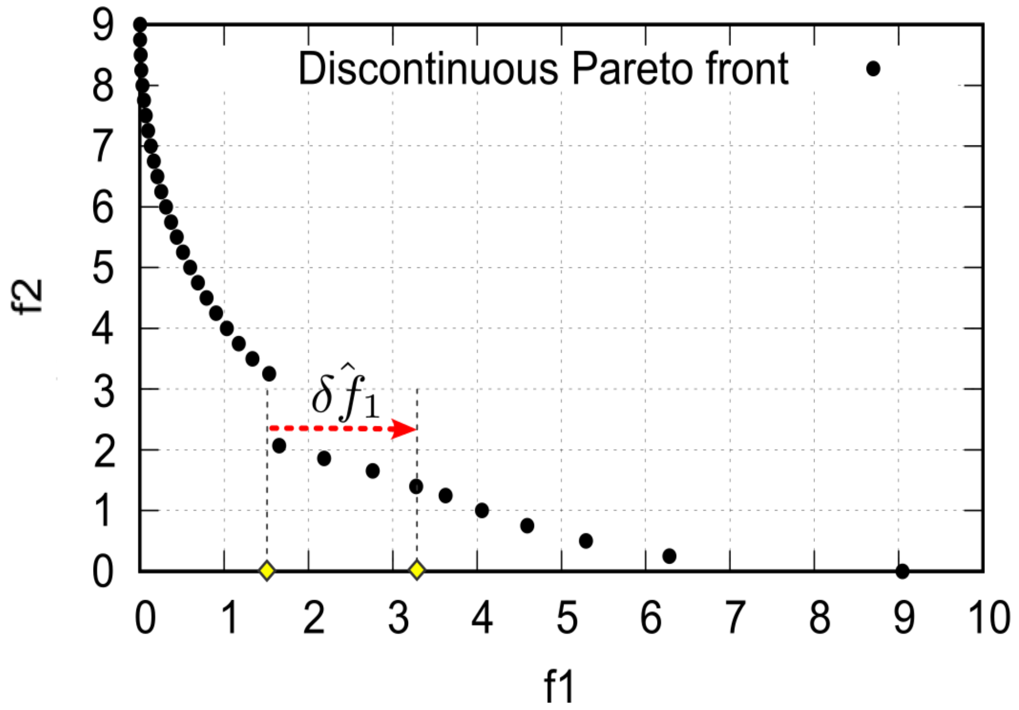
Move-on-(discontinuous) Pareto Front (1/3)

Target-objective Jump: Select a different $\delta\hat{f}_2$ step.



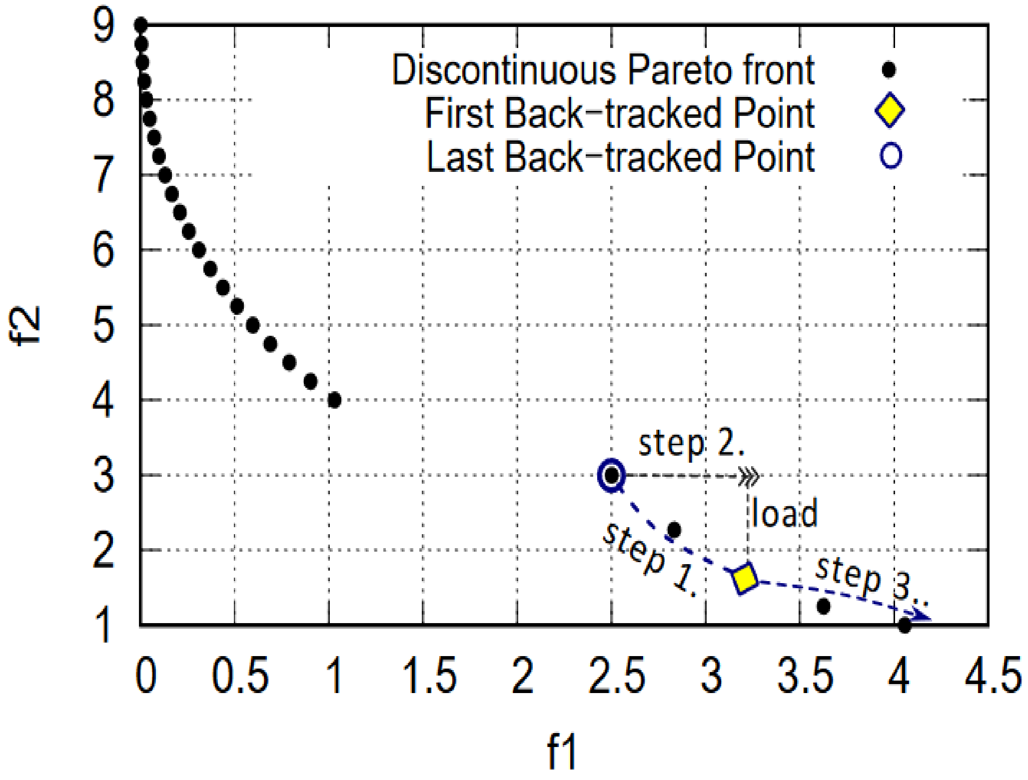
Move-on-(discontinuous) Pareto Front (2/3)

<u>Swap Target-objective</u>: Swap the objective and target of the Lagrangian function.



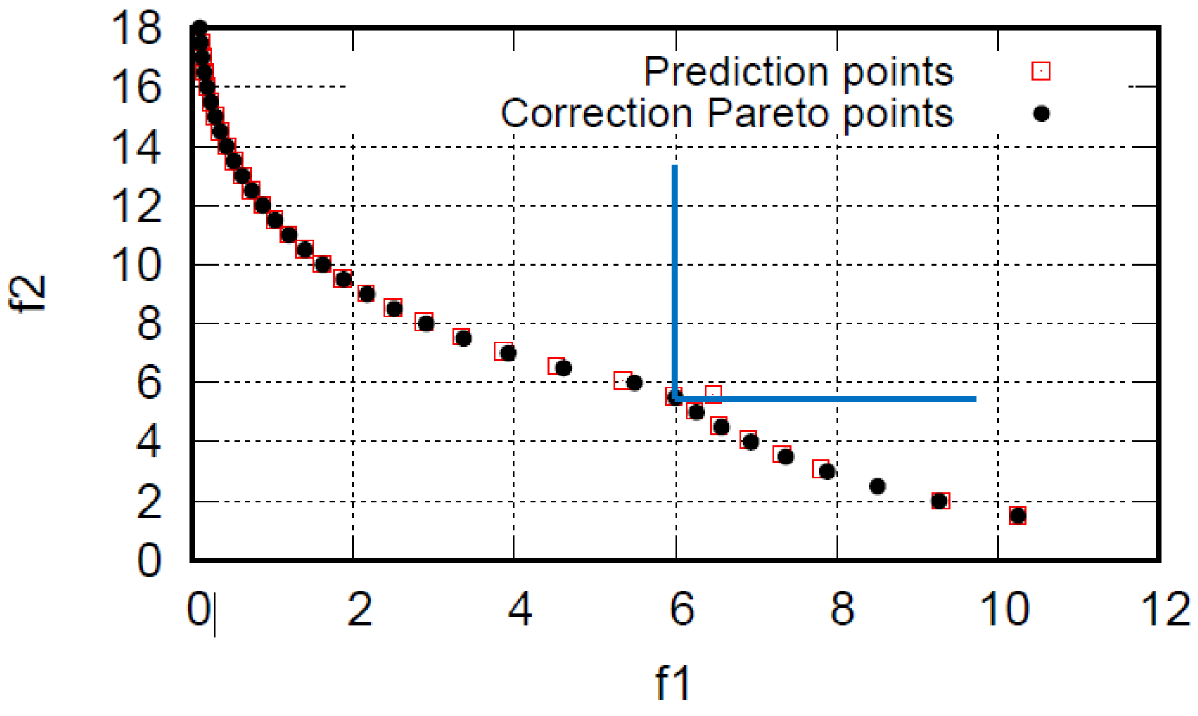
Move-on-(discontinuous) Pareto Front (3/3)

Back-Tracking: Invert the tracking direction of the Pareto front in order to locate Pareto points which could have been omitted during a "large" target-objective jump.

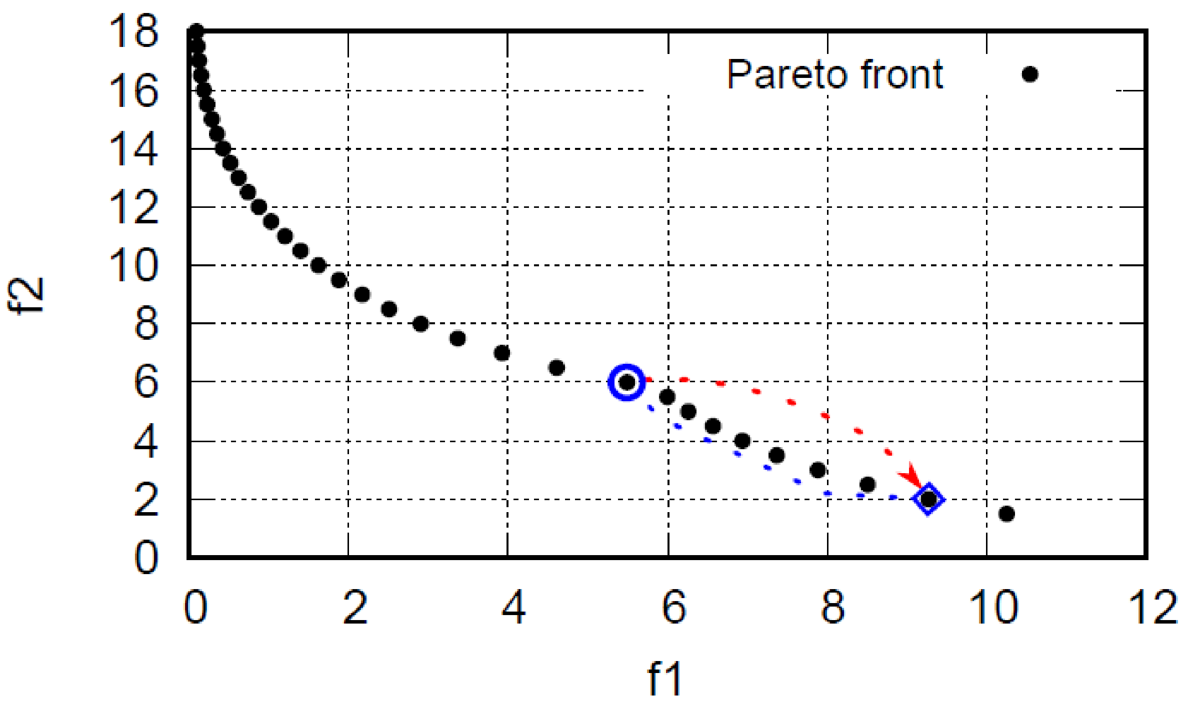


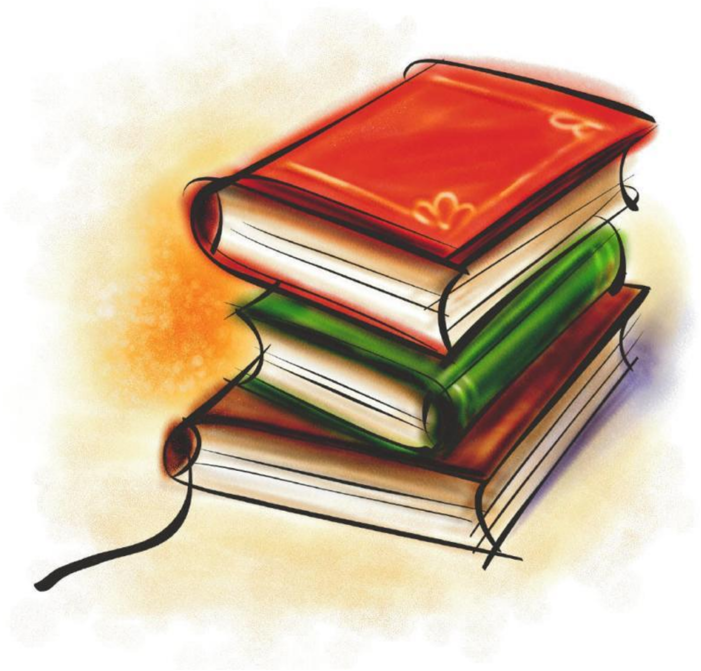
Move-on-(discontinuous) Pareto Front – Example

Discontinuity detection while predicting the 24th Pareto point



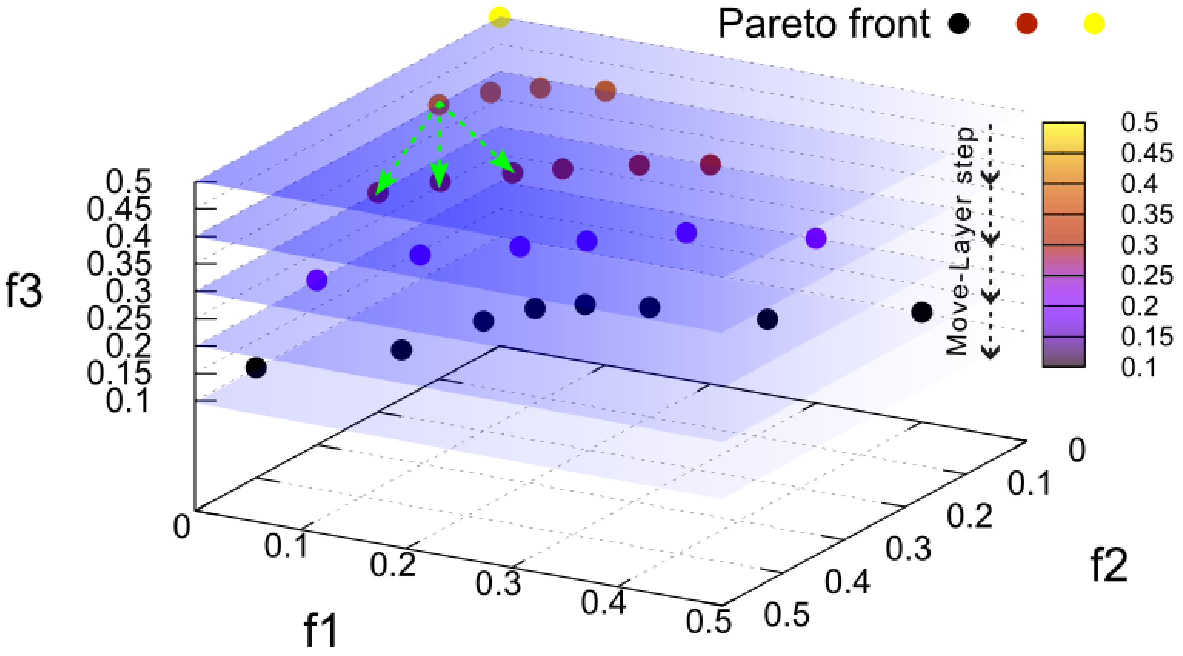
Use a combination of the Target-objective Jump and Back-Tracking





Multi-Dimensional Pareto Fronts

3D Pareto Front Tracing



Read more in:

- I. Vasilopoulos, V.G. Asouti, K.C. Giannakoglou and M. Mayer, “Gradient-based Pareto front approximation applied to turbomachinery shape optimization”, Engineering with Computers 2021; 37:449-459.
- K.T. Gkaragkounis, E.M. Papoutsis-Kiachagias, K.C. Giannakoglou, “Adjoint assisted Pareto Front Tracing in Aerodynamic and Conjugate Heat Transfer Shape Optimization”, Computers & Fluids 2021; 214: 104753.