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Bayesian Quality-Diversity approaches for constrained optimization problems with mixed variables

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Joint work with L. Baraton (Ph.D. thesis, ONERA/ISAE-SupAéro), N. Piatte (intership)

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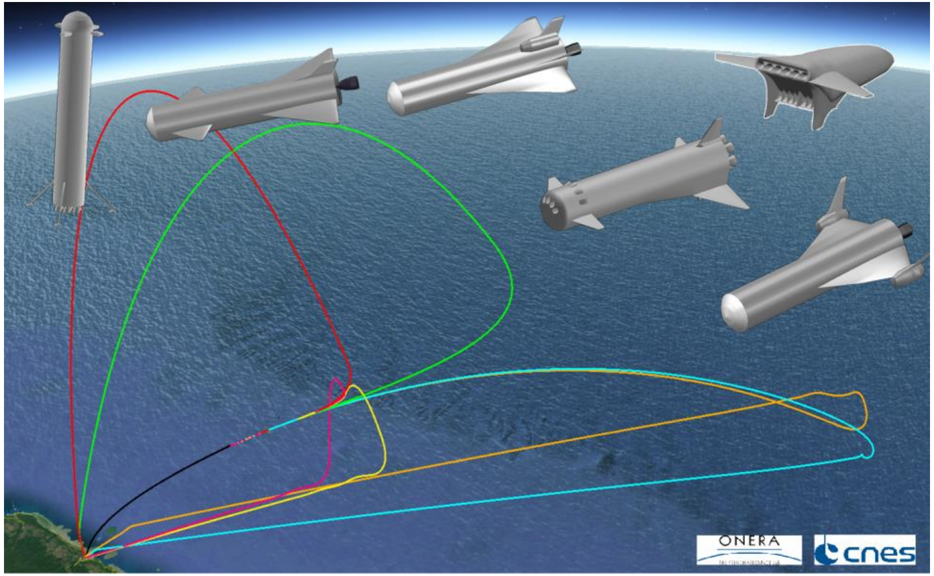
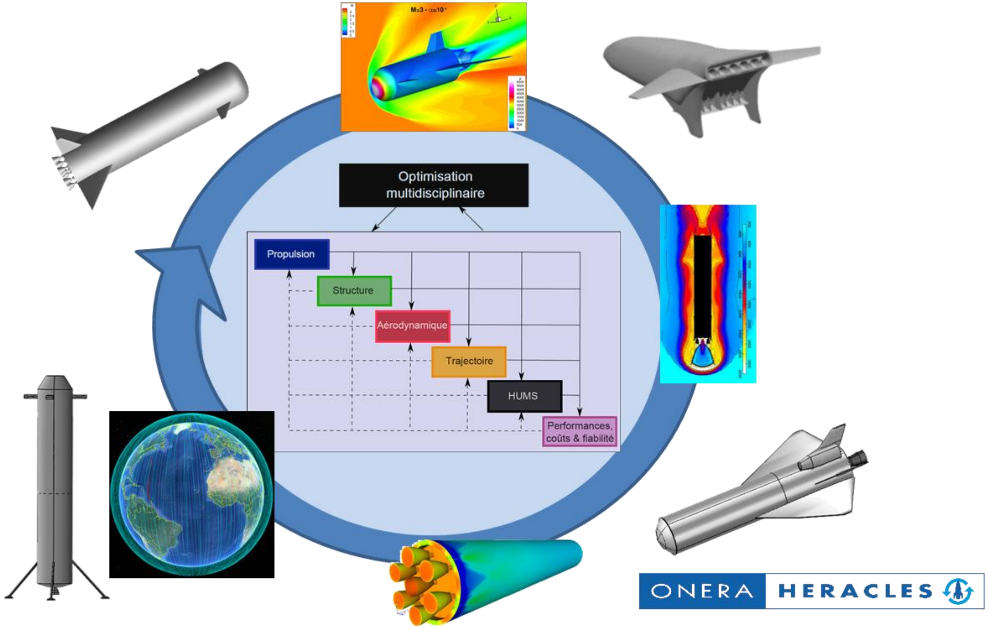
General context: early design of aerospace systems

- Design in early phases :
  - Need to explore a large number of candidate architectures (continuous, discrete and categorical variables)
  - Specifications are not fully defined / frozen



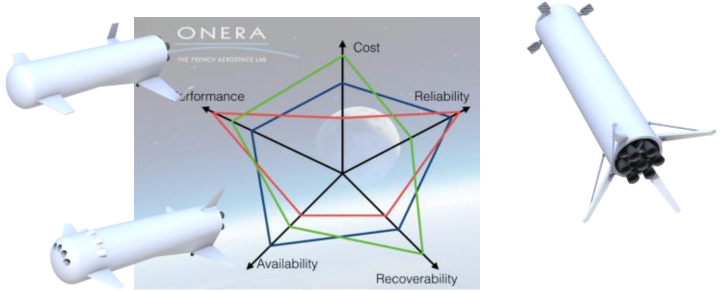
General context: multi-physics system optimization

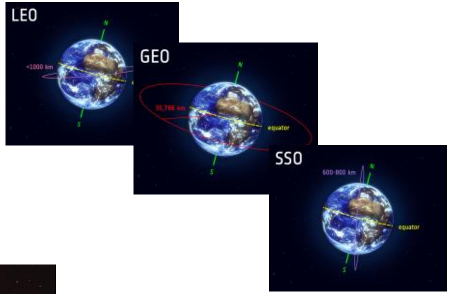
- Multi-physics system optimization
  - Use of multi-physics design process to assess performance and reliability of proposed concepts
  - Mixed-variable constrained optimization problem
  - Computationally intensive simulation models

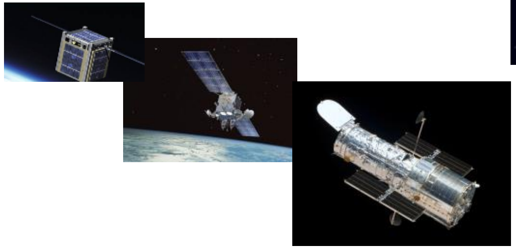


Motivations

- In early design phases:
  - promote a set of diversified optimums for decision makers and not just « *a single optimal solution* »
  - Specifications (expressed through constraints) are not necessarily frozen in early design phases and can change during the overall design process
  - Diversity with respect to non antagonistic criteria (*e.g.*, different possible specifications)







→ Need to extend classical optimization problem formulation (and algorithms)

Content of the presentation

- Quality – Diversity (QD) in a nutshell
- Classical population-based algorithms for QD
- Adaptation of Bayesian Optimization for mixed variable QD
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Mixed-variables optimization problem

$$
\begin{aligned}
\min_{\mathbf{x},\mathbf{z}} \quad & f(\mathbf{x},\mathbf{z}) \\
\text{s.t.} \quad & g_i(\mathbf{x},\mathbf{z}) \leqslant 0 \quad \text{for } i = 1,\ldots,n_g \\
& h_j(\mathbf{x},\mathbf{z}) = 0 \quad \text{for } j = 1,\ldots,n_h \\
& \mathbf{x}_{\text{lb}} \leqslant \mathbf{x} \leqslant \mathbf{x}_{\text{ub}} \\
& \mathbf{z} \in \mathcal{Z}
\end{aligned}
$$

- $f(\cdot)$ is the objective function
- $g_i(\cdot)$ and $h_j(\cdot)$ are the constraints
- $\boldsymbol{x}$, $\boldsymbol{z}$ are respectively the continuous, discrete / categorical variable vector
- $\mathcal{Z}$ is the definition domain of the discrete / categorical variable vector
- $n_{\boldsymbol{x}}$, $n_{\boldsymbol{z}}$ are the dimension of the respective vectors

Mixed-variables optimization problem

$$
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& \mathbf{x}_{\mathrm{lb}} \leqslant \mathbf{x} \leqslant \mathbf{x}_{\mathrm{ub}} \\
& \mathbf{z} \in \mathcal{Z}
\end{aligned}
$$

Rocket design example

- $f(\cdot)$: the cost of the rocket
- $g_i(\cdot)$ and $h_j(\cdot)$ orbit specification (*e.g.*, altitude, velocity), thrust-to-weigth ratio, *etc.*
- $\boldsymbol{x}$: propellant masses, chamber pressures, stage diameters, *etc.*
- $\boldsymbol{z}$: number of engines, type of propellant, type of materials, *etc.*

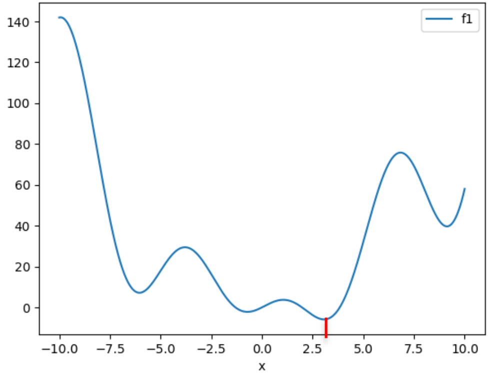
In this optimization problem:

- payload mass and target orbit are frozen → specifications of the optimization problem

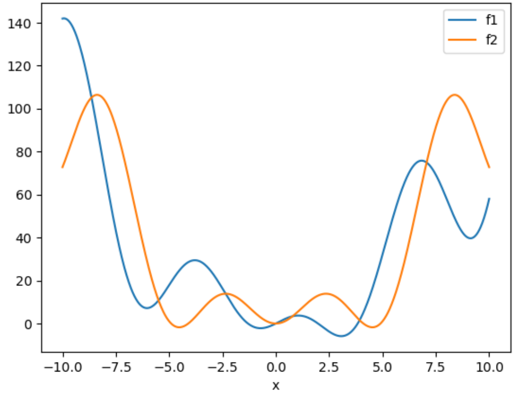
How to generate a set of optimal solutions for a series of specifications ?

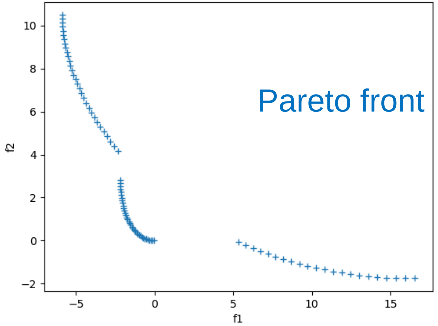
Single and multi-objective optimization

Single objective optimization



Multi-objective optimization



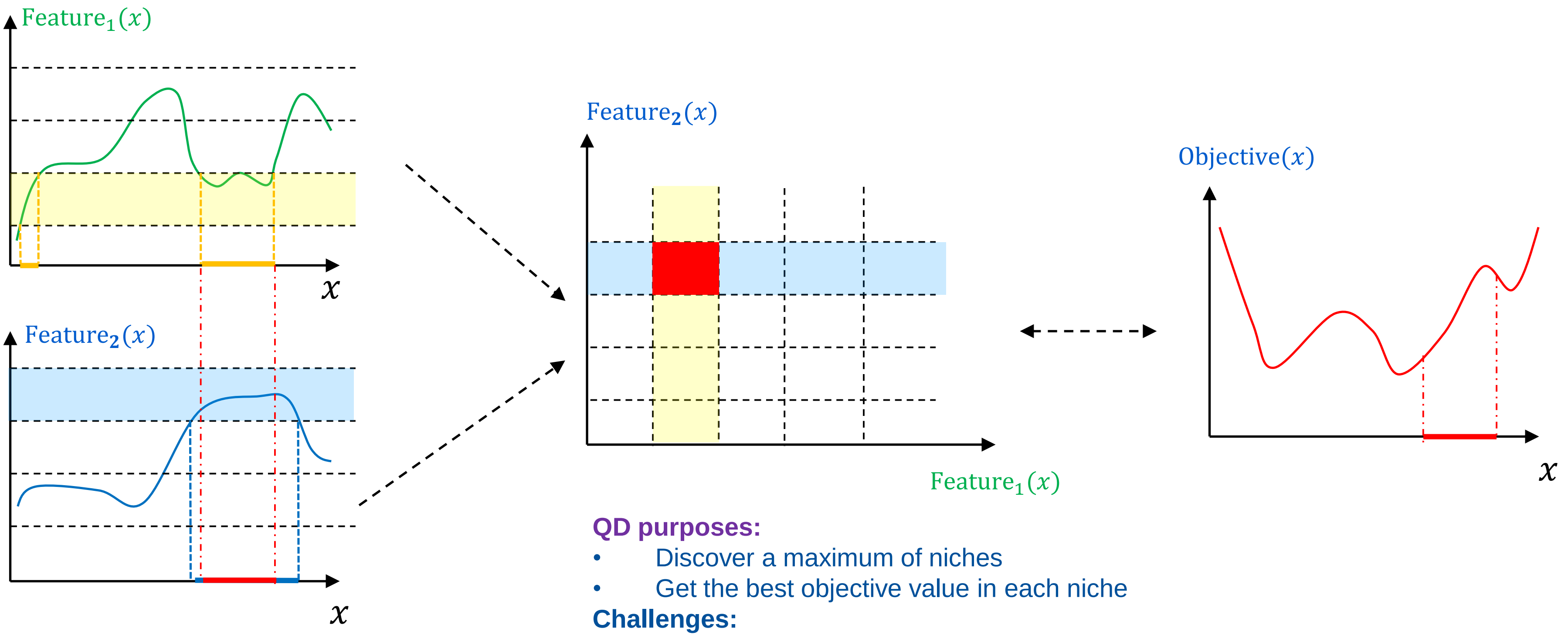


Multi-objective optimization finds a set of solution between **antagonistic objectives**

Quality-diversity (QD)

- Quality-diversity approaches [Mouret et al., 2015] find a set of solutions that are:
  - Optimal with respect to an objective function →quality
  - Diverse with respect to some characteristics called features → diversity
- Feature functions:
  - Inform about interesting characteristics of the candidate solutions → for instance specifications that are not fixed in the current design phase
  - Are not objective functions → they are not optimized
  - May define a low-dimensional space (the feature space) useful to map the design space
- Example of feature functions:
  - Rocket: payload mass, target orbit, *etc*.
  - Aircraft: number of passagers, wing aspect/taper ratio, target range, stealth, *etc*.

How to define a feature map



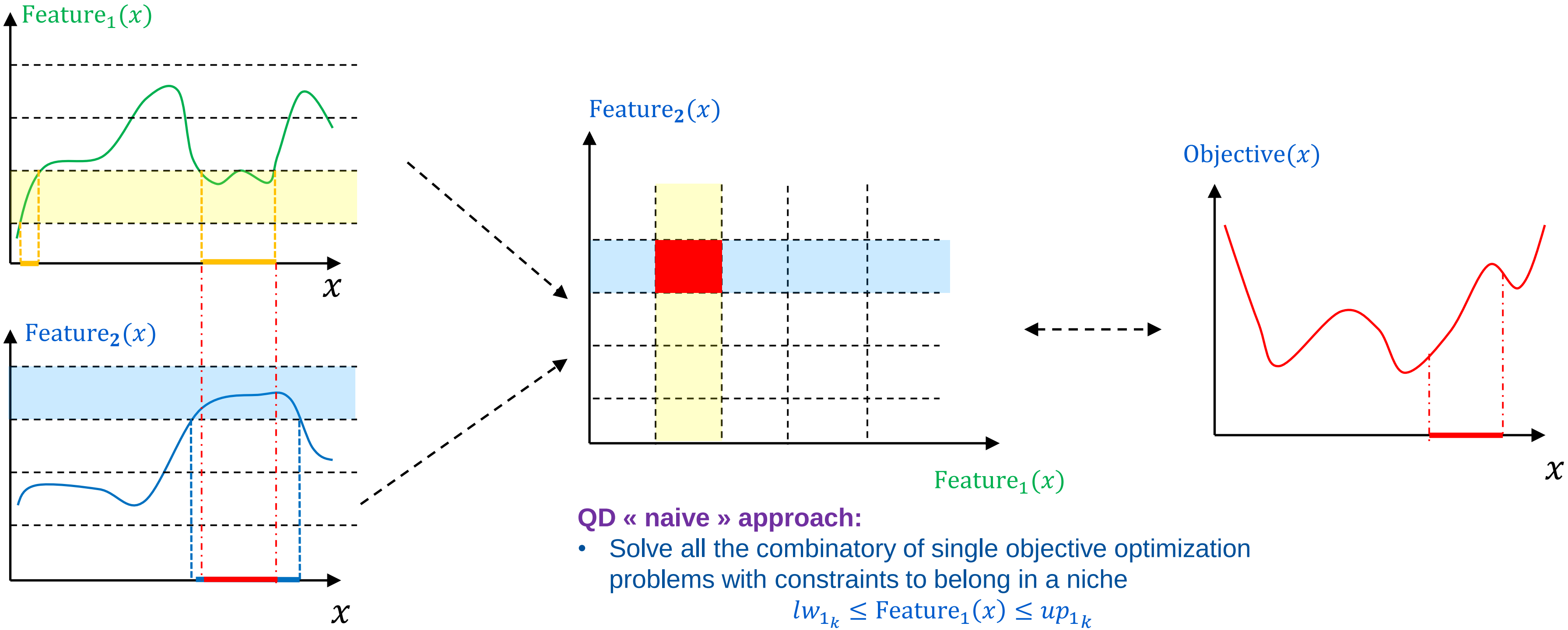
QD purposes:

- Discover a maximum of niches
- Get the best objective value in each niche

Challenges:

- The mapping between $\boldsymbol{x}$, $feature_1$, $feature_2$, and $objective$ is not « explicit »

Solve QD problem



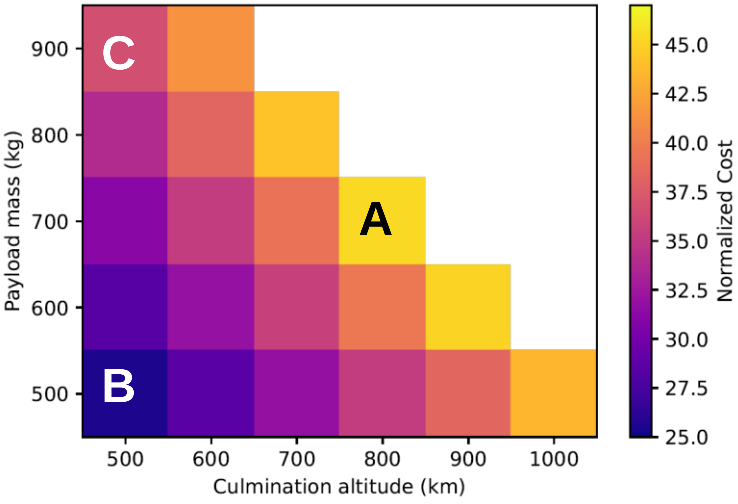
QD « naive » approach:

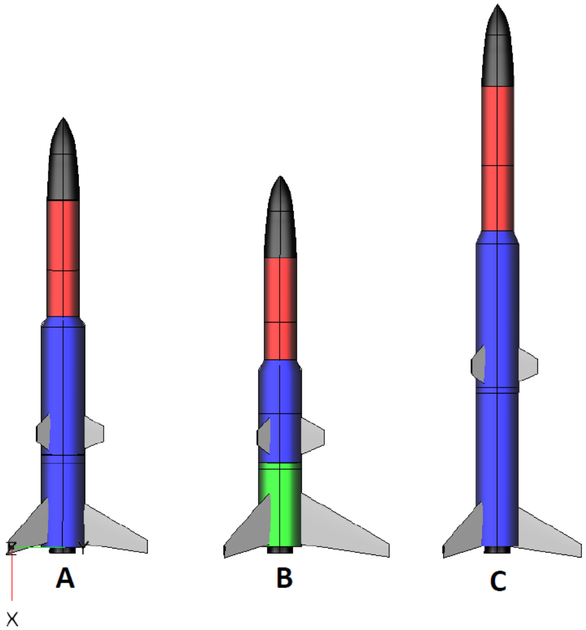
- Solve all the combinatory of single objective optimization problems with constraints to belong in a niche

$$lw_{1_k} \leq \text{Feature}_1(x) \leq up_{1_k}$$
$$lw_{2_k} \leq \text{Feature}_2(x) \leq up_{2_k}$$

for $k \in \{1, \dots, N\}$

QD « optimal map »





Quality-diversity mixed-variables problem

$$
\begin{aligned}
\boxed{}\ \min_{\mathbf{x},\mathbf{z}} \quad & f(\mathbf{x},\mathbf{z}) \\
\text{s.t.} \quad & g_i(\mathbf{x},\mathbf{z}) \leqslant 0 \quad \text{for } i = 1,\ldots,n_g \\
& h_j(\mathbf{x},\mathbf{z}) = 0 \quad \text{for } j = 1,\ldots,n_h \\
& \boxed{} \\
& \mathbf{x}_{\mathrm{lb}} \leqslant \mathbf{x} \leqslant \mathbf{x}_{\mathrm{ub}} \\
& \mathbf{z} \in \mathcal{Z}
\end{aligned}
$$

with:

- $\boldsymbol{f}_t(\cdot,\cdot)$ the feature function vector
- $\widetilde{\boldsymbol{f}}$ a niche inside the map

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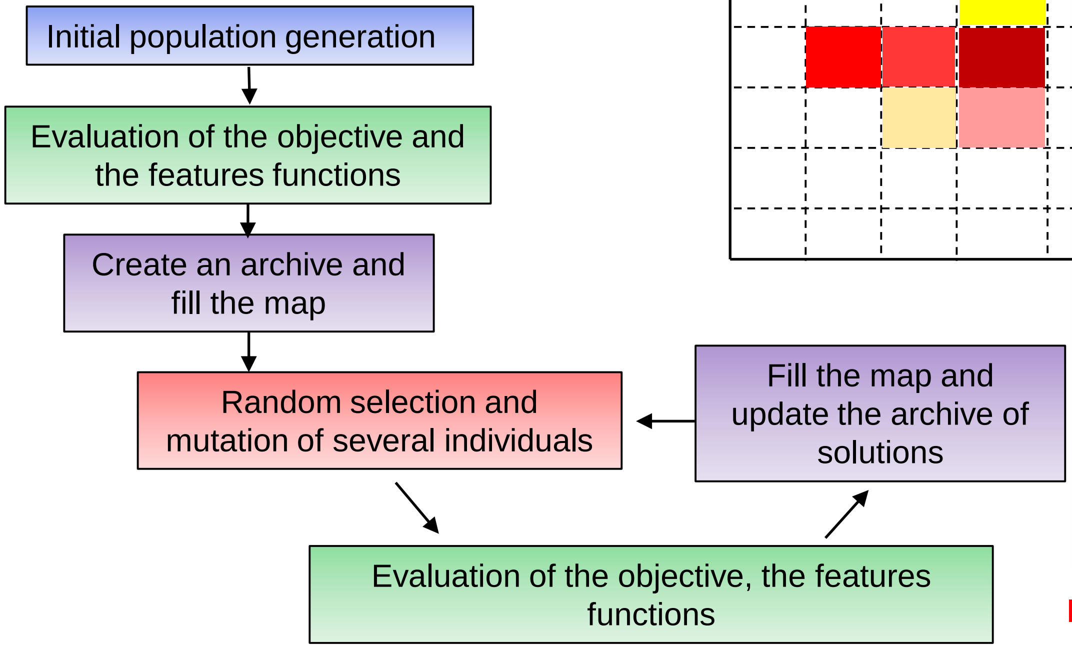
Quality-diversity algorithms

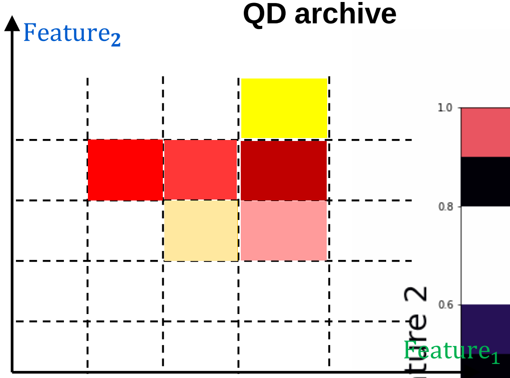
- Population-based algorithms
  - Novelty Search with Local Competition (NSLC) [Lehman et al., 2011]
  - Multidimensional Archive of Phenotypic - Elites (MAP-Elites) [Mouret et al., 2015] and variants :
    - MAP-Elites + Novelty [Pugh et al., 2016],
    - Centroidal Voronoi Tessellation (CVT)-MAP-Elites [Vassiliades et al., 2017], *etc*.
  - Covariance Matrix Adaptation - Evolutionary Strategy (CMA-ES) based algorithms :
    - CMA-MAP-Elites (CMA-ME) [Fontaine et al., 2020] ,
    - CMA-MAE (CMA – MAP Annealing) [Fontaine et al., 2023]
  - Multi-Emitters : ME-MAP-Elites [Cully, 2021]

MAP-Elites [Mouret et al., 2015]

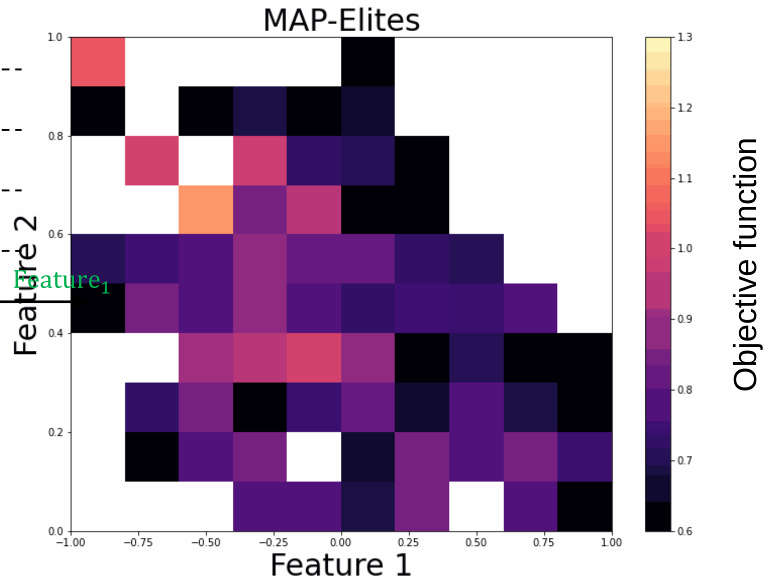
- Evolutionary algorithm



QD archive



Map for maximization problem

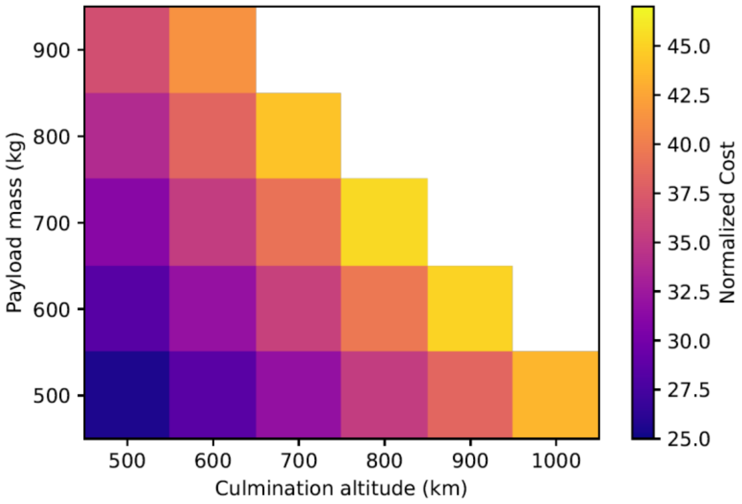


Issue: large number of function evaluations to converge

How to assess the performance of a QD algorithm

Two main performance metrics :

- The filling factor : number of discovered niches in the map → quantifies the diversity
- The QD score : sum of the objective functions in the discovered niches → quantifies the quality of the solutions found in the different niches



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Bayesian QD algorithms

Different Bayesian QD algorithms have been proposed for **continuous unconstrained** problem:

- SAIL (Surrogate-Assisted Illumination) [Gaier et al., 2017, Gaier et al., 2017b]
- SPHEN (Surrogate-Assisted Phenotypic Niching) [Hagg, 2020]
- BOP-Elites (Bayesian Optimization of Elites) [Kent et al., 2020]
- Deep Surrogate Assisted MAP-Elites [Zhang, 2022]

- Limits of existing QD-BO algorithms
  - Do not handle constraints
  - Do not handle mixed variables (continuous, discrete, categorical)

- Proposition of an new QD-BO algorithm to handle such problems

Brevault, L., & Balesdent, M. (2024). Bayesian Quality-Diversity approaches for constrained optimization problems with mixed continuous, discrete and categorical variables. *Engineering Applications of Artificial Intelligence*, 133, 108118, Elsevier.

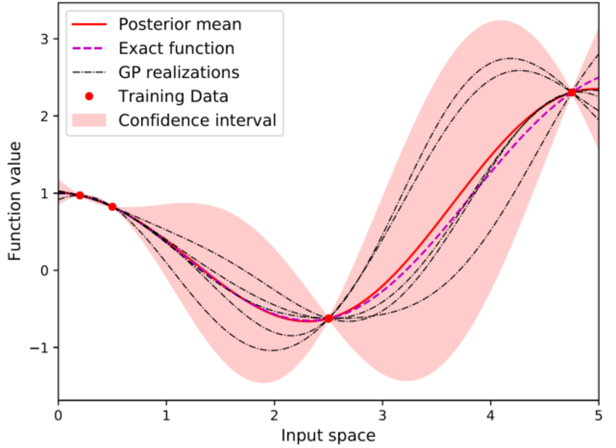
Gaussian process

- A Gaussian process (GP):
  - is a stochastic process corresponding to an infinite collection of random variables such that any finite subset collection follows a multivariate Normal distribution
  - caracterized by a mean function $m(\cdot)$ and a covaraince function $k_\theta(\cdot,\cdot)$

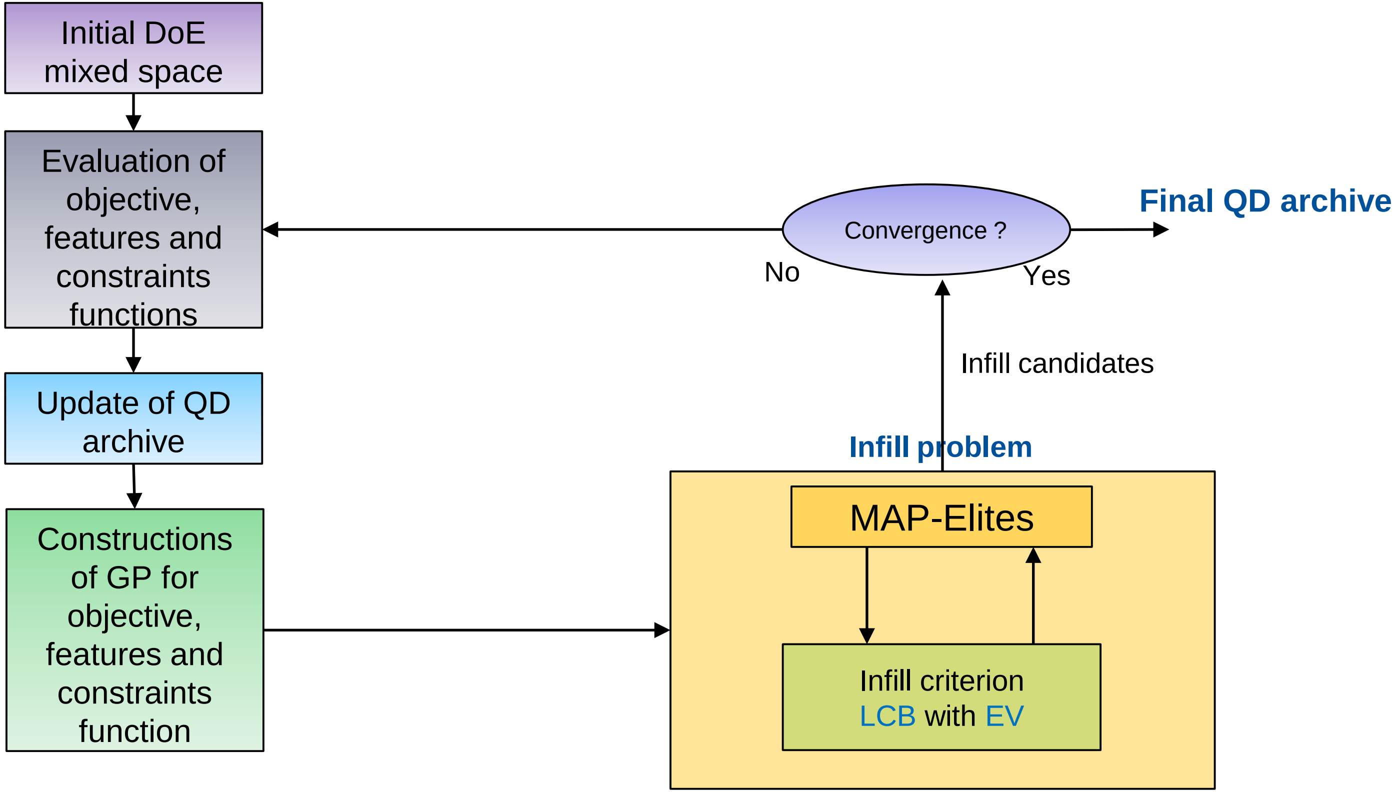
- Construction of a GP $f \sim GP\big(m(\cdot), k_\theta(\cdot,\cdot)\big)$:
  - A prior is defined for the mean and covariance functions (parametric kernel)
  - From a design of experiments (inputs, outputs), GP is trained to maximize the log-likelihood of the data
  - The posterior distribution of GP is obtained by conditionning the GP prior (with optimal parameters) on the data

- The posterior distribution of GP provides :
  - A prediction model $\hat{f}(\cdot)$
  - A « confidance » model $\hat{\sigma}(\cdot)$ associated to the prediction under the corresponding hypotheses

- It is possible to use such « confidence » model in an adaptive enrichment strategy to improve the accuracy of the prediction model and the confidence level



Proposed algorithm: Bayesian Optimization for mixed constrained Quality Diversity problems



LCB: Lower Confidence Bound
EV : Expected Violation

Proposed algorithm

- Use of dedicated **mixed covariance functions** in BO [Halstrup et al., 2016, Pelamatti et al., 2021, Saves et al., 2023] :

$$k_{\Theta}(\{x,z\},\{x',z'\}) = k_{\gamma}(x,x') \times k_{\theta}(z,z')$$

with (x, x') continuous scalar variables and (z, z') discrete/categorical scalar variables

  – Compound Symmetry (Gower distance) [Halstrup et al., 2016, Pelamatti et al., 2021, Saves et al., 2023]

$$k_{\theta}(z,z') = \sigma_z^2 \exp\left(-\theta d_{gow}(z,z')\right)$$ with $d_{gow}(z,z')$=0 if $z = z'$, 1 otherwise

  – Hypersphere decomposition [Zhou et al., 2011, Pelamatti et al., 2021, Saves et al., 2023]

Covariance matrix $\boldsymbol{C}_{\theta}$ associated to the hypersphere kernel $k_{\theta}(z,z')$ is defined by: $\boldsymbol{C}_{\boldsymbol{\theta}} = \sigma_z^2 \boldsymbol{L}^T \boldsymbol{L}$ via Cholesky decomposition with:

$$\mathbf{L} = \sigma_z \begin{bmatrix} 1 & 0 & \dots & \dots & 0 \\ \cos\theta_{2,1} & \sin\theta_{2,1} & 0 & \dots & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \cos\theta_{l,1} & \sin\theta_{l,1}\cos\theta_{l,2} & \dots & \cos\theta_{l,l-1}\prod_{d=1}^{l-2}\sin\theta_{l,d} & \prod_{d=1}^{l-1}\sin\theta_{l,d} \end{bmatrix}$$

Proposed algorithm

- Bayesian optimization for Quality-Diversity through Lower Confidence Bound (LCB) with Expected Violation (EV)

$$\forall \tilde{\boldsymbol{f}} \in \mathcal{F}_t, \ \min_{\boldsymbol{x},\boldsymbol{z}} \ \hat{f}(\boldsymbol{x},\boldsymbol{z}) - k * \hat{\sigma}(\boldsymbol{x},\boldsymbol{z}) \qquad k > 0$$

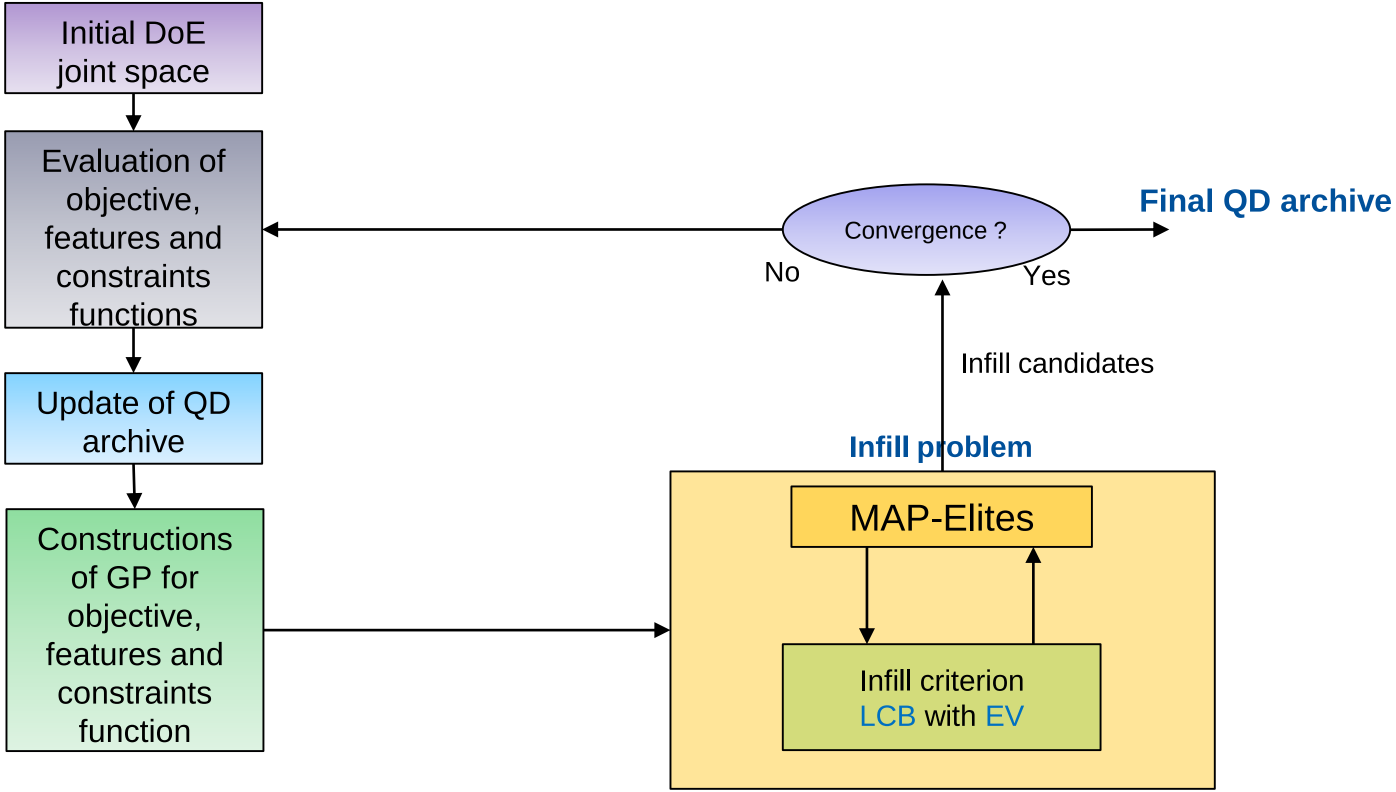
$$s.t. \ EV_{\hat{g}_i}(\boldsymbol{x},\boldsymbol{z}) \leq t_i \qquad \text{for i} = 1, \dots, \text{n}_\text{g}$$

$$\boldsymbol{f}_t(\boldsymbol{x},\boldsymbol{z}) \in \tilde{\boldsymbol{f}}$$

with $EV_{\hat{g}_i}(\boldsymbol{x},\boldsymbol{z}) = \hat{g}_i(\cdot) \times \Phi\left(\frac{\hat{g}_i(\cdot)}{\hat{\sigma}_{g_i}(\cdot)}\right) + \hat{\sigma}_{g_i}(\cdot) \times \phi\left(\frac{\hat{g}_i(\cdot)}{\hat{\sigma}_{g_i}(\cdot)}\right)$ and $\Phi(\cdot), \phi(\cdot)$ CDF and PDF of standard Normal distribution

- Adaptation of MAP-Elites algorithm for the infill optimization problem
  - Derivation of a discrete mutation operator to handle discrete/categorical variables $\boldsymbol{z}$
  - Use of constraint dominance operator to generate feasible solutions [Coello, 2002]
    1. A feasible solution is always preferred to an infeasible solution,
    2. Between two feasible solutions, the solution with the best fitness is preferred.
    3. Between two infeasible solutions, the solution that violates the less the constraints is preferred.

Proposed algorithm: Bayesian Optimization for mixed constrained Quality Diversity problems



LCB: Lower Confidence Bound
EV : Expected Violation

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- Application to aerospace optimization problems
  - Comparison with respect to multi-objective optimization and MAP-Elites
  - Application to sounding rocket design

Numerical experiments

- Evaluation of the algorithm performances on 5 problems
  - 3 analytical problems
  - 2 aerospace problems

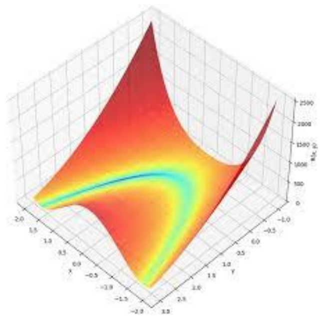
- Comparison with:
  - MAP-Elites algorithm (with two population sizes)
  - Mixed QD-BO with Compound Symmetry kernel
  - Mixed QD-BO with Hypersphere decomposition kernel

- 10 repetitions, metrics of comparison: QD-score, Filling factor

- Use of SMT [Saves, 2024] for surrogate modeling

Illustration on Rosenbrock-like problem

$$
\begin{aligned}
\forall \tilde{\mathbf{f}} \in \mathcal{F}_t, \quad \min_{\mathbf{x},\mathbf{z}} \quad & f(\mathbf{x},\mathbf{z}) \\
\text{s.t.} \quad & g_1(\mathbf{x},\mathbf{z}) \leqslant 0 \\
& \mathbf{f}_t(\mathbf{x},\mathbf{z}) \in \tilde{\mathbf{f}} \\
& -5. \leqslant \mathbf{x} \leqslant 5. \\
& \mathbf{z}^q = [z_1, z_2]^T \in \{0,1,2,3,4,5\} \times \{0,1\}
\end{aligned}
$$



Modification of classical Rosenbrock problem for quality-diversity optimization

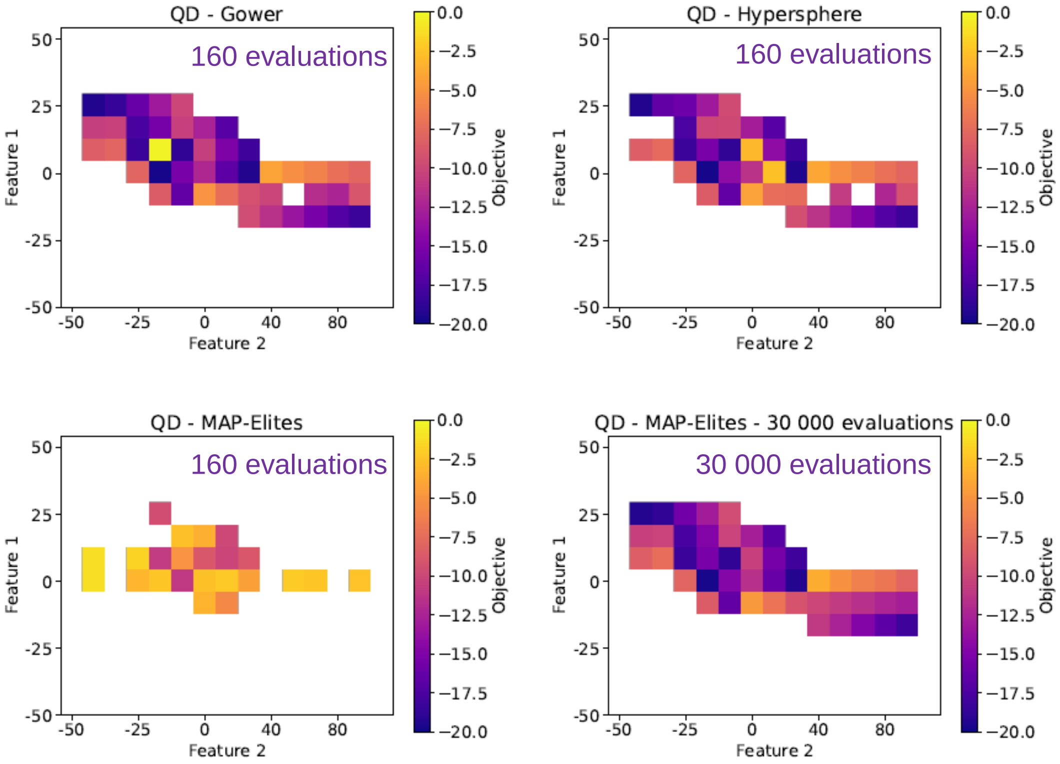
- Dimension continuous variables: 2
- Dimension discrete variables: 2
- Number of feature functions: 2

Antagonistic objective and feature functions :

- Possible comparison with multi-objective optimization

- Budget: 160 exact function evaluations (objective, constraints, features)

Illustration on Rosenbrock-like problem



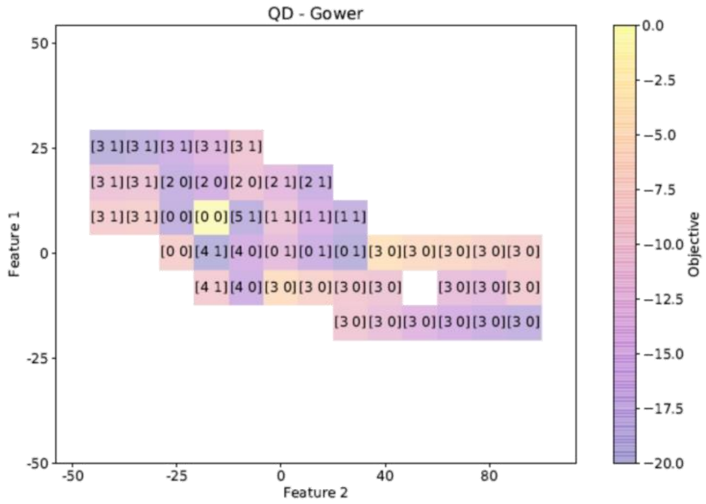
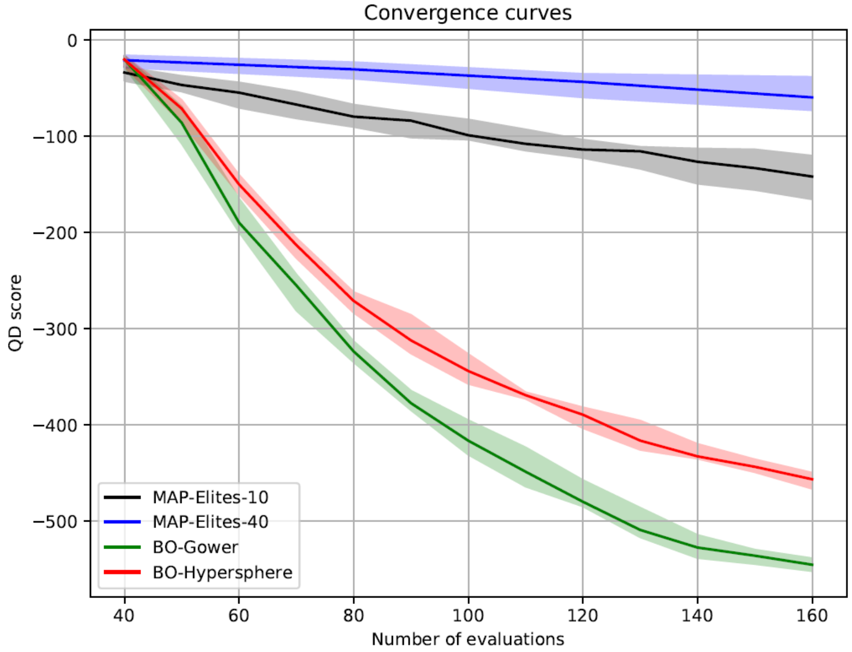
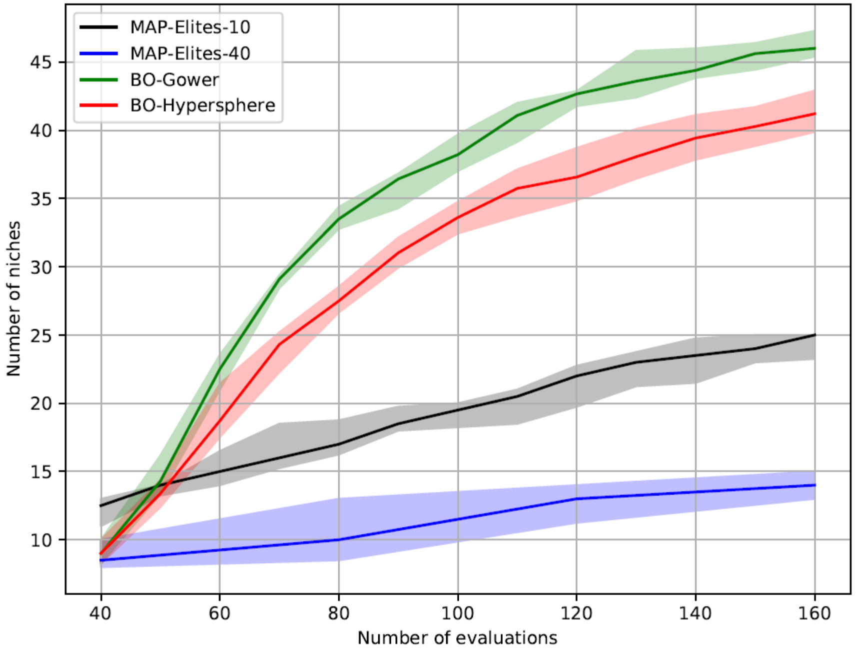


Illustration on Rosenbrock-like problem





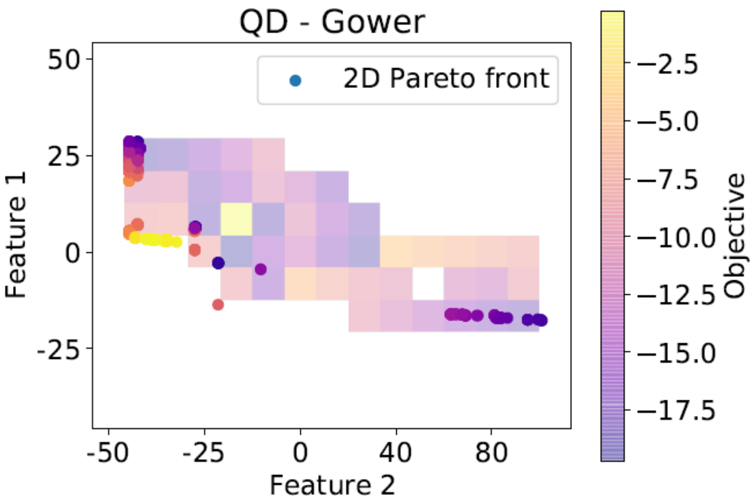
Better convergence of QD-BO approaches

Illustration on Rosenbrock-like problem

Comparison with **multi-objective optimization** :

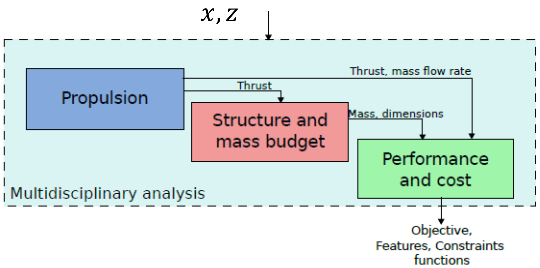
- Pareto-front is only a « part » of the QD-map

- QD-map provides the « consequences » of change in features in terms of objective function without notion of « dominance »

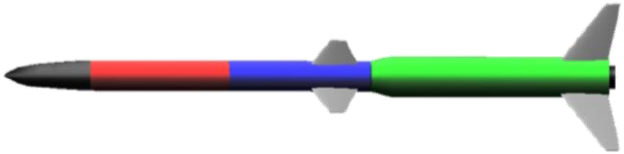


Sounding rocket design optimization

$$
\begin{aligned}
\forall \tilde{\mathbf{f}} \in \mathcal{F}_t, \quad \min_{\mathbf{x},\mathbf{z}} \quad & C(\mathbf{x},\mathbf{z}) \\
\text{s.t.} \quad & g_i(\mathbf{x},\mathbf{z}) \leqslant 0 \quad i = 1,\dots,8 \\
& [f_{m_{CU}}(\mathbf{x},\mathbf{z}), f_{alt}(\mathbf{x},\mathbf{z})]^T \in \tilde{\mathbf{f}} \\
& \mathbf{x}_{\text{lb}} \leqslant \mathbf{x} \leqslant \mathbf{x}_{\text{ub}} \\
& \mathbf{z} \in \mathcal{Z}
\end{aligned}
$$



$C(\cdot)$: objective →normalized cost
$f_{m_{CU}}(\cdot)$: feature →payload mass
$f_{alt}(\cdot)$: feature →culmination altitude



Continuous design variables :

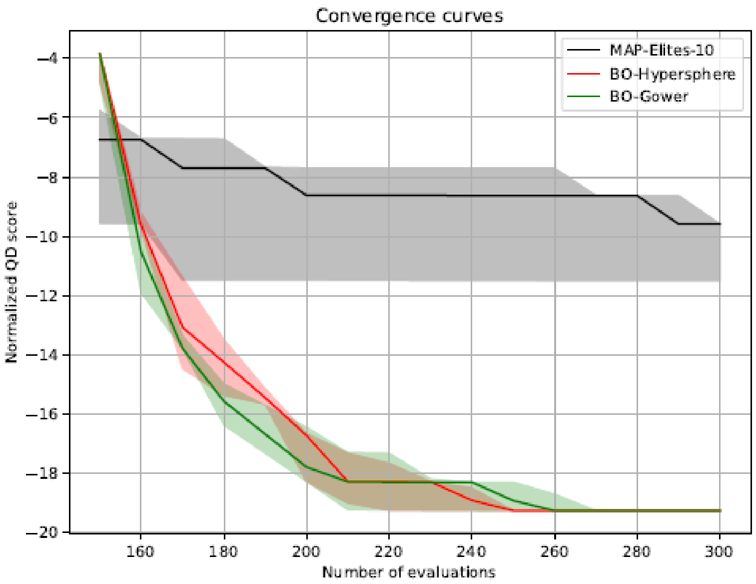
- ratios between the throat diameter and the nozzle exit diameter,
- propellant masses,
- the combustion pressures,
- the nozzle exit diameters,
- the payload mass.

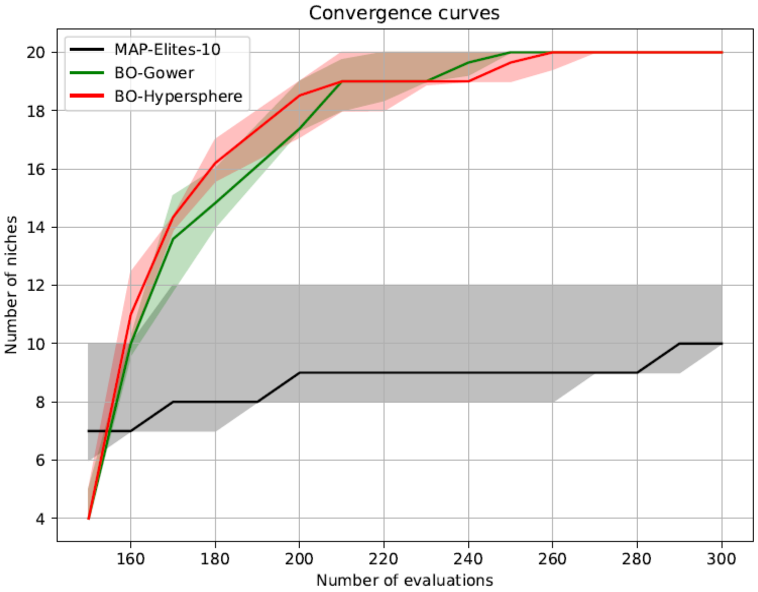
Table 1: Categorical design variables and their definition domains

Variable	Definition domain
Propellant stage 1	{Butalane, Butalite, Nitramite, p-AIM120}
Casing material stage 1	{Steel, Aluminum, Composite}
Engine type stage 1	{Type 1, Type 2, Type 3}
Propellant stage 2	{Butalane, Butalite, Nitramite, p-AIM120}
Casing material stage 2	{Steel, Aluminum, Composite}
Engine type stage 2	{Type 1, Type 2, Type 3}
Number of possible combinations	1296

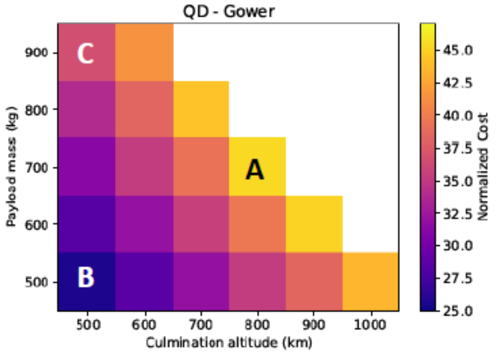
Budget: 300 exact function evaluations (objective, constraints, features)

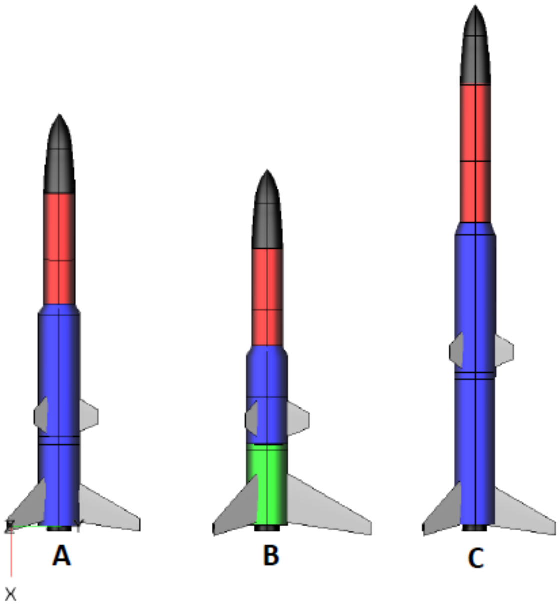
Sounding rocket design optimization

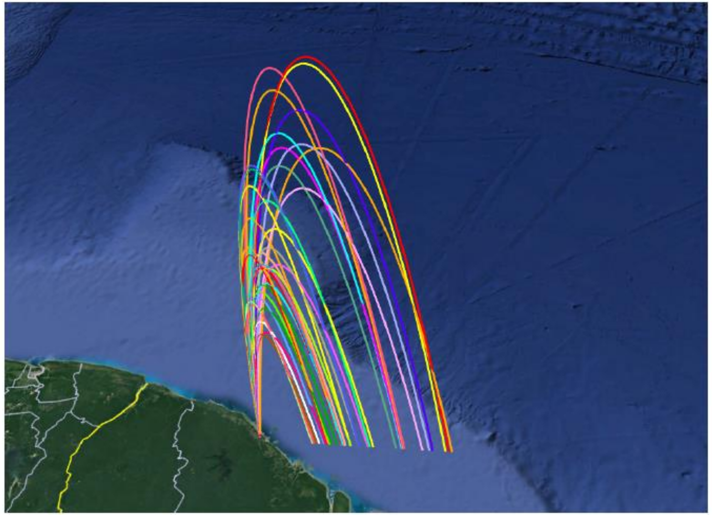




Sounding rocket design optimization







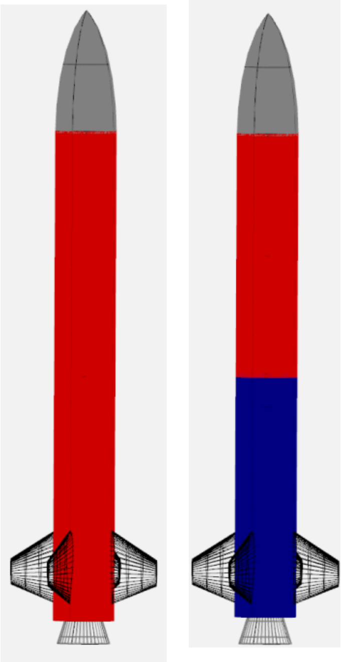
Conclusions

- Quality-diversity allows to extend the design optimization and promote diversity of solutions,
- Classical QD algorithms require a large number of evaluations and are not suitable for practical industrial optimization problems,
- Bayesian optimization can be adapted to Quality-Diversity with to handle mixed continuous/discrete/categorical constrained problems,
- Current works / perspectives :
  - Extension of QD-BO to **conditional search space problems (CSSP)** → Ph.D. thesis of Lucas Baraton with ISAE-SupAéro (2022-2025)
  - Extension of MAP-Elites to CSSP → internship of Nathan Piatte (April-August 2024) + Ph.D. thesis of Lucas Baraton

CSSP for launch vehicle design

Number of segments ?

1

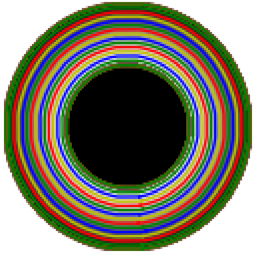


2

For each segment, which grain ?

Star

Finocyl



Circular

Thank you !

Questions ?

More details about this work:

- Brevault, L., & Balesdent, M. (2024). Bayesian Quality-Diversity approaches for constrained optimization problems with mixed continuous, discrete and categorical variables. *Engineering Applications of Artificial Intelligence*, 133, 108118, Elsevier.

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