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Targeting Well-Balanced Solutions in Multi-Objective Bayesian Optimization under a Restricted Budget

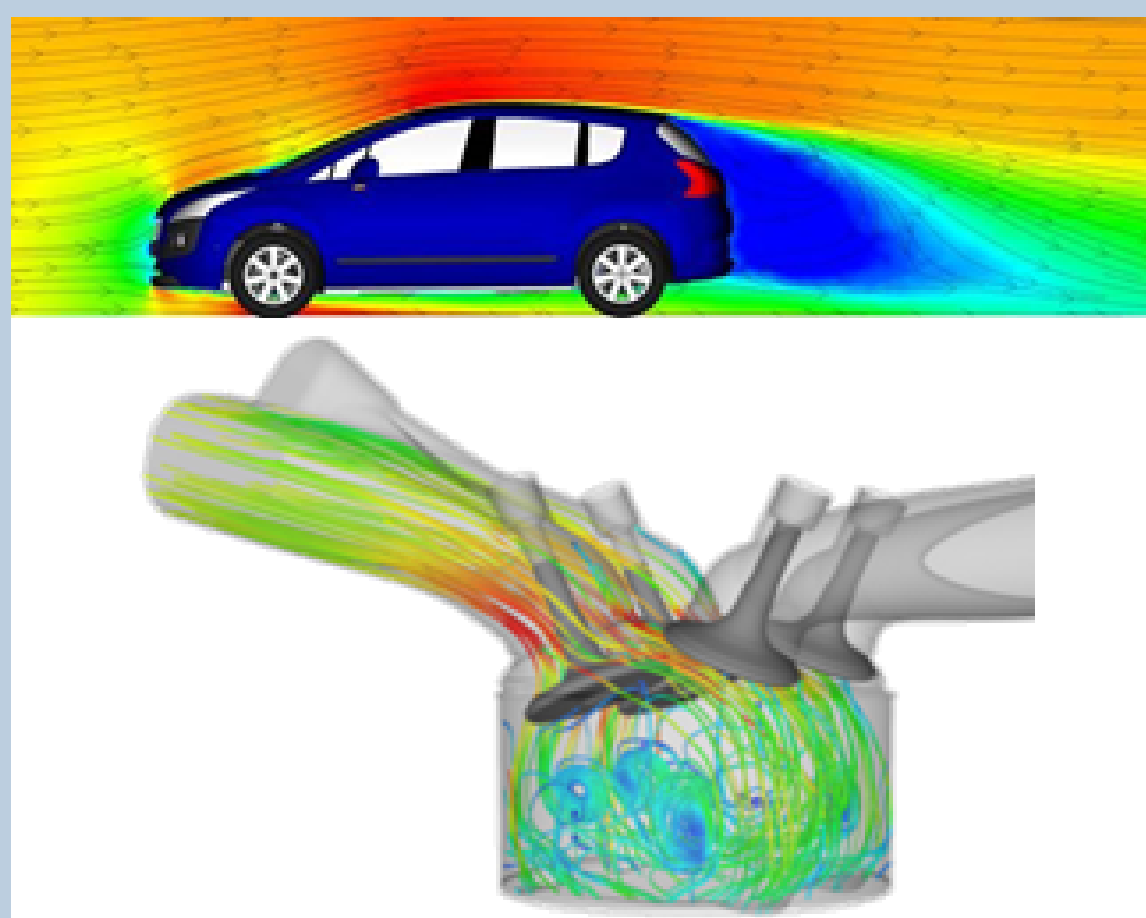
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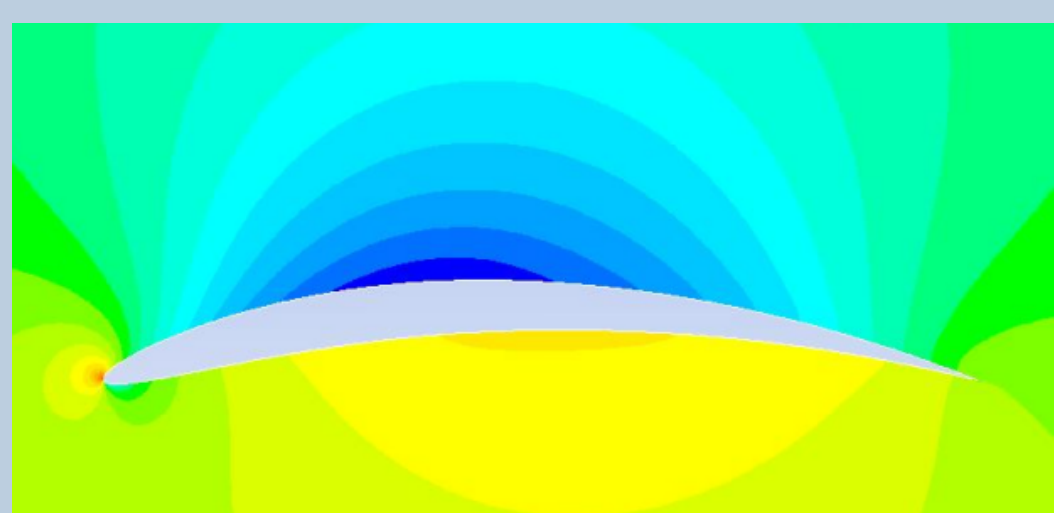
Industrial context

Multi-objective optimization (up to 6-8 objectives) of high dimensional systems (d up to 40)

Complex systems and physics \Rightarrow use of computationally expensive CFD codes (12-24 hours per simulation) \Rightarrow optimization under (very) restricted budget (≈ 200 evaluations) \Rightarrow metamodel-based optimization : multi-objective EGO [1]



Test case : aerodynamic optimization of a NACA airfoil (3, 8 or 22 parameters, 2 to 4 objectives)

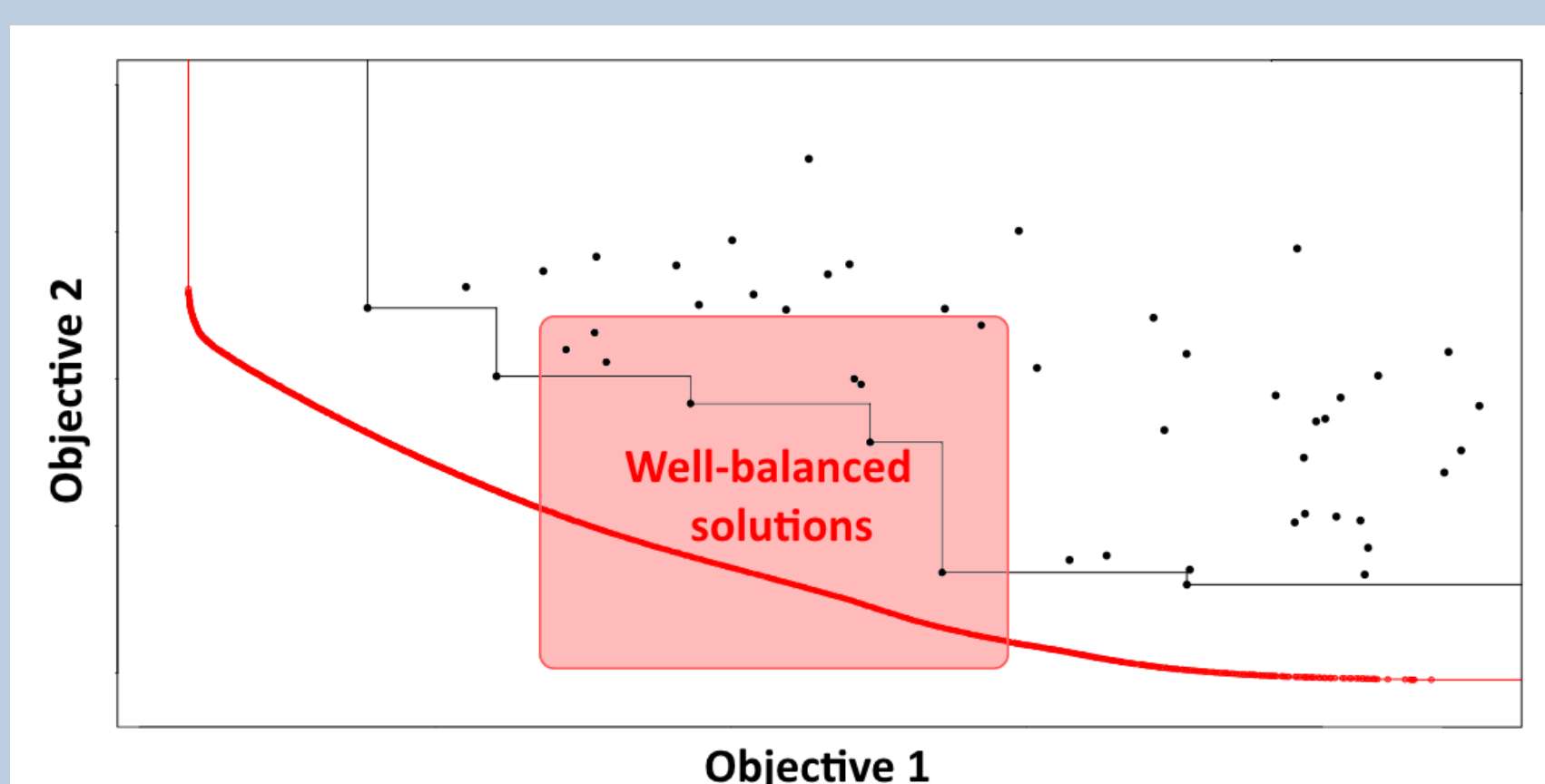


Multi-criteria decision-aid : choice among the optimal solutions made by a Decision Maker

How to obtain several *optimal* trade-off solutions in spite of an extremely parsimonious use of the computer code?

Targeting : motivations

- Restricted budget \Rightarrow Uncovering the whole Pareto Front \mathcal{P}_Y in a "region of interest"
- Growing size of \mathcal{P}_Y with m
- Shrink search to a smaller subset \Rightarrow faster convergence
- Emphasize on solutions that *equilibrate* the objectives : (unknown) central part of the Pareto Front (PF)



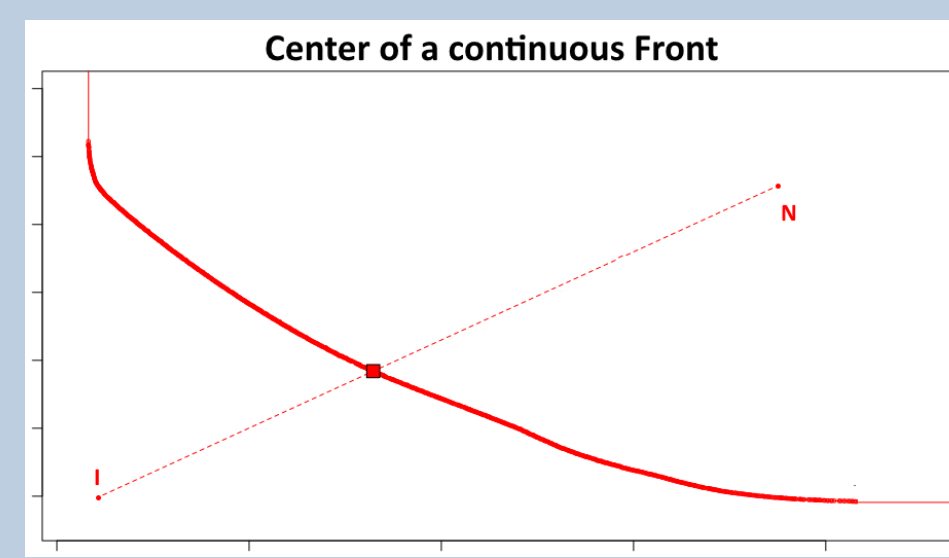
- Interesting solutions for Decision Maker

References

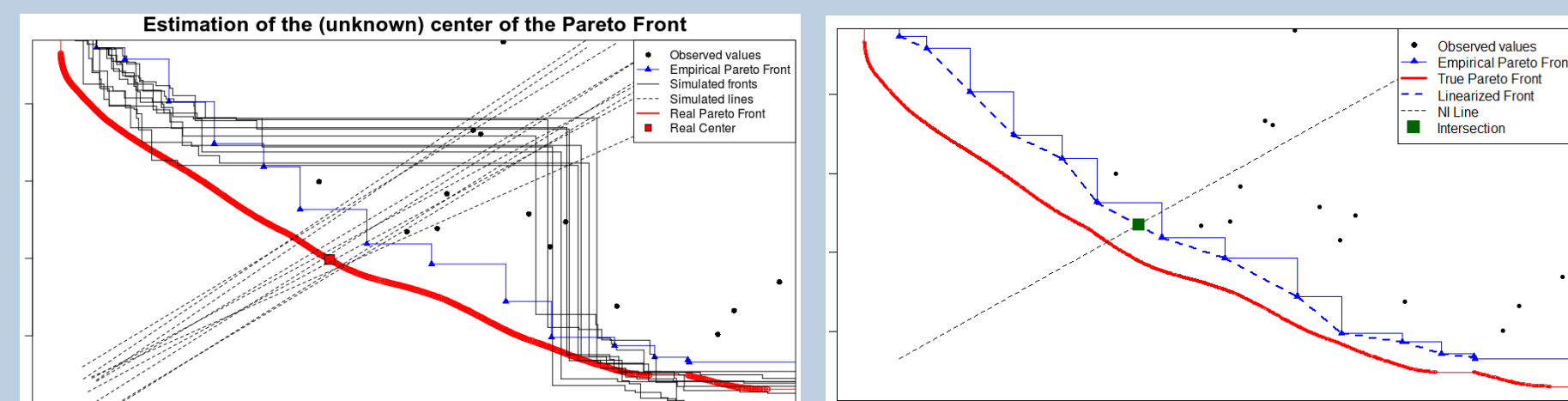
- [1] D. R. Jones, M. Schonlau, and W. J. Welch, *Efficient global optimization of expensive black-box functions*, Journal of Global Optimization, 13, 455–492 (1998)
- [2] E. Zitzler and L. Thiele, *Multiobjective Optimization Using Evolutionary Algorithms - A Comparative Case Study*, Conference on Parallel Problem Solving from Nature (PPSN V), pages 292–301 (1998)
- [3] M. Emmerich, K. Giannakoglou, B. Naujoks, *Single and Multiobjective Evolutionary Optimization Assisted by Gaussian Random Field Metamodels*, IEEE Transactions on Evolutionary Computation, 10 (2006)

Central part of the Pareto Front

Center : Intersection with Nadir-Ideal line \mathcal{L}



- GP simulations \Rightarrow estimated NI line $\hat{\mathcal{L}}$
- Intersection with empirical PF $\hat{\mathcal{P}}_Y$ \Rightarrow estimation of the center

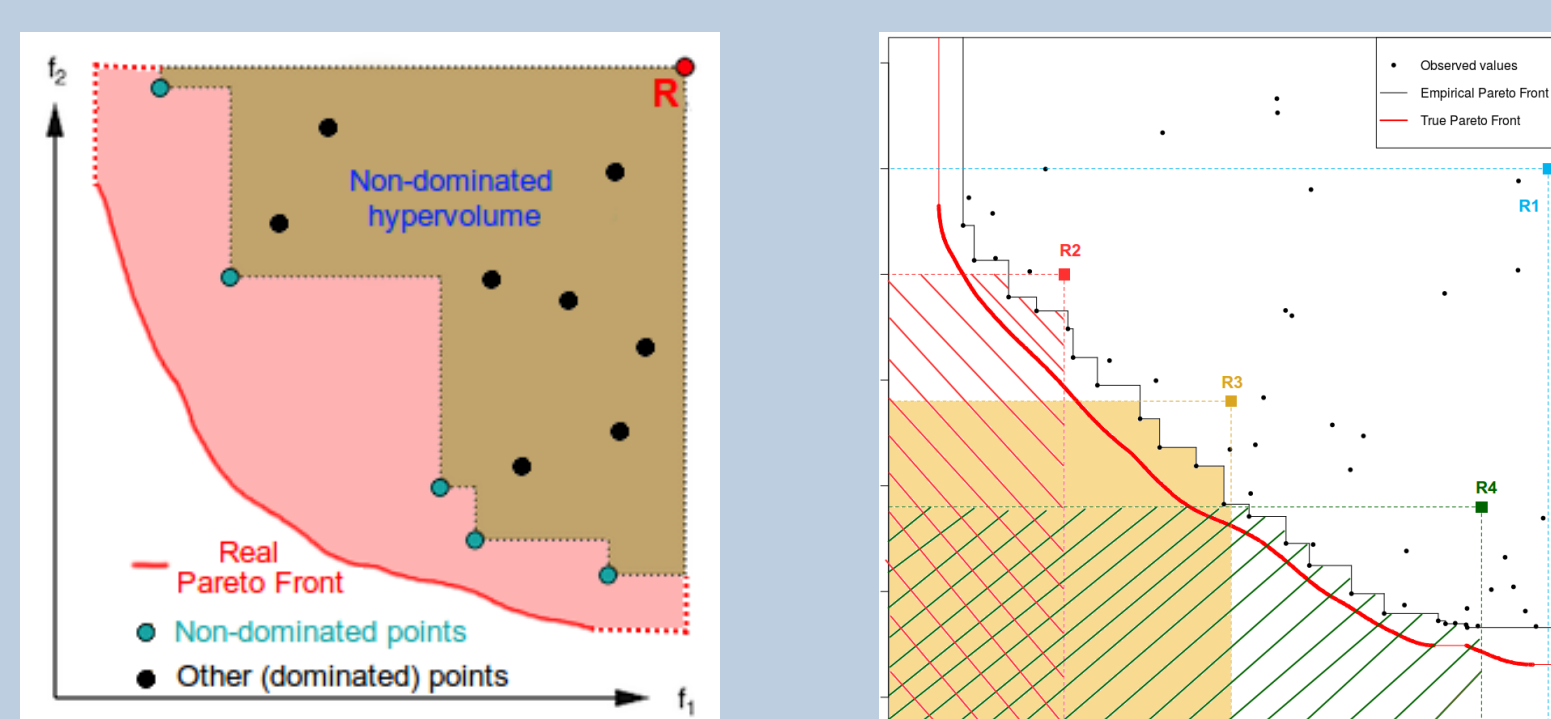


Infill Criteria for targeting the center

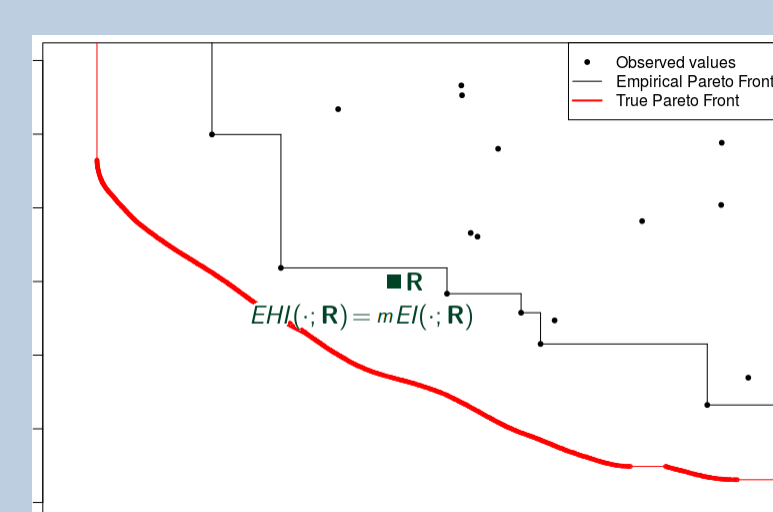
$IC = f(Y_1(\cdot), \dots, Y_m(\cdot); \mathbf{x}; \Theta)$: directs the search towards attractive new designs \mathbf{x}^*

Modify existing IC through Θ to direct the search towards the estimated central area

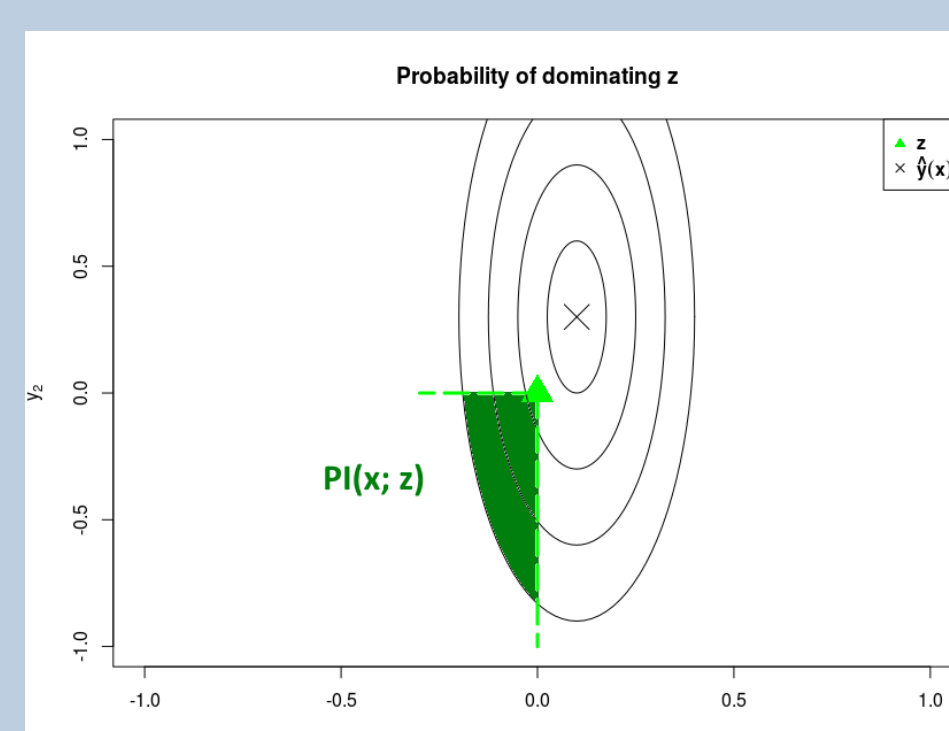
- Hypervolume Indicator [2] : $H(\hat{\mathcal{P}}_Y; \mathbf{R}) = \Lambda \left(\bigcup_{\mathbf{y} \in \hat{\mathcal{P}}_Y} \{ \mathbf{z} : \mathbf{y} \preceq \mathbf{z} \preceq \mathbf{R} \} \right)$
- EHI : Expected Improvement of the Hypervolume [3] (relatively to \mathbf{R}), if adding design \mathbf{x} . $EHI(\mathbf{x}; \mathbf{R}) = \mathbb{E}[H(\hat{\mathcal{P}}_Y \cup \{\mathbf{Y}(\mathbf{x})\}; \mathbf{R}) - H(\hat{\mathcal{P}}_Y; \mathbf{R})]$



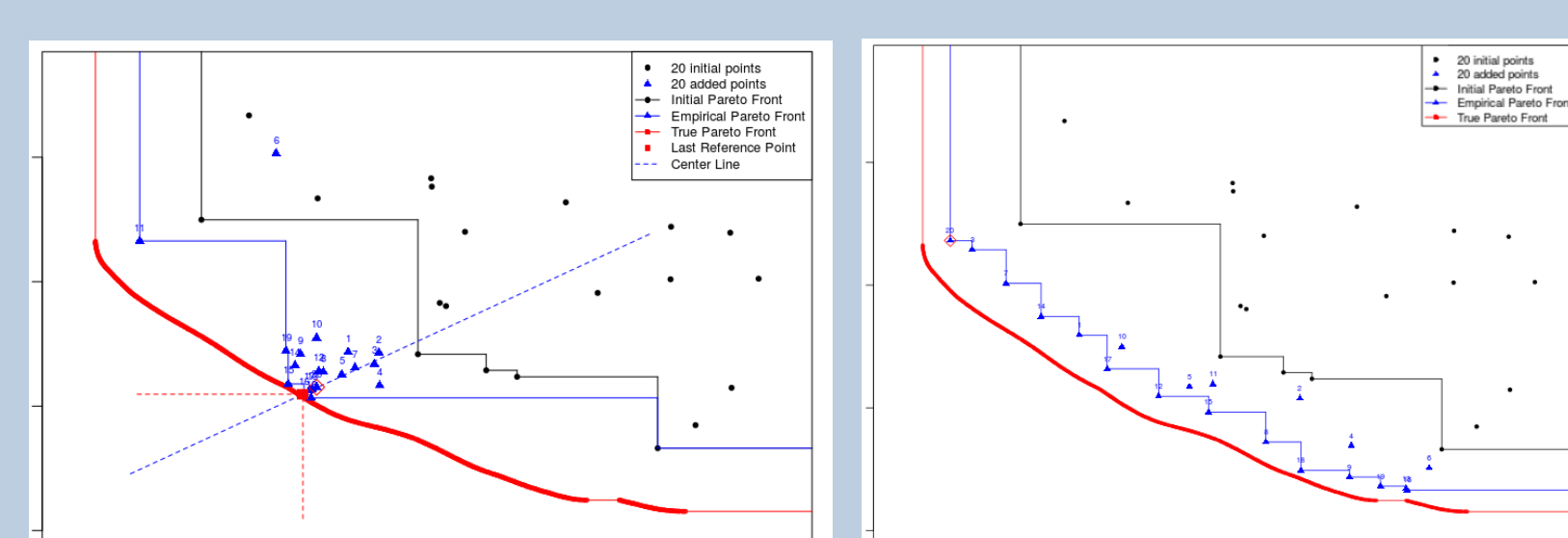
- Product of Expected Improvement w.r.t. $\mathbf{z} \in Y$: $mEI(\mathbf{x}; \mathbf{z}) = \prod_{i=1}^m EI_i(\mathbf{x}; z_i)$, $EI_i(\cdot, z)$: EI in objective i considering z as the current minimum
- If $\mathbf{R} \notin \hat{\mathcal{P}}_Y$, $EHI(\cdot; \mathbf{R}) = mEI(\cdot; \mathbf{R})$



- $PI(\mathbf{x}; \mathbf{z})$: probability that $\mathbf{Y}(\mathbf{x})$ dominates \mathbf{z} . $PI(\mathbf{x}; \mathbf{z}) = \prod_{i=1}^m \Phi \left(\frac{z_i - \hat{y}_i(\mathbf{x})}{s_i(\mathbf{x})} \right)$



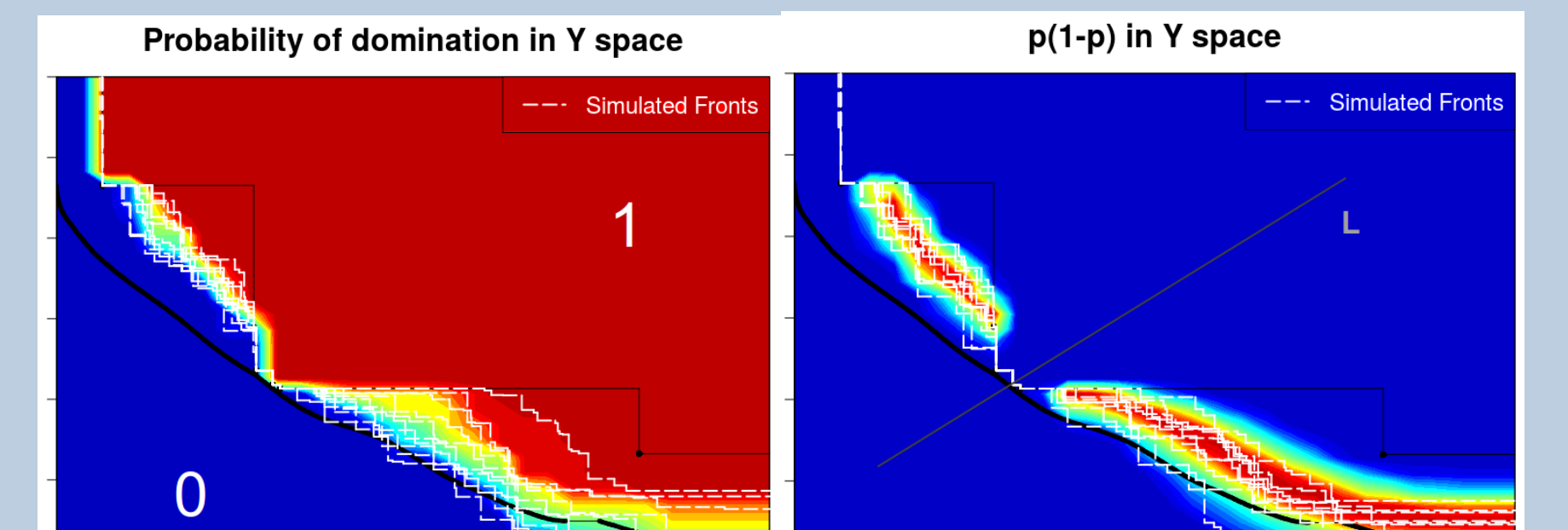
Use the estimated center as reference point \mathbf{R} \Rightarrow Optimization directed towards the center



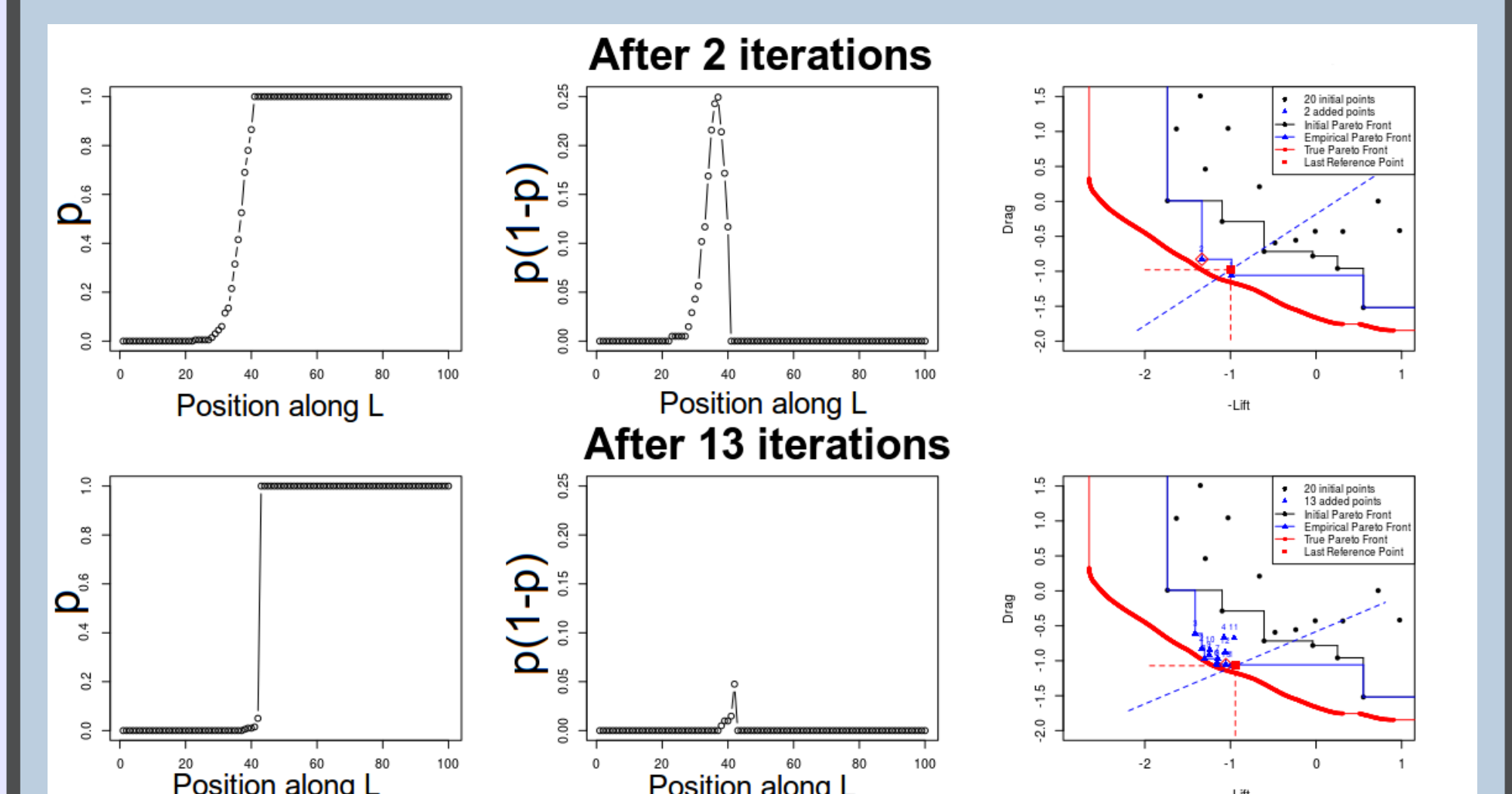
Convergence towards the center of the PF

When to stop the targeting of the center?

- $p : Y \rightarrow [0, 1]$: probability that \mathbf{y} is dominated
- Estimated using GP simulations
- Information about (local) convergence towards the Pareto Front

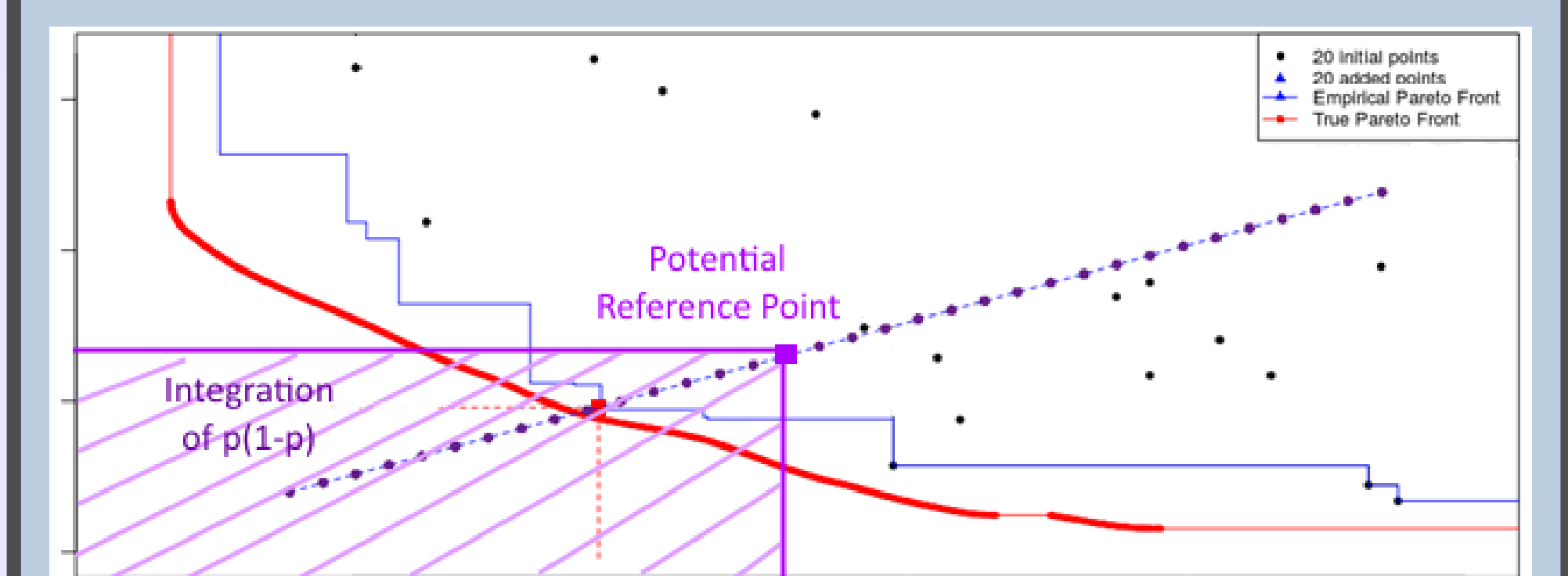


Assume local convergence towards the central part of the PF when $\int_{\hat{\mathcal{L}}} p(1-p) d\mathbf{y} \leq \epsilon$

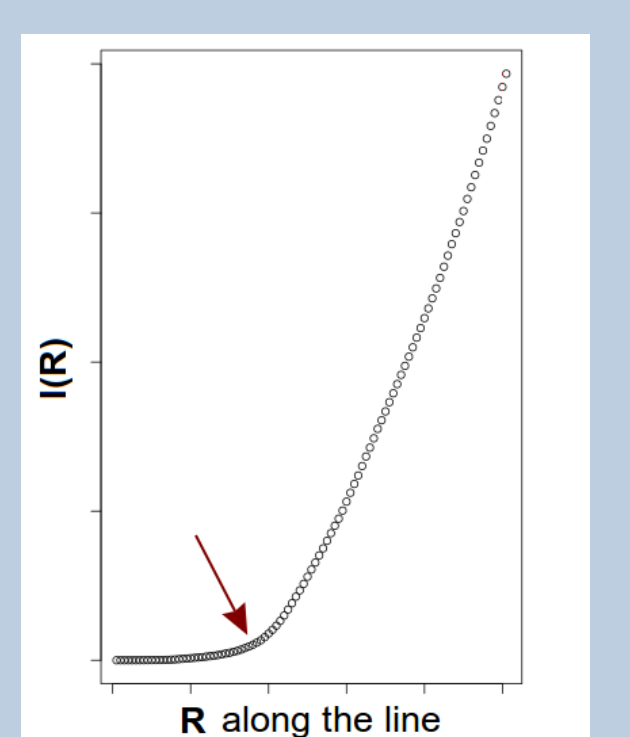


Remaining budget \Rightarrow what to do next?

- Expansion around converged area
- Well-balanced solutions : use $EHI(\cdot, \mathbf{R})$ with \mathbf{R} along $\hat{\mathcal{L}}$
- Choice of \mathbf{R} ?
- $\int_{\mathbf{y} \preceq \mathbf{R}} p(1-p) d\mathbf{y}$ for \mathbf{R} varying along $\hat{\mathcal{L}}$



Elbow : increase of uncertainty \Rightarrow attractive choice for \mathbf{R}



Summary

A two-step algorithm for targeting well-balanced solutions within a few iterations :

- Estimate the NI line $\hat{\mathcal{L}}$, on which the center of the PF is expected to be located
- Define a reference point \mathbf{R} combining $\hat{\mathcal{L}}$ and the current approximation front $\hat{\mathcal{P}}_Y$
- Target the estimated central part of the PF using \mathbf{R} and a targeting infill criterion
- When convergence is detected, widen $\hat{\mathcal{P}}_Y$ defining \mathbf{R} in an adequate way

