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► **To cite this version:**

David Gaudrie, Rodolphe Le Riche, Victor Picheny, Benoît Enaux, Vincent Herbert. Targeting Well-Balanced Solutions in Multi-Objective Bayesian Optimization under a Restricted Budget. Journées du GdR Mascot-Num 2018, Mar 2018, Nantes, France. hal-01803844

HAL Id: hal-01803844

<https://hal.science/hal-01803844v1>

Submitted on 31 May 2018

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

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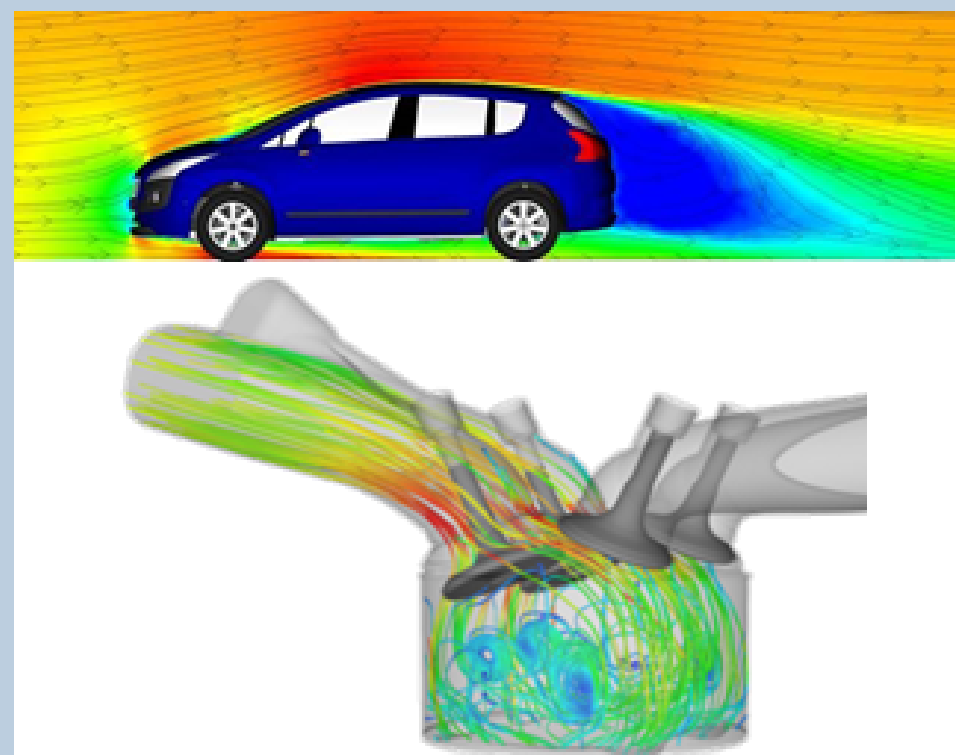


Industrial context

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

$$\min_{\mathbf{x} \in X \subset \mathbb{R}^d} (f_1(\mathbf{x}), \dots, f_m(\mathbf{x}))$$

Computationally expensive CFD codes (24 hours per simulation) \Rightarrow optimization under restricted budget \Rightarrow metamodel-based optimization: Multi-Objective EGO [1]



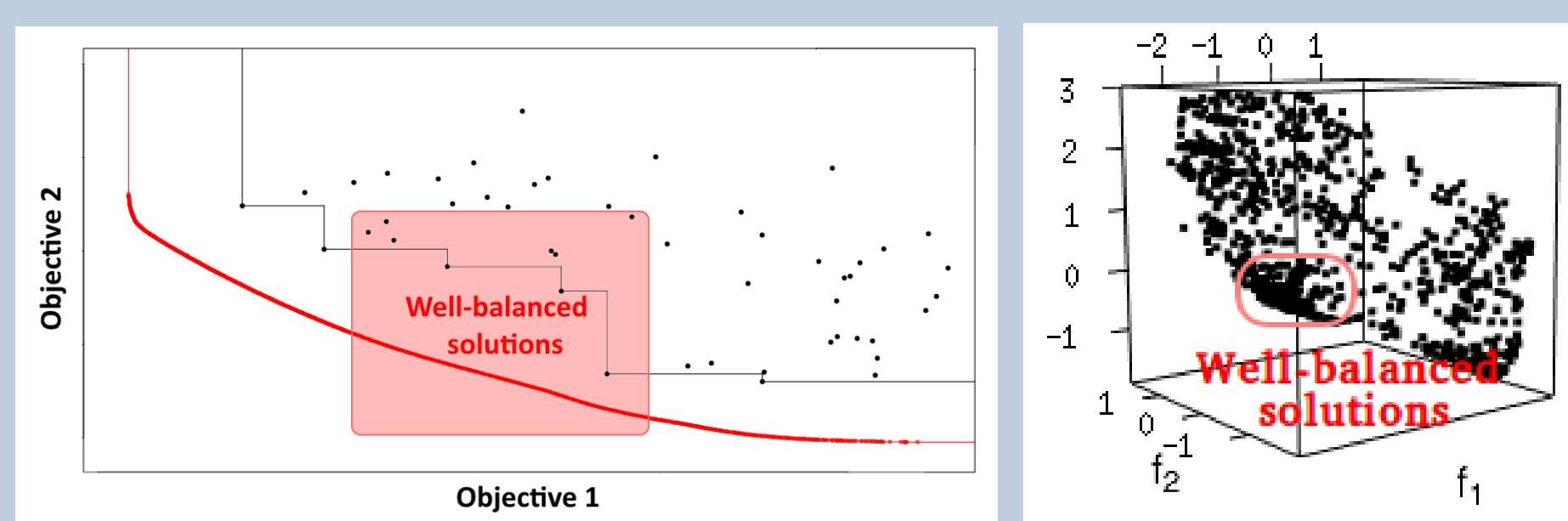
Multi-criteria decision-aid: choice among the optimal solutions made by a Decision Maker

Very tiny budget (≈ 100 evaluations), many objectives ($m \approx 6-8$) \Rightarrow impossible for classical MO-EGO approaches to uncover the Pareto Front (growing size of \mathcal{P}_Y with m)

How to obtain several optimal trade-off solutions in spite of the extremely parsimonious use of the computer code, and the multiple conflicting objectives?

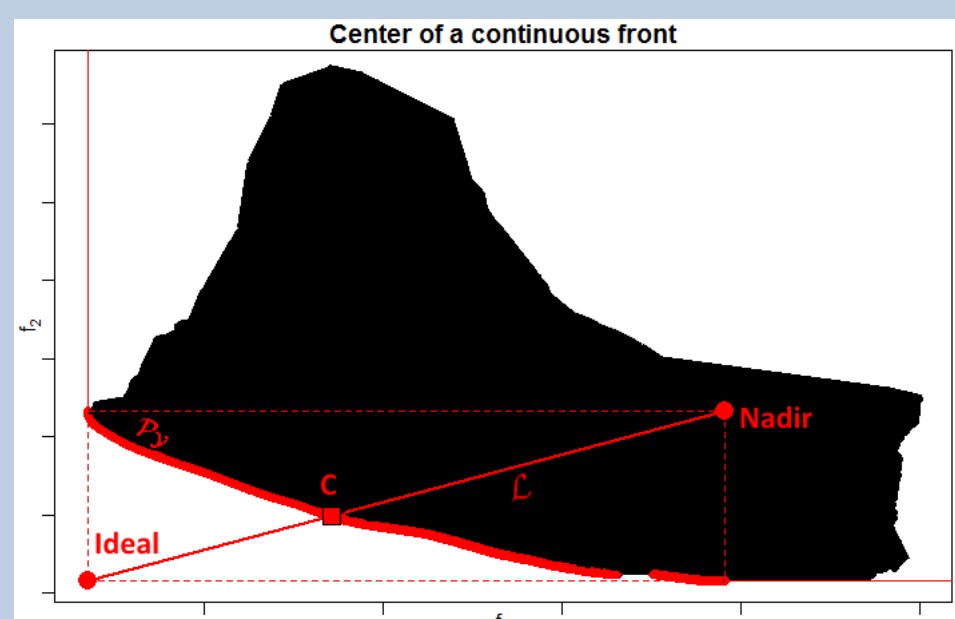
Targeting: motivations

- Restricted budget and large number of objectives \Rightarrow Uncovering the whole Pareto Front \mathcal{P}_Y in a "region of interest"
- Shrink search to a smaller subset \Rightarrow faster convergence
- Emphasize solutions that *equilibrate* the objectives: (unknown) central part of the Pareto Front (PF) \Rightarrow interesting solutions for Decision Makers

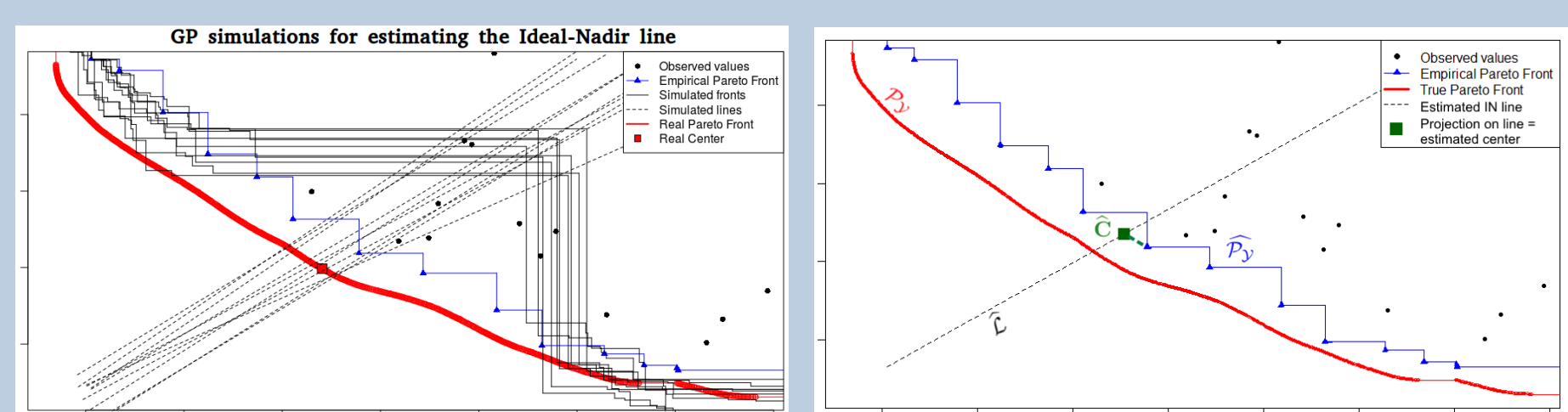


Center of the Pareto Front

Center \mathbf{C} = Projection of closest non-dominated point on Ideal-Nadir line \mathcal{L}



- Low dependence to variations of \mathbf{I} and \mathbf{N} : $|\frac{\partial C_i}{\partial I_i}|$ and $|\frac{\partial C_i}{\partial N_i}| < 1$ for a continuous front
- Insensitive to a linear scaling of the objectives in a bi-objective case, and when \mathcal{L} intersects \mathcal{P}_Y
- Computationally cheap, even for large m
- Estimation: GP simulations emphasizing the edges of the PF \Rightarrow estimated Ideal, Nadir and $\hat{\mathcal{L}} \Rightarrow$ estimated center $\hat{\mathbf{C}}$

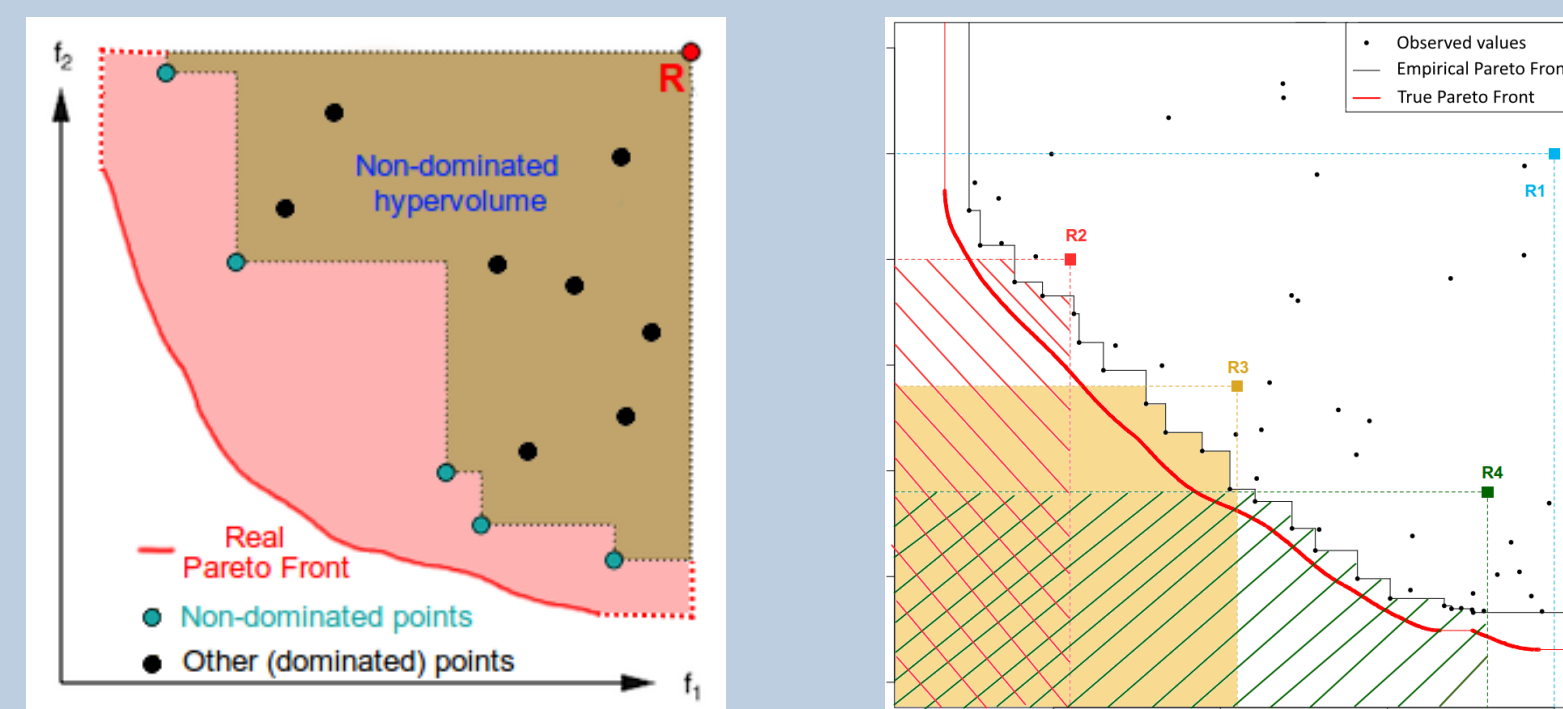


Infill Criteria for targeting the center

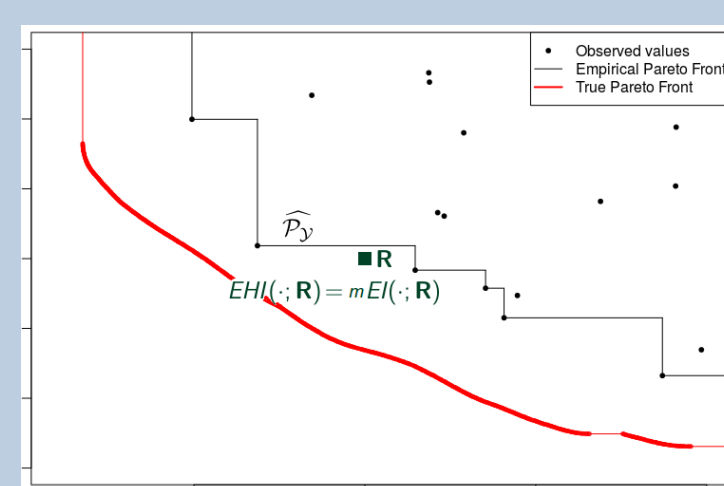
$IC = f(Y_1(\cdot), \dots, Y_m(\cdot); \mathbf{x}; \Theta)$: directs the search towards attractive new designs \mathbf{x}^*

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 Indicator [3] (relatively to \mathbf{R}), if adding design \mathbf{x}

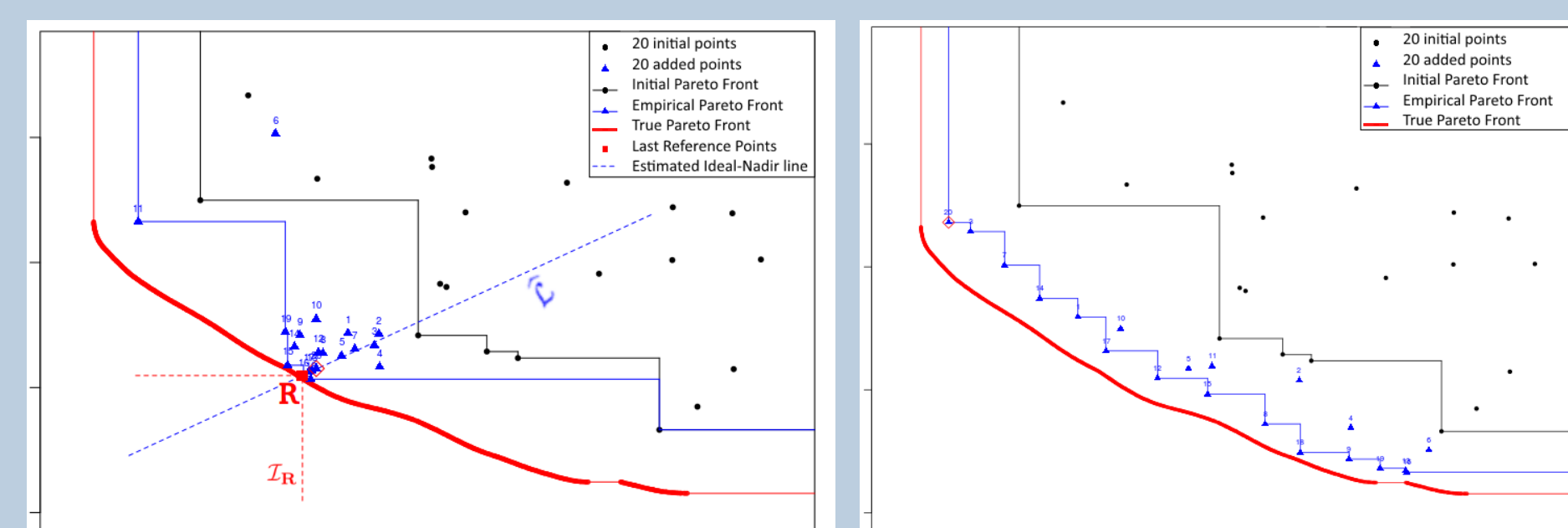


- Subspace targeted by \mathbf{R} : $\mathcal{I}_{\mathbf{R}} = \{\mathbf{y} \in \mathbb{R}^m : \mathbf{y} \preceq \mathbf{R}\}$
- Product of Expected Improvement w.r.t. $\hat{\mathbf{C}}$: $mEI(\mathbf{x}; \hat{\mathbf{C}}) = \prod_{i=1}^m EI_i(\mathbf{x}; \hat{C}_i)$, $EI_i(\cdot, \hat{C}_i)$: EI in objective i considering \hat{C}_i as the current minimum
- If $\mathbf{R} \notin \hat{\mathcal{P}}_Y$, $EHI(\cdot; \mathbf{R}) = mEI(\cdot; \mathbf{R})$



- Still cheap for large m
- Analytical expression
- Parallelizable

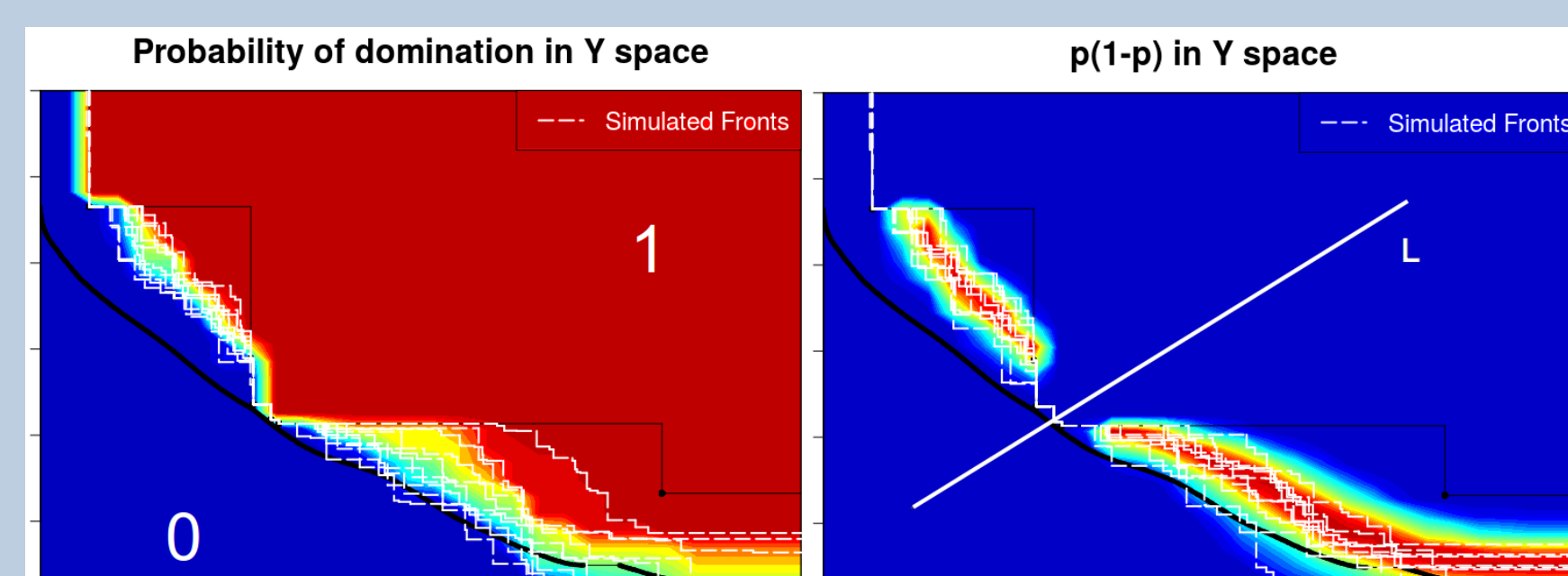
Use the estimated center $\hat{\mathbf{C}}$ as reference point \mathbf{R} \Rightarrow Optimization directed towards the center



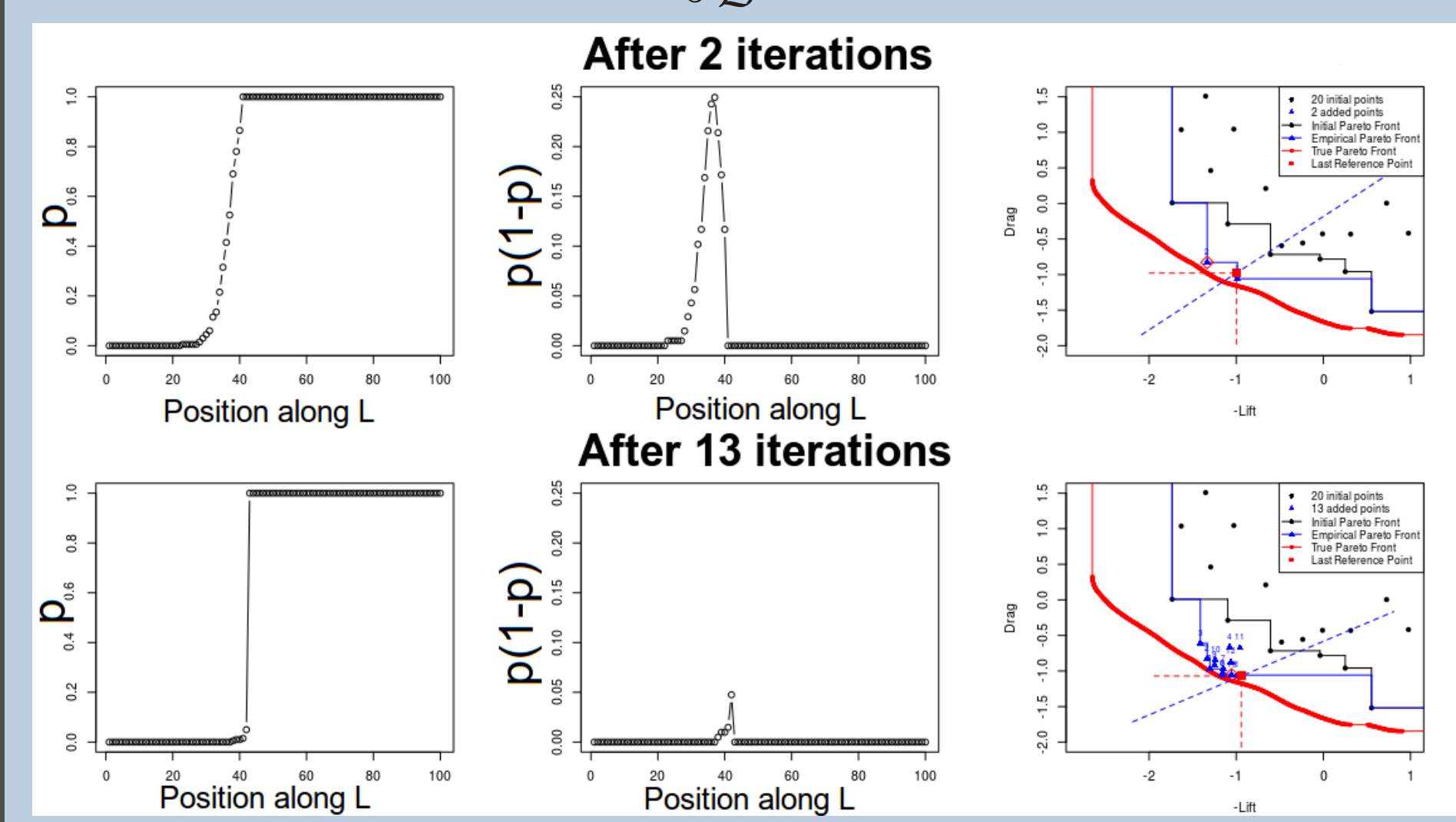
Convergence towards the center of the PF

When to stop the targeting of the center?

- Probability of domination $p(\mathbf{y})$: probability that objective vector \mathbf{y} can be dominated by any $(f_1(\mathbf{x}), \dots, f_m(\mathbf{x})), \mathbf{x} \in X$
- Estimated using Pareto Fronts from GP draws: $p(\mathbf{y}) = \frac{1}{n_{sim}} \sum_{i=1}^{n_{sim}} \mathbb{1}_{\hat{\mathcal{P}}_Y^{(i)} \preceq \mathbf{y}}$
- Information about (local) uncertainty and convergence towards the PF



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

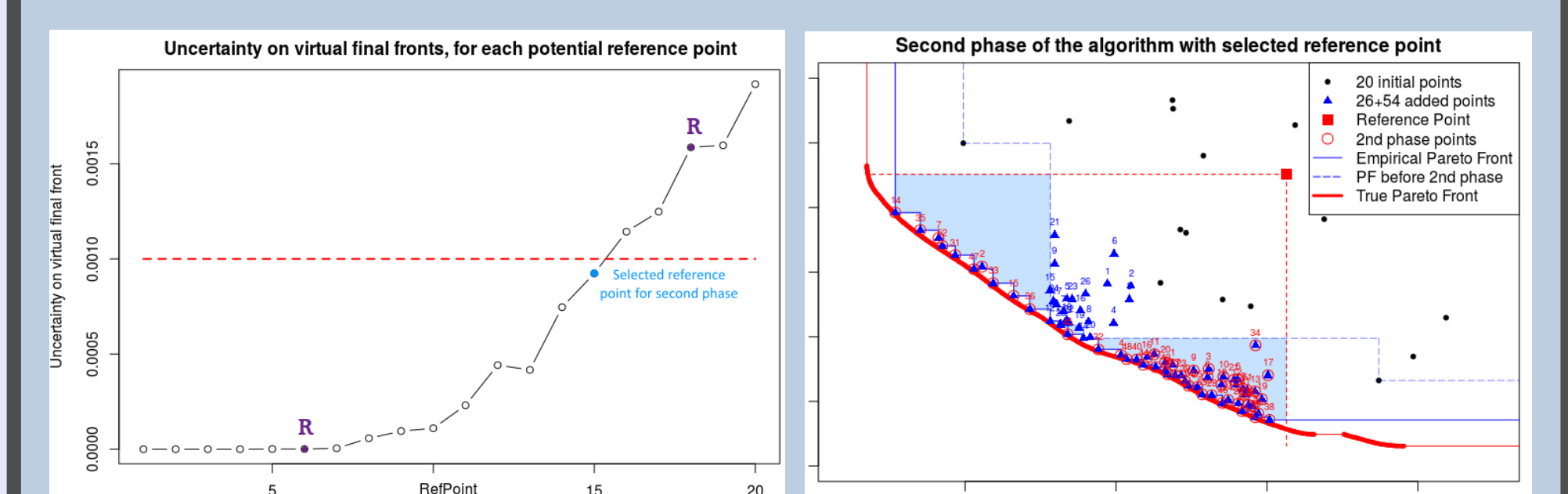
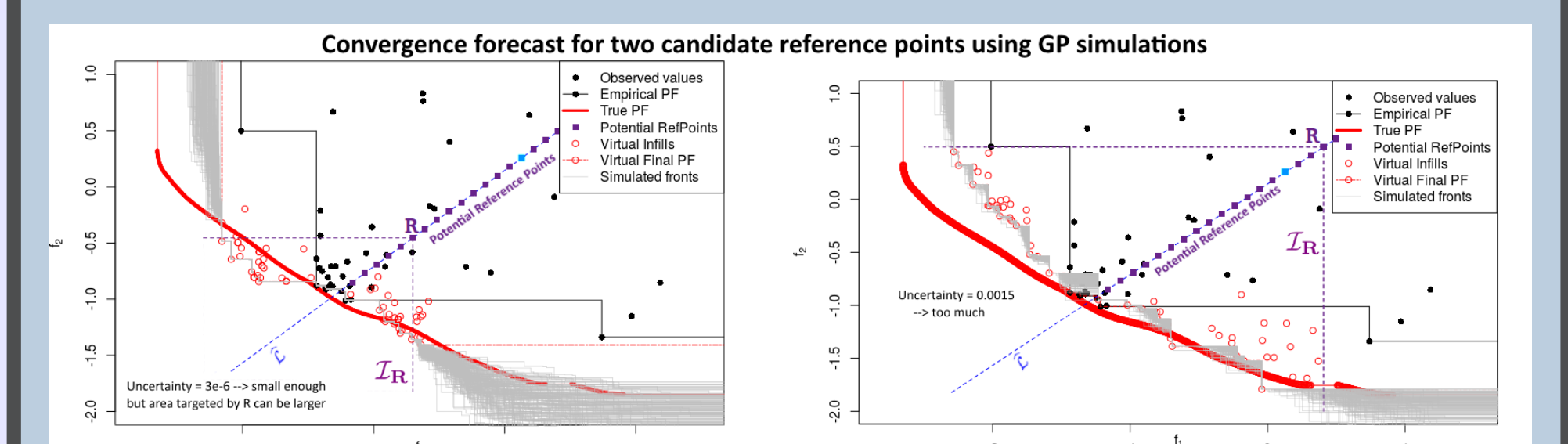


After local convergence: expansion of the PF

b iterations remaining \Rightarrow what to do next?

- Local convergence detected
- Use the remaining budget b to converge towards \mathcal{P}_Y in a wider but attainable central part
- $EHI(\cdot, \mathbf{R})$, with \mathbf{R} on $\hat{\mathcal{L}} \Rightarrow$ focus on central part of \mathcal{P}_Y , size of targeted subspace depending on distance between \mathcal{P}_Y and \mathbf{R}
- Anticipate the algorithm's behavior in the next iterations and the final PF via *virtual infills* that depend on \mathbf{R} : forecast the width of the PF that can be accurately discovered in the last b steps
- *Virtual infills*: either through a Kriging Believer strategy (anticipated \mathbf{y} 's are the kriging mean) or through GPs realizations (anticipated \mathbf{y} 's are samples)
- Small uncertainty on virtual final Pareto Front = convergence in $\mathcal{I}_{\mathbf{R}} \Rightarrow$ choose farthest \mathbf{R} such that

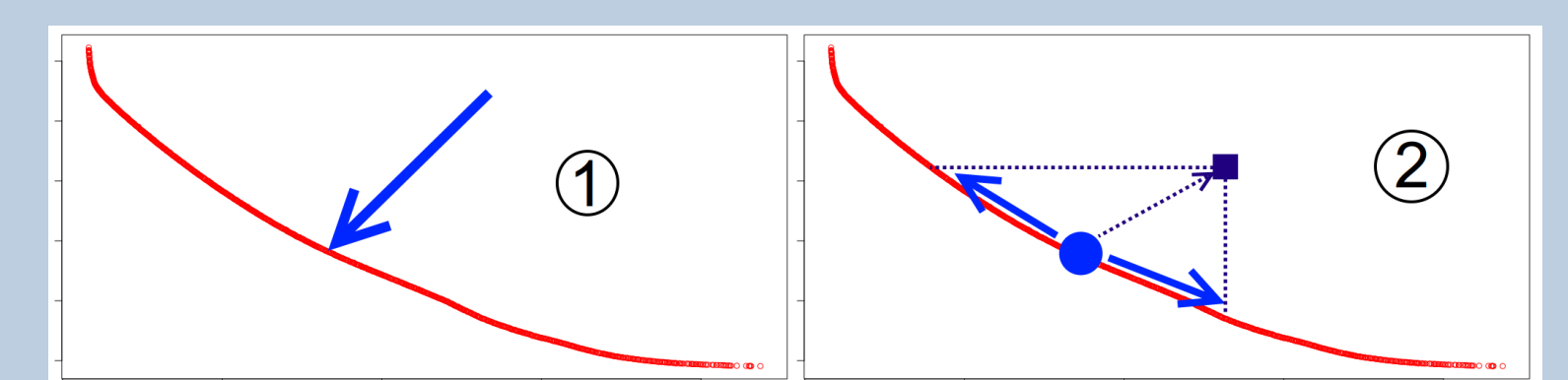
$$\frac{1}{Vol(\mathcal{I}, \mathbf{N})} \int_{\mathbf{y} \preceq \mathbf{R}} p(\mathbf{y})(1-p(\mathbf{y}))d\mathbf{y} \leq \varepsilon$$



Summary

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

- Estimate the Ideal-Nadir line $\hat{\mathcal{L}}$, on which the expected center of the PF is 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 the region of interest $\mathcal{I}_{\mathbf{R}}$ by a backward step of \mathbf{R} calculated through virtual infills.



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)
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