Dimensionality Reduction Applied to Mechanical Design and Optimization

LMA2S Seminar, ONERA – 14/03/2025

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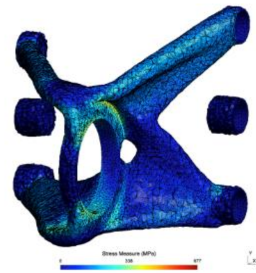
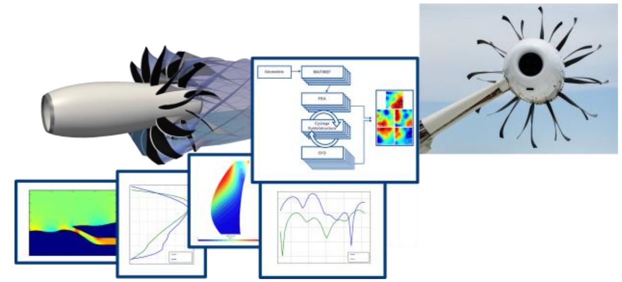
Outline

- Introduction
- Dimensionality Reduction
- Application to design optimization
- Conclusions and future prospects
- References

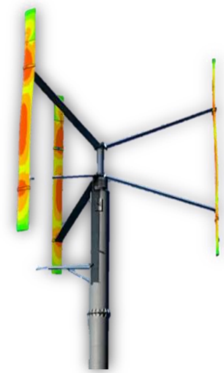
Introduction

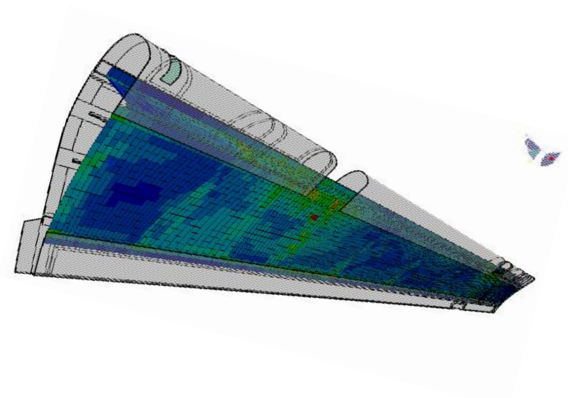
Cenaero





- Private research center, specialized in numerical simulations
- Two locations
  - Non-profit organization in Charleroi (BE)
  - Subsidiary in Moissy-Cramayel (FR)
- 80+ researchers
- Started in 2002 with the support of the European Regional Development Funds and the impulse of the Walloon aeronautical sector and universities





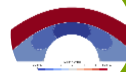
- Operational missions: collaborative research in close collaboration with industry and academia + services for companies (HPC supercomputing facilities, consultancy)

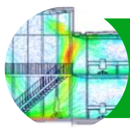
Research Themes at Cenaero

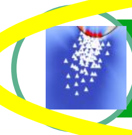

Aerostructures Design & Development

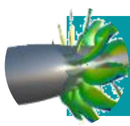

High Performance Computing

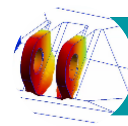

Aerostructures Engineering Environment

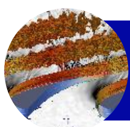

Hypersonic Flows & Phase-changing Materials

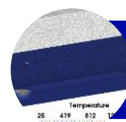

Buildings and Smart Cities

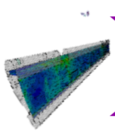

Machine Learning for Modeling, Optimization & Data Mining

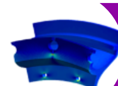

Turbomachinery Design


Manufacturability & Multidisciplinary Design for Manufacturing


High-Fidelity CFD & CAA for Aeronautical Applications

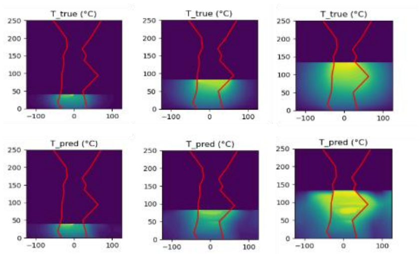

Metallic Manufacturing Processes Modeling


High Performance Composites

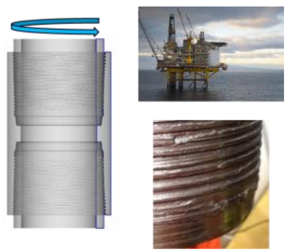

Multiscale Mechanics through Lifetime

Machine Learning & Optimization

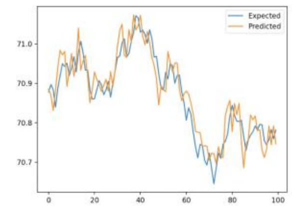
- **Machine Learning (ML) activities in various scientific and industrial projects**



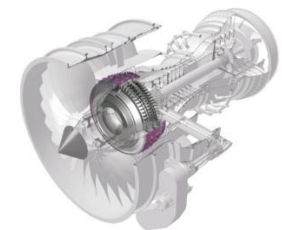
Prediction of physical fields



Detection of defects

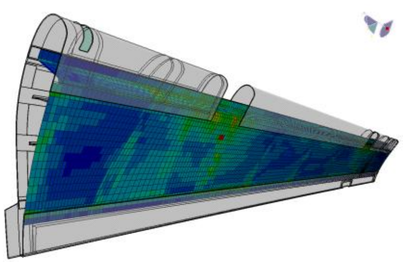


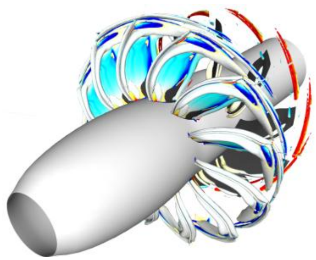
Time series prediction

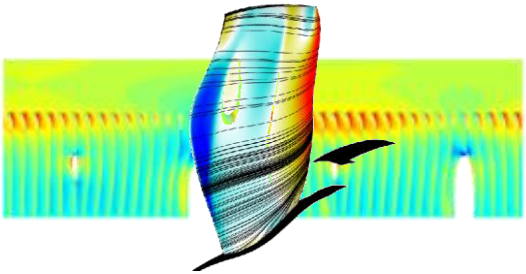


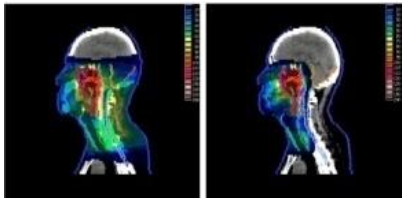
Dimensionality Reduction

- **In addition to ML activities, we also develop Minamo software for optimization and parametric studies**





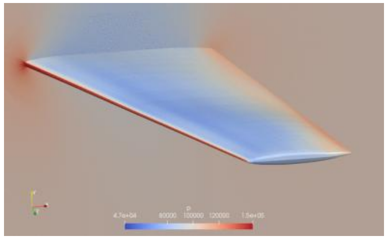


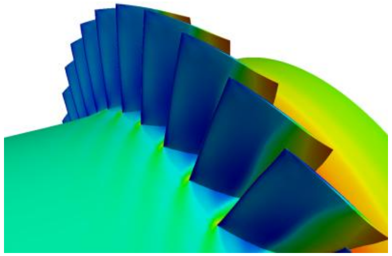


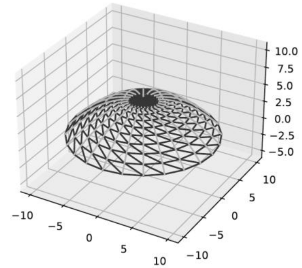
Cenaero

Dimensionality reduction in simulation-based problems

- **Dimensionality reduction in the case of Cenaero's activities:**
  - **Need to cope with high-dimensonal design spaces**
  - **Data coming from physics-based simulations**
  - **Application: engineering design and optimization (fields: aeronautics, biomedical, buildings, …)**







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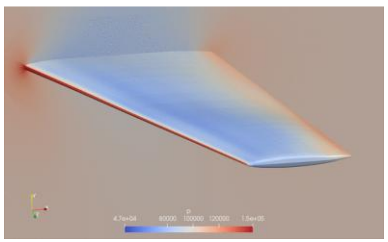
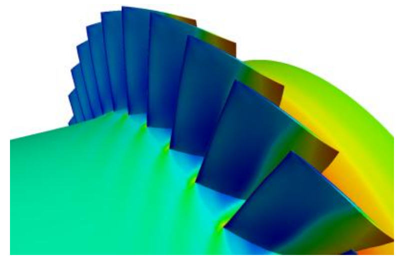
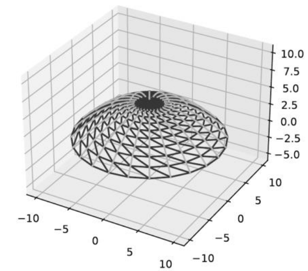




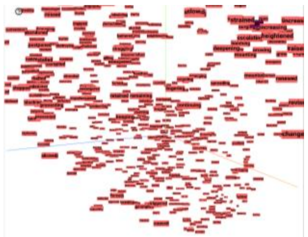


- **Context of this research:**
  - **WINGS project funded by the Walloon Region, with HPC resources from Lucia Tier 1 supercomputer (hosted by Cenaero and also funded by the Walloon Region)**
  - **Goal: develop dimensionality reduction methods for mechanical design examples characterized by highly flexible parametrizations**

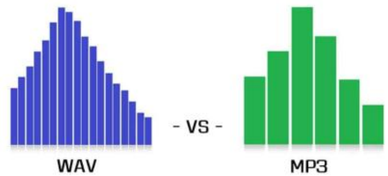
Dimensionality Reduction

Motivation for dimensionality reduction

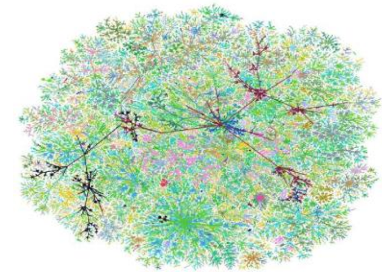
Text categorization of massive document resources



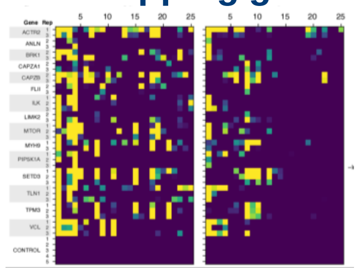
Acoustic signal compression



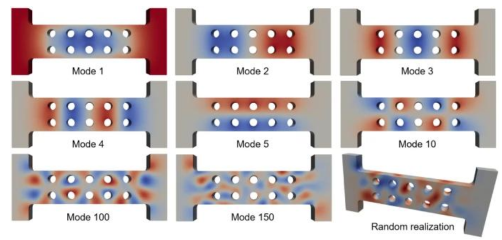
Data visualization of the internet network map



Identification of overlapping genes



Model reduction in physics-based simulations



- **Dimensionality reduction: popular in various application fields**
- **Black-box simulations ⇒ no analytical properties can be *a priori* assumed**
- **Restricted to continuous features (no integer, discrete, or categorical var.)**

Cenaero

Dimensionality reduction in design optimization

- **Three main paradigms:**

$\mathbf{x} = [\, x_1 \ldots x_N \,]^T$

Input space (e.g. CAD or FFD parameters)

Simulation

(CFD, CAA, FEA, ...)

$\mathbf{y} = [\, y_1 \ldots y_M \,]^T$

Output space (e.g. scalar responses extracted from velocity field, stresses, …)

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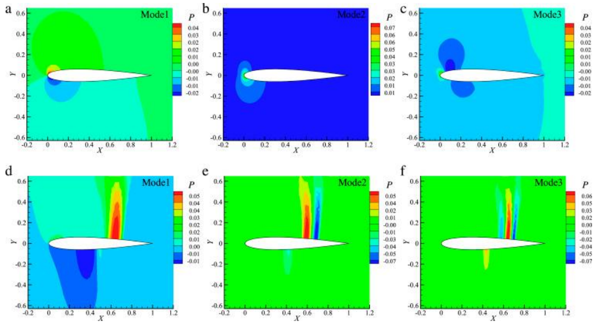
Model reduction on the **output space**
Ex.: POD on the CFD flow field



[Li & Zhang, 2016; Benamara *et al.*, 2017; etc.]

Dimensionality reduction in design optimization

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(CFD, CAA, FEA, ...)

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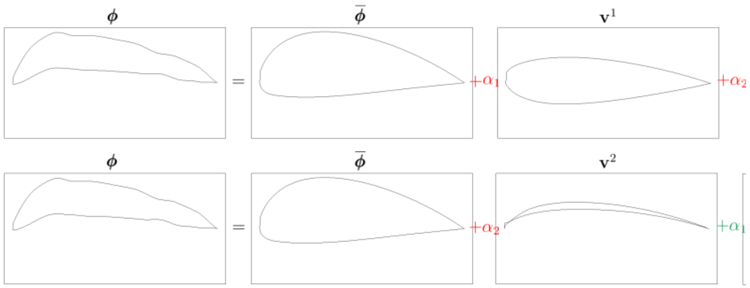
Output space (e.g. scalar responses extracted from velocity field, stresses, …)

Model reduction on the **input space**
Ex.: PCA on the airfoil geometries



[Gaudrie, Le Riche *et al.*, 2019]

Dimensionality reduction in design optimization

- ## Three main paradigms:

$\mathbf{x} = [\, x_1 \ldots x_N \,]^T$

Simulation

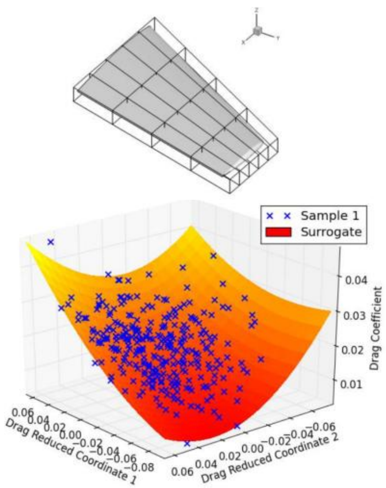
$\mathbf{y} = [\, y_1 \ldots y_M \,]^T$

Input space (e.g. CAD or FFD parameters)

(CFD, CAA, FEA, ...)

Output space (e.g. scalar responses extracted from velocity field, stresses, …)

Model reduction on the **input space**, taking the **ouputs** into account
Ex.: Active subspaces [Lucaczyk *et al.*, 2014]
⇒ Drag-reduced coordinates
⇒ Surrogate on a limited set of variables

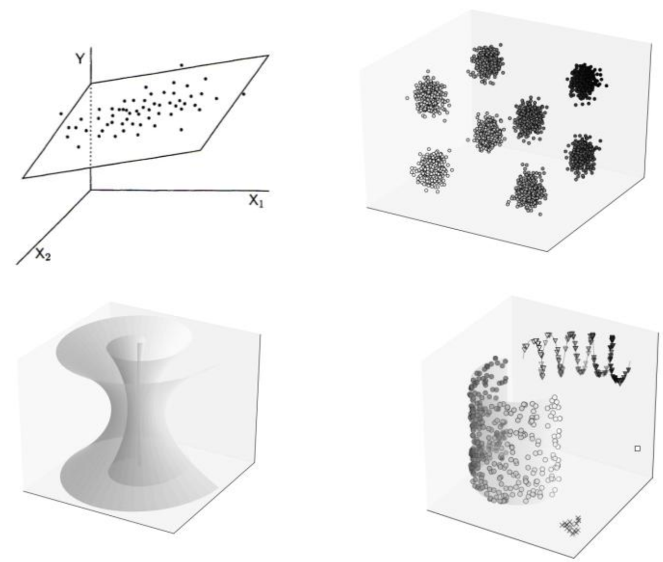


- Efficient, but often CPU expensive and not always flexible enough (need for adjoints, ...)
- **Our goal: develop an alternative *generic* and *affordable* dimensionality reduction methodology (on the input space)**

Dimensionality reduction

- **Generally speaking, data management issues involve:**
  - **Size (= number of samples)**
  - **Complexity (e.g., non-linearities, singularities, ...)**
  - **Dimensionality (= number of features/parameters/variables/inputs)**

- **To address these issues, several dimensionality reduction techniques have been proposed to:**
  - **Transform the original dataset into a new dataset representing low dimensionality...**
  - **… while maintaining as much as possible the original meanings of the data [Zebari *et al.*, 2020]**
  - **Their performances vary in the way they can capture or (not) the inner complexity of the data**

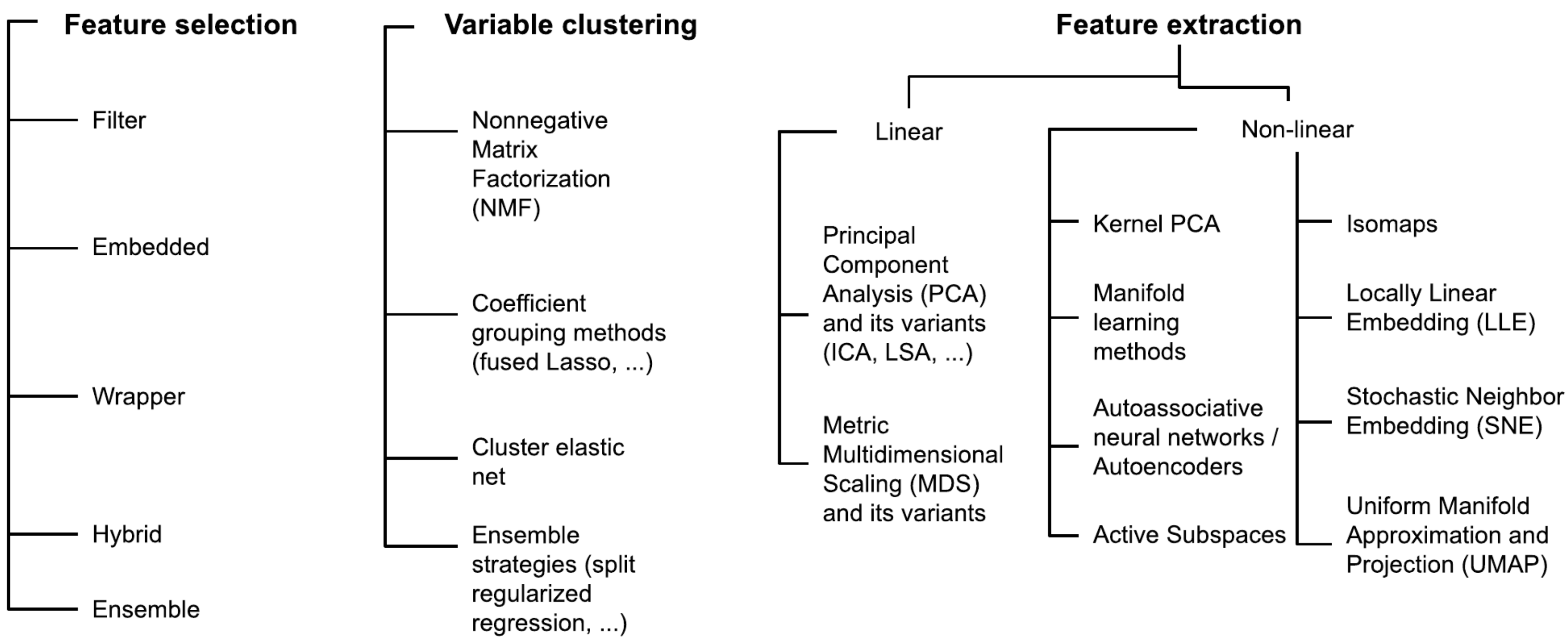


Dimensionality reduction: benefits expected

- **Benefits expected:**
  - **Reduction of the computational time and complexity of the subsequent approximation and optimization process**
  - **Avoids overfitting and noise**
  - **Better data visualization and interpretation**

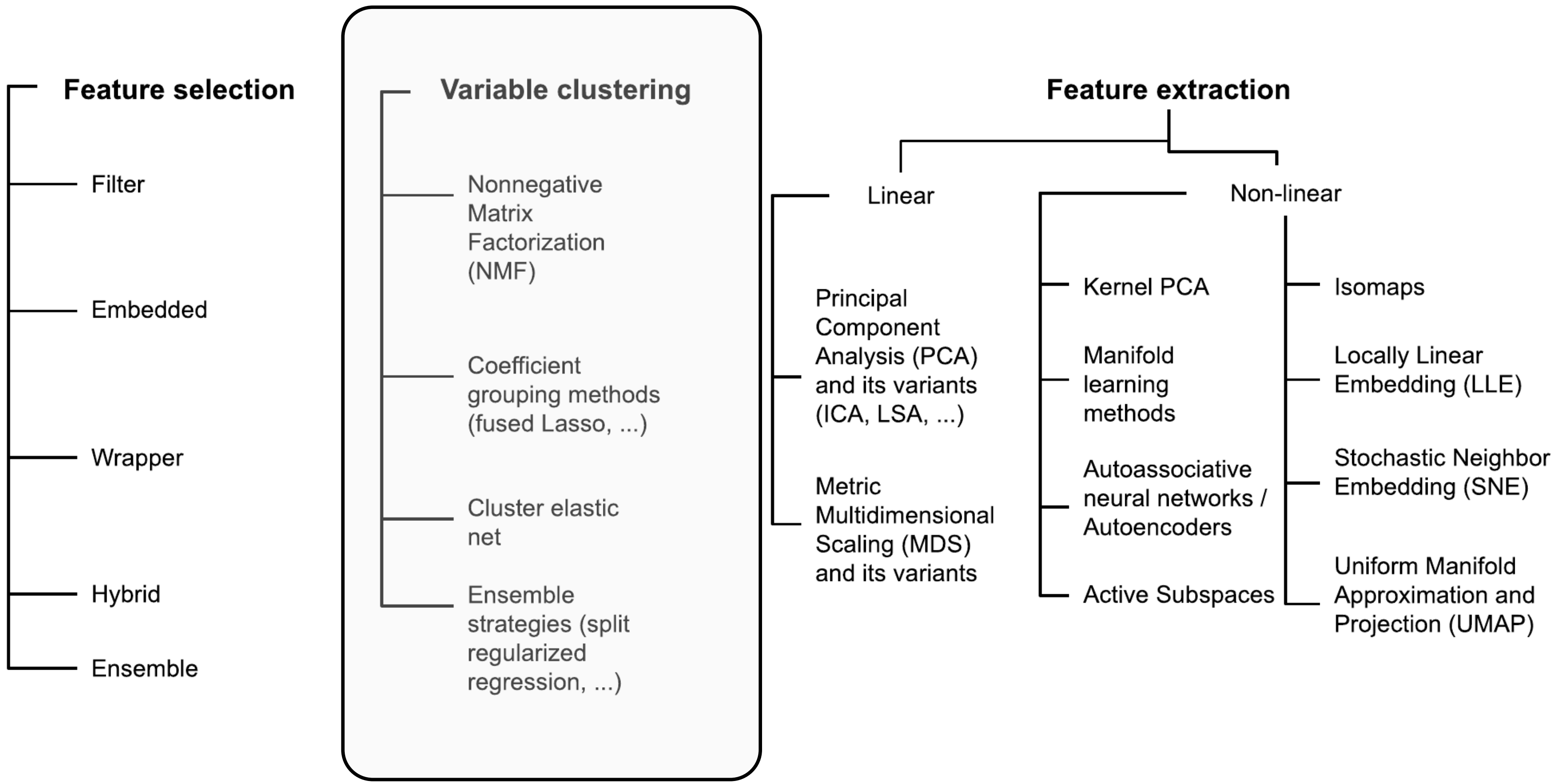
- **Active area of research**
  - **Lots of papers recently published**
    - In various fields (engineering, biotech, finance, etc.)
    - For several applications (image and text processing, data visualization, etc.)
  - **Historical trend of research**
    - First methods focus on global projections (typically: preserve covariance between dimensions, like Principal Component Analysis or PCA)
    - Now: more localized approaches (i.e. preserve pairwise distances or proximities as much as possible)

Taxonomy of dimensionality reduction techniques



Hou, C. K. J. and Behdinan, K. Dimensionality reduction in surrogate modeling: A review of combined methods. Data Science and Engineering, 7(4):402–427, 2022.

Taxonomy of dimensionality reduction techniques



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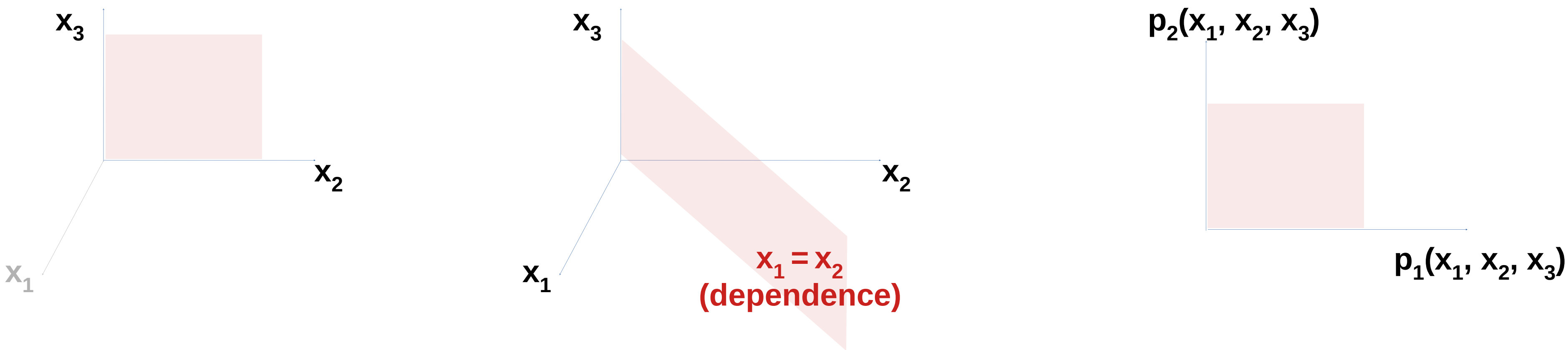
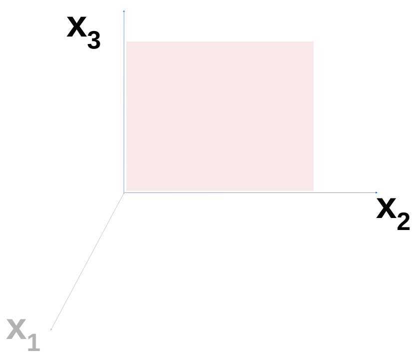
- **Visual comparison of dimensionality reduction paradigms:**

Feature selection **Variable clustering** **Feature extraction**

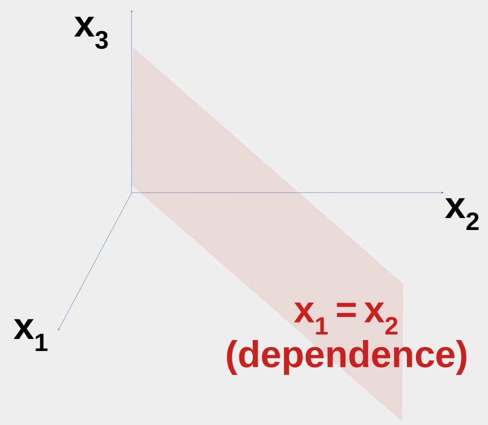


- **Visual comparison of dimensionality reduction paradigms:**

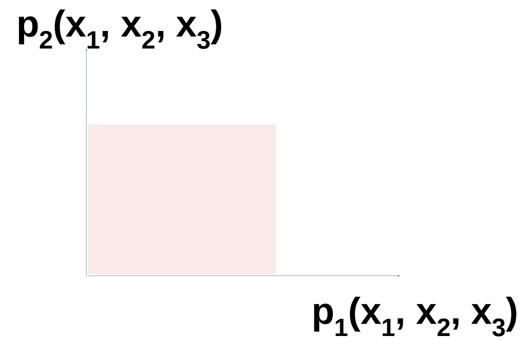
Feature selection



Variable clustering



Feature extraction



Focus on variable clustering:
⇒ **The original parameter space is preserved**
⇒ **Parameters are grouped according to a given criterion, but no one is discarded**

- **Analysis on the state-of-the-art in variable clustering:**
  - **Most methods imply the resolution of a minimization problem expressed as a linear regression or matrix factorization process, coupled with additional penalty functions to deal with grouping**
  - **Techniques directly or remotely inspired by data clustering (k-means, ...) are frequently integrated within the search for variable groups**
  - **Most methods work like in a black-box mode: no visualization tool is proposed to help the user apprehending the high-dimensional space**
  - **In structural and multidisciplinary optimization, the methods proposed usually involve, in one way or another, a significant level of user's expertise, or imply strong physical assumptions**

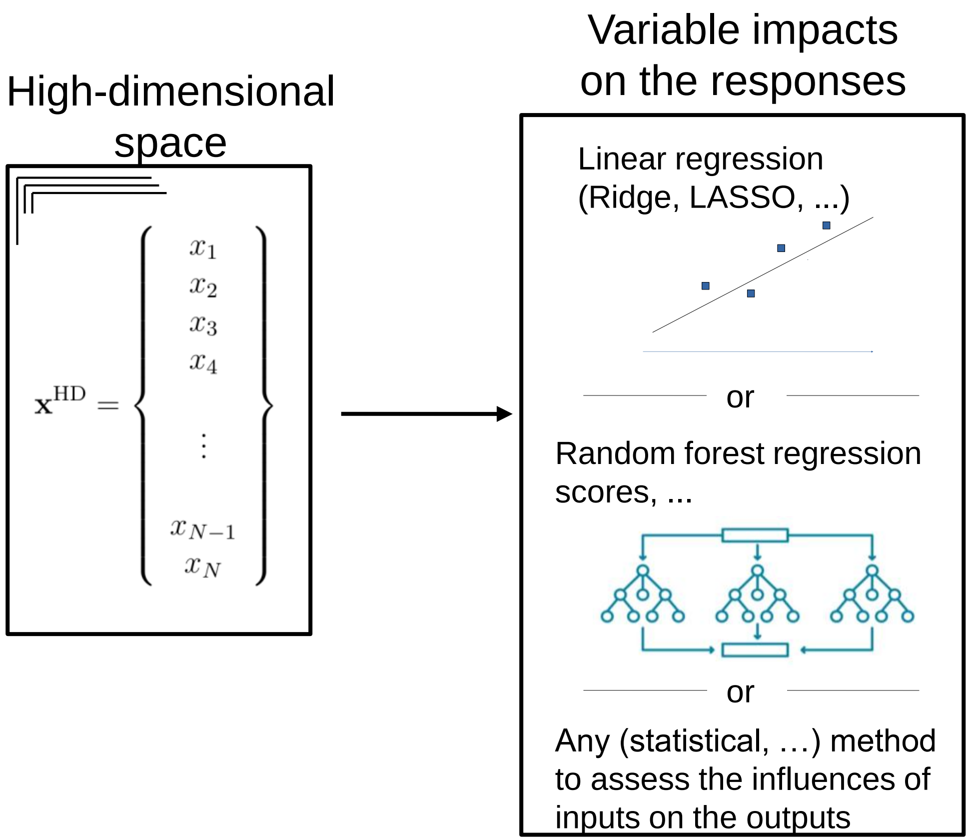
- **Let's remind our objective: devise a generic and flexible variable clustering strategy, with visualization functionalities**

- **Hypothesis: variables with similar impact on the responses are grouped together**

High-dimensional space

$$\mathbf{x}^{\mathrm{HD}} = \left\{ \begin{array}{c} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \vdots \\ x_{N-1} \\ x_N \end{array} \right\}$$

- **Hypothesis: variables with similar impact on the responses are grouped together**



Variable clustering methodology

- **Hypothesis: variables with similar impact on the responses are grouped together**

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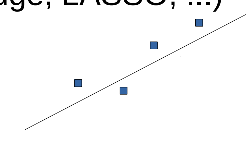
$$\mathbf{x}^{\mathrm{HD}} = \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ \\ \vdots \\ \\ x_{N-1} \\ x_N \end{Bmatrix}$$

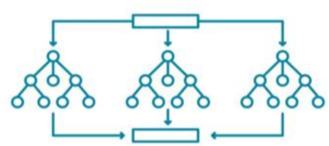
Variable impacts on the responses

Linear regression (Ridge, LASSO, ...)



or

Random forest regression scores, ...

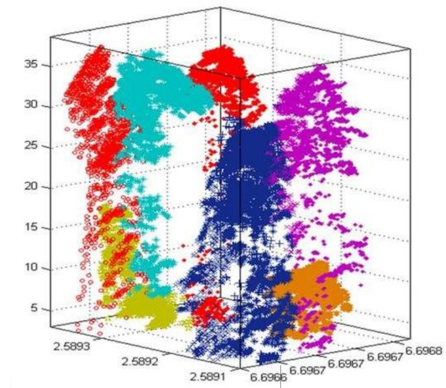


or

Any (statistical, …) method to assess the influences of inputs on the outputs

Variable clustering

DBSCAN, K-MEANS, ...



Variables grouped by importance

$$\mathbf{x}^{\mathrm{grouped}} = \begin{Bmatrix} x_1 \equiv p_1 \\ x_2 \equiv p_2 \\ x_3 \equiv p_2 \\ x_4 \equiv p_1 \\ \\ \vdots \\ \\ x_{N-1} \equiv p_n \\ x_N \equiv p_1 \end{Bmatrix}$$

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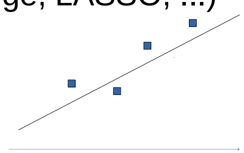

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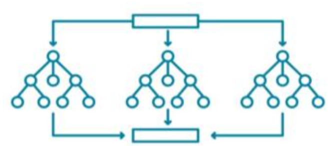

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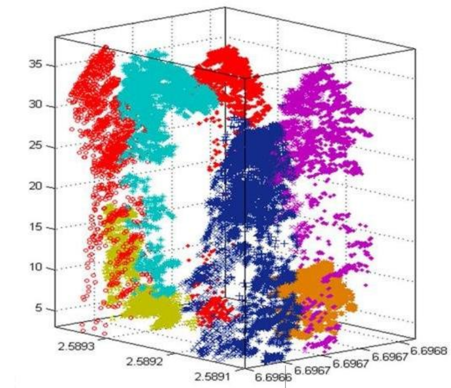
Issue: poor results observed with (even moderately) high number of variables and responses

Variable clustering

DBSCAN, K-MEANS, ...



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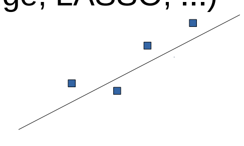

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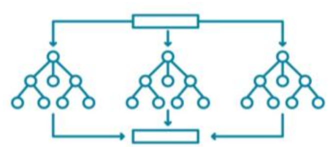
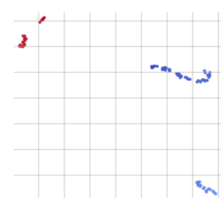


or

Any (statistical, …) method to assess the influences of inputs on the outputs

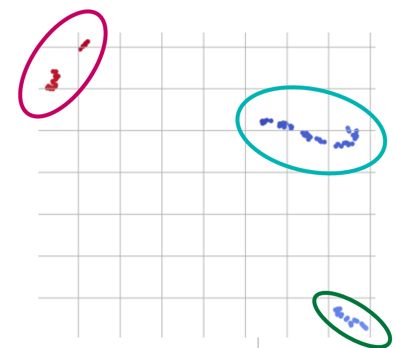
2

Solution: projection on an intermediate latent space, as a pre-conditioner of the clustering



3 Variable clustering

DBSCAN, K-MEANS, ...

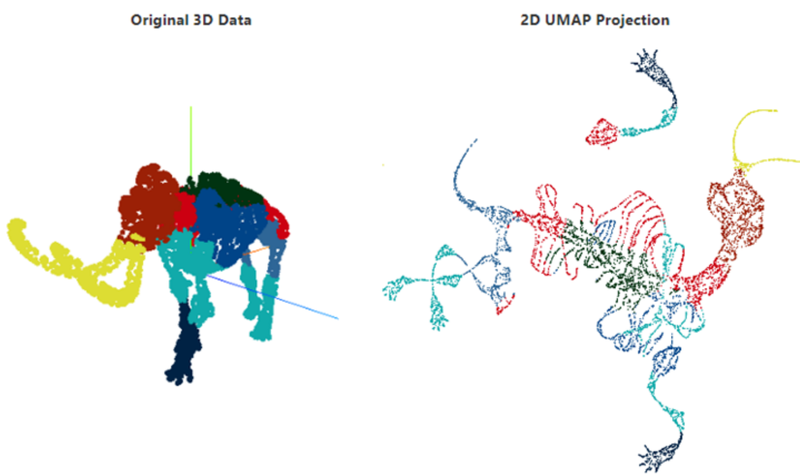


Variables grouped by importance

$$\mathbf{x}^{\text{grouped}} = \left\{ \begin{array}{c} x_1 \equiv p_1 \\ x_2 \equiv p_2 \\ x_3 \equiv p_2 \\ x_4 \equiv p_1 \\ \vdots \\ x_{N-1} \equiv p_n \\ x_N \equiv p_1 \end{array} \right\}$$

Three-step methodology

- **Idea: decomposition in three distinct steps 1, 2, and 3, using the UMAP dimensionality reduction technique at step 2:**
  - **UMAP (Uniform Manifold Approximation and Projection, by McInnes et al., 2018) has gained popularity in recent years in various DR contexts**
  - **Based on fuzzy algebraic topology and Riemannian geometry, UMAP constructs a graph in high dimensions to connect the data, and then performs an optimization to find the most similar graph in lower dimensions**



McInnes, L., Healy, J., Saul, N., and Großberger, L. *UMAP: Uniform Manifold Approximation and Projection*. Journal of Open Source Software, 3(29):861, 2018.

UMAP-based variable clustering

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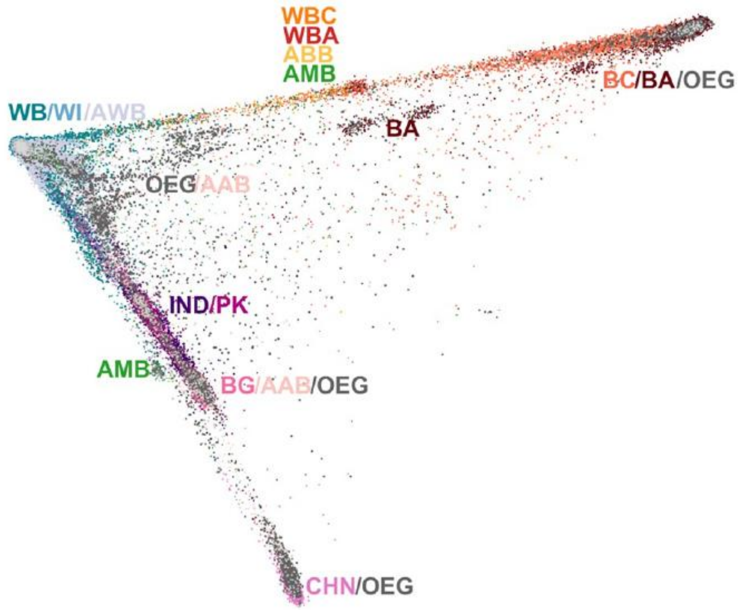
Applications of UMAP

- **Various fields of applications (genetics, image processing, ...)**
- **Example: analyzing genotype data among 488,377 individuals in the UK, according to ethnicity [Diaz-Papkovitch *et al.*, 2018]**
  - **Method: dimension reduction of genomic data combining Principal Component Analysis (PCA) with UMAP to illustrate population structure in large cohorts, and capture their relationships on local and global scales**
  - **Aims:**
    - Detect correlations between genetic diseases and ethnic origins
    - Genetic anthropology



PCA (first 2 modes)

Legend: BA, Black African; BC, Black Caribbean; BG, Bangladeshi; CHN, Chinese; IND, Indian; PK, Pakistani; WB, White British; WI, White Irish; WBC, White and Black Caribbean; WBA, White and Black African; WAA, White and Asian; AAB, Any other Asian Background; ABB, Any other Black Background; AWB, Any other White Background; AMB, Any other Mixed Background; OEG, Other ethnic group.

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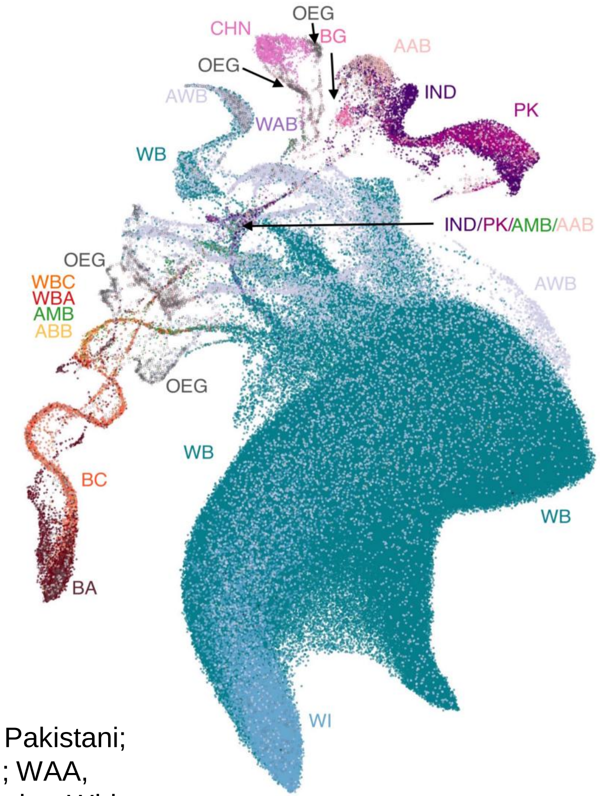


UMAP on first 10 PCA modes

Legend: BA, Black African; BC, Black Caribbean; BG, Bangladeshi; CHN, Chinese; IND, Indian; PK, Pakistani; WB, White British; WI, White Irish; WBC, White and Black Caribbean; WBA, White and Black African; WAA, White and Asian; AAB, Any other Asian Background; ABB, Any other Black Background; AWB, Any other White Background; AMB, Any other Mixed Background; OEG, Other ethnic group.

- **Step 0: design of experiments (dataset)**
- **Step 1: compute a k-neighbor connected graph in the high-dimensional space**

- **Step 2: define a symmetric *measure of similarity* for each pair of data points *i* and *j*:**

$$p_{ij} := p_{j|i} + p_{i|j} - p_{j|i} \cdot p_{i|j}$$

$$p_{j|i} := \begin{cases} \exp\left(-\frac{\left\|\mathbf{x}^{(i)}-\mathbf{x}^{(j)}\right\|_2 - \rho_i}{\sigma_i}\right) & \text{if } \mathbf{x}^{(j)} \in \mathcal{N}_i \\ 0 & \text{otherwise} \end{cases}$$

- **Step 3: compute a k-neighbor connected graph for the embedded points y*(i)* with a similarity measure in the latent space**

$$q_{ij} := \frac{1}{\left(1 + a\,\|\mathbf{y}^{(i)} - \mathbf{y}^{(j)}\|_2^{2b}\right)}$$

- **Step 4: the discrepancy between the similarity measures in the high- and low-dimensional spaces is computed by the fuzzy cross-entropy, to be minimized:**

$$c_1 := \sum_{i=1}^{N} \sum_{j=1, j\neq i}^{N} \left(p_{ij} \ln\left(\frac{p_{ij}}{q_{ij}}\right) + (1 - p_{ij}) \ln\left(\frac{1 - p_{ij}}{1 - q_{ij}}\right)\right)$$

- **Additional mathematical developments lead to a more tractable function to be minimized:**

$$\min_{\{\mathbf{y}_i\}_{i=1}^{n}} c_2 \quad := \quad \sum_{i=1}^{N} \sum_{j=1, j\neq i}^{N} \left[p_{ij} \ln\left(q_{ij}\right) + (1 - p_{ij}) \ln\left(1 - q_{ij}\right)\right]$$

UMAP algorithm: remarks

- UMAP has demonstrated its effectiveness when compared to other techniques like t-SNE or LargeVis in terms of CPU time and resources

- Further modifications have been proposed in the literature (DenseMap algorithm to regularize the cost function, variant for time series, etc.)

- UMAP can be used in high dimensions (not limited to 2D/3D visualization)

- UMAP is a stochastic algorithm: randomness used both when speeding up approximation steps, and when solving hard optimization problems

- UMAP has been promoted as an efficient pre-conditioner for clustering in a few studies [Allaoui et al., 2020; Hozumi et al., 2021]

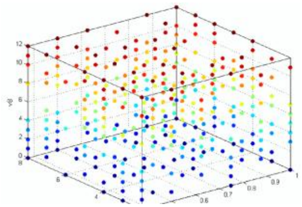
Application to design optimization

Let's go back to our original problem

- **Goal: optimize highly parametrized structural and mechanical systems**
- **Algorithm: surrogate-based optimizer (SBO) from Minamo**
- **Sequential approach followed:**

Design of Experiments

to evaluate the responses on a representative subset of the design space



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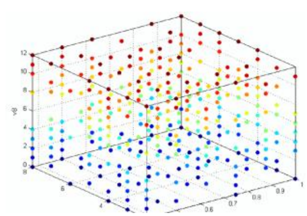

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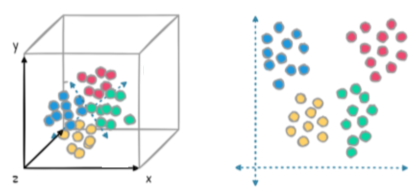
Dimensionality reduction to group variables by importance

(using UMAP)



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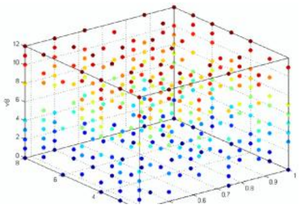
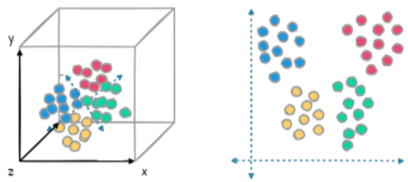
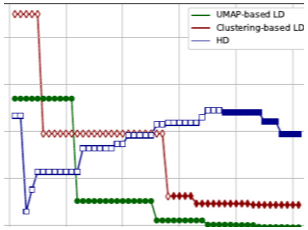
Dimensionality reduction to group variables by importance

(using UMAP)

Surrogate-based optimization (SBO) using Minamo







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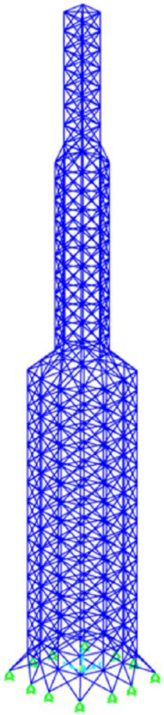
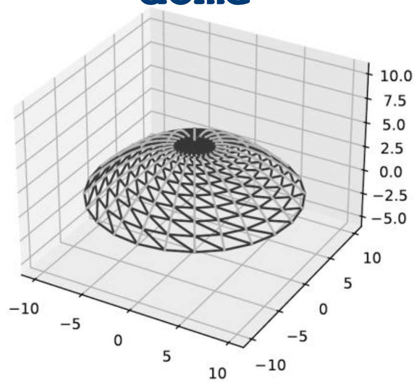
First validation: on structural test cases

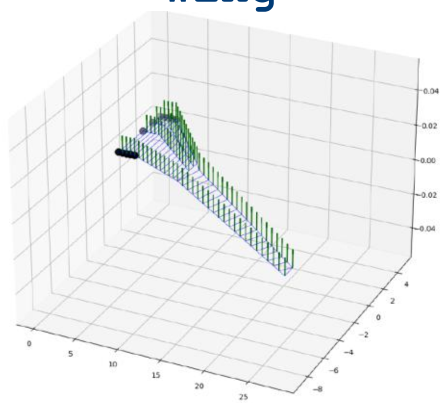
bldg



dome



wing



- **Variables: cross-sectional diameters of beams**
- **Dimensionality:**

Example	Number of variables
`dome`	$np = 696$
`bldg`	$np = 942$
`wing`	$np = 162$

- **Responses: outputs from a finite element analysis [FEAP program, by Taylor *et al.*, 2008]**

$$\left\{\begin{array}{l} \mathrm{mass}(\mathbf{x}) \\ \sigma^{\text{max, external load}}(\mathbf{x}) \\ d^{\text{max, external load}}(\mathbf{x}) \\ s^{\text{max, external load}}(\mathbf{x}) \\ \sigma^{\text{max, dead load}}(\mathbf{x}) \\ d^{\text{max, dead load}}(\mathbf{x}) \\ s^{\text{max, dead load}}(\mathbf{x}) \end{array}\right.$$

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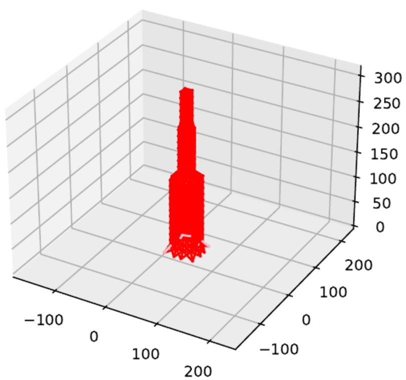
Is the UMAP step really useful?

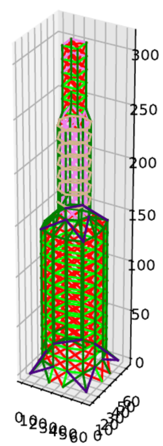
- **Direct clustering vs. UMAP-preconditioned clustering**
  - **Variable impacts on responses estimated by Ridge linear regression coefficients, clustering performed by DBSCAN**

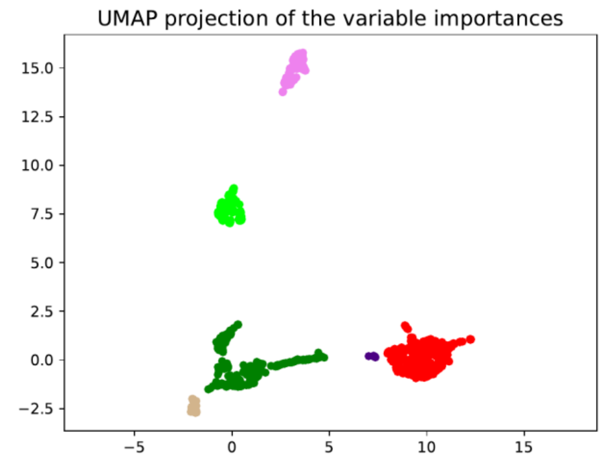
Average number of clusters found	Direct clustering	UMAP-based clustering
bldg	1	7
dome	2	4
wing	1	3

  - **Illustration on the skyscraper test case (`bldg`):**



Direct: 1 cluster found





UMAP-based: 6 clusters found

  - **DBSCAN without UMAP-preconditioning fails to identify meaningful clusters of variables (caveat: no hyperparameter tuning)**

Complex structural application: Dutch Maritime Museum

- **Industrial case: structural optimization of the Dutch Maritime Museum [Descamps *et al.*, 2014 – ULB / Princeton University / Ney & Partners]**
  - **1954 design variables (cross-section areas)**
  - **Objective: mass – Constraints: on stresses, buckling, and displacements**

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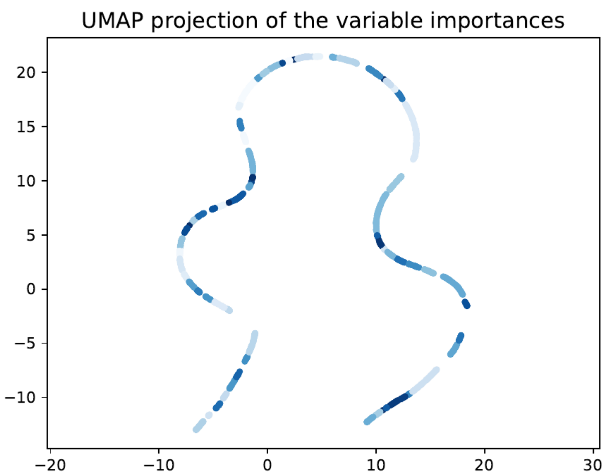
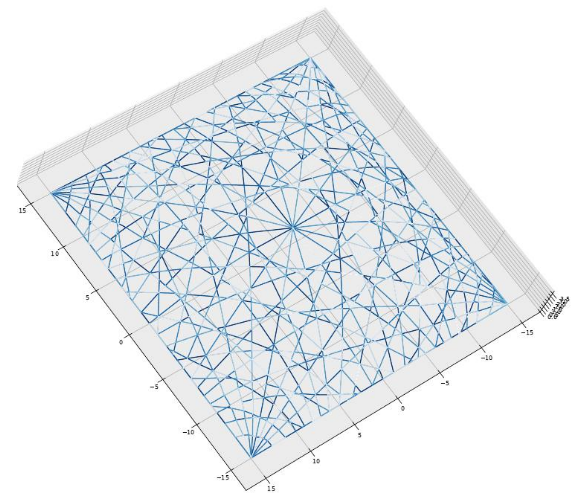
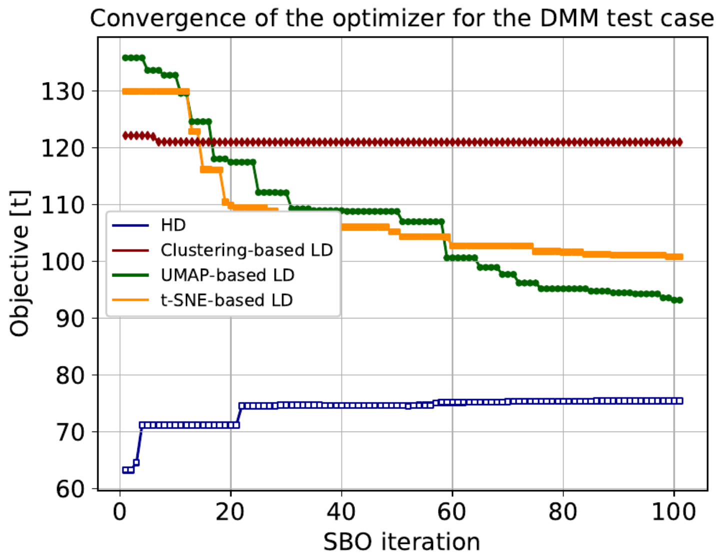


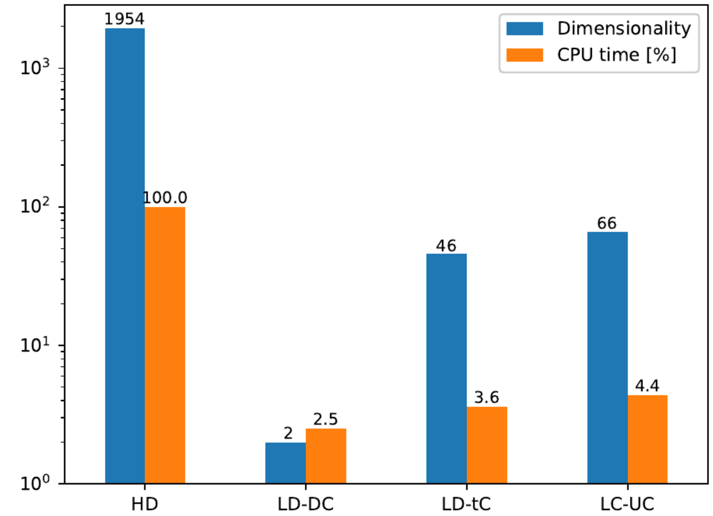


66 clusters detected by UMAP + DBSCAN

Complex structural application: Dutch Maritime Museum

- ## SBO results

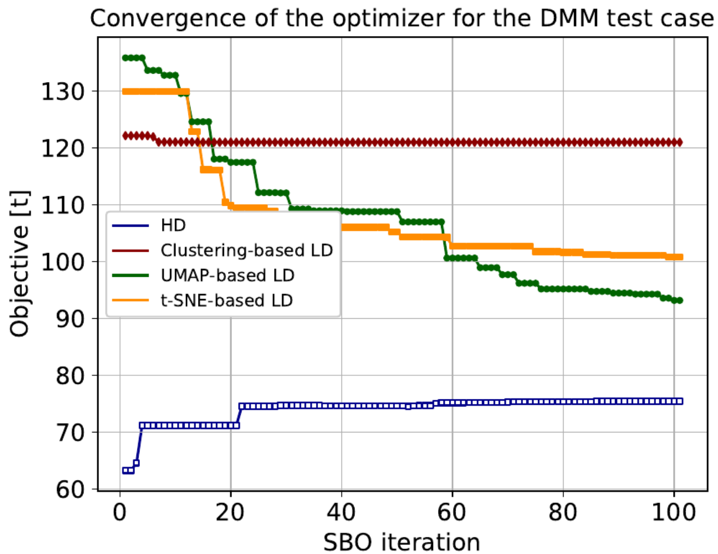


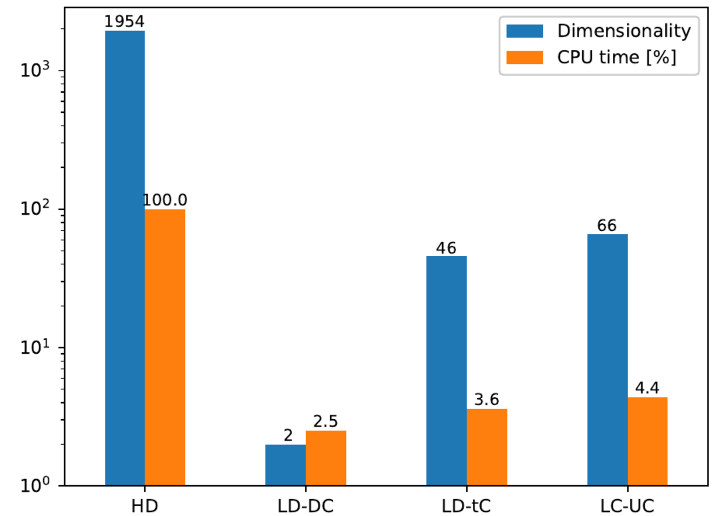


Filomeno Coelho, R., Sainvitu, C., and Benamara, T. *UMAP-based Dimensionality Reduction for Variable Grouping: Application to the Design Optimization of Truss Structures*. In 13th ASMO UK / 2nd ASMO-EUROPE / ISSMO Conference on Engineering Design Optimization Product and Process Improvement, Cenaero, Belgium, July 8-9, 2024.

Complex structural application: Dutch Maritime Museum

- **SBO results**





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- **Take aways from these first results:**
  - **Strategy successfully tested on cases up to 1954 design variables, but on structural design cases only with symmetry / repeatibility patterns**
  - **What about different mechanical systems like compressors?**
  - **Should the same variable grouping be used during the whole SBO?**

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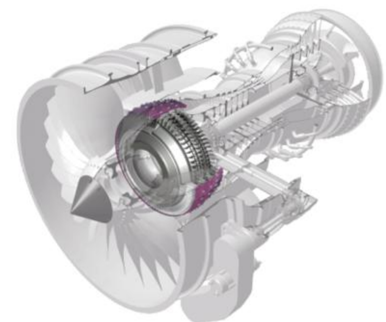
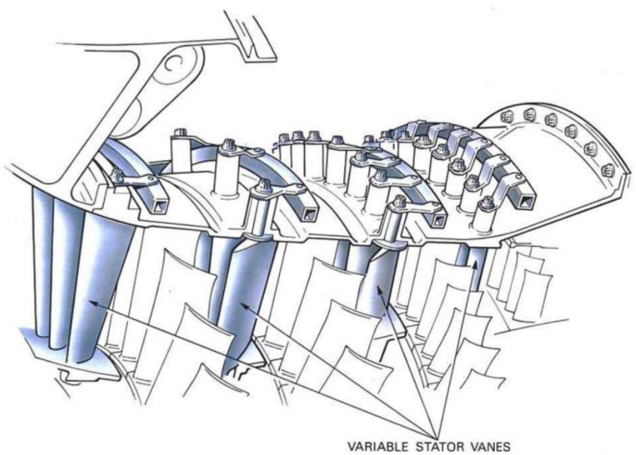
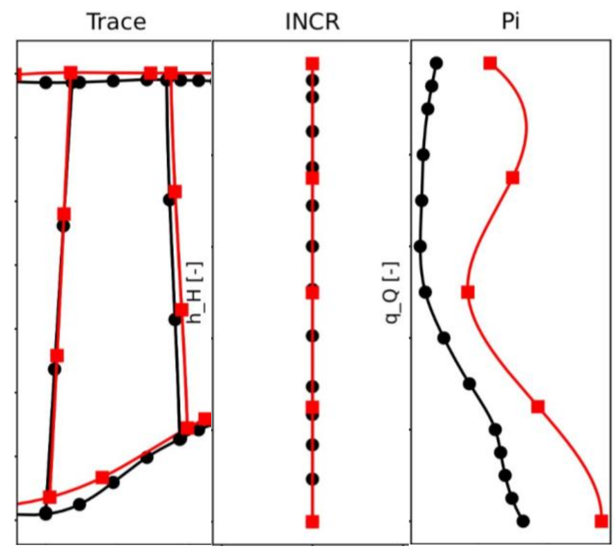
Multi-stage compressor (Safran Aero Boosters)

- **Number of input parameters:**
  - **N = 144 design variables**
  - **Simulation: axisymmetric throughflow CFD solver, widely used at the preliminary design stage in turbomachinery [Simon, 2007]**
  - **Rate of successful simulations: ~55%**



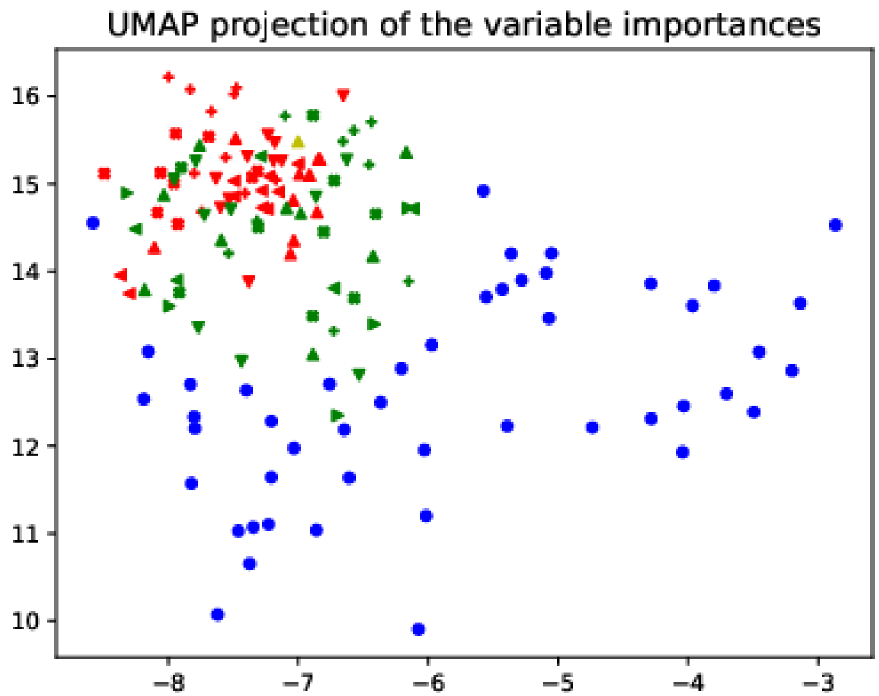




Nigro, R., Baert, L., Nyssen, F., de Cazenove, J., Dominique, J., Lepot, I., Veglio, M., and Princivalle, R. *Multi-fidelity aeromechanical design framework for high flow speed multistage axial compressors*. In: Proceedings of the ASME TurboExpo 2024 conference, London, UK, June 23-28, 2024.

Multi-stage compressor (Safran Aero Boosters)

- **Preliminary results on a multi-stage compressor (SAB)**
  - **Design of Experiments of 5 N = 720 geometries (LHS – Latin Hypercube Sampling)**
  - **Dimensionality reduction performed on 1175 responses**
  - **Agglomerative clustering better adapted to this configuration**



Color:

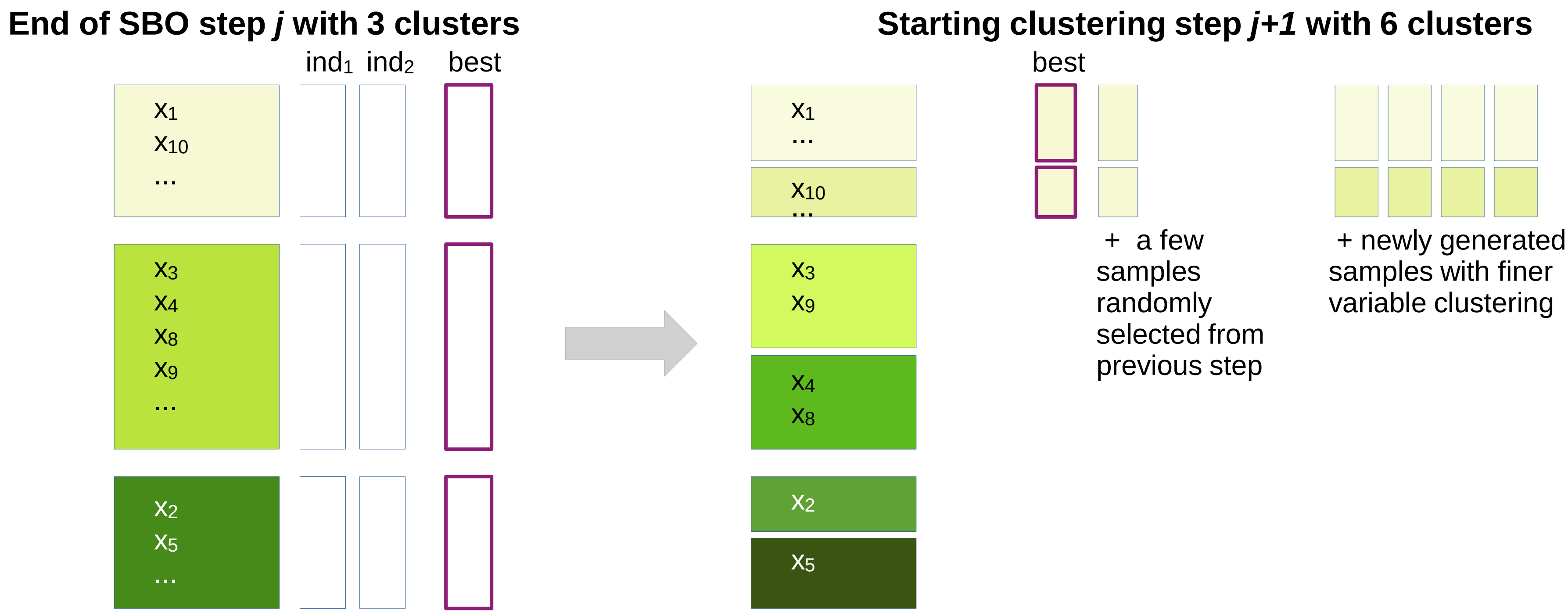
- If "flow_path": blue
- If "aero": red
- If "geom": green
- Otherwise: yellow

Marker:

- S1: v
- S2: ^
- S3: <
- ST: >
- R2: +
- R3: x

Multi-stage compressor (Safran Aero Boosters)

- **Idea: update the clustering of variables during the SBO**
  - **Caution: when switching from a “coarse-grained” to a “fine-grained” variable clustering, there must be a mapping between levels, in order to re-use points from previous SBO iterations:**



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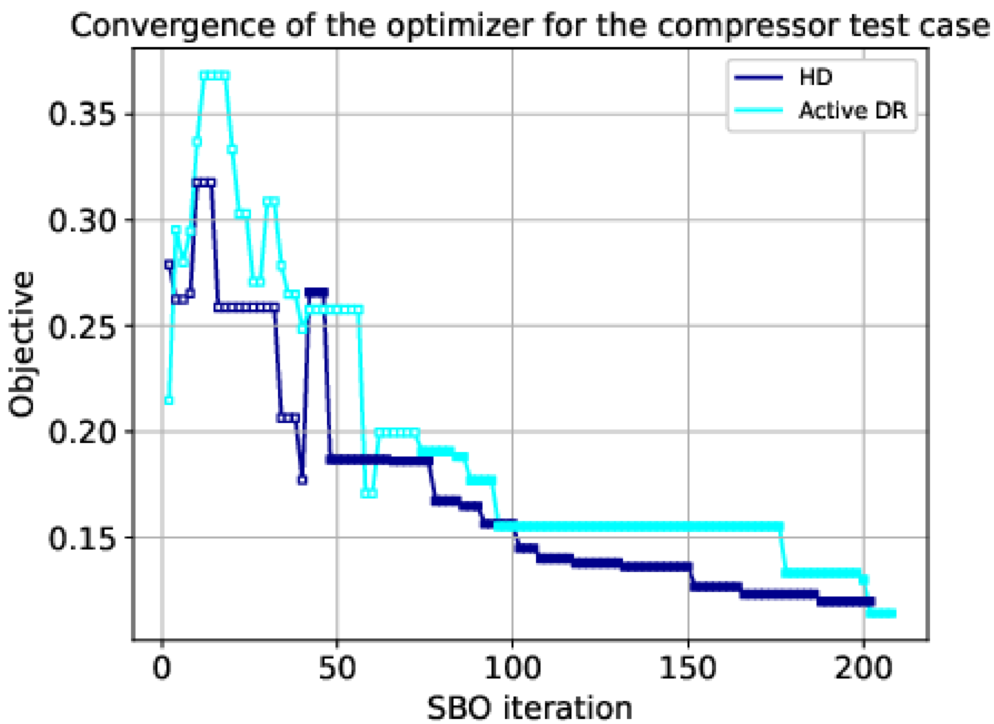
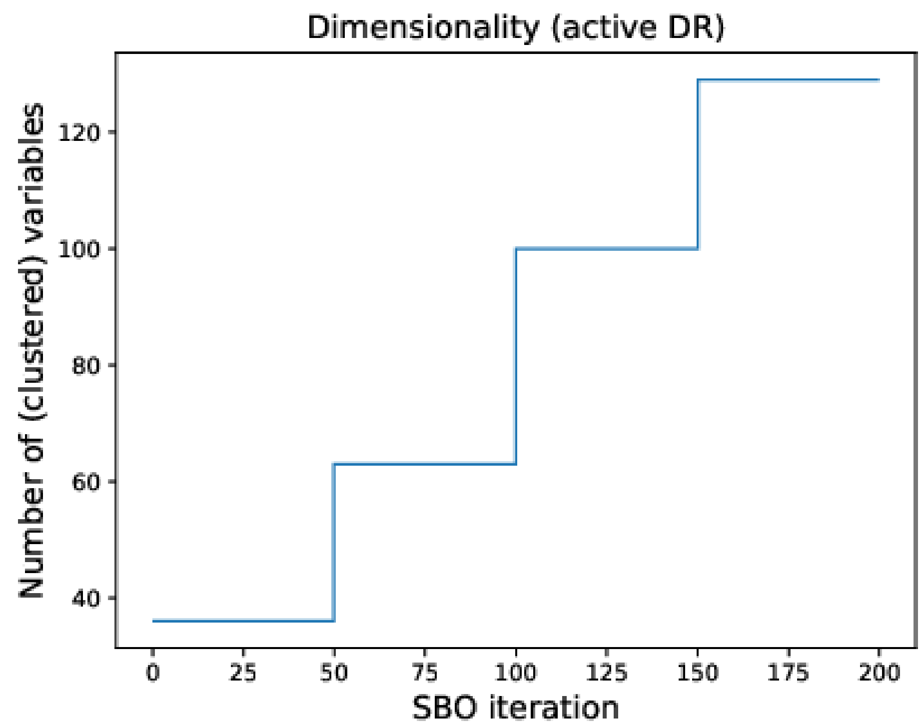
Multi-stage compressor (Safran Aero Boosters)

- **Preliminary results on a multi-stage compressor (SAB)**
  - **SBO: 1 objective (minimize fuel burn) and 122 aerodynamical constraints**
  - **Similar performances obtained, but with a decrease of ~50% CPU time required (faster training of the surrogates due to reduced dimensionalities)**





Conclusions and future prospects

Discussion

- **Design of Experiments**
  - Size of the design of experiments: compromise between accuracy of the results and cost of the simulations

- **Variable importances:**
  - Ridge regression: computationally inexpensive and often acceptable [Grömping, 2009], but might be insufficient in some cases
  - Currently investigated: Random forests (RF), Mutual information (MI) scores [Université de Namur]
  - Grouping dependent on active constraints only?

- **UMAP for variable clustering**
  - UMAP useful to pre-condition data for clustering
  - Strategy efficiently combined to surrogate-based optimization
  - Ongoing developments on active learning strategies

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