Multiobjective Bayesian Optimization under uncertainties

Victor Trappler, Céline Helbert, Christophette Blanchet-Scalliet, Rodolphe Le Riche

(Multi)objective Bayesian Optimization under uncertainties

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December 6, 2024

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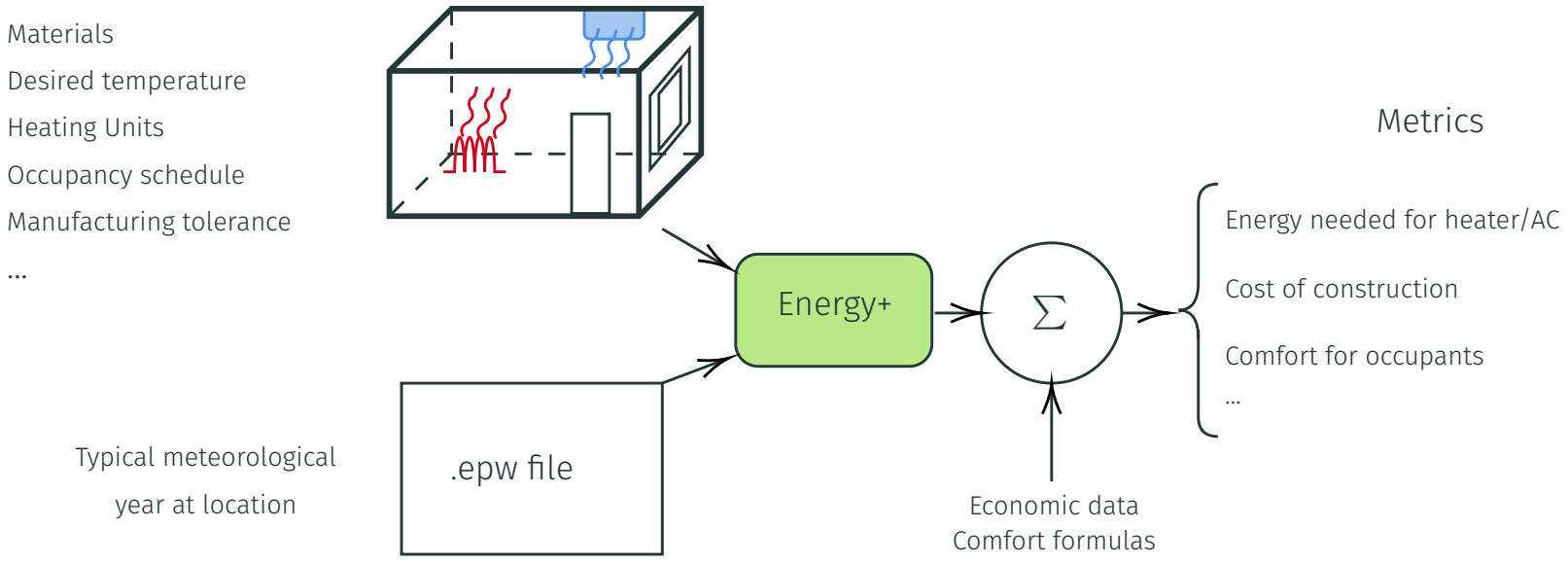
[2]LIMOS

vtrappler.github.io

How to design buildings: EnergyPlus



- $x \in \mathcal{X} \to$ Materials (type and quantity), Heating/AC, Rate of air change...

Desirable building:

- Low cost of construction
- Low energy consumption
- High comfort for occupants

Sadly, no design optimizes simultaneously all objectives.

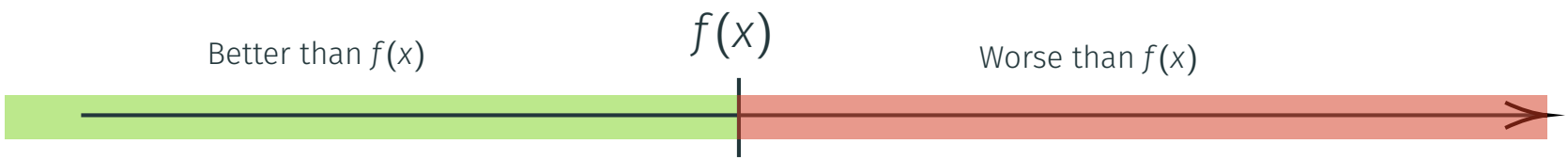
Back to basics

How to compare if x is better than x' ?

Order relation on $\mathbb{R}$: $\leq$

Let $a, b \in \mathbb{R}$. a is not worse than b if $a \leq b$

$f(x')$ *not worse* than $f(x)$ if $f(x') \leq f(x)$



$$\min_{x \in \mathcal{X}} f(x) = y \text{ verifies } y \leq f(x), \quad \forall x \in \mathcal{X}$$

What if f is very expensive to evaluate ?

Bayesian Optimization

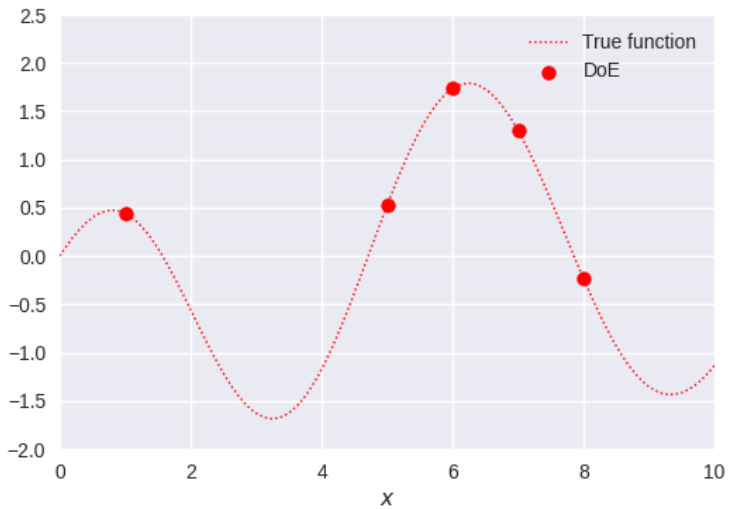
GP modelling

BO relies on Gaussian Process Regression:

GP modelling in very short

Gaussian Process F: Surrogate model of (the expensive to evaluate) f, conditioned on a Design of Experiment

$$F(x) \sim \mathcal{N}(\underbrace{m_F(x)}_{\text{prediction}}, \underbrace{\sigma_F^2(x)}_{\text{uncertainty}})$$



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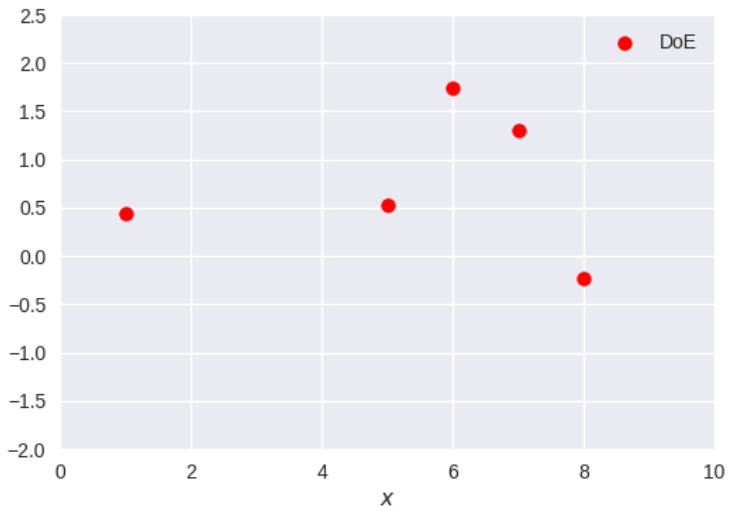

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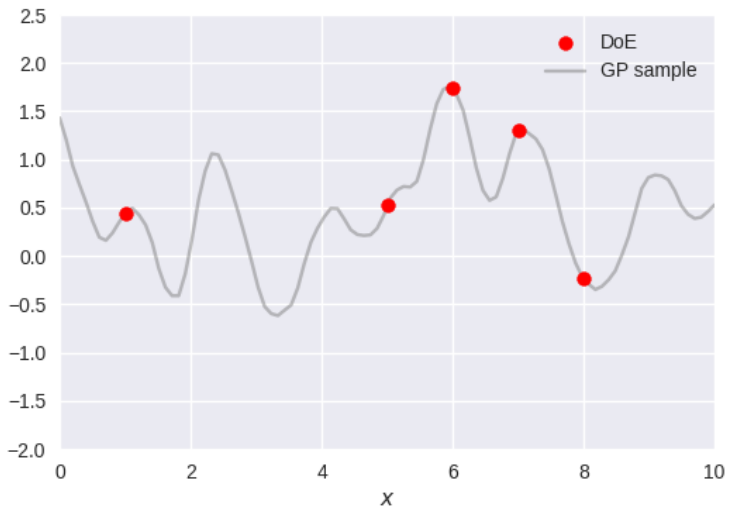

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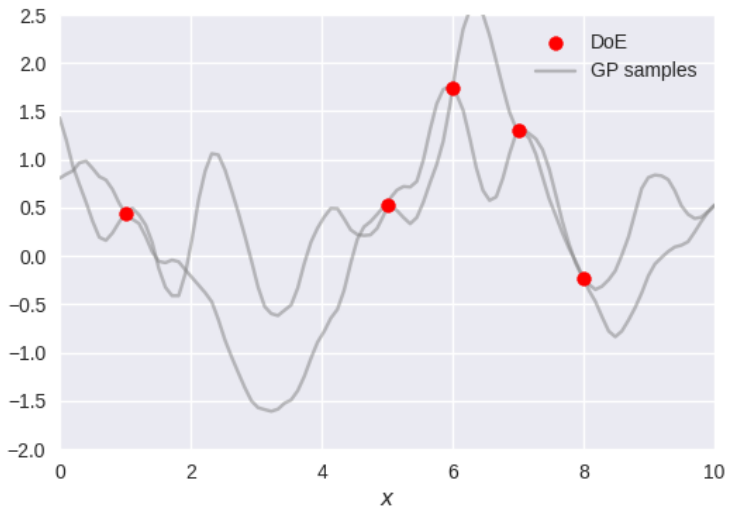

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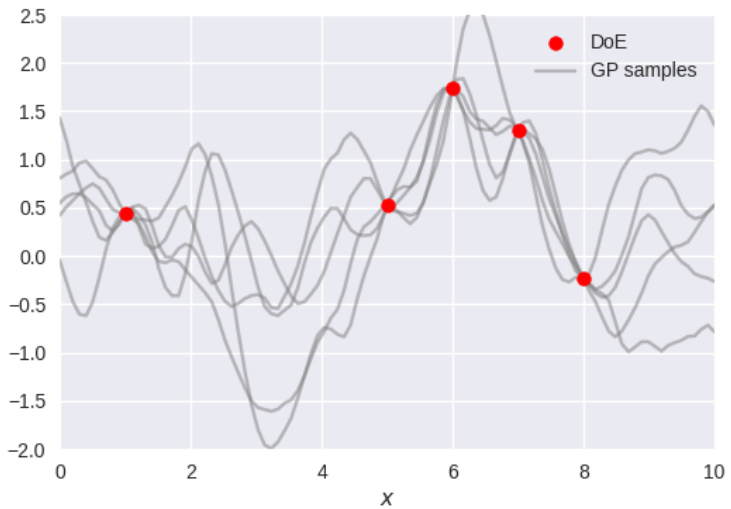

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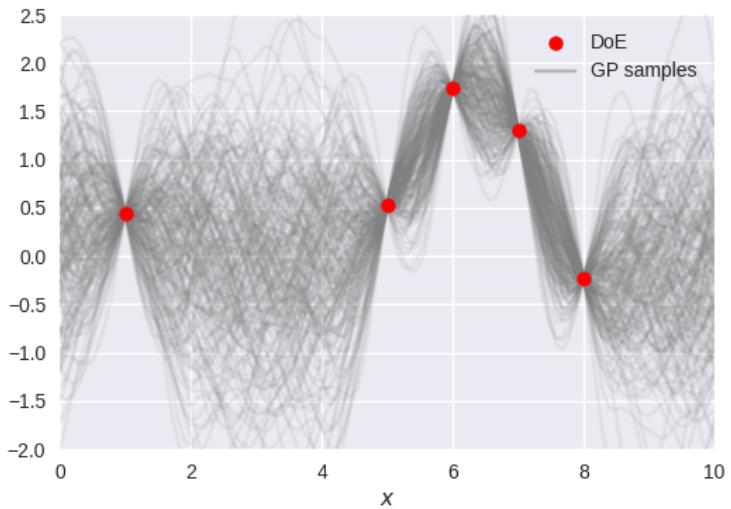

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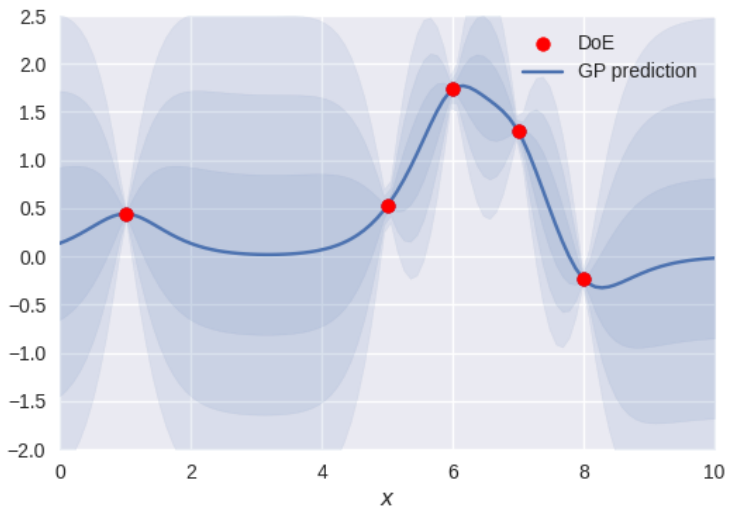
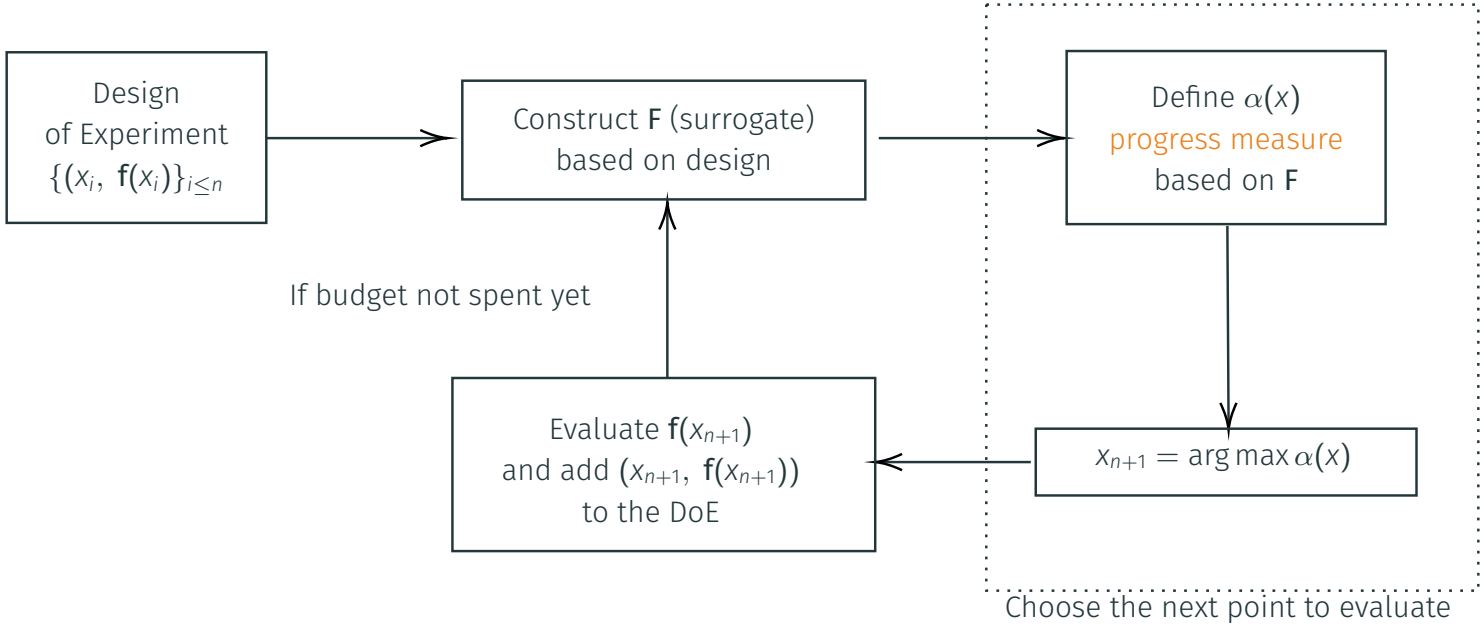


Works well for noisy evaluations of the function !

Bayesian Optimization Loop: Active Learning



- Different Acquisition methods for different objectives
  - EGO, EFI(SUR), LCB, Entropy-based acquisitions...

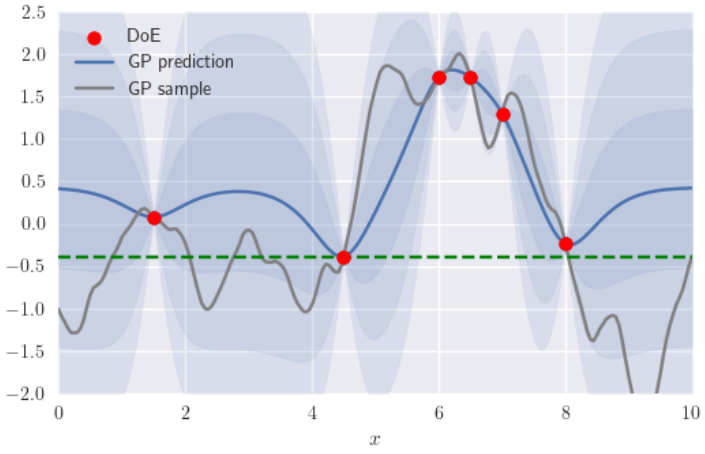
Efficient Global Optimization [JS98]

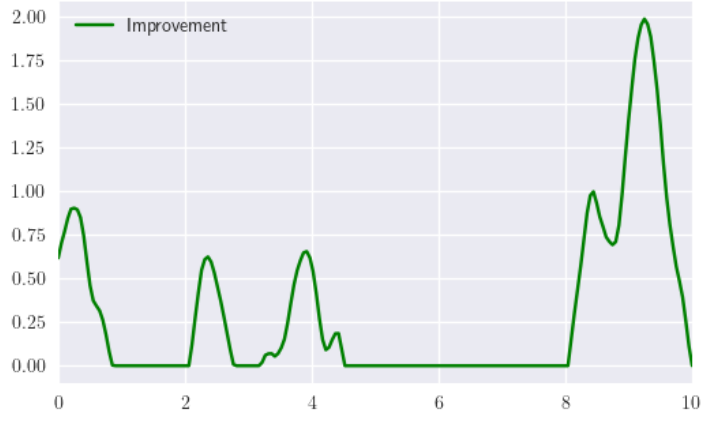
Improvement

How much does $F(x)$ improves the current best value $f_{\min}$?

$$I(x) = \begin{cases} f_{\min} - F(x) & \text{if } f_{\min} \geq F(x) \\ 0 & \text{elsewhere} \end{cases}$$

r.v.





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Progress Measure: Expected Improvement

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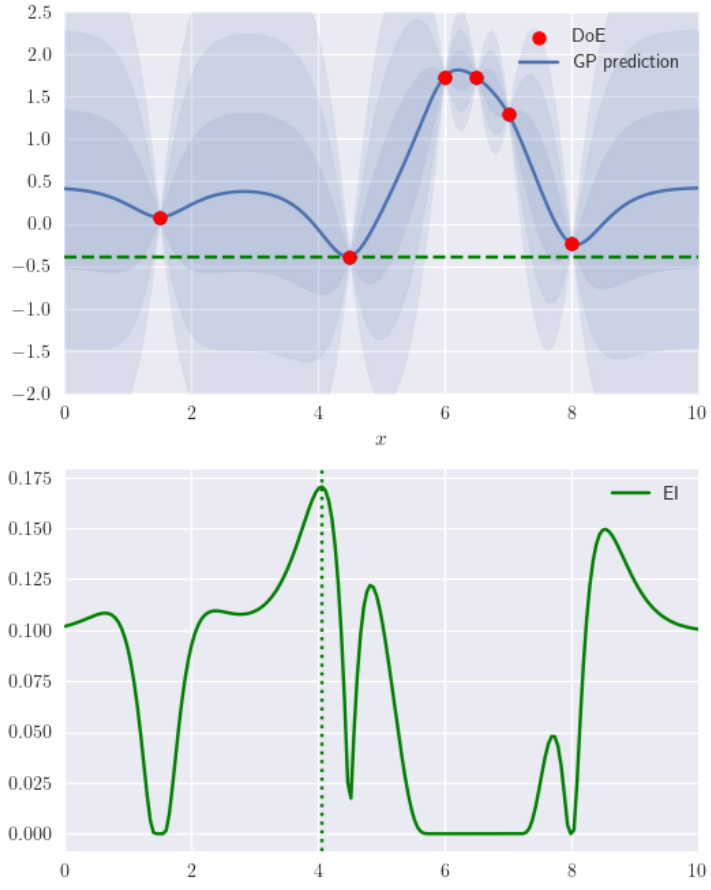
$$x_{n+1} = \arg\max_x \alpha(x)$$

Analytical expression exists for EI (and its gradient) since F is a GP !



$\rightarrow$ Tradeoff exploration vs exploitation

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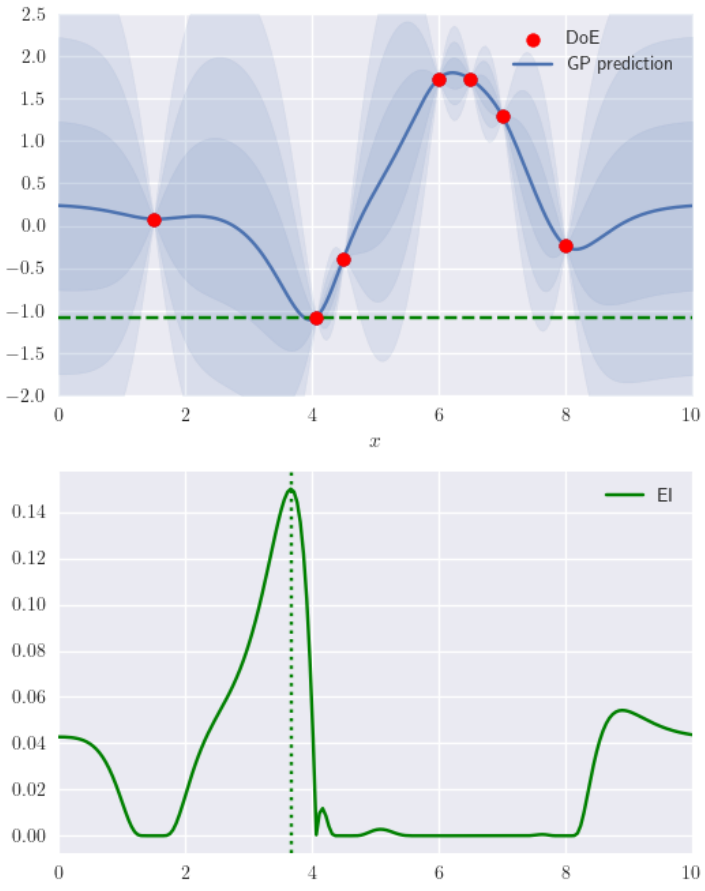

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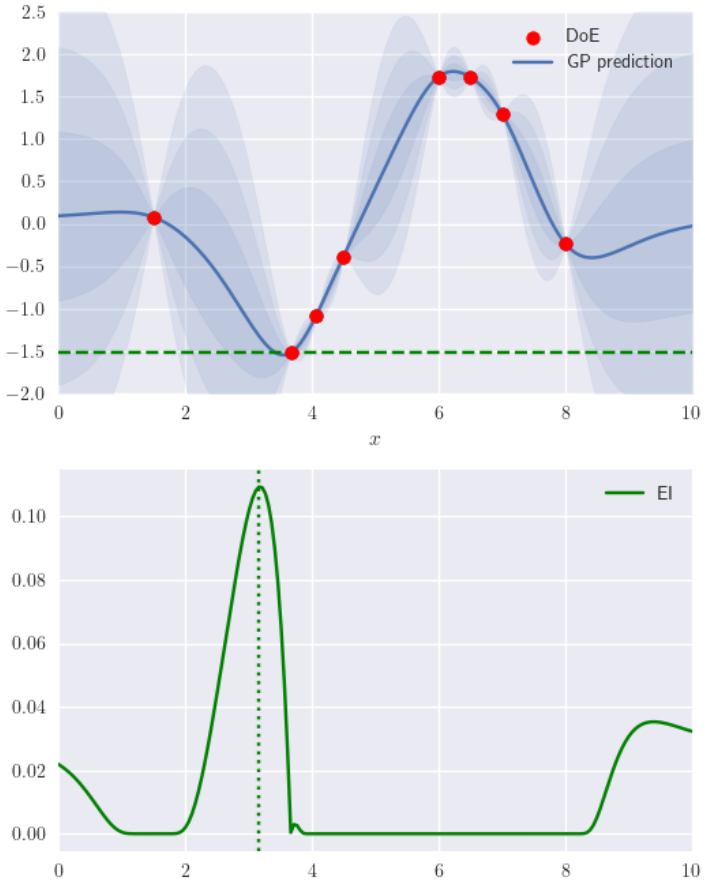

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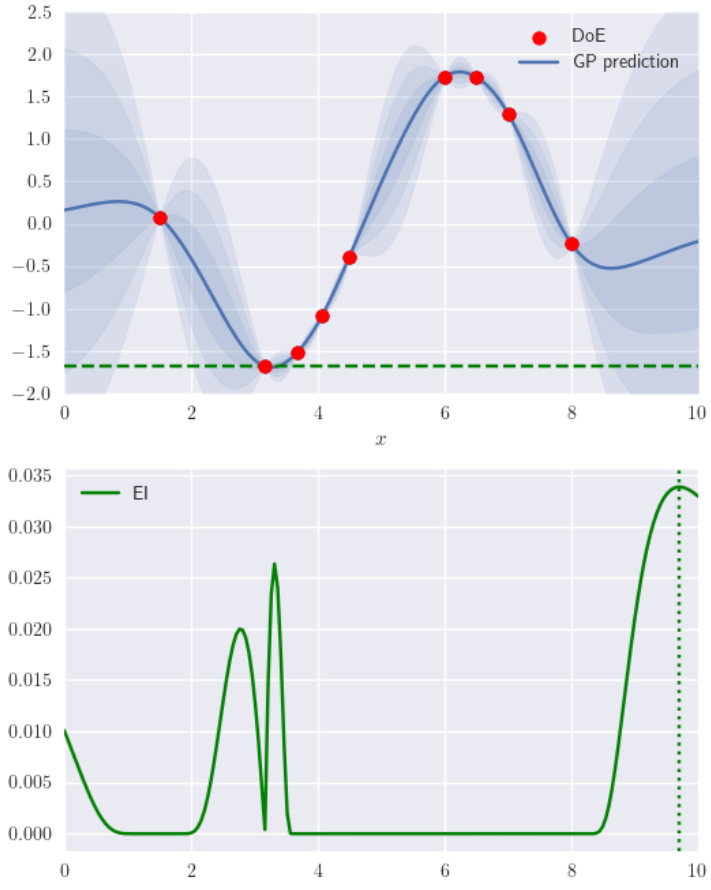

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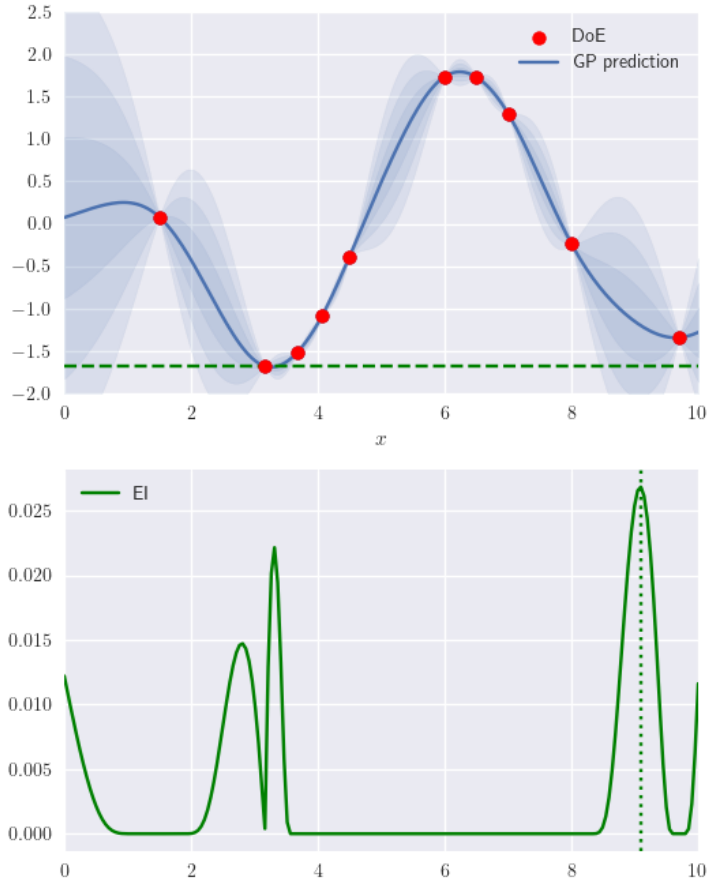

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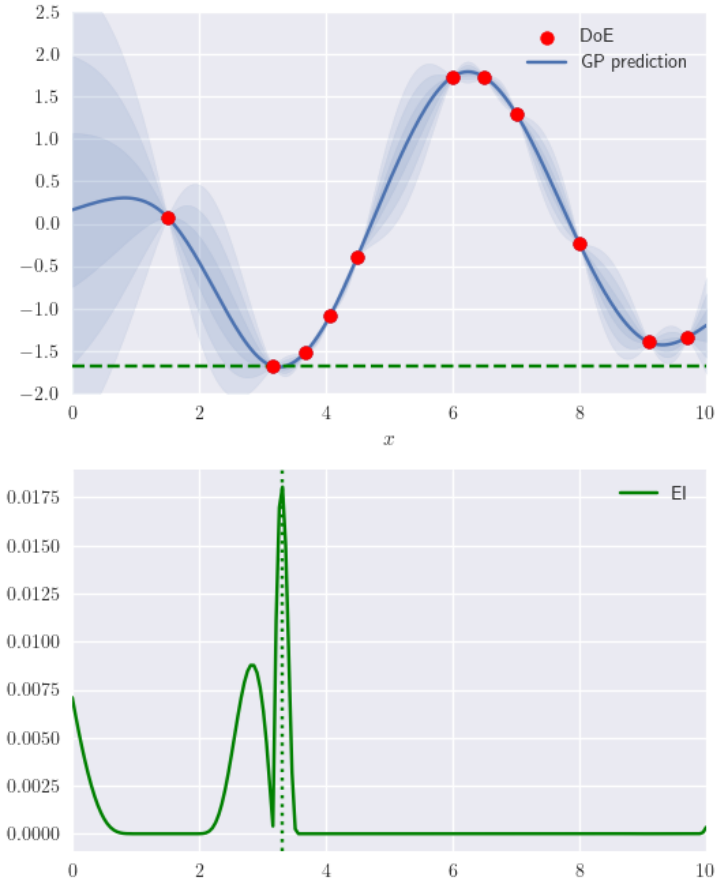

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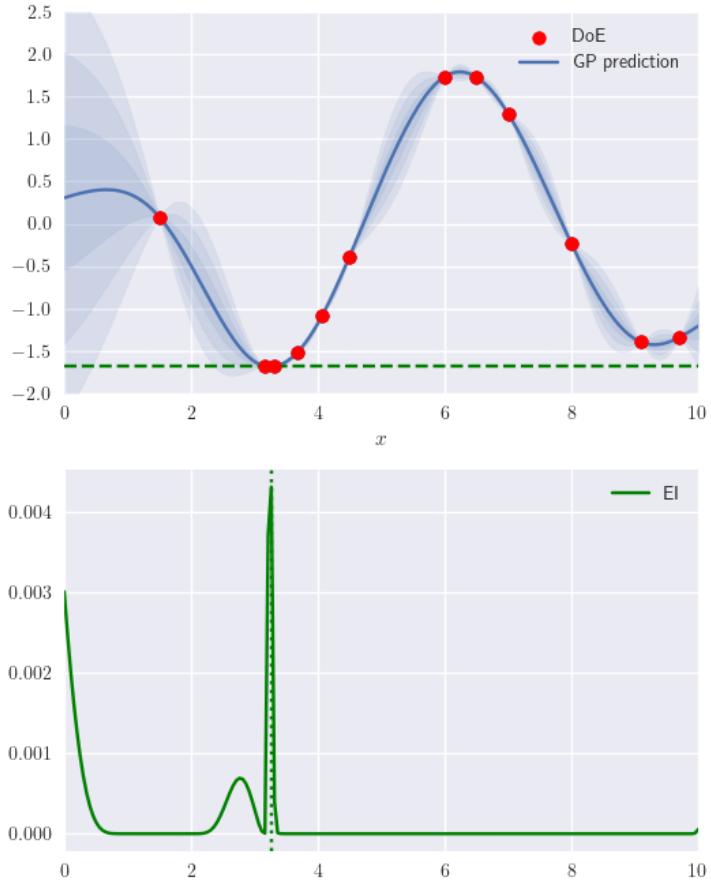

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Multiobjective Optimization

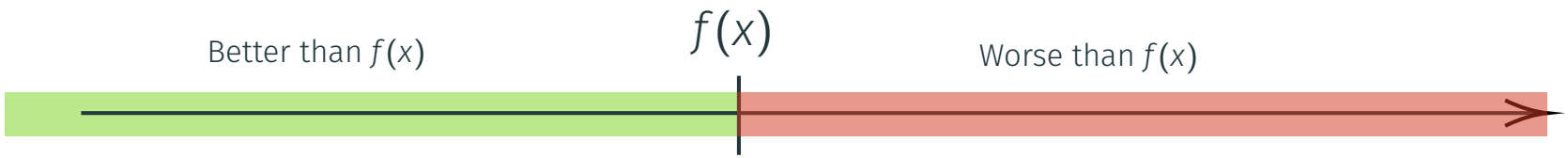
Back to "Back to basics"

How to compare if x is better than x' ?

Order relation on $\mathbb{R}$: $\leq$

Let $a, b \in \mathbb{R}$. a is not worse than b if $a \leq b$

$f(x')$ *not worse* than $f(x)$ if $f(x') \leq f(x)$



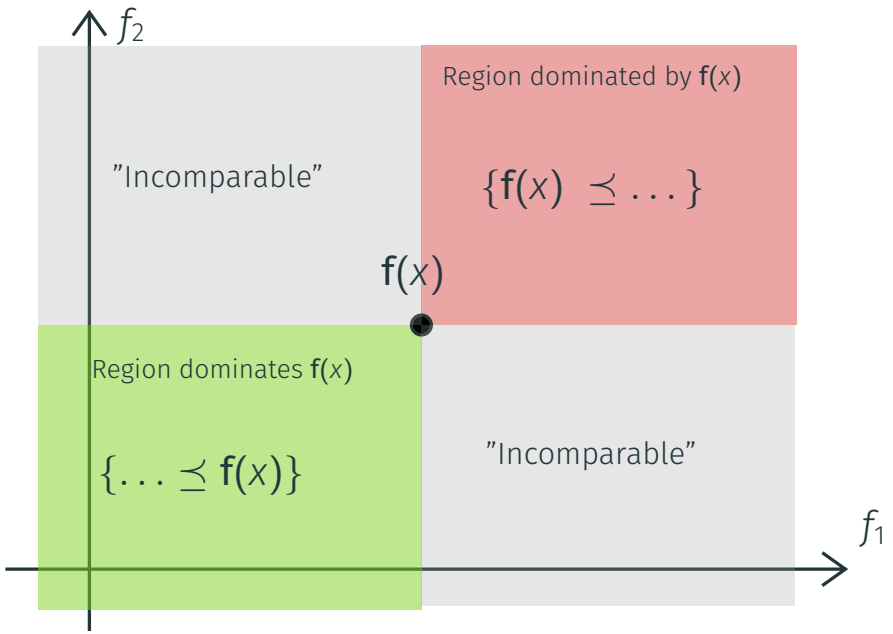
$$\min_{x \in \mathcal{X}} f(x) = y \text{ verifies } y \leq f(x), \quad \forall x \in \mathcal{X}$$

Pareto Domination relation

Partial order relation on $\mathbb{R}^2$: $\preceq$

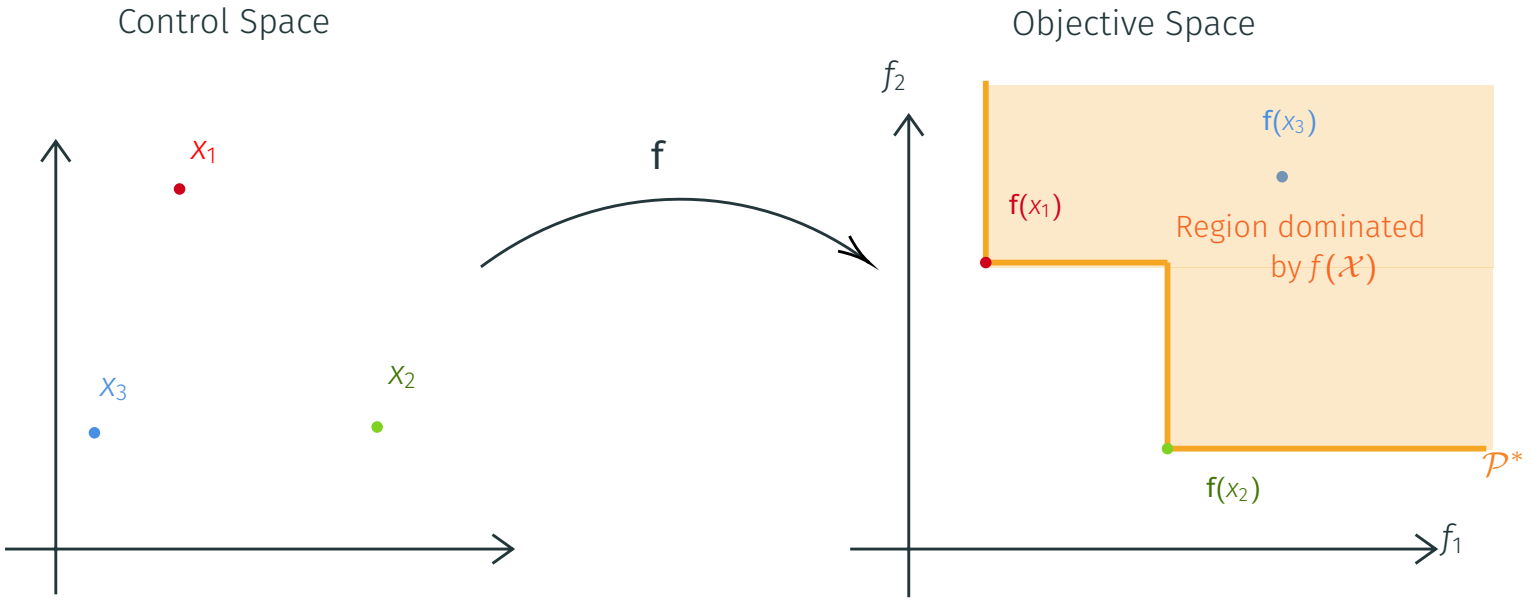
Let $\mathbf{a}, \mathbf{b} \in \mathbb{R}^2$.

$\mathbf{a} \preceq \mathbf{b} \iff a_i \leq b_i \quad \forall i$: all components of $\mathbf{a}$ are *not worse* than those of $\mathbf{b}$



"Incomparable"
$\rightarrow$ some components are better, some worse

Pareto Front, Pareto Set



- Pareto Front $\mathcal{P}^*$: Set of **non-dominated** point of $\mathbf{f}(\mathcal{X})$. Subset of objective space
- Pareto set $\mathcal{P}^*_{\mathcal{X}}$: Preimage of Pareto front. Subset of control space

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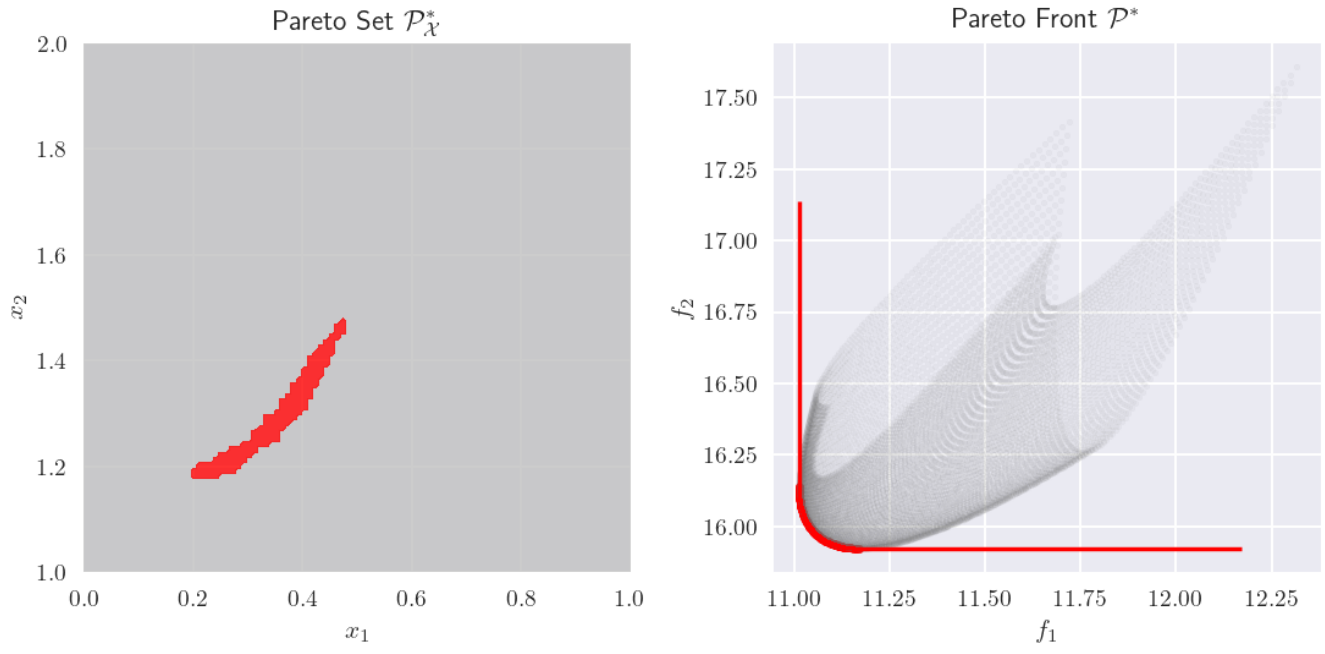

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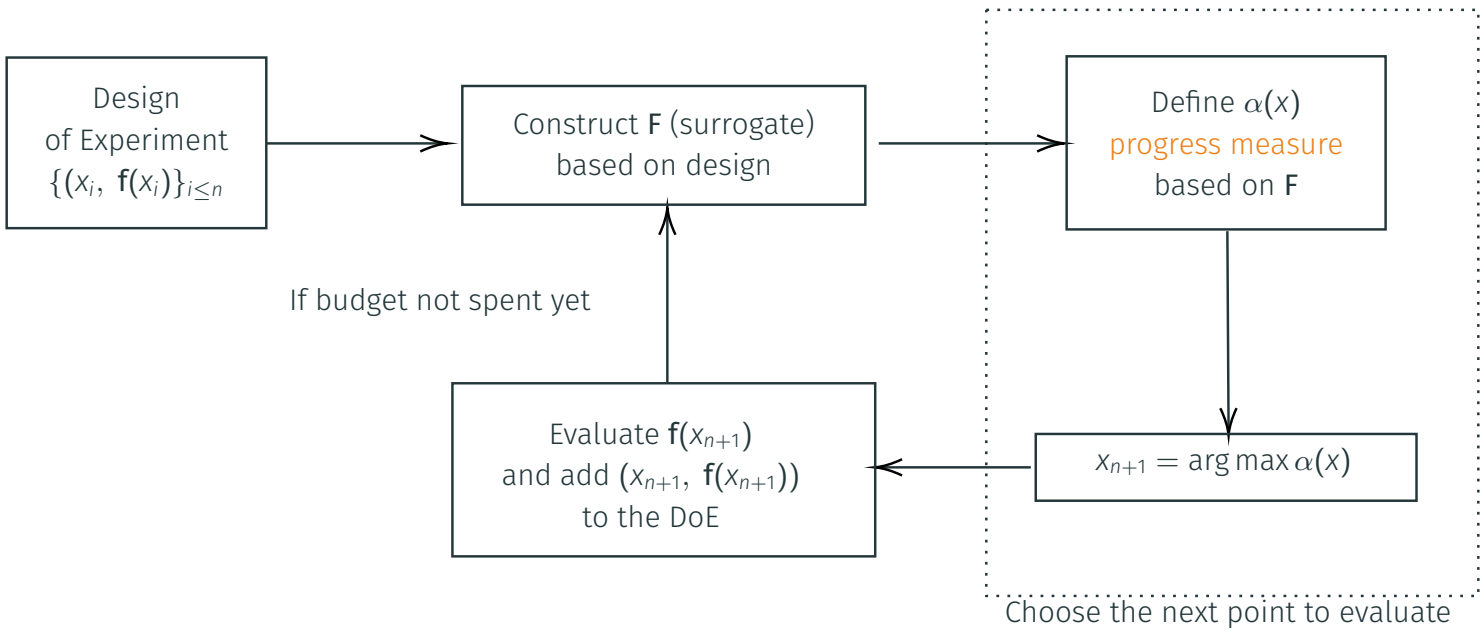
Typical Bayesian Optimization Loop

Multidim GP

$$\mathbf{F} \sim \mathrm{GP}(\mathbf{m}, \mathbf{k})$$

$$\mathbf{F}(x,u) \sim \mathcal{N}\left(\begin{bmatrix} m_1(x,u) \\ m_2(x,u) \end{bmatrix}, \begin{bmatrix} \sigma_1(x,u) & 0 \\ 0 & \sigma_2(x,u) \end{bmatrix}\right)$$



Multiobjective Bayesian Optimisation

Bayesian Optimisation methods exist to find non dominated points !

EHVI, SUR, $\star$-ESMO . . . [Pic13, HHSA16]

Hypervolume Improvement

$$\mathrm{HVI}(x_1) = \mathrm{Vol}\left(\square \cup \square\right) - \mathrm{Vol}\left(\square\right)$$

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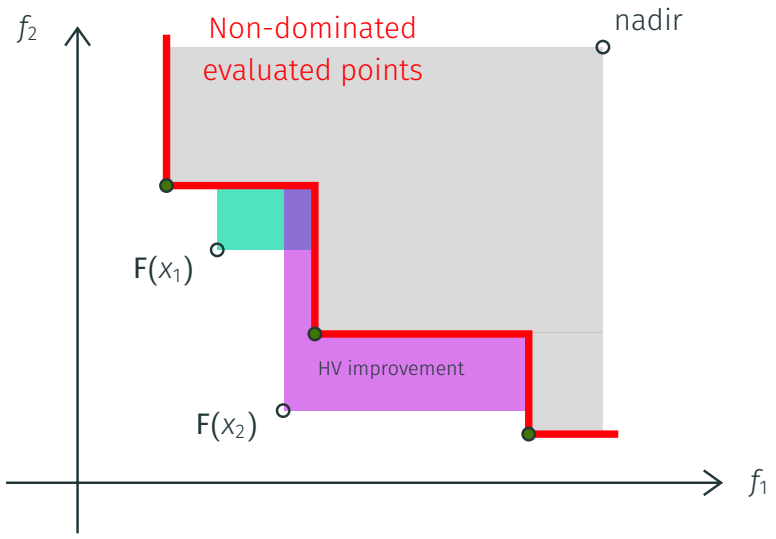
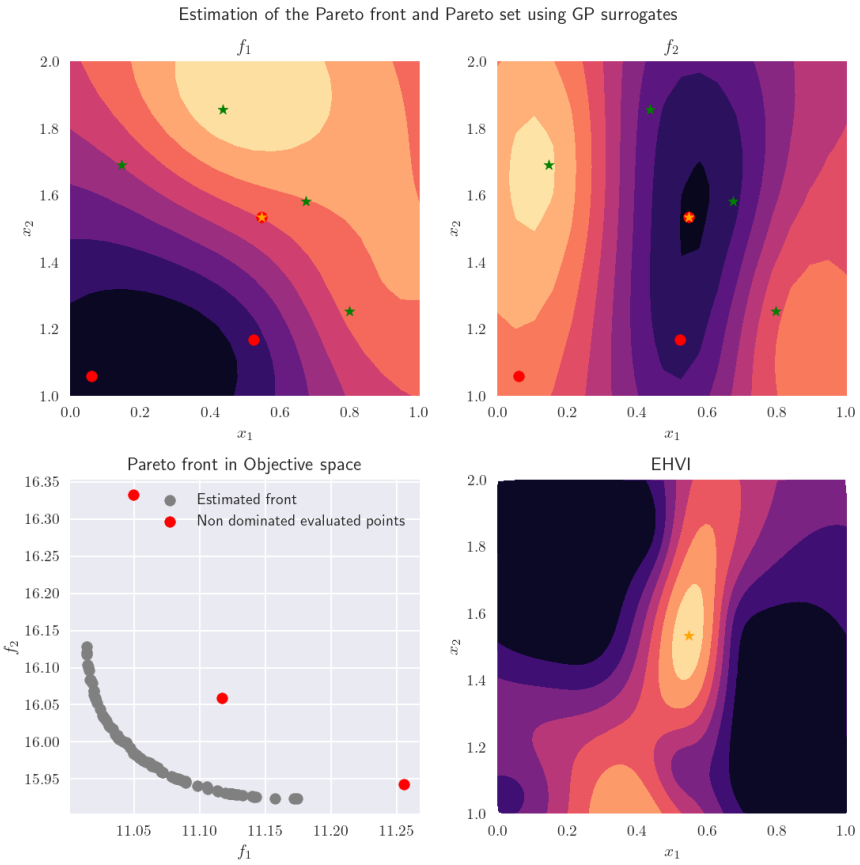
$$\alpha(x) = \mathbb{E}\left[HVI(x)\right]$$





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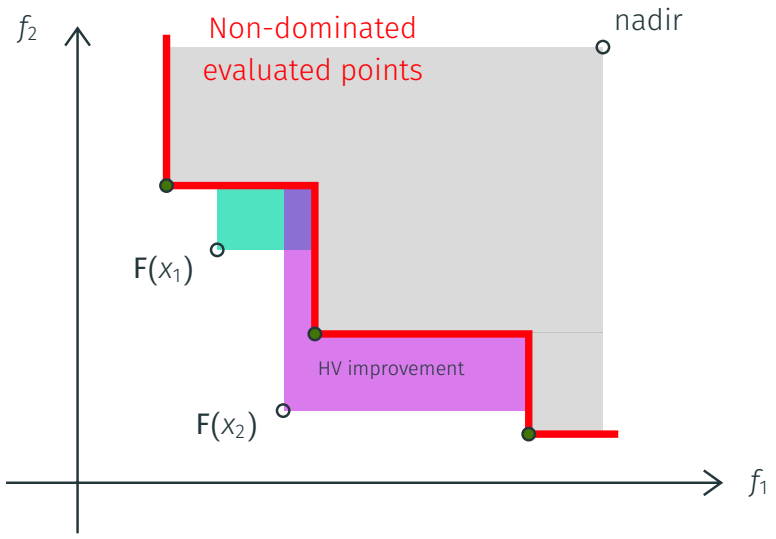

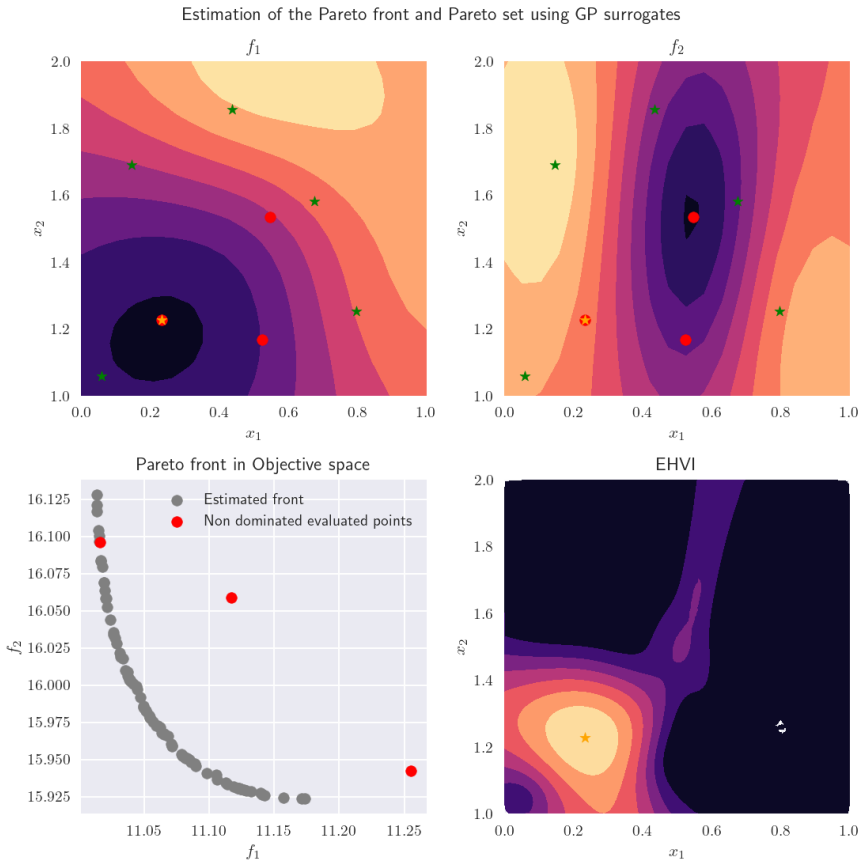

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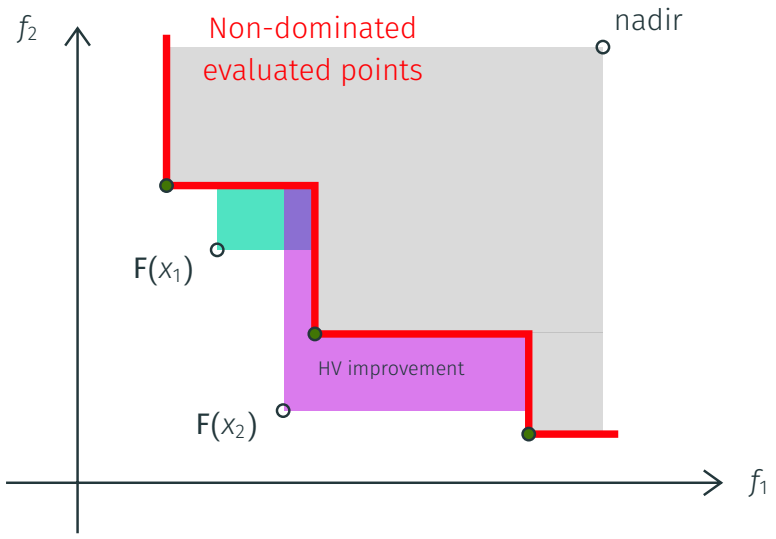

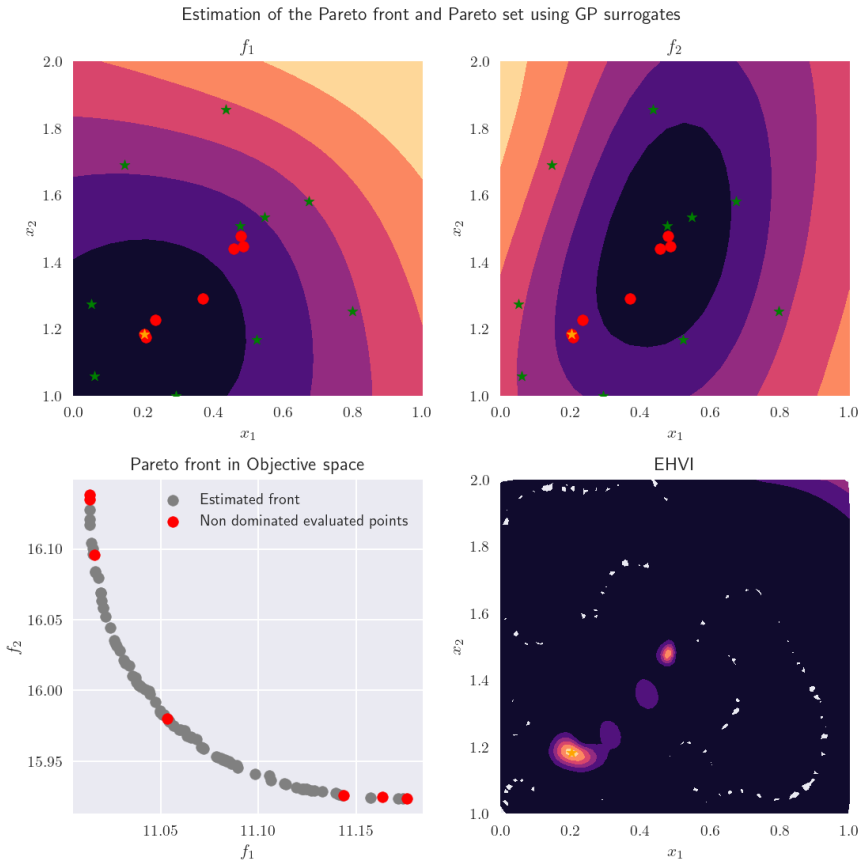

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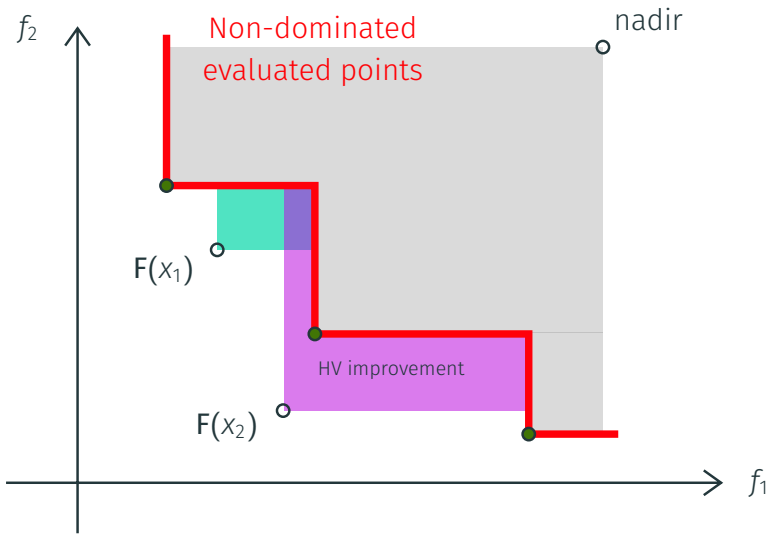

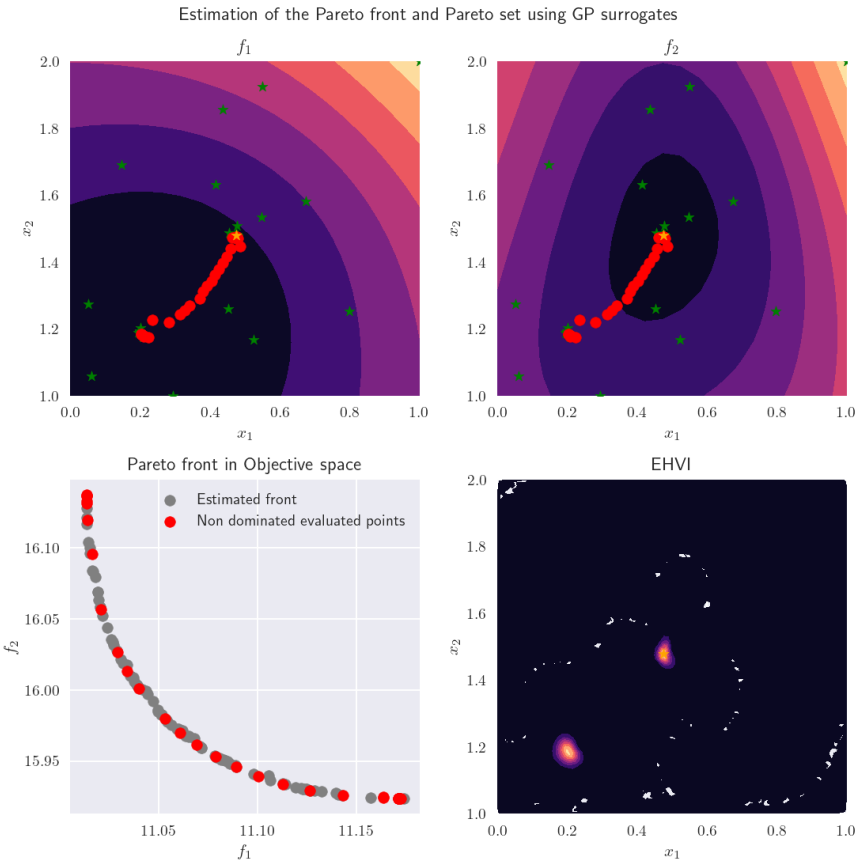

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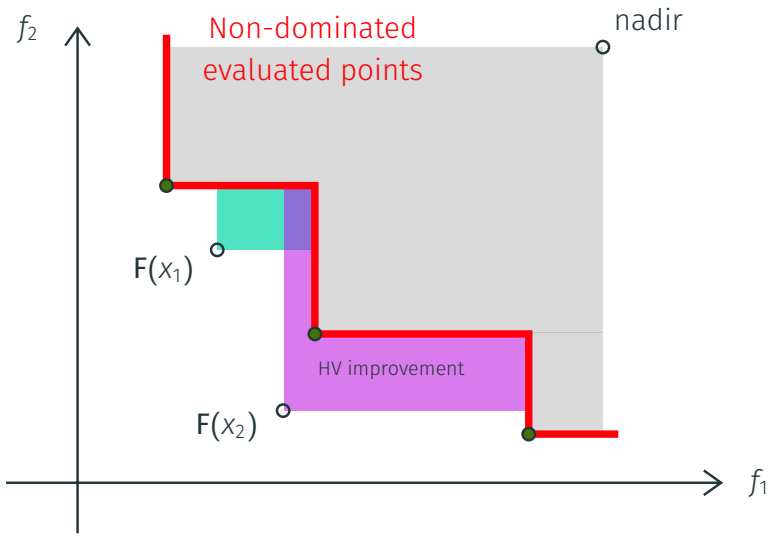
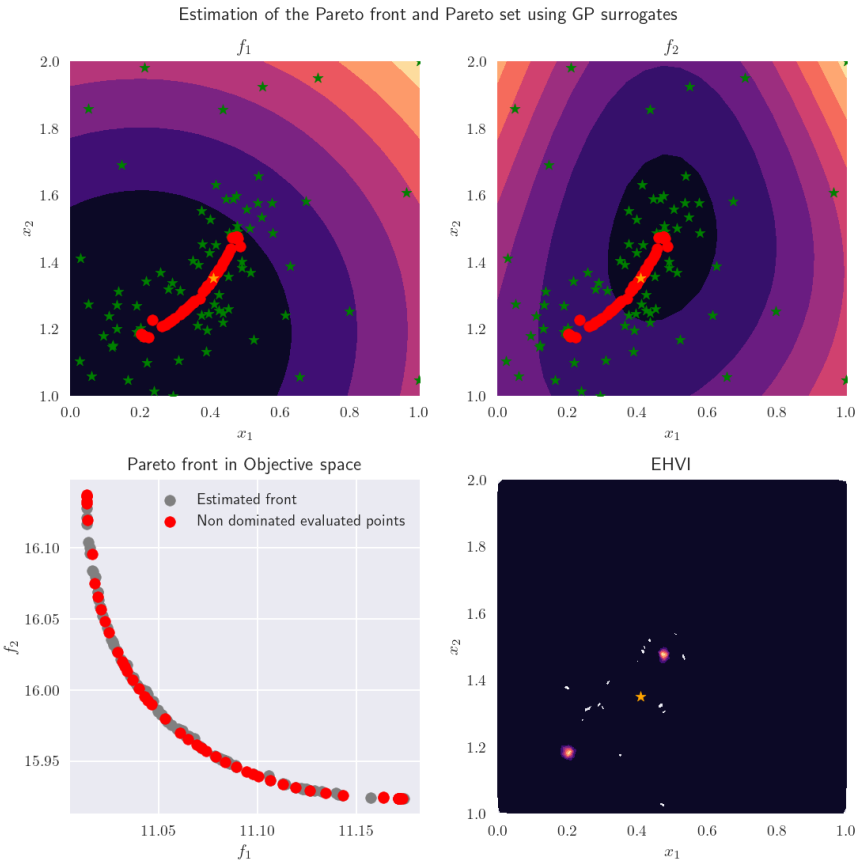




Optimal Conditions today ?

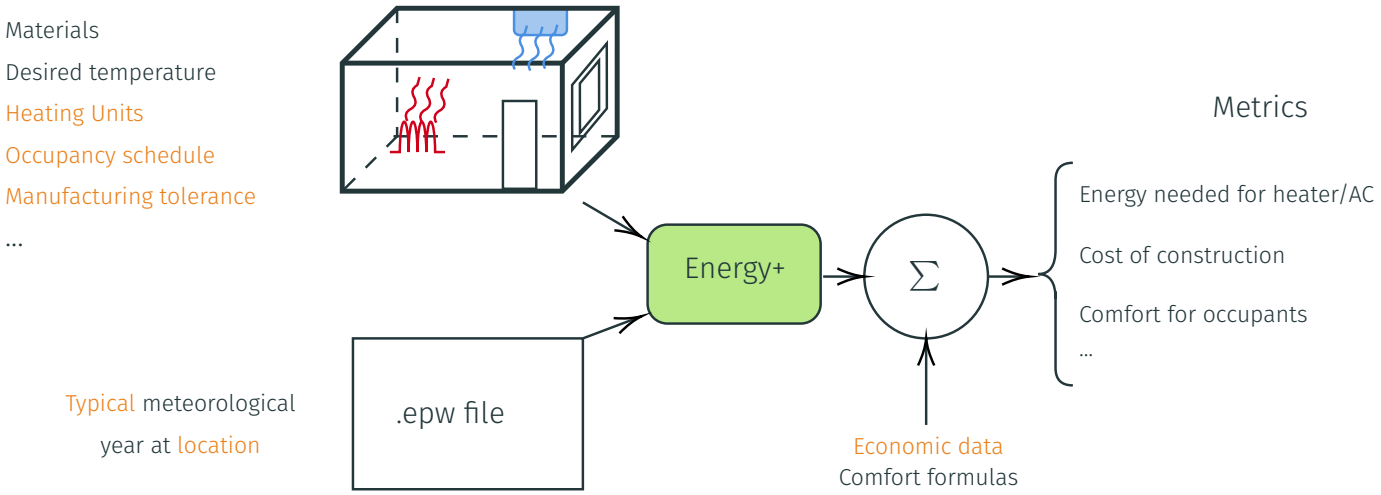
Buildings have a lifespan > 20 years.

If the building is ”optimal” today, how about in 5 years, 10 years or 20+ years ?

$\Rightarrow$ Many uncertainties can be taken into account for this modelling !

Multiobjective Optimization under uncertainties

Introducing uncertainties



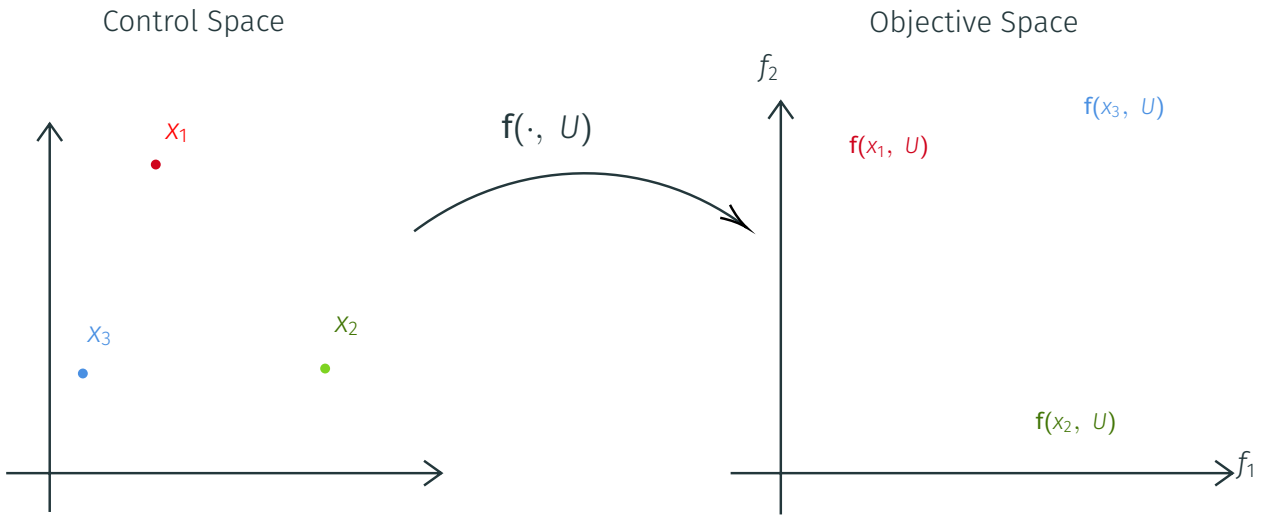
Let $u \sim U$ with support $\mathcal{U}$ which models

- Nominal vs real physical properties
- Energy prices / Environmental impact
- Climate Change
- Time variability of materials properties
- Occupancy schedules...

$\mathbf{f}(x, U)$: Multivariate random variable to *optimize* ?

Comparing sets ?

$\mathbf{f}(x, U)$: Multivariate random variable

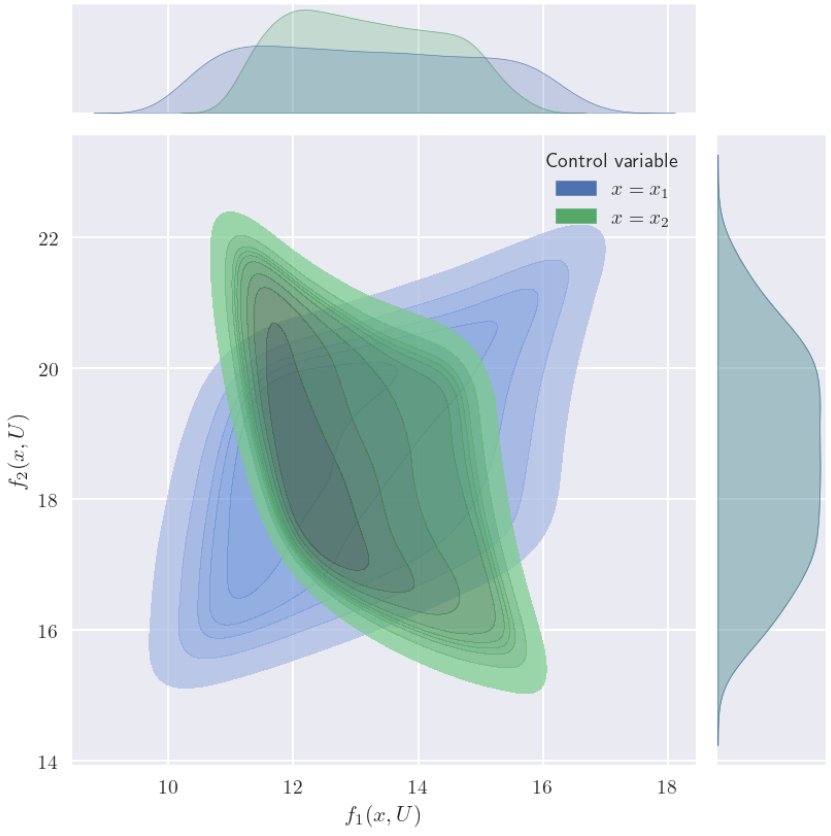


What does it mean to be better/not worse in this context ?

How to deal with U ?

Comparing sets ?

$\mathbf{f}(x_1, U)$ vs $\mathbf{f}(x_2, U)$



What does it mean to be better/not worse in this context ?

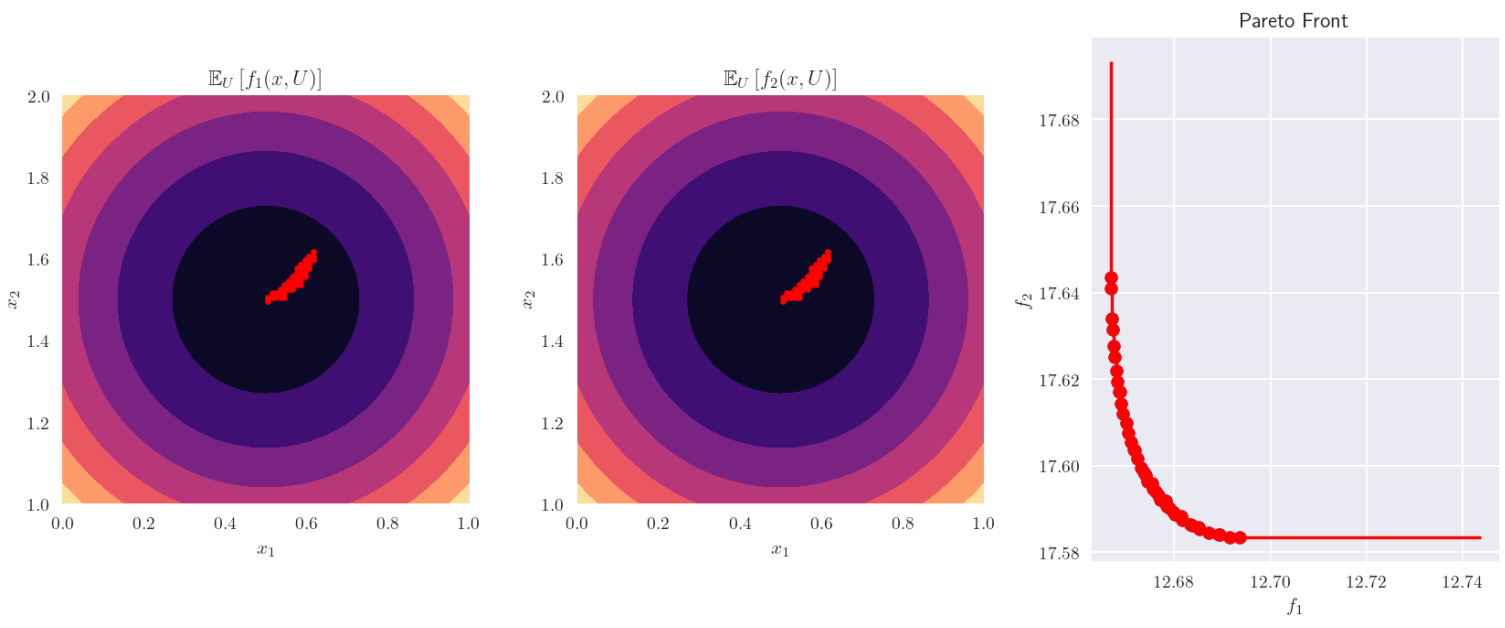
How to deal with U ?

Mean Objective Optimization

We can look for statistics of $\mathbf{f}(x, U)$.

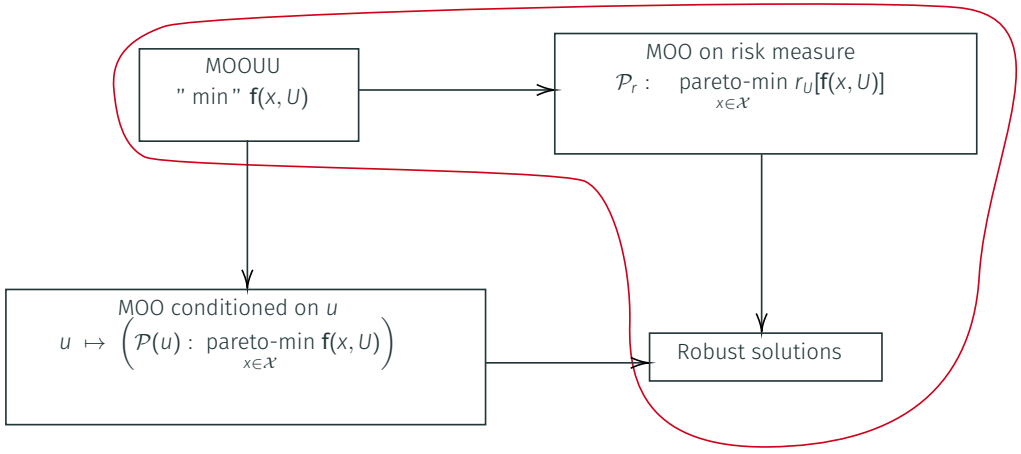
Mean Objective Optimization

Non dominated points of $\mathbb{E}_U[\mathbf{f}(x, U)] = (\mathbb{E}_U[f_1(x, U)], \ldots, \mathbb{E}_U[f_m(x, U)])$



$\Rightarrow$ We can construct an acquisition function (like in EFISUR, or Noisy EHVI)

Robustify or Solve first ?



"Robustify then Solve"

$$r_U[\mathbf{f}(x,U)] = \begin{cases} \mathbb{E}_U\left[\mathbf{f}(x,U)\right] & \text{[QCD23, DG05]} \\ \text{Multivariate VaR} & \text{[TKLS24, DCB}^+\text{22]} \\ \text{Bounding boxes approaches} & \text{[RC22]} \end{cases}$$

"Solve then Robustify"

- For a given u, MOO problem $\rightarrow$ Conditional Pareto front $\mathcal{P}^*(u)$
- Do some things using $\mathcal{P}^*(U)$ and $\mathcal{P}^*_{\mathcal{X}}(U)$?

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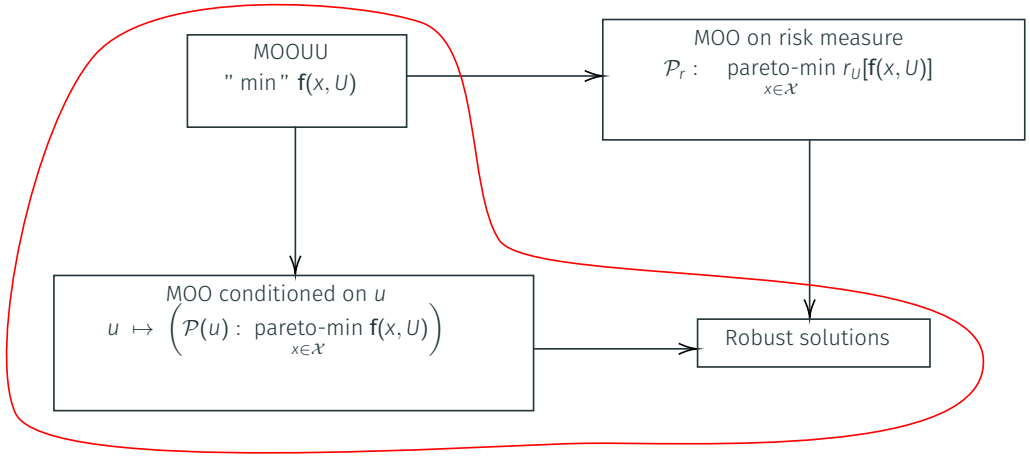

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Conditional Pareto Front/Set – Contextual Optimization

Given $u \in \mathcal{U}$, we have a deterministic MOO problem:

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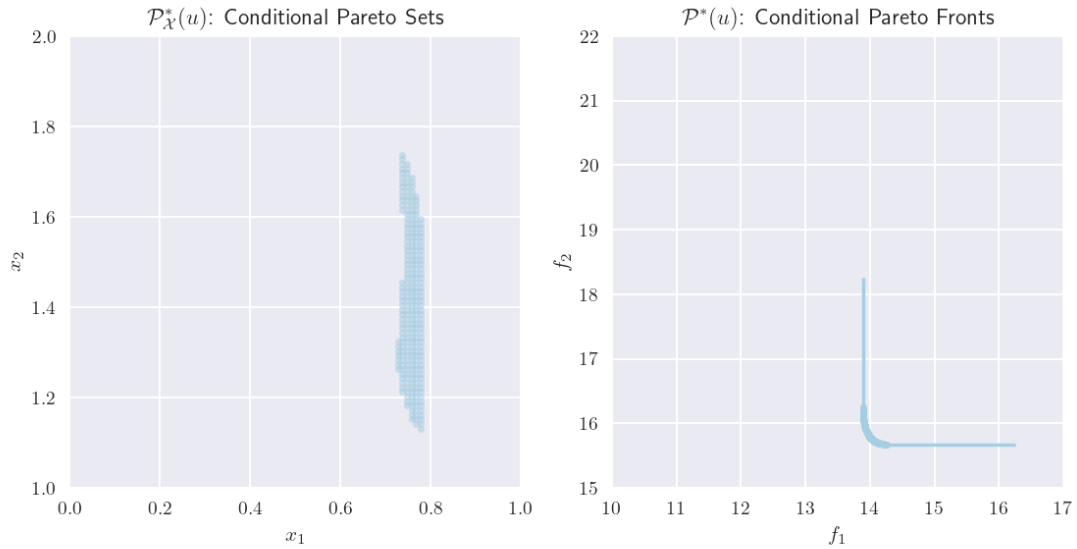

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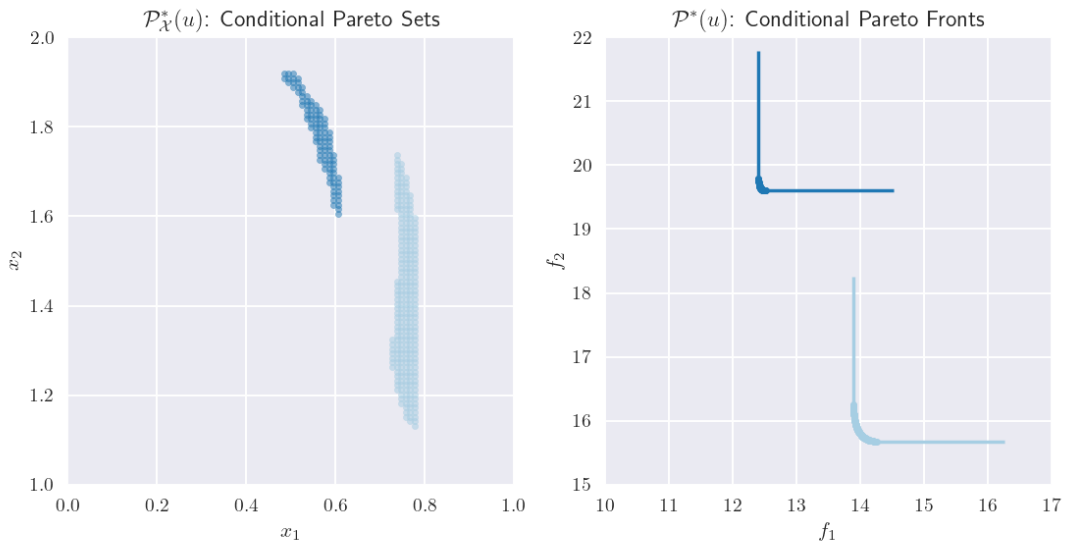

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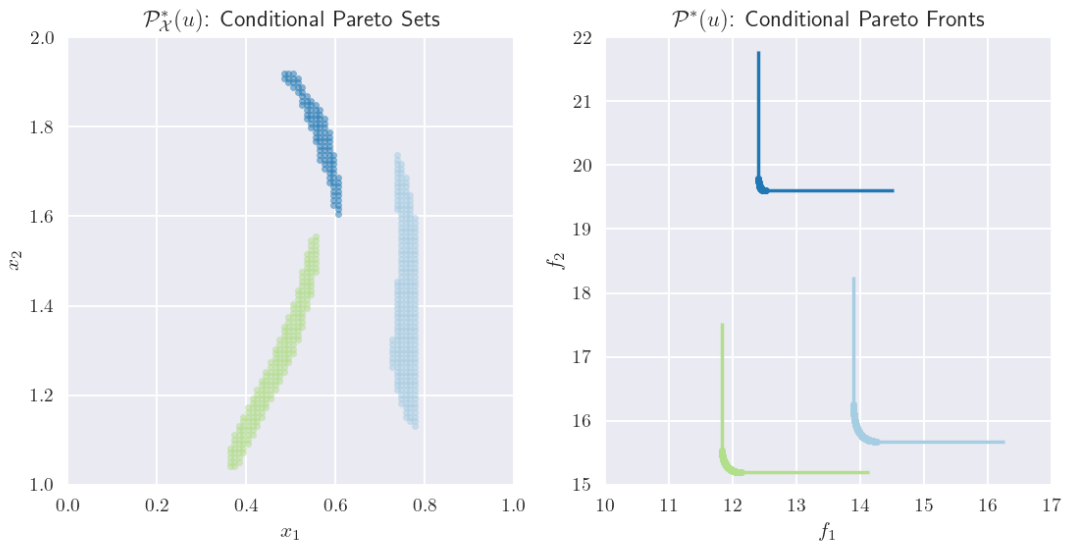

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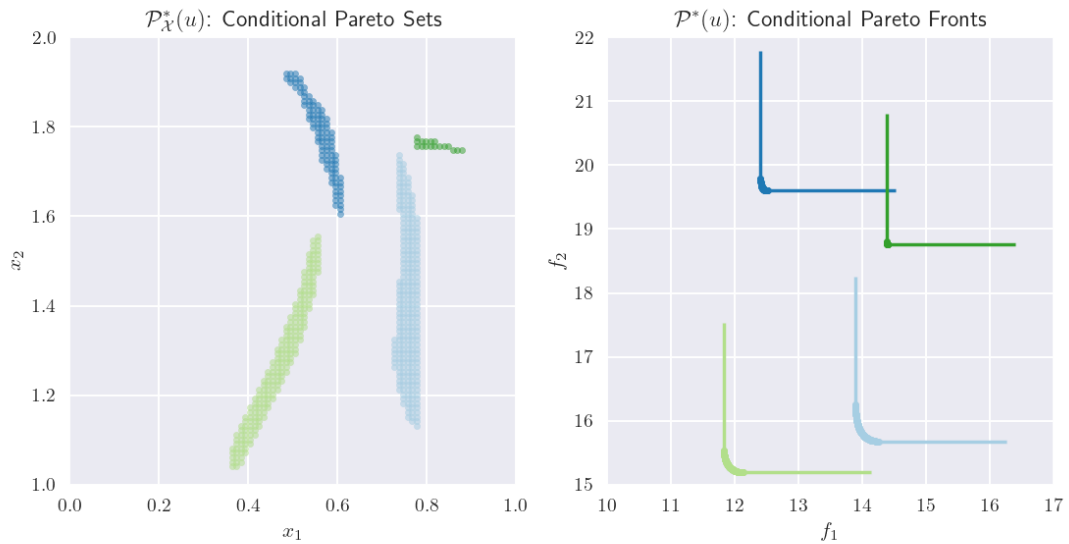

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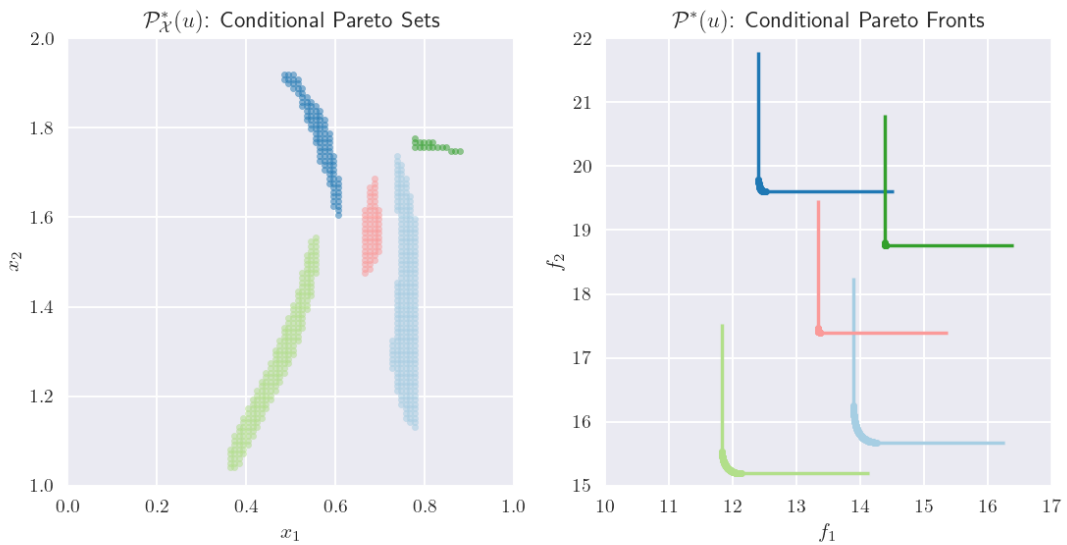

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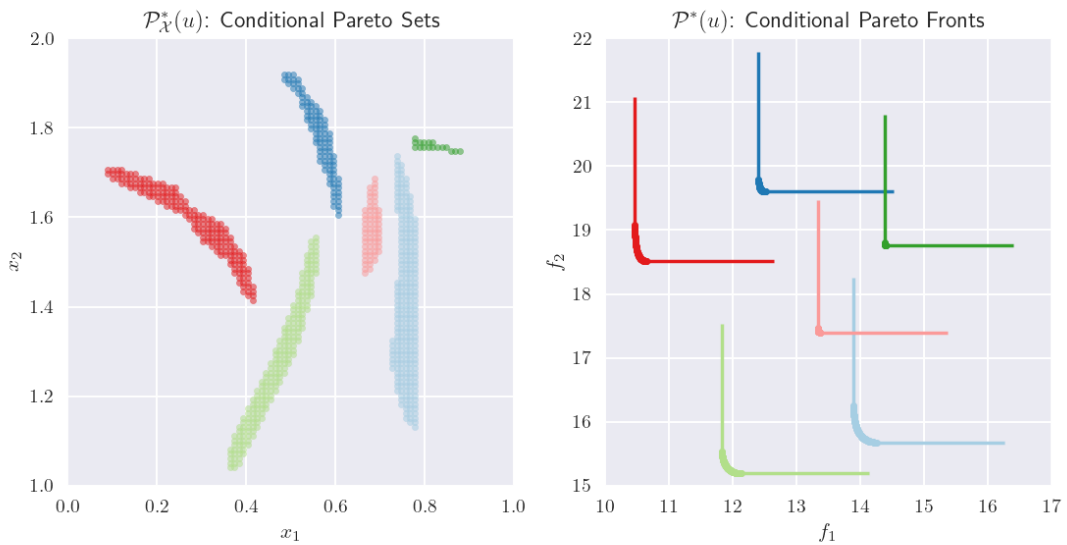

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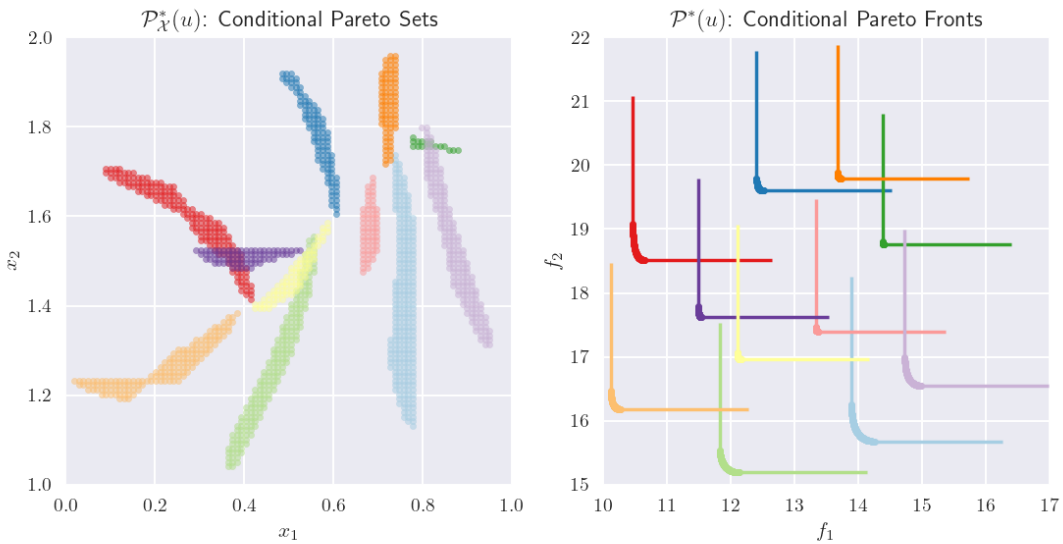

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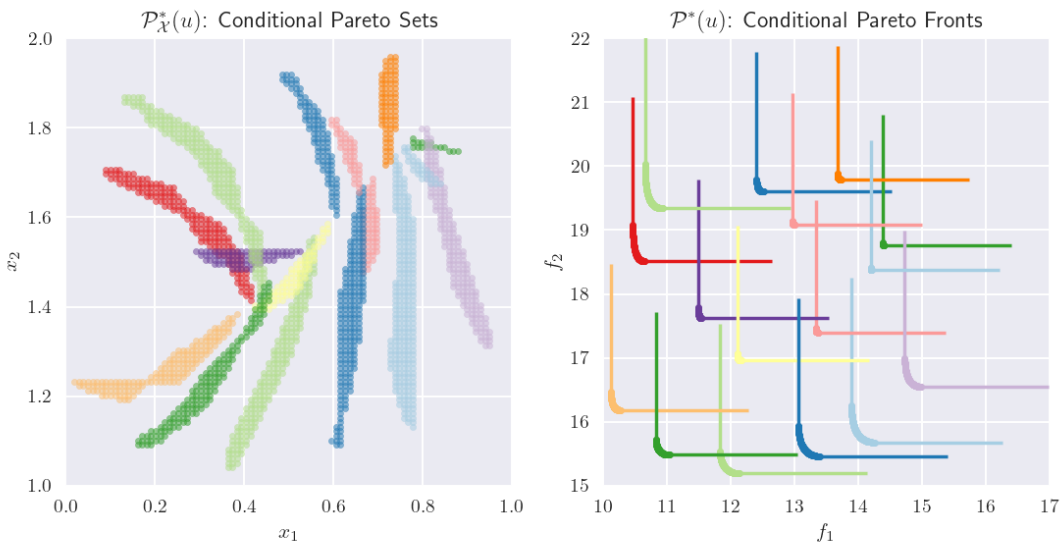

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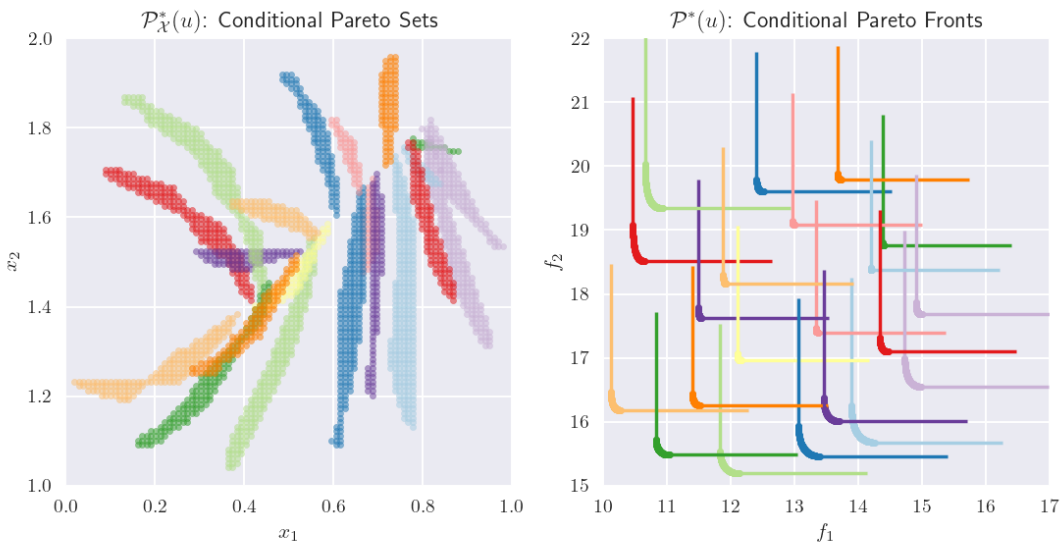
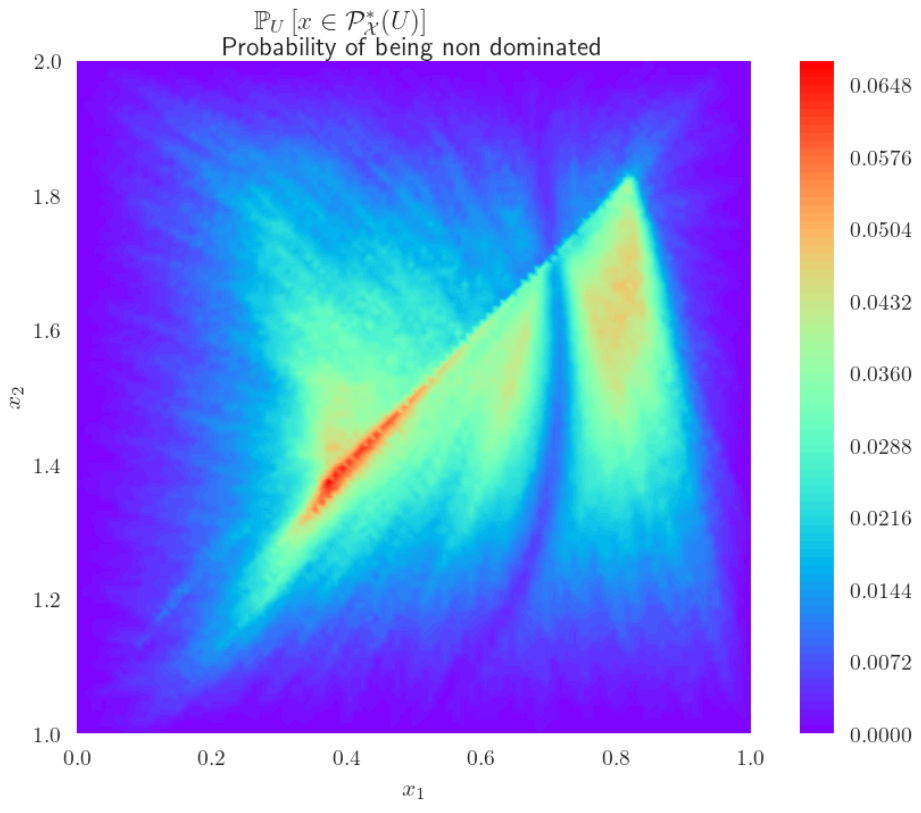


Probability of being non-dominated

$\rightarrow \mathbb{P}_U\left[x \in \mathcal{P}^*_{\mathcal{X}}(U)\right]$ the probability of being "Pareto-optimal"



- $\max \mathbb{P}_U\left[x \in \mathcal{P}^*_{\mathcal{X}}(U)\right]$
- Get subset of $\mathcal{X}$ which corresponds to the top k% of values

How to estimate $u \mapsto \mathcal{P}^*_{\mathcal{X}}(u)$?

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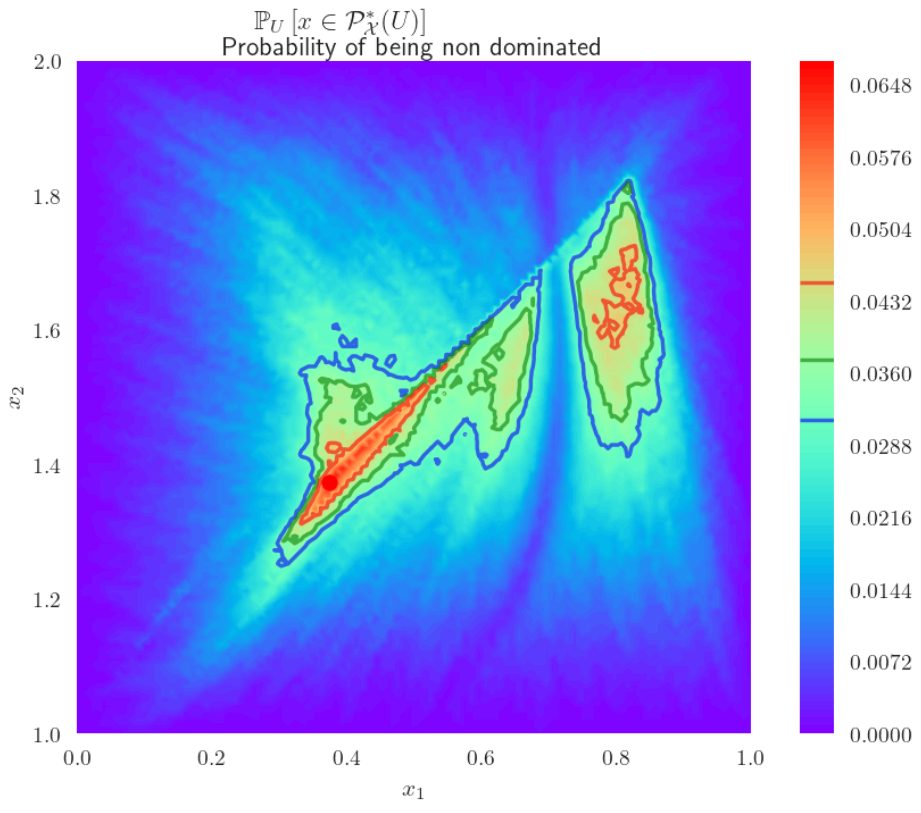

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How to estimate $u \mapsto \mathcal{P}^*_{\mathcal{X}}(u)$?

GP framework

$\mathsf{f}(x, u)$ is expensive to evaluate once, it is even worse when taking into account the random nature of $u \sim U$

We consider the joint input space $\mathcal{X} \times \mathcal{U}$:

$$\mathsf{F}(x, u) \sim \mathcal{N}(\mathsf{m}(x, u), \Sigma(x, u)) \tag{1}$$

Since F is a GP, it works well with linear operators, ie $\mathsf{Z}(x) = \mathbb{E}[\mathsf{F}(x, U)]$ still a GP !

Modify the EHVI for CPF estimation

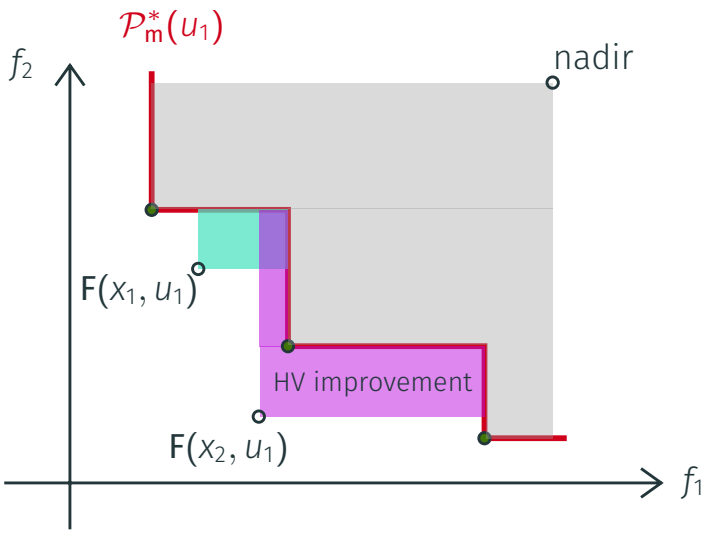
We want to estimate $u \mapsto \mathcal{P}^*(u), \mathcal{P}^*_{\mathcal{X}}(u)$ using the GP

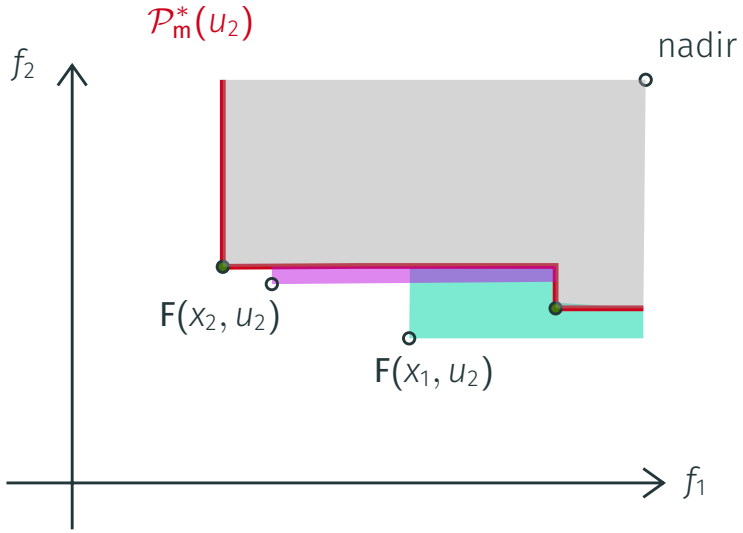
Profile-EHVI

Similar to the PEI defined in [GBC+14], acquisition defined on $\mathcal{X} \times \mathcal{U}$

$$\mathrm{PEHVI}(x, u) = \mathbb{E}_{\mathsf{F}}\left[\underbrace{\mathrm{HV}(\mathcal{P}^*_{\mathsf{m}}(u) \cup \mathsf{F}(x, u)) - \mathrm{HV}(\mathcal{P}^*_{\mathsf{m}}(u))}_{\text{HVI of } \mathcal{P}^*_{\mathsf{m}}(u)}\right]$$

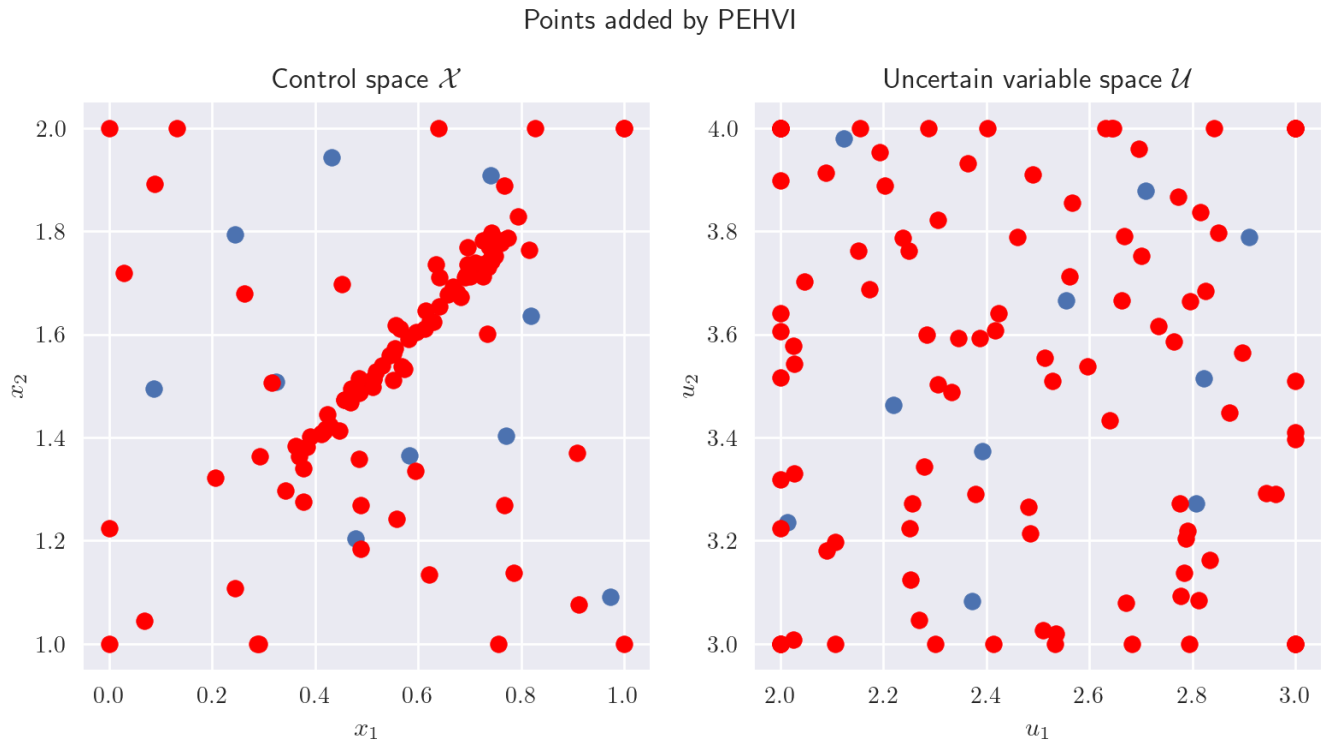
Estimation of $\mathcal{P}^*_{\mathsf{m}}(u)$ based on GP means





Design of Experiment using PEHVI

- PEHVI relies on a single optimization in the joint space $\mathcal{X} \times \mathcal{U}$
- This acquisition function leads to an intensification around the diagonal on $\mathcal{X}$, while exploring $\mathcal{U}$.
- Depending on the estimation of $\mathcal{P}^*_{\text{m}}(u)$, we can tend toward more exploration $\Rightarrow$ Better quality metrics



Use the metamodel to estimate $\mathbb{P}_U\left[x \in \mathcal{P}^*_{\mathcal{X}}(U)\right]$

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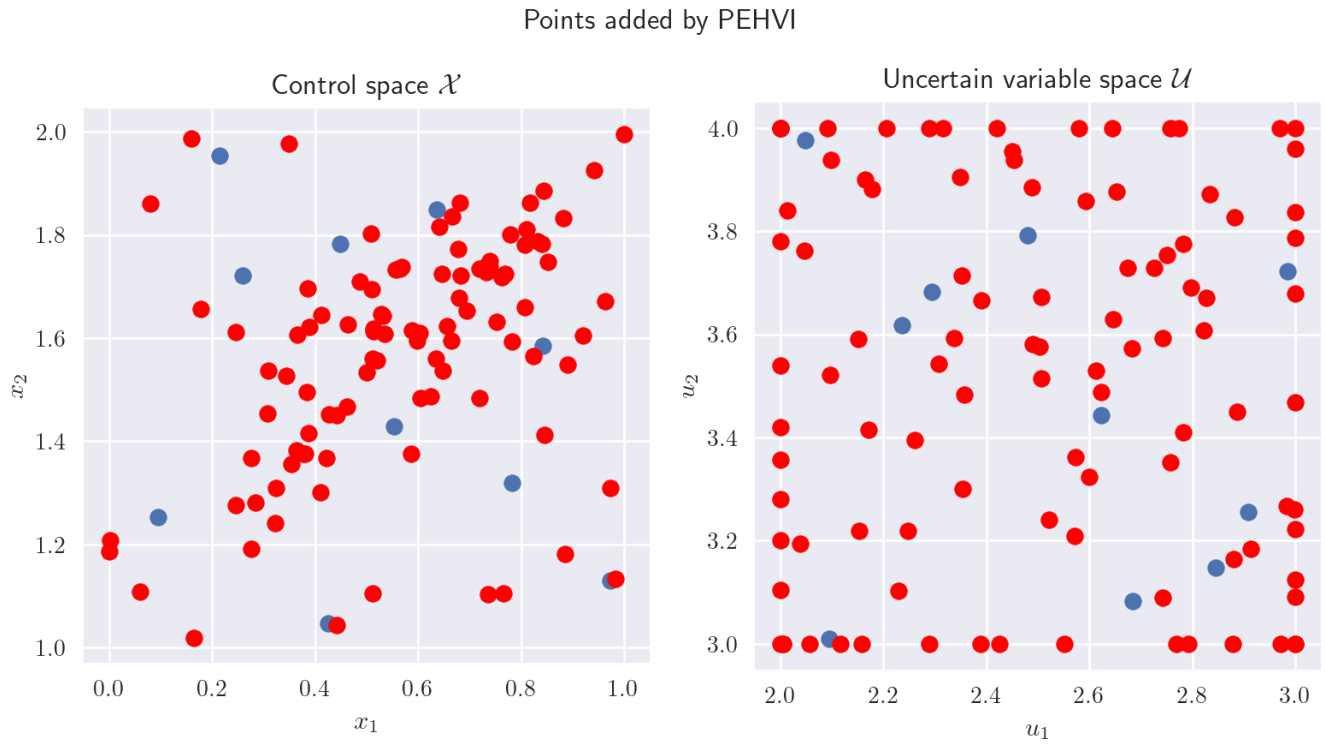

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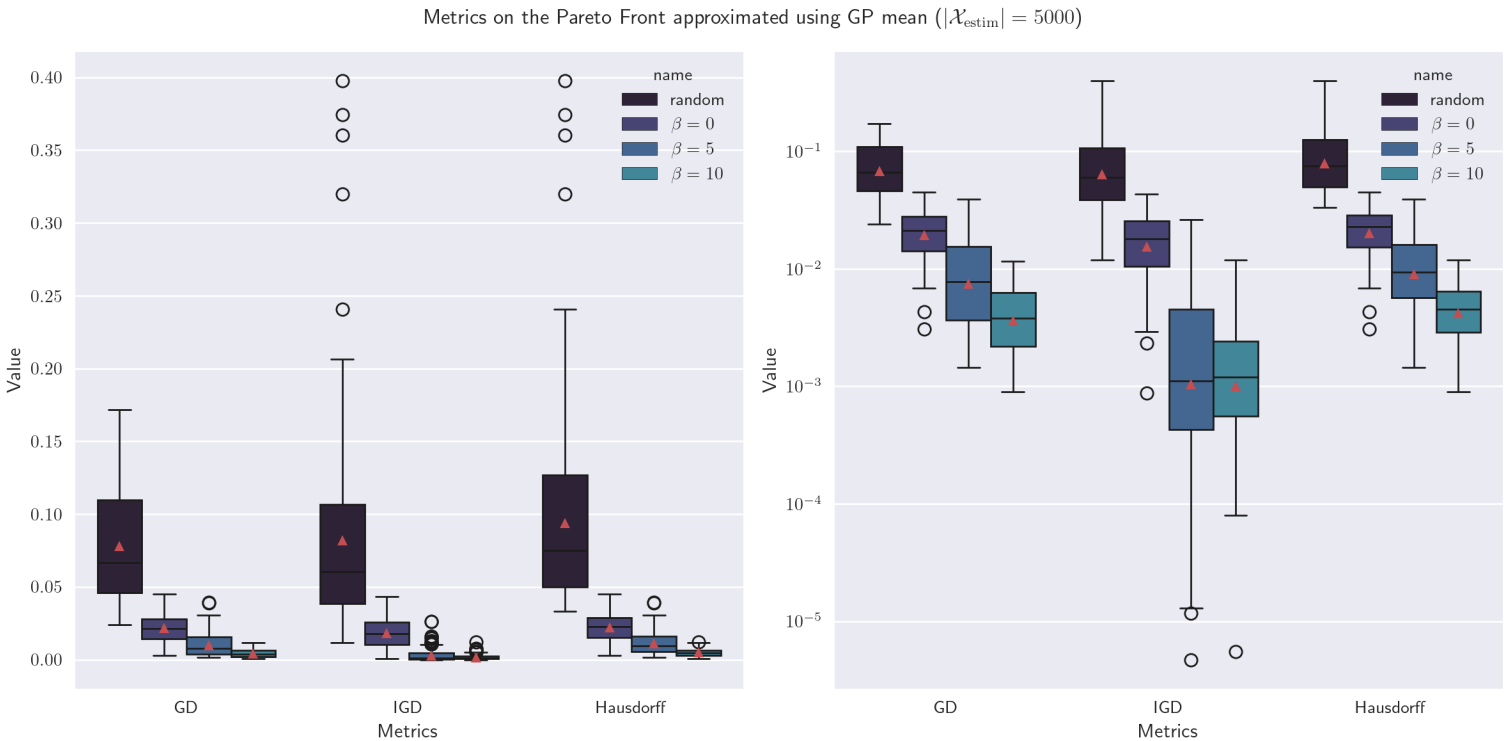

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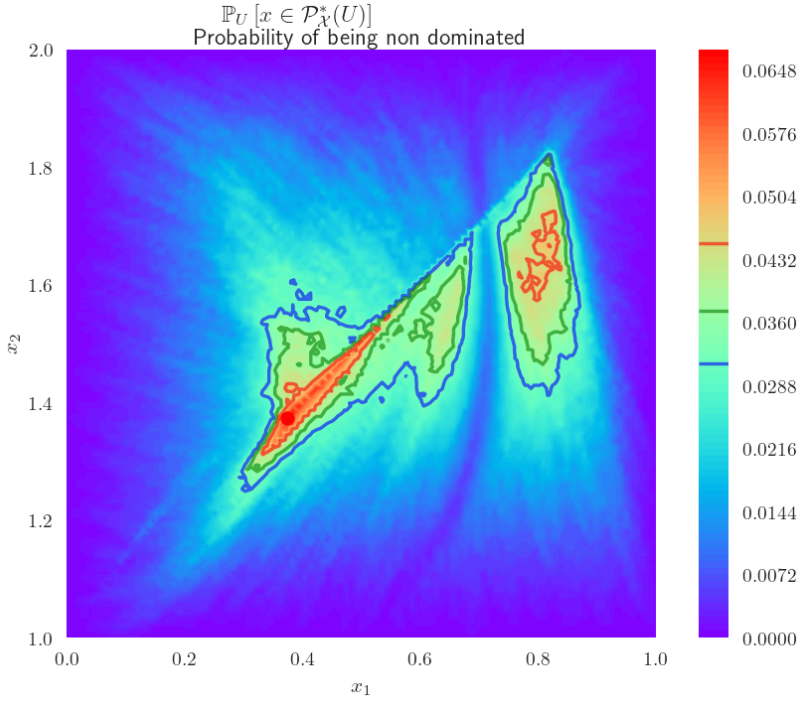
Limitations of CPF



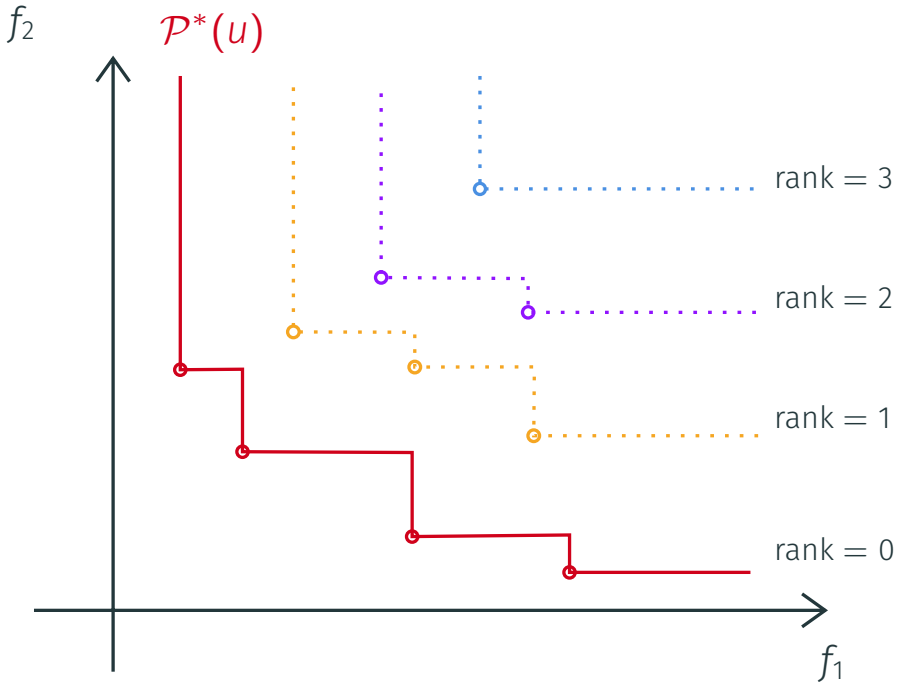
But

- No control on the probability of optimality: what if no x has a "high" probability of being optimal
- If $x \notin \mathcal{P}^*_{\mathcal{X}}(u)$, is it still a reasonable solution or not ?

How to quantify the proximity to the CPF, while keeping some notion of "incommensurability" (don't compare apples to oranges) ?

Non-dominated Sorting

Let $u \in \mathcal{U}$, let us say that we evaluated $\mathbf{f}(\mathfrak{X}, u)$. At the heart of NSGA-II ([DPAM02])



- $r(x, u) =$ rank of $\mathbf{f}(x, u)$ among $\mathbf{f}(\mathfrak{X} \cup \{x\}, u)$
- $r(x, u) = 0 \iff x \in \mathcal{P}^*_{\mathcal{X}}(u)$
- Look for points which have low $\mathbb{E}_U[r(x, U)]$?

Proximity indicator ρ

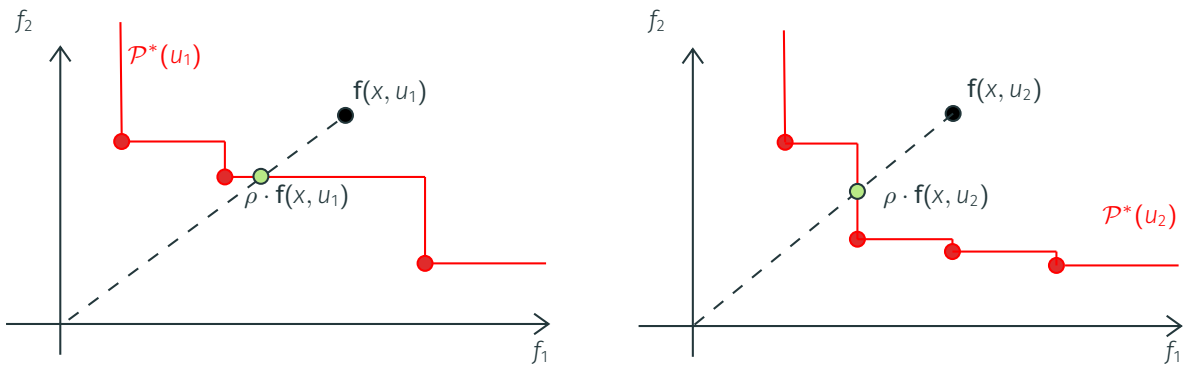
Let us assume that $\forall x, u$, $\mathbf{f}(x, u) > 0$, and that $\mathbf{0}$ is a "nice" ideal point

Definition of ρ

Let $x \in \mathcal{X}, u \in \mathcal{U}$

$$\text{largest } \rho \text{ such that } \rho \cdot \mathbf{f}(x, u) \preceq \mathcal{P}^*(u)$$

- $0 < \rho \leq 1$
- $\rho = 1$ means $\mathbf{f}(x, u)$ not dominated thus $x \in \mathcal{P}^*_{\mathcal{X}}(u)$
- Invariant to linear scaling of one or more objectives



We can define $(x, u) \mapsto \rho(x, u)$.

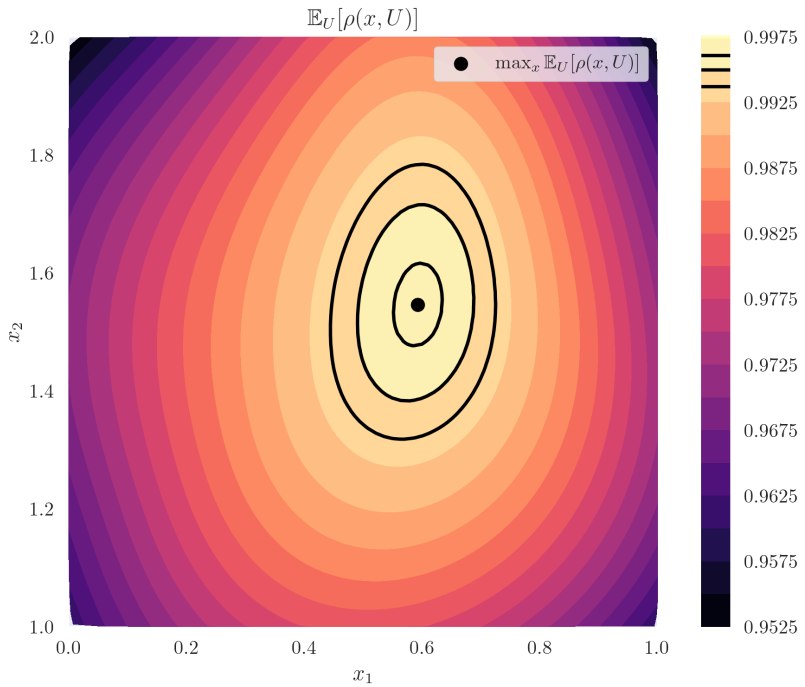
$\rightarrow$ Maximize average proximity ?

ρ-based designs

Definition of ρ

$$\rho(x, u) = \sup_{\rho} \{\rho \cdot \mathbf{f}(x, u) \preceq \mathcal{P}^*(u)\} = \ell(\mathbf{f}(x, u), \mathcal{P}^*(u))$$

We are interested in high values of $\mathbb{E}_U[\rho(x, U)]$



- $\max \mathbb{E}_U[\rho(x, U)]$
- get top k% of values

Estimation of ρ using GP

Definition of ρ

$$\rho(x,u) = \sup_{\rho} \{\rho \cdot \mathbf{f}(x,u) \preceq \mathcal{P}^*(u)\} = \ell(\mathbf{f}(x,u), \mathcal{P}^*(u))$$

ρ can not be modelled directly as a GP using $\mathbf{F}$.

Estimation of $\rho(x,u)$ using GP samples:

- Samples of the GP at $\underbrace{\mathbf{F}_\omega(x,u)}_{\text{for } \mathbf{f}(x,u)}, \underbrace{\mathbf{F}_\omega(\xi_1,u),\ldots,\mathbf{F}_\omega(\xi_N,u)}_{\text{for } \mathcal{P}^*_\omega(u)}$ to get $\rho_\omega(x,u)$

Estimation of $\mathbb{E}_U[\rho(x,U)]$ using GP samples and samples of U

- Using a finite set of samples $\{u^{(i)}\}_i$, we can approach $\mathbb{E}_U[\rho_\omega(x,U)]$ as $\hat{\rho}_\omega(x)$

$\Rightarrow$ using enough GP samples, and doing this (hopefully) in parallel, we can have a prediction + measure of uncertainty $\rightarrow$ Bayesian Optimization

Optimization of ρ ?

Definition of ρ

$$\rho(x,u) = \sup_{\rho} \{\rho \cdot \mathbf{f}(x,u) \preceq \mathcal{P}^*(u)\} = \ell(\mathbf{f}(x,u), \underbrace{\mathcal{P}^*(u)}_{\text{does not depend on } x})$$

Uncertainty on $U \neq$ Uncertainty ω from the GP

To optimize $\mathbb{E}_U[\rho(x,U)]$ using GP: we decouple choice of x and u

- Construct and optimize UCB acquisition function using GP samples, to get x_{target} (where we aim at reducing the uncertainty)
- ... but lookahead methods in the joint space on $\mathbb{V}\text{ar}_\omega[\mathbb{E}_U[\rho_\omega(x,U)]]$ is too expensive
- ... reducing uncertainty at x_{target} does not necessarily means evaluating at some $\mathbf{f}(x_{\text{target}}, \tilde{u})$

  $\rightarrow$ uncertainty might come from the estimation of $\mathcal{P}^*(u)$.

Comparison between MOOUU methods

$\mathbb{E}_U[\mathbf{f}(x, U)]$

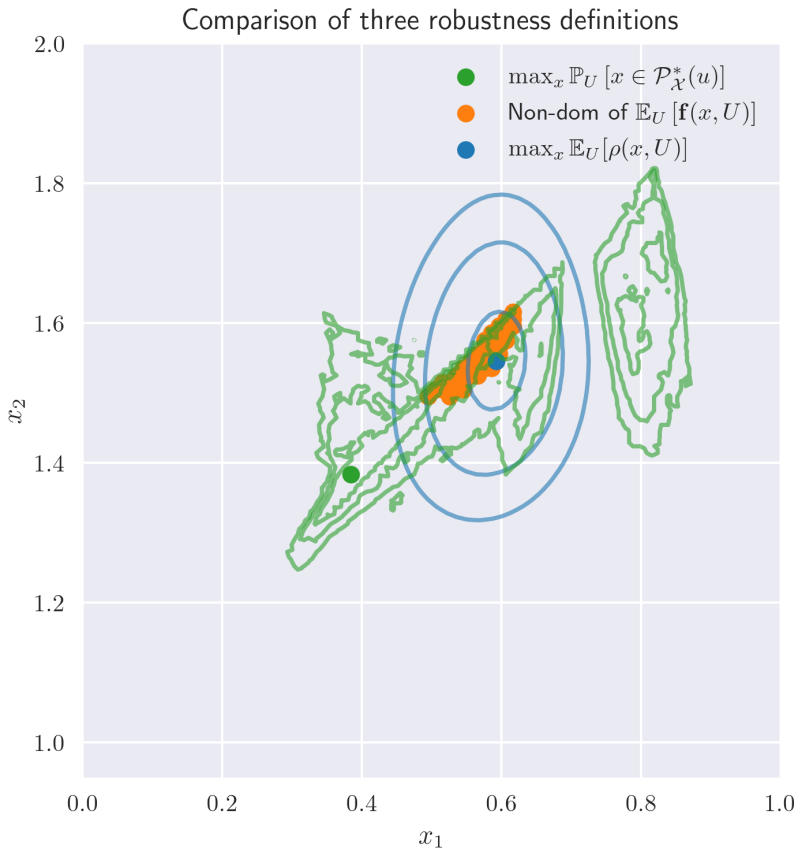
- Mean performances
- Ease of implementation
- Information on marginals, not on dependence

$\mathbb{P}_U[x \in \mathcal{P}^*_{\mathcal{X}}(u)]$

- Probability of being non-dominated
- PEHVI
- No control on performance outside of this optimality

$\mathbb{E}_U[\rho(x, U)]$ / Average NDS Rank

- Average "proximity" with $\mathcal{P}^*(u)$
- More expensive to estimate
- Tricky acquisition procedure



Wrapping-up/Take-Home messages

What does it mean to be robust in a MO setting ?

- What does it mean to be robust in my problem ?
- Comparing multivariate random variables is not trivial
- Conditional Pareto Front: Solve then Robustify strategy
- Profile-EHVI helps improve the estimation of $u \mapsto \mathcal{P}^*(u)$
- ρ is more challenging, and acquisition function is not easy to construct

What is next ?

- Continue numerical experiments
- Metrics to compare acquisitions functions
- Application to EnergyPlus

Three steps optimization

- Identify the x_{target} where we want to reduce the variance of the estimation (UCB)

$$x_{\text{target}} = \arg\max_{x \in \mathcal{X}} \hat{\rho}(x) + \beta \hat{v}(x)^{1/2}$$

- Identify the env. var. which brings the most uncertainty at x_{target}

$$u_{\text{target}} = \arg\max_{u \in \mathcal{U}} \mathbb{V}\text{ar}_{\omega} \left[\rho_{\omega}(x_{\text{target}}, u) \right]$$

  Find which MOO problem (dependent on u) carries the most uncertainty on the estimation of $\hat{\rho}(x_{\text{target}})$

- Minimize lookahead variance

$$x_{n+1} = \arg\min_{x \in \mathcal{X}} \mathbb{V}\text{ar}_{\omega} \left[\rho^{(n+1)}_{\omega,(x,u_{\text{target}})}(x_{\text{target}}, u_{\text{target}}) \right]$$

- Finally, the next point to evaluate is $(x_{n+1}, u_{n+1}) \leftarrow (x_{n+1}, u_{\text{target}})$

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