Gaussian process for Bayesian optimization with mixed hierarchical variables: Application to aircraft eco-design

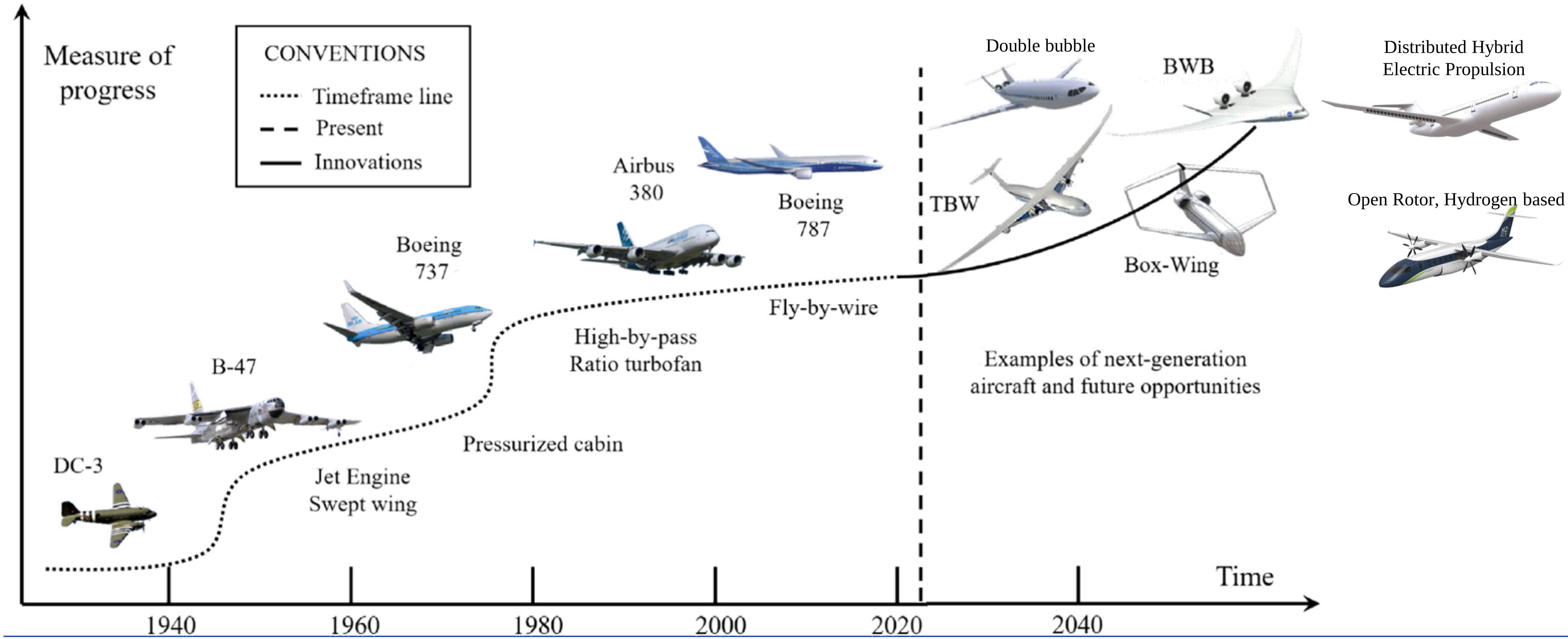
Paul Saves, *Eric Nguyen Van, Nathalie Bartoli, Thierry Lefebvre, Youssef Diouane, Joseph Morlier*

Thursday, June 20, 2024

Future aircraft concepts

Goals:

- Extend design space exploration and bring to light « unexpected » concepts
- Avoid the definition of sub optimal configurations



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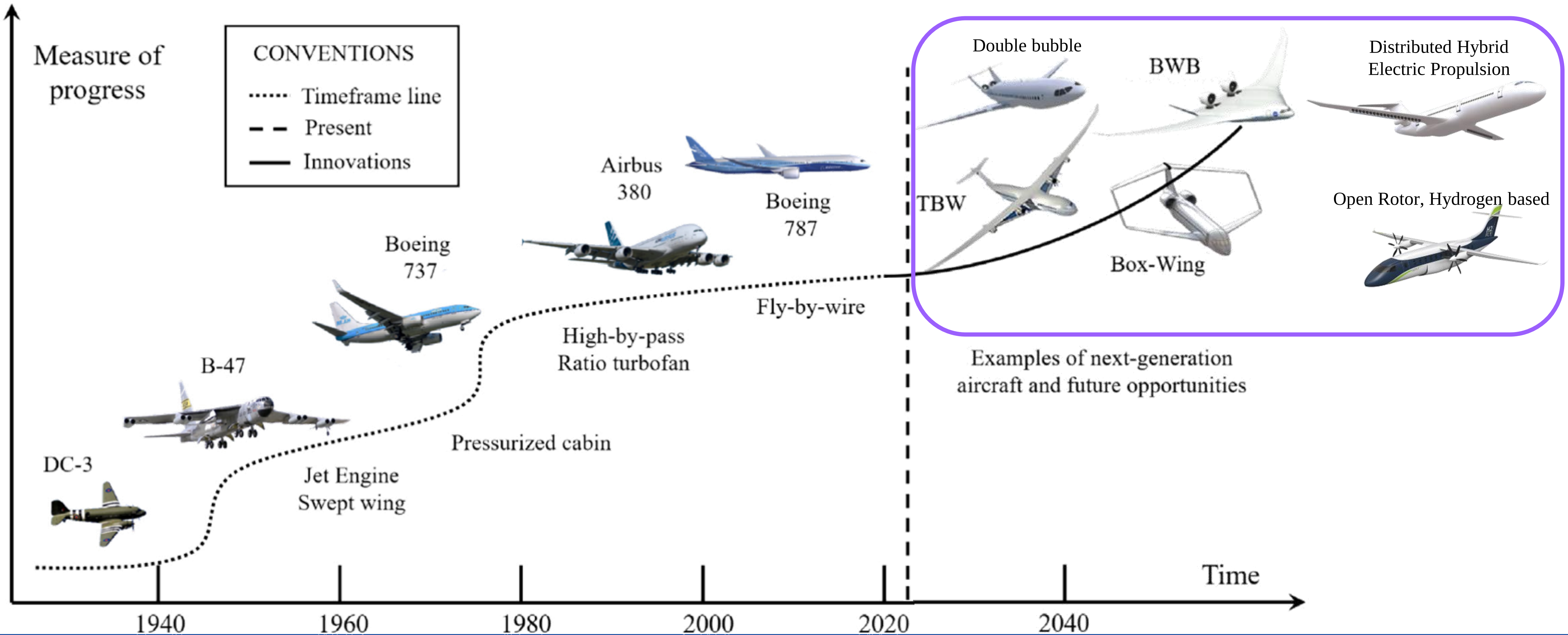

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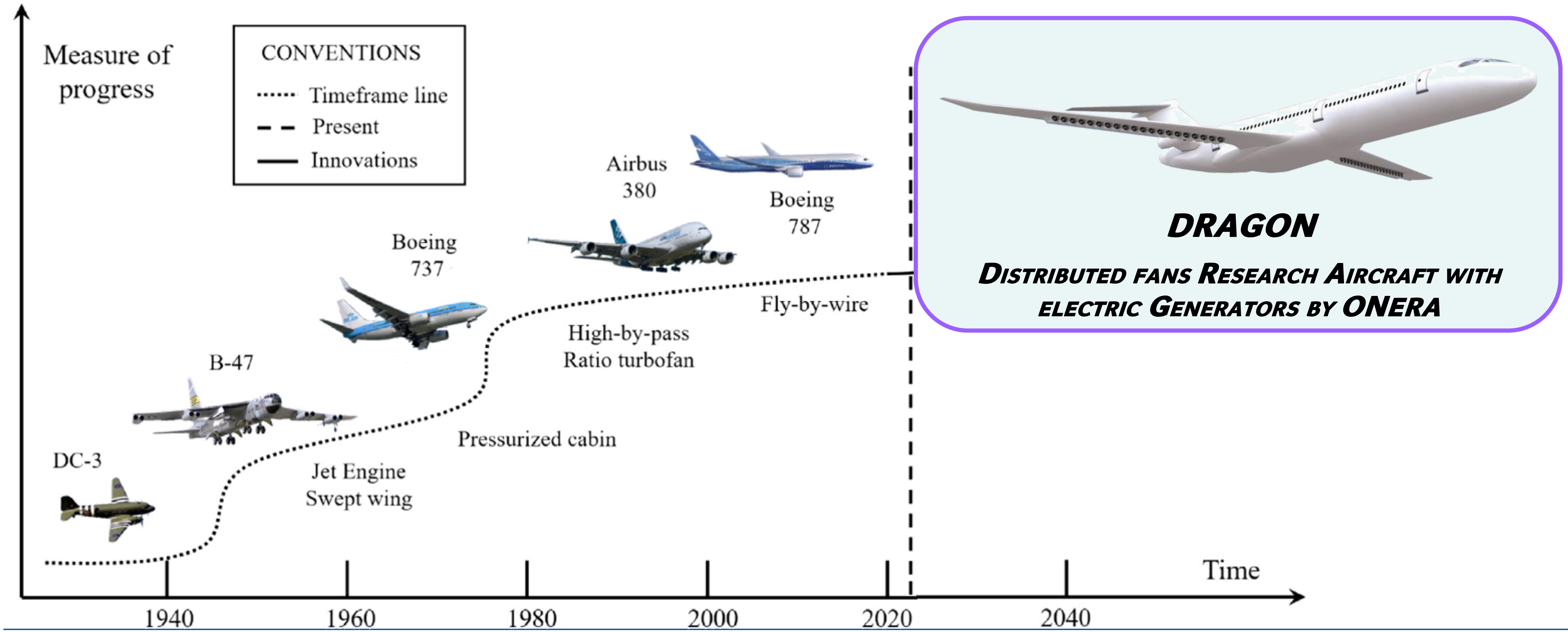

DRAGON

DISTRIBUTED FANS RESEARCH AIRCRAFT WITH ELECTRIC GENERATORS BY ONERA

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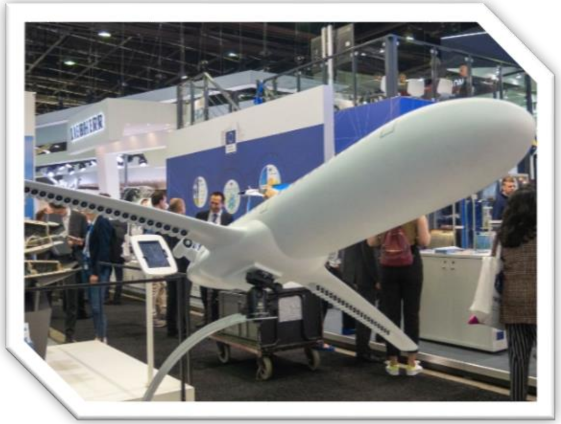
Towards a green aircraft design: DRAGON concept



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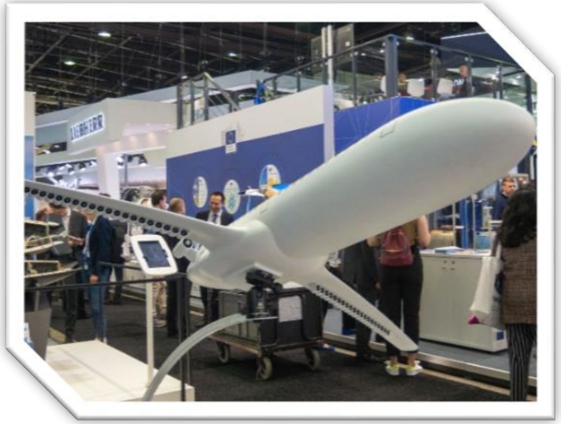
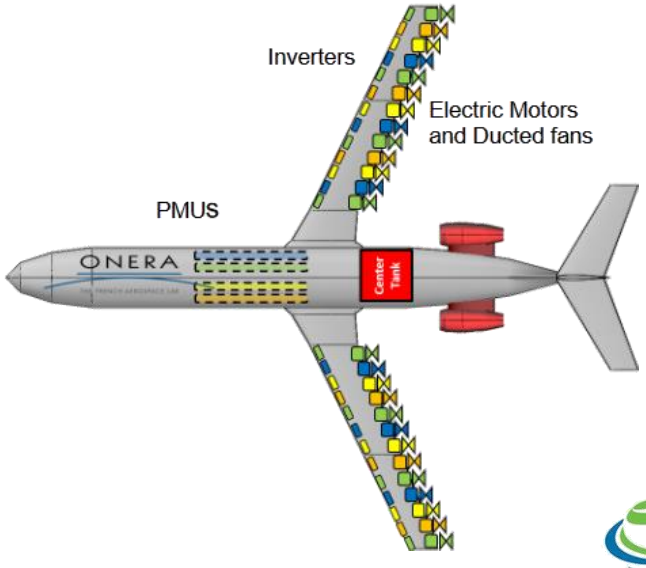
- 150 passengers over 2750 nautical miles
- Transonic cruise speed (Mach 0.78)





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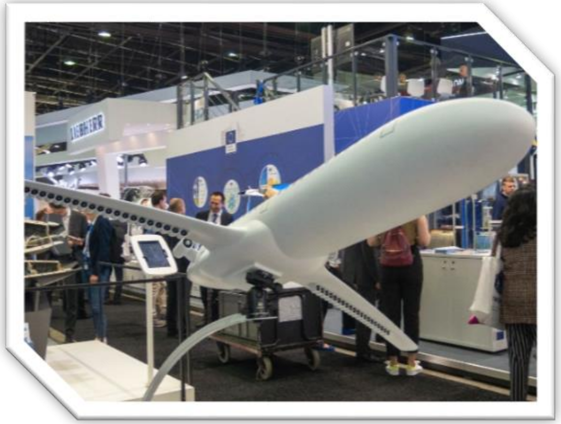

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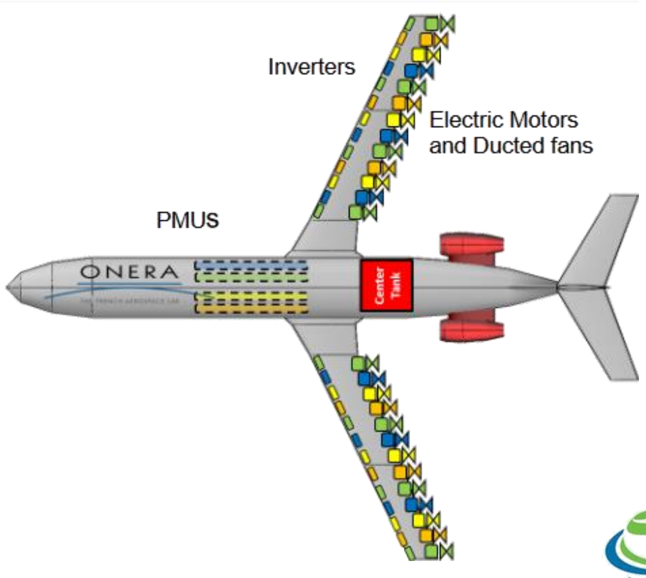

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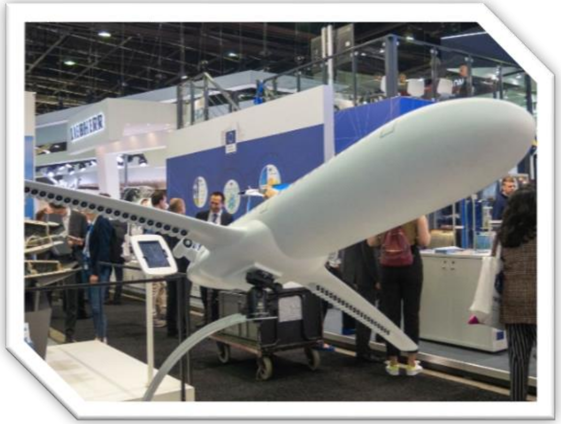

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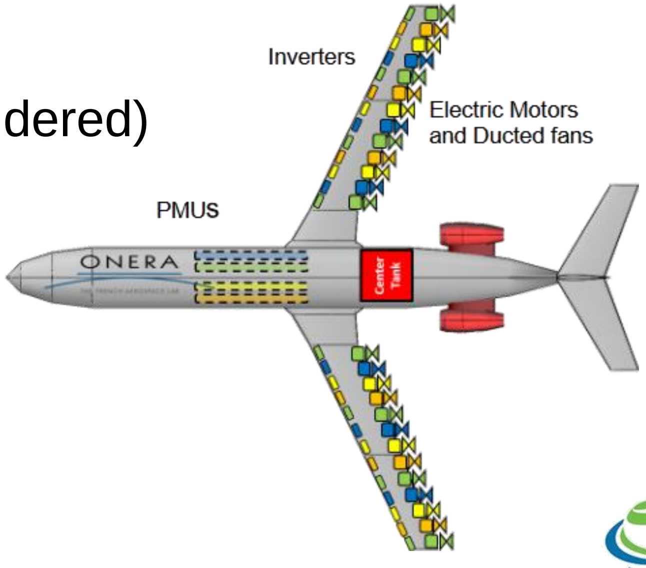
- 30% reduction of CO_2 emissions by 2035 (NO_x or contrails not considered)



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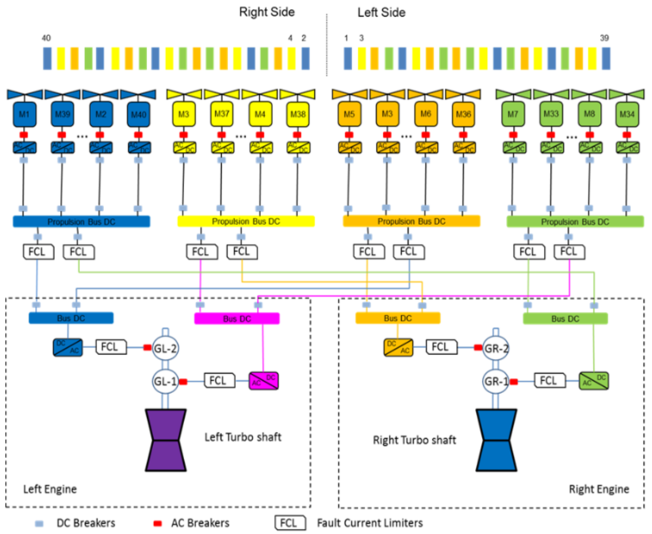
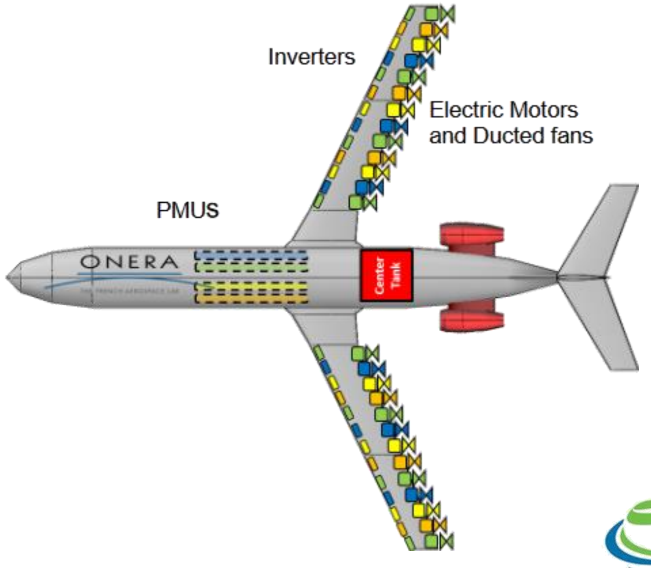
DRAGON optimization test case





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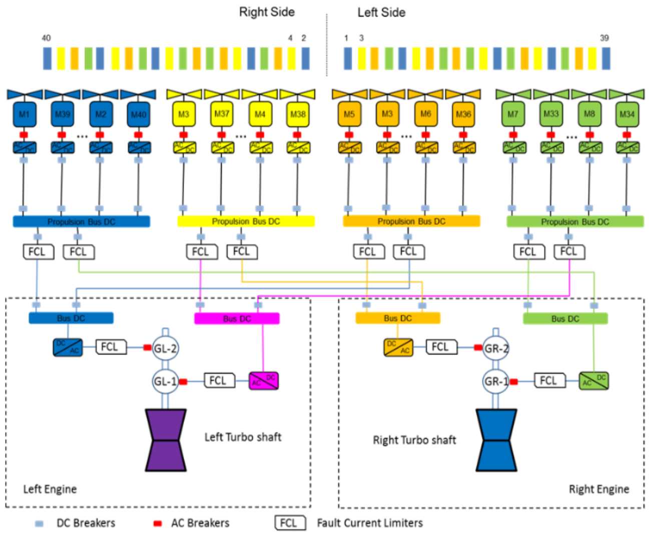

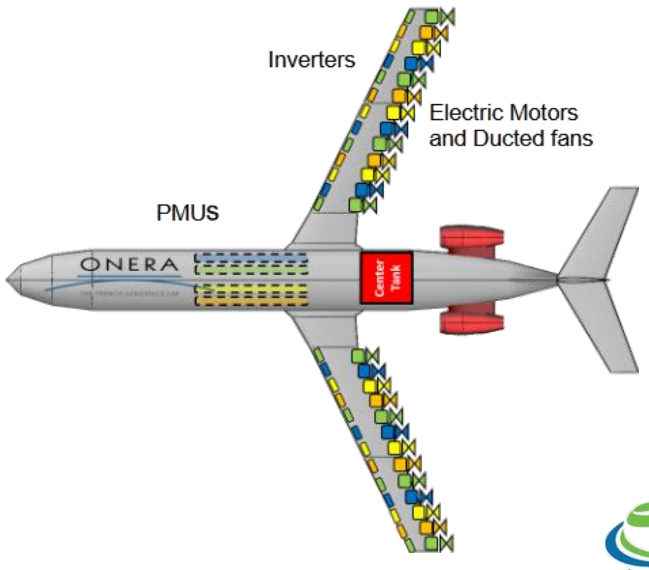

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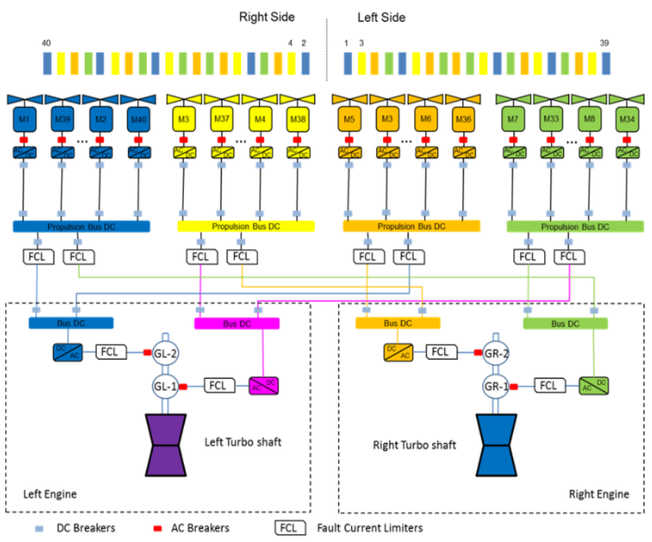

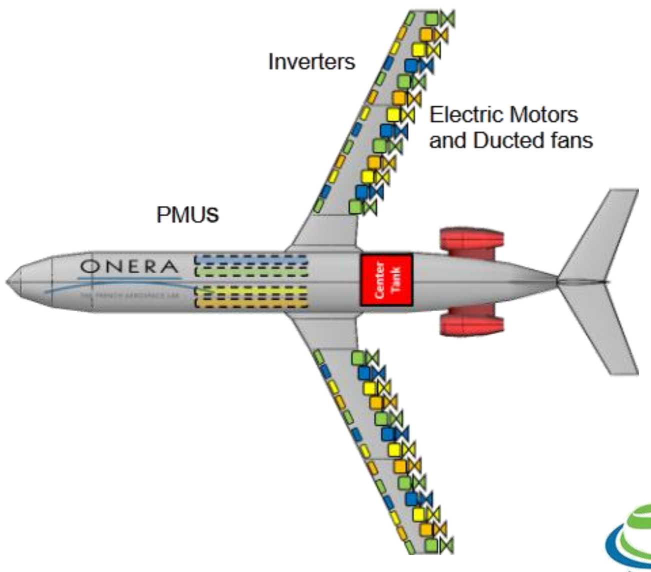

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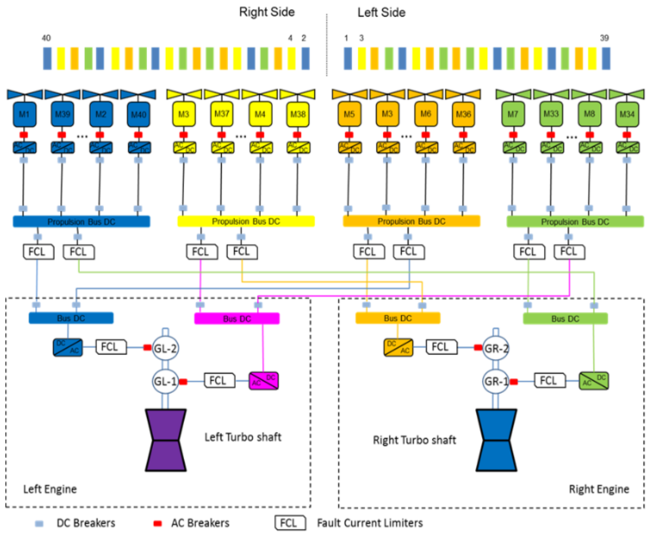

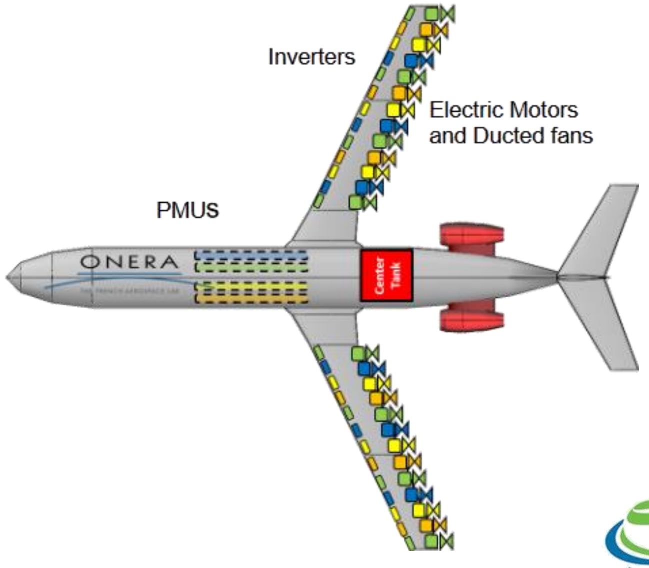

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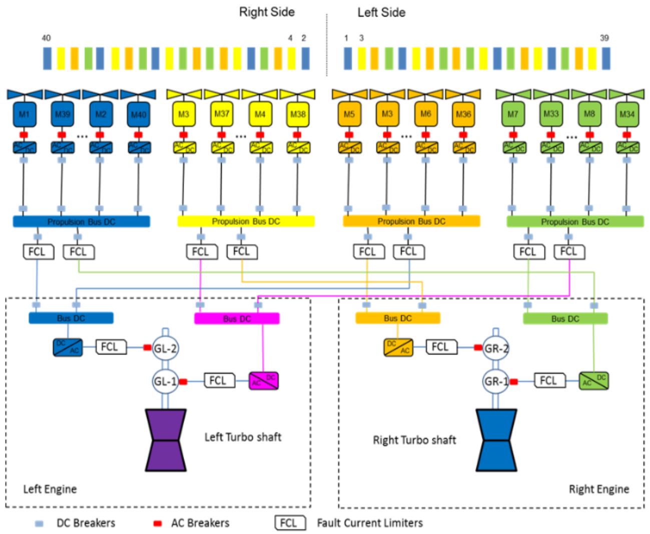

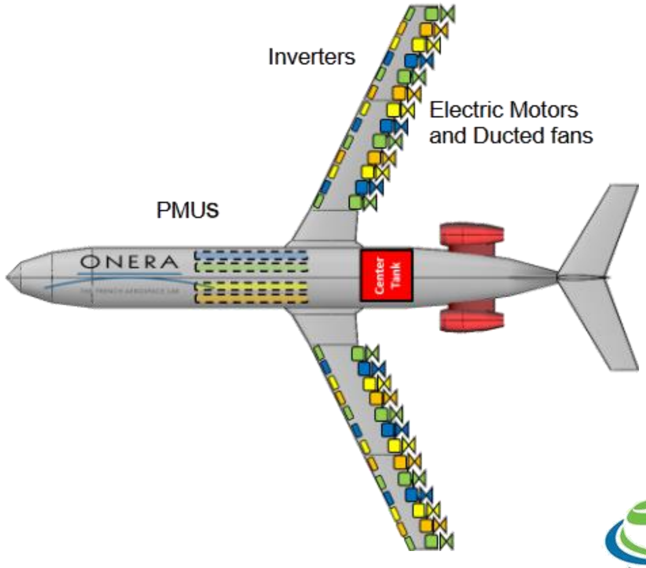

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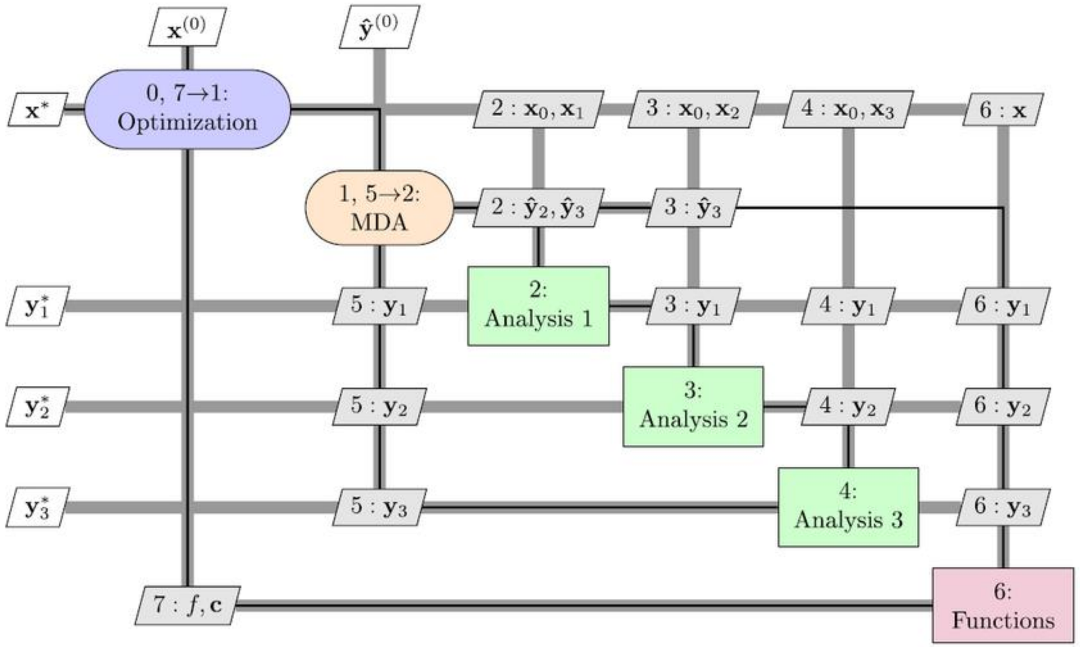

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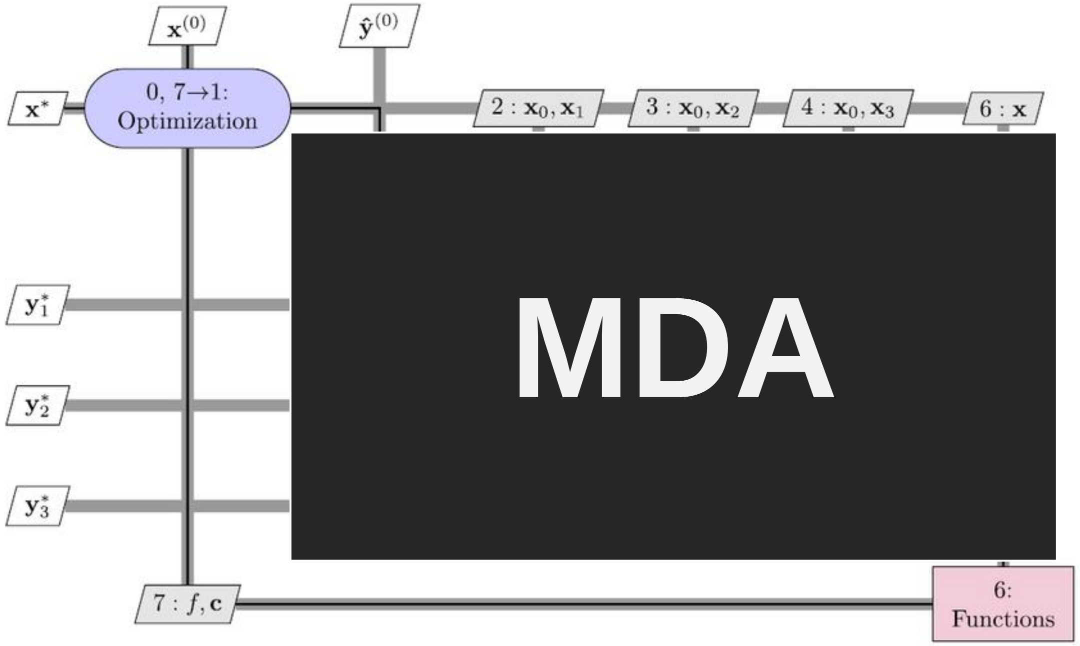

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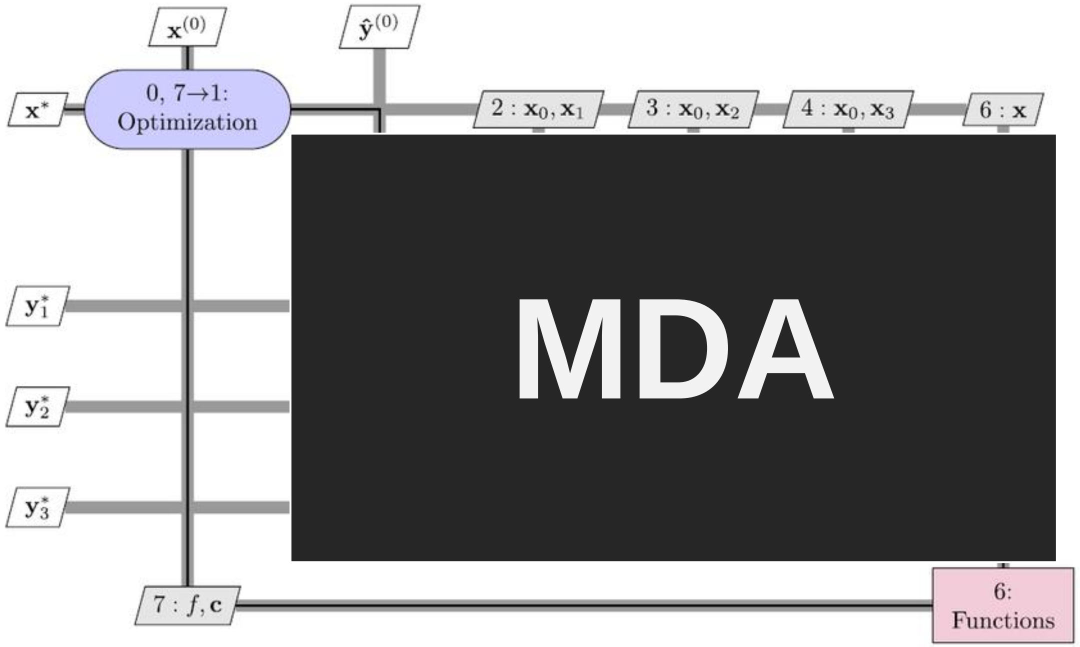

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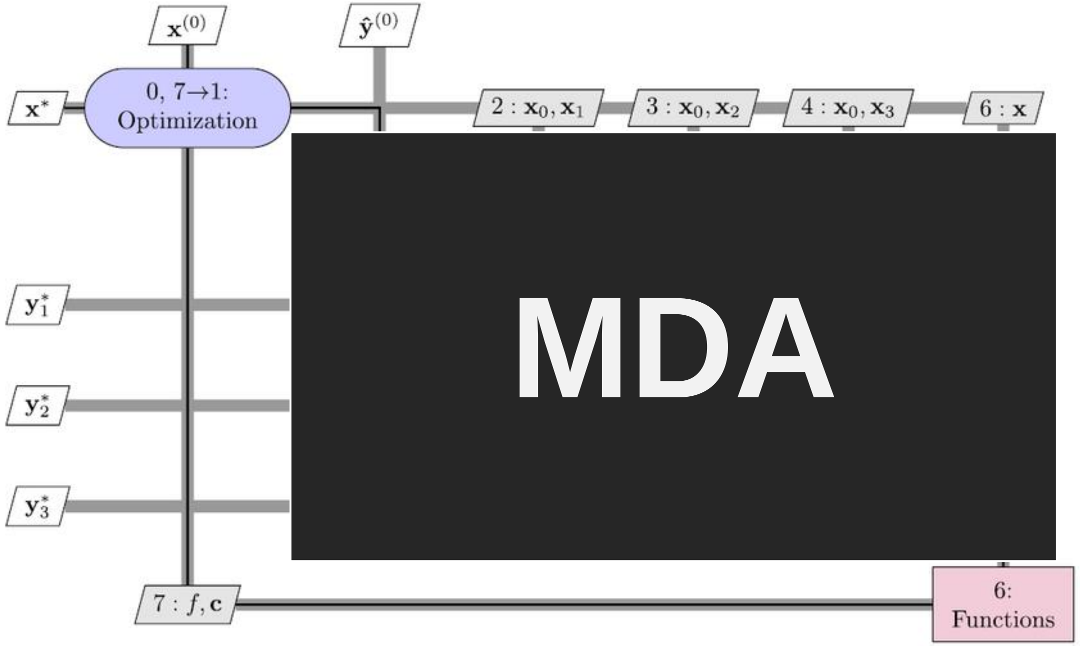

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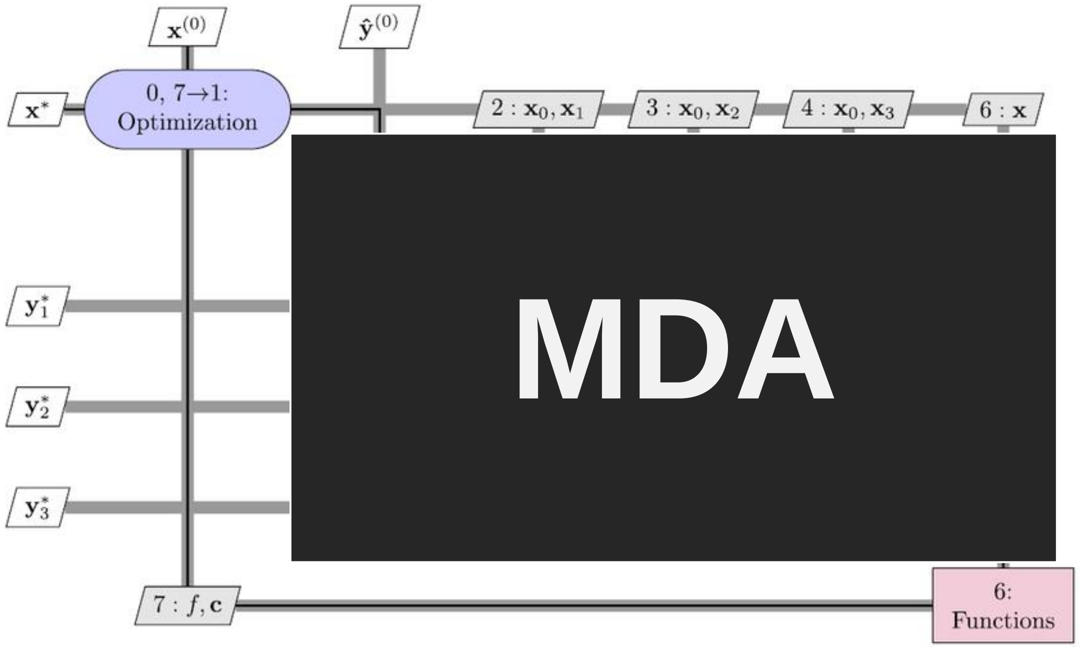

Overall objective:

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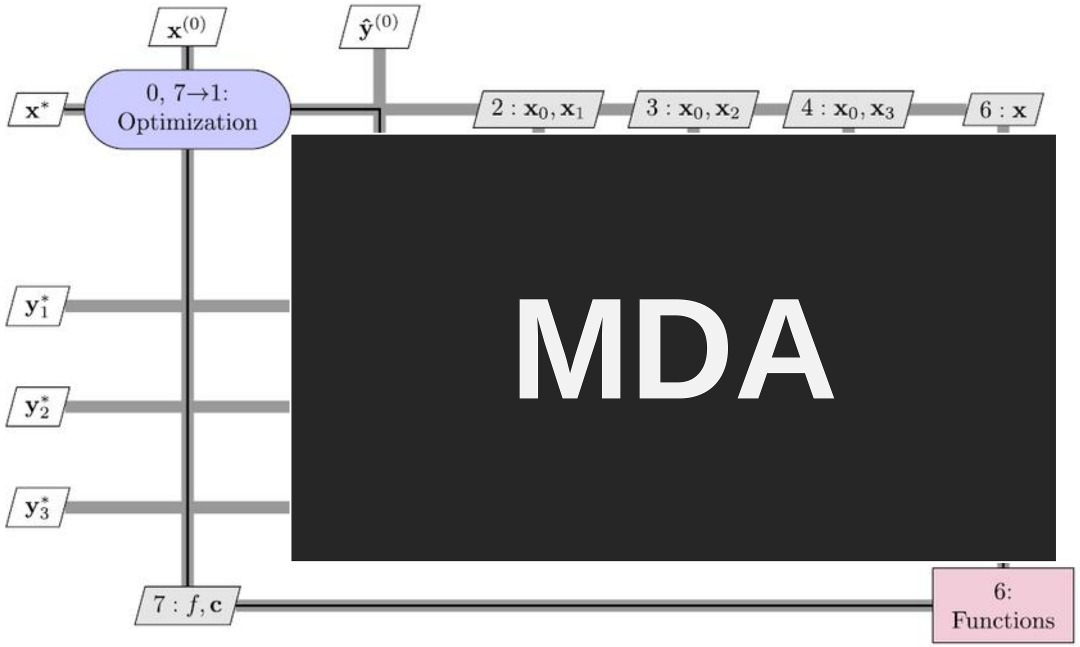

Overall objective:

- **Optimize a high-dimensional mixed discrete hierarchical expensive-to-evaluate black-box simulation**

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Expensive black-box optimization

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	Search		Algorithm		Function evaluation		Stochasticity	
	Local	Global	Mathematical	Heuristic	Direct	Surrogate	Deterministic	Stochastic
Nelder–Mead	•			•	•		•	
GPS		•	•		•		•	
MADS		•	•		•			•
Trust region	•		•			•	•	
Implicit filtering	•		•			•	•	
DIRECT		•	•		•		•	
MCS		•	•		•		•	
EGO		•	•			•	•	
Hit and run		•		•	•			•
Evolutionary		•		•	•			•

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GPS		•	•		•		•	
MADS		•	•		•			•
Trust region	•		•			•	•	
Implicit filtering	•		•			•	•	
DIRECT		•	•		•		•	
MCS		•	•		•		•	
EGO		•	•			•	•	
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Nelder–Mead	•			•	•		•	
GPS		•	•		•		•	
MADS		•	•		•			•
Trust region	•		•			•	•	
Implicit filtering	•		•			•	•	
DIRECT		•	•		•		•	
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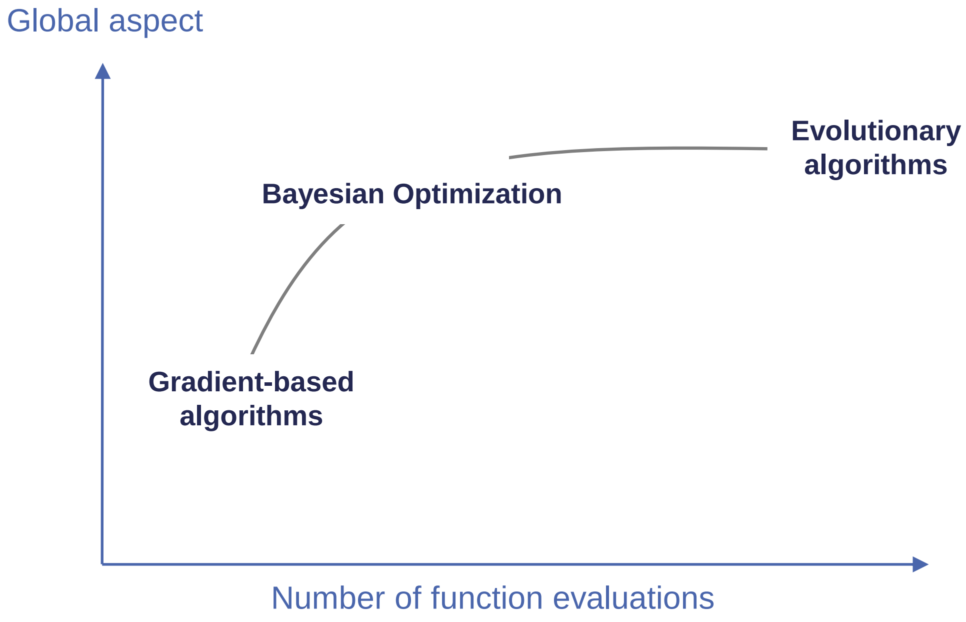

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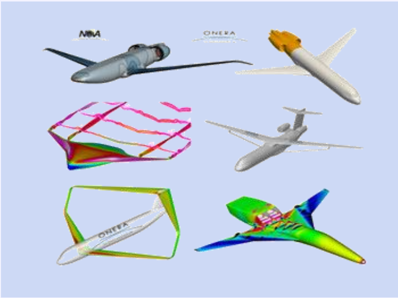
Methodology

New concepts



Ω

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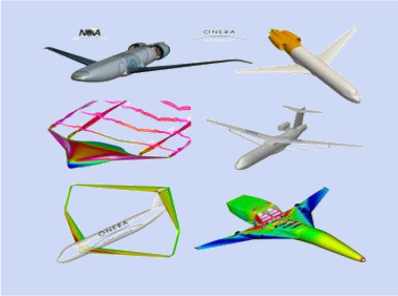
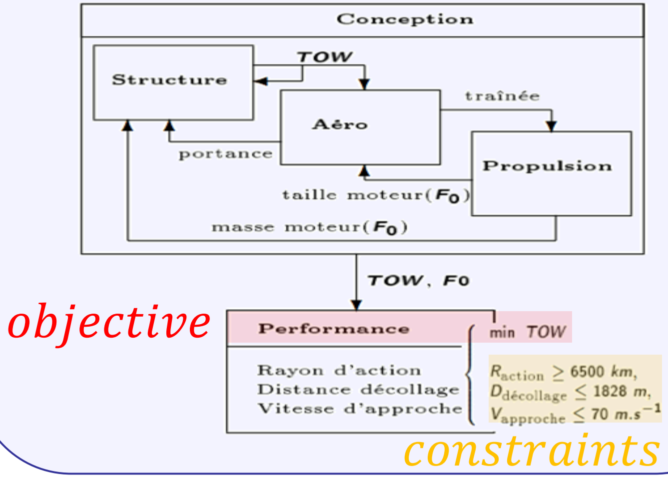


Ω

Analyze

Multidisciplinary design analysis



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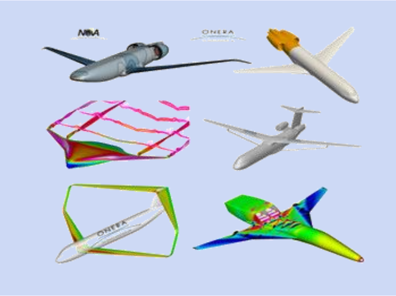
Methodology

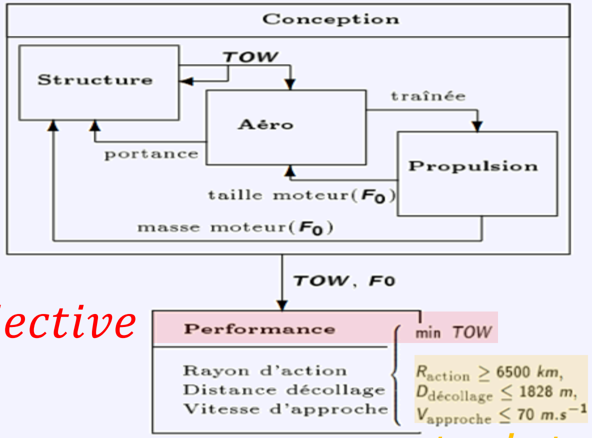
New concepts



Ω

Analyze

Multidisciplinary design analysis



objective

constraints

Improvements

Global optimization

$$\min_{\text{inputs} \in \Omega} \ objective\,(\text{inputs})$$
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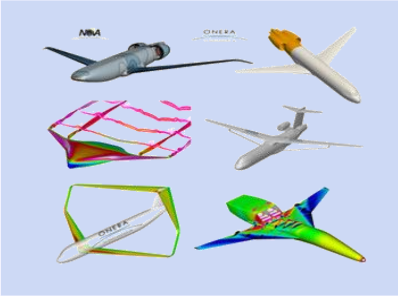

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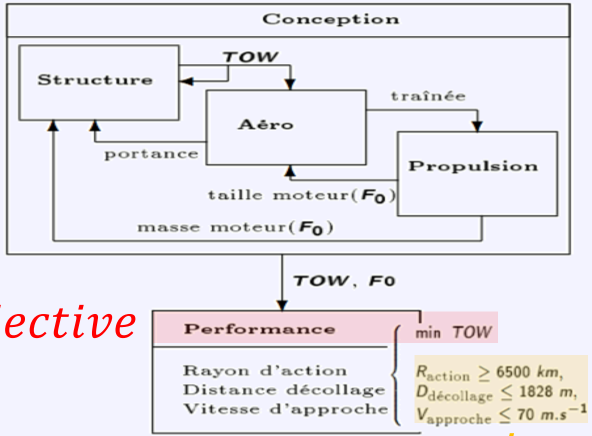

Improvements

Global optimization

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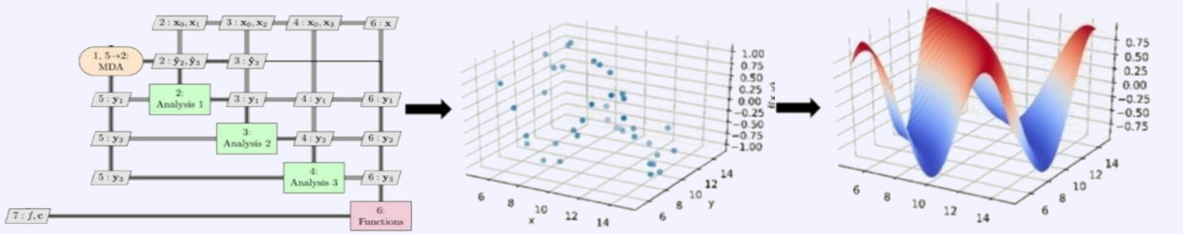
Expensive computations

Surrogate model



Expensive black-box — Design of experiments — Gaussian processes

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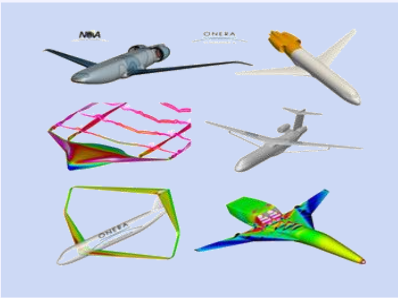

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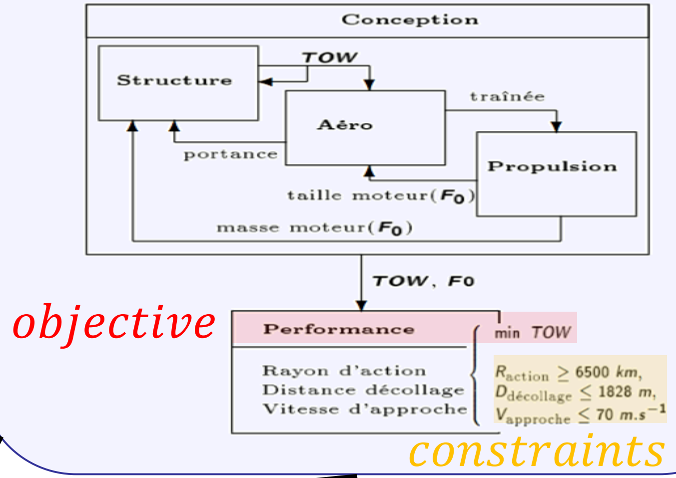

Improvements

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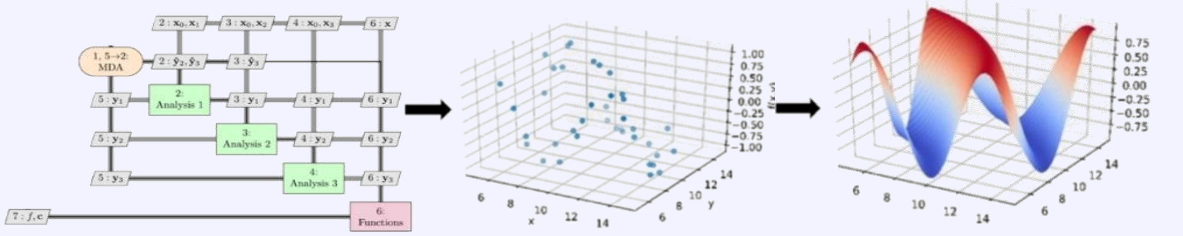
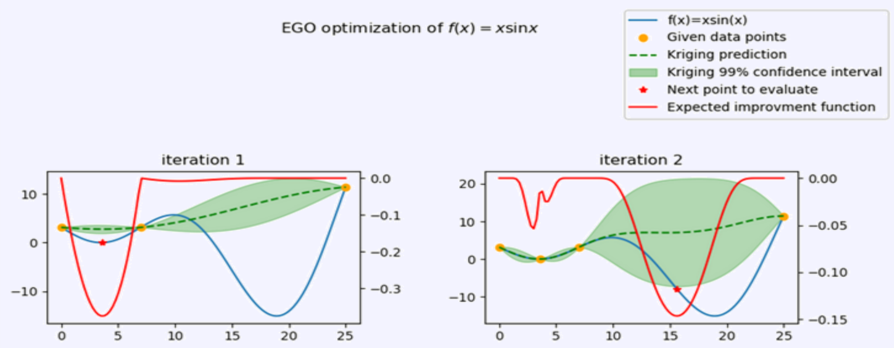


Expensive black-box

Design of experiments

Gaussian processes

Bayesian optimization



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Overall objective:

- Optimize a high-dimensional mixed discrete hierarchical expensive-to-evaluate black-box simulation

→ **Surrogate modeling**

Global optimization

$$\min_{\text{inputs} \in \Omega} \; objective\,(\text{inputs})$$
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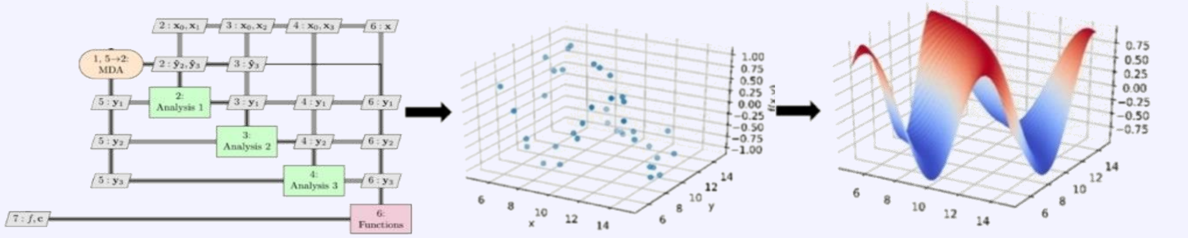
Expensive black-box optimization

Surrogate model



Expensive black-box | Design of experiments | Gaussian processes

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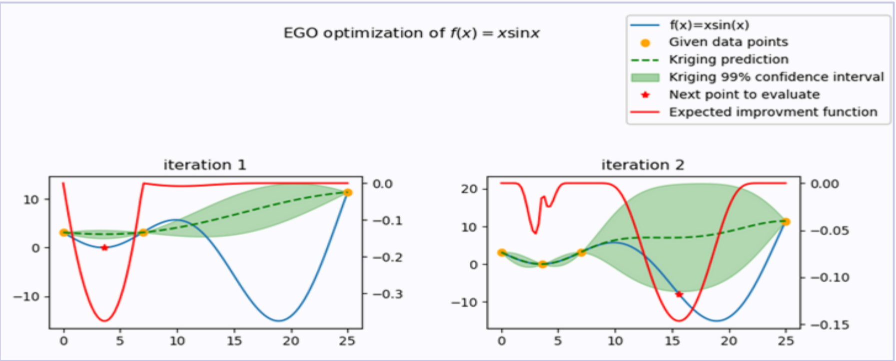

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→ **Surrogate modeling**

Need for Gaussian process to handle:

- Mixed variables (continuous, integer or categorical)
- A high number of variables
- Hierarchical variables

Global optimization

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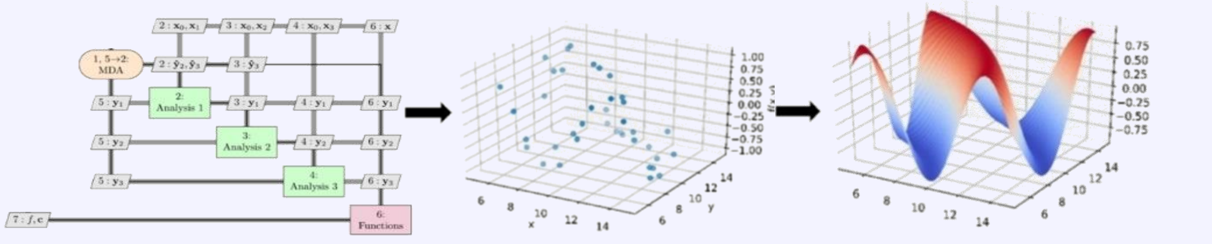
Expensive black-box optimization

Surrogate model



Expensive black-box Design of experiments Gaussian processes

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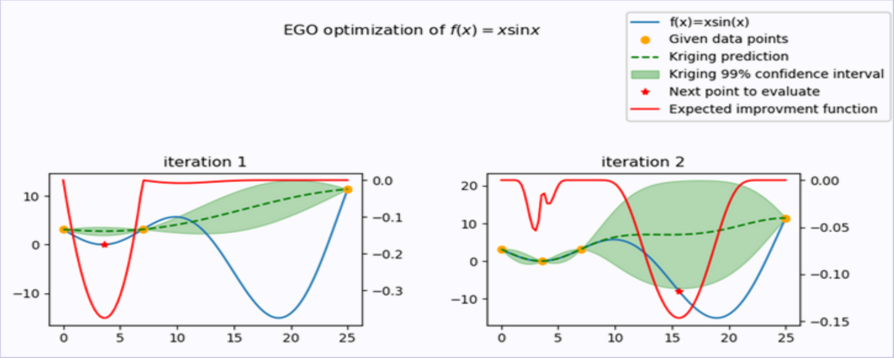

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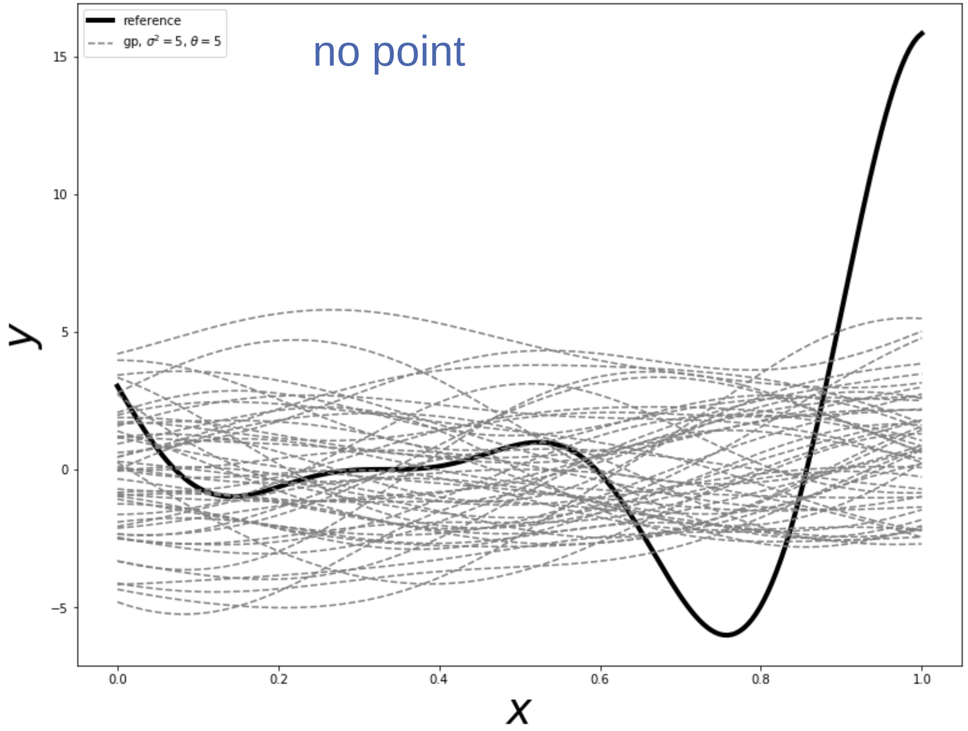
Gaussian process (or Kriging model)



$(x^r, x^s) \in (\mathbb{R}^n)^2 \quad f(x) \in \mathbb{R}$

A Gaussian process (GP) is characterized by:

- its trend
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Estimation of hyperparameters $\theta_i, i = 1, \ldots, n$ by MLE

➔ Hyperparameters tuning

➔ The number of hyperparameters increases with the dimension n

➔ Curse of dimensionality (n large)

$$f(x) \Rightarrow Y(x) = \mathcal{N}(\hat{y}(\boldsymbol{x}), \mathrm{s}^2(\boldsymbol{x}))$$

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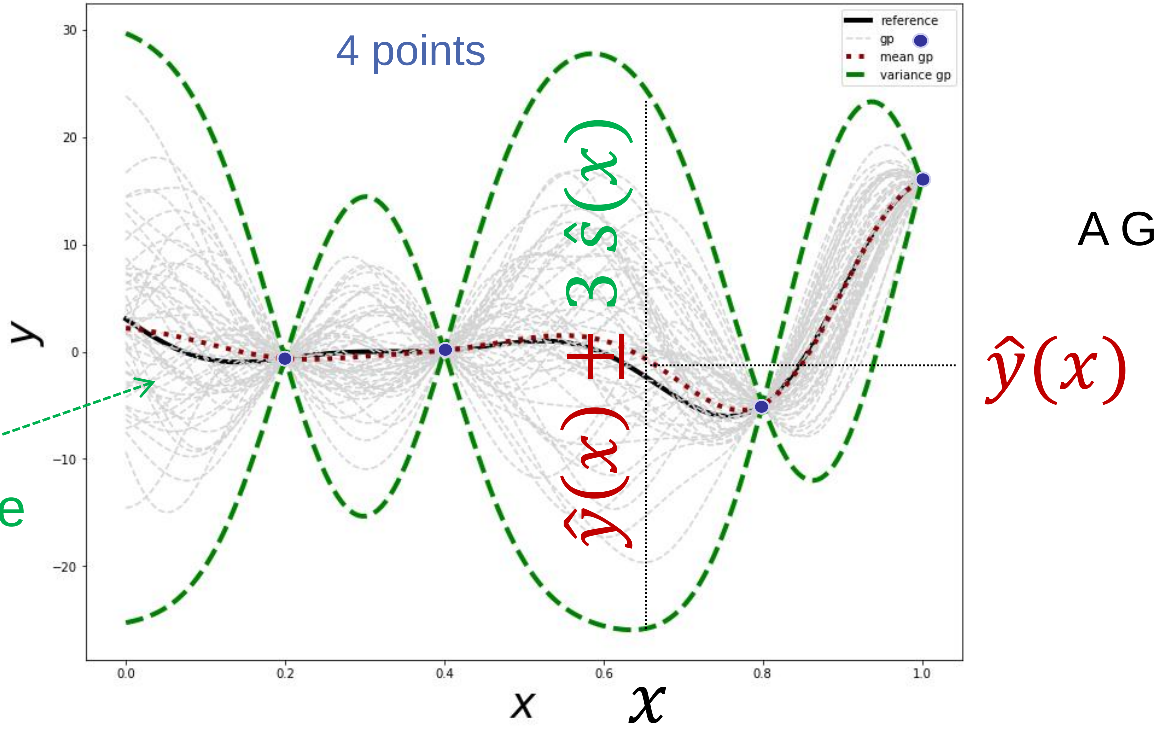

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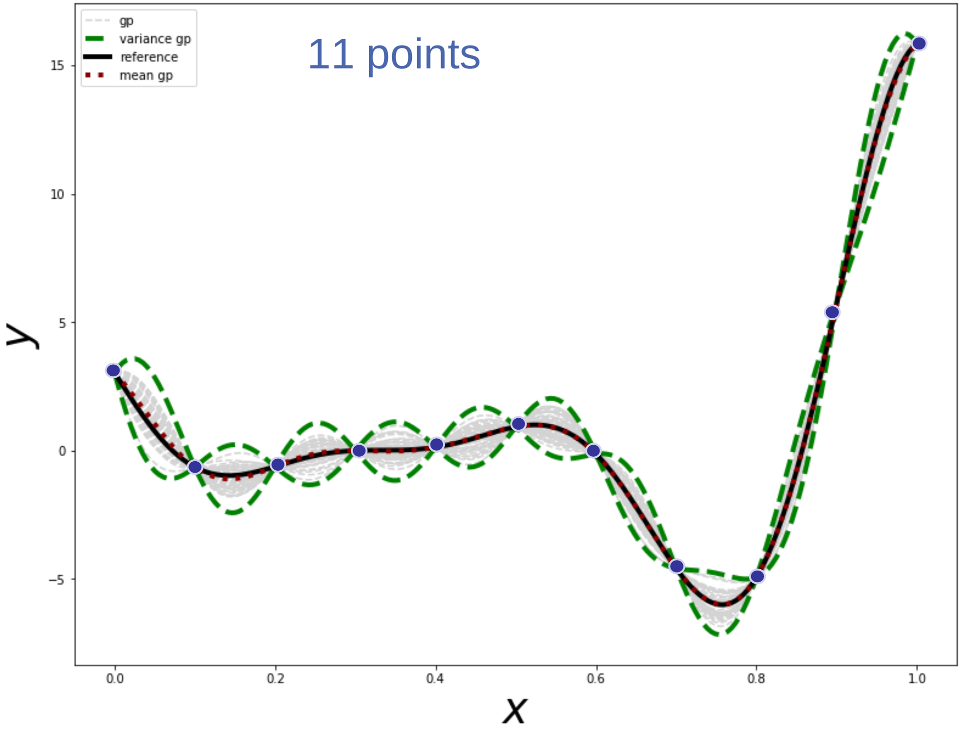

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From continuous to mixed-integer Gaussian process

Exponential kernels

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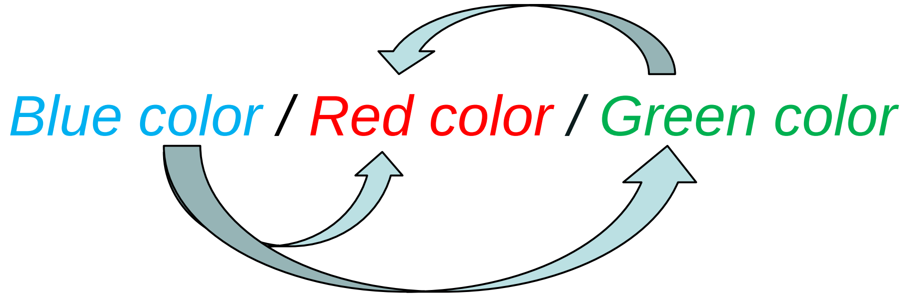

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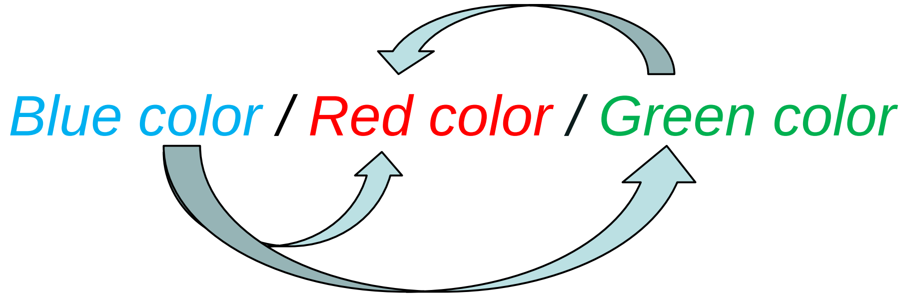

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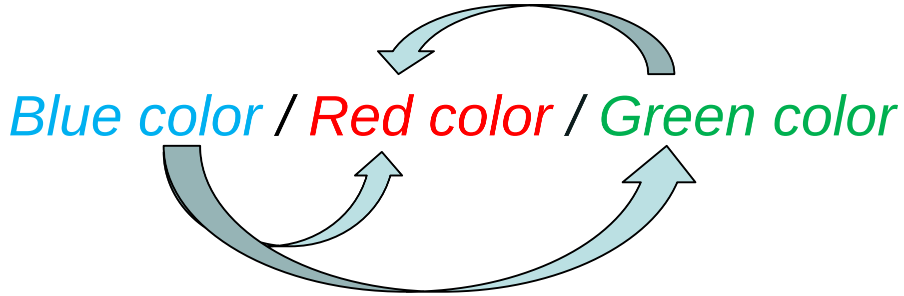

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Correlation matrix

$$\boldsymbol{\Theta}_{color} = \begin{pmatrix} \mathbf{1} & \boldsymbol{\theta}_{Blue/Red} & \boldsymbol{\theta}_{Blue/Green} \\ & \mathbf{1} & \boldsymbol{\theta}_{Red/Green} \\ \boldsymbol{Sym} & & \mathbf{1} \end{pmatrix}$$

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To estimate

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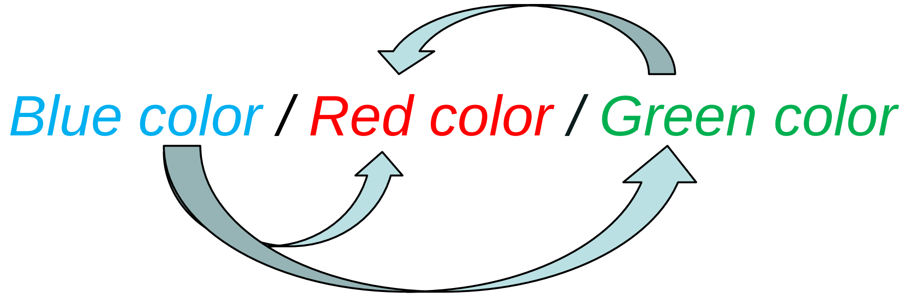

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State-of-the-art: Mixed-integer GP

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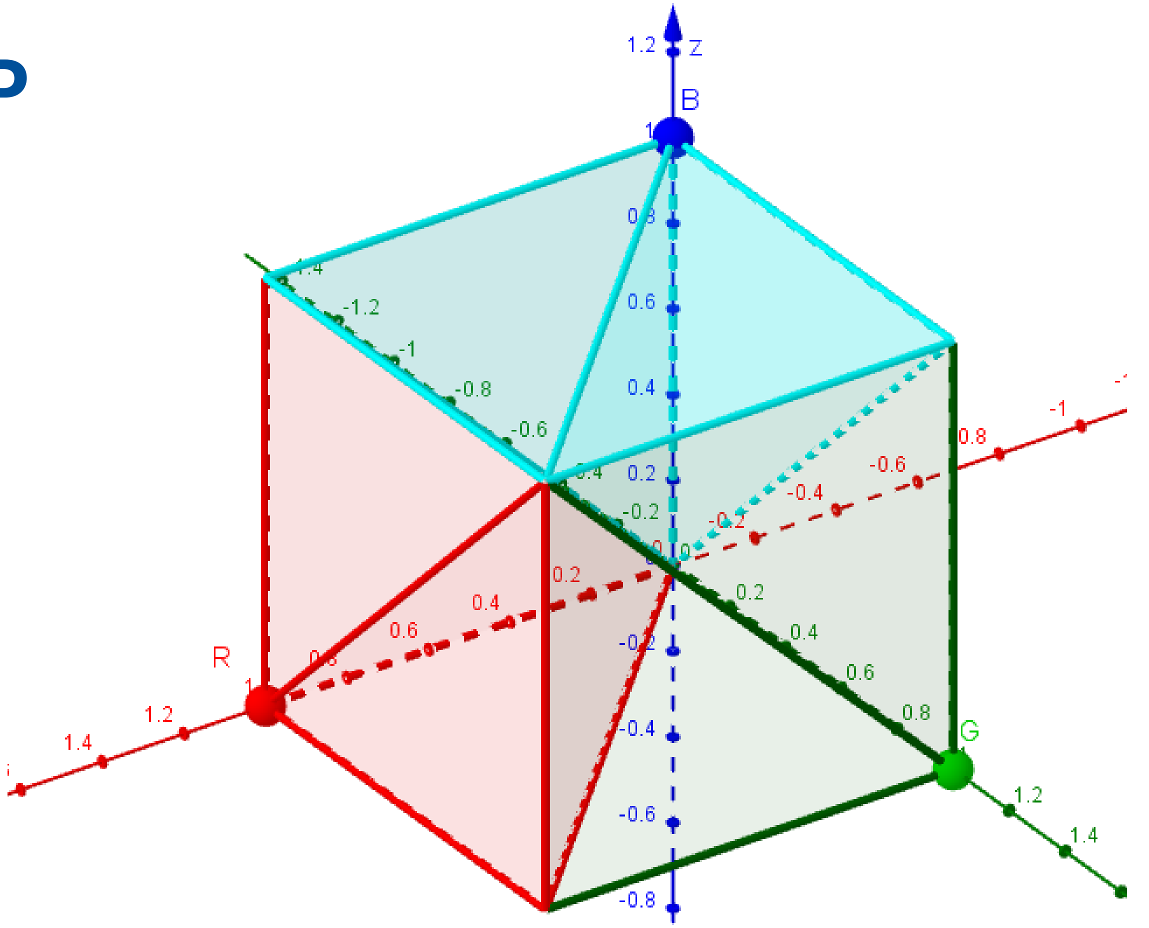

Relaxed dimension: $\boldsymbol{L_1 = 3}$

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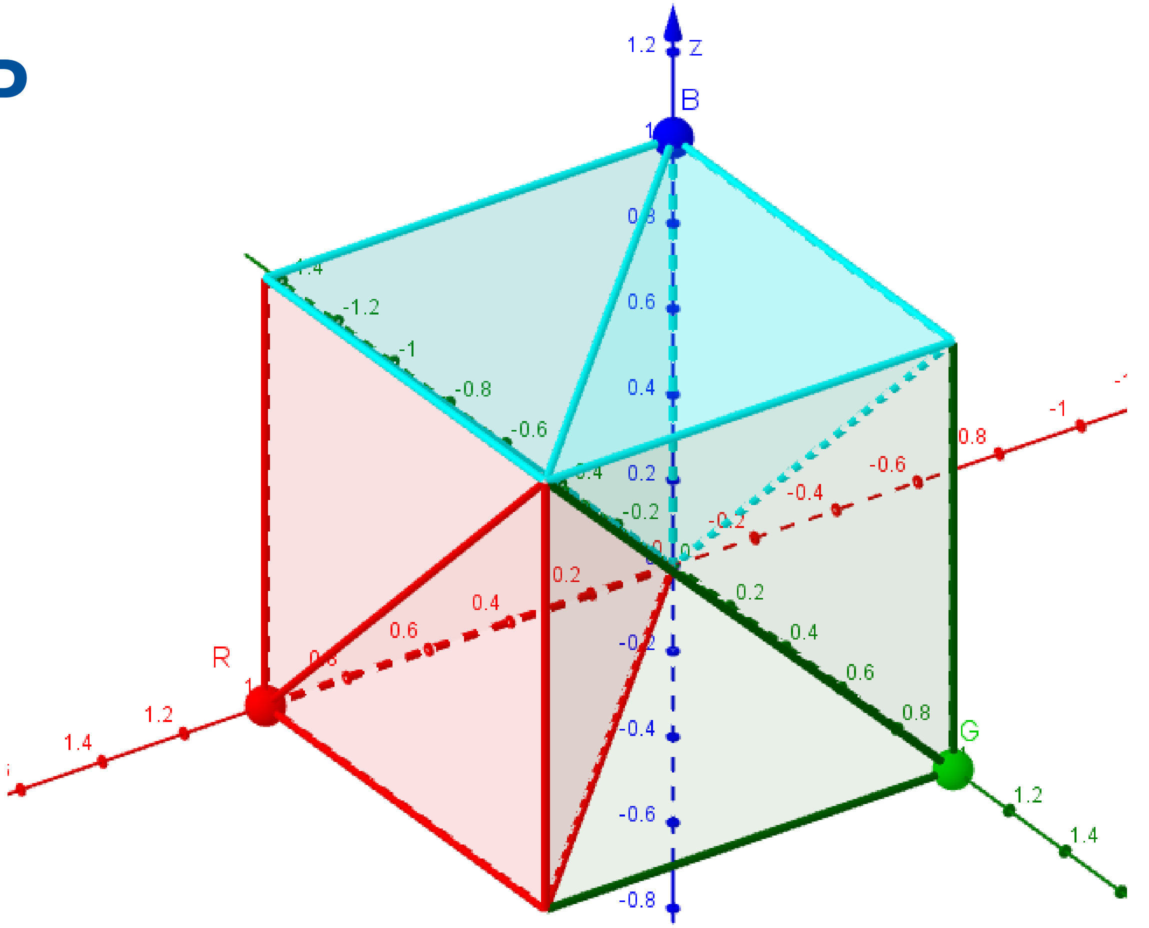

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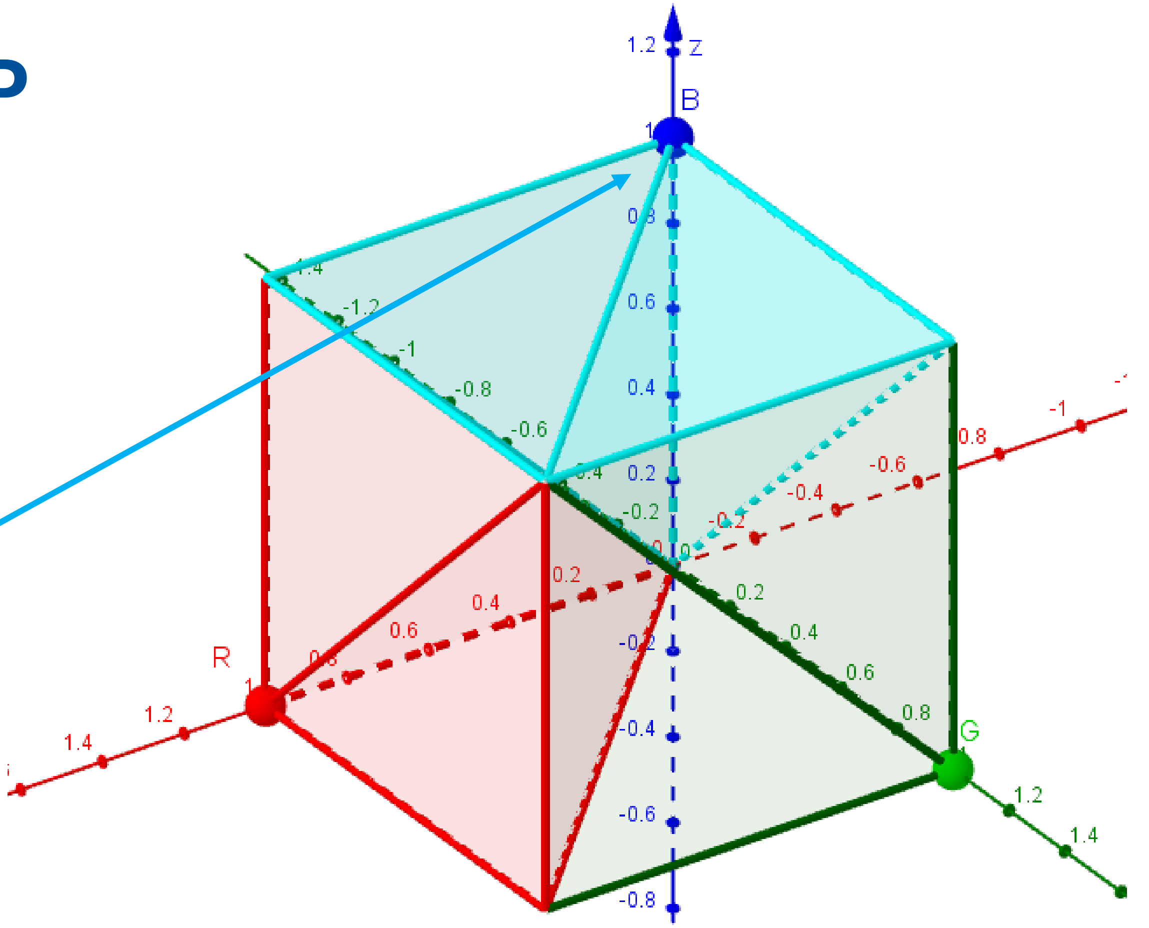

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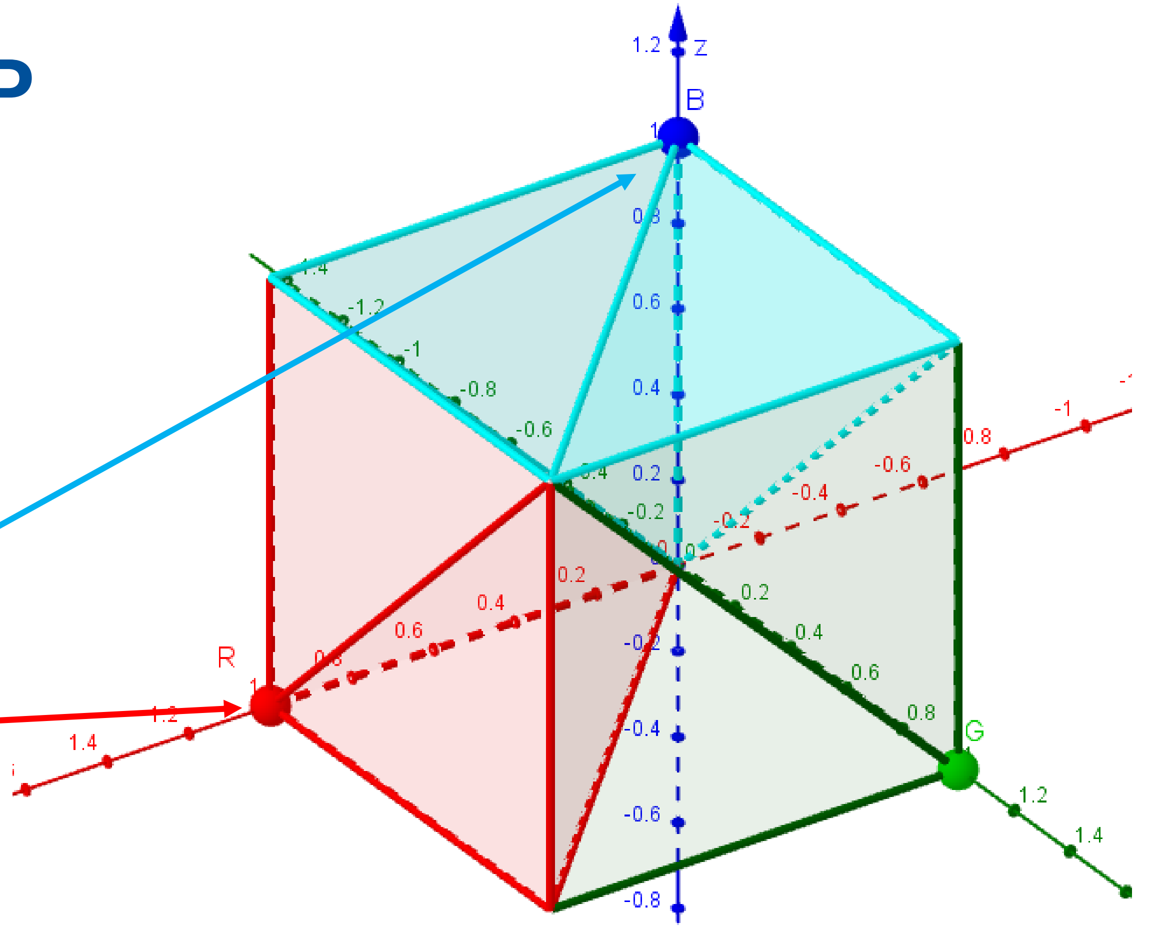

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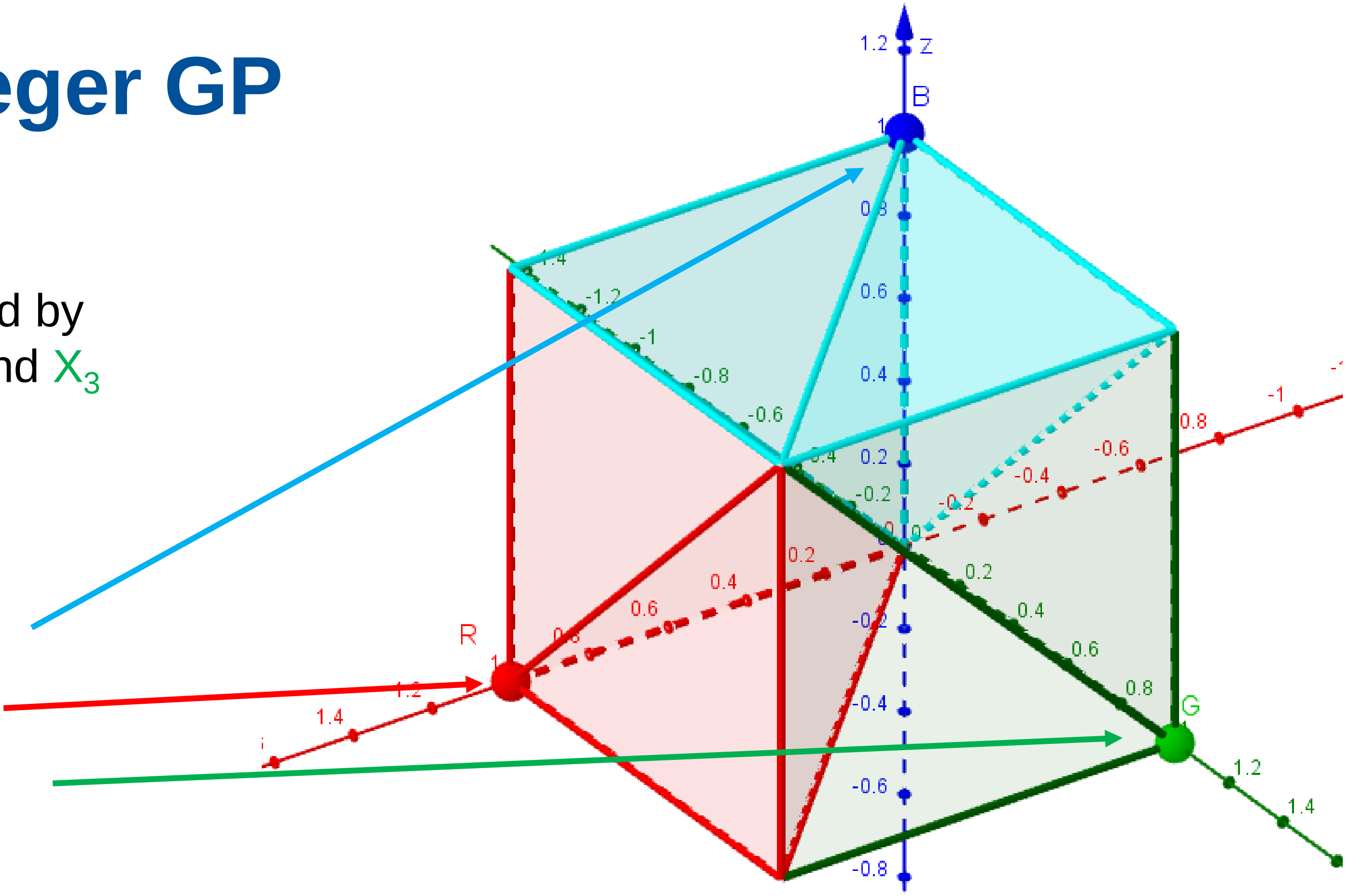

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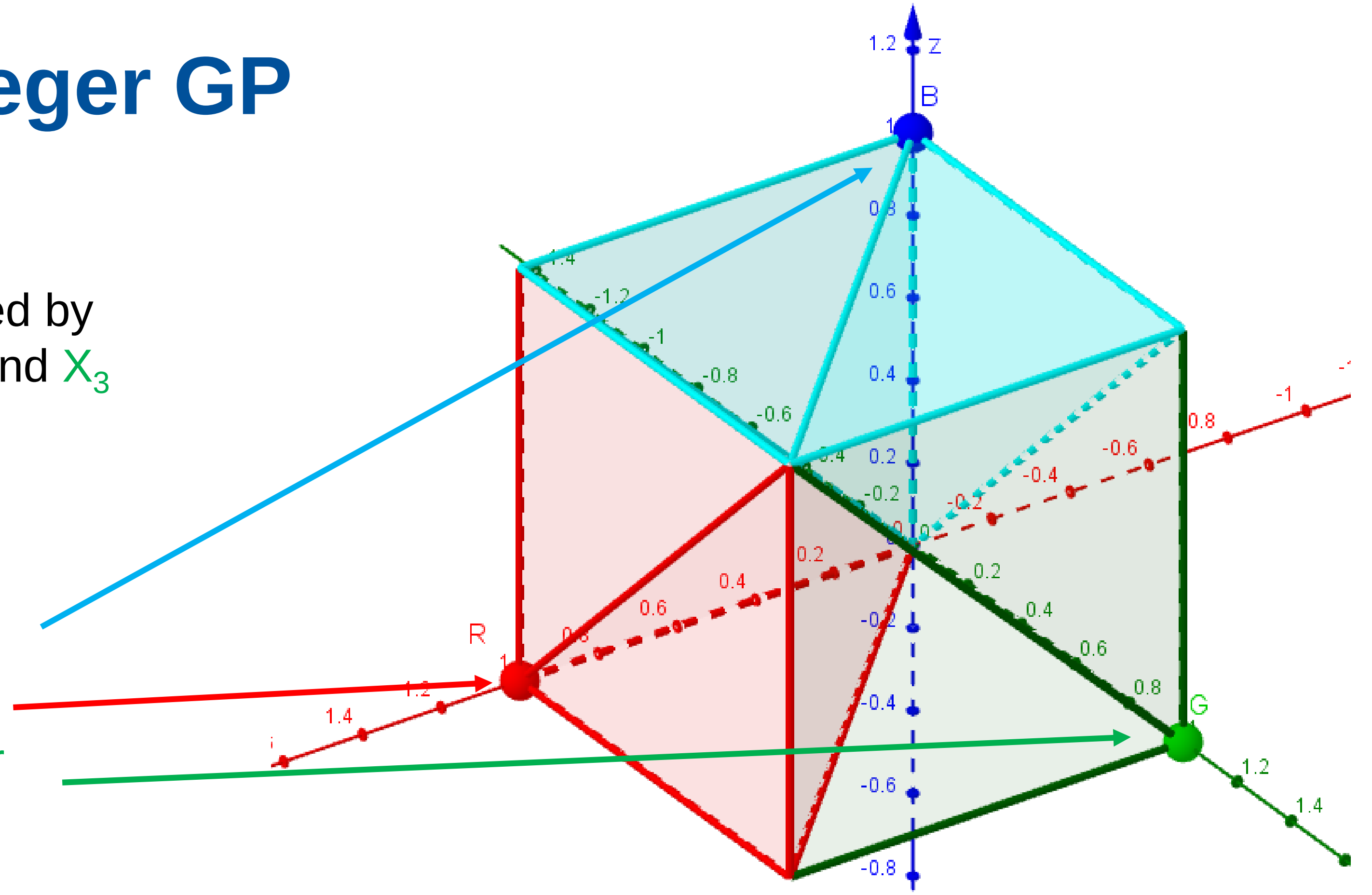

Relaxed dimension: $\boldsymbol{L_1 = 3}$

$\boldsymbol{x^r, x^s} \in \mathbb{R}^3$

A continuous kernel

State-of-the-art: Mixed-integer GP

- *Gower distance*

M. Halstrup, **Black-Box Optimization of Mixed Discrete-Continuous Optimization Problems**, 2016, TU Dortmund, PhD thesis.

State-of-the-art: Mixed-integer GP

- *Gower distance*

$$\Delta_{gow}(c_1^r, c_1^s) = \begin{cases} \mathbf{0}, \text{if } c_1^r = c_1^s \\ \mathbf{1}, \text{if } c_1^r \neq c_1^s \end{cases}$$

- $\Delta_{gow}(\text{Red}, \text{Red}) = 0$
- $\Delta_{gow}(\text{Red}, \text{Blue}) = 1$
- $\Delta_{gow}(\text{Red}, \text{Green}) = 1$
- $\Delta_{gow}(\text{Blue}, \text{Blue}) = 0$
- $\Delta_{gow}(\text{Blue}, \text{Green}) = 1$
- $\Delta_{gow}(\text{Green}, \text{Green}) = 0$

M. Halstrup, **Black-Box Optimization of Mixed Discrete-Continuous Optimization Problems**, 2016, TU Dortmund, PhD thesis.

State-of-the-art: Mixed-integer GP

- *Gower distance*

$$\Delta_{gow}(c_1^r, c_1^s) = \begin{cases} \mathbf{0}, \text{if } c_1^r = c_1^s \\ \mathbf{1}, \text{if } c_1^r \neq c_1^s \end{cases}$$

- $\Delta_{gow}(\text{Red}, \text{Red}) = 0$
- $\Delta_{gow}(\text{Red}, \text{Blue}) = 1$
- $\Delta_{gow}(\text{Red}, \text{Green}) = 1$
- $\Delta_{gow}(\text{Blue}, \text{Blue}) = 0$
- $\Delta_{gow}(\text{Blue}, \text{Green}) = 1$
- $\Delta_{gow}(\text{Green}, \text{Green}) = 0$

➔ Integer encoding: Categorical variable replaced by one continuous variable $X_1 \in [1, L_i]$

- $X_1 := \ell^1_{blue} = 1 \Rightarrow$ Blue color
- $X_1 := \ell^1_{red} = 2 \Rightarrow$ Red color
- $X_1 := \ell^1_{green} = 3 \Rightarrow$ Green color

$$\Delta_{gow}(c_1^r, c_1^s) = \begin{cases} \mathbf{0}, \text{if } \ell^1_r = \ell^1_s \\ \mathbf{1}, \text{if } \ell^1_r \neq \ell^1_s \end{cases}$$

1 relaxed dimension

$\boldsymbol{x^r}, \boldsymbol{x^s} \in \mathbb{R}$

M. Halstrup, **Black-Box Optimization of Mixed Discrete-Continuous Optimization Problems**, 2016, TU Dortmund, PhD thesis.

State-of-the-art: Mixed-integer GP

- *Gower distance*

$$\Delta_{gow}(c_1^r, c_1^s) = \begin{cases} \mathbf{0}, \text{if } c_1^r = c_1^s \\ \mathbf{1}, \text{if } c_1^r \neq c_1^s \end{cases}$$

- $\Delta_{gow}(\text{Red}, \text{Red}) = 0$
- $\Delta_{gow}(\text{Red}, \text{Blue}) = 1$
- $\Delta_{gow}(\text{Red}, \text{Green}) = 1$
- $\Delta_{gow}(\text{Blue}, \text{Blue}) = 0$
- $\Delta_{gow}(\text{Blue}, \text{Green}) = 1$
- $\Delta_{gow}(\text{Green}, \text{Green}) = 0$

➔ Integer encoding: Categorical variable replaced by one continuous variable $X_1 \in [1, L_i]$

- $X_1 := \ell_{blue}^1 = 1 \Rightarrow$ Blue color
- $X_1 := \ell_{red}^1 = 2 \Rightarrow$ Red color
- $X_1 := \ell_{green}^1 = 3 \Rightarrow$ Green color

$$\Delta_{gow}(c_1^r, c_1^s) = \begin{cases} \mathbf{0}, \text{if } \ell_r^1 = \ell_s^1 \\ \mathbf{1}, \text{if } \ell_r^1 \neq \ell_s^1 \end{cases}$$

1 relaxed dimension

$\boldsymbol{x^r}, \boldsymbol{x^s} \in \mathbb{R}$

A continuous kernel

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State-of-the-art: Mixed-integer GP

- *Homoscedastic hypersphere mixed kernel*

R. Rebonato, P. Jaeckel, **The most general methodology to create a valid correlation matrix for risk management and option pricing purposes**, 2001, Journal of Risk.

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State-of-the-art: Mixed-integer GP

- *Homoscedastic hypersphere mixed kernel*

$$\boldsymbol{\Theta}_1 = \begin{pmatrix} \mathbf{1} & \boldsymbol{\theta}_{Blue/Red} & \boldsymbol{\theta}_{Blue/Green} \\ & \mathbf{1} & \boldsymbol{\theta}_{Red/Green} \\ \boldsymbol{Sym} & & \mathbf{1} \end{pmatrix}$$

R. Rebonato, P. Jaeckel, **The most general methodology to create a valid correlation matrix for risk management and option pricing purposes**, 2001, Journal of Risk.

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$$k(c_1^r, c_1^s) = [\boldsymbol{\Theta}_1]_{\ell_r^1, \ell_s^1}$$

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$$k(c_1^r, c_1^s) = [\boldsymbol{\Theta}_1]_{\ell_r^1,\, \ell_s^1}$$

The matrix $\boldsymbol{\Theta}_1$ should be
Symmetric Positive Definite (SPD)

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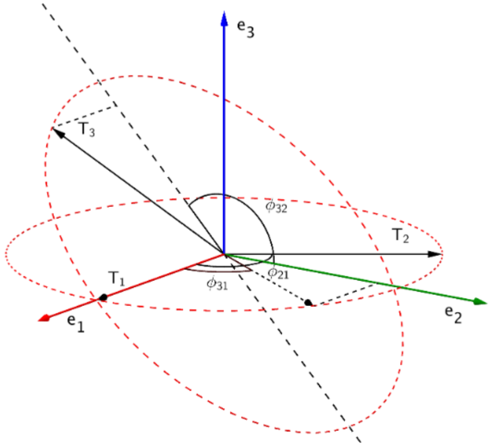
State-of-the-art: Mixed-integer GP

- *Homoscedastic hypersphere mixed kernel*

$$\boldsymbol{\Theta}_1 = \begin{pmatrix} 1 & \theta_{Blue/Red} & \theta_{Blue/Green} \\ & 1 & \theta_{Red/Green} \\ Sym & & 1 \end{pmatrix} \qquad k(c_1^r, c_1^s) = [\boldsymbol{\Theta}_1]_{\ell_r^1, \ell_s^1}$$

The matrix $\boldsymbol{\Theta}_1$ should be
Symmetric Positive Definite (SPD) → Hypersphere Decomposition

$$[\boldsymbol{\Theta}_1] = CC^T$$



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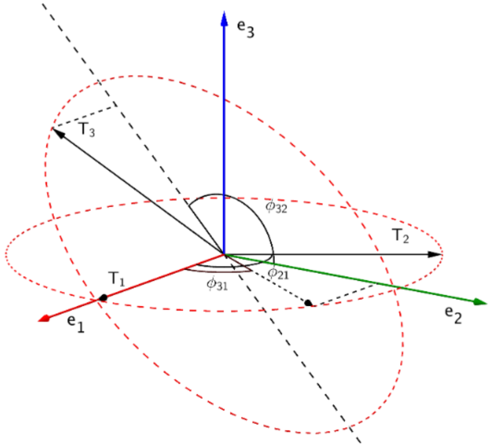
$$k(c_1^r, c_1^s) = [\boldsymbol{\Theta_1}]_{\ell_r^1, \ell_s^1}$$

The matrix $\boldsymbol{\Theta_1}$ should be
Symmetric Positive Definite (SPD)

Hypersphere Decomposition

$$[\boldsymbol{\Theta_1}] = CC^T$$



No relaxed dimension

$\boldsymbol{c_1^r}, \boldsymbol{c_1^s} \in \{Blue, Red, Green\}$

A categorical kernel

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Modeling categorical kernels

Model	Θ_i (example with 3 levels)	$K_i(c_i^r, c_i^s, \Theta_i)$	# of parameters
Homoscedastic Hypersphere (HH)	$\begin{pmatrix} 1 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 1 & [\Theta_i]_{23} \\ \text{Sym.} & & 1 \end{pmatrix}$	$[\Theta_i]_{c_i^r, c_i^s}$	$\frac{1}{2} L_i(L_i - 1)$

P. Saves, Y. Diouane, N. Bartoli, T. Lefebvre, J. Morlier, **A mixed-categorical correlation kernel for Gaussian process**, 2023, Neurocomputing.

Modeling categorical kernels

Model	Θ_i (example with 3 levels)	$K_i(c_i^r, c_i^s, \Theta_i)$	# of parameters
Homoscedastic Hypersphere (HH)	$\begin{pmatrix} 1 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 1 & [\Theta_i]_{23} \\ \text{Sym.} & & 1 \end{pmatrix}$	$[\Theta_i]_{c_i^r, c_i^s}$	$\frac{1}{2} L_i (L_i - 1)$
Reference: Our full model (FE)	$\begin{pmatrix} [\Theta_i]_{11} & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & [\Theta_i]_{22} & [\Theta_i]_{23} \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$	$\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s})) \exp(-2 [\Theta_i]_{c_i^r, c_i^s})$	$\frac{1}{2} L_i (L_i + 1)$

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Modeling categorical kernels

Model	Θ_i (example with 3 levels)	$K_i(c_i^r, c_i^s, \Theta_i)$	# of parameters
Homoscedastic Hypersphere (HH)	$\begin{pmatrix} 1 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 1 & [\Theta_i]_{23} \\ \text{Sym.} & & 1 \end{pmatrix}$	$[\Theta_i]_{c_i^r, c_i^s}$	$\frac{1}{2} L_i(L_i - 1)$
Reference: Our full model (FE)	$\begin{pmatrix} [\Theta_i]_{11} & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & [\Theta_i]_{22} & [\Theta_i]_{23} \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$	$\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s})) \exp(-2 [\Theta_i]_{c_i^r, c_i^s})$	$\frac{1}{2} L_i(L_i + 1)$
Our model as Exponential Homoscedastic Hypersphere (EHH)	$\begin{pmatrix} 0 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 0 & [\Theta_i]_{23} \\ \text{Sym.} & & 0 \end{pmatrix}$	$\exp(-2 [\Theta_i]_{c_i^r, c_i^s})$	$\frac{1}{2} L_i(L_i - 1)$

P. Saves, Y. Diouane, N. Bartoli, T. Lefebvre, J. Morlier, **A mixed-categorical correlation kernel for Gaussian process**, 2023, Neurocomputing.

Modeling categorical kernels

Model	Θ_i (example with 3 levels)	$K_i(c_i^r, c_i^s, \Theta_i)$	# of parameters
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Reference: Our full model (FE)	$\begin{pmatrix} [\Theta_i]_{11} & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & [\Theta_i]_{22} & [\Theta_i]_{23} \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$	$\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s})) \exp(-2 [\Theta_i]_{c_i^r, c_i^s})$	$\frac{1}{2} L_i(L_i + 1)$
Our model as Exponential Homoscedastic Hypersphere (EHH)	$\begin{pmatrix} 0 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 0 & [\Theta_i]_{23} \\ \text{Sym.} & & 0 \end{pmatrix}$	$\exp(-2 [\Theta_i]_{c_i^r, c_i^s})$	$\frac{1}{2} L_i(L_i - 1)$
Our model as Continuous Relaxation (CR)	$\begin{pmatrix} [\Theta_i]_{11} & 0 & 0 \\ & [\Theta_i]_{22} & 0 \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$	$\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s}))$	L_i

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Modeling categorical kernels

Model	Θ_i (example with 3 levels)	$K_i(c_i^r, c_i^s, \Theta_i)$	# of parameters
Homoscedastic Hypersphere (HH)	$\begin{pmatrix} 1 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 1 & [\Theta_i]_{23} \\ \text{Sym.} & & 1 \end{pmatrix}$	$[\Theta_i]_{c_i^r, c_i^s}$	$\frac{1}{2} L_i (L_i - 1)$
Reference: Our full model (FE)	$\begin{pmatrix} [\Theta_i]_{11} & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & [\Theta_i]_{22} & [\Theta_i]_{23} \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$	$\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s}))\ \exp(-2\, [\Theta_i]_{c_i^r, c_i^s})$	$\frac{1}{2} L_i (L_i + 1)$
Our model as Exponential Homoscedastic Hypersphere (EHH)	$\begin{pmatrix} 0 & [\Theta_i]_{12} & [\Theta_i]_{13} \\ & 0 & [\Theta_i]_{23} \\ \text{Sym.} & & 0 \end{pmatrix}$	$\exp(-2\, [\Theta_i]_{c_i^r, c_i^s})$	$\frac{1}{2} L_i (L_i - 1)$
Our model as Continuous Relaxation (CR)	$\begin{pmatrix} [\Theta_i]_{11} & 0 & 0 \\ & [\Theta_i]_{22} & 0 \\ \text{Sym.} & & [\Theta_i]_{33} \end{pmatrix}$	$\exp(-([\Theta_i]_{c_i^r, c_i^r} + [\Theta_i]_{c_i^s, c_i^s}))$	L_i
Our model as Gower distance (GD)	$[\Theta_i]_{cov} \begin{pmatrix} 0 & 1 & 1 \\ & 0 & 1 \\ \text{Sym.} & & 0 \end{pmatrix}$	$\exp(-2\, [\Theta_i]_{cov})$	1

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Modeling categorical kernels

Theorem

1. GD is the particular case of CR in which all hyperparameters are equal.
2. CR is a particular case of FE in which all non-diagonal hyperparameters are equal to zero.
3. FE and EHH kernels lead to the same GP model (all diagonal terms are redundant).
4. EHH is a particular case of HH in which the modeled correlations are positive.

P. Saves, Y. Diouane, N. Bartoli, T. Lefebvre, J. Morlier, **A mixed-categorical correlation kernel for Gaussian process**, 2023, Neurocomputing.

State-of-the-art: GP for high-dimension

Gaussian Process (GP) or Kriging

- Exponential kernel $k(x^r, x^s) = \exp\left(-\sum_{i=1}^{n} \theta_i |x_i^r - x_i^s|^2\right)$ with n parameters θ_i to estimate

H. Wold, **Estimation of Principal Components and Related Models by Iterative Least squares**, 1966, Multivariate analysis.

M.-A. Bouhlel, N. Bartoli, A. Otsmane, J. Morlier, **Improving kriging surrogates of high-dimensional design models by Partial Least Squares dimension reduction**, 2016, Structural and Multidisciplinary Optimization.

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- Exponential kernel $k(x^r, x^s) = \exp\left(-\sum_{i=1}^{n} \theta_i |x_i^r - x_i^s|^2\right)$ with n parameters θ_i to estimate

Kriging with Partial Least Squares (KPLS)

- $\forall i = 1, \cdots, n, \forall j = 1, \cdots, h, \left|W_{i,j}\right|$ describes how sensitive the *j*-th principal component is to each design variable *i*

n_t *DATA:* $(x \in \mathbb{R}^{\boldsymbol{n}}, f(\boldsymbol{x}) \in \mathbb{R})$ *PLS* → $\eta_i = \sum_{j=1}^{h} \theta_j \left|W_{i,j}\right|$

- θ_j describes how sensitive the function is to each principal component ($h \ll n$)

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n_t *DATA:* $(x \in \mathbb{R}^{\boldsymbol{n}}, f(\boldsymbol{x}) \in \mathbb{R})$ —*PLS*→ $\eta_i = \sum_{j=1}^{h} \theta_j |W_{i,j}|$

- θ_j describes how sensitive the function is to each principal component ($h \ll n$)

- Exponential kernel $k(x, x') = \exp\left(-\sum_{i=1}^{n} \eta_i |x_i^r - x_i^s|^2\right)$ with h parameters θ_j to estimate

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New KPLS models for mixed variables

Model	# of parameters	Relaxation	KPLS?
GD	1	—	—
CR	L_i		
HH	$\frac{1}{2} L_i (L_i - 1)$		
EHH			

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New KPLS models for mixed variables

Model	# of parameters	Relaxation	KPLS?
GD	1	—	—
CR	L_i	One-hot encoding	$h \ll L_i, h \in \mathbb{N}$
HH	$\frac{1}{2} L_i (L_i - 1)$		
EHH			

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New KPLS models for mixed variables

Model	# of parameters	Relaxation	KPLS?
GD	1	—	—
CR	L_i	One-hot encoding	$h \ll L_i, h \in \mathbb{N}$
HH	$\frac{1}{2} L_i (L_i - 1)$	Cross-level encoding	$h = \frac{1}{2} \ell_i (\ell_i - 1), \ell_i \ll L_i \in \mathbb{N}$
EHH			

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Multi-Layer Perceptron: hierarchical variables

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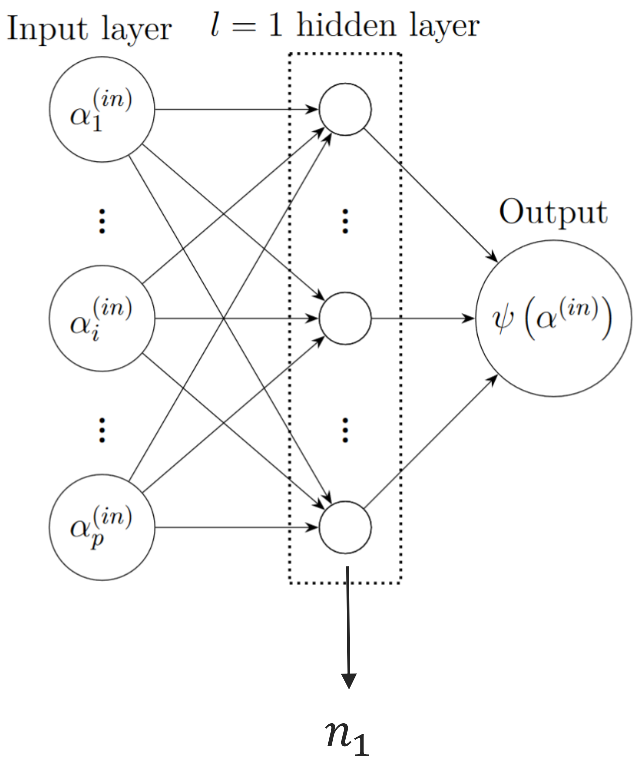
Multi-Layer Perceptron: hierarchical variables



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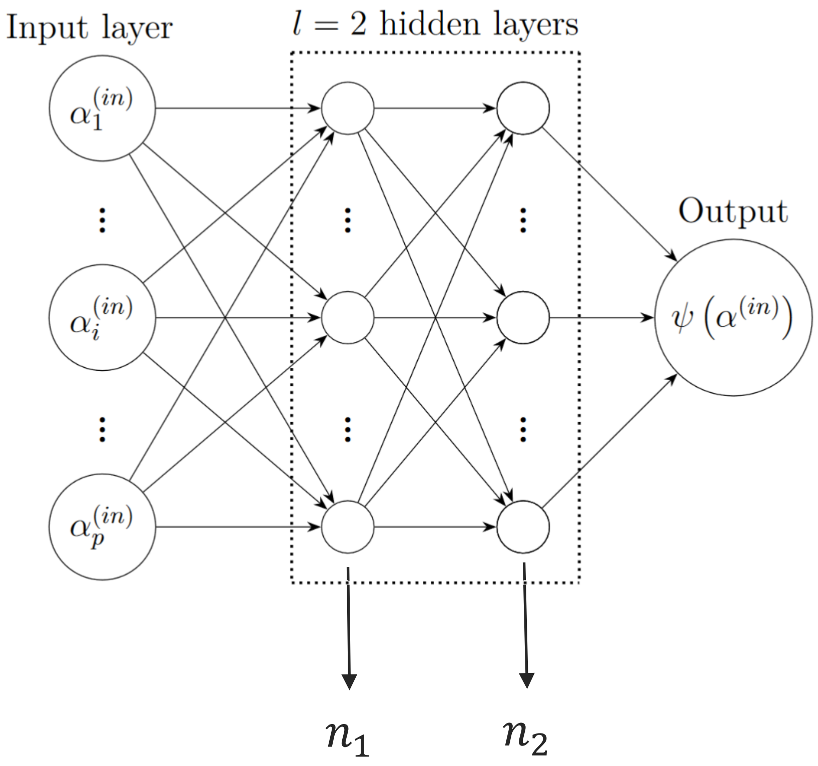

MLP Hyperparameters	Variable	Domain	Type	Role
Learning rate	r	$[10^{-5}, 10^{-2}]$	FLOAT	NEUTRAL
Momentum	α	$[0, 1]$	FLOAT	NEUTRAL
Activation function	a	{ReLU, Sigmoid, Tanh}	ENUM	NEUTRAL
Batch size	b	$\{8, 16, \ldots, 128, 256\}$	ORD	NEUTRAL
# of hidden layers	l	$\{1, 2, 3\}$	ORD	META
# of neurons hidden layer k	n_k	$\{50, 51, \ldots, 55\}$	ORD	DECREED

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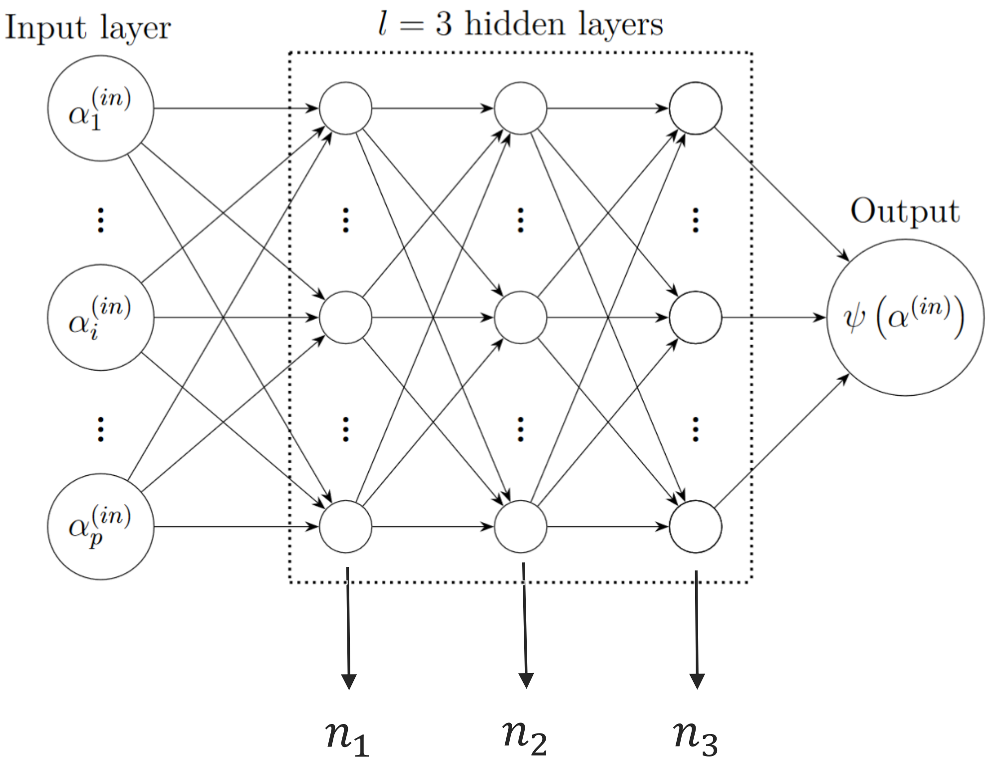

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Batch size	b	$\{8, 16, \ldots, 128, 256\}$	ORD	NEUTRAL
# of hidden layers	l	$\{1, 2, 3\}$	ORD	META
# of neurons hidden layer k	n_k	$\{50, 51, \ldots, 55\}$	ORD	DECREED

J. Bussemaker, P. Saves, N. Bartoli, T. Lefebvre, R. Lafage, **System Architecture Optimization Strategies: Dealing with Expensive Hierarchical Problems**, 2024, JOGO, *Under review.*

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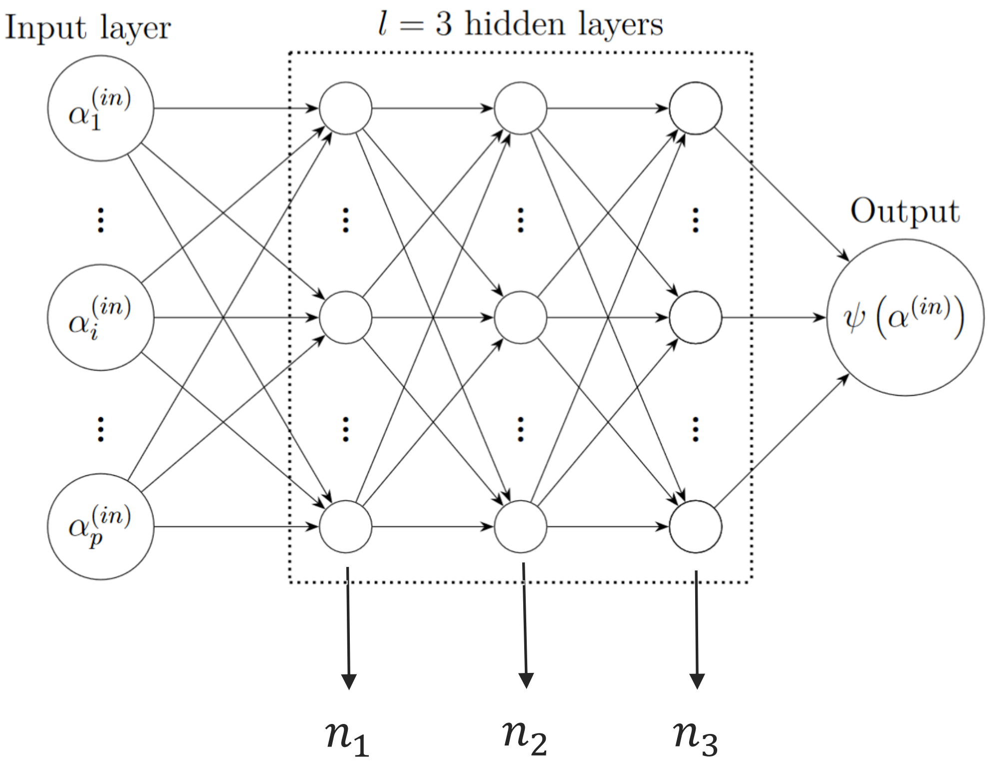
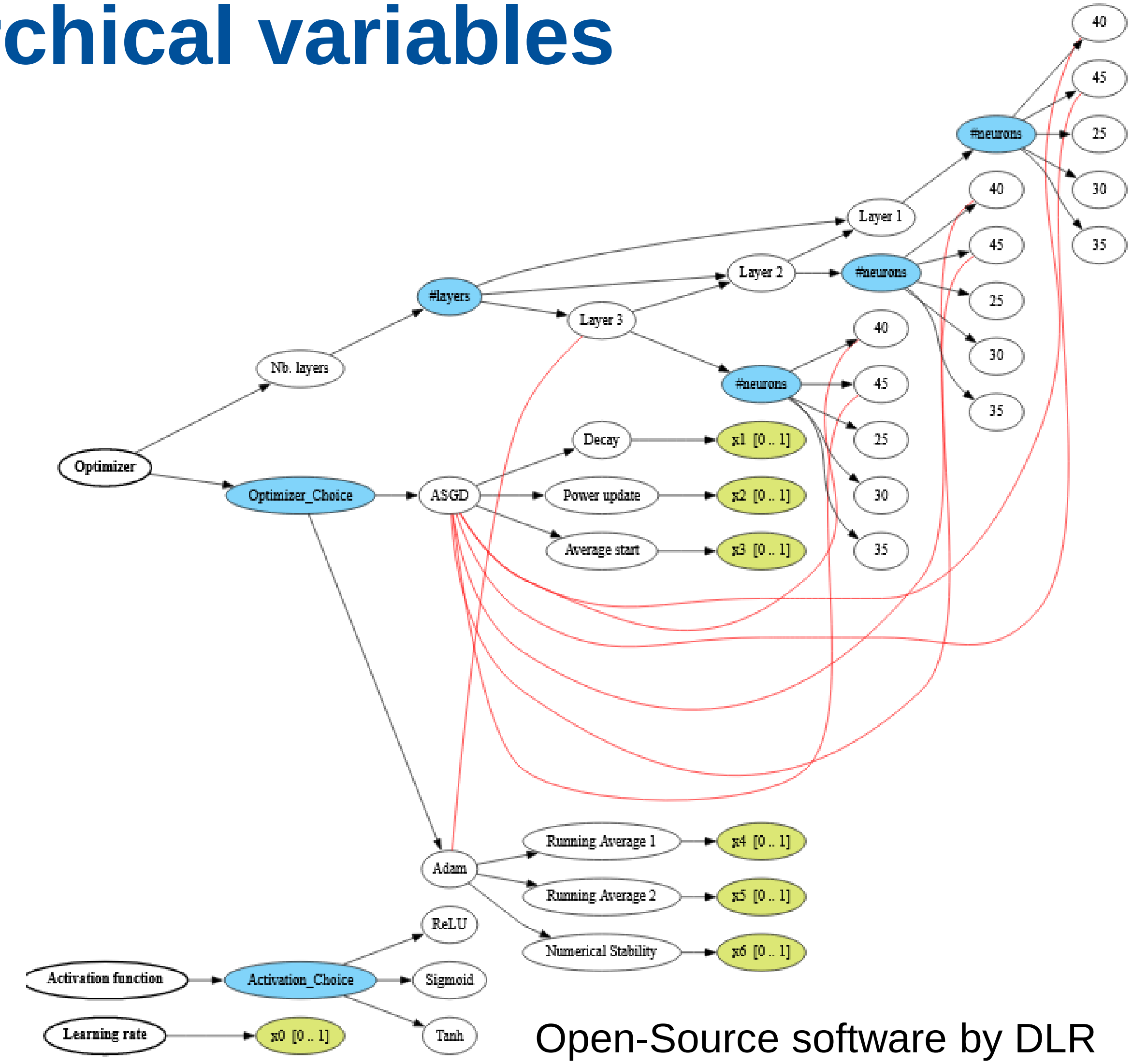
Multi-Layer Perceptron: hierarchical variables





MLP Hyperparameters	Variable	Domain	Type	Role
Learning rate	r	$[10^{-5}, 10^{-2}]$	FLOAT	NEUTRAL
Momentum	α	$[0, 1]$	FLOAT	NEUTRAL
Activation function	a	{ReLU, Sigmoid, Tanh}	ENUM	NEUTRAL
Batch size	b	$\{8, 16, \ldots, 128, 256\}$	ORD	NEUTRAL
# of hidden layers	l	$\{1, 2, 3\}$	ORD	META
# of neurons hidden layer k	n_k	$\{50, 51, \ldots, 55\}$	ORD	DECREED

Open-Source software by DLR
Architecture Design Space Graph
https://github.com/jbussemaker/adsg-core

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GP for hierarchical variables

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GP for hierarchical variables

- Activeness vector δ

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GP for hierarchical variables

- Activeness vector δ
  - A vector associated with a hierarchical input whose dimension is the size of the "full space".
    - $w^r = (10^{-3}, ReLU, 16, 1, 55) \Rightarrow \delta^r = (1,1,1,1,1,0,0)$

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- Distance d

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  - Any distance can be used for d, e.g $d(a,b) = |a - b|^2$

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- State-of-the-art: Imputation method

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- Distance d
  - Any distance can be used for d, e.g $d(a,b) = |a-b|^2$

- State-of-the-art: Imputation method
  - Inactive variables take ground value
    - $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55) \Rightarrow (10^{-3}, ReLU, 16, \mathbf{1}, 55, 50,50)$
    - $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
    - $w^s = (10^{-3}, ReLU, 64, \mathbf{2}, 55, 52) \Rightarrow (10^{-4}, ReLU, 64, \mathbf{2}, 55, 52,50)$
    - $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$

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- Distance d
  - Any distance can be used for d, *e.g* $d(a,b) = |a-b|^2$
- State-of-the-art: Imputation method
  - Inactive variables take ground value
  - Full dimension mixed integer kernel

- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55) \Rightarrow (10^{-3}, ReLU, 16, \mathbf{1}, 55, 50, 50)$
- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $w^s = (10^{-3}, ReLU, 64, \mathbf{2}, 55, 52) \Rightarrow (10^{-4}, ReLU, 64, \mathbf{2}, 55, 52, 50)$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$

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- Distance d
  - Any distance can be used for d, e.g $d(a,b) = |a-b|^2$

d = 0: no effect

$\omega_i = 50$

- State-of-the-art: Imputation method
  - Inactive variables take ground value
  - Full dimension mixed integer kernel

- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55) \Rightarrow (10^{-3}, ReLU, 16, \mathbf{1}, 55, 50, 50)$
- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $w^s = (10^{-3}, ReLU, 64, \mathbf{2}, 55, 52) \Rightarrow (10^{-4}, ReLU, 64, \mathbf{2}, 55, 52, 50)$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$

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GP for hierarchical variables

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    - $w^r = (10^{-3}, ReLU, 16, 1, 55) \Rightarrow \delta^r = (1,1,1,1,1,0,0)$
- Distance d
  - Any distance can be used for d, e.g $d(a,b) = |a-b|^2$

d = 2: residual distance

d = 0: no effect

$\omega_i = 50$

- State-of-the-art: Imputation method
  - Inactive variables take ground value
  - Full dimension mixed integer kernel

- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55) \Rightarrow (10^{-3}, ReLU, 16, \mathbf{1}, 55, 50, 50)$
- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $w^s = (10^{-3}, ReLU, 64, \mathbf{2}, 55, 52) \Rightarrow (10^{-4}, ReLU, 64, \mathbf{2}, 55, 52, 50)$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$

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GP for hierarchical variables

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    - $w^r = (10^{-3}, ReLU, 16, 1, 55) \Rightarrow \delta^r = (1,1,1,1,1,0,0)$

- Distance d
  - Any distance can be used for d, e.g $d(a,b) = |a-b|^2$

d = 1: residual distance

d = 0: no effect

$\omega_i = 51$

- State-of-the-art: Imputation method
  - Inactive variables take ground value
  - Full dimension mixed integer kernel

- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55) \Rightarrow (10^{-3}, ReLU, 16, \mathbf{1}, 55, 51, 51)$
- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $w^s = (10^{-3}, ReLU, 64, \mathbf{2}, 55, 52) \Rightarrow (10^{-4}, ReLU, 64, \mathbf{2}, 55, 52, 51)$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$

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- Distance d
  - Any distance can be used for d, e.g $d(a,b) = |a-b|^2$

d = 1: residual distance

d = 0: no effect

$\omega_i = 51$

- State-of-the-art: Imputation method
  - Inactive variables take ground value
  - Full dimension mixed integer kernel

- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55) \Rightarrow (10^{-3}, ReLU, 16, \mathbf{1}, 55, 51, 51)$
- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $w^s = (10^{-3}, ReLU, 64, \mathbf{2}, 55, 52) \Rightarrow (10^{-4}, ReLU, 64, \mathbf{2}, 55, 52, 51)$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$

$$d_{Imp}(w_i^r, w_i^s) = \begin{cases} 0 & \text{both inactive} \\ |w_i^r - \omega_i|^2 & \text{only one active} \\ |w_i^r - w_i^s|^2 & \text{both active} \end{cases}$$

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  - Any distance can be used for d, e.g $d(a,b) = |a-b|^2$

d = 1: residual distance

d = 0: no effect

- State-of-the-art: Imputation method
  - Inactive variables take ground value
  - Full dimension mixed integer kernel

- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55) \quad \Rightarrow (10^{-3}, ReLU, 16, \mathbf{1}, 55, 51, 51)$
- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $w^s = (10^{-3}, ReLU, 64, \mathbf{2}, 55, 52) \Rightarrow (10^{-4}, ReLU, 64, \mathbf{2}, 55, 52, 51)$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$

$$d_{Imp}(w_i^r, w_i^s) = \begin{cases} 0 & \text{both inactive} \\ |w_i^r - \omega_i|^2 & \text{only one active} \\ |w_i^r - w_i^s|^2 & \text{both active} \end{cases}$$

User-defined

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GP for hierarchical variables

- State-of-the-art: Arc-Kernel

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GP for hierarchical variables

- State-of-the-art: Arc-Kernel
  - Inactive variables are excluded

- $\delta^r = (1,1,1,1,\mathbf{1,0,0})$
- $\delta^s = (1,1,1,1,\mathbf{1,1,0})$
- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55)$
- $w^s = (10^{-3}, ReLU, 16, \mathbf{2}, 55, 52)$

d = 0: no effect

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GP for hierarchical variables

- State-of-the-art: Arc-Kernel
  - Inactive variables are excluded
  - Dedicated kernel

d = 1: residual distance

- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$
- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55)$
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$$d_{Arc}(w_i^r, w_i^s) = \begin{cases} 0 & \text{both inactive} \\ 1 & \text{only one active} \\ \sqrt{2 - 2\cos\left(\frac{\rho_i \, |w_i^r - w_i^s|^2}{u_i - l_i}\right)} & \text{both active} \end{cases}$$

- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$
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ρ_i: Parameter to estimate

$u_i - l_i$: Bounds-dependent

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$$d_{Arc}(w_i^r, w_i^s) = \begin{cases} 0 & \text{both inactive} \\ 1 & \text{only one active} \\ \sqrt{2 - 2\cos\left(\rho_i \frac{|w_i^r - w_i^s|^2}{u_i - l_i}\right)} & \text{both active} \end{cases}$$

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$u_i - l_i$: Bounds-dependent

- New Alg-Kernel

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d = 1: residual distance

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- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$
- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55)$
- $w^s = (10^{-3}, ReLU, 16, \mathbf{2}, 55, 52)$

d = 0: no effect

$$d_{Arc}(w_i^r, w_i^s) = \begin{cases} 0 & \text{both inactive} \\ 1 & \text{only one active} \\ \sqrt{2 - 2\cos\left(\rho_i \frac{|w_i^r - w_i^s|^2}{u_i - l_i}\right)} & \text{both active} \end{cases}$$

ρ_i: Parameter to estimate

$u_i - l_i$: Bounds-dependent

- New Alg-Kernel
  - Normalized data

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  - Inactive variables are excluded
  - Dedicated kernel

$$d_{Arc}(w_i^r, w_i^s) = \begin{cases} 0 & \text{both inactive} \\ 1 & \text{only one active} \\ \sqrt{2 - 2\cos\left(\frac{\rho_i \left|w_i^r - w_i^s\right|^2}{u_i - l_i}\right)} & \text{both active} \end{cases}$$

ρ_i: Parameter to estimate

$u_i - l_i$: Bounds-dependent

- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$
- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55)$
- $w^s = (10^{-3}, ReLU, 16, \mathbf{2}, 55, 52)$

d = 1: residual distance

d = 0: no effect

- New Alg-Kernel
  - Normalized data
  - New algebraic kernel

P. Saves, R. Lafage, N. Bartoli, Y. Diouane, J. Bussemaker, T. Lefebvre, J. Hwang, J. Morlier, J. Martins, **SMT 2.0: A Surrogate Modeling Toolbox with a focus on Hierarchical and Mixed Variables Gaussian Processes**, 2024, Advances in Engineering Software.

D. Horn, J. Stork, N. Schüßler, M. Zaefferer, **Surrogates for hierarchical search spaces: The wedge-kernel and an automated analysis**, 2019, Proceedings of the genetic and evolutionary computation conference.

GP for hierarchical variables

- State-of-the-art: Arc-Kernel
  - Inactive variables are excluded
  - Dedicated kernel

$$d_{Arc}(w_i^r, w_i^s) = \begin{cases} 0 & \text{both inactive} \\ 1 & \text{only one active} \\ \sqrt{2 - 2\cos\left(\rho_i \frac{|w_i^r - w_i^s|^2}{u_i - l_i}\right)} & \text{both active} \end{cases}$$

ρ_i → Parameter to estimate

$u_i - l_i$ → Bounds-dependent

- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$
- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55)$
- $w^s = (10^{-3}, ReLU, 16, \mathbf{2}, 55, 52)$

d = 1: residual distance

d = 0: no effect

- New Alg-Kernel
  - Normalized data
  - New algebraic kernel

$$d_{Alg}(w_i^r, w_i^s) = \begin{cases} 0 & \text{both inactive} \\ 1 & \text{only one active} \\ \frac{2\,|w_i^r - w_i^s|^2}{\sqrt{w_i^r + 1}\sqrt{w_i^s + 1}} & \text{both active} \end{cases}$$

- $\delta^r = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $\delta^s = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$
- $w^r = (10^{-3}, ReLU, 16, \mathbf{1}, 55)$
- $w^s = (10^{-3}, ReLU, 16, \mathbf{2}, 55, 52)$

d = 0: no effect

d = 1: residual distance

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Contents

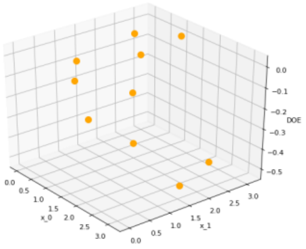
SEGOMOE algorithm

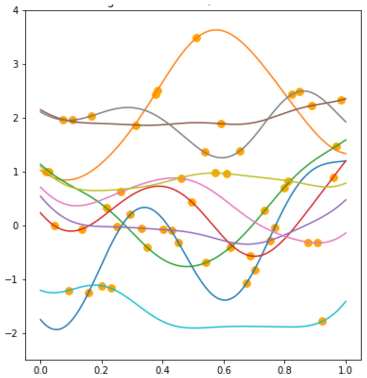
$$\min_{w \in \Omega} \; f(w)$$

$$s.t \begin{cases} c_1(w) \leq 0 \\ \vdots \\ c_m(w) \leq 0 \end{cases}$$

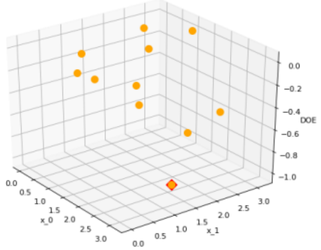
Problem definition

Initial DoE building

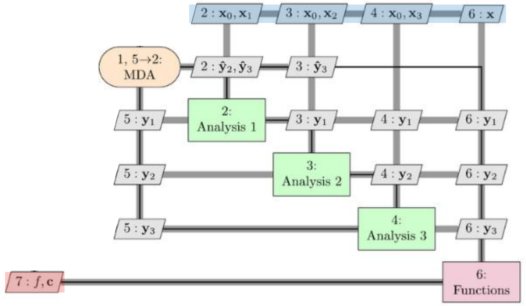




Building / Training Surrogate models

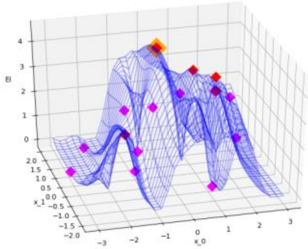


Adding new point to DOE



Evaluation of problem true functions

Optimization criterion



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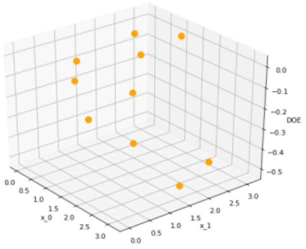
SEGOMOE algorithm

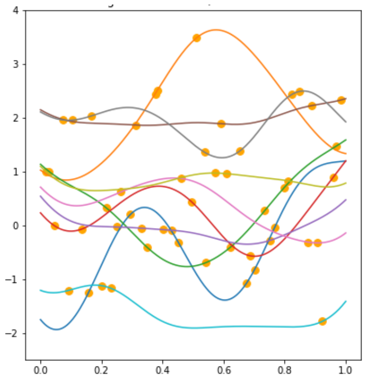
$$\min_{w \in \Omega} \; f(w)$$
$$s.t \begin{cases} c_1(w) \leq 0 \\ \vdots \\ c_m(w) \leq 0 \end{cases}$$

Problem definition ✓

Initial DoE building ✓

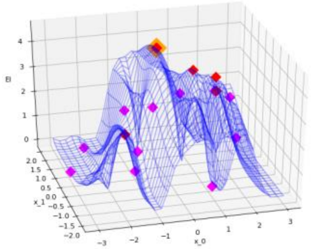


Building / Training Mixed GP ✓

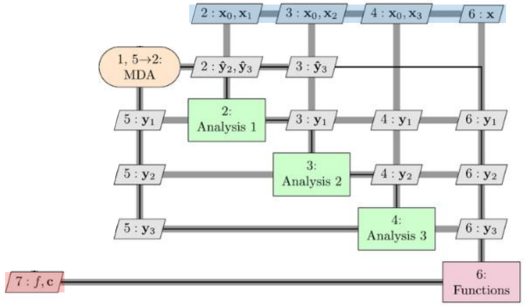


$\hat{y}(w), s(w)$

Optimization criterion



Evaluation of problem true functions



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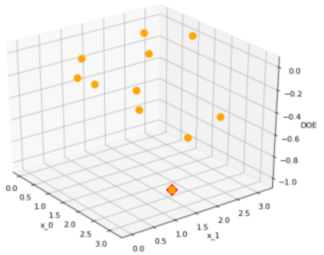

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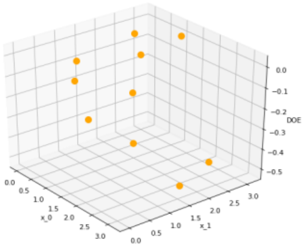
SEGOMOE algorithm

$$\max_{w \in \Omega} \quad (f_{min} - \hat{y}(w))\, \Phi\left(\frac{f_{min} - \hat{y}(w)}{s(w)}\right) + s(w)\phi\left(\frac{f_{min} - \hat{y}(w)}{s(w)}\right)$$

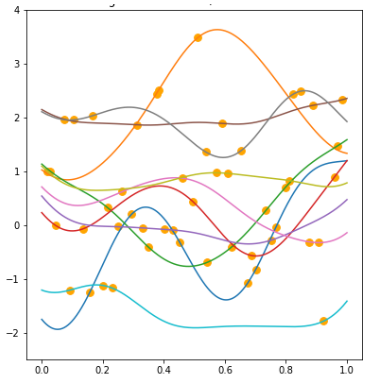
$$s.t \begin{cases} \widehat{c_1}(w) \leq 0 \\ \vdots \\ \widehat{c_m}(w) \leq 0 \end{cases}$$

Problem definition ✓

Initial DoE building ✓

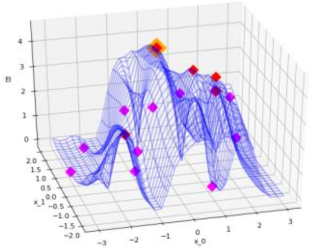


Building / Training Mixed GP ✓

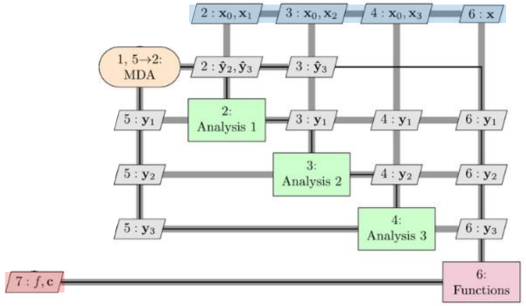


$\hat{y}(w), s(w)$

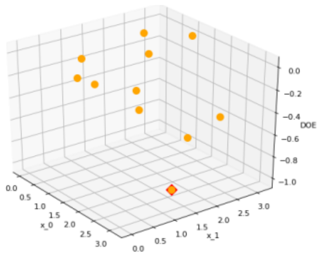
Optimization criterion



Evaluation of problem true functions



Adding new point to DOE



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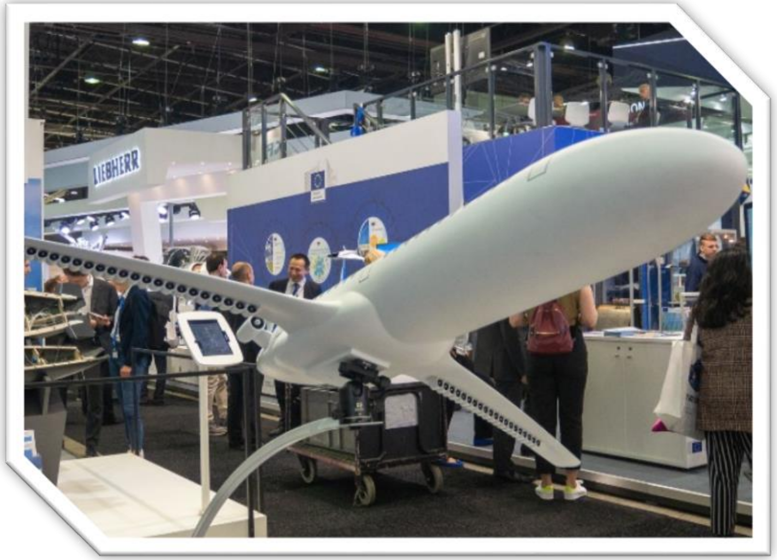
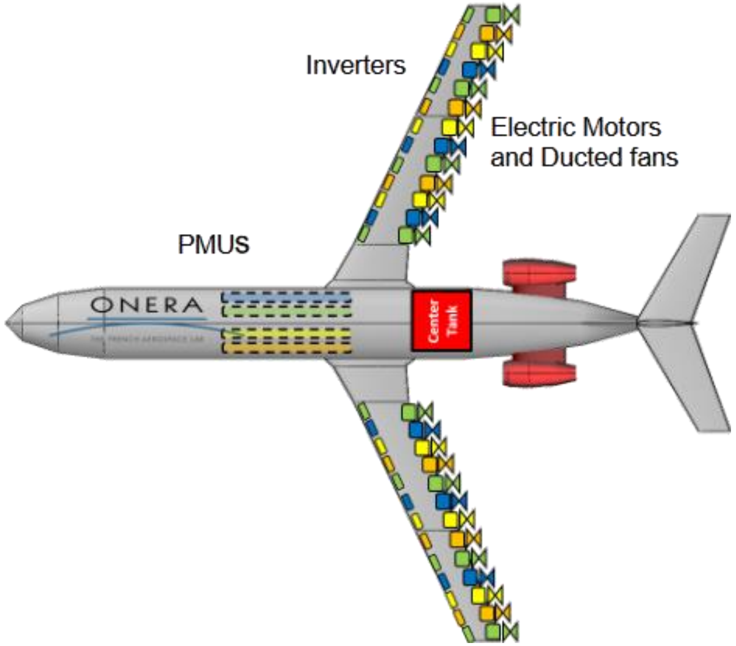
Optimization problem: DRAGON
Towards a green aircraft concept



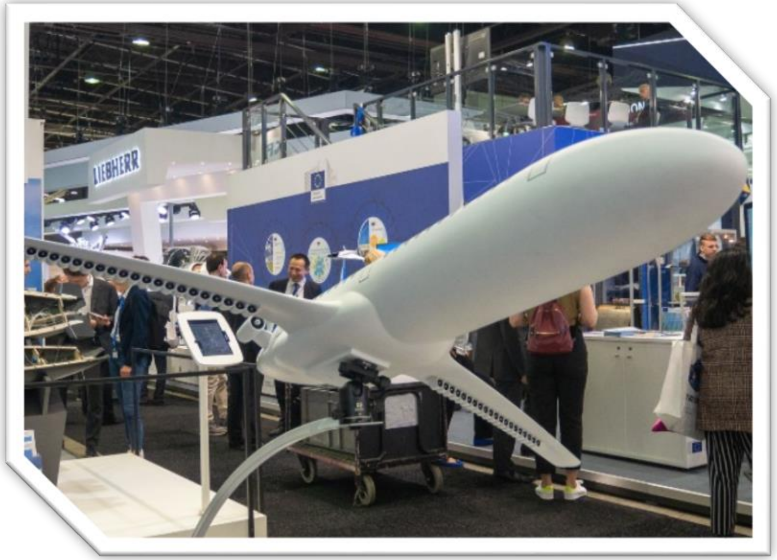


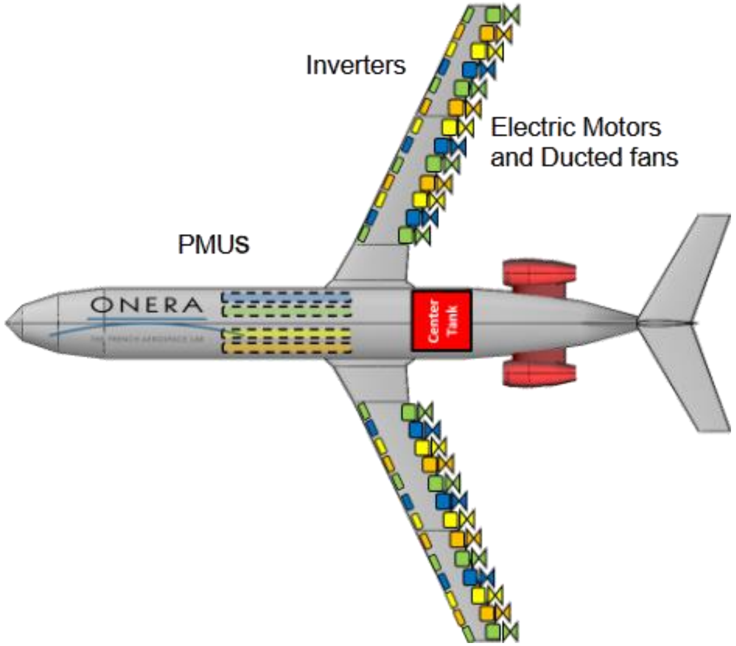
P. Schmollgruber, C. Doll, J. Hermetz, R. Liaboeuf, M. Ridel, I. Cafarelli, O. Atinault, C. Francois, B. Paluch, **Multidisciplinary Exploration of DRAGON: an ONERA Hybrid Electric Distributed Propulsion Concept**, 2019, AIAA SciTech Forum.

Optimization problem: DRAGON

Towards a green aircraft concept

- 30% reduction of CO_2 emissions by 2035





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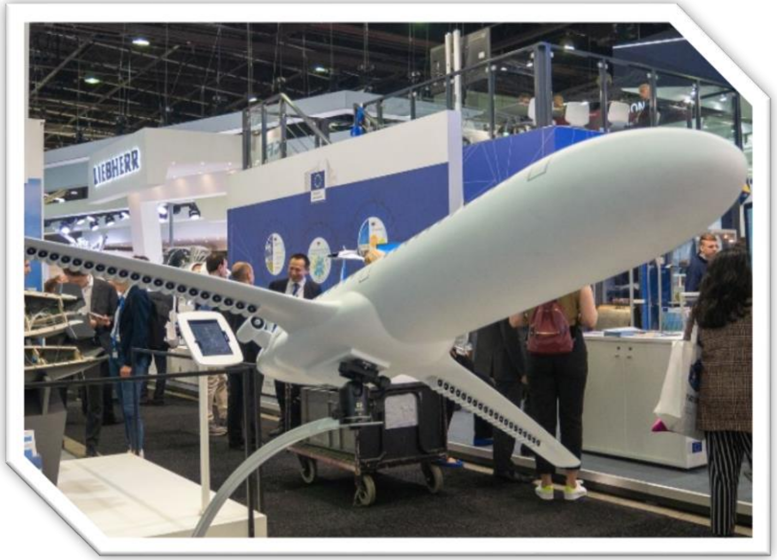
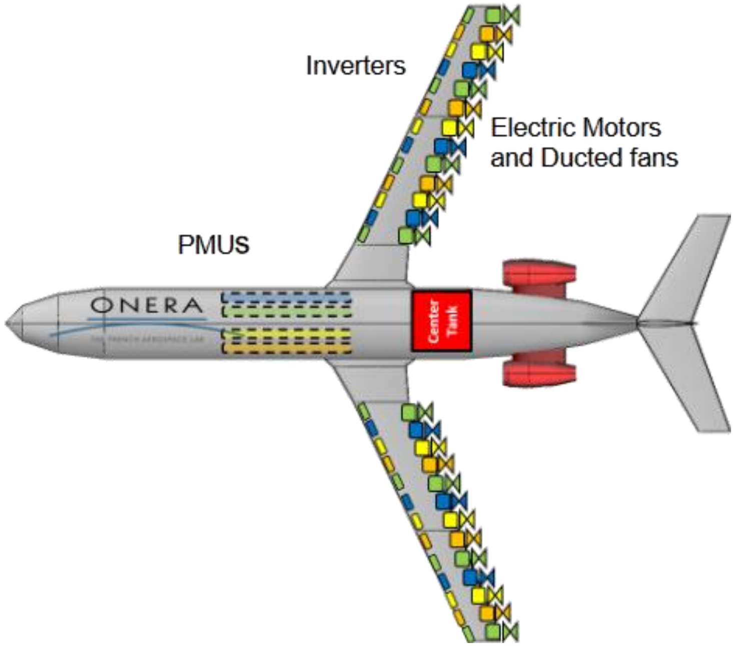
Optimization problem: DRAGON
Towards a green aircraft concept

- 30% reduction of CO_2 emissions by 2035

→ Reduce fuel consumption





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DRAGON optimization test case

	Function/variable	Nature	Quantity	Range
Minimize	Fuel mass	cont	1	
	Total objectives		**1**	
with respect to	Fan operating pressure ratio	cont	1	$[1.05, 1.3]$
	Wing aspect ratio	cont	1	$[8, 12]$
	Angle for swept wing	cont	1	$[15, 40]$ (°)
	Wing taper ratio	cont	1	$[0.2, 0.5]$
	HT aspect ratio	cont	1	$[3, 6]$
	Angle for swept HT	cont	1	$[20, 40]$ (°)
	HT taper ratio	cont	1	$[0.3, 0.5]$
	TOFL for sizing	cont	1	$[1800., 2500.]$ (m)
	Top of climb vertical speed for sizing	cont	1	$[300., 800.](ft/min)$
	Start of climb slope angle	cont	1	$[0.075., 0.15.](rad)$
	Total continuous variables		10	
	Turboshaft layout	cat	2 levels	{1,2}
	Architecture_cat	cat	17 levels	{1,2,3, ...,15,16,17}
	Number of cores	int	1	{2,4,6}
	Number of motors*	int	1	{8,12,16,20,...,40}
	*graph-structure dependence to the core value			
subject to	Wing span < 36 (m)	cont	1	
	TOFL < 2200 (m)	cont	1	
	Wing trailing edge occupied by fans < 14.4 (m)	cont	1	
	Climb duration < 1740 (s)	cont	1	
	Top of climb slope > 0.0108 (rad)	cont	1	
	Total constraints		**5**	

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	Function/variable	Nature	Quantity	Range
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	TOFL for sizing	cont	1	$[1800., 2500.]$ (m)
	Top of climb vertical speed for sizing	cont	1	$[300., 800.](ft/min)$
	Start of climb slope angle	cont	1	$[0.075., 0.15.](rad)$
	Total continuous variables		10	
	Turboshaft layout	cat	2 levels	{1,2}
Categorical	Architecture_cat	cat	17 levels	{1,2,3, . . . ,15,16,17}
or	Number of cores	int	1	{2,4,6}
Hierarchical	Number of motors*	int	1	{8,12,16,20,. . . ,40}
	*graph-structure dependence to the core value			
subject to	Wing span < 36 (m)	cont	1	
	TOFL < 2200 (m)	cont	1	
	Wing trailing edge occupied by fans < 14.4 (m)	cont	1	
	Climb duration < 1740 (s)	cont	1	
	Top of climb slope > 0.0108 (rad)	cont	1	
	Total constraints		**5**	

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DRAGON optimization test case

	Function/variable	Nature	Quantity	Range
Minimize	Fuel mass	cont	1	
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	Wing aspect ratio	cont	1	$[8, 12]$
	Angle for swept wing	cont	1	$[15, 40]$ ($°$)
	Wing taper ratio	cont	1	$[0.2, 0.5]$
	HT aspect ratio	cont	1	$[3, 6]$
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	HT taper ratio	cont	1	$[0.3, 0.5]$
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	Top of climb vertical speed for sizing	cont	1	$[300., 800.](ft/min)$
	Start of climb slope angle	cont	1	$[0.075., 0.15.](rad)$
	Total continuous variables		10	
	Turboshaft layout	cat	2 levels	{1,2}
Categorical or Hierarchical	Architecture_cat	cat	17 levels	{1,2,3, . . . ,15,16,17}
	Number of cores	int	1	{2,4,6}
	Number of motors*	int	1	{8,12,16,20,. . . ,40}
	*graph-structure dependence to the core value			
subject to	Wing span < 36 (m)	cont	1	
	TOFL < 2200 (m)	cont	1	
	Wing trailing edge occupied by fans < 14.4 (m)	cont	1	
	Climb duration < 1740 (s)	cont	1	
	Top of climb slope > 0.0108 (rad)	cont	1	
	Total constraints		**5**	

- *10 continuous design variables*
- *2 categorical design variables*
  - *Electric propulsion Architecture: 17 choices*
  - *Turboshaft layout: 2 choices*

Categorical or Hierarchical:

➔ 29 variables in relaxed dimension
➔ 13 variables in relaxed dimension

- 5 inequality constraints (MC)
- Fuel mass to minimize

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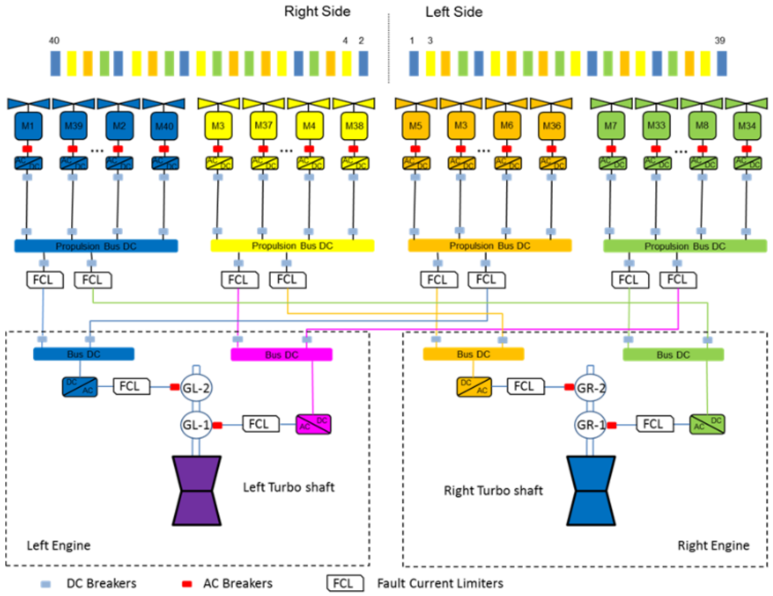
DRAGON optimization test case

Architecture	cat	17 levels	{1,2,3, . . . ,15,16,17}
Turboshaft layout	cat	2 levels	{1,2}
Total categorical variables		2	
Total relaxed variables		**29**	

Architecture number	number of motors	number of generators
1	8	2
2	12	2
3	16	2
4	20	2
5	24	2
6	28	2
7	32	2
8	36	2
9	40	2
10	8	4
11	16	4
12	24	4
13	32	4
14	40	4
15	12	6
16	24	6
17	36	6



layout	position	y ratio	tail	VT aspect ratio	VT taper ratio
1	under wing	0.25	without T-tail	1.8	0.3
2	behind	0.34	with T-tail	1.2	0.85

- *10 continuous design variables*
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  - *Electric propulsion Architecture: 17 choices*
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➔ 13 variables in relaxed dimension

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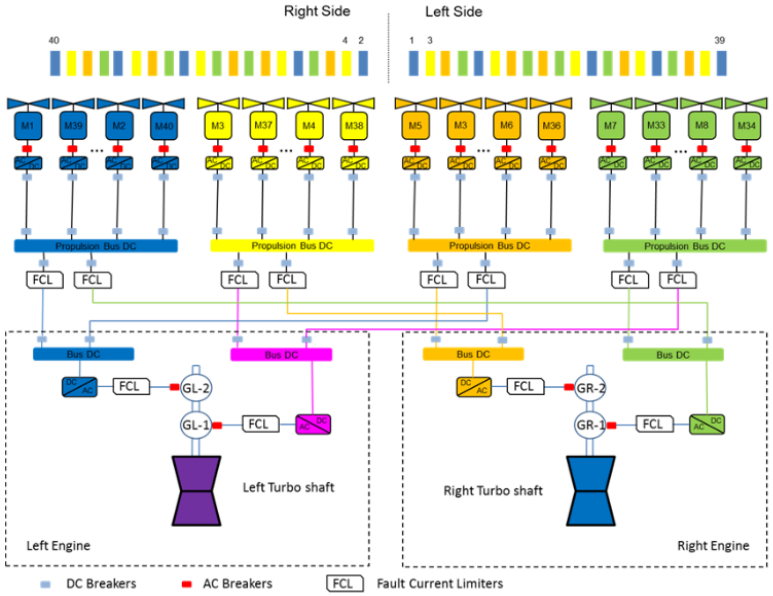
DRAGON optimization test case



Architecture	cat	17 levels	{1,2,3, . . . ,15,16,17}
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Total categorical variables		2	
Total relaxed variables		**29**	

Architecture number	number of motors	number of generators
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3	16	2
4	20	2
5	24	2
6	28	2
7	32	2
8	36	2
9	40	2
10	8	4
11	16	4
12	24	4
13	32	4
14	40	4
15	12	6
16	24	6
17	36	6

layout	position	y ratio	tail	VT aspect ratio	VT taper ratio
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- *10 continuous design variables*
- *2 categorical design variables*
  - *Electric propulsion Architecture: 17 choices*
  - *Turboshaft layout: 2 choices*

Categorical
or
Hierarchical

➔ 29 variables in relaxed dimension
➔ 13 variables in relaxed dimension

- 5 inequality constraints (MC)
- Fuel mass to minimize

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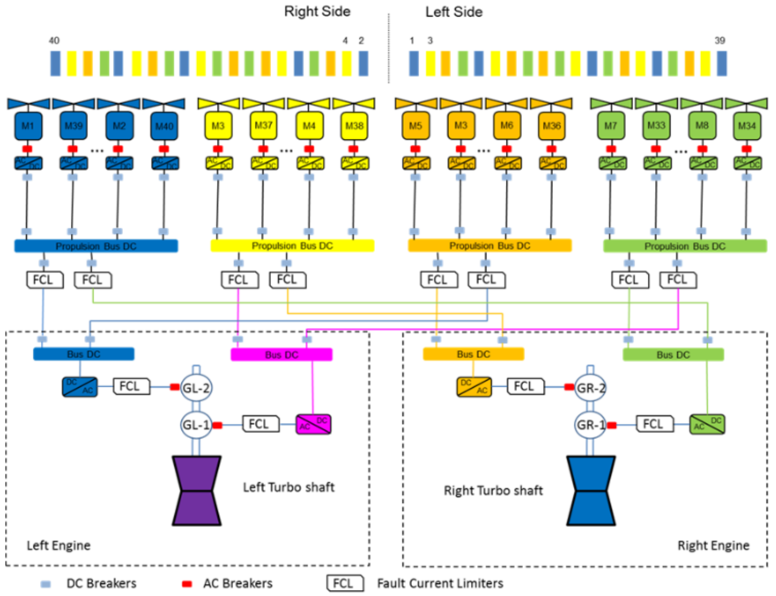
DRAGON optimization test case



Architecture	cat	17 levels	{1,2,3, . . . ,15,16,17}
Turboshaft layout	cat	2 levels	{1,2}
Total categorical variables		2	
Total relaxed variables		**29**	

Architecture number	number of motors	number of generators
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9	40	2
10	8	4
11	16	4
12	24	4
13	32	4
14	40	4
15	12	6
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  - *Turboshaft layout: 2 choices*

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➔ 29 variables in relaxed dimension
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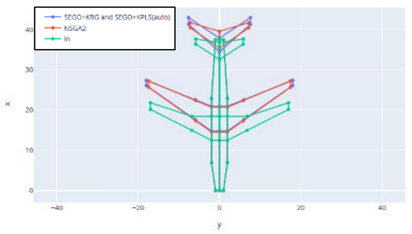
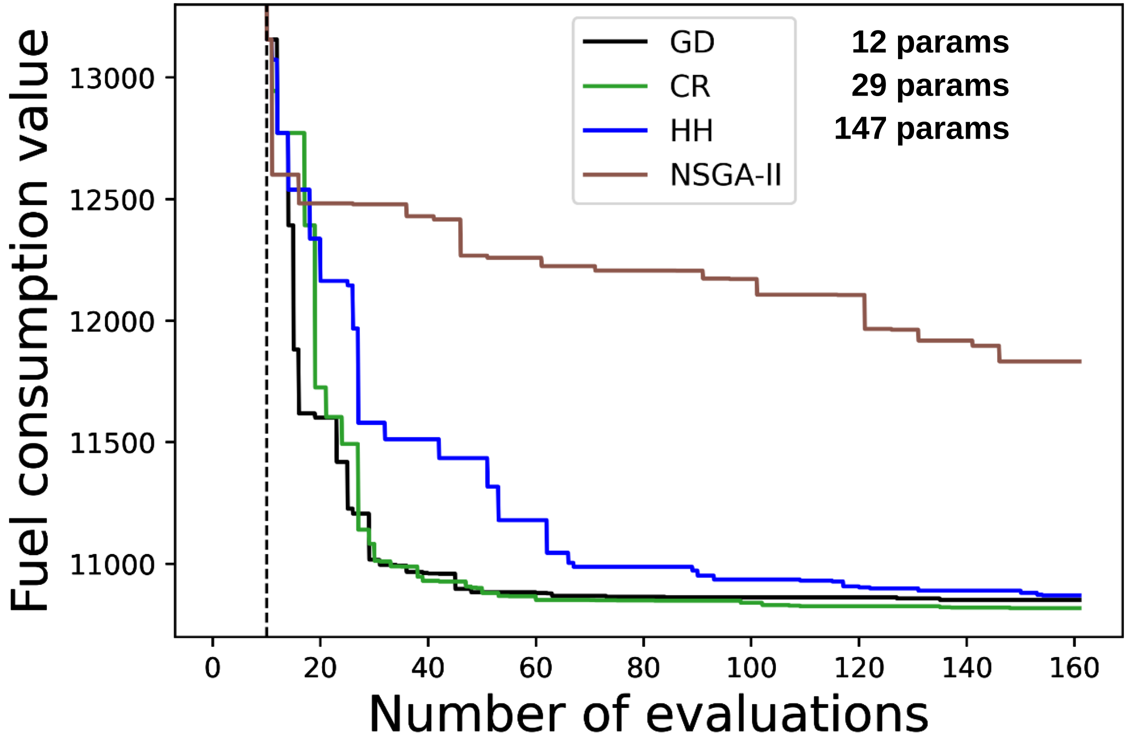


DRAGON optimization results

Without PLS

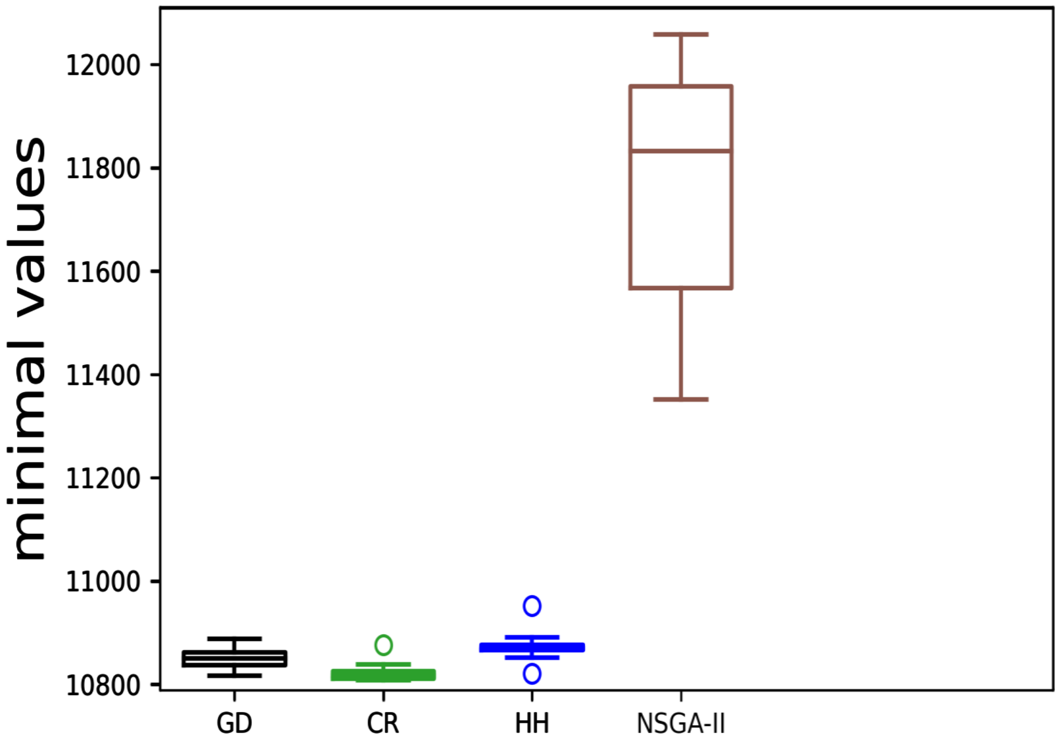
Convergence plots

10 runs of 10 + 150 iterations



Boxplots after 160 evaluations

10 runs of 10 + 150 iterations



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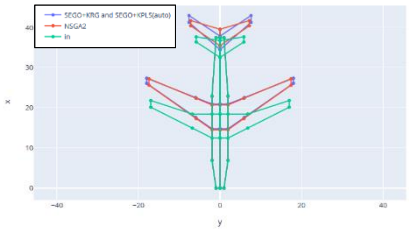
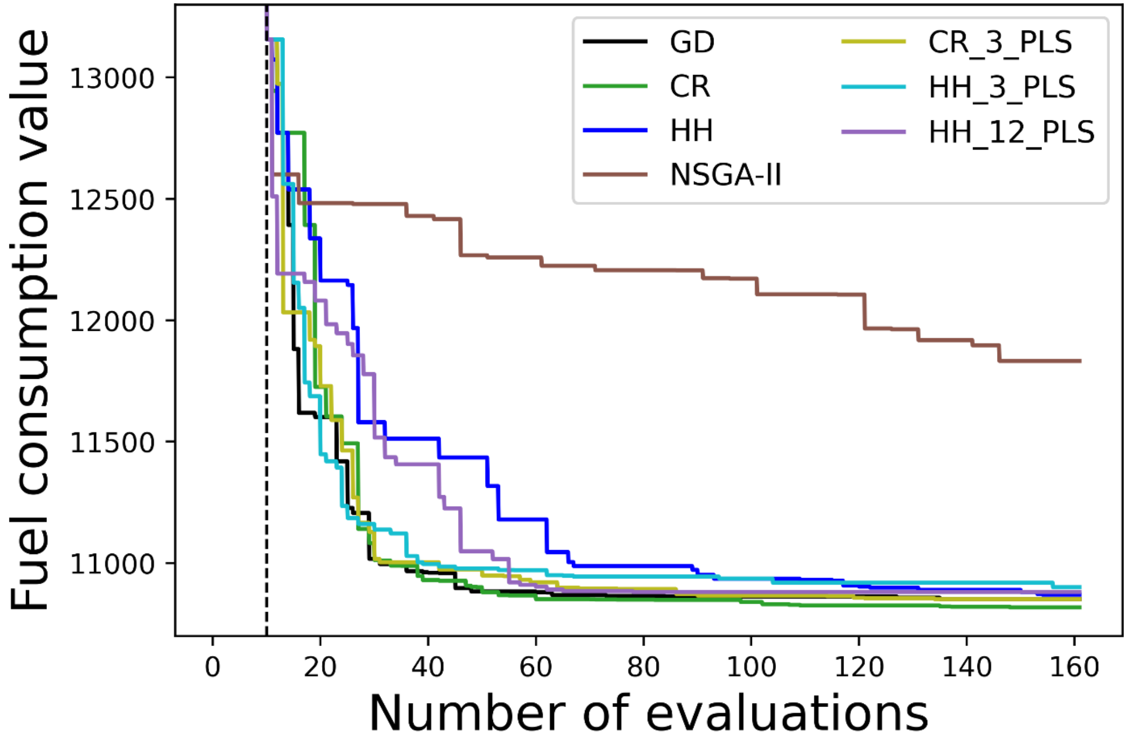
DRAGON optimization results



With PLS

Convergence plots

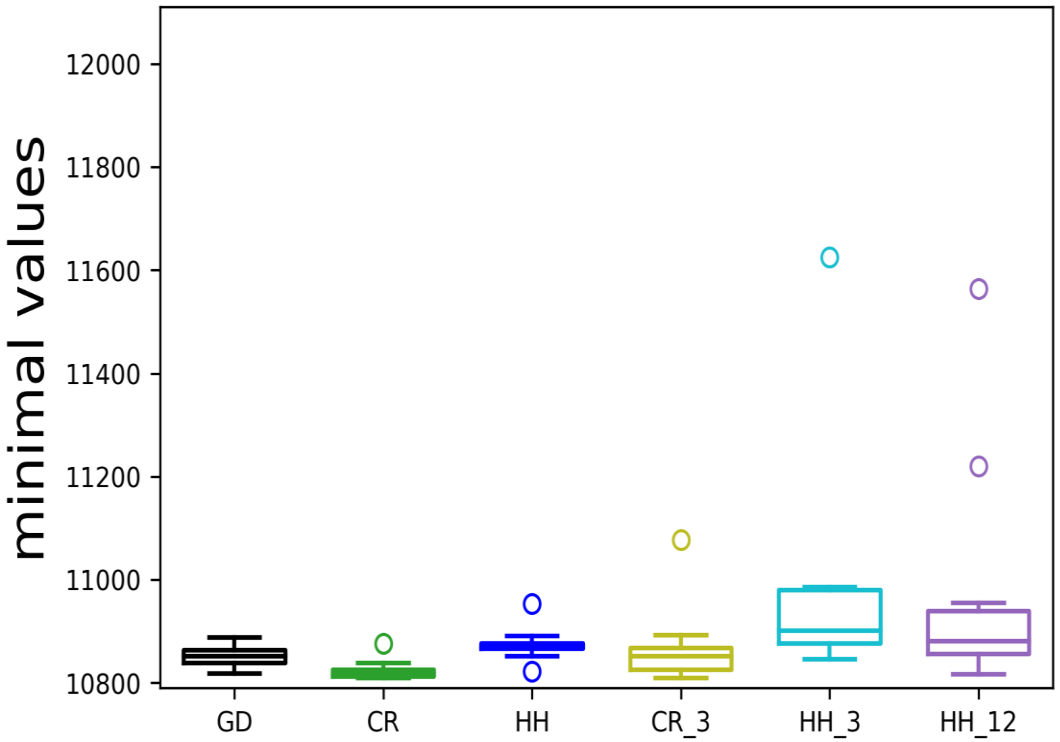
10 runs of 10 + 150 iterations



3 params
3 params
12 params

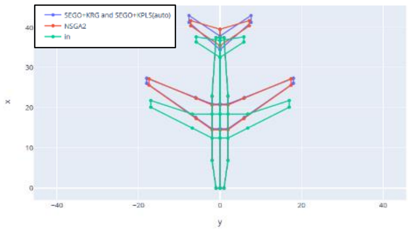
Boxplots after 160 evaluations

10 runs of 10 + 150 iterations



P. Saves, E. Nguyen Van, N. Bartoli, Y. Diouane, T. Lefebvre, J. Morlier, C. David, S. Defoort, **Bayesian optimization for mixed variables using an adaptive dimension reduction process: applications to aircraft design**, 2022, AIAA SciTech Forum.

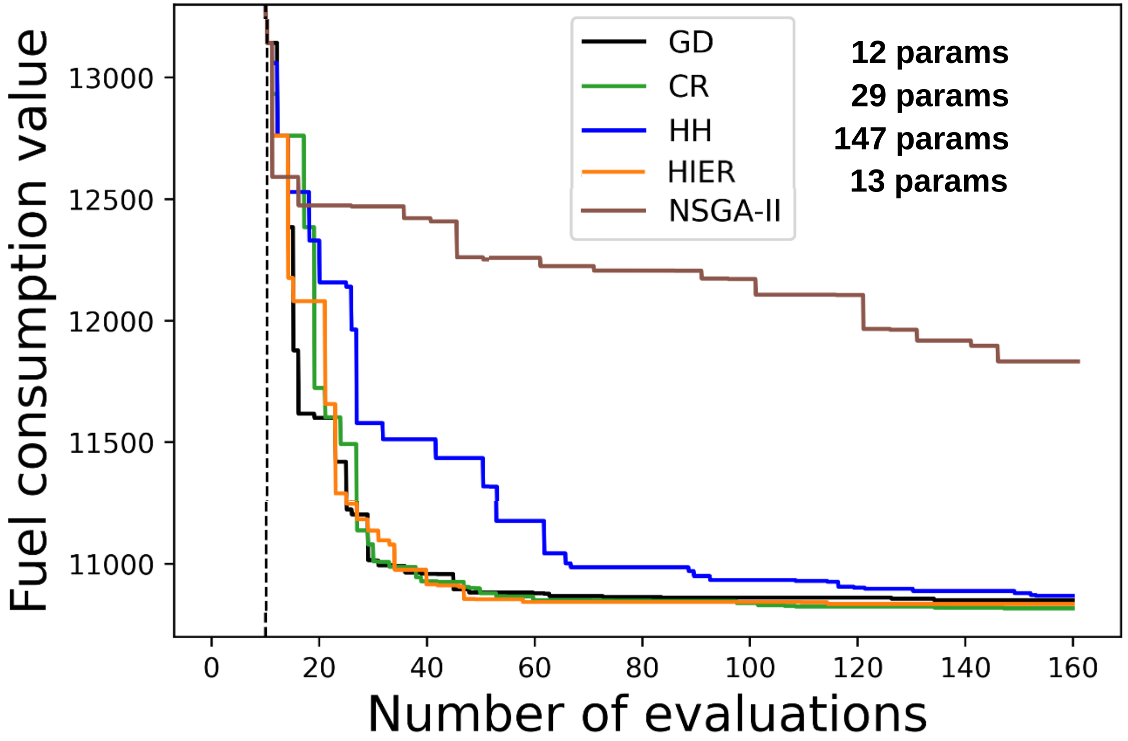
DRAGON optimization results



With Hierarchy

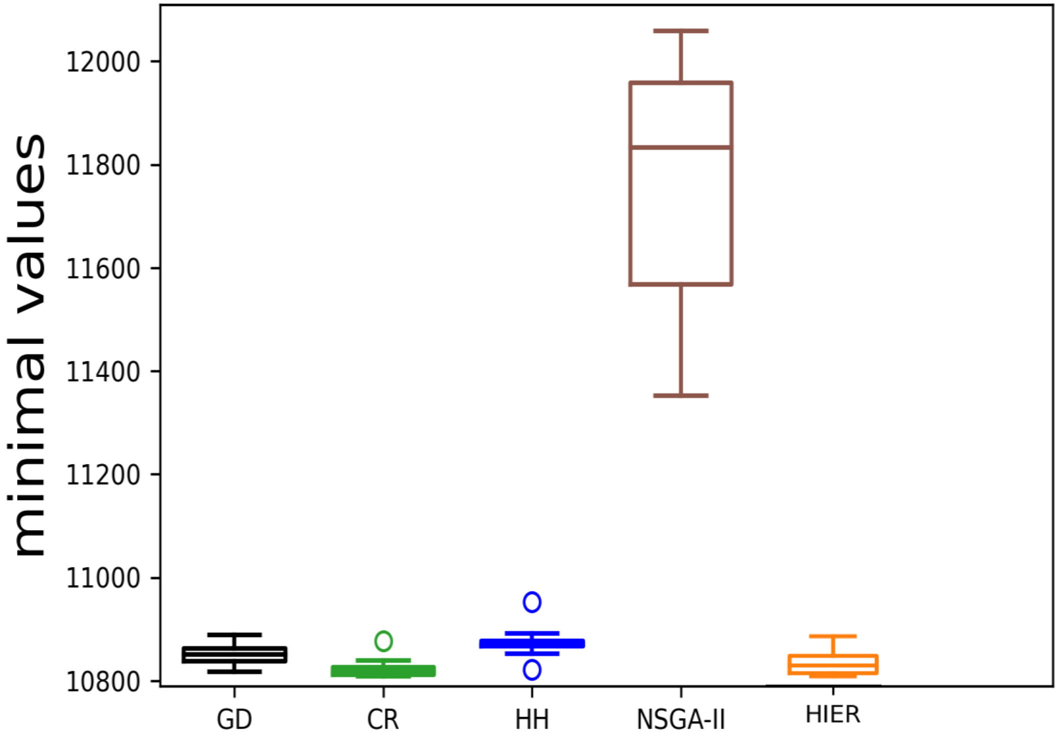
Convergence plots

10 runs of 10 + 150 iterations



Boxplots after 160 evaluations

10 runs of 10 + 150 iterations



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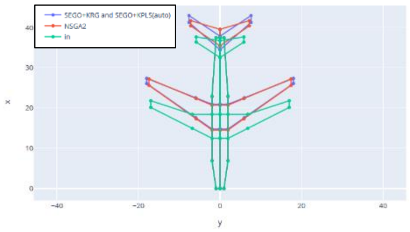


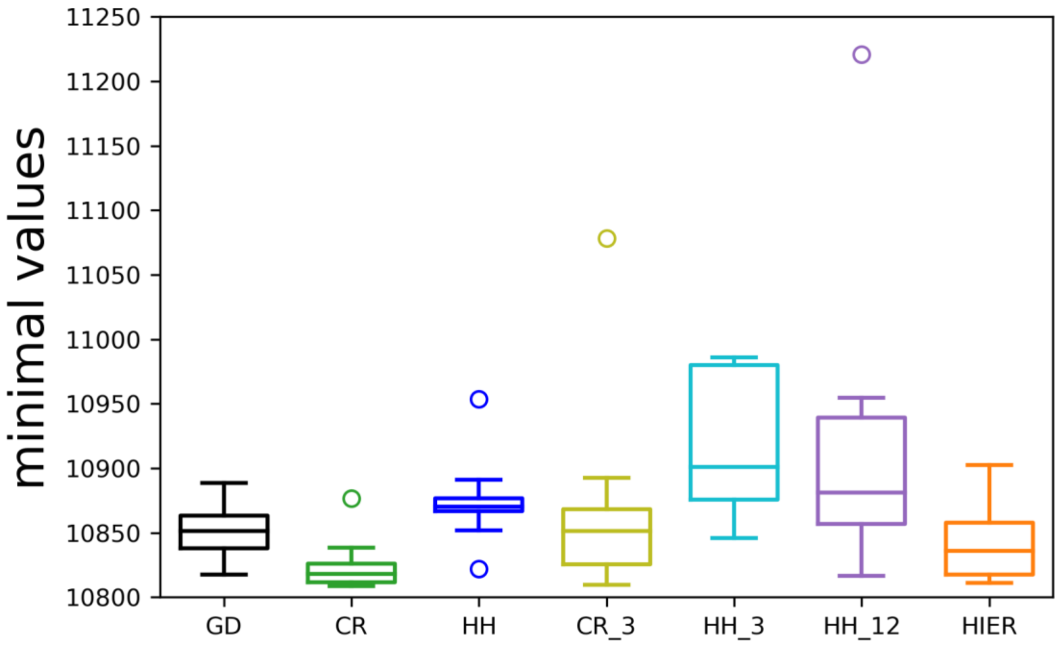
- **DRAGON MDA run time ~ 3min*160 = 8h**

Name	# of cat. params	# of cont. params	Total # of params
GD	2	10	12
CR	19	10	29
CR with PLS 3D	Not applicable	Not applicable	3
HH	137	10	147
HH with PLS 3D	2	1	3
HH with PLS 12D	2	10	12
NSGA-II	Not applicable	Not applicable	Not applicable
HIER	1	12	13

- **GD ~ 36h** → Good but HIER is better
- **CR ~ 62h** → Best convergence
- **CR with PLS 3D ~ 14h** → Best speed
- **HH ~ 320h**
- **HH with PLS 3D ~ 102h**
- **HH with PLS 12D ~ 258h**
- **NSGA-II ~ 16h**
- **HIER ~ 40h** → Best trade-off

Boxplots after 160 evaluations

10 runs of 10 + 150 iterations



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Contents

Contents

Open-source toolbox for surrogate models

python

SMT 2.6 features:

- Models to handle a large number of design variables (KPLS – KPLSK – MGP): automatic number of components
- Mixture of experts to handle heterogeneous functions (MOE)
- Different covariance kernels added
- Multi-fidelity models (MFK – MFKPLS – MFKPLSK)
- Noisy kriging to handle uncertainties on data
- Kriging models for **mixed variables** (continuous, discrete, categorical) & associated kernels, sampling and optimization
- Kriging models for **hierarchical variables** (meta, neutral, decreed) & associated kernels, sampling and optimization
- Benchmarking problems

➔ Included some Jupyter notebooks & documentation

github.com/SMTorg/smt

P. Saves, R. Lafage, N. Bartoli, Y. Diouane, J. Bussemaker, T. Lefebvre, J. Hwang, J. Morlier, J. Martins, **SMT 2.0: A Surrogate Modeling Toolbox with a focus on Hierarchical and Mixed Variables Gaussian Processes**, 2024, Advances in Engineering Software.

M.-A. Bouhlel, J. Hwang, N. Bartoli, R. Lafage, J. Morlier, J. Martins, **A Python surrogate modeling framework with derivatives**, 2019, Advances in Engineering Software.

Conclusions

- Developed Gaussian process for:
  - ➔ Mixed variables (continuous, integer, categorical) ✓
  - ➔ Hierarchical variables / variable-size problems (Meta, decreed, neutral) ✓
  - ➔ High dimensional problems (a high number of variables) ✓
- Implement models in an open-source software ✓

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- Several Bayesian optimization extensions have been implemented:
  - ❑ SEGOMOE for **multi-objective** optimization (with R. Grapin, ISAE) ✓
  - ❑ SEGOMOE for **multi-fidelity** optimization (with R. Charayron, ISAE/ONERA) ✓
  - ❑ SEGOMOE for **architecture** (hierarchical) optimization (with J. Bussemaker, DLR) ✓
  - ❑ SEGOMOE for very **high dimension** (*up to 1000*) optimization (with R. Priem, ISAE/ONERA) ✓

N. Bartoli, T. Lefebvre, R. Lafage, P. Saves, Y. Diouane, J. Morlier, J. Bussemaker, G. Donelli, J. Gomes de Mello, M. Mandorino, P. Della Vecchia, **Multi Objective Bayesian Optimization with mixed integer variables for Aeronautical applications**, 2023, Aerobest 2023.

Future steps

- Coupling ADSG with SMT (with J. Bussemaker, DLR)
- Generalize the hierarchical mathematical framework (with E. Hallé-Hannan, Polytechnique Montréal)

J. Bussemaker, P. Saves, N. Bartoli, T. Lefebvre, R. Lafage, **System Architecture Optimization Strategies: Dealing with Expensive Hierarchical Problems**, 2024, JOGO, *Under review.*

E. Hallé-Hannan, C. Audet, Y. Diouane, S. Le Digabel, P. Saves, **A graph-structured distance for heterogeneous datasets with meta variables**, 2024, SIMODS, *Under review.*

P. Saves, J. Bussemaker, R. Lafage, T. Lefebvre, N. Bartoli, Y. Diouane, J. Morlier, **System-of-systems Modeling and Optimization: An Integrated Framework for Intermodal Mobility**, 2024, ODAS 2024.

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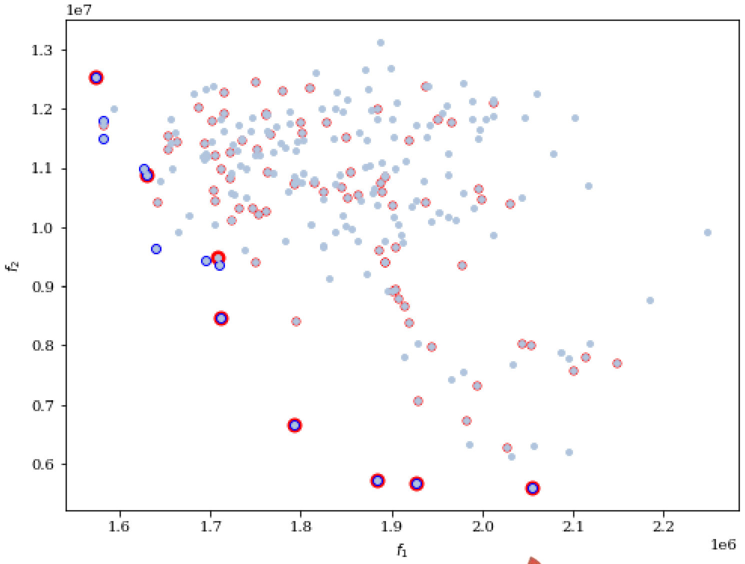
COLLABORATIVE SYSTEM OF SYSTEMS

European Commission

- ❑ Coupling ADSG with SMT (with J. Bussemaker, DLR)
- ❑ Generalize the hierarchical mathematical framework (with E. Hallé-Hannan, Polytechnique Montréal)

- In the frame of COLOSSUS
  - ❑ ONERA SEGOMOE has been successfully applied to wildfire fighting case
  - ❑ Urban air mobility within an intermodal optimization will be the next step!



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Thank you for your attention!

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