

BAYESIAN MULTI-OBJECTIVE OPTIMIZATION WITH CONSTRAINTS

APPLICATION TO THE DESIGN OF A COMMERCIAL AIRCRAFT ENVIRONMENT CONTROL SYSTEM

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TAKING INTO ACOUNT STOCHASTICS IN OPTIMIZATION PROBLEMS

PAUL FELIOT (IRT SYSTEMX), JULIEN BECT (L2S), EMMANUEL VAZQUEZ (L2S)









IRT SYSTEMX & SUPELEC

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Multi-objective optimization problem with constraints:

$$\left\{\begin{array}{ll} \mathsf{Minimize} & f(x) \\ \mathsf{Subject to} & x \in \mathbb{X} \quad \mathsf{and} \quad c(x) \leq \mathsf{0} \end{array}\right.$$

with

 $\begin{array}{lll} o & \mathbb{X} \subset \mathbb{R}^d & \to & \text{search space} \\ o & f = (f_j)_{1 \leq j \leq p} & \to & \text{vector of objective functions to be minimized} \\ o & c = (c_i)_{1 \leq i \leq q} & \to & \text{vector of constraint functions} \end{array}$

Sequentially approximate the set of feasible and non-dominated solutions:

 $\Gamma = \{x \in \mathbb{X} : c(x) \leq 0 \text{ and } \nexists x' \in \mathbb{X} \text{ such that } c(x') \leq 0 \text{ and } f(x') \prec f(x)\}$

Assumptions:

- Both f and c are smooth, nonlinear, expensive-to-evaluate functions (black-box)
- The available simulation budget is very limited (\approx 10*d*)



Positioning:

- We adopt a Bayesian approach to this optimization problem.
- We focus on highly constrained problems. Tipically it is assumed that no feasible observation is available at the start of the optimization procedure.

Main contributions:

- Proposal of an Expected Improvement (EI) criterion for the constrained multi-objective optimization problem.
- Study on the use of Sequential Monte Carlo techniques for the optimization of improvement based sampling criteria.
- Implementation of the associated algorithm, which we call BMOO.



Associated publications:

- P. Feliot, J. Bect, and E. Vazquez. A bayesian approach to constrained single- and multi-objective optimization. Journal of Global Optimization, 2016.
- P. Feliot, Y. Le Guennec, J. Bect, and E. Vazquez. Design of a commercial aircraft environment control system using Bayesian optimization techniques. ENGOPT, 2016 (to appear).



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Expected Hypervolume Improvement (EHVI) criterion Extending the EHVI to handle constraints Criterion calculation and optimization Structure of the algorithm Illustration



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We first consider the multi-objective optimization problem without constraints.

Expected Hypervolume Improvement (EHVI) sampling criterion:

• Given evaluation results $(f(X_1), \ldots, f(X_n))$, with $f(X_l) = (f_1(X_l), \ldots, f_p(X_l)), 1 \le i \le n$, define:

$$\begin{cases} \mathbb{B} &= \{y \in \mathbb{R}^p; \ y \le y^{\mathsf{upp}}\}, y^{\mathsf{upp}} \in \mathbb{R}^r \\ H &= \{y \in \mathbb{B}; \exists x \in \mathbb{X}, f(x) \prec y\} \\ H_n &= \{y \in \mathbb{B}; \exists i \le n, f(X_i) \prec y\} \end{cases}$$

Loss function:

$$arepsilon_n(\underline{X},f) = |H \setminus H_n| \; ,$$

Hypervolume improvement:

$$I_n(X_{n-1}) = \varepsilon_n(\underline{X}, f) - \varepsilon_{n+1}(\underline{X}, f)$$

= $|H_{n+1}| - |H_n|$

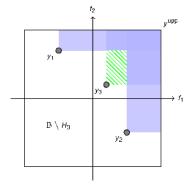


Figure: Hypervolume improvement yielded by the observation of y_3



Expected Hypervolume Improvement (EHVI) sampling criterion:

- Assume a vector-valued Gaussian random process model ξ = (ξ₁,..., ξ_ρ) of f = (f₁,..., f_ρ)
- The EHVI^a comes from taking the expectation of the improvement with respect to the posterior probability of ξ:

$$\begin{aligned} \mathsf{EI}_n(x) &= & \mathbb{E}_n \left(|H_{n+1}| - |H_n| \right) \\ &= & \mathbb{E}_n \left(\int_{\mathbb{D} \setminus H_n} \mathbb{1}_{\xi(x) \prec y} \, \mathrm{d}y \right) \\ &= & \int_{\mathbb{B} \setminus H_n} \mathbb{P}_n \left(\xi(x) \prec y \right) \, \mathrm{d}y \end{aligned}$$

◆ The next sample is chosen as X_{n+1} = argmax El_n(x), which requires solving an auxiliary optimization problem at each iteration.



• We now consider the multi-objective problem with constraints.

Constraint handling in the literature:^b

- Emmerich [2005] and Couckuyt et al. [2014] propose to multiply the EHVI by $\mathbb{P}_n(\xi_c(x) \leq 0)$
 - This corresponds to $I_n = (|H_{n+1}| |H_n|) \|_{c(x) \le 0}$ under the independence assumption.
 - The progress on constraint resolution is not measured.
- Gramacy et al. [2015] recently proposed to use the Augmented Lagrangian approach.
- Our proposal is to extend the Pareto domination rule to handle the constraints.

^b<u>References:</u> See e.g. Conn et al. [1991], Sasena [2002], Parr et al. [2012], Gelbart [2015]



Extended domination rule definition:

- Denote $\mathbb{Y}_{o} = \mathbb{R}^{p}$, the objective space and $\mathbb{Y}_{c} = \mathbb{R}^{q}$ the constraint space, and let $\mathbb{Y} = \mathbb{Y}_{o} \times \mathbb{Y}_{c}$.
- We shall say that $y_1 \in \mathbb{Y}$ dominates $y_2 \in \mathbb{Y}$, which will be written as $y_1 \triangleleft y_2$, if $\psi(y_1) \prec \psi(y_2)$, where \prec is the usual Pareto domination rule.

- Properties of the extended domination rule:
 - Feasible solutions are compared wrt their objectives values.
 - Non-feasible solutions are compared wrt their component wise constraint violations.
 - Feasible solutions always dominate non-feasible ones.

 $^{\circ}$ <u>References:</u> Ray et al. [2001], Fonseca and Fleming [1998], Oyama et al. [2007]



Similarly to the EHVI derivation, we can define the following sets.

 $\begin{cases} \mathbb{B} &= \mathbb{B}_{o} \times \mathbb{B}_{c}, \text{ where } \mathbb{B}_{o} \subset \mathbb{Y}_{o} \text{ and } \mathbb{B}_{c} \subset \mathbb{Y}_{c} \text{ are bounded hyper-rectangles} \\ H &= \{y \in \mathbb{B}; \exists x \in \mathbb{X} (f(x), c(x)) \lhd y\} \\ H_{o} &= \{y \in \mathbb{B}; \exists i \leq n (f(X_{i}), c(X_{i})) \lhd y\} \end{cases}$

Expected hypervolume improvement criterion with constraints:

$$\begin{split} \mathsf{E}\mathsf{I}_n(x) &= & \mathbb{E}_n\left(|H_{n-1}| - |H_n|\right) \\ &= & \mathbb{E}_n\left(\int_{\mathbb{R}\setminus H_n} \mathbf{1}_{\xi(x) < y} \, \mathrm{d}y\right) \\ &= & \int_{\mathbb{R}\setminus H_n} \mathbb{P}_n\left(\xi(x) \lhd y\right) \, \mathrm{d}y, \end{split}$$

• where $\xi = (\xi_o, \xi_c)$, with $\xi_o = (\xi_{o,1}, \ldots, \xi_{o,\rho})$ and $\xi_c = (\xi_{c,1}, \ldots, \xi_{c,q})$.



Criterion calculation:

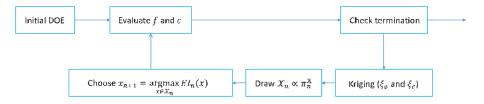
- The criterion takes the form of a multi-dimensional integral for which no closed form solution exists.
- The BMOO algorithm implements a Monte Carlo approximation of the integral using sequential Monte Carlo techniques.

Criterion optimization:

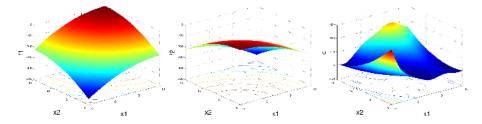
- The criterion optimization is performed using sequential Monte Carlo techniques as well.
- At time *n*, the next sample is chosen out of a population X_n of particles distributed according to a density of interest π_n^K.

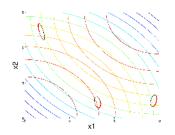


Structure of the algorithm:

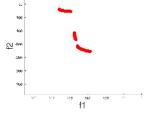




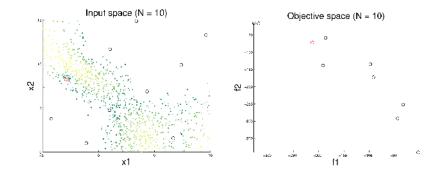




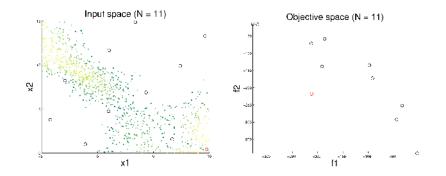




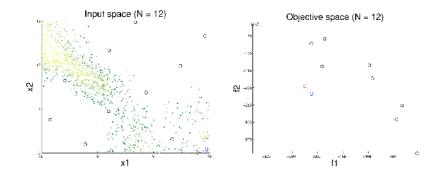




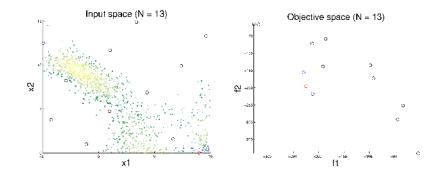




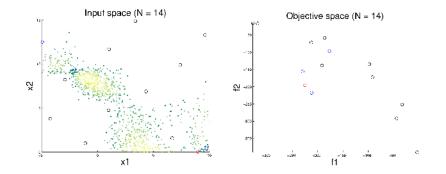




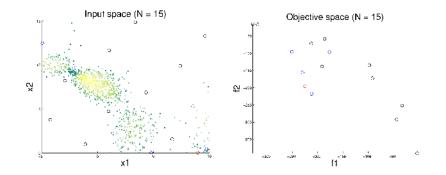




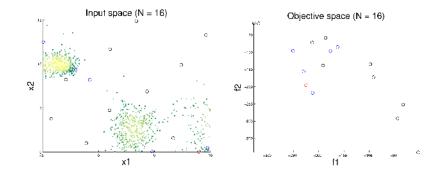




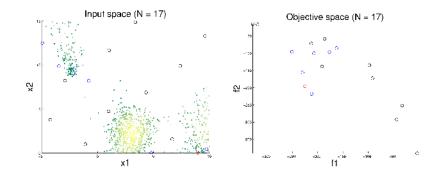




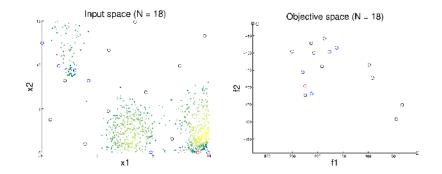




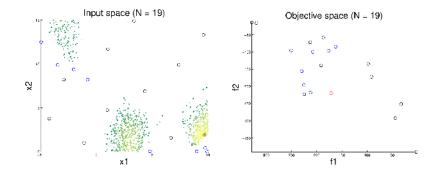




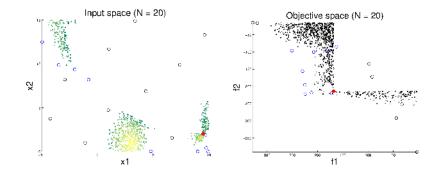




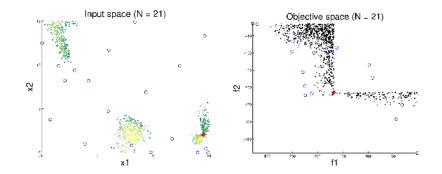




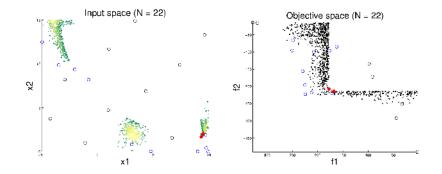




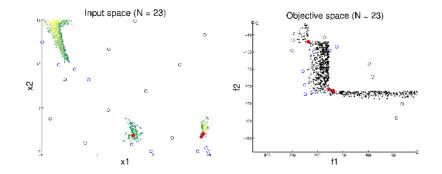




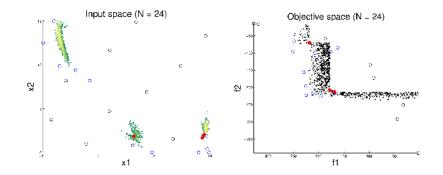




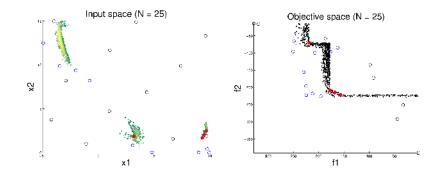




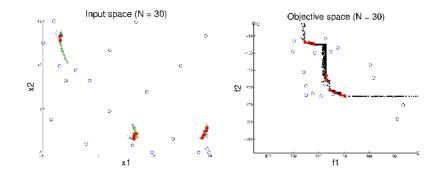




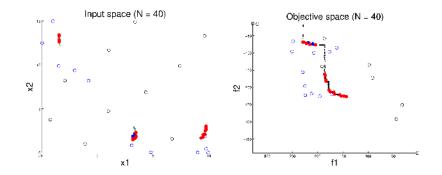




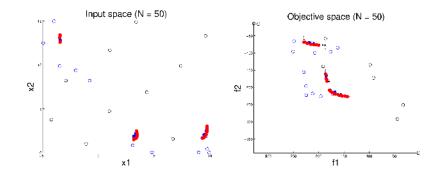












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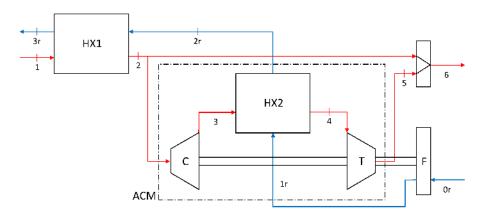
Presentation of the problem One dimensional model of the system Formulation of an optimization problem

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Architecture of the ECS:





Sizing scenario:

Aircraft-on-ground, full of passengers, with 50°C outside.

 $\mathcal{P}_{HT} = \mathcal{P}_{out} + \mathcal{P}_{eq} + N_{pax}\mathcal{P}_{pax} + N_{crew}\mathcal{P}_{crew}$

• Keep the cabin temperature at $T_c = 24^{\circ}$ C.

$$\mathcal{P}_{HT} \leq \dot{m}c_p \left(T_c - T_5\right)$$

Keep the cabin pressure close to the atmospheric pressure.

$$P_{min} \leq P_5 \leq P_{max}$$

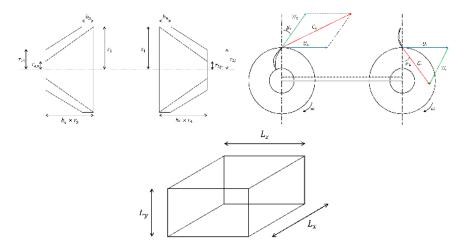
• The air injected into the cabin must lie between $T_{min} = 15^{\circ}$ C and $T_{max} = 25^{\circ}$ C.

Objectives:

- Minimize the mass of the system.
- Minimize its entropy generation rate.



Parametrization:



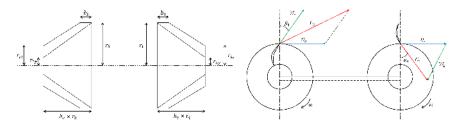
18 variables: m, m_r, r₃, r_{2p}, r_{2t}, b₃, β₃, r₄, r_{5p}, r_{5t}, b₄, α₄, L_{x1}, L_{y1}, L_{z1}, L_{x2}, L_{y2}, L_{z2}.



• The system is ruled by a non-linear system of 13 equations with 13 unknowns: T_{t2} , T_{t3} , T_{t4} , T_{t5} , T_{t2r} , T_{t3r} , P_{t2} , P_{t3} , P_{t4} , P_{t5} , P_{t2r} , P_{t3r} and ω .

ĺ	$\dot{m}c_p(T_{l1}-T_{l2})$		$\dot{m}_r c_p (T_{i3r} - T_{i2r})$
	$\dot{m}c_p(T_{t3}-T_{t4})$	=	$\dot{m}_r c_p (T_{t2r} - T_{t1r})$
	$c_p(T_{t1}-T_{t2})$	=	$\epsilon_1 c_p (T_{t1} - T_{t2r})$
	$c_p(T_{t3}-T_{t4})$	—	$\epsilon_2 c_p (T_{t3} - T_{t1r})$
	$P_{l2} - P_{l1}$	=	ΔP_{HX}
	$P_{t4} - P_{t3}$	=	ΔP_{HX}
	P _{r3}		$P_{t2}\left(1+\eta_{c}\frac{T_{t3}-T_{t2}}{T_{t2}}\right)^{\frac{\gamma}{\gamma-1}}$
	P _{t5}	=	$P_{t4}\left(1+\tfrac{1}{\eta_{7}}\tfrac{T_{t5}-T_{t4}}{T_{t4}}\right)^{\frac{\gamma}{\gamma-1}}$
	Ŵc	=	$\dot{m}\left(r_{3}^{2}\omega^{2}-\frac{\dot{m}\tan(\beta_{3})}{2\pi\rho b_{3}}\omega\right)$
	Ŵτ	—	$-rac{\dot{m}^2 \tan(lpha_2)}{2\pi ho b_4}\omega$
	$\dot{W}_{C}+\dot{W}_{T}+rac{1}{\eta_{F}}rac{\dot{m}_{t}^{3}}{2 ho^{2}A_{r}^{2}}$	=	0
	Ŵ _c	=	$\eta_{G}\dot{m}c_{P}(T_{t3}-T_{t2})$
	Ŵŗ		$rac{1}{\eta_T}\dot{m}c_p(T_{t5}-T_{t4})$





Design constraints:



Simulation constraints:



Summary:

- 18 variables: m, m, r₃, r_{2p}, r_{2t}, b₃, β₃, r₄, r_{5p}, r_{5t}, b₄, α₄, L_{x1}, L_{y1}, L_{z1}, L_{x2}, L_{y2}, L_{z2}.
- Bound constraints on the variables.
- 9 design constraints: d₁₋₉.
- 15 simulation constraints: c_{1-15} .
- 2 objectives: \mathcal{M} and $\dot{\mathcal{S}}$.

Remarks:

- The design space is not hypercubic.
- Possibility of simulation failures (hidden constraints).

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Hidden constraints management:

- There are two cases where the model fails to produce a result:
 - The system can not be inverted.
 - The air flowrate becomes supersonic.
- This is taken into account in BMOO by multiplying the Expected improvement by a probability of observability^d.
 - A nearest-neighbour classifier is built on the observed/non-observed data to this end.
- The sampling density $\pi_0^{\mathbb{X}}$ is also multiplied by the probability of observability.



Initial DoE:

Denote D the domain delimited by the bound constraints and define:

$$\mathbb{X} = \mathbb{D} \setminus \{x \in \mathbb{D}; d(x) > 0\}$$

- If |X|/|D| is not too small, a pseudo-maximin design on X can be achieved using the following process.
 - Sample a large population uniformly on D.
 - Discard particles falling out of X.
 - Prune the remaining particles to augment the maximin distance until the required number of particles remain.

During the optimization:

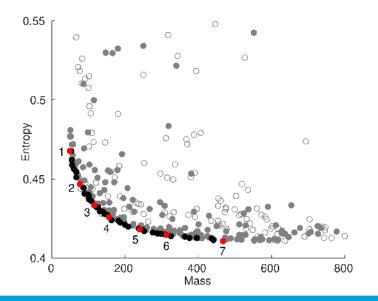
The sampling density π^X_n is multiplied by 1_K.



A few statistics:

- Initial DoE:
 - N_{init} = 90 samples.
 - 44 simulation failures.
 - No feasible observation
- Optimization process:
 - N_{max} = 500 samples.
 - 92 additional simulation failures.
 - First feasible point found after 25 iterations.





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					4 - Optimization results		
	1	2	3	4	5	6	7
<i>ṁ</i>	2.95	2.92	2.94	2.94	2.94	2.95	2.94
m _r	7.74	6.86	5.63	5.06	4.64	4.40	4.27
r ₂₀	0.07	0.05	0.05	0.03	0.03	0.07	0.04
r_{2t}	0.10	0.08	0.08	0.08	0.06	0.09	0.10
r 3	0.10	0.11	0.10	0.10	0.12	0.12	0.13
b_3	0.01	0.01	0.05	0.05	0.04	0.02	0.03
β_3	0.36	0.74	0.97	-0.16	0.61	0.94	0.48
r ₅₀	0.03	0.03	0.03	0.03	0.03	0.03	0.03
r _{5t}	0.05	0.05	0.05	0.05	0.05	0.05	0.05
r 4	0.10	0.10	0.11	0.12	0.11	0.10	0.11
b_4	0.02	0.02	0.04	0.02	0.04	0.03	0.03
α_4	1.04	0.50	0.89	1.01	0.44	0.79	0.30
L_{x1}	0.67	0.65	0.68	0.68	0.63	0.69	0.70
L_{y1}	0.65	0.68	0.61	0.67	0.67	0.66	0.65
L_{z1}	0.03	0.04	0.07	0.12	0.17	0.20	0.32
L_{x2}	0.66	0.69	0.66	0.66	0.70	0.68	0.69
Ly2	0.69	0.53	0.68	0.65	0.65	0.68	0.65
L_{z2}	0.03	0.06	0.09	0.10	0.17	0.25	0.36

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- BMOO: A Bayesian optimization algorithm for single- and multi-objective optimization.
 - Designed to address highly constrained problems.
 - Based on a generalized EHVI criterion defined using an extended domination rule.
 - SMC techniques for the criterion calculation and optimization.
 - Hidden constraints handling capability.
 - Non-hypercubic design spaces handling capability.
- The algorithm is applied to the design of a commercial aircraft environment control system with promising results.
- Directions for future work on this application case.
 - Taking into account uncertainties on key parameters of the simulation.
 - · Sensitivity analysis on non-hypercubic design spaces.
 - Sensitivity analysis in constrained multi-objective optimization.



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Adaptive procedure to set \mathbb{B}_c and \mathbb{B}_o :

Assume that *n* evaluation results ξ(X_i), 1 ≤ i ≤ n, are available. Then, we define the corners of B_o by

$$\left(\begin{array}{cc} y_{\mathbf{o},l,n}^{\mathsf{low}} &=& \min\left(\min_{i\leq n}\xi_{\mathbf{o},l}(X_{l}),\ \min_{x\in\mathcal{X}_{n}}\hat{\xi}_{\mathbf{o},l,n}(x) - \lambda_{\mathbf{o}}\sigma_{\mathbf{o},l,n}(x)\right), \\ y_{\mathbf{o},l,n}^{\mathsf{upo}} &=& \max\left(\max_{i\leq n}\xi_{\mathbf{o},i}(X_{i}),\ \max_{x\in\mathcal{X}_{n}}\hat{\xi}_{\mathbf{o},i,n}(x) + \lambda_{\mathbf{o}}\sigma_{\mathbf{o},i,n}(x)\right). \end{array} \right)$$

for $1 \leq i \leq p$, and the corners of \mathbb{B}_{e} by

$$\begin{cases} y_{c,j,n}^{\text{low}} &= \min\left(0, \min_{l \leq n} \xi_{c,j}(X_l), \min_{x \in \mathcal{X}_n} \hat{\xi}_{c,j,n}(x) - \lambda_c \sigma_{c,j,n}(x)\right), \\ y_{c,j,n}^{\text{upp}} &= \max\left(0, \max_{l \leq n} \xi_{c,j}(X_l), \max_{x \in \mathcal{X}_n} \hat{\xi}_{c,j,n}(x) + \lambda_c \sigma_{c,j,n}(x)\right), \end{cases}$$

for $1 \le j \le q$, where λ_0 and λ_c are positive numbers.



7 - L_2^{opt} density for EHVI calculation

L_2^{opt} density for EHVI calculation:

Let (x_k)_{1≤k≤mg} be a population of candidates on which we want to compute the EHVI value, using a population of particles (y_i)_{1≤i<mg} distributed according to some density π.

$$\hat{l}_k^{\pi} = rac{1}{m_{\mathbb{Y}}}\sum_{i=1}^{m_{\mathbb{Y}}}rac{\mathbb{P}_{\sigma}(\xi(x_k)\prec y_i)}{\pi(y_i)}$$

We want to achieve a good approximation for all particles (x_k)_{1≤k≤m_x}. Using the L₂ norm, we get the following:

$$\mathbb{E}\left(\left\|\hat{l}^{\pi}-l\right\|_{2}^{2}\right) = \mathbb{E}\left(\sum_{k=1}^{m_{2}}(\hat{l}_{k}^{\pi}-l_{k})^{2}\right)$$
$$= \frac{1}{m_{\mathbb{Y}}}\sum_{k=1}^{m_{2}}\left(\int\frac{\mathbb{E}_{n}(\xi(x_{k})\prec y)^{2}}{\pi(y)^{2}}\pi(y)\mathrm{d}y-l_{k}^{2}\right)$$

$$ightarrow L_2^{opt}(y) \propto \sqrt{\sum_{k=1}^{m_{\infty}} \mathbb{P}_n(\xi(x_k) \prec y)^2}$$



7 - A DENSITY FOR HEAVILY CONSTRAINED PROBLEMS

A density for problems with a lot of constraints:

- Suppose q = d, $X = [-1/2, 1/2]^q$ and $c_j : x = (x_1 \dots, x_q) \mapsto |x_j| \frac{\epsilon}{2}, \epsilon \in (0, 1].$
- ◆ Thus, the feasible domain is C = [-ε/2, ε/2]^q and the volume of the subset of X where exactly k constraints are satisfied is

$$V_k pprox \left(rac{q}{k}
ight) \, arepsilon^k \, \left(1 - arepsilon
ight)^{q-k}$$

Assume moreover that the Gaussian process models are almost perfect, i.e.,

$$\mathbb{P}_n\left(\xi_{c,l}(x) \le 0\right) \approx \begin{cases} 1, & \text{if } c_l(x) \le 0, \\ 0, & \text{otherwise,} \end{cases}$$
(1)

- Further assume n = 1 with X₁ = (¹/₂,..., ¹/₂) so that the probability of improvement P_n (ξ(x) ∈ G₁) is close to one everywhere on X.
- The expected number of particles satisfying exactly k constraints is m V_k
- If q is large, the particles thus tend to concentrate in regions where $k \approx q\varepsilon$.
- To compensate for the decrease of V_k, we suggest using the following modified sampling density:

$$\pi_n^{\mathbb{X}} \propto \mathbb{E}_n\left(K(x)! \ \mathbb{1}_{\xi(x)\in G_n}\right),$$

where K(x) is the number of constraints satisfied by ξ at x.



7 - INTERMEDIATE SUBSETS

Parametric construction of intermediate subsets:

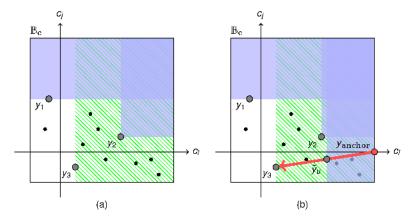


Figure: Procedure to construct intermediate subsets before the observation of a feasible solution.



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Parametric construction of intermediate subsets:

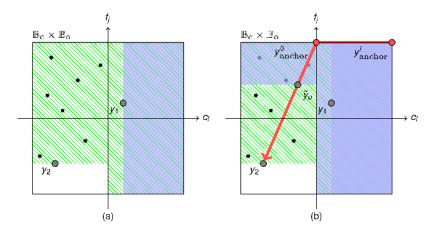


Figure: Procedure to construct intermediate subsets after the observation of a feasible solution.