EFISUR

A sampling criterion for constrained bayesian optimization with uncertainties

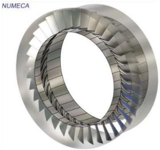
Céline Helbert

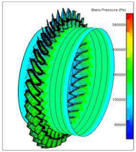
Joint work with **Reda El Amri**, Adrien Spagnol, Delphine Sinoquet (IFPEN), Rodolphe Le Riche (EMSE - LIMOS), **Noé Fellmann**, Christophette Blanchet (ECL - ICJ) and Sébastien Da Veiga (ENSAI).

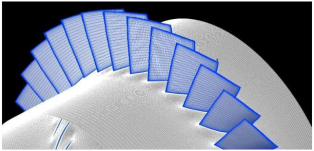
Test case : the NASA rotor 37, a representative transonic axial-flow compressor

Industrial Problem

- How to design the blades to have optimum performances ?
- Under some uncertainties (manufacturing + external conditions)
- And constraints (manufacturing and design practices)



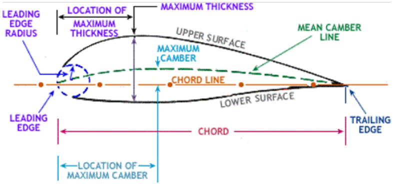


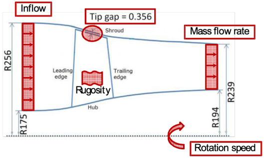


Test case : the NASA rotor 37, a representative transonic axial-flow compressor

Inputs

- 20 design variables, i.e. 5 shape parameters at 4 control points : the chord, the maximum thickness, the location of this maximum, the pitch angle, the sweep (sketched as α)
- 7 uncertain variables : 2 manufacturing uncertainties (tip gap, rugosity on the blade), 3 Inflow uncertainties (pressure, temperature, azimuthal momentum), 2 operational uncertainties (flow rate, rotation speed)





Sketch of the configuration

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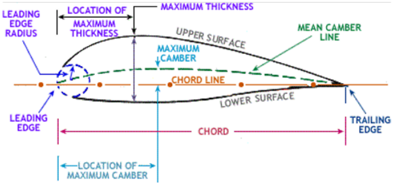
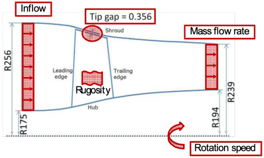
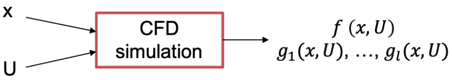




Sketch of the configuration

Scalar outputs

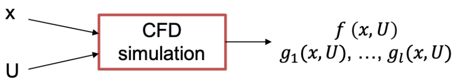
- Objective function : polytropic efficiency (to be maximized)
- Constraints : inlet and outlet flow angles, deceleration, etc.



Problem formulation taking into account uncertainty

$$\min_{\mathbf{x}\in\mathcal{S}_{\mathcal{X}}\subset\mathbb{R}^d} \mathbb{E}[f(\mathbf{x},\mathbf{U})] \quad \text{s.t.} \quad \mathbb{P}(g_1(\mathbf{x},\mathbf{U}) \leq 0, \dots, g_l(\mathbf{x},\mathbf{U}) \leq 0) \geq 1-\alpha$$

with $\alpha = 5\%$ and $\mathbf{U} \sim \rho_{\mathcal{U}}$ with support $\mathcal{S}_{\mathcal{U}} \subset \mathbb{R}^m$



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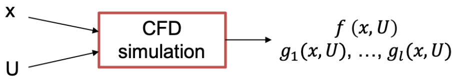
Equivalent formulation

$$\min_{\mathbf{x}\in\mathcal{S}_{\mathcal{X}}} \quad z(\mathbf{x}) \quad \text{s.t.} \quad c(\mathbf{x})\leq 0$$

where $z(\mathbf{x}) = \mathbb{E}[f(\mathbf{x},\mathbf{U})]$ and $c(\mathbf{x}) = 1-\alpha-\mathbb{E}[\mathbb{1}_{\{g_i(\mathbf{x},\mathbf{U})\leq 0,\ i=1,\dots,l\}}]$.



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Objective

- Solve this problem through Bayesian Optimization
- Choose a convenient Gaussian process modeling and a relevant acquisition function

Outline

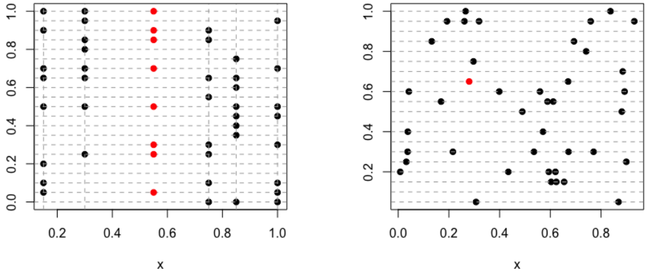
Recall of the problem formulation

$$\min_{\mathbf{x}\in\mathcal{S}_{\mathcal{X}}} \quad z(\mathbf{x}) \quad \text{s.t.} \quad c(\mathbf{x}) \leq 0$$

where $z(\mathbf{x}) = \mathbb{E}[f(\mathbf{x},\mathbf{U})]$ and $c(\mathbf{x}) = 1 - \alpha - \mathbb{E}[\mathbb{1}_{\{g_i(\mathbf{x},\mathbf{U})\leq 0,\ i=1,\ldots,l\}}]$.

Remark

- Building surrogate models for z (espectation over $\mathbf{U}$) and c (probability over $\mathbf{U}$) would need too many computer code evaluations (Monte Carlo).
- We build surrogate models for f and $g_1, \ldots, g_l$ directly in the joint space $\mathcal{S}_{\mathcal{X}} \times \mathcal{S}_{\mathcal{U}}$. Surrogate models for z and c are then deduced.



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Assume: f and $g_1, ..., g_l$ are realization of independent Gaussian processes F and G_i such that

$$F(\mathbf{x},\mathbf{u}) \sim \mathcal{GP}(m_F(\mathbf{x},\mathbf{u}), k_F(\mathbf{x},\mathbf{u},\mathbf{x}',\mathbf{u}')),$$
$$\forall i = \{1,\dots,l\}\ ,\ G_i(\mathbf{x},\mathbf{u}) \sim \mathcal{GP}(m_{G_i}(\mathbf{x},\mathbf{u}), k_{G_i}(\mathbf{x},\mathbf{u},\mathbf{x}',\mathbf{u}')),$$

Let $F^{(t)}$ and $G_i^{(t)}$ denote the Gaussian processes conditioned on the t observations obtained at points $D^{(t)} = \{(\mathbf{x}_k,\mathbf{u}_k)\ ,\ k = 1,..,t\}$.

Surrogate model for z :

$$Z^{(t)}(\mathbf{x}) = \int_{\mathbb{R}^m} F^{(t)}(\mathbf{x}, \mathbf{u}) \rho_{\mathbf{U}}(\mathbf{u}) d\mathbf{u}$$

remark : Z is still a Gaussian process with known mean and known covariance function given by :

$$m_Z^{(t)}(\mathbf{x}) = \int_{\mathbb{R}^m} m_F^{(t)}(\mathbf{x}, \mathbf{u}) \rho_{\mathbf{U}}(\mathbf{u}) d\mathbf{u},$$

$$k_Z^{(t)}(\mathbf{x}, \mathbf{x}') = \iint_{\mathbb{R}^{2m}} k_F^{(t)}(\mathbf{x}, \mathbf{u}, \mathbf{x}', \mathbf{u}') \rho_{\mathbf{U}}(\mathbf{u}, \mathbf{u}') d\mathbf{u} d\mathbf{u}'.$$

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Surrogate model for c :

$$C^{(t)}(\mathbf{x}) = 1 - \alpha - \int_{\mathbb{R}^m} \mathbb{1}_{\cap_{i=1}^{l} \{ G_i^{(t)}(\mathbf{x}, \mathbf{u}) \leq 0 \}} \rho_{\mathbf{U}}(\mathbf{u}) d\mathbf{u}$$

remark : $C^{(t)}$ is not Gaussian anymore !

Algorithm Data-driven optimization in the joint space

Create an initial Design of Experiments (DoE) of size t in the joint space and calculate simulator responses:
$D^{(t)} = \{(\mathbf{x}_i, \mathbf{u}_i)\ ,\ i = 1, \ldots, t\}$, and associated $f^{(t)}$ and $g_i^{(t)}$
while $t\ \leq$ maximum budget **do**
    Create the GPs of the objective and the constraints in the joint space: $F^{(t)}$ and $(G_i^{(t)})_{i=1}^{l}$
    Calculate the processes $Z^{(t)}$ and $C^{(t)}$ in the search space $\mathcal{S}_{\mathcal{X}}$
    Select $(\mathbf{x}_{t+1}, \mathbf{u}_{t+1})$ based on $Z^{(t)}$ and $C^{(t)}$
    Calculate simulator responses at the next point $(\mathbf{x}_{t+1}, \mathbf{u}_{t+1})$
    Update the DoE:
    $D^{(t+1)} = D^{(t)} \cup (\mathbf{x}_{t+1}, \mathbf{u}_{t+1})\ ,\ f^{(t+1)} = f^{(t)} \cup f(\mathbf{x}_{t+1}, \mathbf{u}_{t+1}),$
    $g_i^{(t+1)} = g_i^{(t)} \cup g_i(\mathbf{x}_{t+1}, \mathbf{u}_{t+1})\ ,\ i = 1, \ldots, l\ ,\ t \leftarrow t + 1$
end while
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    Set $n = n + 1$
end while
end

Outline

General principle for robust global optimization algorithms

Define a progress measure $P(x)$ in relation with the problem formulation and calculated from the GPs trajectories

- $\mathbf{x}_{\text{targ}} = \arg\max_{\mathbf{x} \in \mathcal{S}_{\mathcal{X}}} \mathbb{E}\left(P^{(t)}(\mathbf{x})\right)$
- $(\mathbf{x}_{t+1}, \mathbf{u}_{t+1}) = \arg\min_{(\tilde{\mathbf{x}}, \tilde{\mathbf{u}}) \in \mathcal{S}_{\mathcal{X}} \times \mathcal{S}_{\mathcal{U}}} \mathbb{VAR}\left(P^{(t+1)}(\mathbf{x}_{\text{targ}})\right)$ where $P^{(t+1)}$ is evaluated with GPs updated according to $D^{(t+1)} = D^{(t)} \cup \{(\tilde{\mathbf{x}}, \tilde{\mathbf{u}})\}$.

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What is a natural choice for $P(x)$?

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What is a natural choice for $P(x)$? Feasible Improvement

$$FI^{(t)}(\mathbf{x}) = I^{(t)}(\mathbf{x})\ \mathbb{1}_{\{C^{(t)}(\mathbf{x})\leq 0\}}\ ,$$

where $I^{(t)}(x) = \left(z_{\min}^{\text{feas}} - Z^{(t)}(\mathbf{x})\right)^{+}$ denotes the improvement over the current feasible minimum value defined as $z_{\min}^{\text{feas}} = \min_{\mathbf{x}\in\mathcal{X}_t} m_Z^{(t)}(\mathbf{x})$ s.t. $\mathbb{E}[C^{(t)}(\mathbf{x})] \leq 0$.

Main steps of the EFISUR algorithm - first step

$$\mathbf{x}_{\text{targ}} = \arg\max_{\mathbf{x}\in\mathcal{S}_{\mathcal{X}}} \mathbb{E}\left(FI^{(t)}(\mathbf{x})\right). \quad (1)$$

Because of the independence of Z and C,

$$\mathbb{E}\left(FI^{(t)}(\mathbf{x})\right) = \mathrm{EI}^{(t)}(\mathbf{x})\mathbb{P}(C^{(t)}(\mathbf{x}) \leq 0)$$

.

- $\mathrm{EI}^{(t)}(\mathbf{x}) = (z_{\min}^{\text{feas}} - m_Z^{(t)}(\mathbf{x}))\Phi\left(\frac{z_{\min}^{\text{feas}} - m_Z^{(t)}(\mathbf{x})}{\sigma_Z^{(t)}(\mathbf{x})}\right) + \sigma_Z^{(t)}(\mathbf{x})\phi\left(\frac{z_{\min}^{\text{feas}} - m_Z^{(t)}(\mathbf{x})}{\sigma_Z^{(t)}(\mathbf{x})}\right)$,
- $\mathbb{P}(C^{(t)}(\mathbf{x}) \leq 0)$ can be approximated with available numerical methods.

Main steps of the EFISUR algorithm - second step

Minimize the variance of the one-step-ahead feasible improvement

$$(\mathbf{x}_{t+1}, \mathbf{u}_{t+1}) = \arg \min_{(\tilde{\mathbf{x}},\tilde{\mathbf{u}}) \in \mathcal{S}_{\mathcal{X}} \times \mathcal{S}_{\mathcal{U}}} \mathbb{VAR}\left(I^{(t+1)}(\mathbf{x}_{\text{targ}}) \; \mathbb{1}_{\{C^{(t+1)}(\mathbf{x}_{\text{targ}}) \leq 0\}} \right),$$

As it is too difficult, this problem is replaced by the following

$$\mathbf{u}_{t+1} = \arg \min_{\tilde{u} \in \mathcal{S}_{\mathcal{U}}} \; \mathbb{VAR}\big(\big(z_{\min}^{\text{feas}} - Z^{(t+1)}(\mathbf{x}_{\text{targ}})\big)^+\big) \int_{\mathbb{R}^m} \mathbb{VAR}\big(\mathbb{1}_{\cap_{i=1}^{l}\{G_i^{(t+1)}(\mathbf{x}_{\text{targ}},\mathbf{u}) \leq 0\}}\big) \rho_{\mathbf{U}}(\mathbf{u}) d\mathbf{u}$$

with GPs updated according to $D^{(t+1)} = D^{(t)} \cup \{(\mathbf{x}_{\text{targ}}, \tilde{\mathbf{u}})\}$.

Our algorithm : EFISUR

Algorithm Data-driven optimization in the joint space

Create an initial Design of Experiments (DoE) of size t in the joint space and calculate simulator responses:
$D^{(t)} = \{(\mathbf{x}_i, \mathbf{u}_i)\ ,\ i = 1, \dots, t\}$, and associated $f^{(t)}$ and $g_i^{(t)}$
while $t\ \leq$ maximum budget **do**
    Create the GPs of f and $g_1, ..., g_l$ in the joint space: $F^{(t)}$ and $(G_i^{(t)})_{i=1}^{l}$
    Calculate the processes $Z^{(t)}$ and $C^{(t)}$ in the search space $\mathcal{S}_{\mathcal{X}}$
    Optimize $\mathbb{E}\left(FI^{(t)}\right)$ and set $\mathbf{x}_{t+1} = \mathbf{x}_{\text{targ}}$ such that

$$\mathbf{x}_{\text{targ}} = \arg\max_{\mathbf{x} \in \mathcal{S}_{\mathcal{X}}} \text{EFI}^{(t)}(\mathbf{x})$$

    Sample the next uncertain point by solving

$$\mathbf{u}_{t+1} = \arg\min_{\tilde{u} \in \mathcal{S}_{\mathcal{U}}} S(\mathbf{x}_{\text{targ}}, \tilde{u})$$

    Calculate simulator responses at the next point $(\mathbf{x}_{t+1}, \mathbf{u}_{t+1})$
    Update the DoE:
    $D^{(t+1)} = D^{(t)} \cup (\mathbf{x}_{t+1}, \mathbf{u}_{t+1})\ ,\ f^{(t+1)} = f^{(t)} \cup f(\mathbf{x}_{t+1}, \mathbf{u}_{t+1}),$
    $g_i^{(t+1)} = g_i^{(t)} \cup g_i(\mathbf{x}_{t+1}, \mathbf{u}_{t+1})\ ,\ i = 1, \dots, l\ ,\ t \leftarrow t+1$
end while

Outline

A first competitive algorithm : EFIrand

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$$\mathbf{x}_{\text{targ}} = \arg\max_{\mathbf{x} \in \mathcal{S}_{\mathcal{X}}} \text{EFI}^{(t)}(\mathbf{x})$$

    Sample the next uncertain point randomly, $\mathbf{u}_{t+1} \sim \rho_{\mathbf{U}}$
    Calculate simulator responses at the next point $(\mathbf{x}_{t+1}, \mathbf{u}_{t+1})$
    Update the DoE:
        $D^{(t+1)} = D^{(t)} \cup (\mathbf{x}_{t+1}, \mathbf{u}_{t+1})\ ,\ f^{(t+1)} = f^{(t)} \cup f(\mathbf{x}_{t+1}, \mathbf{u}_{t+1})$,
        $g_i^{(t+1)} = g_i^{(t)} \cup g_i(\mathbf{x}_{t+1}, \mathbf{u}_{t+1})\ ,\ i = 1, \dots, l\ ,\ t \leftarrow t + 1$
end while
end

A second competitive algorithm : cEIdevNum

Algorithm Data-driven optimization in the joint space

1: Create an initial Design of Experiments (DoE) of size t in the joint space and calculate simulator responses:
2: $D^{(t)} = \{(\mathbf{x}_i, \mathbf{u}_i)\ ,\ i = 1, \ldots, t\}$, and associated $f^{(t)}$ and $g_i^{(t)}$
3: **while** $t \leq$ maximum budget **do**
4: Create the GPs of f and $g_1, ..., g_l$ in the joint space: $F^{(t)}$ and $(G_i^{(t)})_{i=1}^{l}$
5: Calculate the GP of the mean objective, $Z^{(t)}$, in the search space $\mathcal{S}_{\mathcal{X}}$
6: **Optimize** the EI under quantile constraints :

$$\mathbf{x}_{t+1} = \arg\max_{\mathbf{x} \in \mathcal{S}_{\mathcal{X}}} \mathrm{EI}^{(t)}(\mathbf{x}) \text{ s. t. } \forall i \in \{1, \ldots, l\},\ q_{1-\alpha/l}(m_{G_i}^{(t)}(\mathbf{x}, \mathbf{U})) \leq 0$$

7: **Sample** the next uncertainty by minimizing the deviation number,

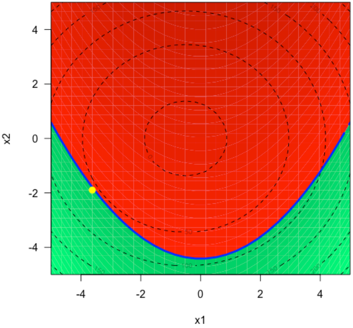
$$\mathbf{u}_{t+1} = \arg\min_{\mathbf{u}} \min_{i=1,\ldots,l} \frac{|m_{G_i^{(t)}}(\mathbf{x}_{t+1}, \mathbf{u})|}{\sigma_{G_i}^{(t)}(\mathbf{x}_{t+1}, \mathbf{u})}$$

8: Calculate simulator responses at the next point $(\mathbf{x}_{t+1}, \mathbf{u}_{t+1})$
9: Update the DoE:
10: **end while**
11: **end**

The problem is the following:

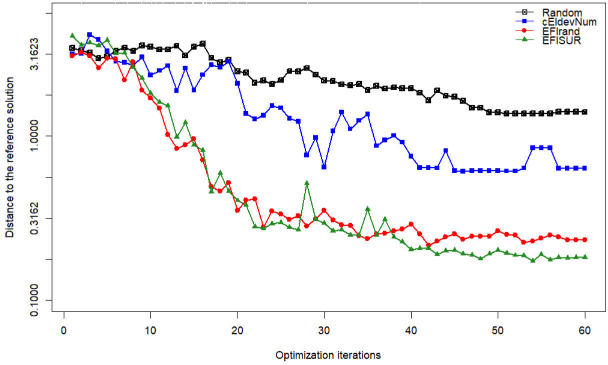
$$f(\mathbf{x},\mathbf{u}) = 5(x_1^2+x_2^2) - (u_1^2+u_2^2) + x_1(u_2-u_1+5) + x_2(u_1-u_2+3)$$

$$g(\mathbf{x},\mathbf{u}) = -x_1^2 + 5x_2 - u_1 + u_2^2 - 1$$

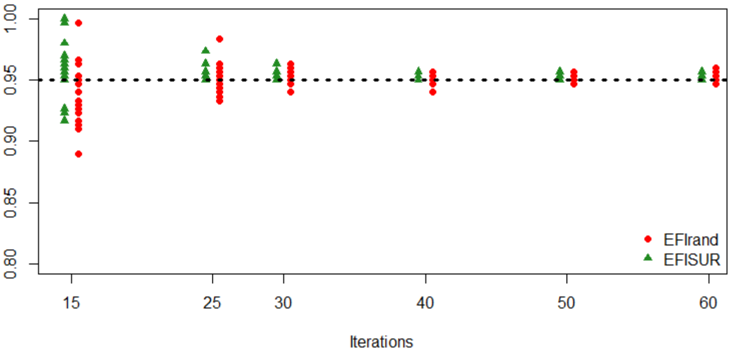


$$\text{minimize} \quad \mathbb{E}[f(\mathbf{x},\mathbf{U})] \text{ such that } \mathbb{P}(g(\mathbf{x},\mathbf{U}) \leq 0) \geq 1-\alpha$$

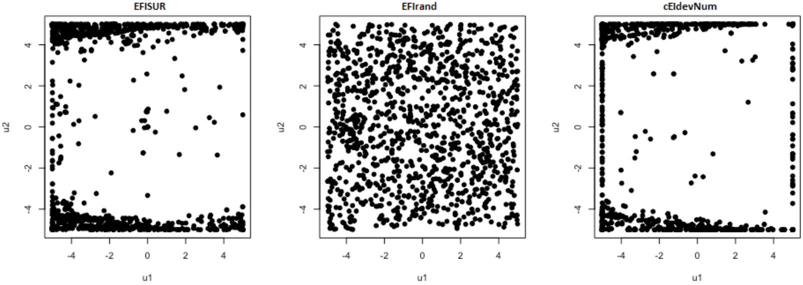
$$\text{with } \mathbf{x} \in [-5,5]^2, \mathbf{U} \sim \mathcal{U}([-5,5]^2)$$



Distance to the reference solution. The mean is calculated from 30 replications of the runs. Initial DOE are composed of 8 points.

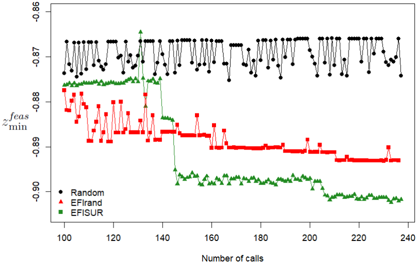


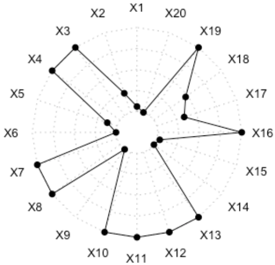
A posteriori probability of satisfying the constraint at the current "feasible" point $z_{\text{min}}^{\text{feas}}$ for different iterations of the `EFISUR` and `EFIrand` strategies. $z_{\text{min}}^{\text{feas}} = \min_{\mathbf{x} \in \mathcal{X}_t} m_Z^{(t)}(\mathbf{x})$ s.t. $\mathbb{E}[C^{(t)}(\mathbf{x})] \leq 0$.



Enrichment in the uncertain space, $\mathcal{S}_{\mathbf{U}}$, for the three methods.

SAFRAN test case:

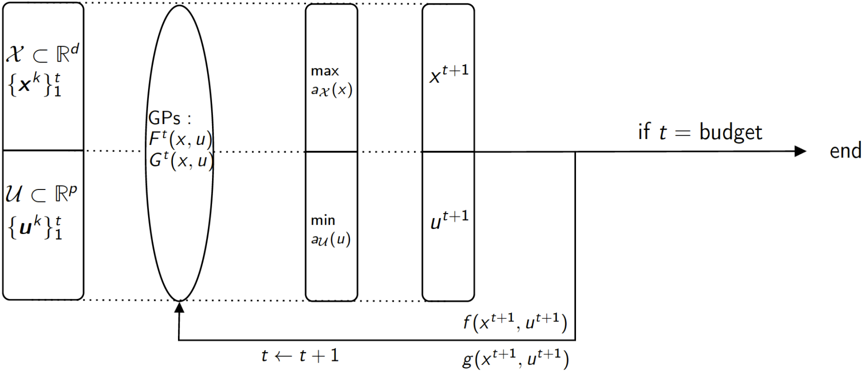




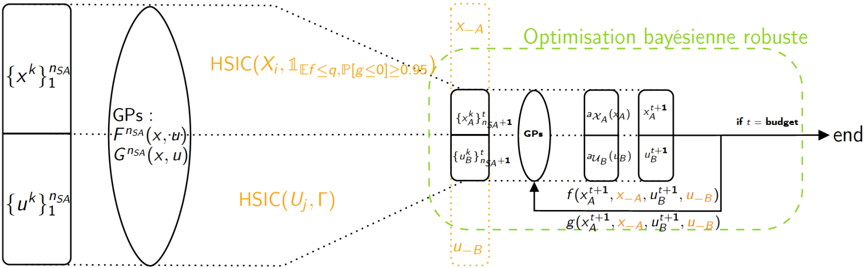
- Convergence history of the average objective function of the current feasible minimum, $z_{\text{min}}^{\text{feas}}$. Initial DOE are composed of 100 points in dimension 27.
- Relative coordinates of the optimal design with respect to their respective lower and upper bounds.

Outline

EFISUR global Schema



AS offline : dimension reduction before optimization



AS goal-oriented for x

$$HSIC(X_i, \mathbf{1}_{\mu_Z(X)\leq q, \mu_C(X)\leq 0})$$

where $Z_{\mathbf{x}}^{(t)} = \mathbb{E}[F_{(\mathbf{x},\mathbf{U})}^{(t)}]$

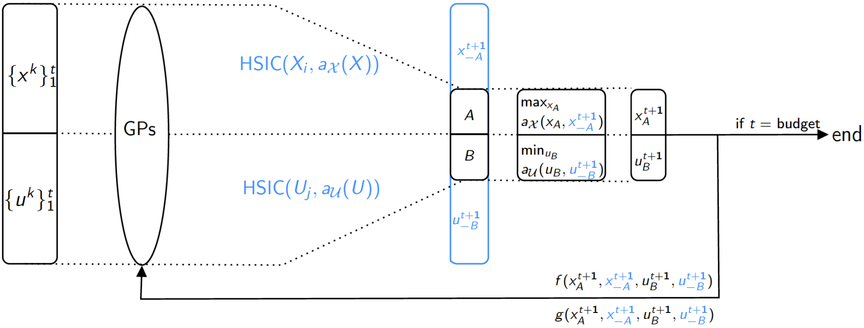
AS goal-oriented for U

$$HSIC(U_j, \tilde{\Gamma})$$

where
$\tilde{\Gamma} = \{\mathbf{x}, \mu_F(\mathbf{x},\mathbf{U}) \leq q, \mu_G(\mathbf{x},\mathbf{U}) \leq 0\}$

AS seq offline : One step of AS each 10 iterations

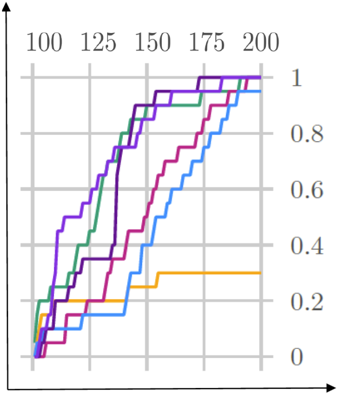
AS online - dimension reduction inside the optimization loop



Acquisition functions are the following :

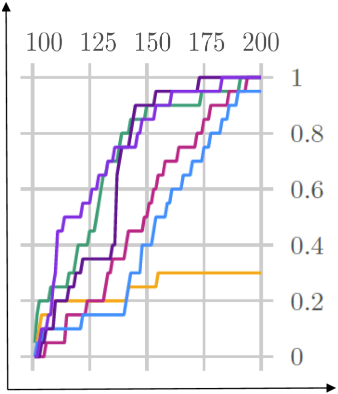
- $a_{\mathcal{X}}(\mathbf{x}) = \mathbb{E}[FI(\mathbf{x})]$
- $a_{\mathbf{U}} = S(\mathbf{U}) \approx \mathbb{VAR}[FI(\mathbf{U})]$

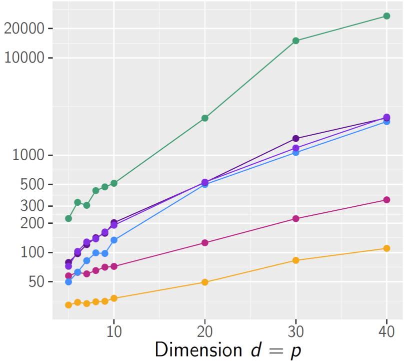
Comparison on a toy function - 10 design variables - 10 uncertain variables
EFISUR - AS offline - AS seq offline - AS online -



Percentage of runs (out of 20 runs) which have reached the target (95% of the lowest value) at iteration n.

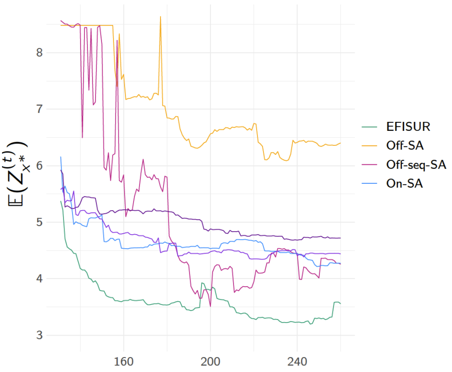
Comparison on a toy function - 10 design variables - 10 uncertain variables
EFISUR - AS offline - AS seq offline - AS online -





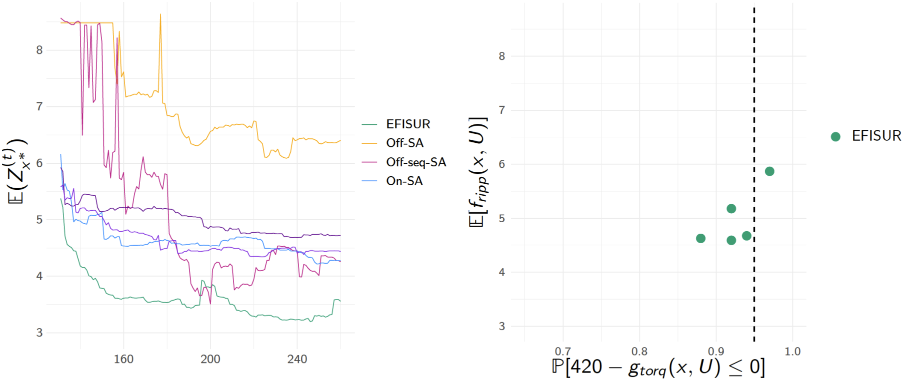
Percentage of runs (out of 20 runs) which have reached the target (95% of the lowest value) at iteration n.

Electrical machine - 12 design variables - 14 uncertain variables



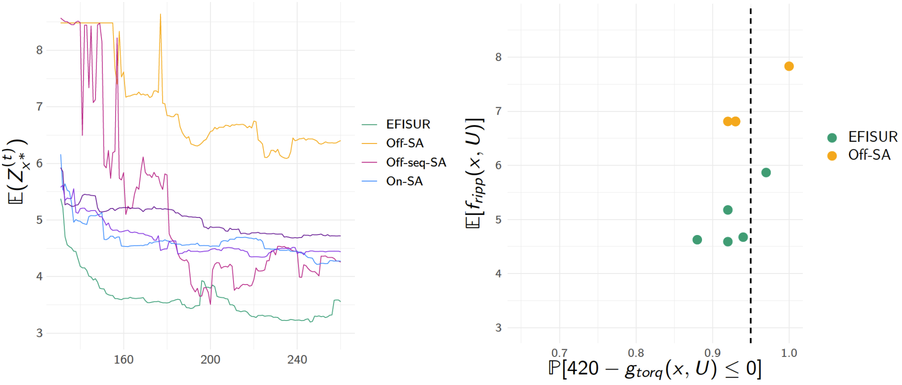
- Initial DOE : 130 points
- Number of iterations : 130 points

Electrical machine - 12 design variables - 14 uncertain variables



- Initial DOE : 130 points
- Number of iterations : 130 points
- Validation step : 100 model evaluations per design solution

Electrical machine - 12 design variables - 14 uncertain variables



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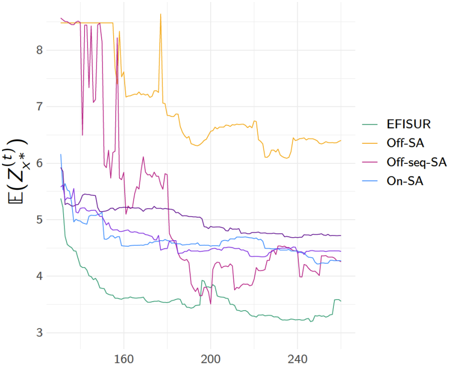

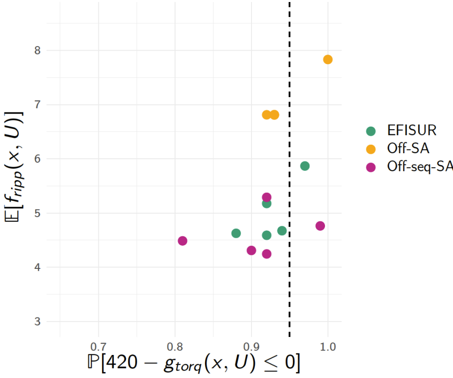

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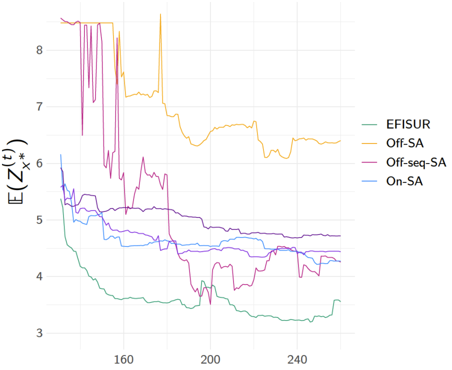

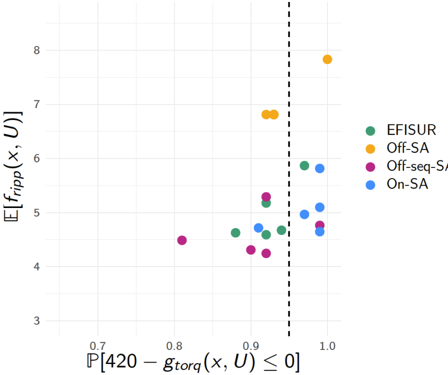

- Initial DOE : 130 points
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Conclusion and futur work

- GP in the joint space coupled to well designed acquisition functions leads to an efficient methodology
- Warning : too few samples in the uncertain space leads to a poor probability estimation. A validation step is necessary.
- In high dimension sensitivity analysis helps when applied sequentially.
- Futur Work : how to combine this complex optimization problem with multifidelity approaches ?

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Thank you for your attention