A graph-structured distance for heterogeneous datasets with meta variables

Advancing Toward Architecture Modeling

Paul Saves, Edward Hallé-Hannan

Jasper Bussemaker, Eric Nguyen Van, Nathalie Bartoli, Youssef Diouane, Rémi Lafage, Charles Audet, Sébastien Le Digabel, Thierry Lefebvre, Joseph Morlier

Tuesday, October 1st, 2024

Heterogeneous Data and Large Representation Models in Sciences

Toulouse

30 sep - 03 oct 2024

AI for science, science for AI

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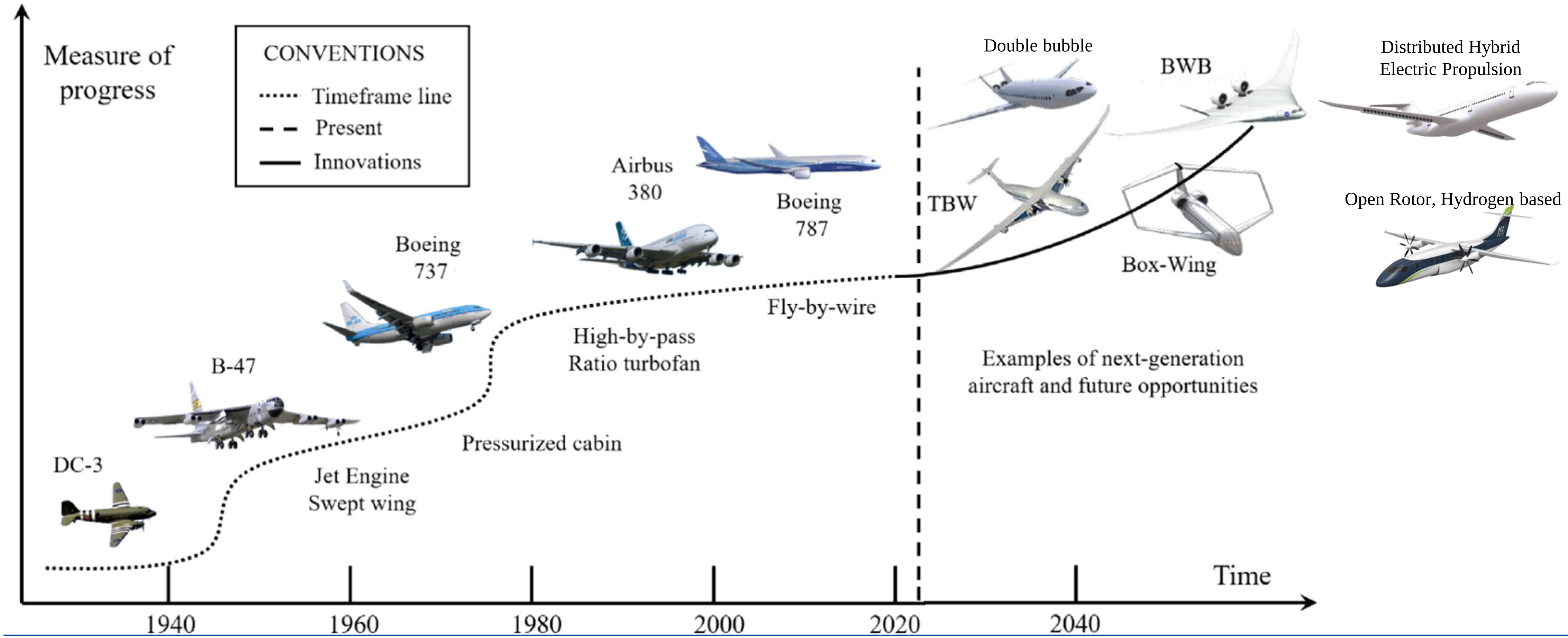
Future aircraft concepts

Goals:

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



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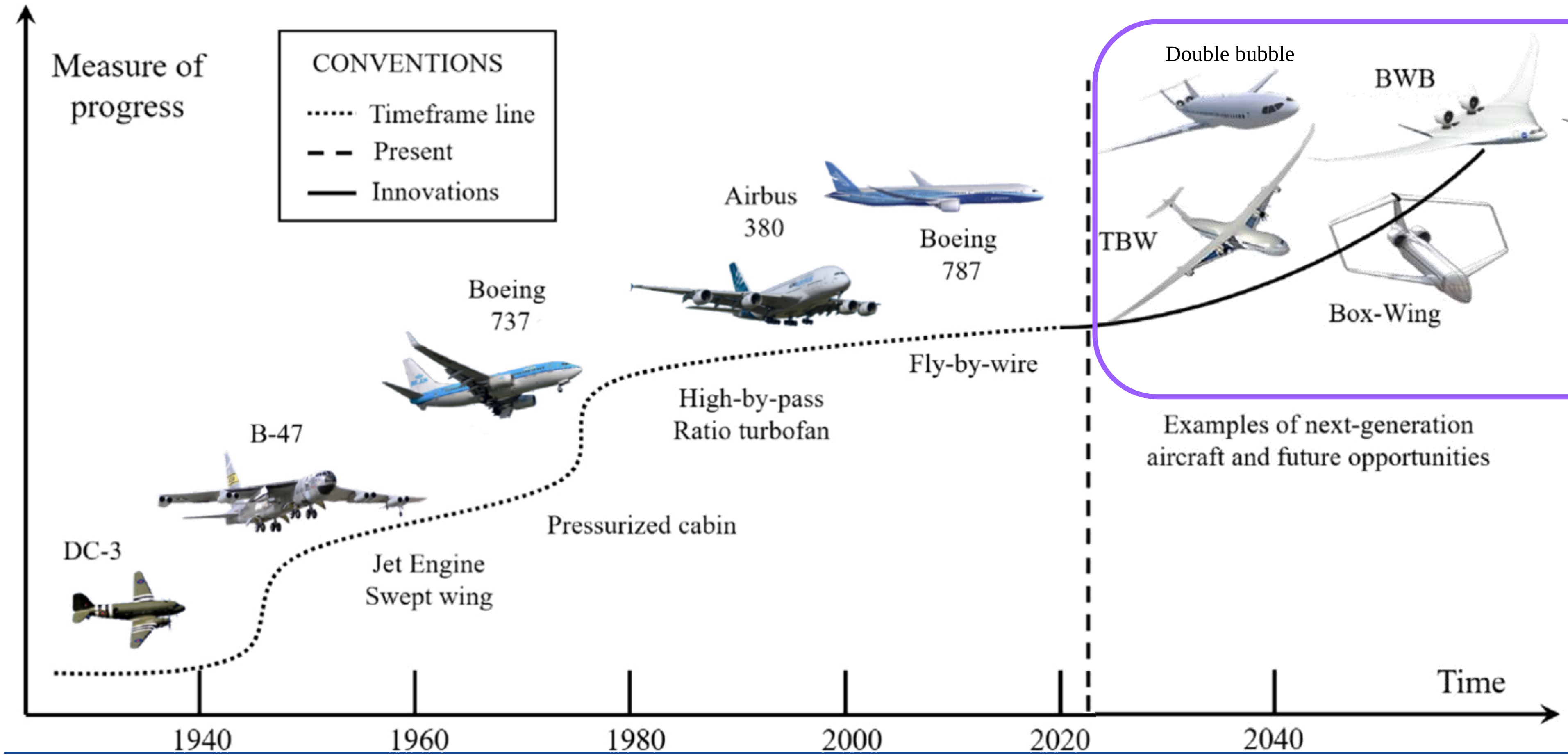

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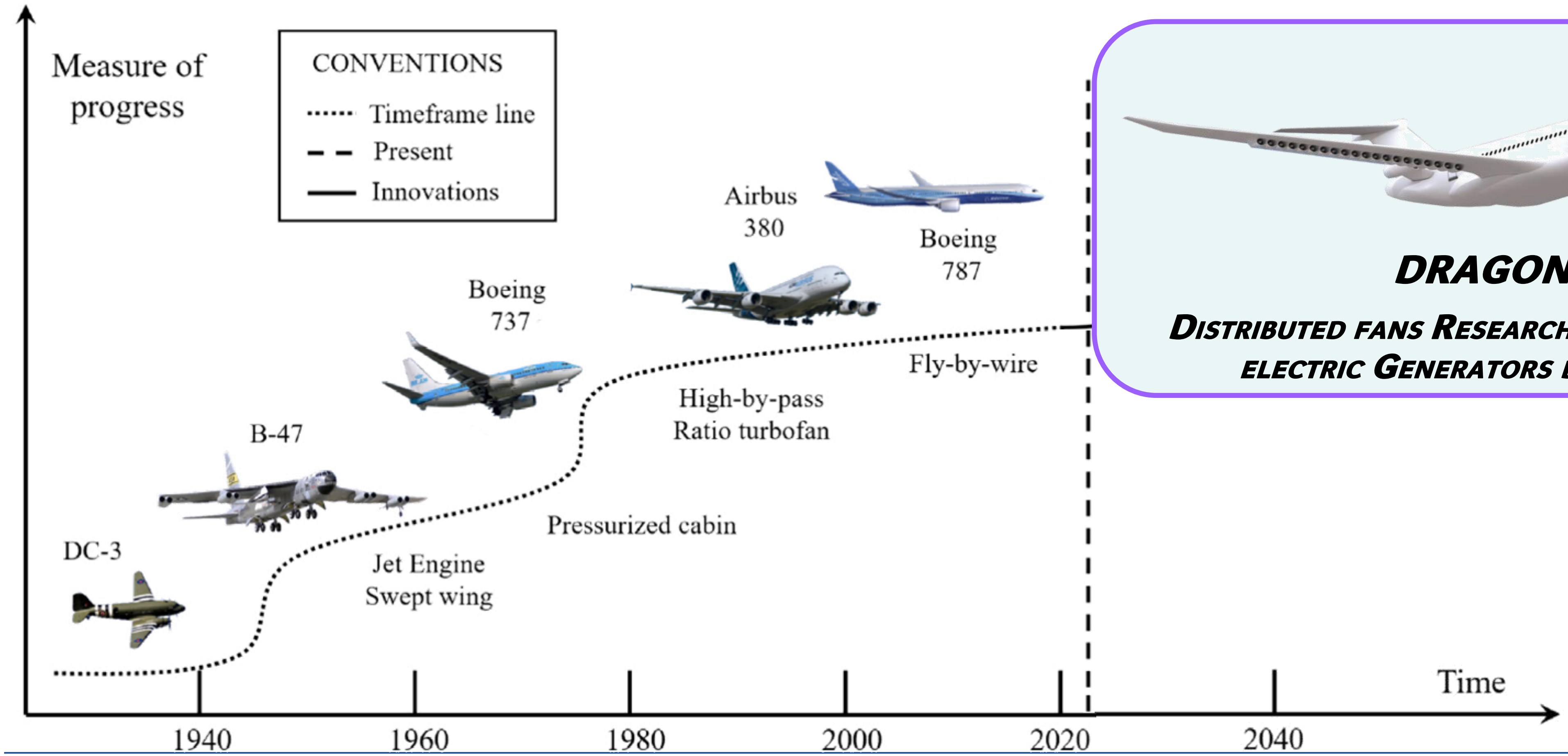

DRAGON

Distributed fans Research Aircraft with electric Generators by ONERA

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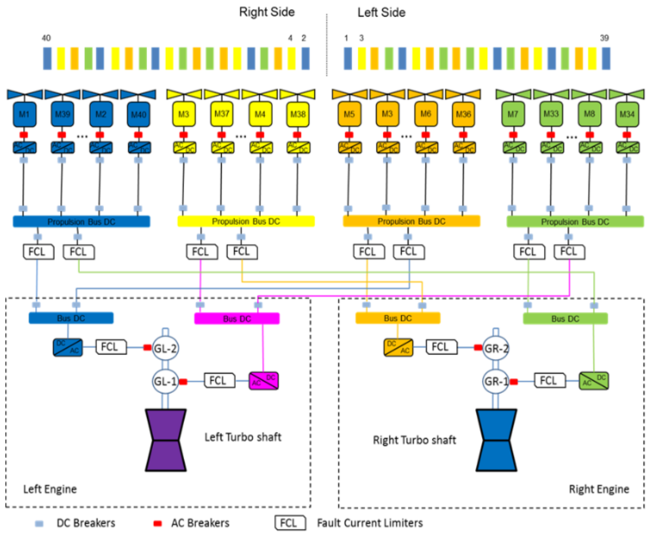
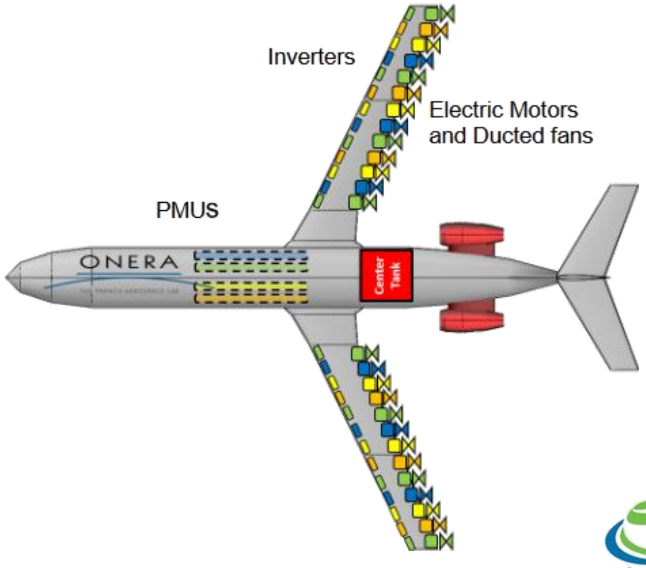
DRAGON optimization test case





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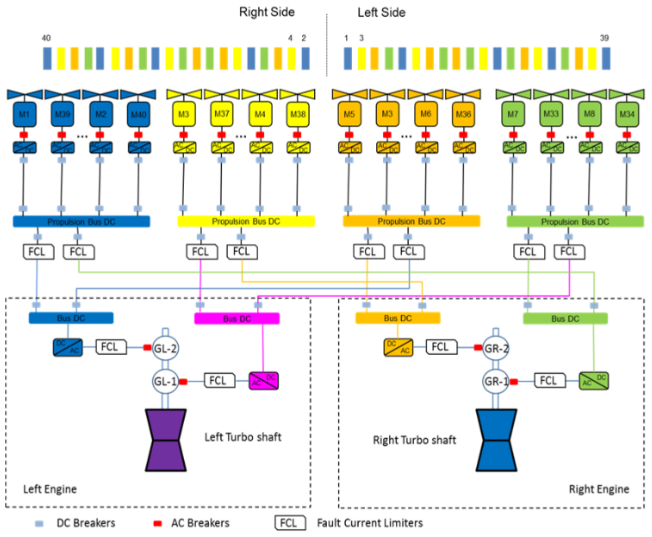

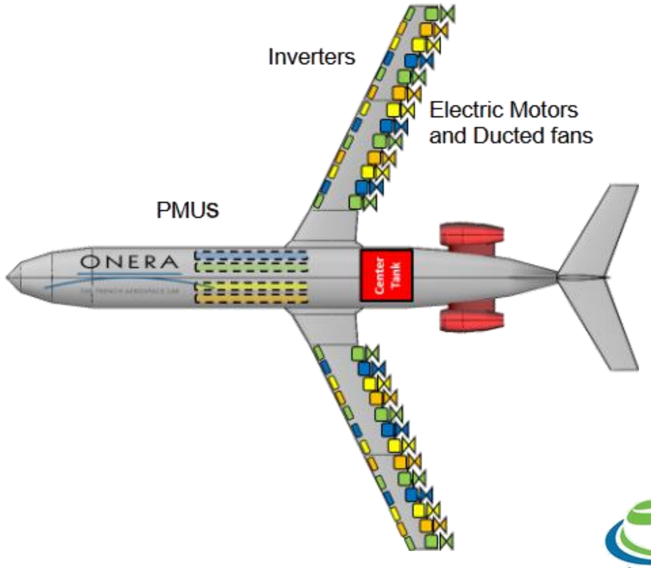

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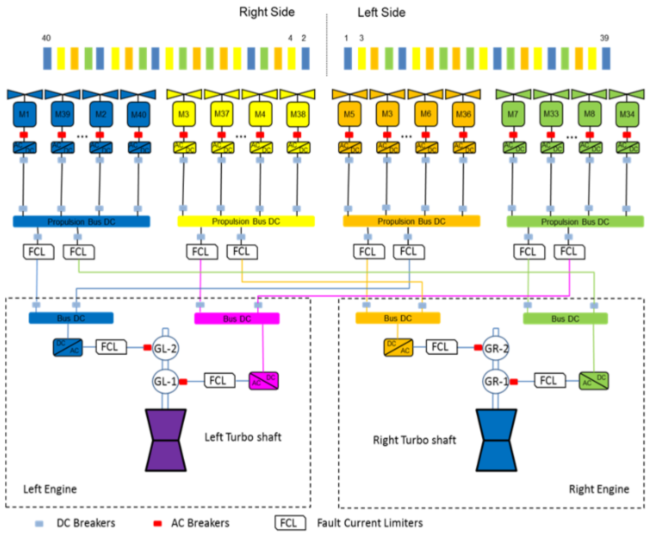

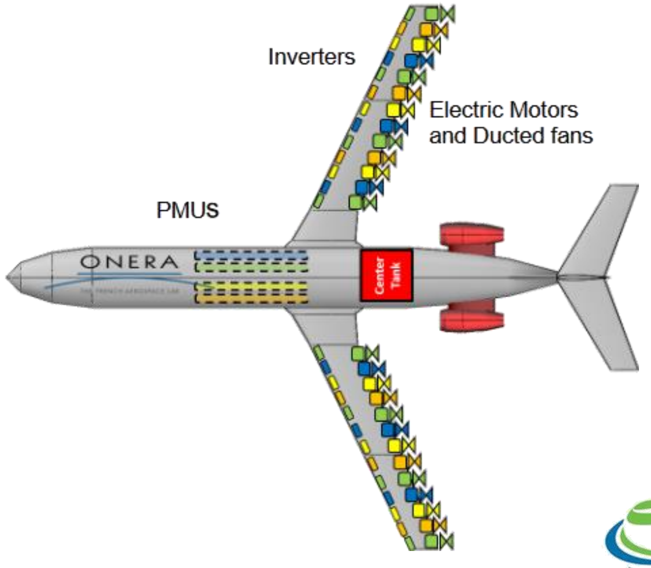

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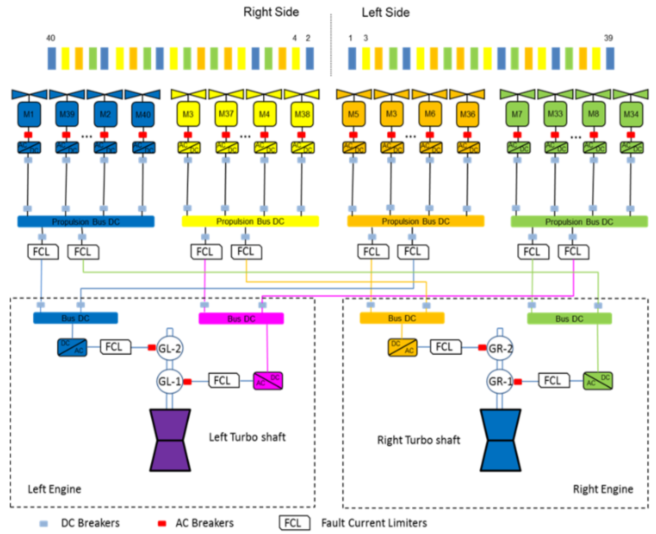

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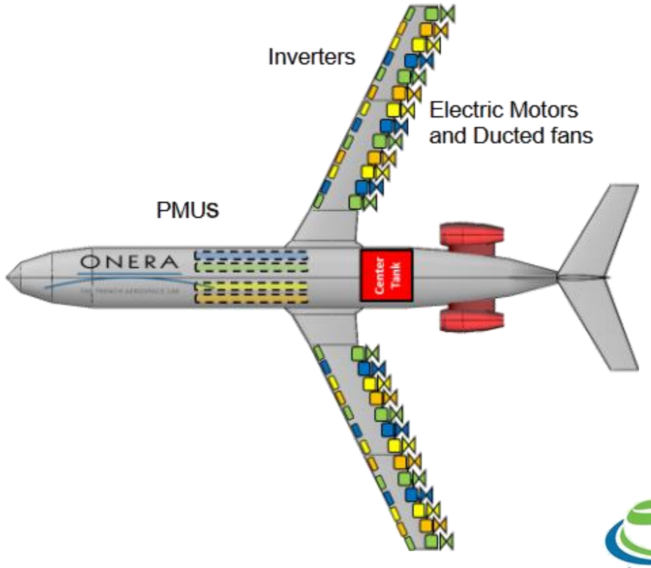

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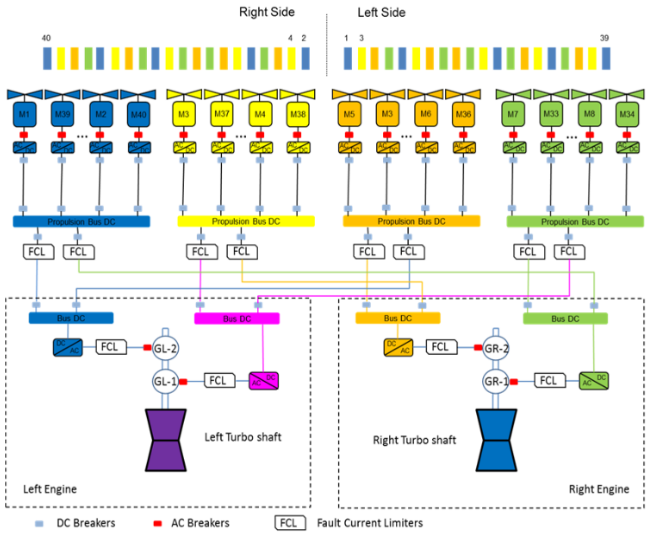

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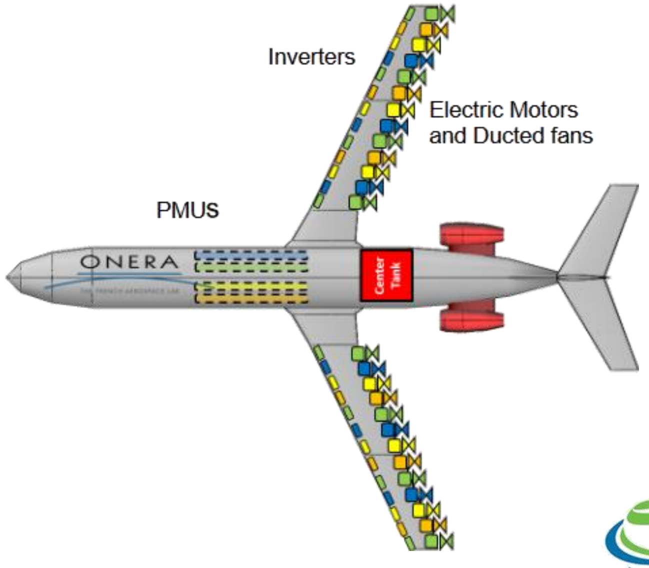

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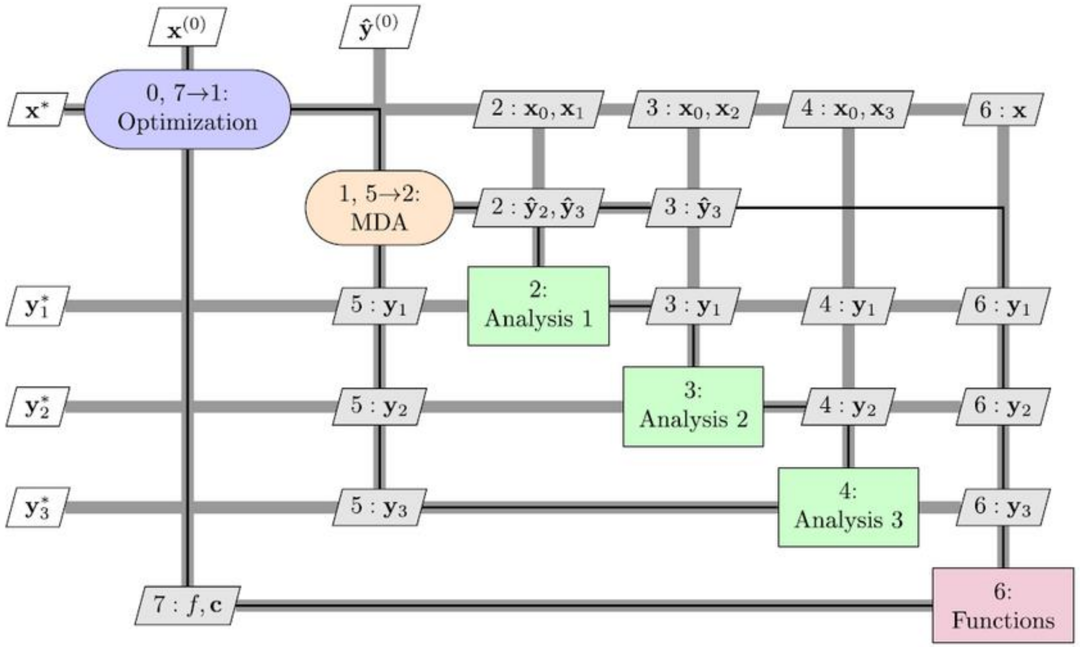

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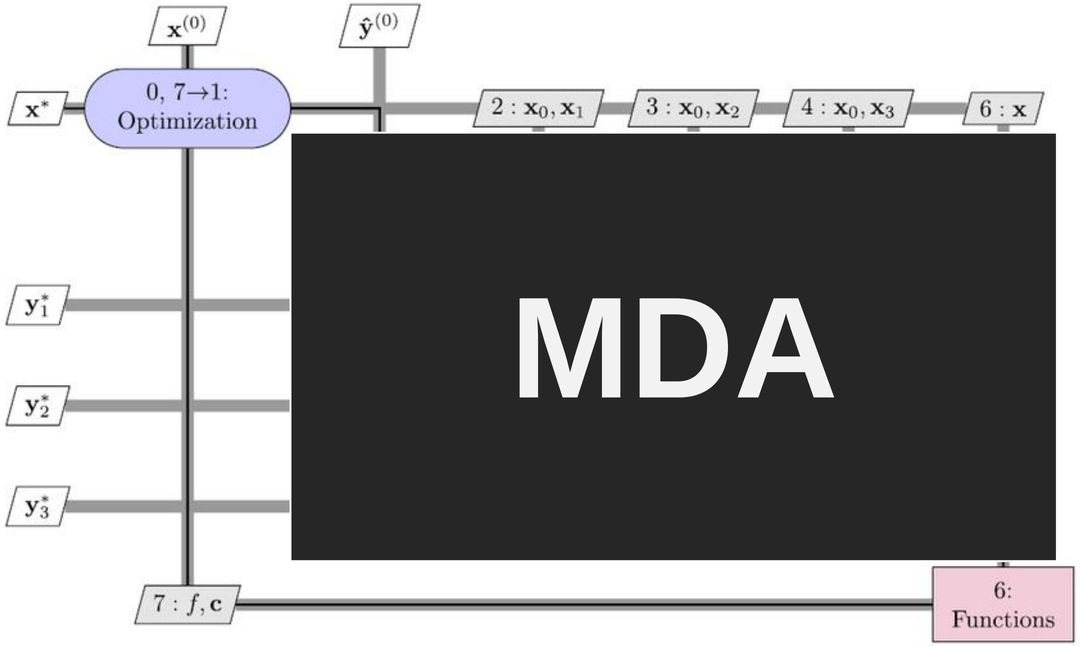

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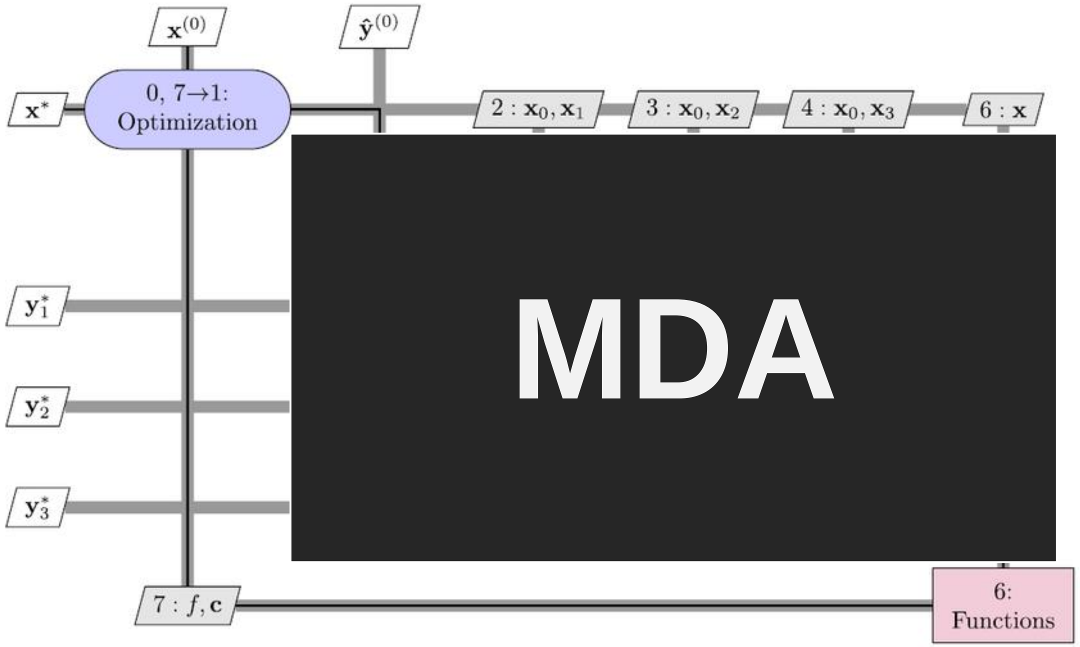

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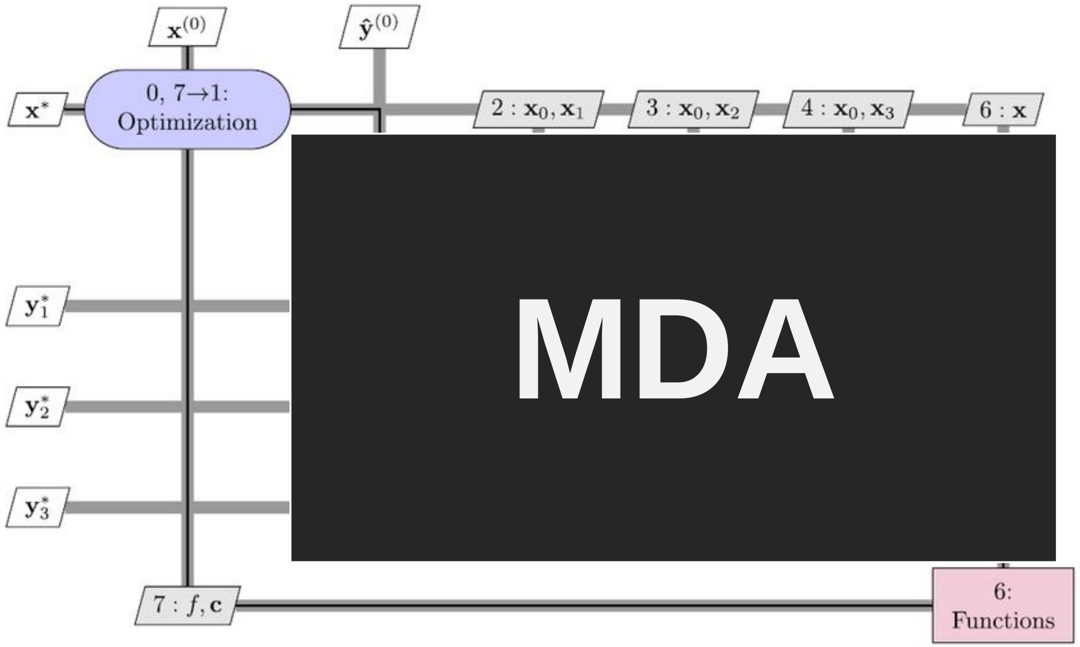

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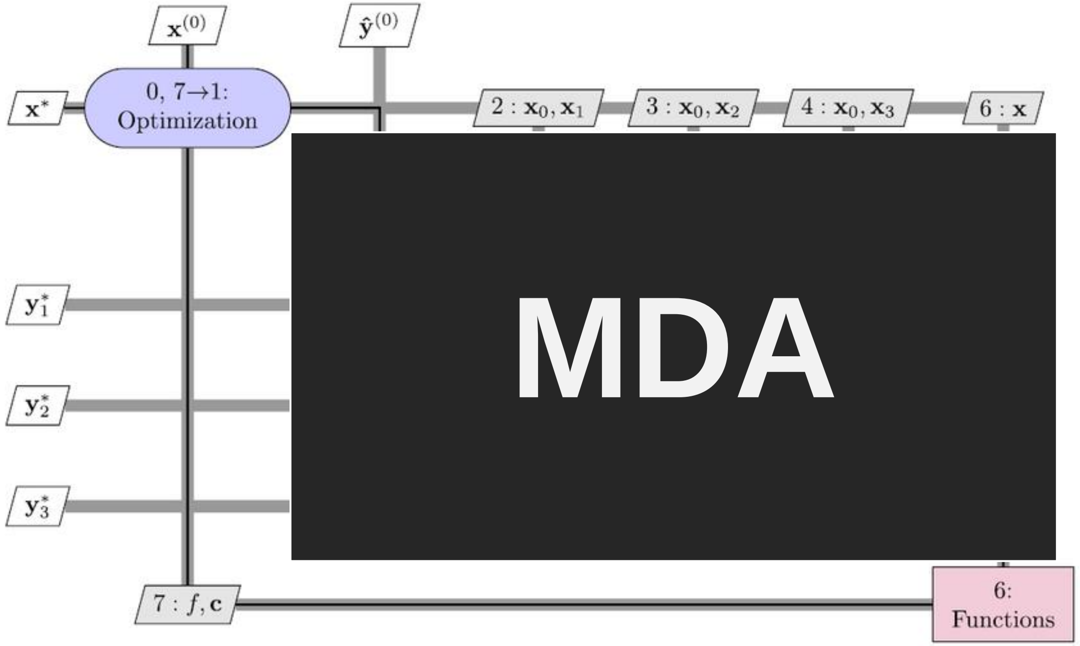

Overall objective:

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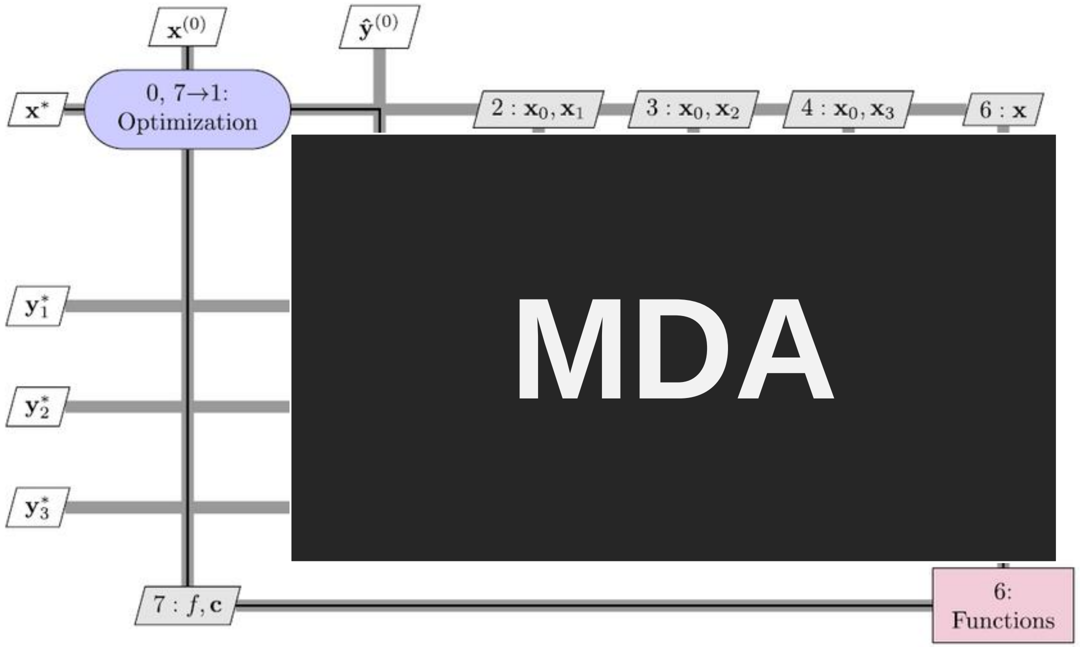

Overall objective:

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

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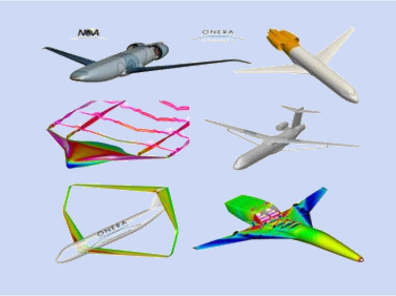
Methodology

New concepts



Ω

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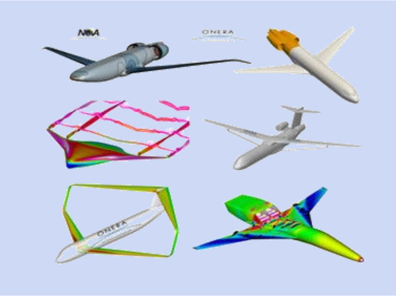
Methodology

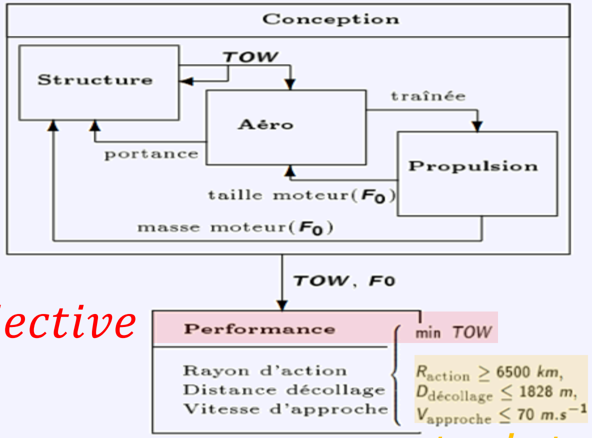
New concepts



Ω

Analyze

Multidisciplinary design analysis



objective

constraints

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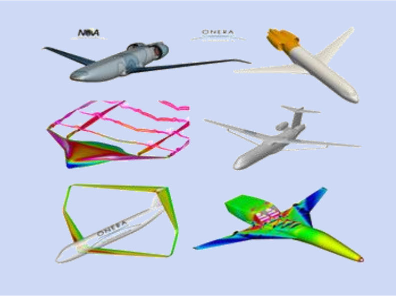

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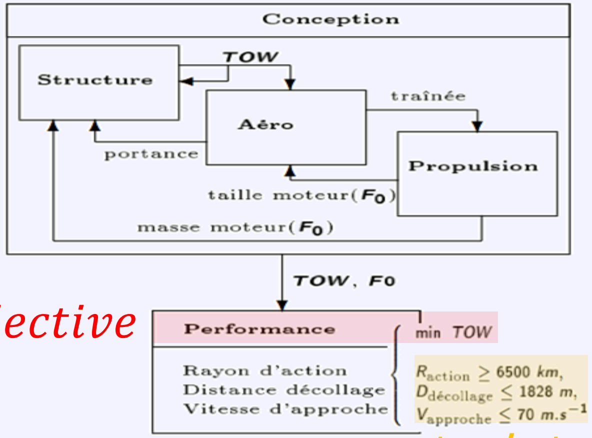
Analyze

Multidisciplinary design analysis



objective

constraints

Improvements

Global optimization

$$\min_{\text{inputs} \in \Omega} \ objective\,(\text{inputs})$$
$$s.t \quad constraints\,(\text{inputs})$$

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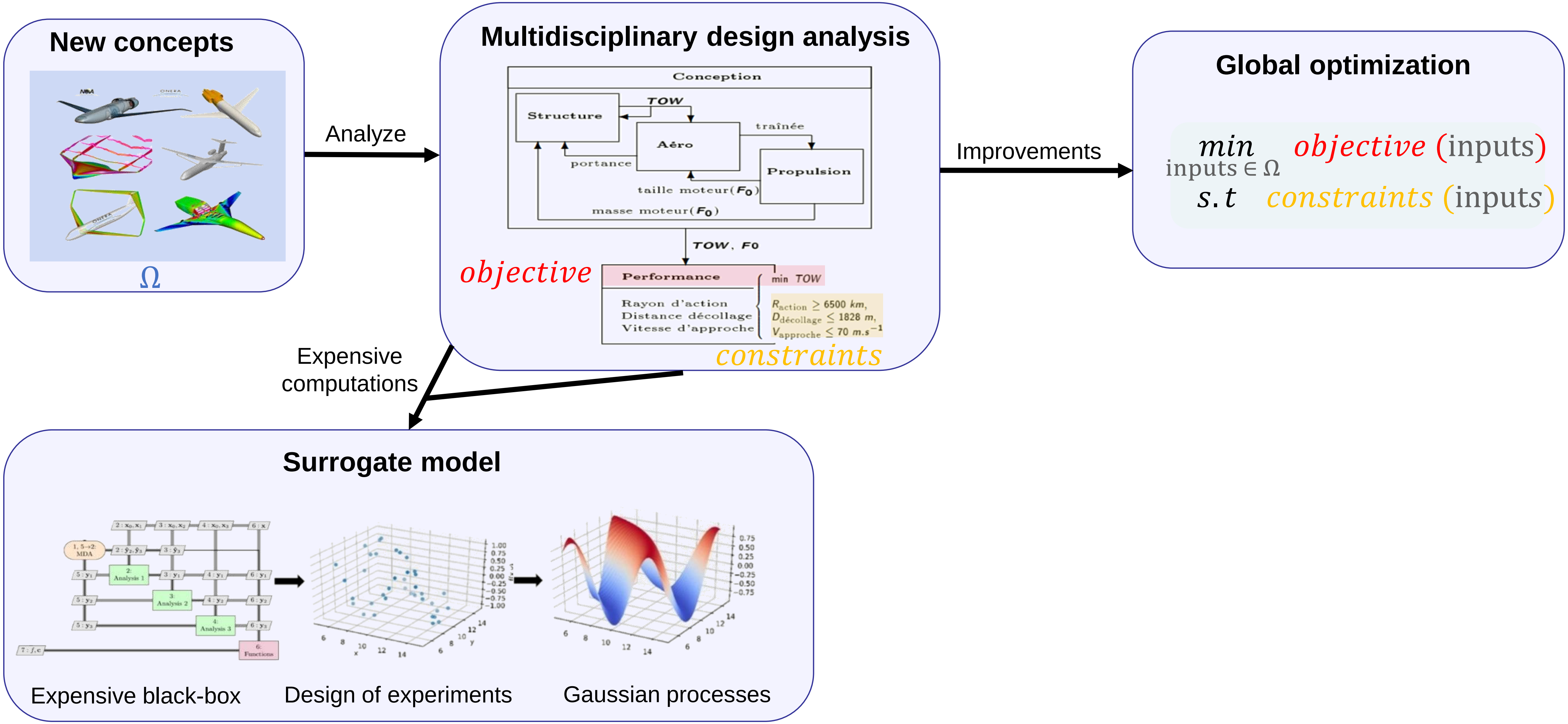

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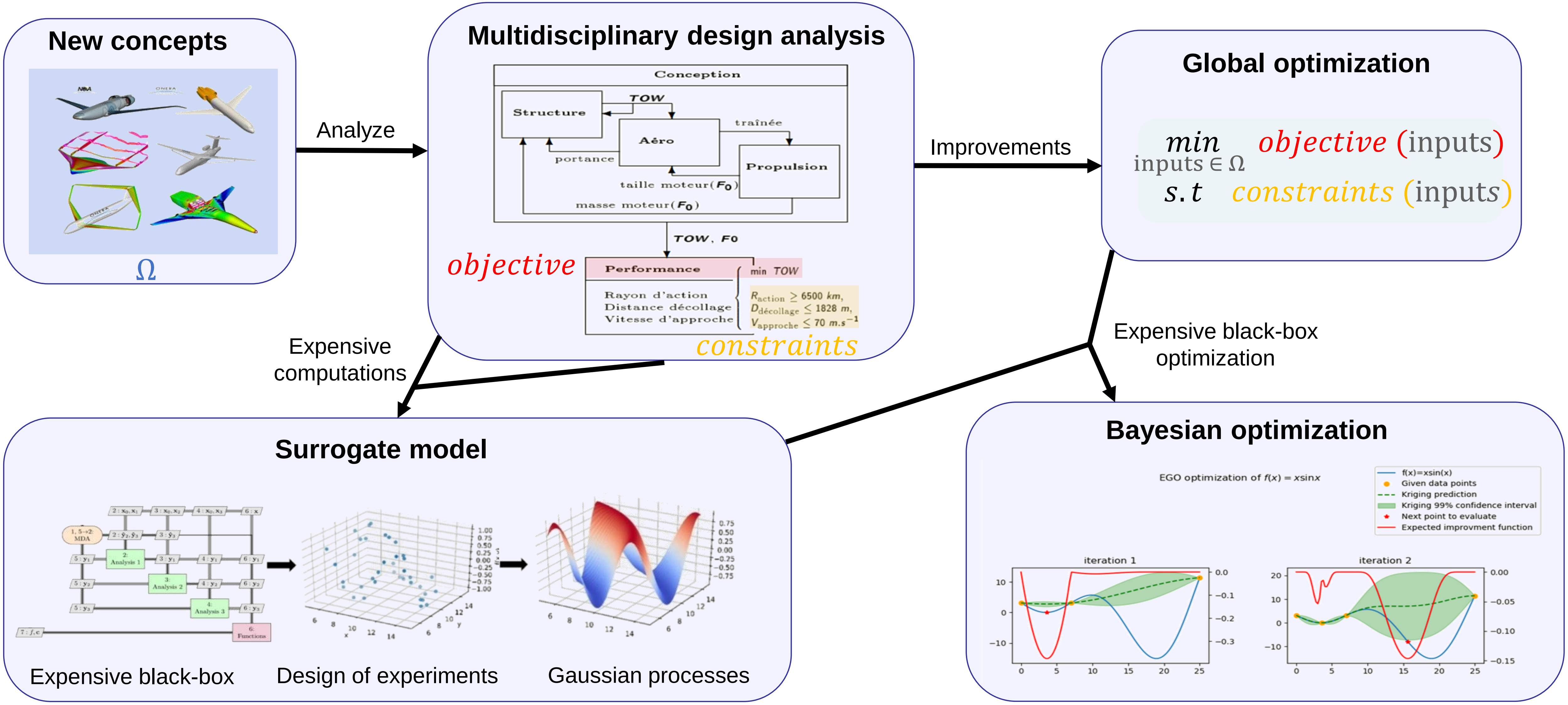

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Methodology

Overall objective:

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

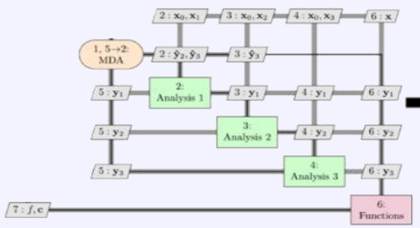
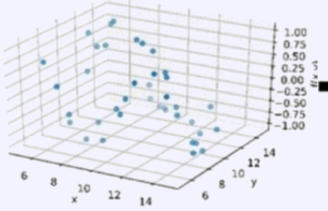
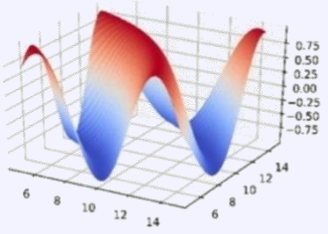
  ⇨ **Surrogate modeling**

Global optimization

$$\min_{\text{inputs} \in \Omega} \; objective\,(\text{inputs})$$
$$s.t \quad constraints\,(\text{inputs})$$

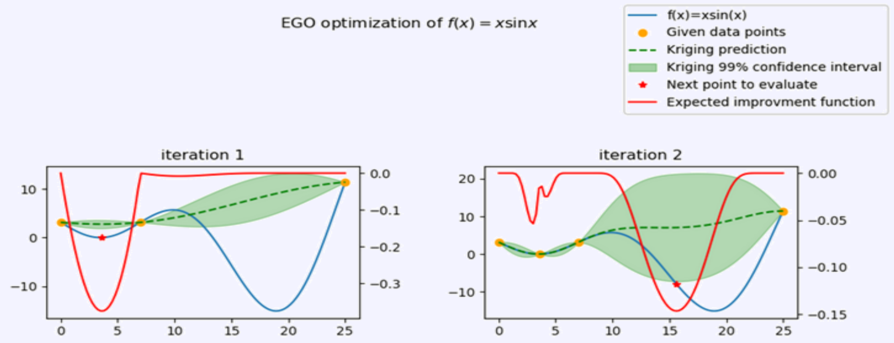
Expensive black-box optimization

Surrogate model

Expensive black-box | Design of experiments | Gaussian processes

Bayesian optimization



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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

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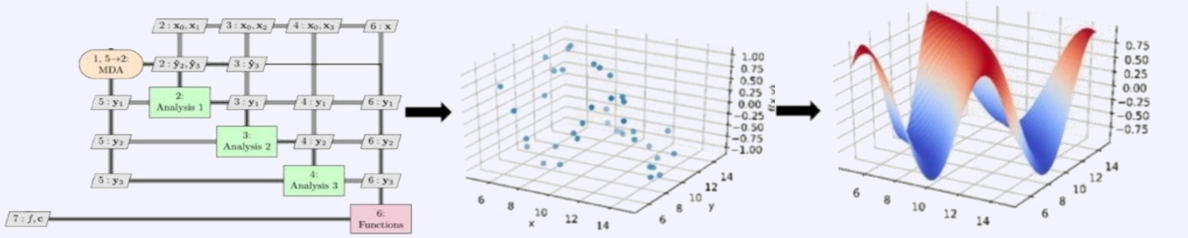
Expensive black-box optimization

Surrogate model



Expensive black-box   Design of experiments   Gaussian processes

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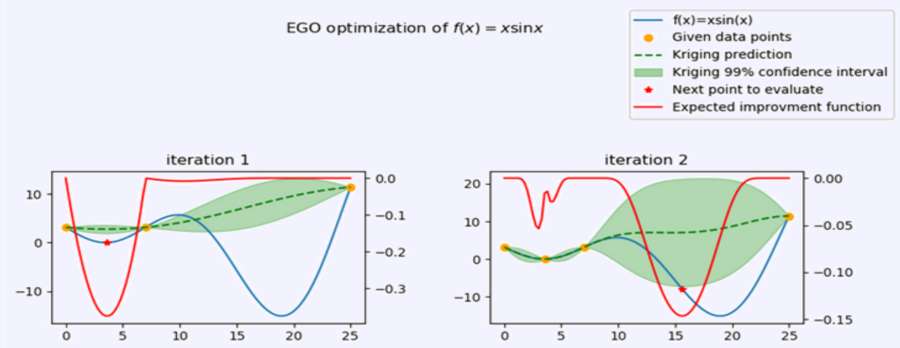

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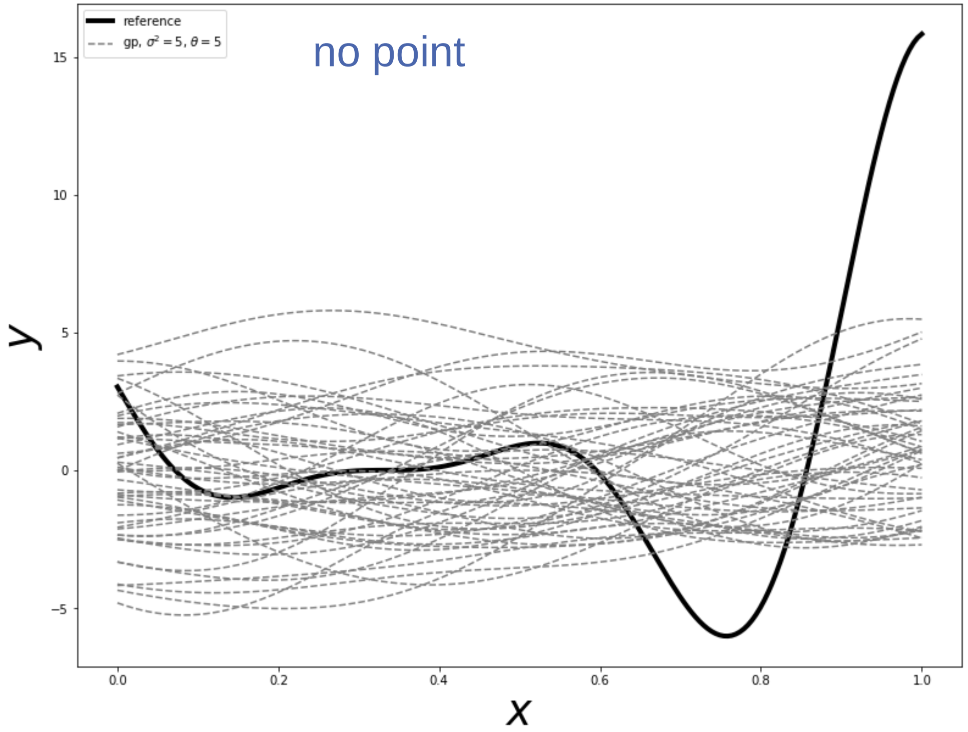
Gaussian process (or Kriging model)



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

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

A Gaussian process (GP) is characterized by:

- its trend

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- its correlation kernel

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D. Krige, **A statistical approach to some basic mine valuation problems on the Witwatersrand,** 1951, Journal of the Southern African Institute of Mining and Metallurgy.

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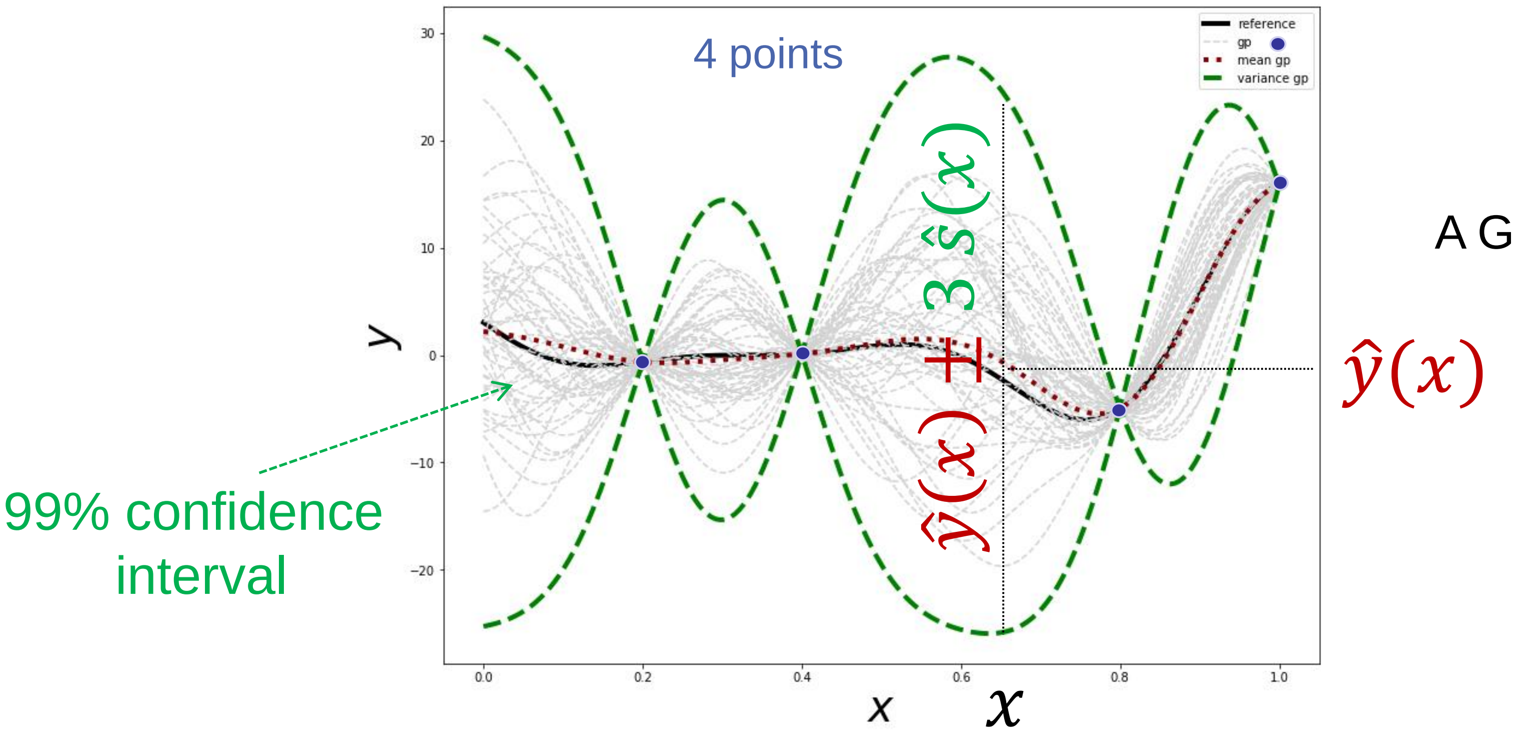

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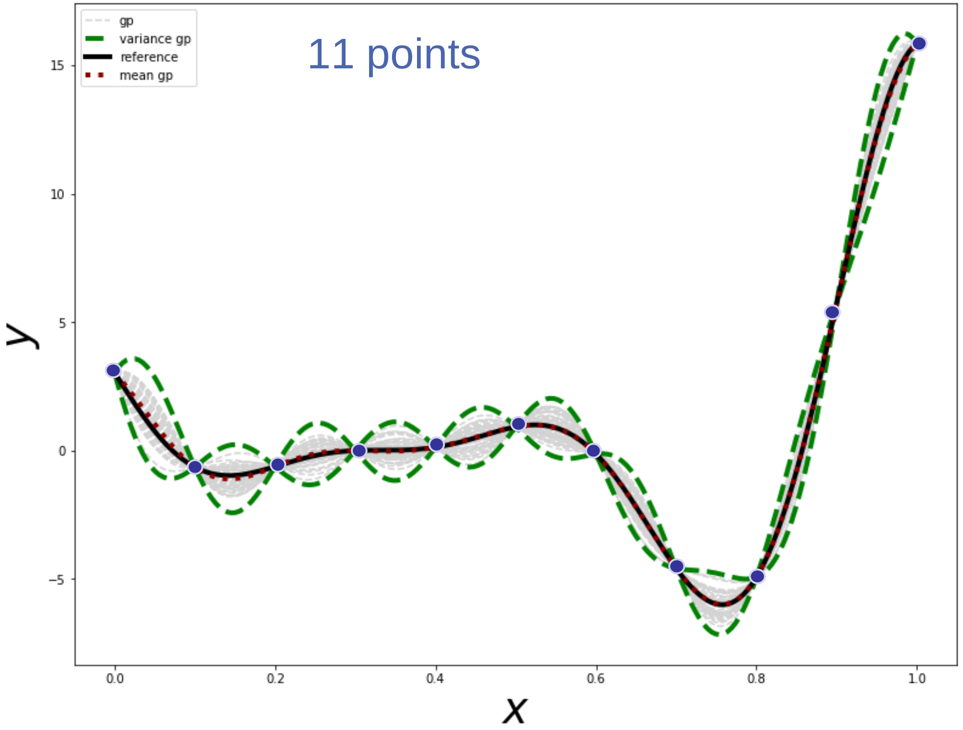

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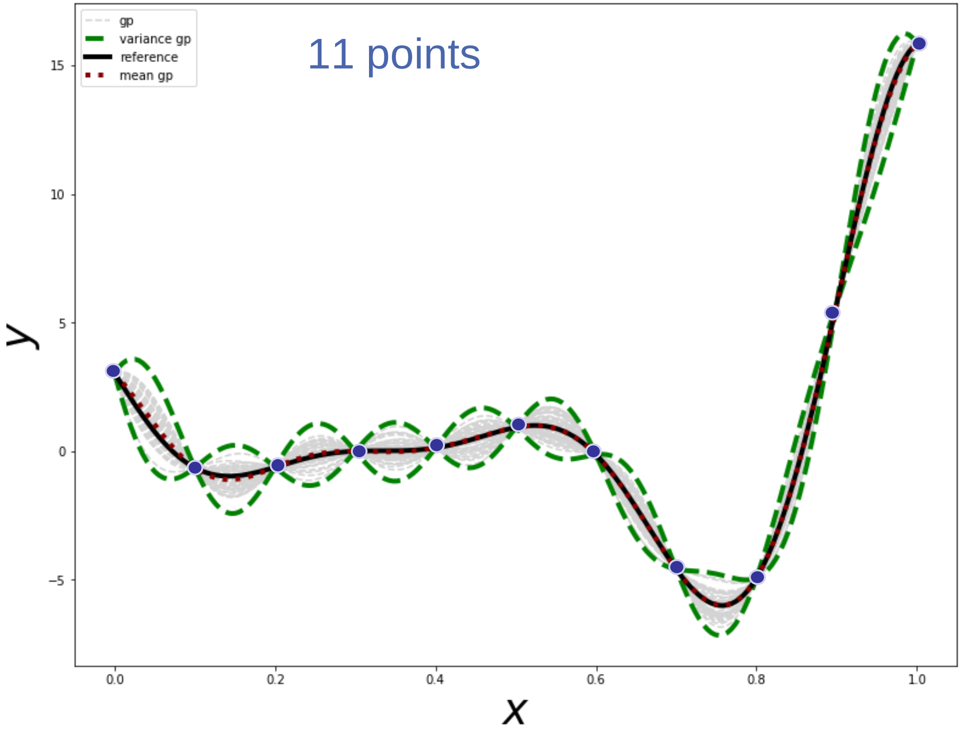
Gaussian process (or Kriging model)



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

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

A Gaussian process (GP) is characterized by:

- its trend
  $\mu(x^p) \in \mathbb{R}$
- its correlation kernel
  $k(x^p, x^q) \in \mathbb{R}$

- **Need a hierarchical distance**
  $$\boldsymbol{k(x^p, x^q) = f[d_{hier}(\theta, x^p, x^q)]}$$
  - Estimation of hyperparameters $\theta_i, i = 1, \ldots, n$ by MLE

➔ Hyperparameters tuning

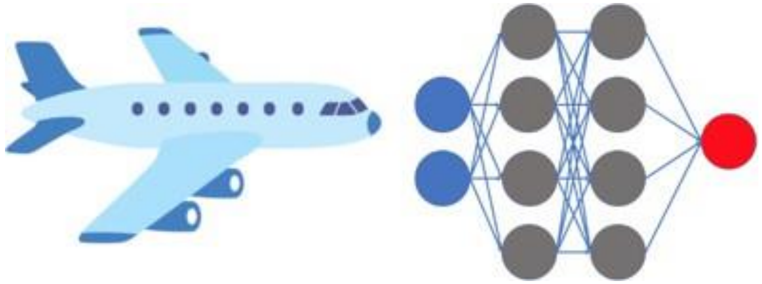
➔ The number of hyperparameters increases with the dimension n

D. Krige, **A statistical approach to some basic mine valuation problems on the Witwatersrand,** 1951, Journal of the Southern African Institute of Mining and Metallurgy.

Objectives of this work

➔ **What:** allow accessible ML models & optimization methods to efficiently tackle heterogeneous datasets

- Mixed-variable
- Points do not share same variables
- Bounds of variables may change



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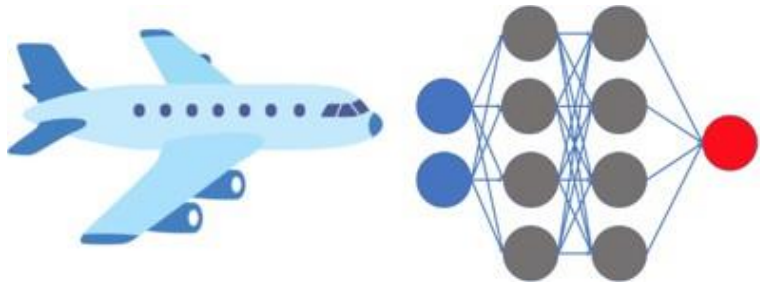
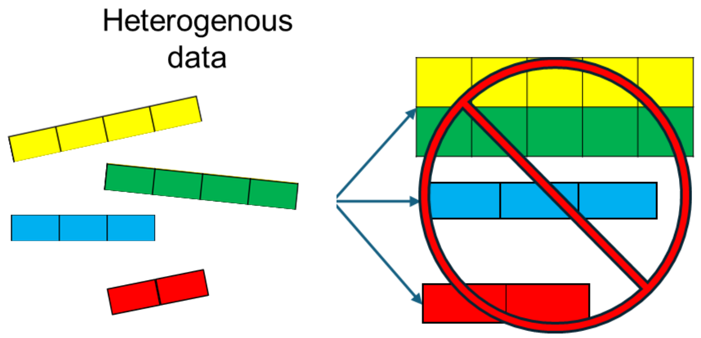
- Limited data (generalizability)
- Structure/information lost (optimization)





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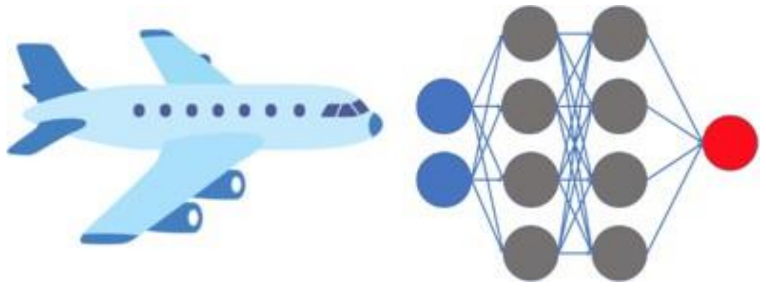
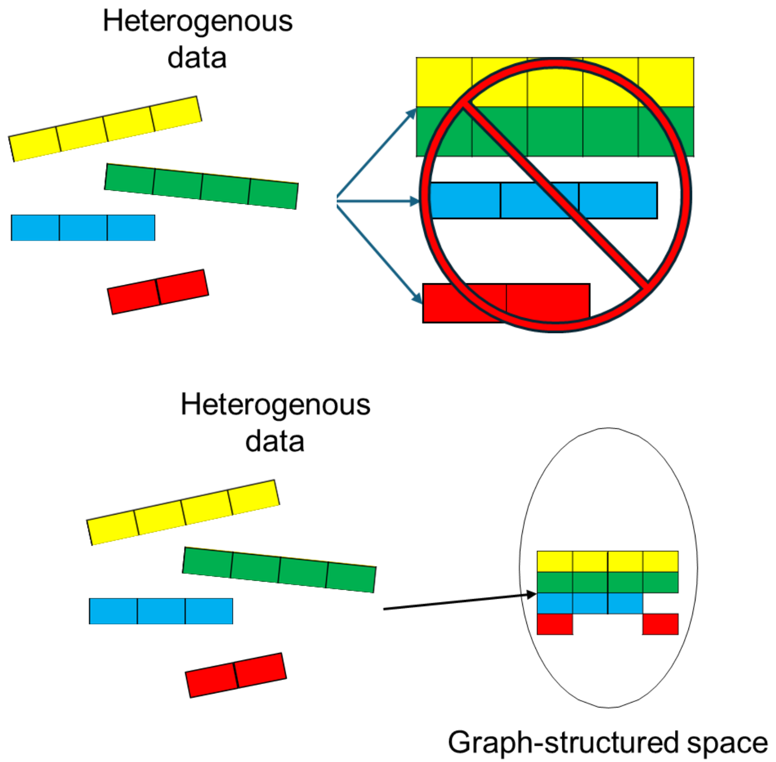
➔ **How:** formalize domains & distances, because (most) ML & optimization are fundamentally distance-based





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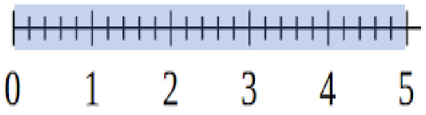
Contents

Mixed variables

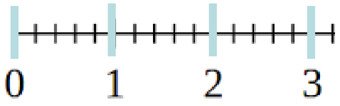
Hybrid variables

Variables types:

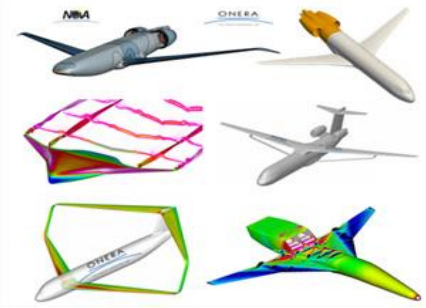
- Continuous (Cont) Ex: wing length



- Integer (Int) Ex: winglet number



- Categorical (Cat) Ex: Plane shape / material properties



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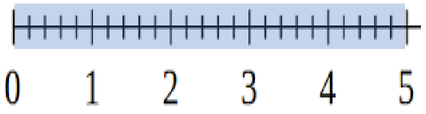

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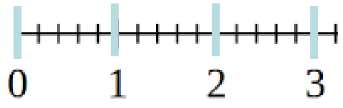

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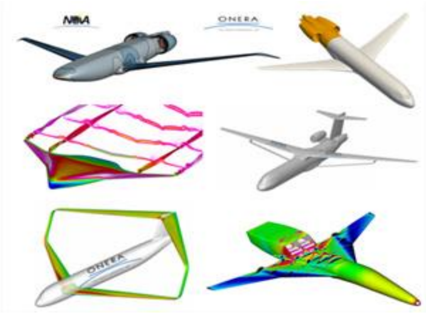

Categorical variables: n variables, n=2
u1= shape
u2= color

Levels: L_i levels for I in 1,..n, L_1=3, L_2=2
Levels(u1)= square, circle, rhombus
Levels(u2)= blue, red

Categories: $\prod_{i=1}^{n} L_i$, 2*3=6
- Blue square
- Blue circle
- Blue rhombus
- Red square
- Red circle
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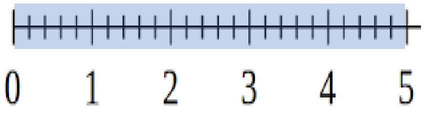

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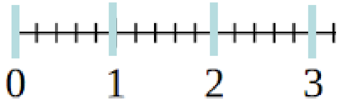

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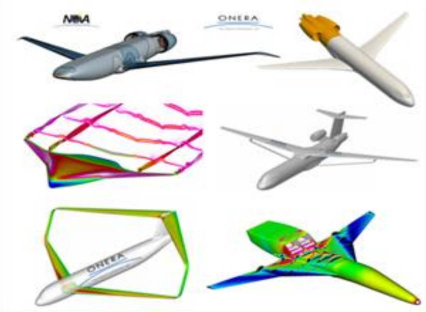

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6 possibilities

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Multi-Layer Perceptron: hierarchical variables

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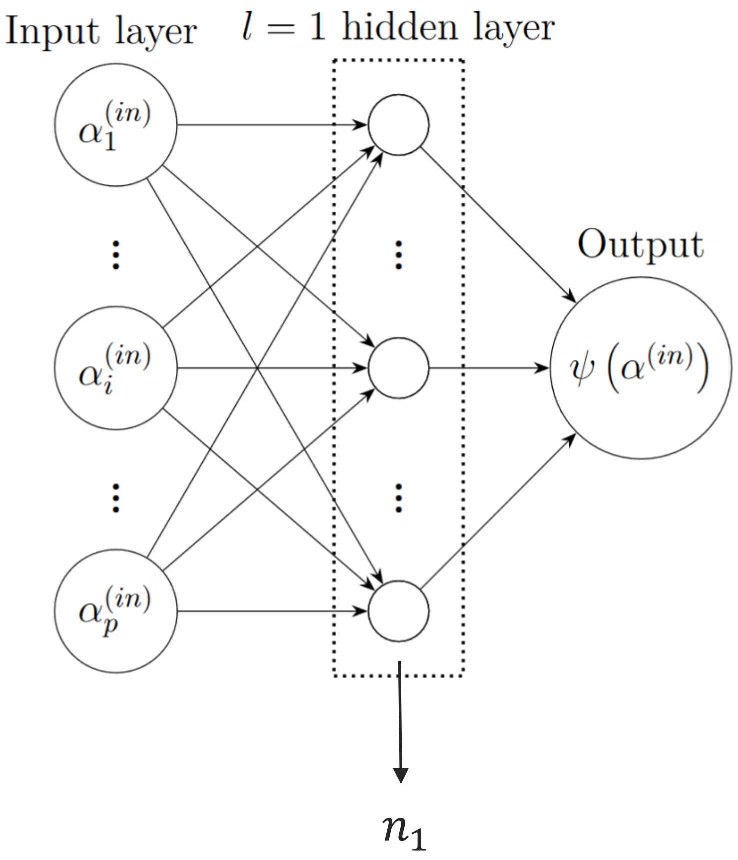

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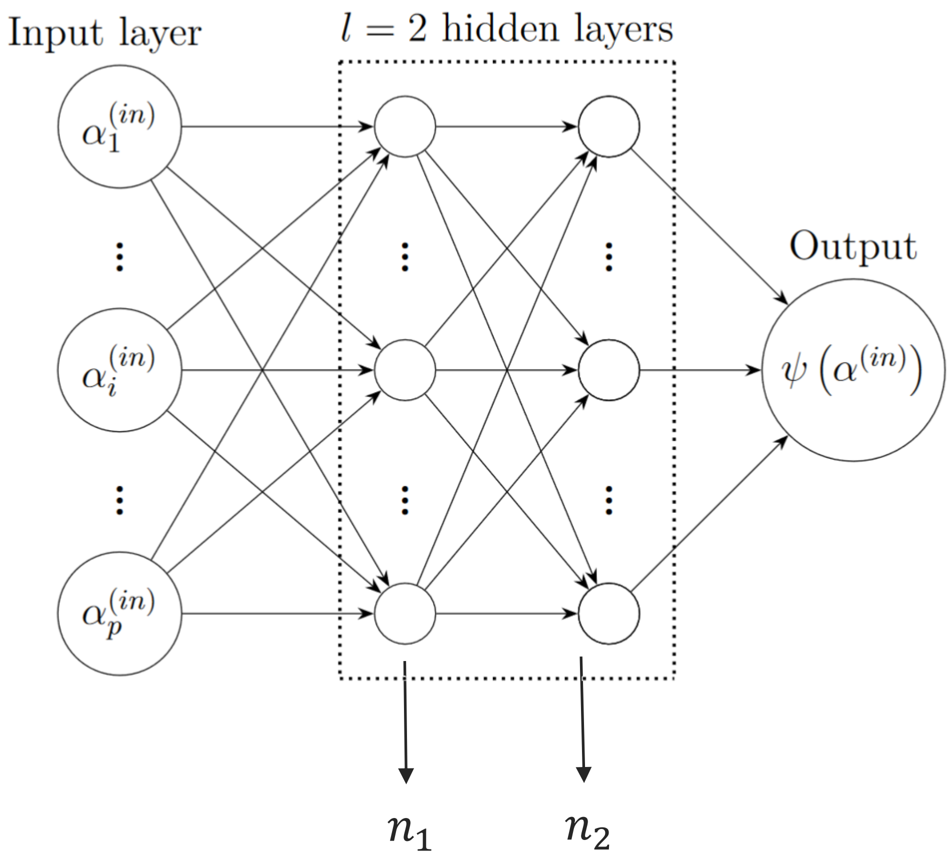

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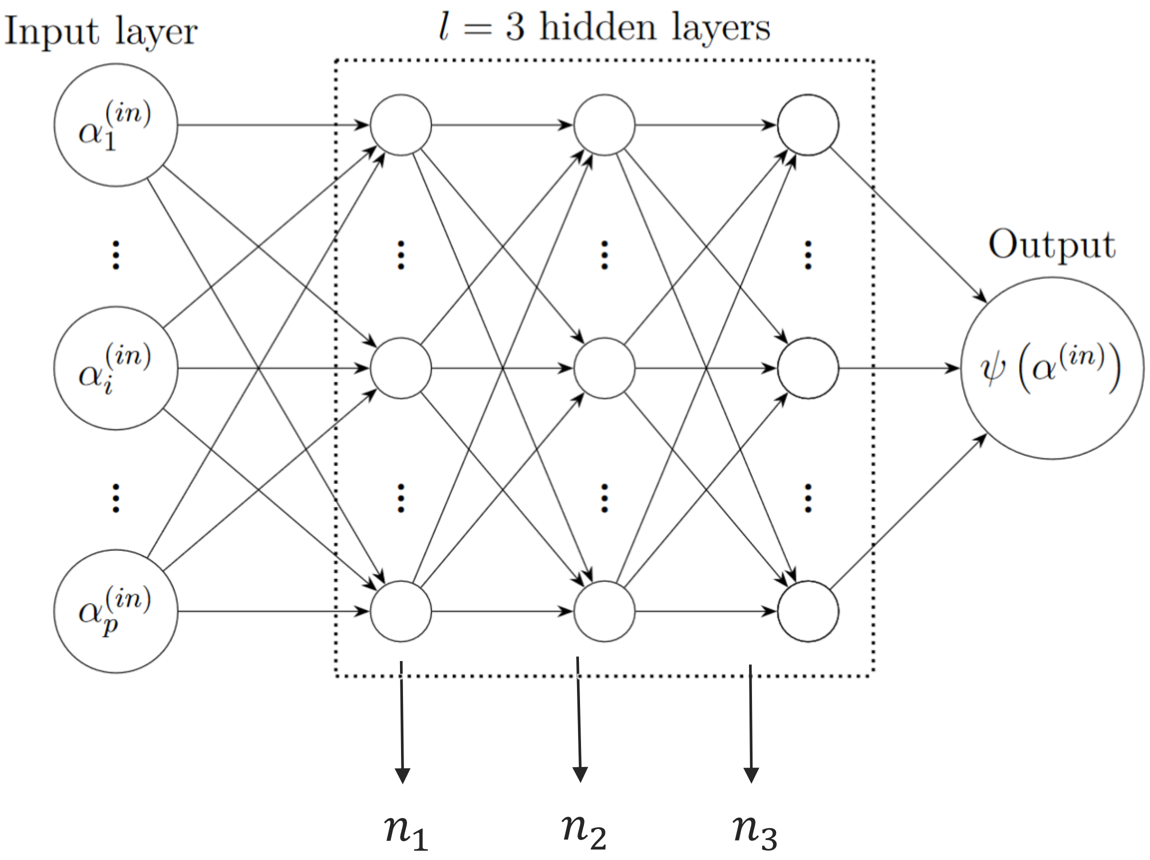

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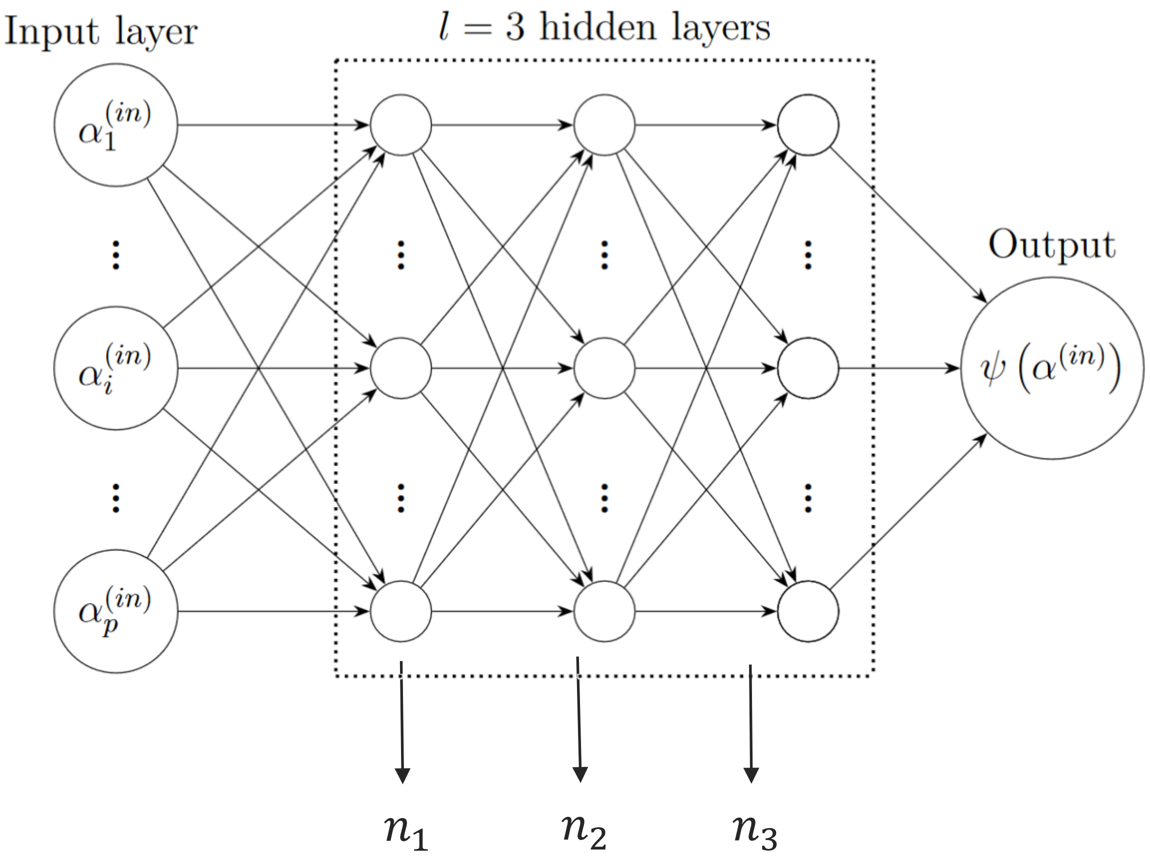

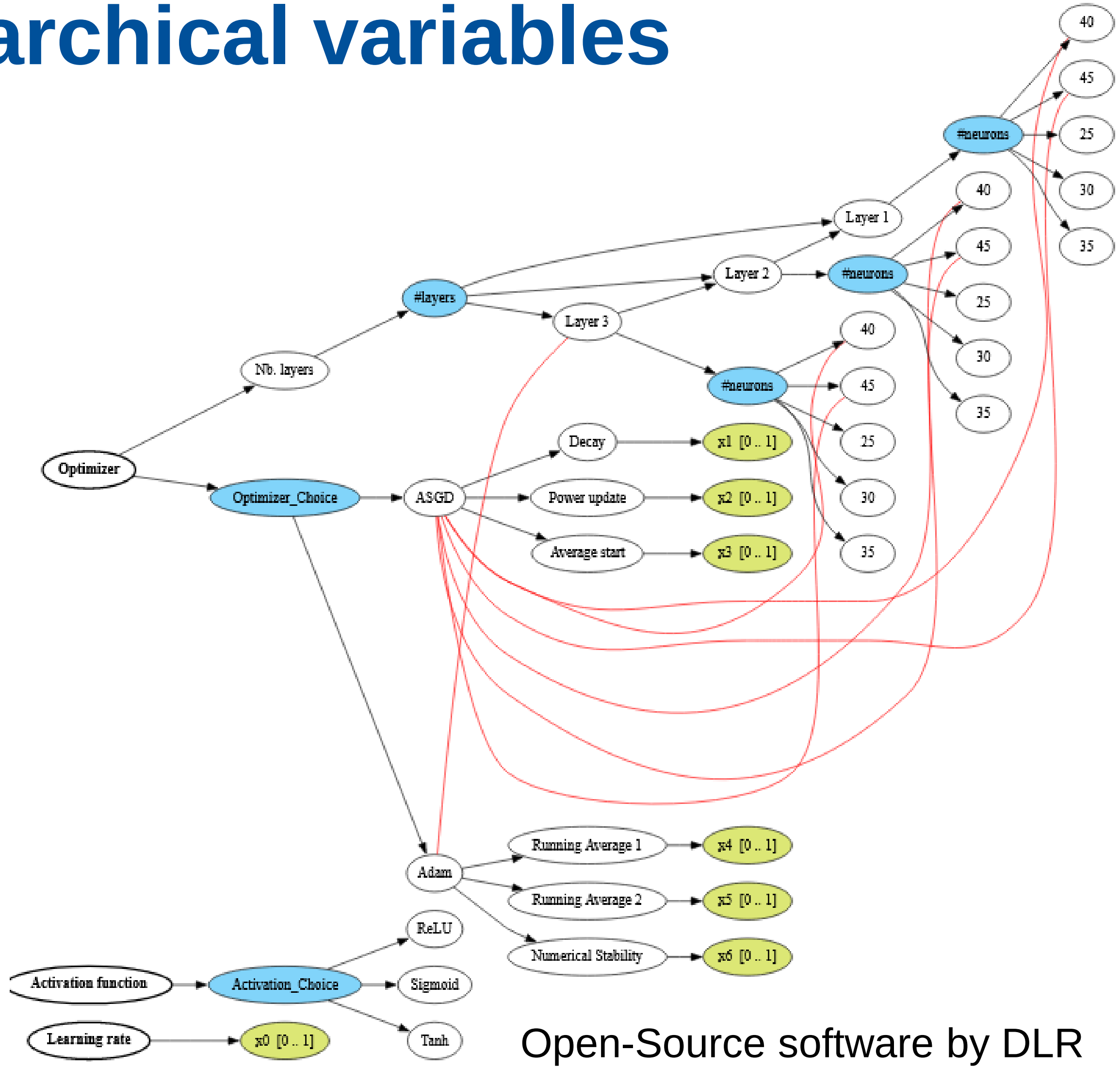

Open-Source software by DLR
Design Space Graph
https://github.com/jbussemaker/adsg-core

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Extended domain and roles

- **Meta** variables control inclusion and/or bounds of **decreed** variables
- **Roles** (meta and/or decreed) are attributed to variables, in addition to their type

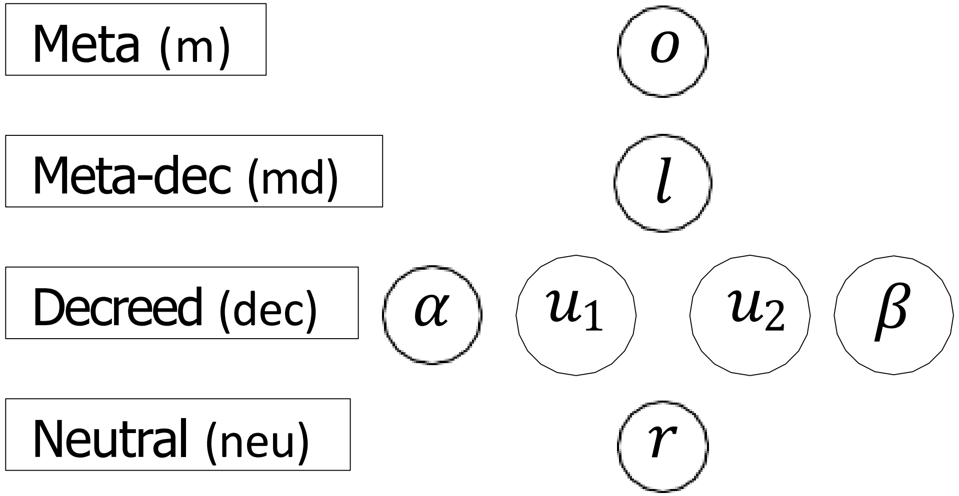
Hyperparam.	Domain	Type
Learning rate (r)	$(0, 1)$	Cont
Optimizer (o)	{ASGD, ADAM}	Cat

if $o =$ ASGD

Hyperparam.	Domain	Type
Update (α)	$(0, 1)$	Cont
# layers (l)	$\{0, 1\}$	Int
# units (u_i)	U_{ASGD}	Int

if $o =$ ADAM

Hyperparam.	Domain	Type
Average (β)	$(0, 1)$	Cont
# layers (l)	$\{0, 1, 2\}$	Int
# units (u_i)	U_{ADAM}	Int



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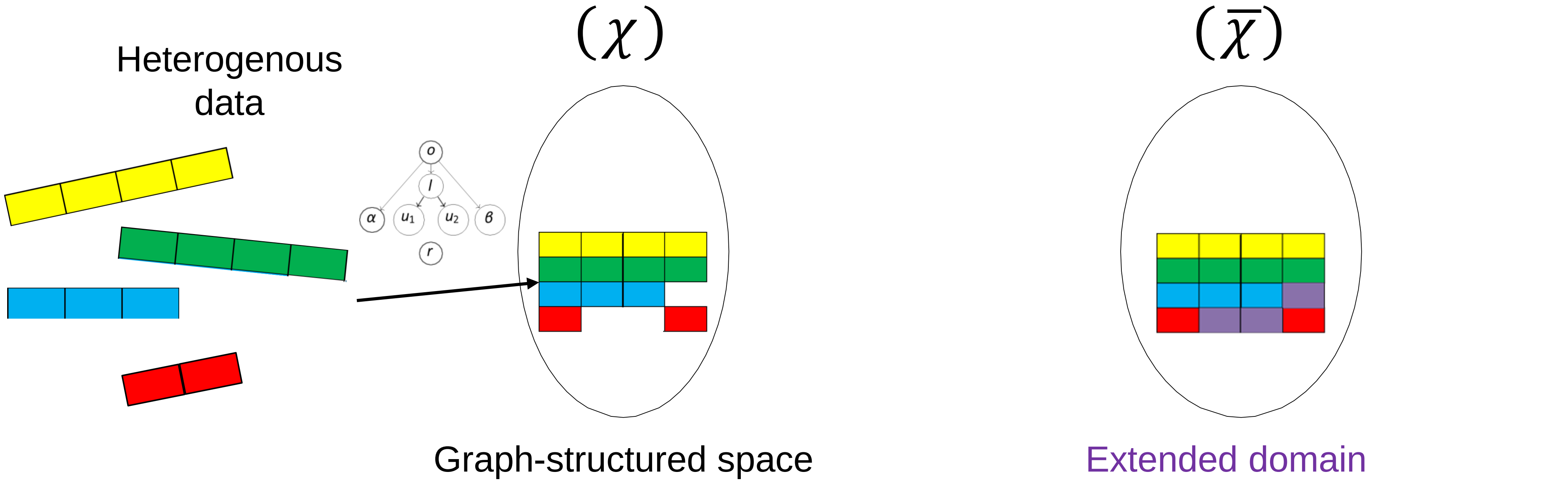
- **Extended domain** $\bar{\chi}$ is the maximal domain of all variables where excluded variable have domain $\{EXC\}$



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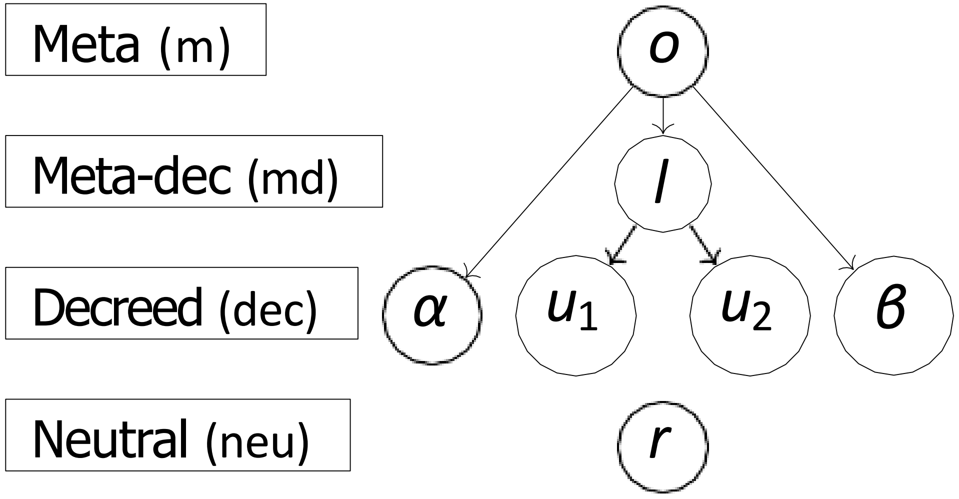
Hyperparam.	Domain	Type
# of layers (l)	{0, 1,2}	Cat

if $l = 1$

Hyperparam.	Domain	Type
# units layer 1 ($u1$)	{50,51,…55}	Cat
# units layer 2 ($u2$)	EXC	Cat

if $l = 2$

Hyperparam.	Domain	Type
# units layer 1 ($u1$)	{50,51,…55}	Cat
# units layer 2 ($u2$)	{50,51,…55}	Cat



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Distance $d(53, 52) = 1$

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Hyperparam.	Domain	Type
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# units layer 2 ($u2$)	{50,51,...55}	Cat

Distance $d(53, 52) = 1$

Distance $d(53, ?)$?

Extended distance $\bar{d}(53, EXC)$?

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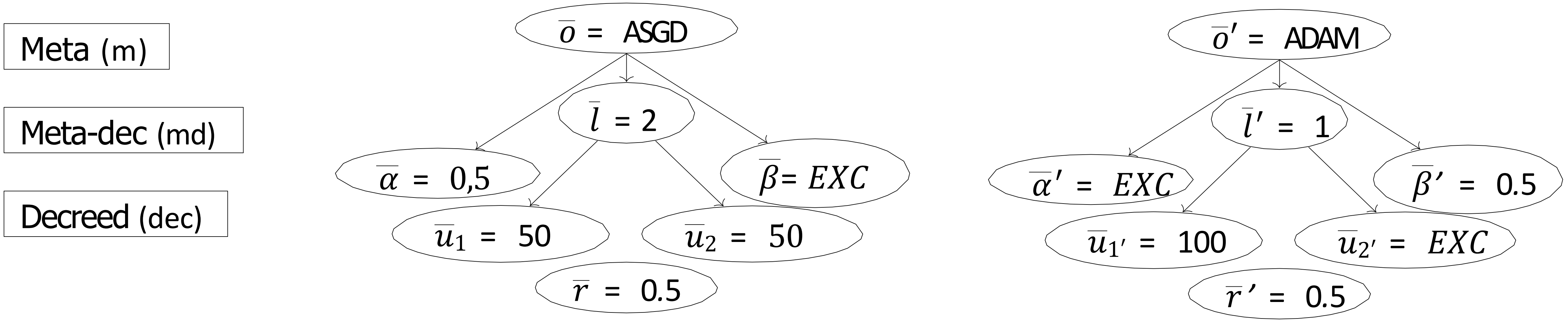
Graph-structured distance

Theorem 1 (Graph-structured distance)

For any $k \geq 1$, the mixed distance $\overline{dist}: \bar{\chi} \times \bar{\chi} \to \mathbb{R}$ is a distance.

$$\overline{dist_p}(\bar{x}, \bar{y}) = \left(\sum_{r \in R} \sum_{i=1}^{n^r} \bar{d}(\bar{x}_i{}^r, \bar{y}_i{}^r)^k \right)^{\frac{1}{k}},$$

Where $R = \{m, md, dec, neu\}$ are the roles and n^r is the dimension of the role r.



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Conditionally active distance

Fundamentally, ML & optimization rely on distances: 1st step for heterogeneity with meta variables

Theorem 2 (conditionally active distance)

The following function, defined for the i-th variable of role r between two extended points $x, y \in X$, is a one-dimensional distance

$$\bar{d}\left(\overline{x_i}^r, \overline{y_i}^r\right) := \begin{cases} 0 & \text{if } \overline{x_i}^r \text{ and } \overline{y_i}^r \text{ are excluded (inactive),} \\ \theta_i^r & \text{if either } \overline{x_i}^r \text{ or } \overline{y_i}^r \text{ is excluded,} \\ d(x_i^r, y_i^r) & \text{if } \overline{x_i}^r \text{ and } \overline{y_i}^r \text{ are included (active),} \end{cases}$$

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- $\theta_i^r \geq \frac{M_i^r}{2} > 0$ is a parameter that guarantees the triangular inequality,
- M_i^r is the largest distance between any pair x^r, y^r of included variables,
- d is a one-dimensional distance of the appropriate variable type.

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

Exemples of conditionally active distance

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.

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Exemples of conditionally active distance

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

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

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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

- $w^p = (10^{-3}, ReLU, 16, \mathbf{1}, 55) \Rightarrow (10^{-3}, ReLU, 16, \mathbf{1}, 55, 50, 50)$
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- 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

- $w^p = (10^{-3}, ReLU, 16, \mathbf{1}, 55) \Rightarrow (10^{-3}, ReLU, 16, \mathbf{1}, 55, 50, 50)$
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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

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

$\omega_i = 51$

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

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

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

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User-defined

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Exemples of conditionally active distance

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

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Exemples of conditionally active distance

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

- $\delta^p = (1,1,1,1,\mathbf{1},\mathbf{0},\mathbf{0})$
- $\delta^q = (1,1,1,1,\mathbf{1},\mathbf{1},\mathbf{0})$
- $w^p = (10^{-3}, ReLU, 16, \mathbf{1}, 55)$
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d = 0: no effect

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Exemples of conditionally active distance

- State-of-the-art: Arc-Kernel
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$$d_{Arc}(w_i^p, w_i^q) = \begin{cases} 0 & \text{both inactive} \\ 1 & \text{only one active} \\ \sqrt{2 - 2\cos\left(\frac{\rho_i \left|w_i^p - w_i^q\right|^2}{u_i - l_i}\right)} & \text{both active} \end{cases}$$

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Parameter to estimate (ρ_i)

Bounds-dependent ($u_i - l_i$)

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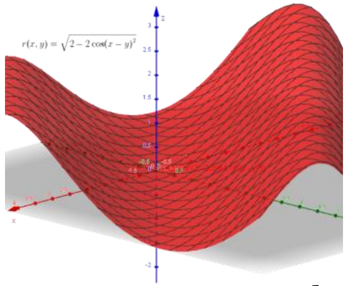

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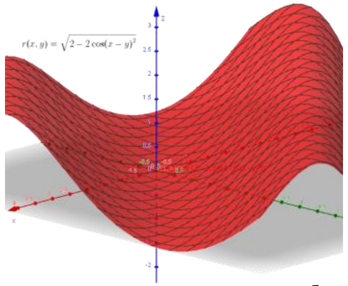

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ρ_i → Parameter to estimate

$u_i - l_i$ → Bounds-dependent

- New Alg-Kernel

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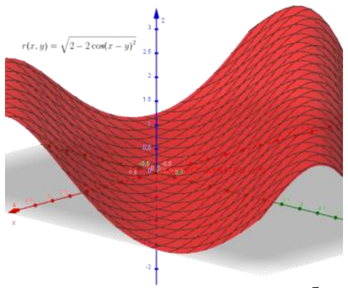

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Parameter to estimate

Bounds-dependent

- New Alg-Kernel
  - Normalized data

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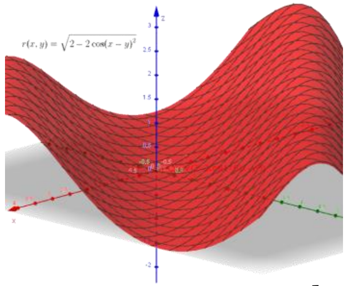

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d = 1: residual distance

d = 0: no effect

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

ρ_i: Parameter to estimate

$u_i - l_i$: Bounds-dependent

- New Alg-Kernel
  - Normalized data
  - 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.

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Exemples of conditionally active distance

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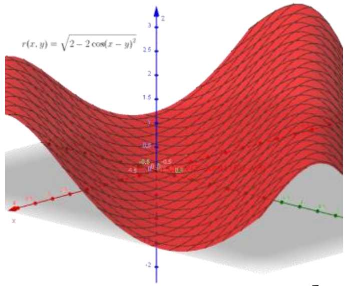

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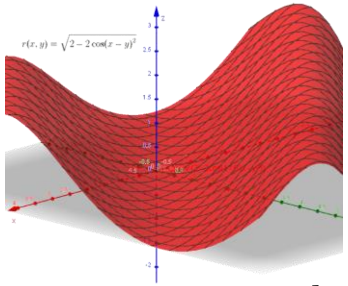

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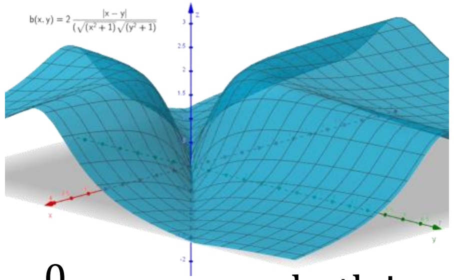

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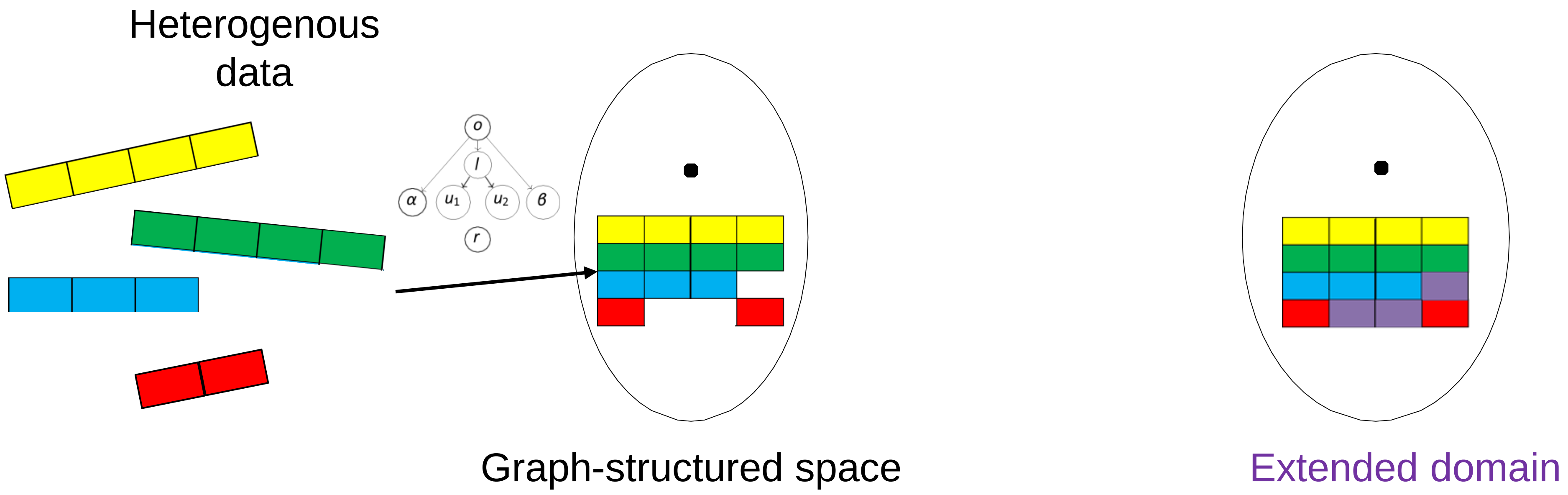
Induced distance

Theorem 3 (One-to-one correspondance)

There is a bijection T_G between the domain χ and the extended domain $\bar{\chi}$.
For any $p \geq 1$, the mixed distance $dist: \chi \times \chi \rightarrow \mathbb{R}$ is a distance.

$$dist_p(x, y) = \overline{dist_p}(T_G(x), T_G(y)) = \overline{dist_p}(\bar{x}, \bar{y})$$



P. Saves, **High-dimensional multidisciplinary design optimization for aircraft eco-design**, 2024, ISAE-SUPAERO.

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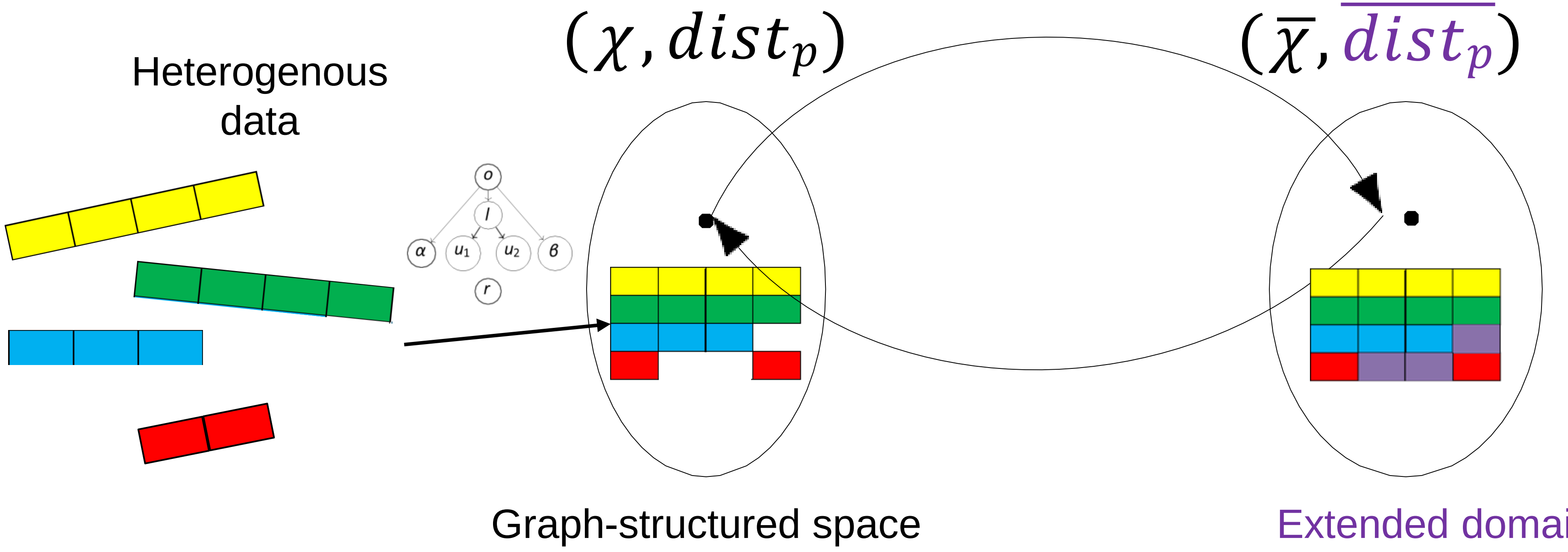

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Open-source toolbox for surrogate models

github.com/SMTorg/smt

SMT 2.0 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

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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.

Contents

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}
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	
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	Total constraints		**5**	

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

➔ 29 variables in relaxed dimension

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

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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	
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Categorical or Hierarchical

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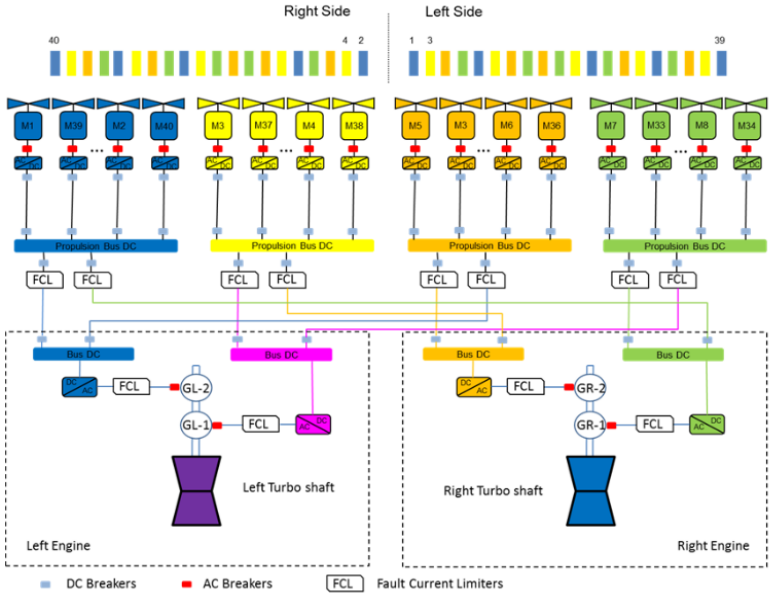
DRAGON optimization test case

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

Neutral Meta Decreed



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

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13		32
14		40
15		12
16	6	24
17		36

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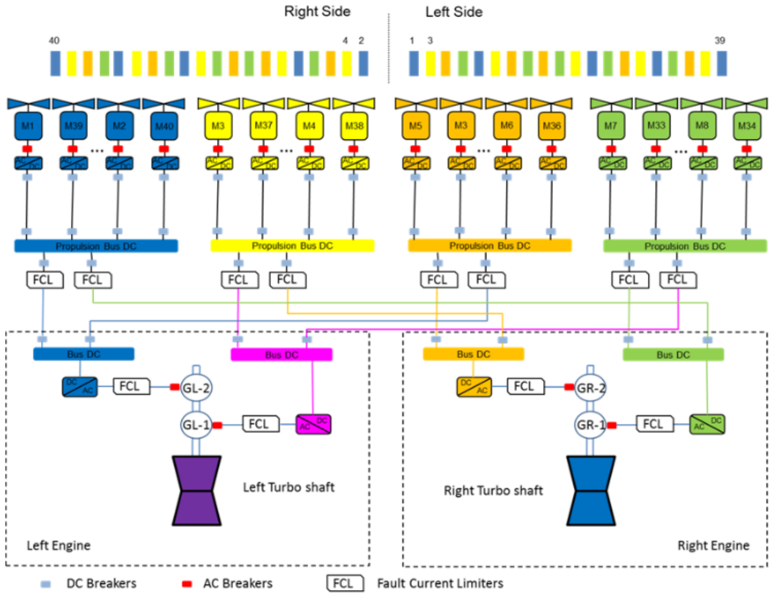

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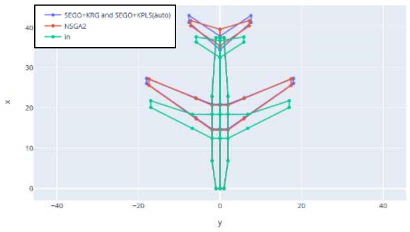
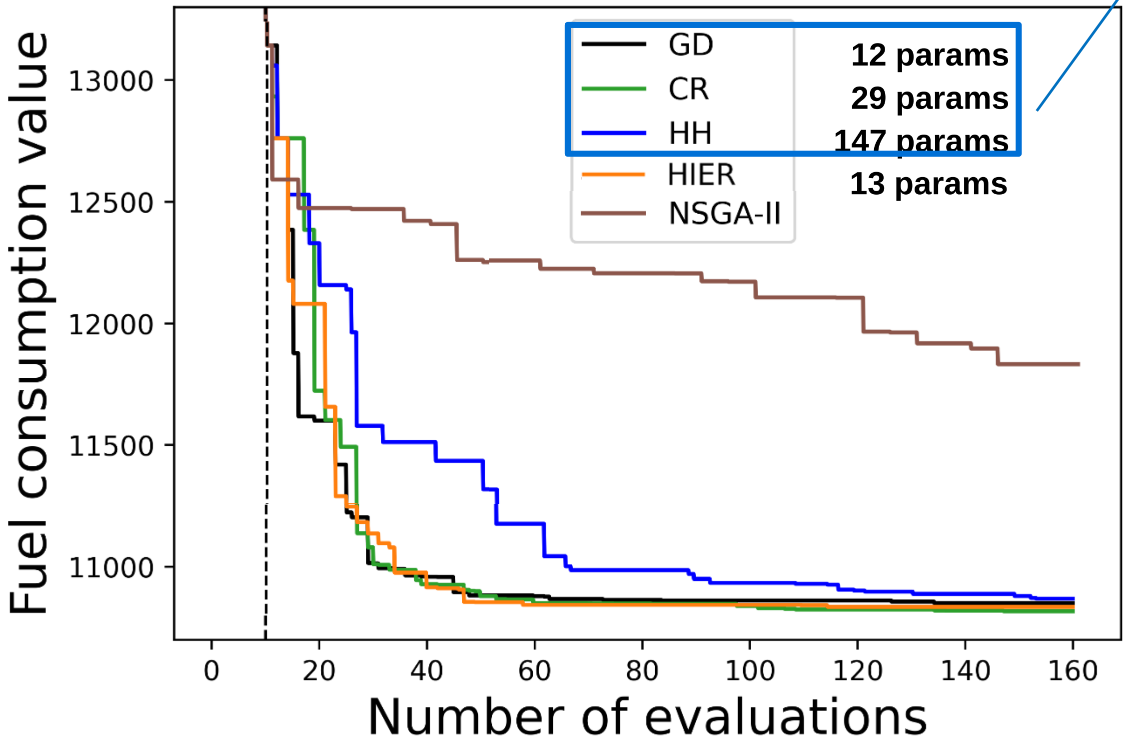
DRAGON optimization results



Categorical variants

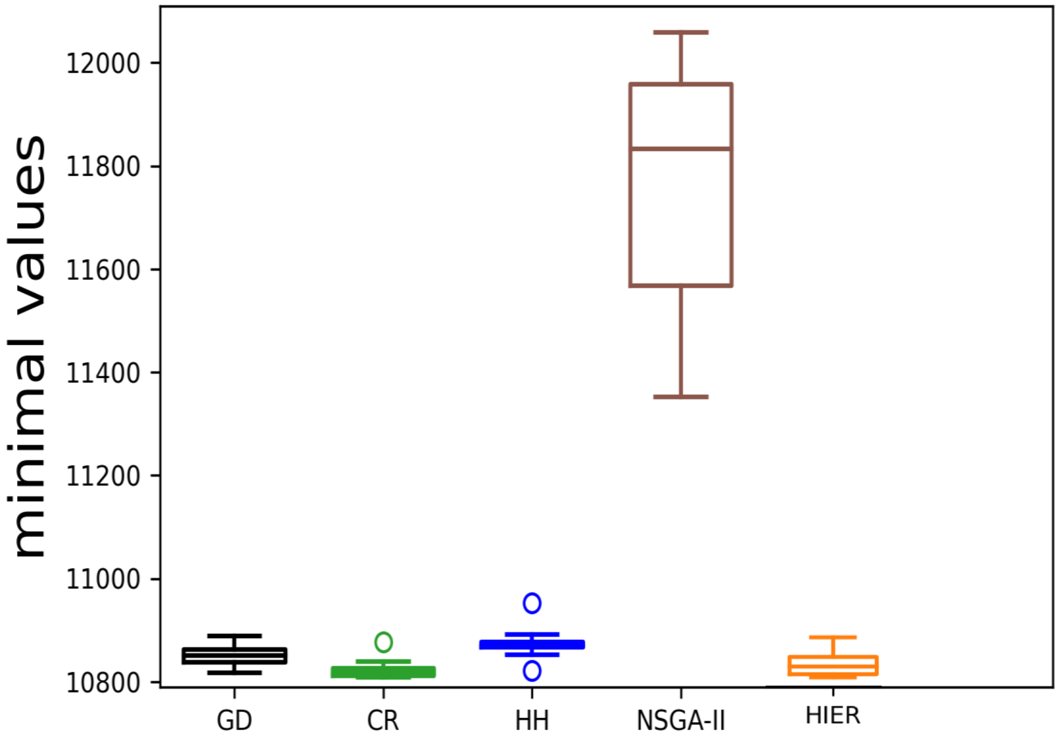
Convergence plots

10 runs of 10 + 150 iterations



Boxplots after 160 evaluations

10 runs of 10 + 150 iterations



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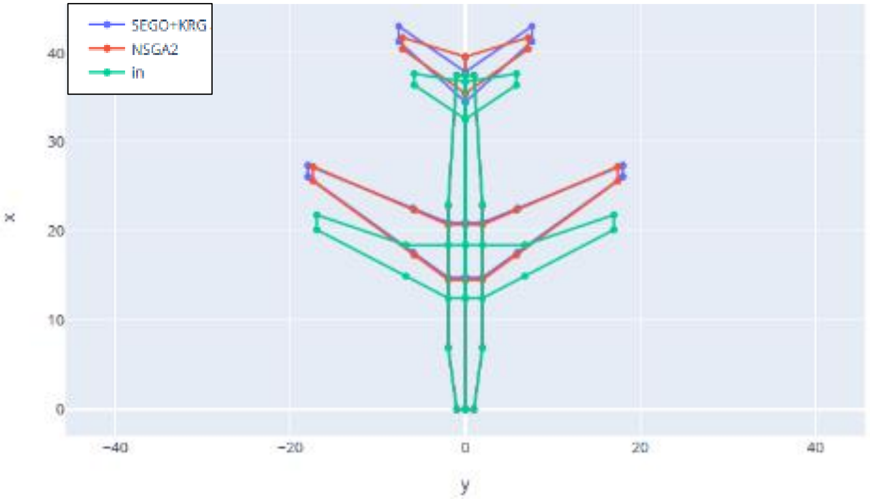
DRAGON optimization results

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

Categorical variants

Method	Rank in time	Rank in precision
Gower Distance	2	3
Continuous Relaxation	4	1
HH	5	4
NSGA II	1	5
HIERARCHICAL	3	2

- GD ~ 36h
- CR ~ 62h
- HH ~ 320h
- NSGA-II ~ 16h
- HIER ~ 40h



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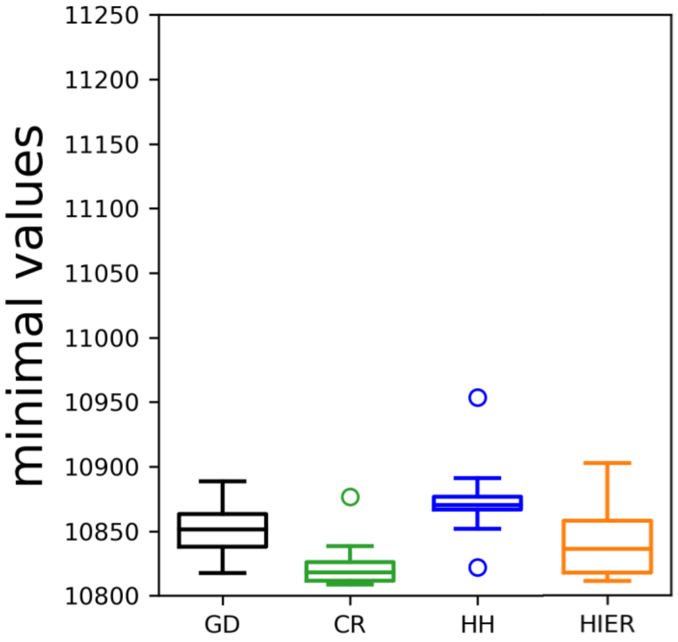

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NSGA II	1	✗ 5
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- CR ~ 62h → Best convergence
- HH ~ 320h
- NSGA-II ~ 16h
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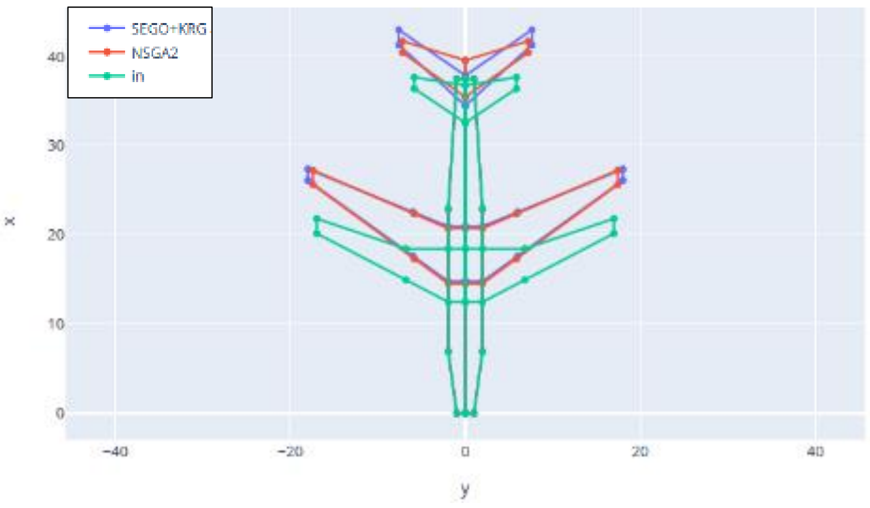
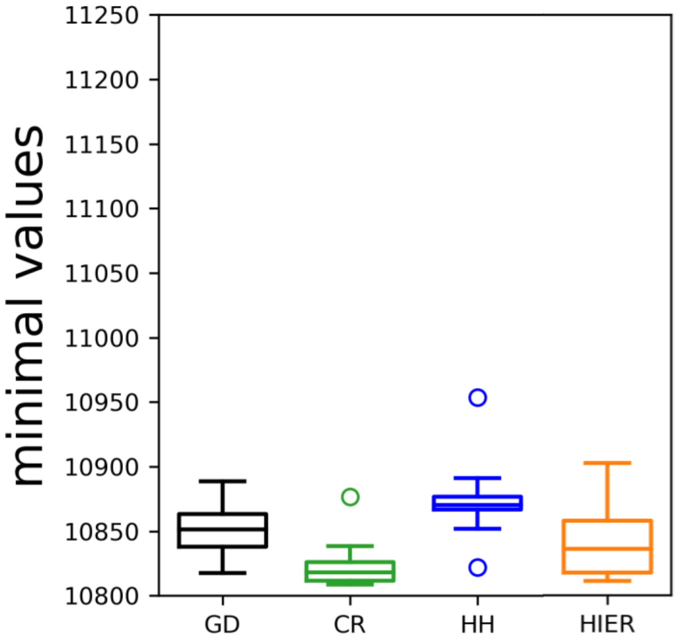


10 runs of 10 + 150 iterations



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Categorical variants

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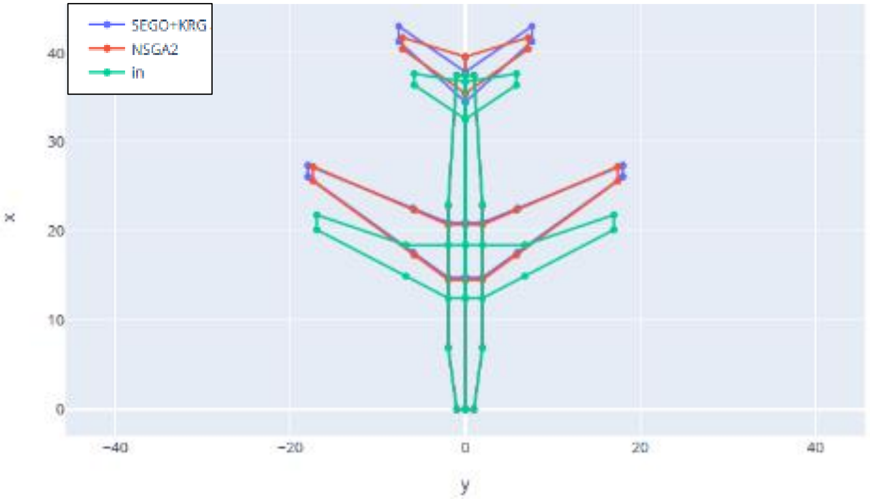
HH	5 ✗	4
NSGA II	1	✗ 5
HIERARCHICAL	3	✓ 2

- GD ~ 36h → Good but HIER is better
- CR ~ 62h → Best convergence
- HH ~ 320h
- NSGA-II ~ 16h
- HIER ~ 40h → Best trade-off



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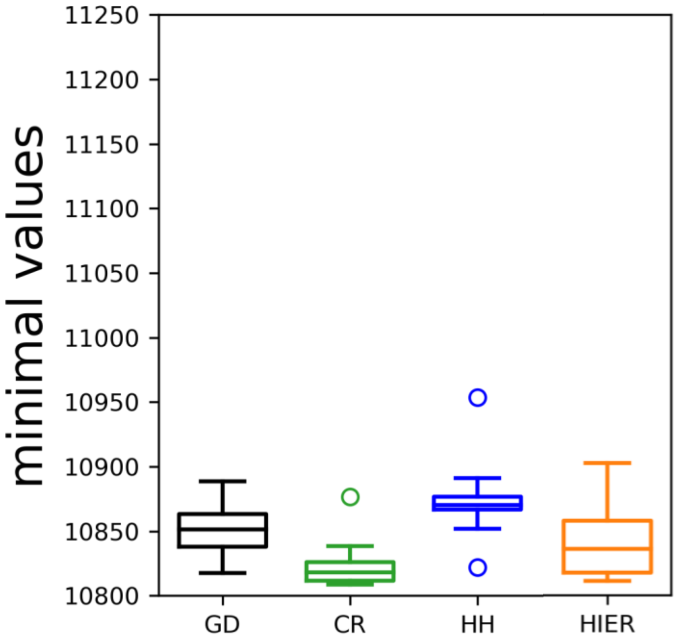

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P. Saves, Y. Diouane, N. Bartoli, T. Lefebvre, J. Morlier, **High-dimensional mixed-categorical Gaussian processes with application to multidisciplinary design optimization for a green aircraft**, 2024, Structural & Multidisciplinary optimization.

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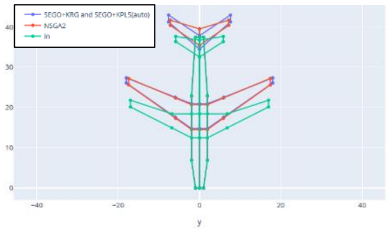
➔ **What:** fundamental tools for ML and optimization with heterogeneous



➔ **Why:** avoid dividing into smaller subproblems

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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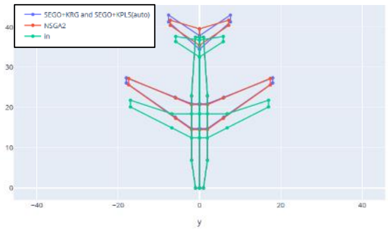

➔ **What:** fundamental tools for ML and optimization with heterogeneous

➔ **Why:** avoid dividing into smaller subproblems

➔ **How:** generalized framework & distances

- Exc. variables, extended point $\bar{x}$ and domain χ
- Included-excluded distance
- Graph-structured distance

github.com/SMTorg/smt

$$\bar{d}\left(\bar{x}_i^{\,r}, \bar{y}_i^{\,r}\right) := \begin{cases} 0 \\ \theta_i^r \\ \bar{d}\left(x_i^r, y_i^r\right) \end{cases}$$

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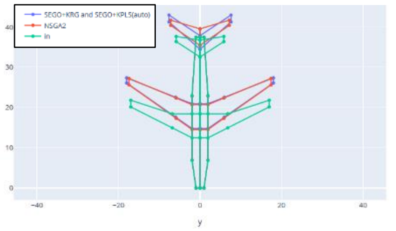

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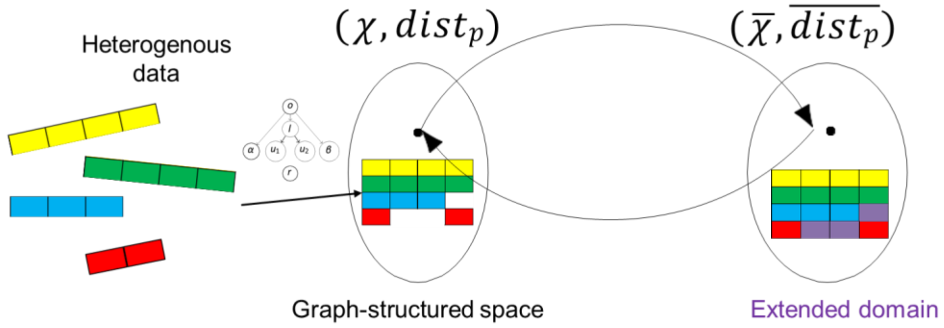
➔ **More computational experiments in the paper: Graph** seems promising

- KNN: neighbors accessible across subproblems
- Better models: random forests, GPs, etc.
- Time: 10 vs 40min on #5 variant-large with IDW

https://arxiv.org/abs/2405.13073



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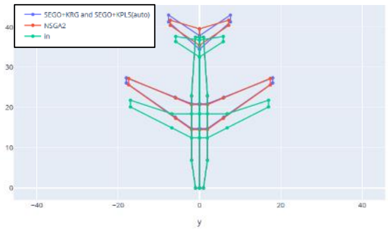

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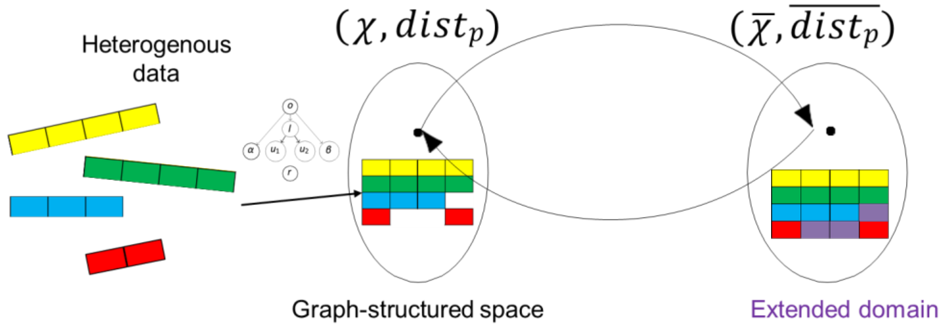

➔ **More to come for System Architecture Optimization**

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Université de Toulouse

COLOSSUS
COLLABORATIVE SYSTEM OF SYSTEMS

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