A Deep Gaussian Process based model for Multi-Objective optimization

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1 SCIENCES ET TECHNOLOGIES

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Context

Resolution of a multi-objective optimization problem characterized by :

- Black box and computationally expensive functions,
- Correlated objectives.

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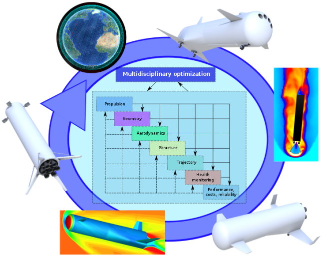


Multi-disciplinary optimization of an aerospace vehicle

Context

Resolution of a multi-objective optimization problem characterized by :

- Black box and computationally expensive functions,
- Correlated objectives.

✗ Gradient based optimization approaches

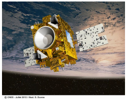
✗ Classic evolutionary algorithms

✓ Bayesian Optimization

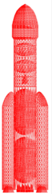
Context

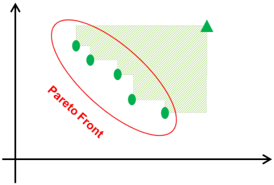
Resolution of a multi-objective optimization problem characterized by :

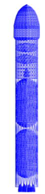
- Black box and computationally expensive functions,
- Correlated objectives.



Maximize f_1 : The payload value.





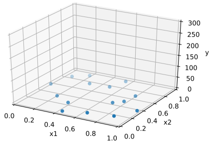


Minimize f_2 : The gross lift off-weight value.

MO-BO framework

Multi-Objective Bayesian Optimization (MO-BO) [Emmerich et al., 2006]

Initial dataset



Design of Experiment depending on the dimension and the nature of the problem

MO-BO framework

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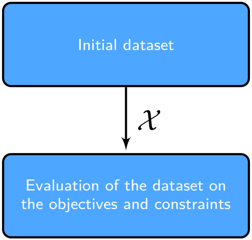
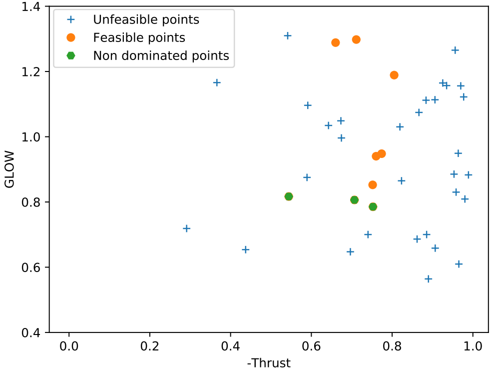




Calls the **expensive** black-box functions

MO-BO framework

Multi-Objective Bayesian Optimization (MO-BO) [Emmerich et al., 2006]

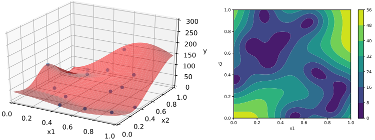
Initial dataset

$\downarrow \mathcal{X}$

Evaluation of the dataset on the objectives and constraints

$\downarrow \mathcal{Y}, \mathcal{G}$

Construction of the GP regression models for the objectives and constraints



Learning the hyperparameters of each surrogate model

MO-BO framework

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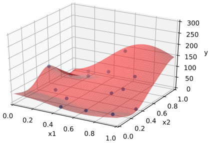
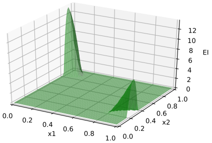
$\hat{\mathbf{y}}, \hat{\mathbf{g}}$

Adding the most promising point(s)





Optimization of a chosen **infill sampling criterion**

MO-BO framework

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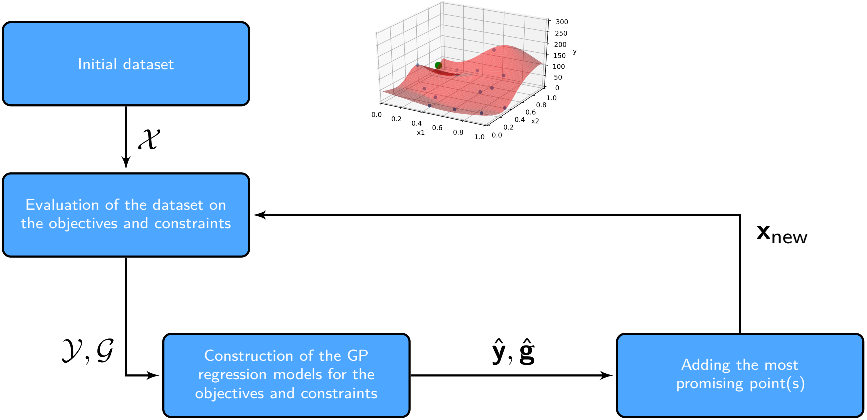
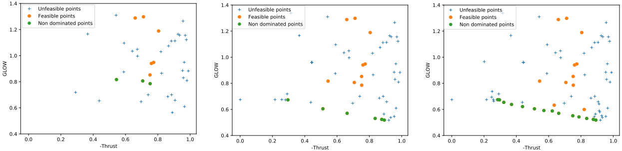


MO-BO framework

Initial DoE 30 added points 50 added points



Initial dataset

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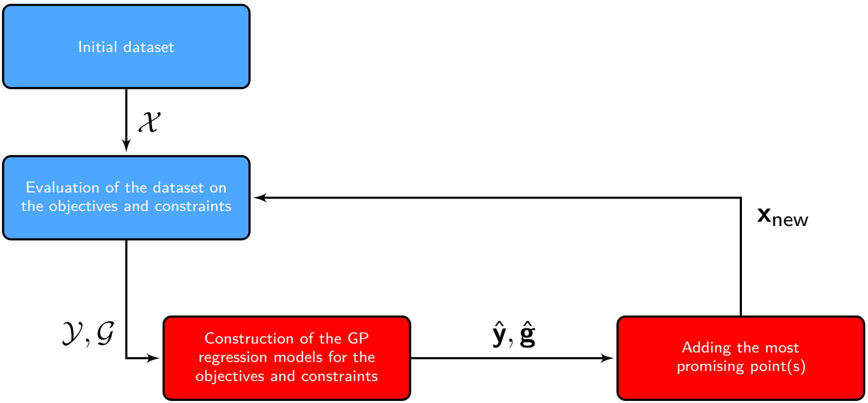
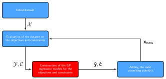
Adding the most promising point(s)

$\mathbf{x}_{\text{new}}$

MO-BO framework

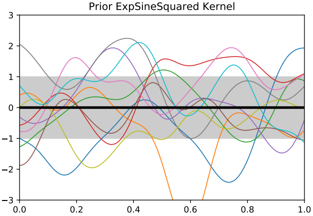


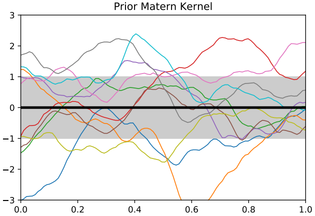
Gaussian Process Regression



Gaussian process [Rasmussen, 2004]

A Gaussian Process is used to describe a distribution over function. It is a collection of infinite random variables, **any finite number of which have a joint Gaussian distribution**.
It is defined by its mean function and covariance function (Kernel) : $f(.) \sim \mathcal{GP}(\mu(.), k^{\Theta}(.))$





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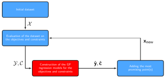

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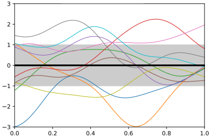
Automatic Relevance Determination (ARD) squared exponential kernel :

$$K^{\Theta}(\mathbf{x}, \mathbf{x'}) = \sigma^2 \exp\left(-\sum_{i=1}^{D} \theta_i . |x_i - x_i'|^2\right)$$

Prior Gaussian Process



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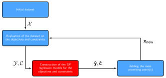

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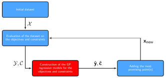
$$\text{Maximize w.r.t } \Theta \ : p(\mathbf{y}|\mathcal{X}) = \mathcal{N}(\mathbf{y}|0, \mathbf{K}^{\Theta}_{NN}\mathbf{I})$$

Gaussian Process Regression



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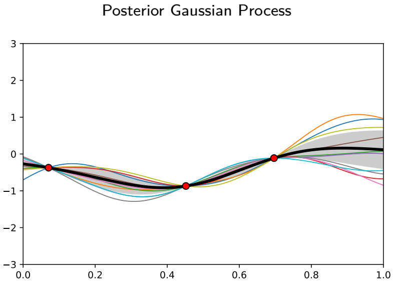
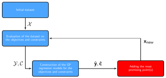


$$y^* | \mathbf{x}^*, \mathcal{X}, \mathcal{Y} \sim \mathcal{N}(\hat{y}^*, \hat{s}^*)$$

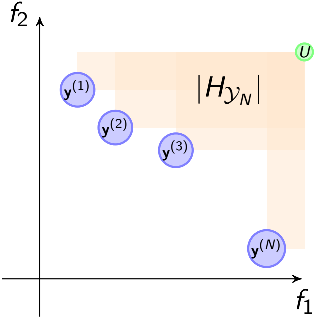
Infill Criteria



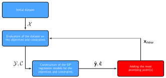
Hypervolume indicator

The hypervolume indicator expresses the hypervolume of the objective space dominated by the approximated Pareto set.

$$H_{\mathcal{Y}_N} = \left\{ \mathbf{y} \in \mathbb{B}; \exists i \in \{1, \ldots, N\}, \mathbf{y}^{(i)} \prec \mathbf{y} \right\}$$



Infill Criteria

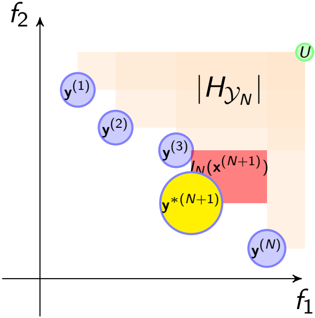


Hypervolume improvement

[Emmerich et al., 2006]

The hypervolume improvement is the improvement of the hypervolume by adding a candidate to the data set

$$I_N(\mathbf{x}^{(N+1)}) = |H\mathcal{Y}_{N+1}| - |H\mathcal{Y}_N|$$



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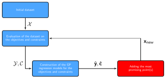
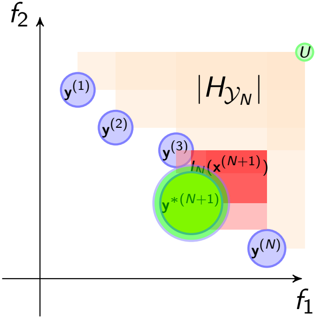


Expected Hypervolume improvement [Emmerich et al., 2006]

The expected hypervolume improvement is the mathematical expected improvement of the hypervolume by adding a candidate to the sample

$$
\begin{aligned}
EHVI_N(\mathbf{x}) &= \mathbb{E}(|H_{\mathcal{Y}_{N+1}}| - |H_{\mathcal{Y}_N}|) \\
&= \int_{\mathbb{B}\setminus H_{\mathcal{Y}_N}} \mathbb{P}(\mathbf{y}^{*(N+1)} \prec p)\mathrm{d}p
\end{aligned}
$$



with $\mathbf{y}^{*(N+1)} = [y_1^{*(N+1)}, y_2^{*(N+1)}]$

and $y_1^{*(N+1)} \sim \mathcal{N}\left(\hat{y}_1^{*(N+1)}, \hat{s}_1^{*(N+1)}\right)$ and $y_2^{*(N+1)} \sim \mathcal{N}\left(\hat{y}_2^{*(N+1)}, \hat{s}_2^{*(N+1)}\right)$

Multi-task GPs

- Classic MO-BO approaches use an independent GP for each objective $\rightarrow$ assumption of independency between the objectives.
- Multi-task GPs [Shah and Ghahramani, 2016] : exhibit correlation between functions by introducing a coregionalization matrix K^{coreg} :

$$\mathrm{Cov}\left(f_i(\mathbf{x}), f_j(\mathbf{x}')\right) = K^{coreg}_{ij} k(\mathbf{x}, \mathbf{x}')$$

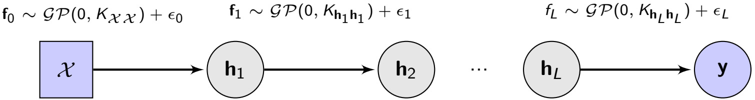
- Each function is marginally identically distributed up to a scaling factor.

Deep Gaussian Processes

Deep Gaussian Processes [Damianou and Lawrence, 2013]

DGPs are a class of surrogate models based on the structure of neural networks, where each layer is a GP. They consider that the statistical relationship between the inputs and the response is expressed by a functional composition of GPs :

$$y = f_L(\mathbf{f}_{L-1}(\dots \mathbf{f}_1(\mathbf{f}_0(\mathbf{x}) + \epsilon_0) + \epsilon_1)\dots) + \epsilon_{L-1}) + \epsilon_L$$



Deep Gaussian Processes

$\mathbf{f}_0 \sim \mathcal{GP}(0, K_{\mathcal{X}\mathcal{X}}) + \epsilon_0$ $\quad$ $\mathbf{f}_1 \sim \mathcal{GP}(0, K_{\mathbf{h}_1\mathbf{h}_1}) + \epsilon_1$ $\quad$ $f_L \sim \mathcal{GP}(0, K_{\mathbf{h}_L\mathbf{h}_L}) + \epsilon_L$

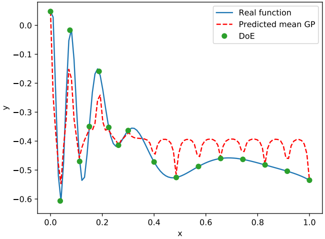
$$\mathcal{X} \longrightarrow \mathbf{h}_1 \longrightarrow \mathbf{h}_2 \quad \cdots \quad \mathbf{h}_L \longrightarrow \mathbf{y}$$

$\mathcal{X}$ A deterministic observed variable

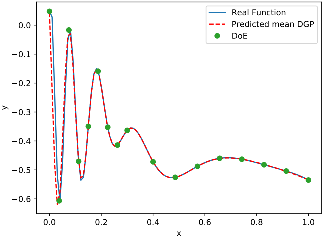
$\mathbf{h}_i$ A distribution with **Non**-observed instantiations

$\mathbf{y}$ A distribution with observed instantiations

Deep Gaussian Processes



GP approximation of a non-stationary 1-D function. The GP model can not capture the stability of the region $[0.4, 1]$ and continues to oscillate [?]

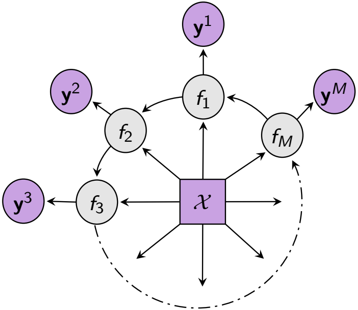


DGP approximation of a non-stationary 1-D function. The DGP model appropriately capture the two regions with different smoothness

MO-DGP model

MO-DGP model

The MO-DGP model is a DGP network where each layer represents an objective. Moreover, a connection is made between the first and the last layer, creating a loop DGP. Propagating through the loop allows to take into account the different correlations between the objectives.



Specifications of the MO-DGP model

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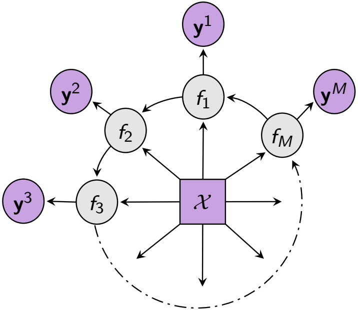

A multi-objective covariance function

$$k_l^{\rho}(\mathbf{x},\mathbf{x}')k_l^{f}\left(f_i^*(\mathbf{x}), f_{i+1}^*(\mathbf{x}')\right) + k_l^{\gamma}(\mathbf{x},\mathbf{x}')$$

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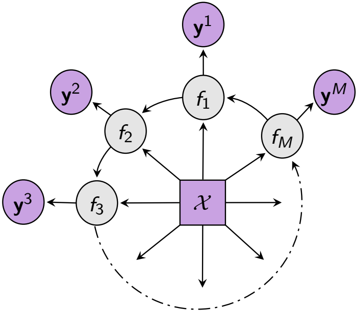

The evidence lower bound

The evidence lower bound is derived using the sparse variational approximation of a GP inference [Salimbeni and Deisenroth, 2017] :

$$P\left(\mathbf{y}^1, \ldots, \mathbf{y}^M | \mathcal{X}\right) \geq ELBO$$

with

$$ELBO = \sum_{t=1}^{M} \sum_{i=1}^{N} \mathbb{E}_{q(f_t^{(i),t})} \left[\log p(y^{(i),t} | f_t^{(i),t})\right] - \sum_{l=1}^{M} KL\left[q(\mathbf{u}_l) || p(\mathbf{u}_l; Z_{l-1})\right]$$

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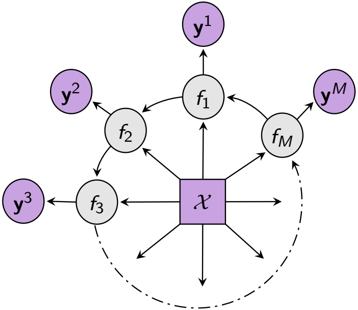

Optimization of the ELBO

An optimization loop is considered :

- An optimization step with the ordinary gradient with respect to the deterministic parameters,
- An optimization step with the natural gradient with respect to the variational distributions.

specifications of the MO-DGP model

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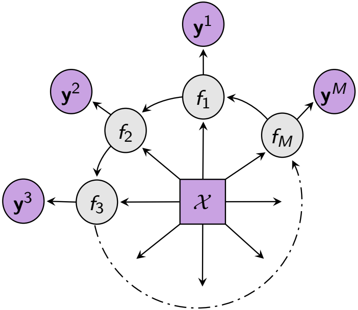

Complexity

The computational complexity of the model is :

$$\mathcal{O}(SMNK^2)$$

where : S is the number of samples used for the evaluation of the ELBO,
M is the number of objectives,
N is the number of training inputs,
K is the number of inducing inputs.

Analytic multi-objective problem

dtlz1a [Deb, 2001] is defined for $\mathbf{x} \in [0,1]^6$:

$$\left|\begin{array}{lll} \text{Min} & f_1(\mathbf{x}) & = -0.5x_1\left(1+g(x)\right) \\ \text{Min} & f_2(\mathbf{x}) & = -0.5(1-x_1)\left(1+g(x)\right) \\ \text{with} & g(\mathbf{x}) & = 100\left[5+\sum_{i=2}^{6}(x_i-0.5)^2+\cos\left(2\pi(x_i-0.5)\right)\right] \end{array}\right.$$

- Initial DoE : 30 initial points using a Latin Hypercube sampling,
- Added points : 60,
- EHVI criterion optimized with a parallel differential evolution algorithm.

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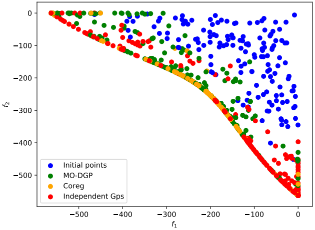

Approximated Pareto Fronts

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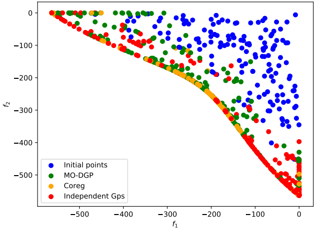
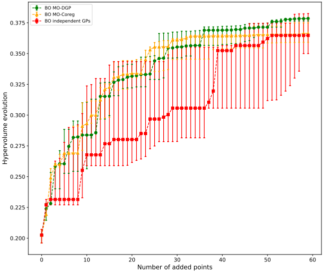
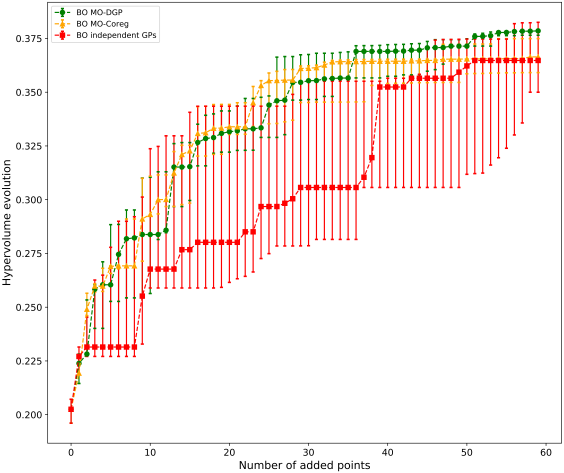


Approximated Pareto Fronts



Hypervolume evolution according to the added points

Analytic multi-objective problem



Hypervolume evolution according to the number of added points

Analytic multi-objective problem

Kursawe [Kursawe, 1990] is defined for $\mathbf{x} \in [-5, 5]^3$:

$$\left| \begin{array}{lll} \text{Min} & f_1(\mathbf{x}) & = \sum_{i=1}^{2} \left[-10 \exp\left(-0.5 \sqrt{x_i - 2 + x_{i+1}^2} \right) \right] \\ \text{Min} & f_2(\mathbf{x}) & = \sum_{i=1}^{3} \left[|x_i|^{0.8} + 5 \sin(x_i^3) \right] \end{array} \right.$$

- Initial DoE : 15 initial points using a Latin Hypercube sampling,
- Added points : 20,
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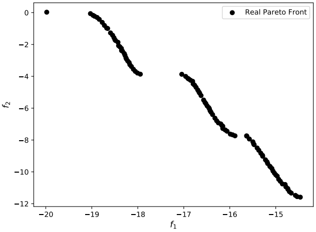

Exact Pareto Front

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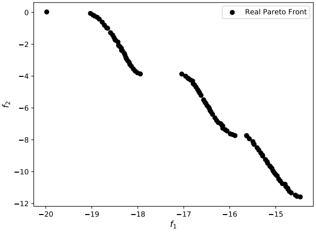

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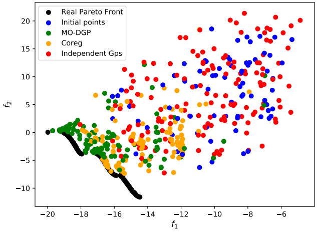
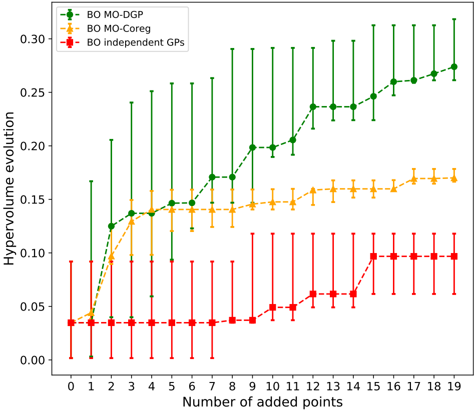


Solutions of the different MO-BO approaches.

Analytic multi-objective problem



Hypervolume evolution according to the number of added points

Analytic multi-objective problem

Kursawe 10D is defined for $\mathbf{x} \in [-5, 5]^10$:

$$\left| \begin{array}{lll} \text{Min} & f_1(\mathbf{x}) & = \sum_{i=1}^{9} \left[-10 \exp \left(-0.5 \sqrt{x_i - 2 + x_{i+1}^2} \right) \right] \\ \text{Min} & f_2(\mathbf{x}) & = \sum_{i=1}^{10} \left[|x_i|^{0.8} + 5 \sin(x_i^3) \right] \end{array} \right.$$

- Initial DoE : 50 initial points using a Latin Hypercube sampling,
- Added points : 85,
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Analytic multi-objective problem

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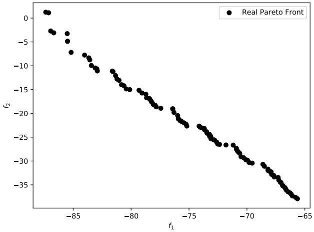

Exact Pareto Front

Analytic multi-objective problem

Kursawe 10D is defined for $\mathbf{x} \in [-5, 5]^{1}0$:

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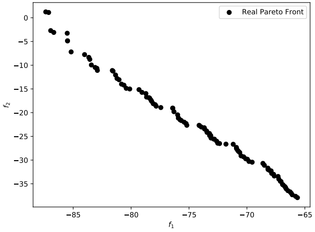

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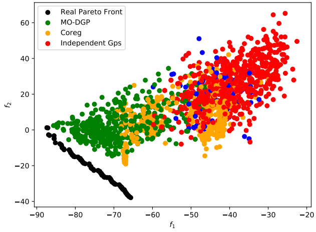

Solutions of the different MO-BO approaches.

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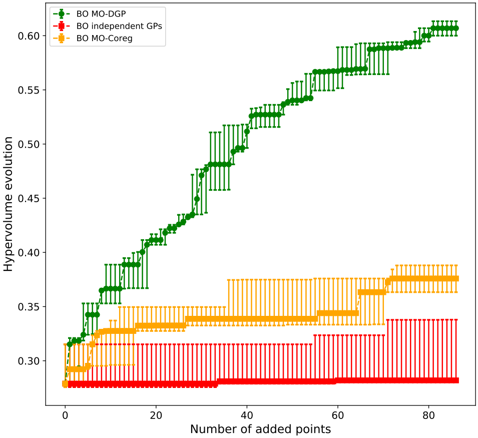

Hypervolume evolution according to the added points

Summary

Comparison of the **average** hypervolume obtained by different approaches and for the same number of evaluations :

Algorithms	dtlz1a (90 eval)	Kursawe 3D (35 eval)	Kursawe 10D (140 eval)
MO-DGP	**0.3791**	**0.2976**	**0.6084**
MO-Coreg	0.3659	0.19429	0.3846
MO-GP	0.3621	0.13361	0.30764

Comparison of the hypervolume **standard deviation** obtained by different approaches and for the same number of evaluations :

Algorithms	dtlz1a (90 eval)	Kursawe 3D (35 eval)	Kursawe 10D (140 eval)
MO-DGP	**0.00407**	0.05213	**0.01127**
MO-Coreg	0.00983	**0.05041**	0.04088
MO-GP	0.02197	0.06034	0.03268

Conclusions

- Proposition of a Deep Gaussian Process multi-objective model, taking into account the correlations between objectives,
- Experimentations on analytical functions confirm the efficiency of the proposed model compared to coregionalization GP approach and independent GPs.
- MO-DGP is a more efficient model but the complexity to train the model is more important that regular GPs. Hence, it is more interesting for computationally expensive problems.

Future works :

- Derivation of an EHVI taking into account the correlations exhibited by the MO-DGP model,
- Application of the model to problems with over three objectives,
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Thank you for your attention !

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