# High Dimensional Efficient Global Optimization via Multi-Fidelity Surrogate Modeling

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# Plan

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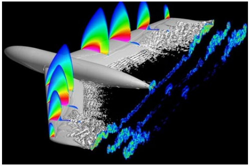
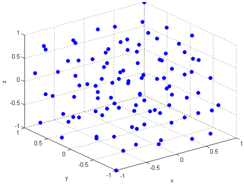
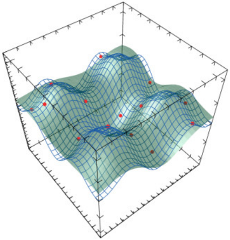
# Introduction



HF simulation [ONERA a]

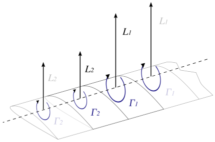


Design of Experiment

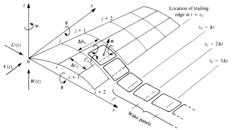


Surrogate model

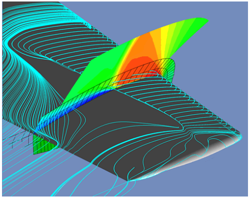
- High-Fidelity computer experiments are too expensive to perform direct Design Optimization, Sensitivity Analysis, Design Exploration...
- Surrogate models can be used to perform these tasks at lower computational costs.



Lifiting Line Theory



Vortex Lattice Method [Katz 2001]



RANS CFD [ONERA b]

– Reduce computational costs further: use lower fidelity knowledge to enhance high-fidelity models.

**Project objective:**

– Global optimization of an aerodynamic shape using multi-fidelity information sources.

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# Kriging

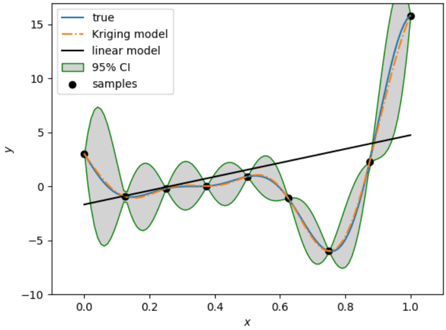



Figure: Mean and variance of a Kriging model

$$\hat{y}(x) = \underbrace{m(x)}_{\text{Regression term}} + Z(x;\theta)$$

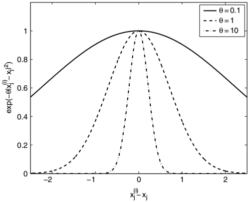



Figure: correlation model [Forrester 2008]

– The Kriging model considers the 'errors' as deviations to be modeled by a Gaussian Process through a correlation function.

# Multi-Fidelity co-Kriging

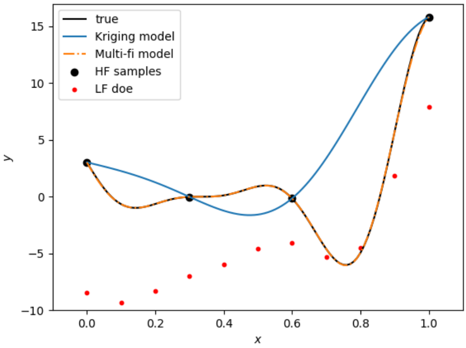
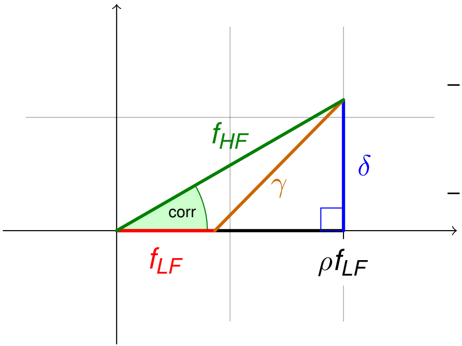



Figure: Multi-fidelity surrogate modeling illustration

– How to best use low-fidelity information to enhance the high-fidelity model?




– Additive formulation [Lewis 2000]

$$f_{HF}(x) = f_{LF}(x) + \gamma(x)$$

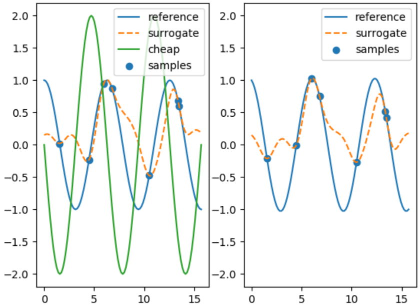
– Kennedy-O'Hagan [Kennedy 2001]

$$\begin{cases} f_{HF}(x) = \rho f_{LF}(x) + \delta(x) \\ f_{LF}(\cdot) \perp \delta(\cdot) \end{cases}$$

– The addition of the term $\rho$ makes the multi-fidelity learning more robust to poor correlation as well as differences in modelization.

Animation: evolution of model for increasing signal correlations

$$f_{HF}(x) = \rho f_{LF}(x) + \delta(x)$$




Functions definition for $\alpha \in [0, \pi/2]$:

$$f_{HF}(x) = \cos(x)$$
$$f_{LF}(x) = 2\cos(x + \alpha)$$

HF-LF correlation:

$$\mathrm{corr}(f_{HF}, f_{LF}) = cos(\alpha)$$

– The use of mutli-fidelity information sources reduces the amount of information to be retrieved by the highest fidelities.

Recursive formulation [Le Gratiet 2013]:

$$\mu_k = \rho_{k-1}\ \mu_{k-1} + \mu_{\delta_k}$$
$$\sigma_k^2 = \rho_{k-1}^2\ \sigma_{k-1}^2 + \sigma_{\delta_k}^2$$

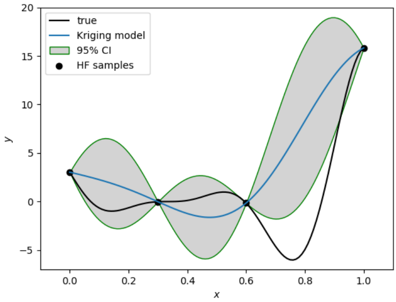
– Nested DOEs:

$$X_{HF} = X_l \subseteq X_{l-1} \ldots \subseteq X_0 = X_{LF}$$

* MFK [Vauclin 2014, OpenMDAO ]
* MFKPLS - MFKPLSK (high dimension)
* Analytical derivatives w.r.t design variables
* Noise Estimation
* Regression/ Re-interpolation
* multi-fidelity data pre-processing

Open source Python library: Surrogate Modeling Toolbox (SMT)
`https://github.com/SMTOrg/smt`

- **Gradient-based**: minimize the objective gradient norm.
- **Bayesian (gradient-free)**: minimize the expected deviation from the extremum of the studied function.



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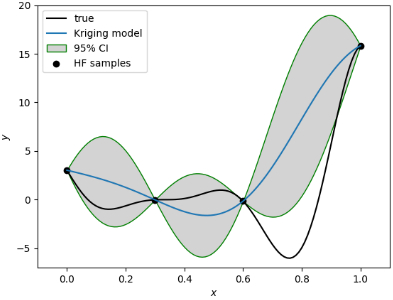
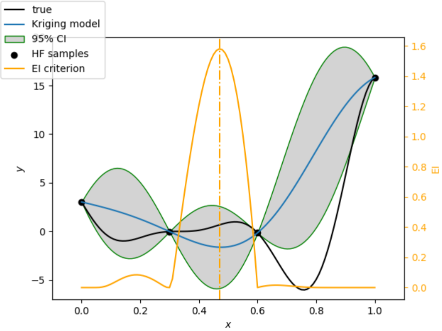



  – Prediction and uncertainty of the model are used in sequential strategies to balance Exploration/Exploitation
  – Bayesian optimization is a global optimization.

Efficient Global Optimization [Jones 1998]

– EI criterion [Močkus 1975]:

$$E[I(x)] = E[\max(f_{min} - Y, 0)]$$




– EI expresses a certain balance between Exploitation and Exploration based on the mean and variance of the Kriging model.

MFEGO:

- most promising point: EI criterion

$$x^* = \underset{x}{\operatorname{argmax}} \left( E[I(x)] \right)$$

- choice of levels of enrichment: trade-off information gain/cost

$$k^* = \underset{k \in (0,\dots,l)}{\operatorname{argmax}} \quad \frac{\sigma^2_{red}(k, x^*)}{f(c_k)}$$

MFEGO:

- most promising point: EI criterion

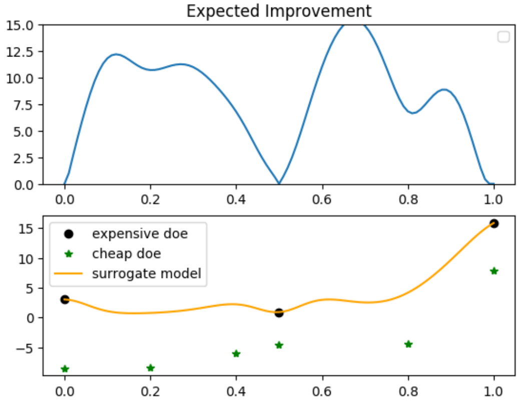
$$x^* = \underset{x}{\text{argmax}}\,(E[I(x)])$$

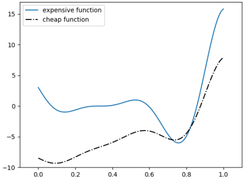
- choice of levels of enrichment: trade-off information gain/cost

$$k^* = \underset{k\in(0,\ldots,l)}{\text{argmax}} \quad \frac{\sigma^2_{red}(k, x^*)}{f(c_k)}$$

$\Rightarrow$ By using low-fidelity to reduce the uncertainty we reduce the Exploration contribution to the EI criterion

$\Rightarrow$ High-fidelity is used for Exploitation and model enhancement




$$f_{HF}(x) = (6x - 2)^2 \times \sin(2(6x - 2))$$
$$f_{LF}(x) = 0.5 f_{HF} + 10(x - 0.5) - 5$$

Cost ratio: 1/1000

| | HF | LF | Cost |
|---|---|---|---|
| MFEGO | 3+2 | 6+9 | 5.015 |
| EGO | 4+11 | - | 15 |

Table: Toy problem optimization summary

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# Airfoil shape optimization – Parametrization

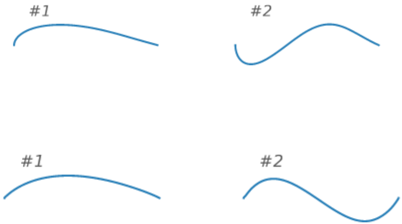


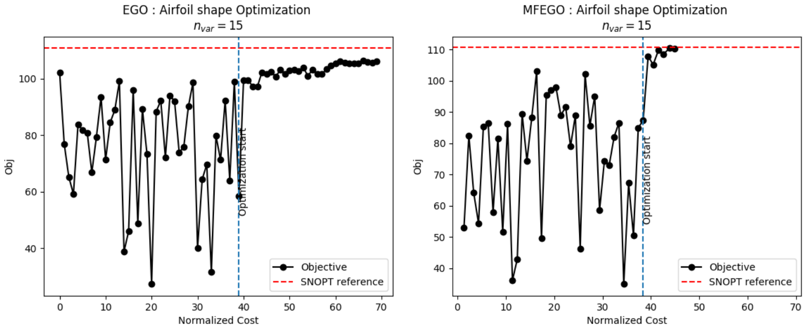

Figure: First thickness (above) and camber (below) modes [Li 2018]

Parametrization [Li 2018]: Mode decomposition of an airfoil database.
Up to 14 modes available (7 camber + 7 thickness modes).

* HF: RANS solver (ADflow)
* LF: Xfoil [Drela 1989]

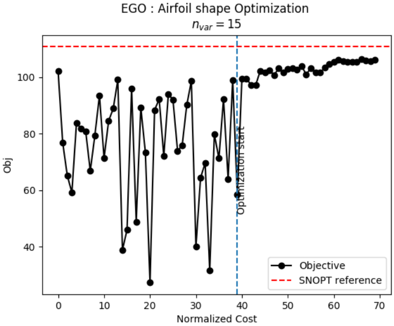
Cost ratio: 1/200
Reference: SNOPT [Gill 2005]

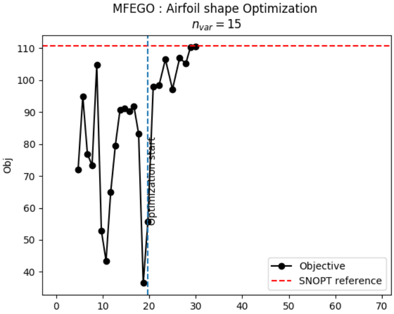
# Airfoil shape – Unconstrained optimization




- L/D maximization
- 15 design variables (7 camber + 7 thickness modes + AoA)

# Airfoil shape – Unconstrained optimization




- L/D maximization
- 15 design variables (7 camber + 7 thickness modes + AoA)

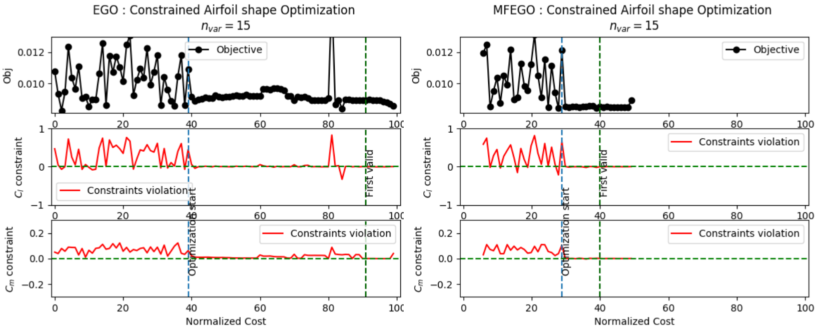
# Airfoil shape – Unconstrained optimization

| | HF | LF | Cost | Obj |
|---|---|---|---|---|
| EGO | 40 + 30 | - | 70 | 104.9 |
| MFEGO | 16 + 8 | 744 + 437 | 29.89 | 110.5 |
| SNOPT | 21 | - | 21 | 110.7 |

Table: Comparison of EGO and MFEGO for unconstrained optimization

- L/D maximization
- 15 design variables (7 camber + 7 thickness modes + AoA)

# Airfoil shape – Constrained optimization




– Use of SEGOMOE framework [Bartoli 2016]

- $C_d$ minimization
- $C_l$, $C_m$ equality constraints
- 15 design variables (7 camber + 7 thickness modes + AoA)

# Airfoil shape – Constrained optimization

| | HF | LF | Cost | Obj | Feasible | RMSCV |
|---|---|---|---|---|---|---|
| EGO | 40 + 60 | - | 100 | 89.188 | Yes | 8.8e-2 |
| MFEGO | 24 + 18 | 964 + 63 | 47.135 | 84.67 | Yes | 4.9e-3 |
| SNOPT | 73 | - | 73 | 84.68 | Yes | - |

Table: Comparison of EGO and MFEGO for constrained optimization

$$RMSCV = \sqrt{\frac{1}{N}\sum_{j=1}^{N}\left(val_j - target\right)^2}$$

– Use of SEGOMOE framework [Bartoli 2016]

- $C_d$ minimization
- $C_l$, $C_m$ equality constraints
- 15 design variables (7 camber + 7 thickness modes + AoA)

# Conclusion & Perspectives

This project has shown it is possible to use multi-fidelity information sources to:

- enhance surrogate models → MFK integration in SMT,
- alleviate dimensionality curse → MFKPLS – MFKPLSK,
- reduce global search cost (global optimizations) → MFEGO,
- find better results with lesser cost compared to EGO (and occasionally SNOPT) for multiple constrained and unconstrained problems → SEGOMOE framework extension.

– In progress: AIAA Aviation 2019 Conference abstract submission, aerostructural optimization test case.

Work can be done to improve the approach:

- hybrid models (a different model adapted to each level of fidelity)
- multi-fidelity mixture of experts,
- ...

Thank you for your attention!
Do you have any questions?

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