Learning Physics from Data

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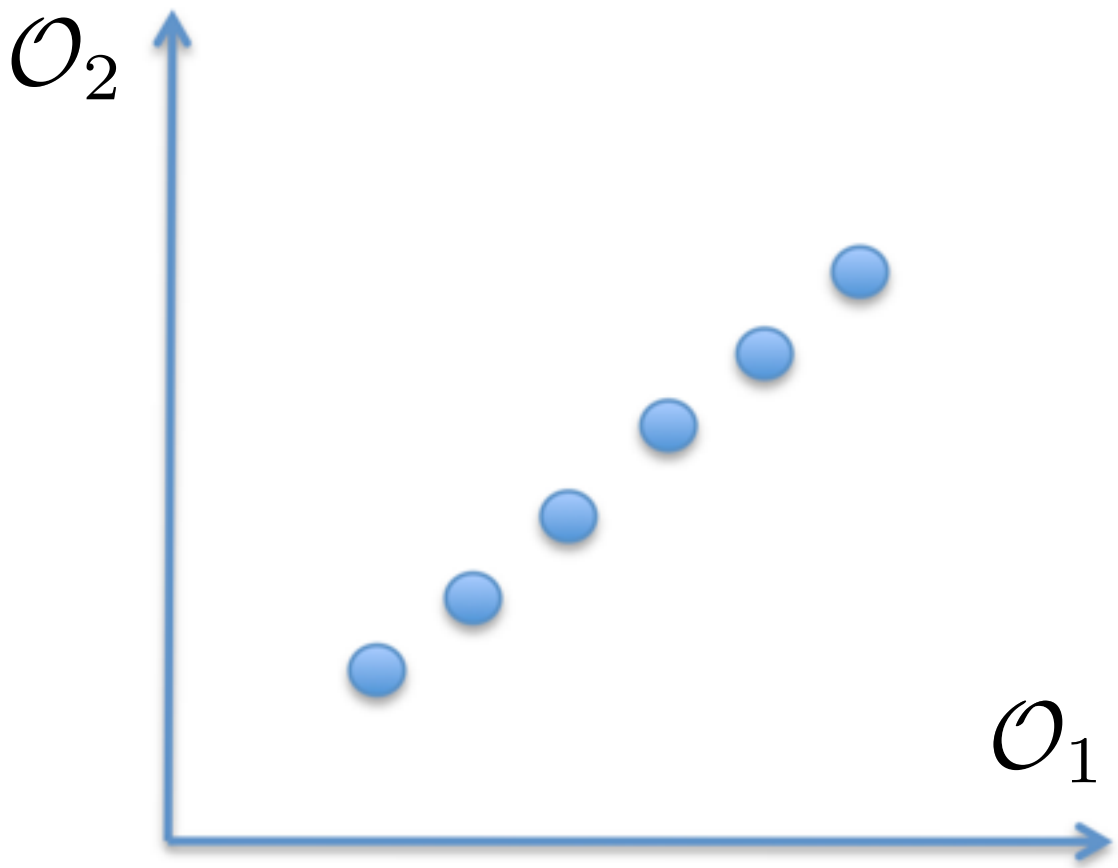
OUTLINE

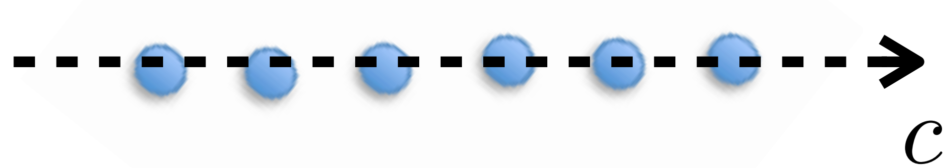
- **DATA REDUCTION**
- **MODELLIG REDUCED DATA**
- **MODEL ORDER REDUCTION**

DATA REDUCTION

From linear to nonlinear dimensionality reduction

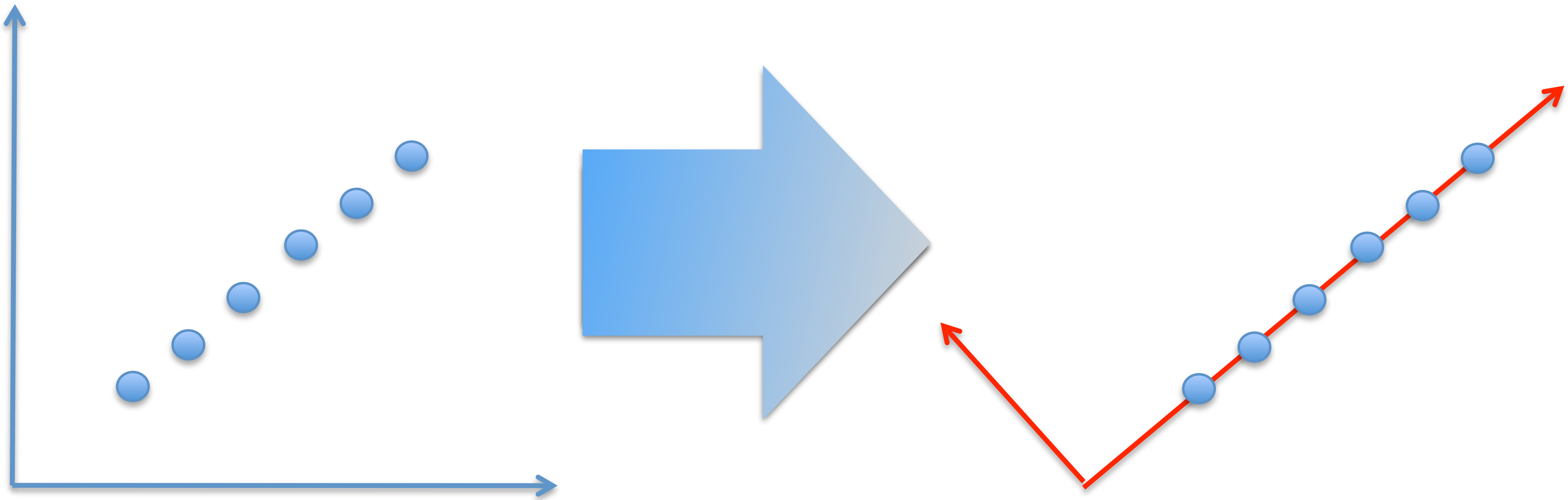
$$(\mu_1^i, \mu_2^i, \dots) \to (\mathcal{O}_1^i, \mathcal{O}_2^i), \quad i = 1, \dots, D$$



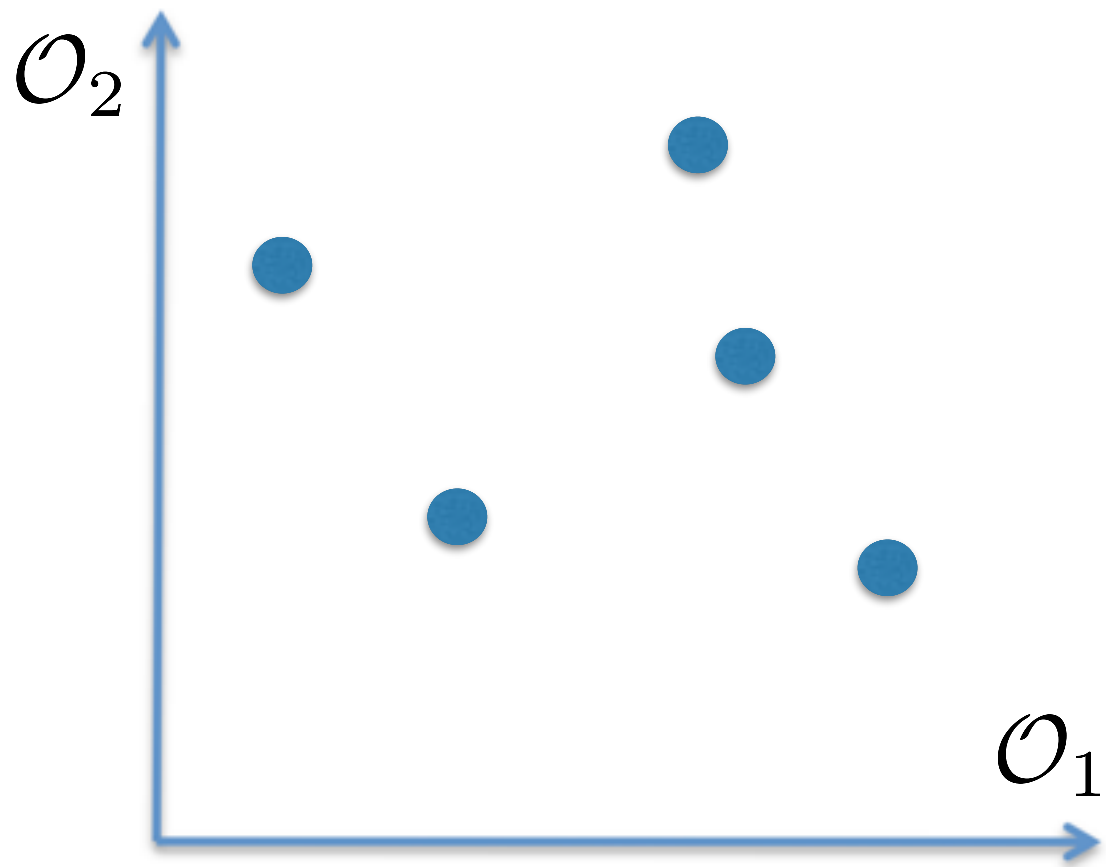


$$\begin{cases} \mathcal{O}_1(c) \\ \mathcal{O}_2(c) \end{cases}$$

Geometrical view



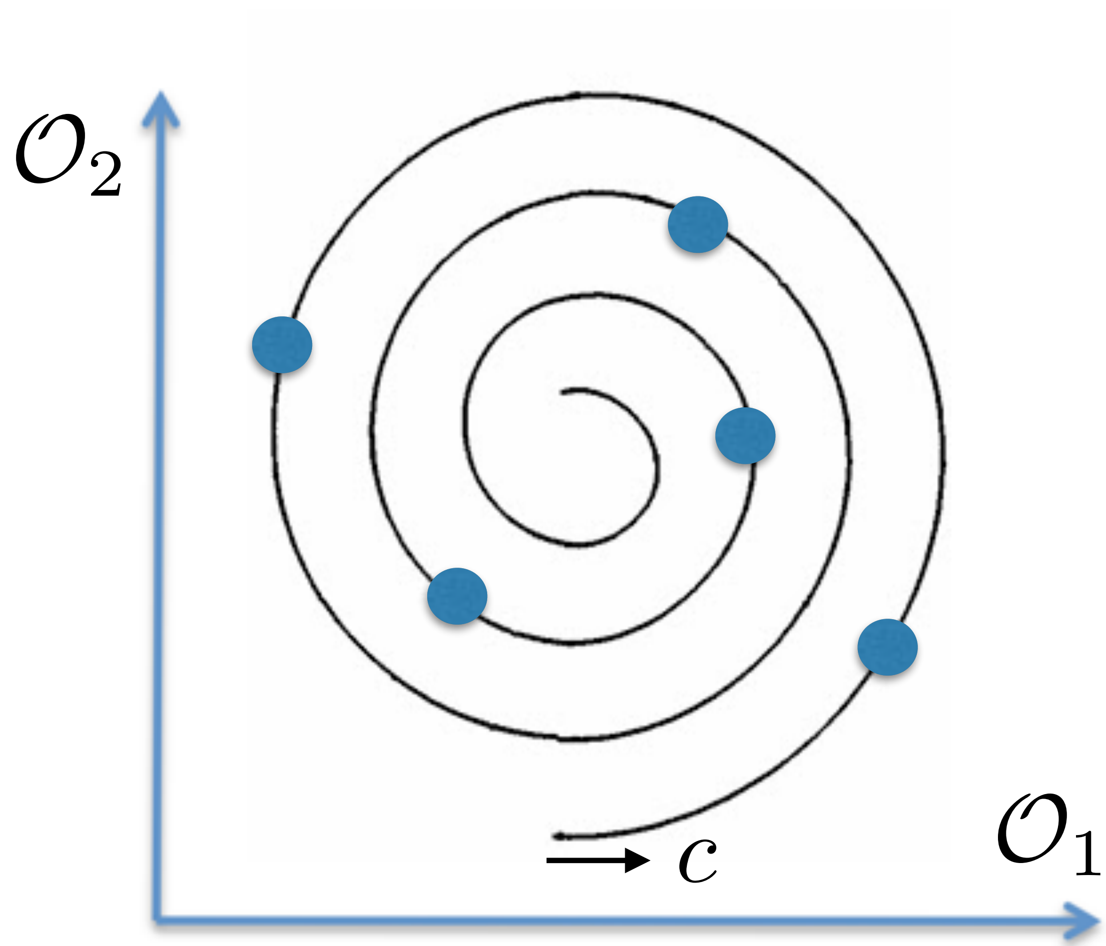
$$(\mu_1^i, \mu_2^i, \dots) \rightarrow (\mathcal{O}_1^i, \mathcal{O}_2^i), \quad i = 1, \dots, D$$

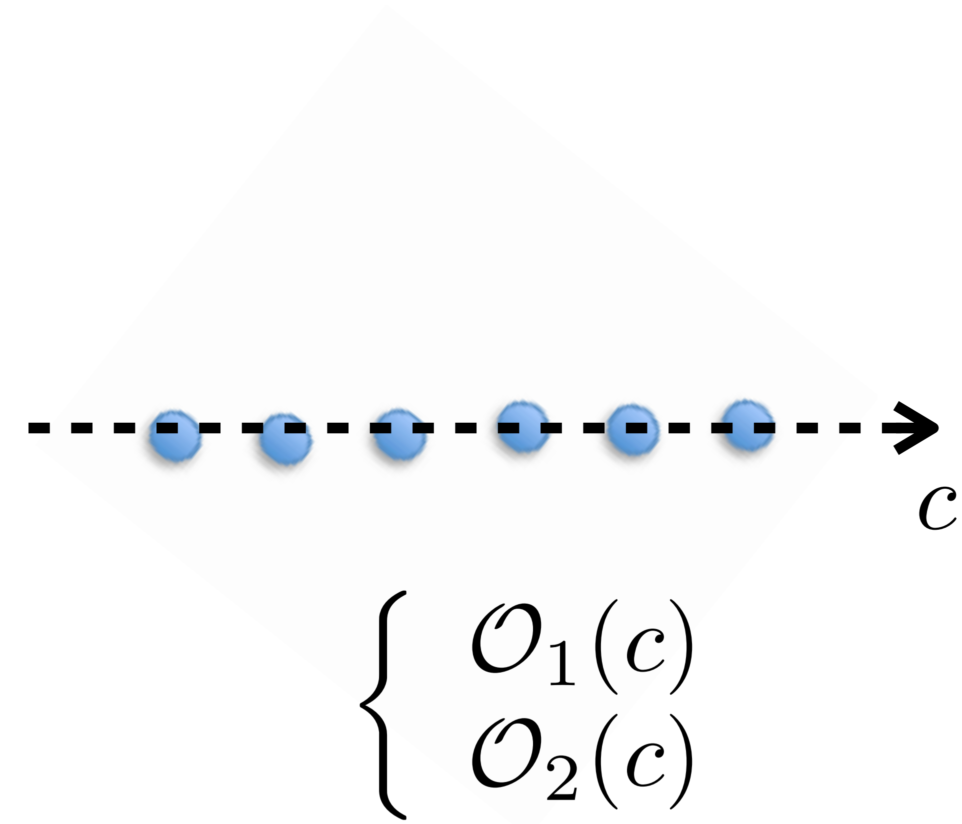


What is the dimensionality ?

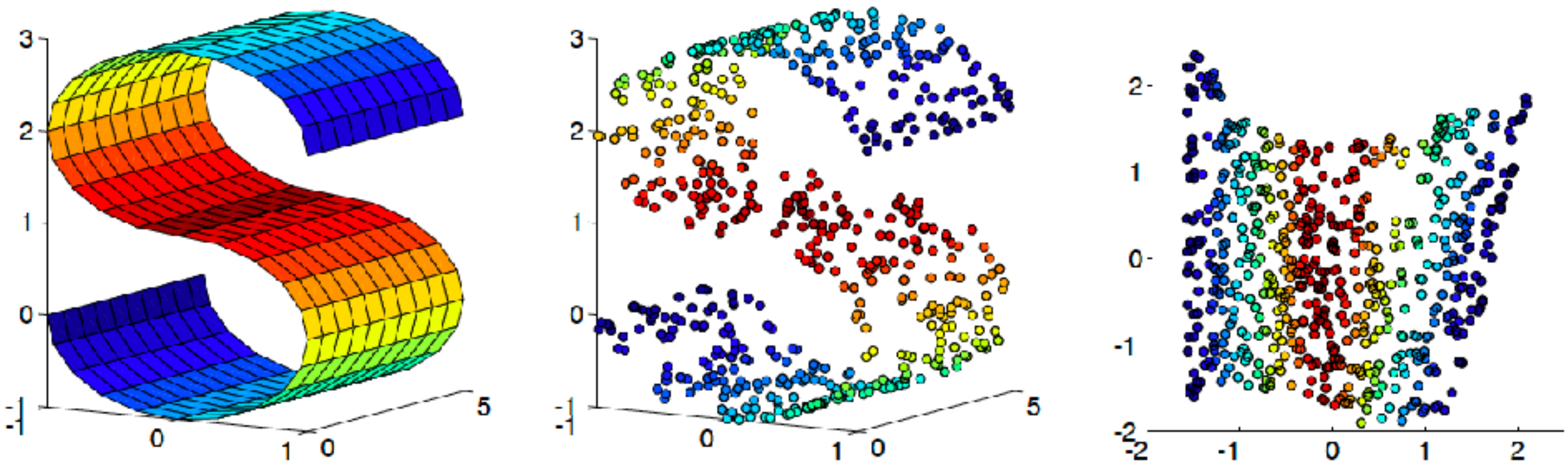
Apparently 2

However it is still 1 !

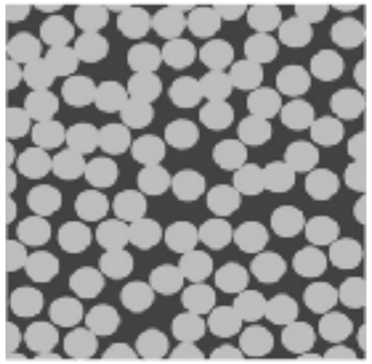


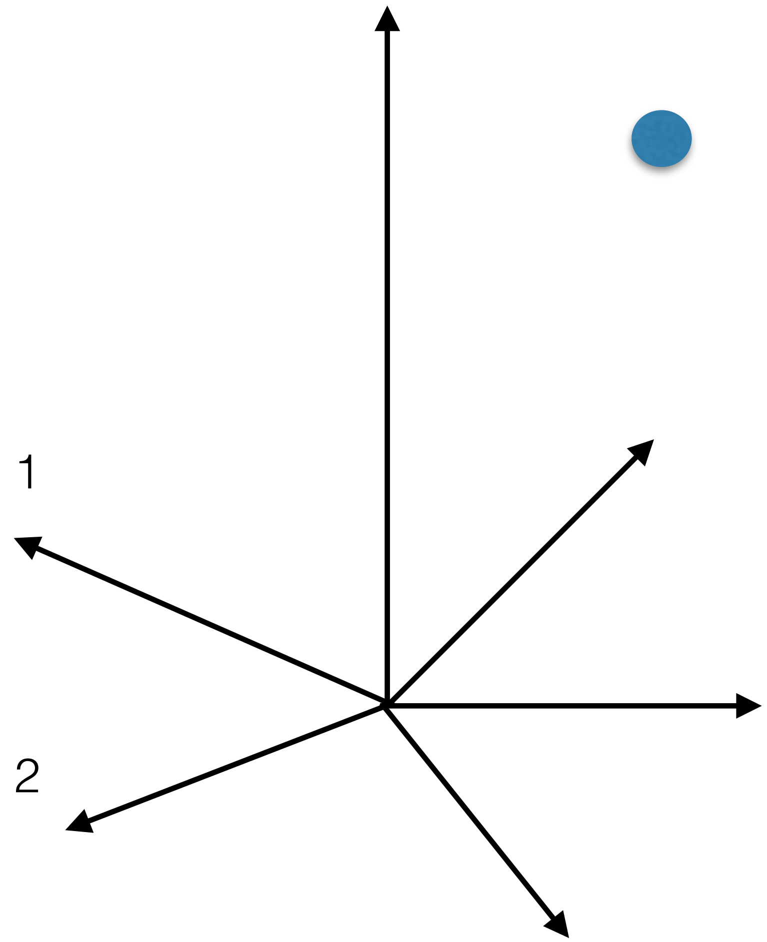


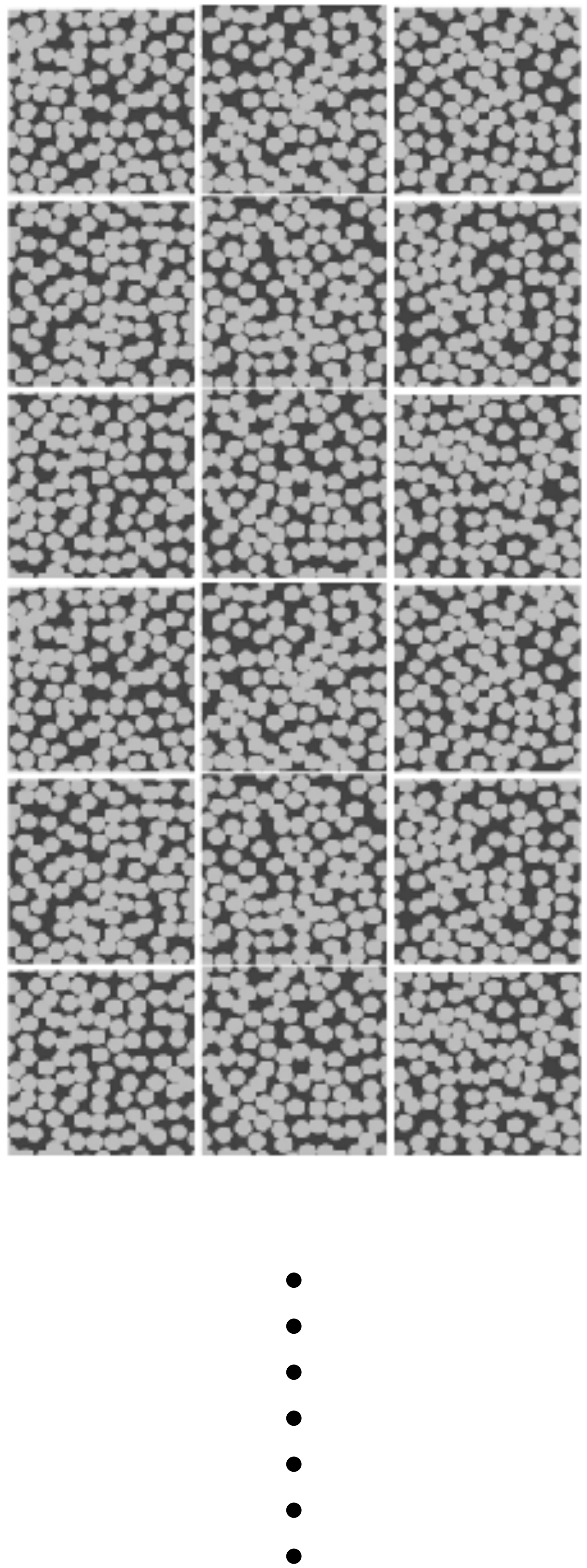
Linear model order reduction (e.g. PCA) fails whereas non-linear ones work (e.g. LLE, kPCA, lPCA,tSNE, …)

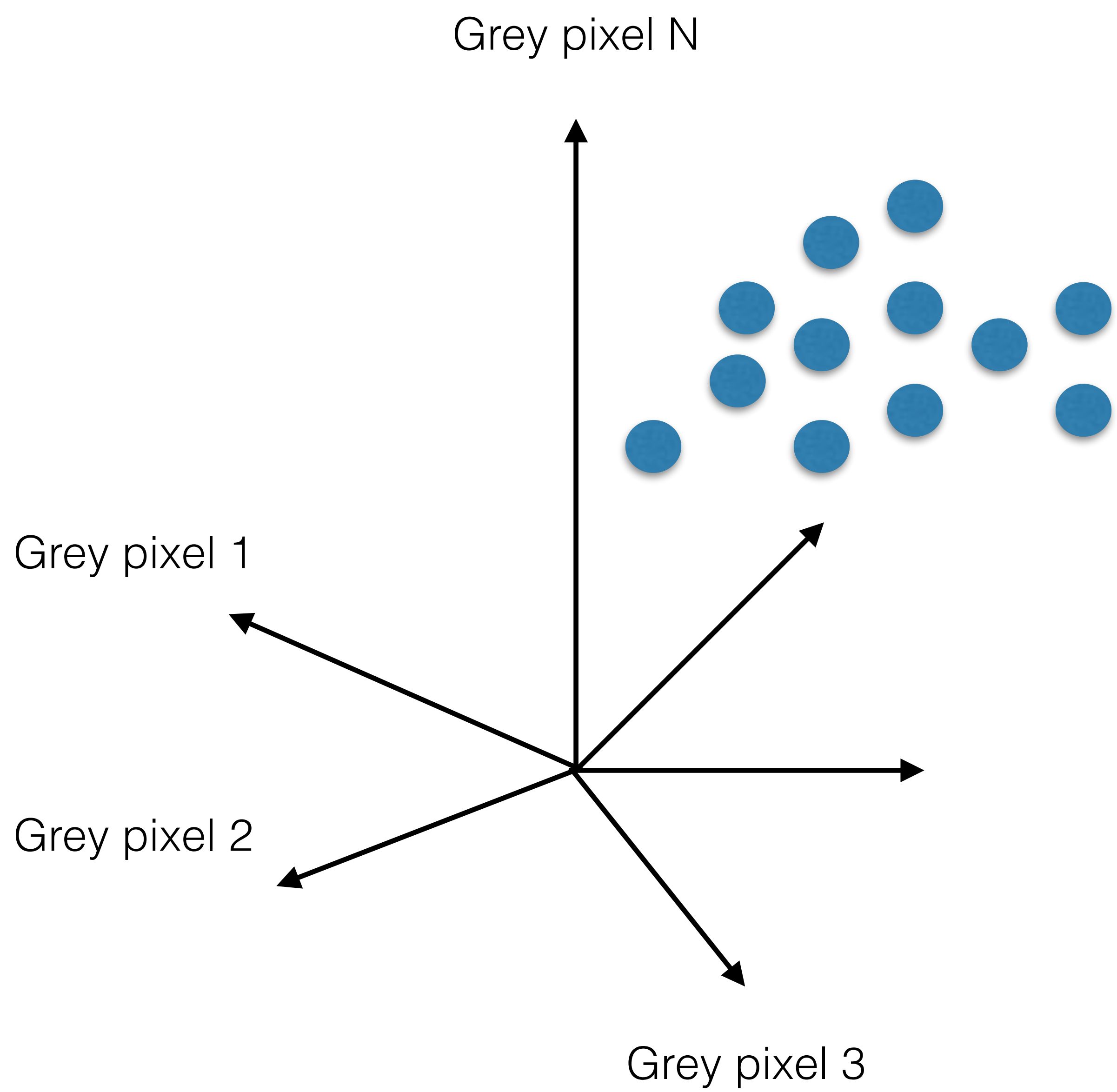

3
2
1
0
-1
-1
0
1
0
5
3
2
1
0
-1
-1
0
1
0
5
2
1
0
-1
-2
-2
-1
0
1
2

Parametrizing Microstructures



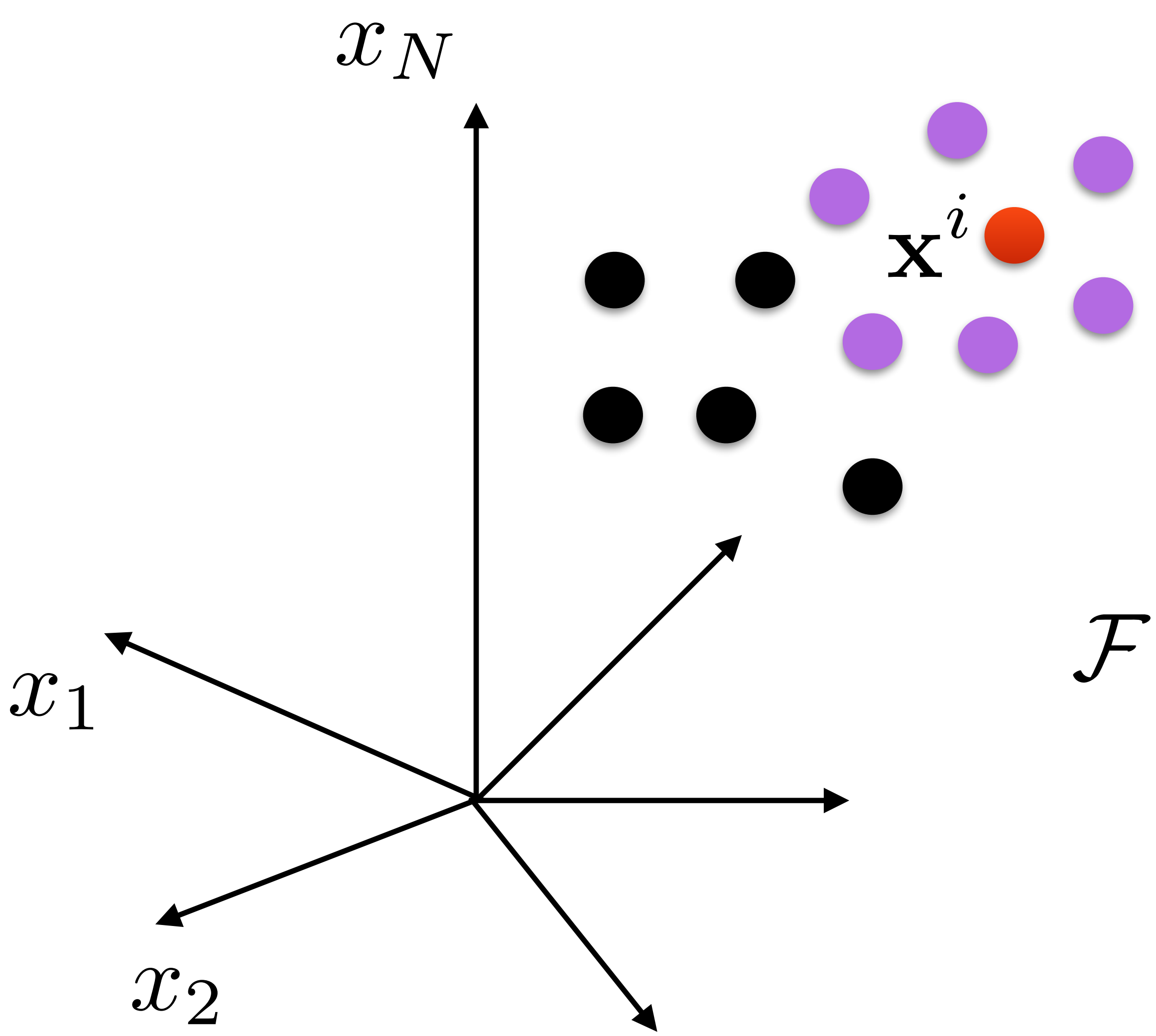






What is the dimensionality ? N ?

Locally Linear Embedding - LLE

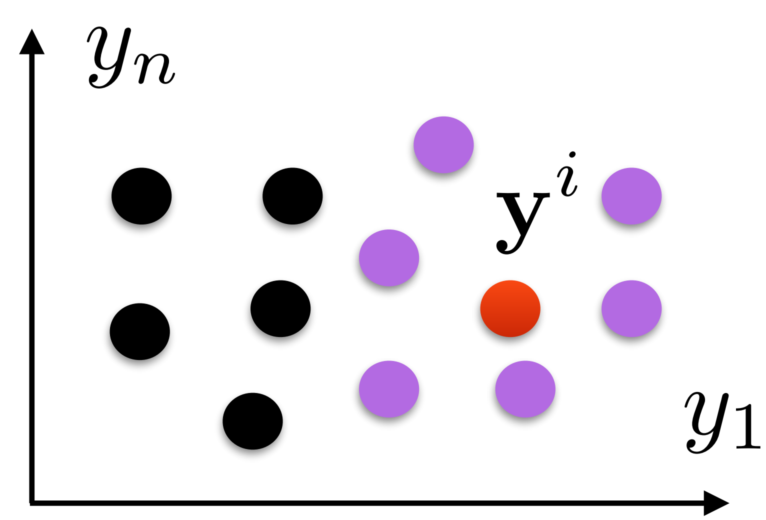


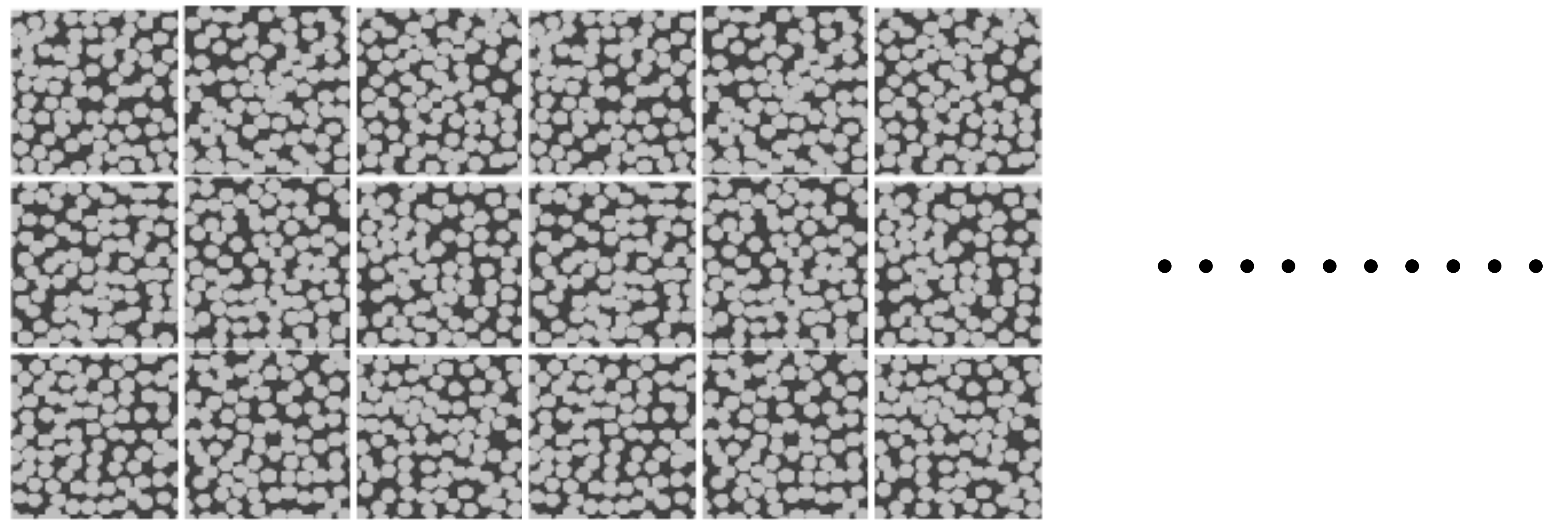
$$\mathbf{x}^i = \sum_{j \in \mathcal{V}_i} W_{ij} \mathbf{x}^j$$

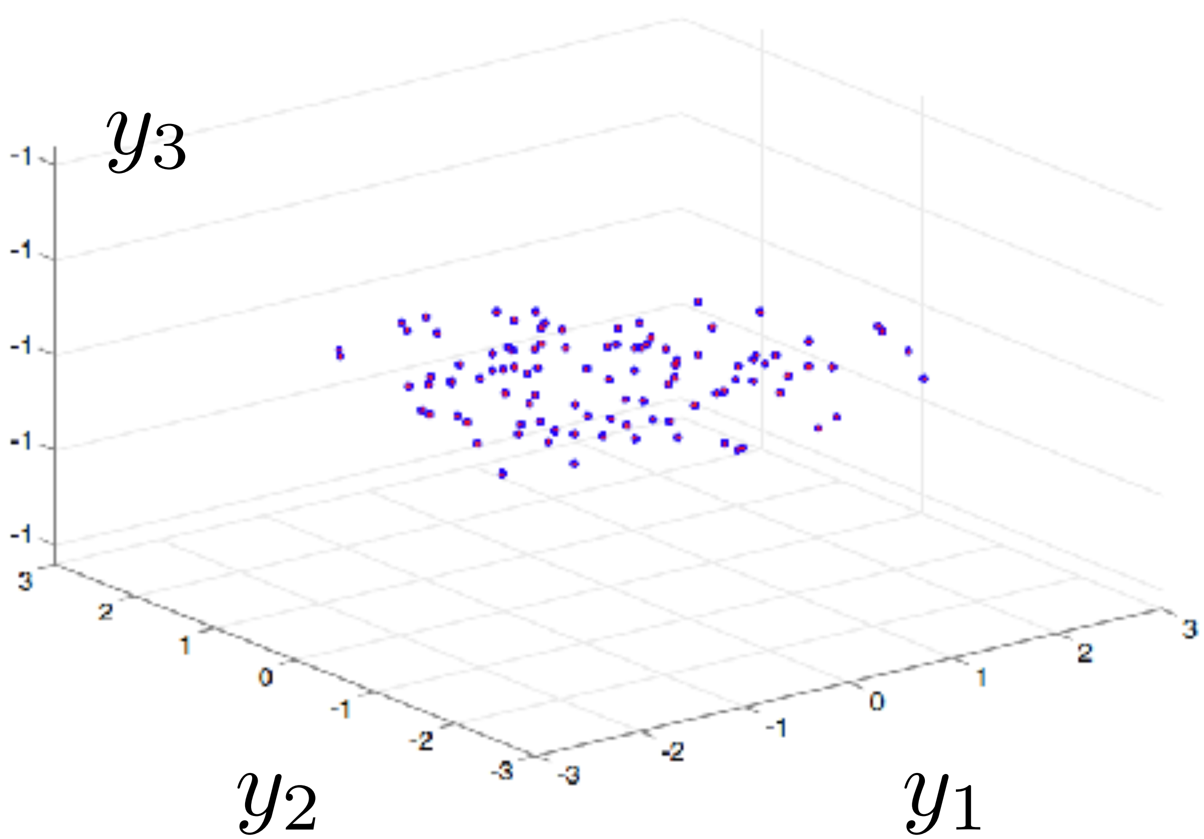
$$\mathcal{F}(W_{ij}) = \sum_i \left\{ \mathbf{x}^i - \sum_{j \in \mathcal{V}_i} W_{ij} \mathbf{x}^j \right\}^2$$

$$\mathbf{y}^i = \sum_{j \in \mathcal{V}_i} W_{ij} \mathbf{y}^j$$

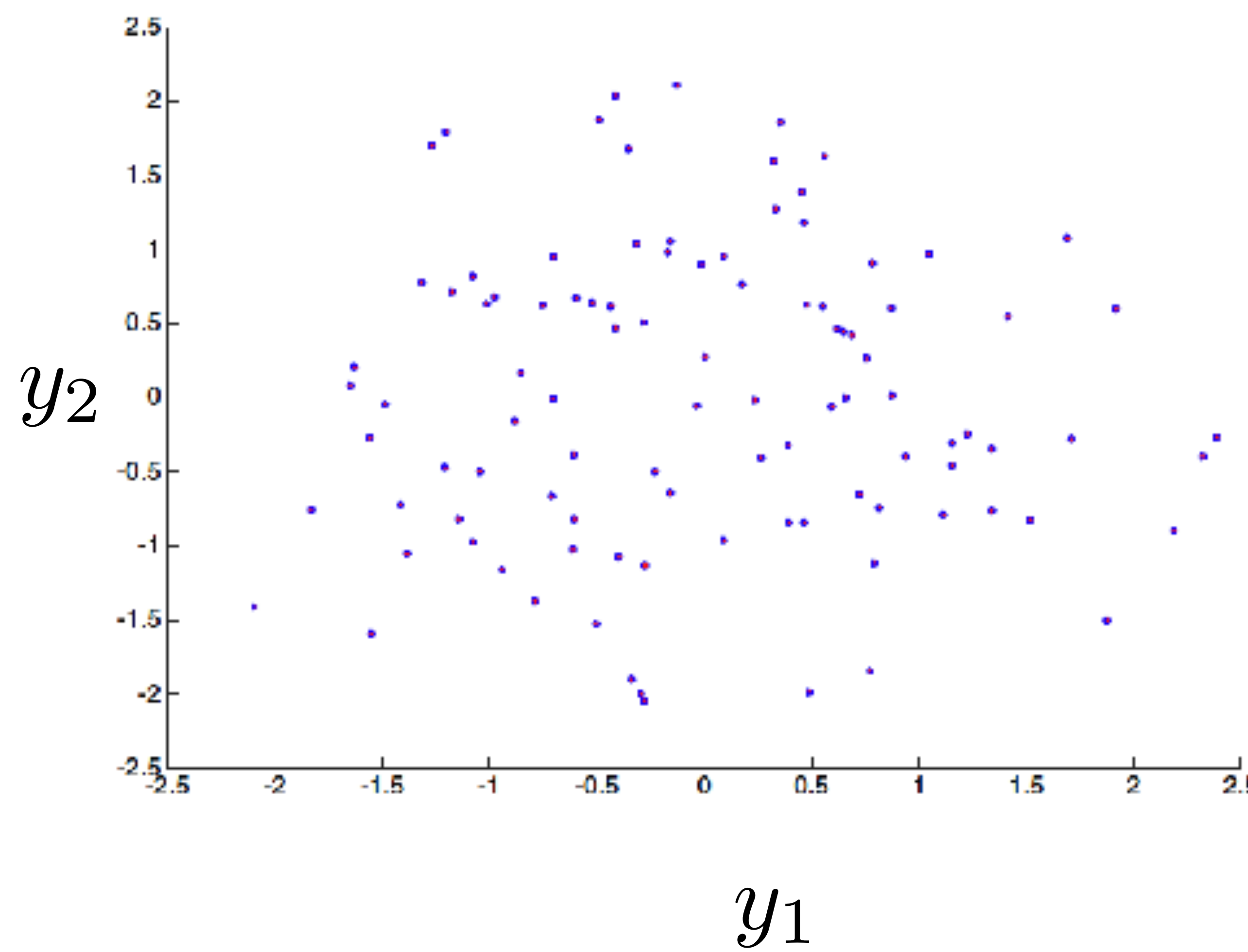
$$\mathcal{G}(\mathbf{y}^i) = \sum_i \left\{ \mathbf{y}^i - \sum_{j \in \mathcal{V}_i} W_{ij} \mathbf{y}^j \right\}^2$$





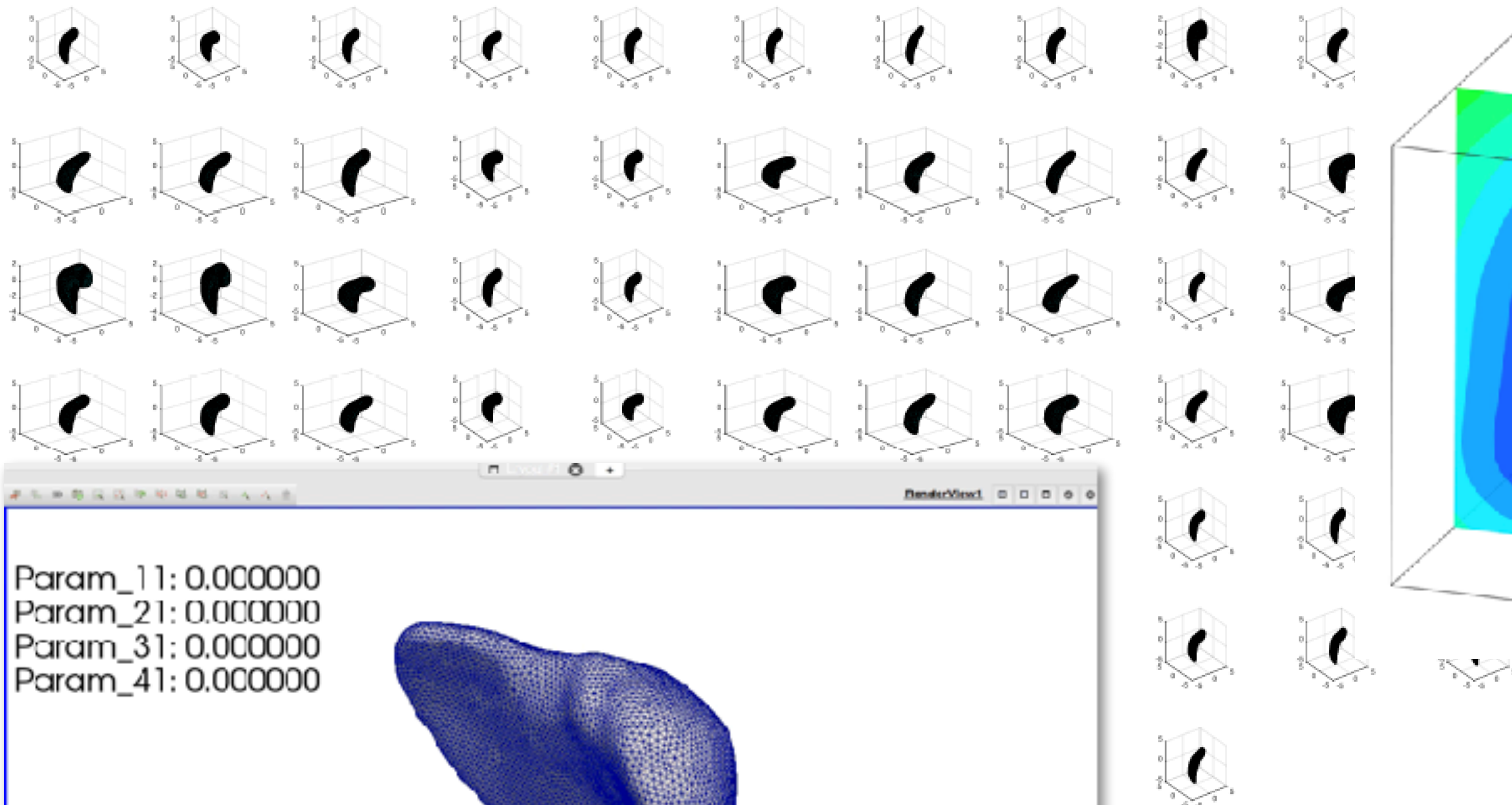


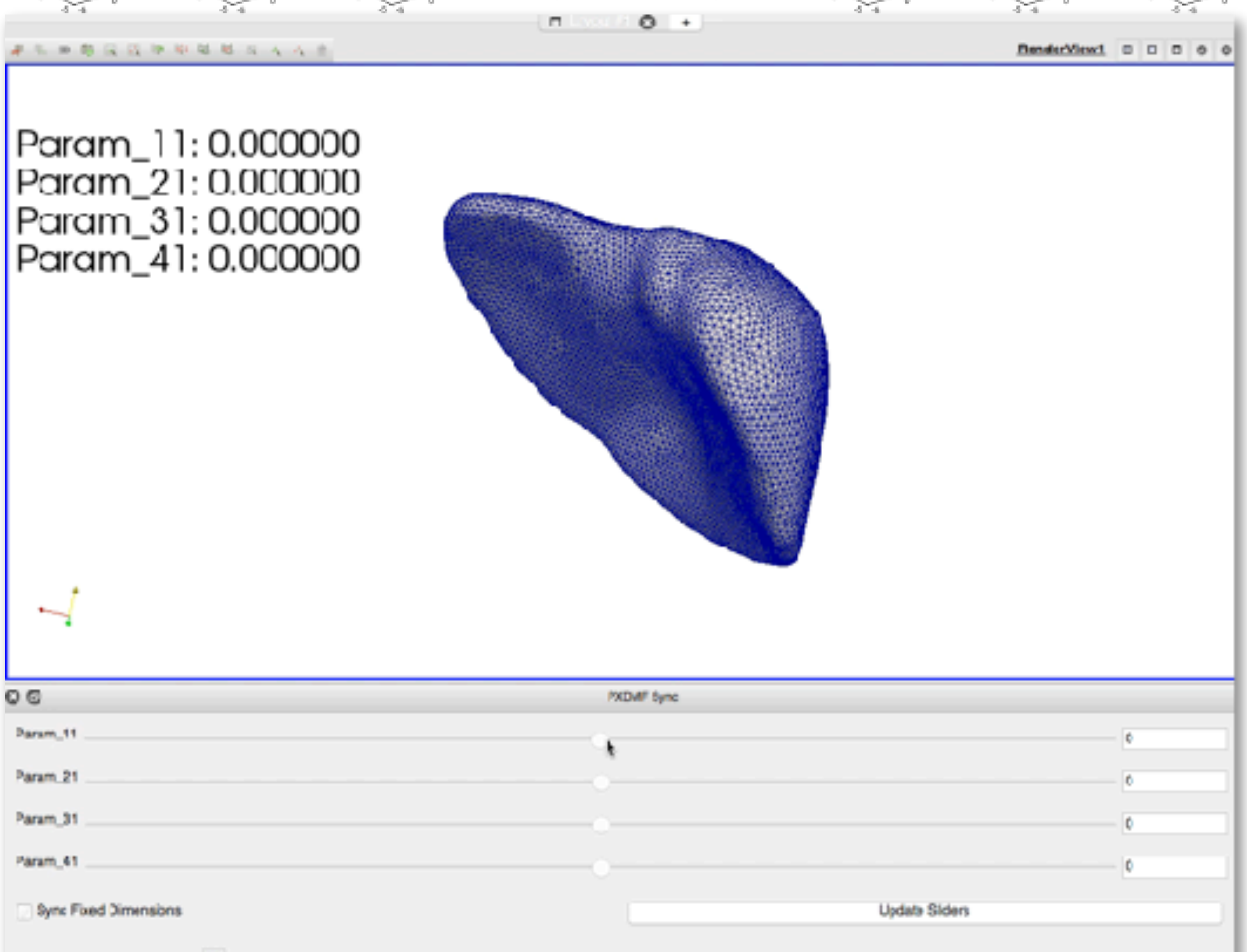
y_3
-1
-1
-1
-1
-1
3
2
1
0
-1
-2
-3
y_2
-3
-2
-1
0
1
2
3
y_1

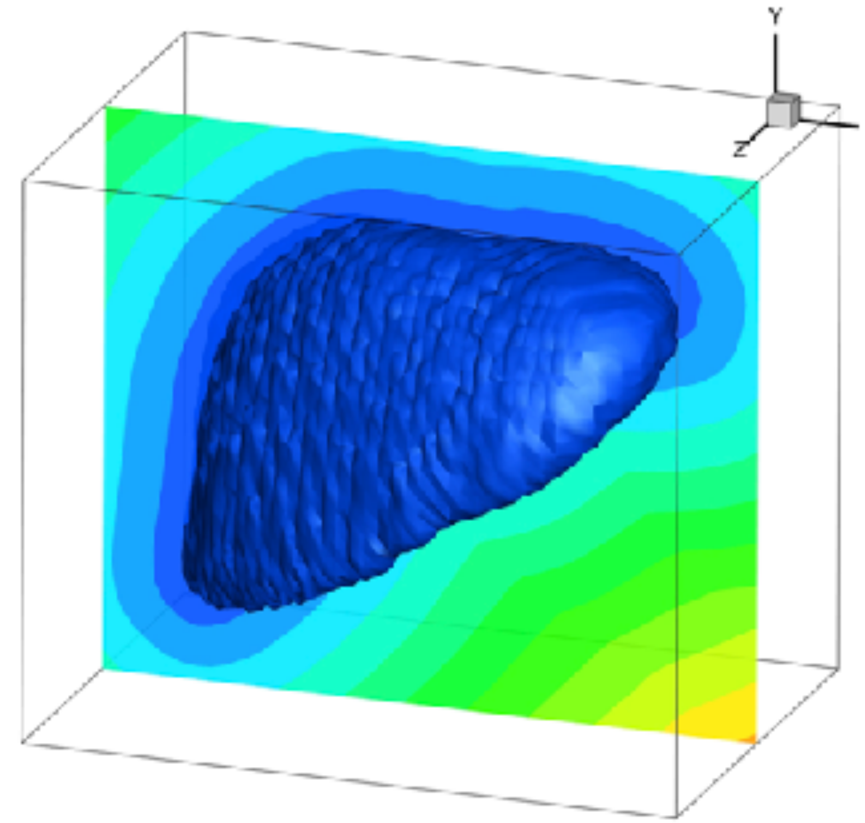


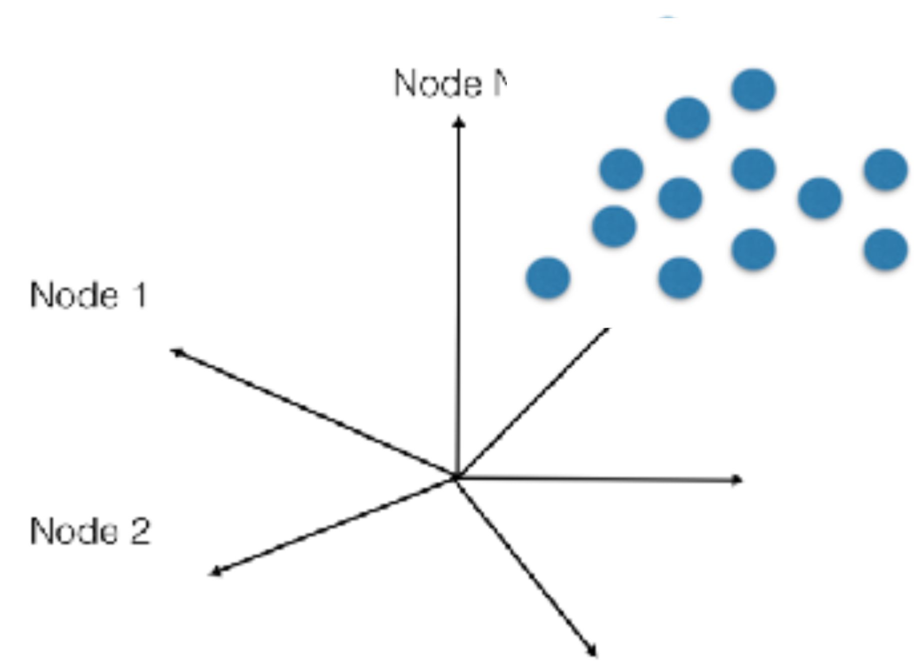
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-2.5
y_2
-2.5
-2
-1.5
-1
-0.5
0
0.5
1
1.5
2
2.5
y_1

Parametrizing Shapes

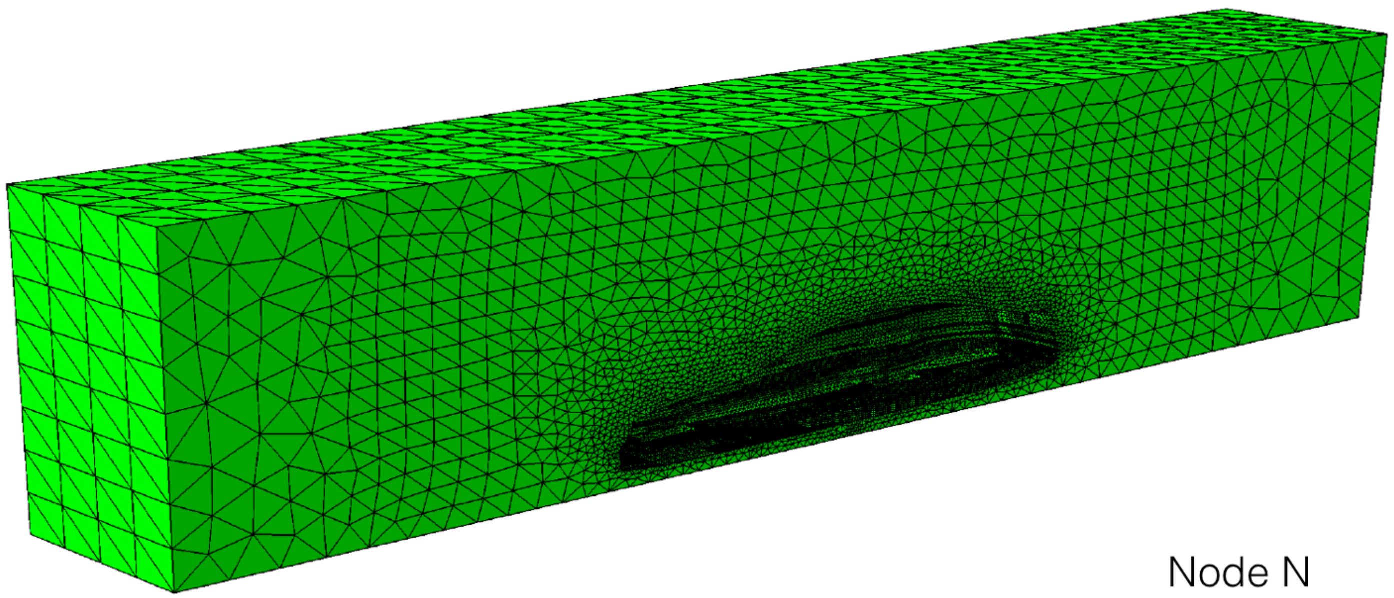






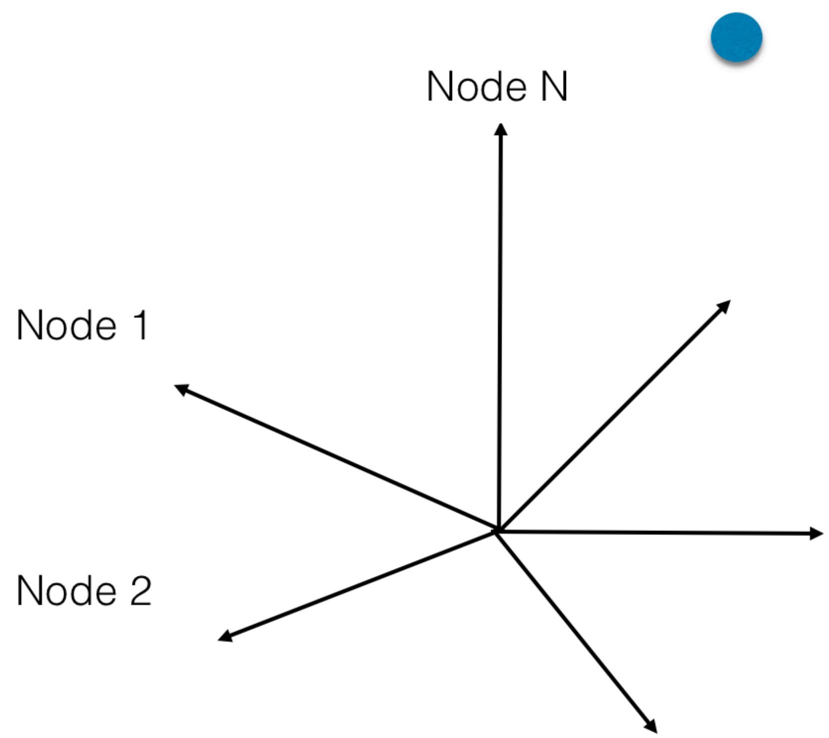


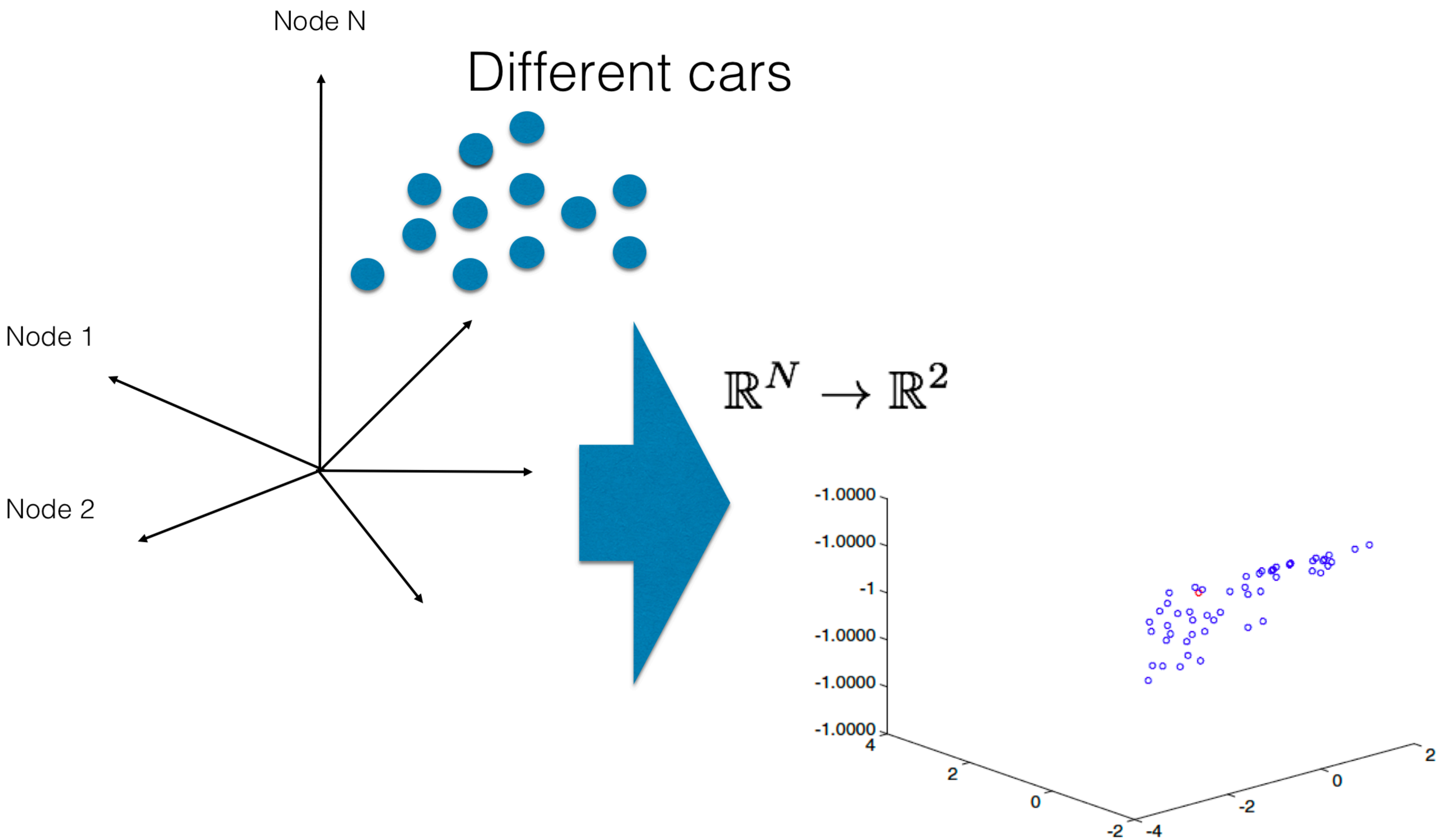
Parametrizing Shapes (Cont)

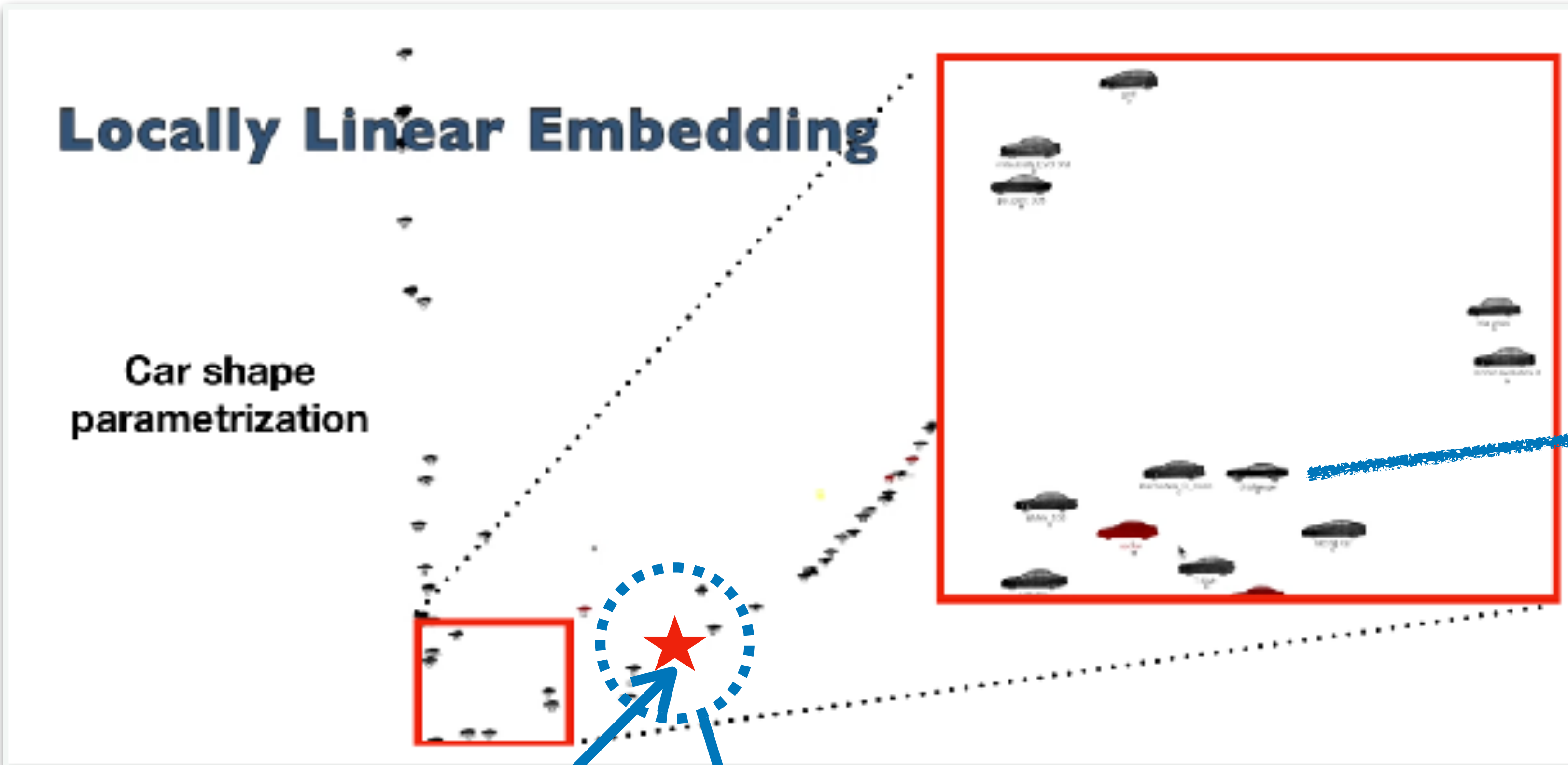


Level set: distance of each node to the car surface

Car 1 represented by its level-set function




Node N
Different cars
Node 1
Node 2
$\mathbb{R}^N \to \mathbb{R}^2$
-1.0000
-1.0000
-1
-1.0000
-1.0000
-1.0000
4
2
0
-2
-4
-2
0
2



New car NEVER SIMULATED

CFD solution interpolated on the manifold from its neighbors

Error in the prediction of lift and drag < 2%

Augmented Reality using High-Fidelity Models

Wind Tunnel

A. Badías, I. Alfaro, D. González, F. Chinesta and E. Cueto

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amb applied mechanics & bioengineering

Instituto Universitario de Investigación en Ingeniería de Aragón Universidad Zaragoza

Universidad Zaragoza 1542

METRICS OR METRICS? THAT IS THE QUESTION

Apparently three trees, apparently !

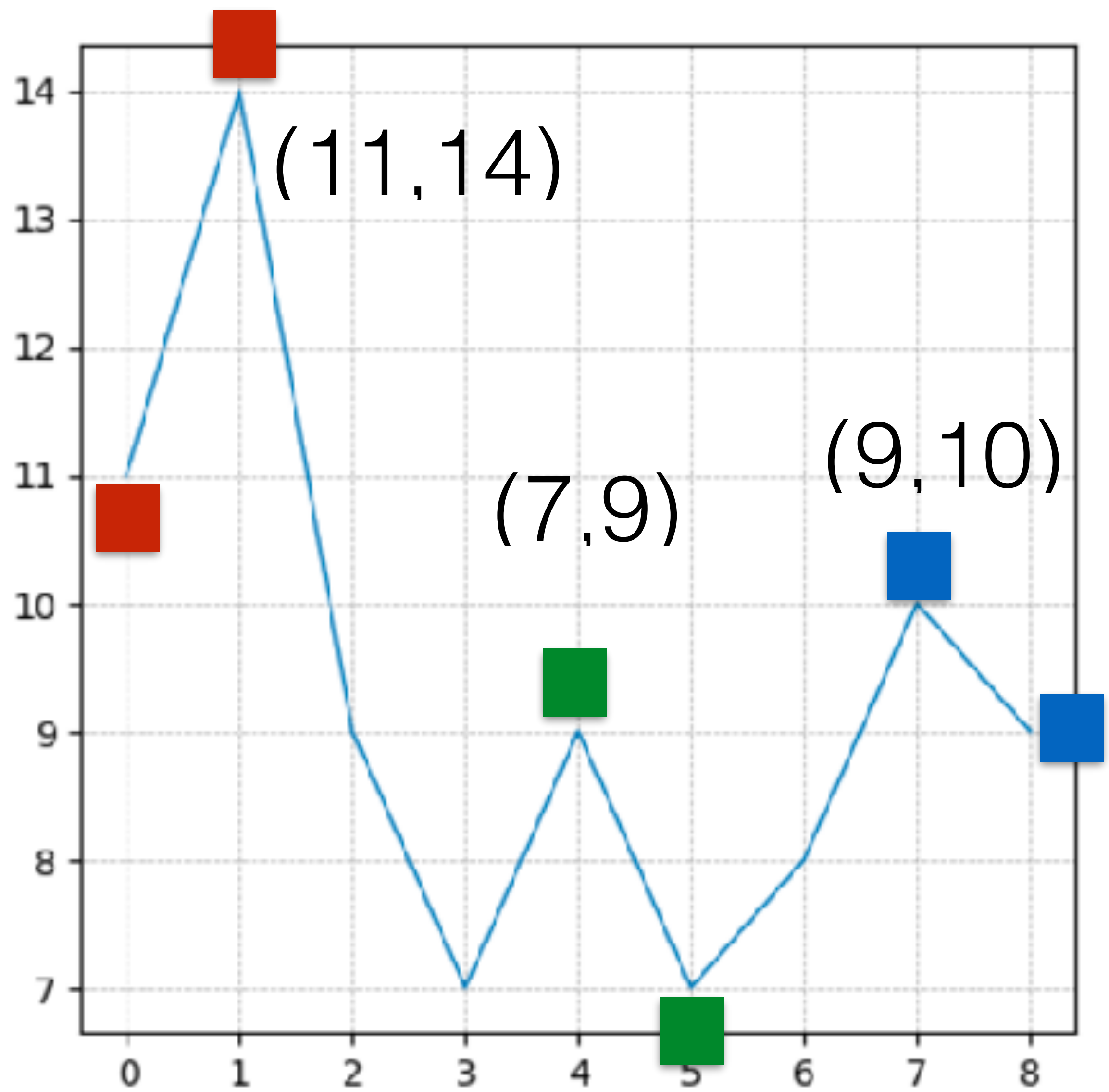
In what sense they are close?
What kind of resemblance?
How many parameters define them?
What is the adequate metric for comparing them?

the Euclidean operating on the pixelated images certainly not ! $||\mathbf{A_i} - \mathbf{A_j}||_\mathbf{2} > \epsilon$

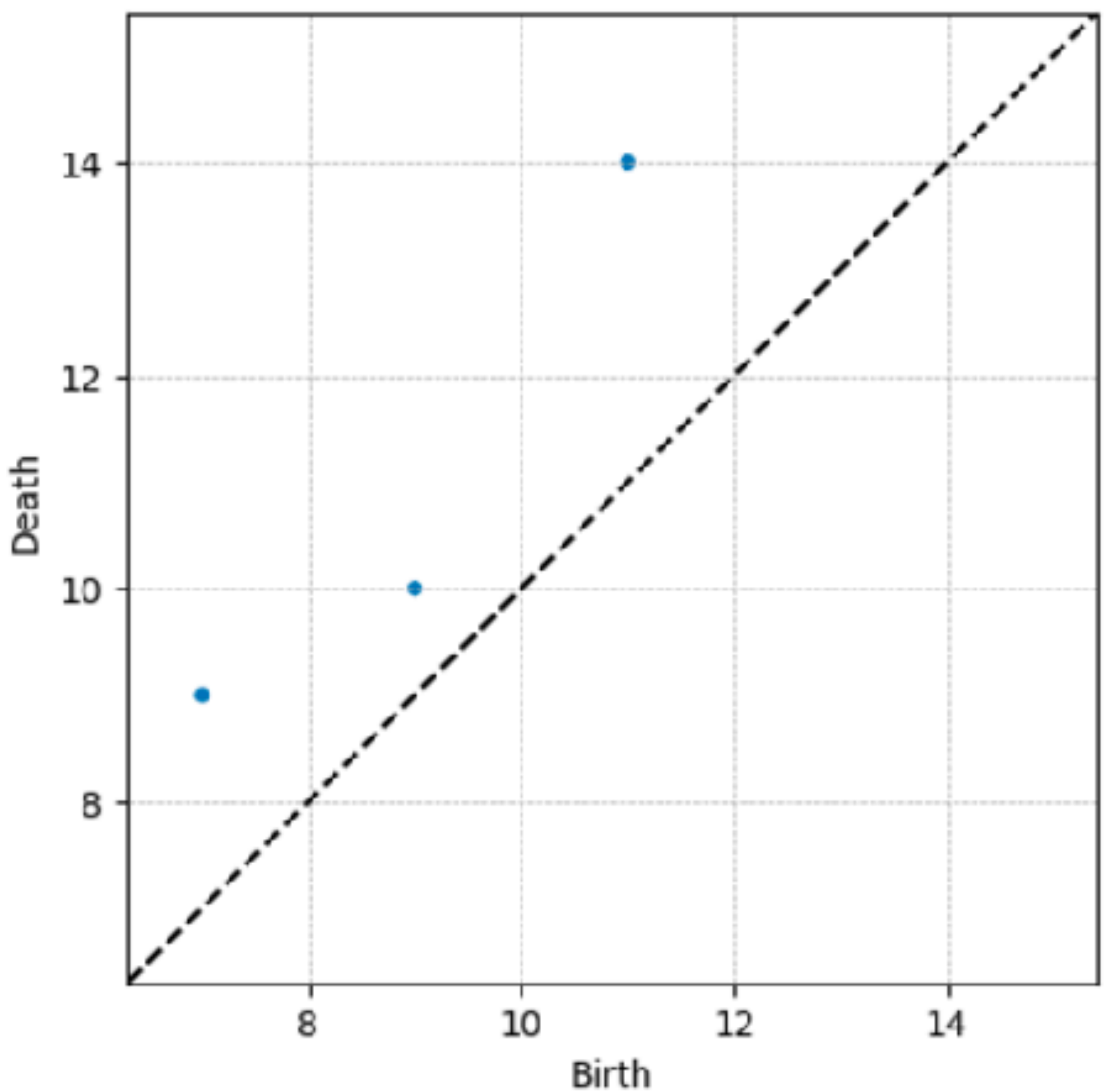
… and registration does not suffice

Topological Data Analysis: Time Series

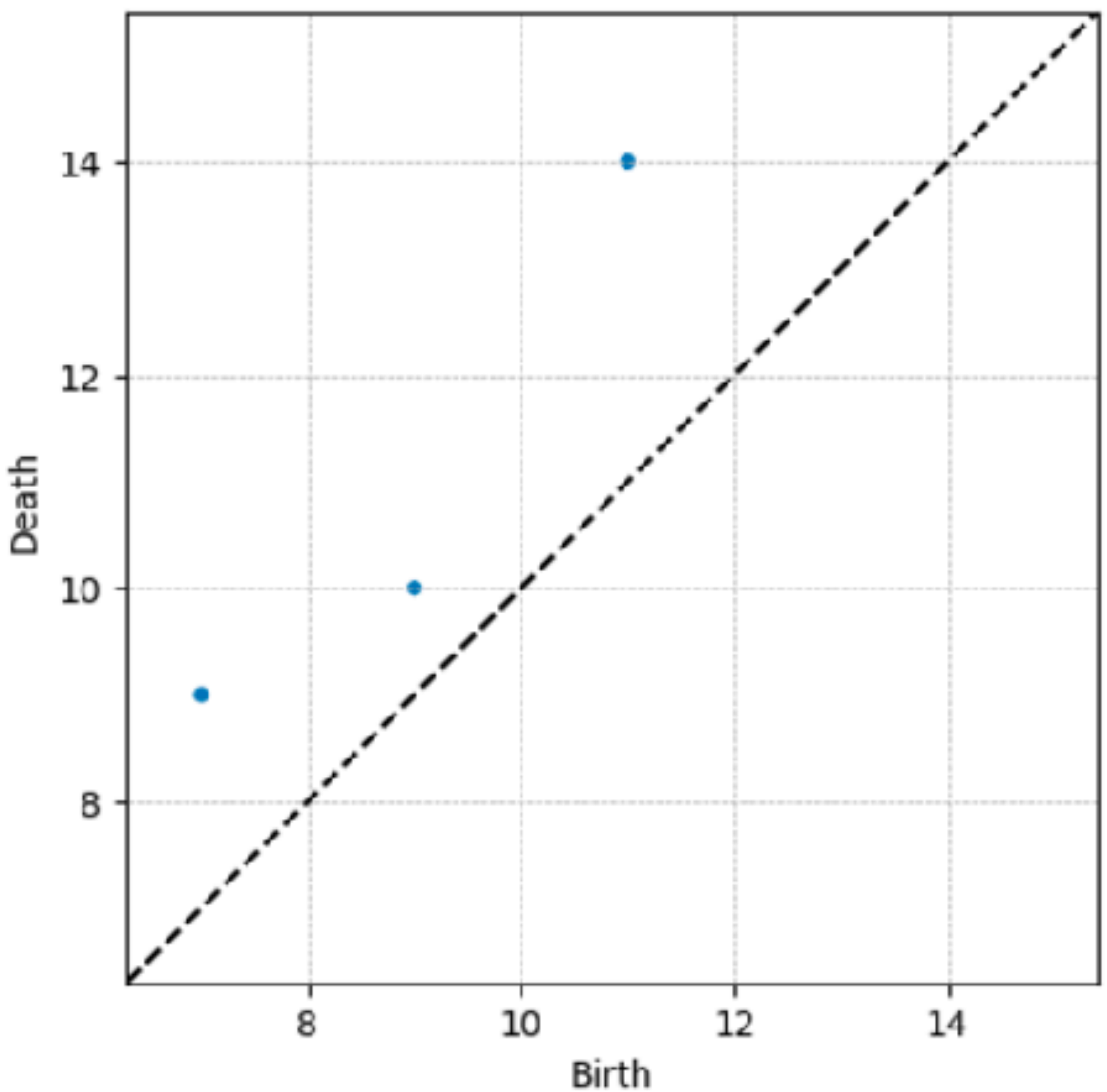
Pairing min-max



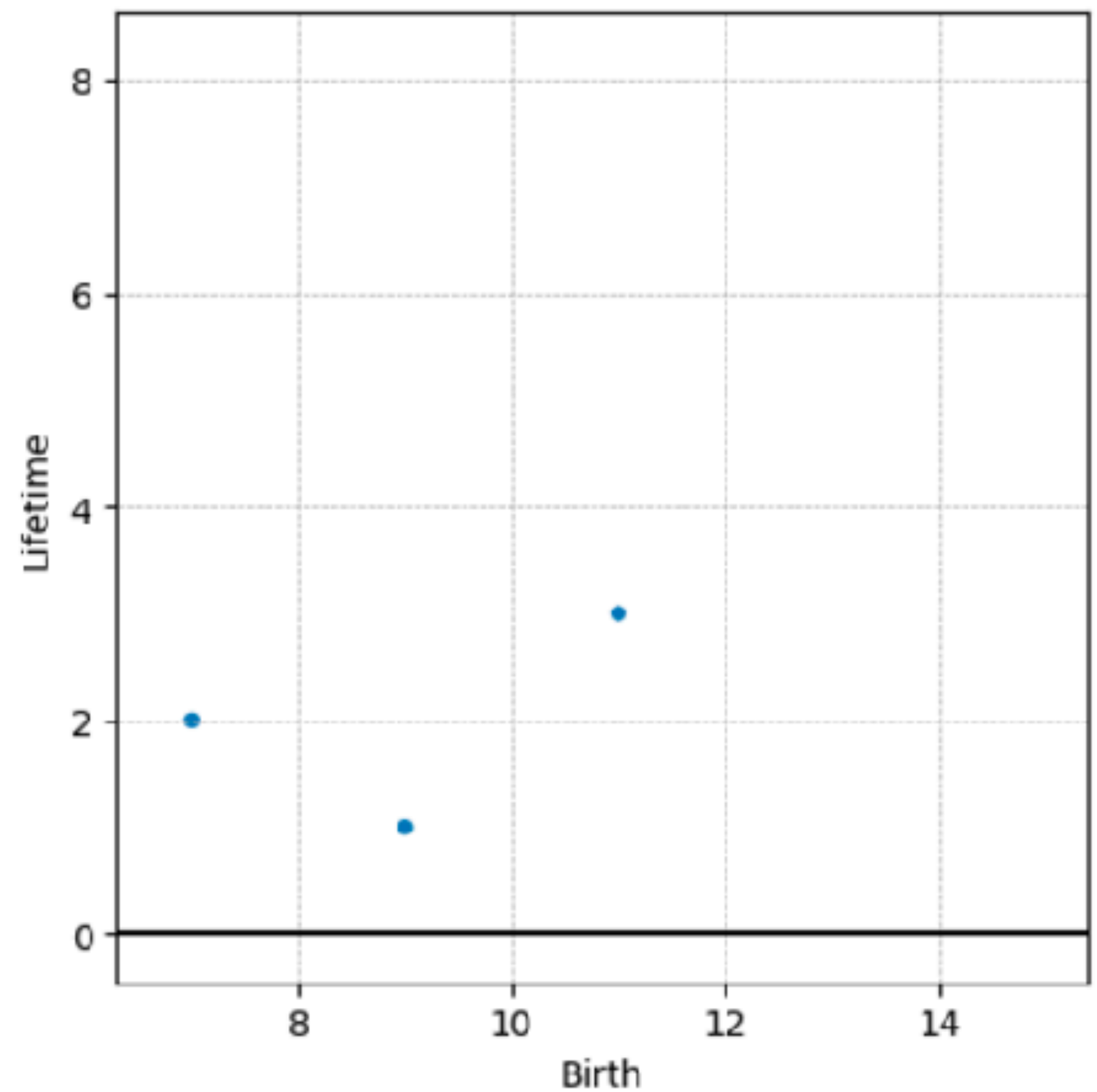
Persistence diagram



Persistence diagram

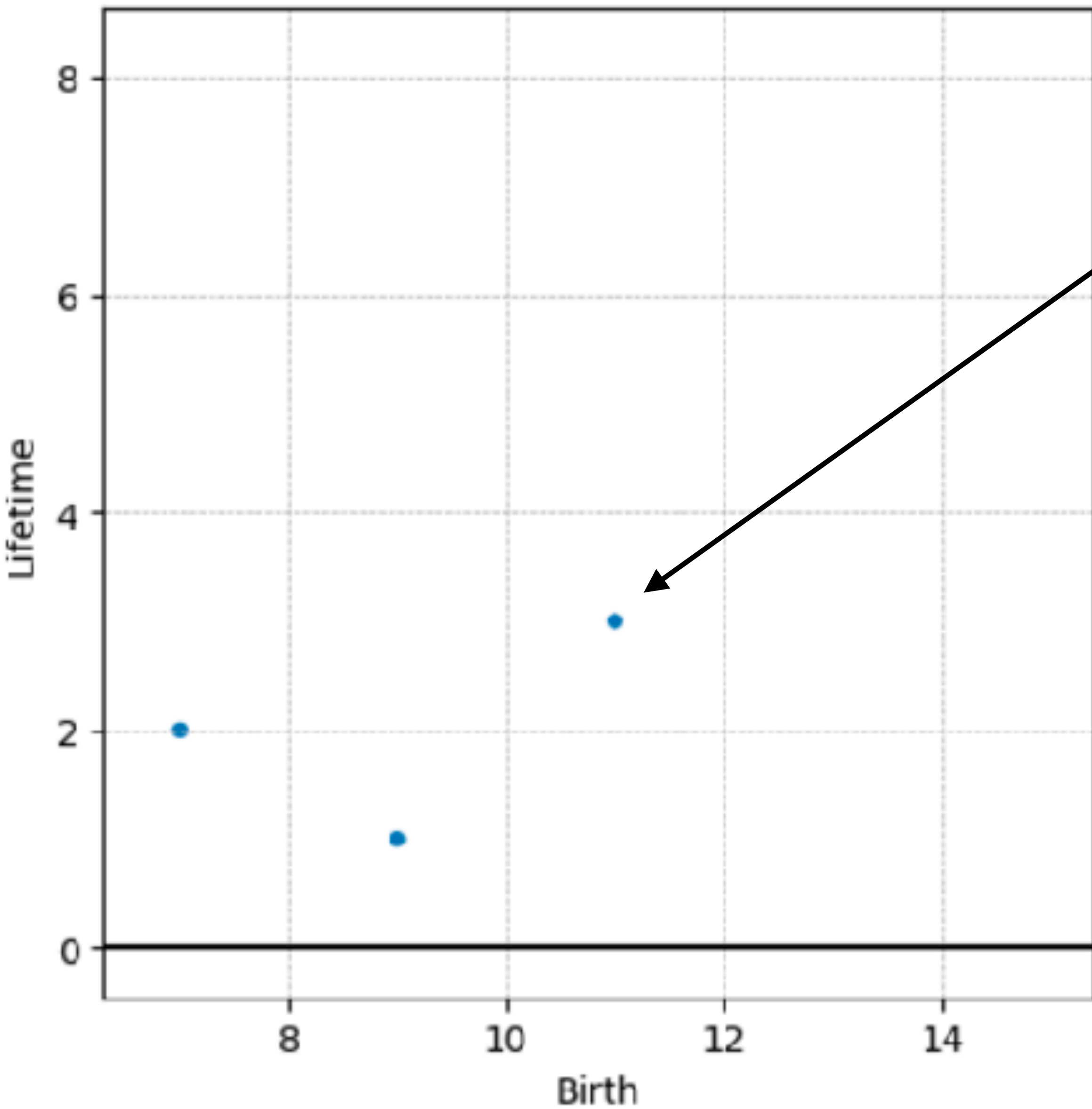


Lifetime diagram

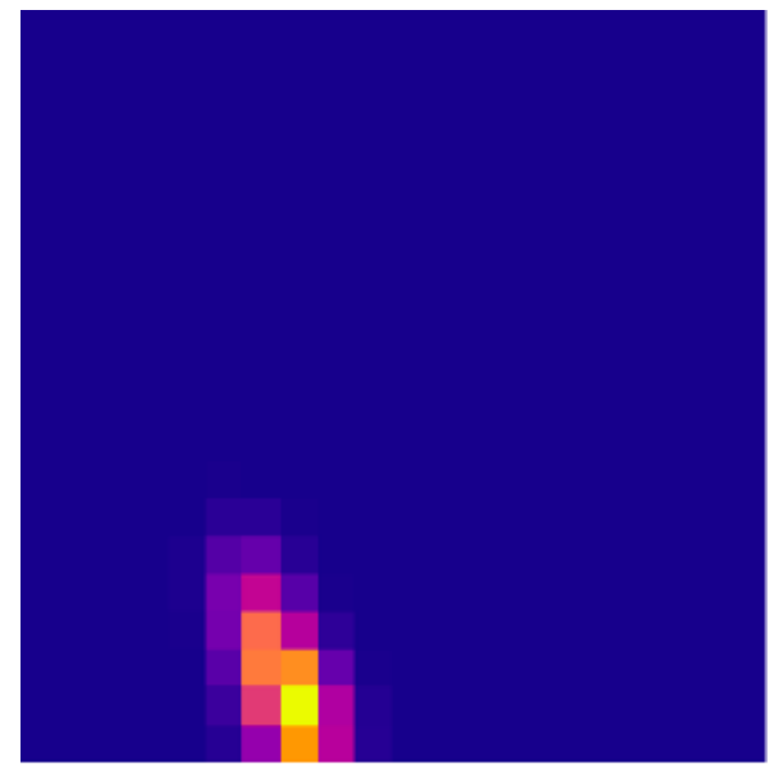


$$\rho_S(u,v) = \sum_{(x,y)\in\mathcal{T}(S)} w(x,y)\, g_{(x,y)}(u,v).$$

Lifetime diagram



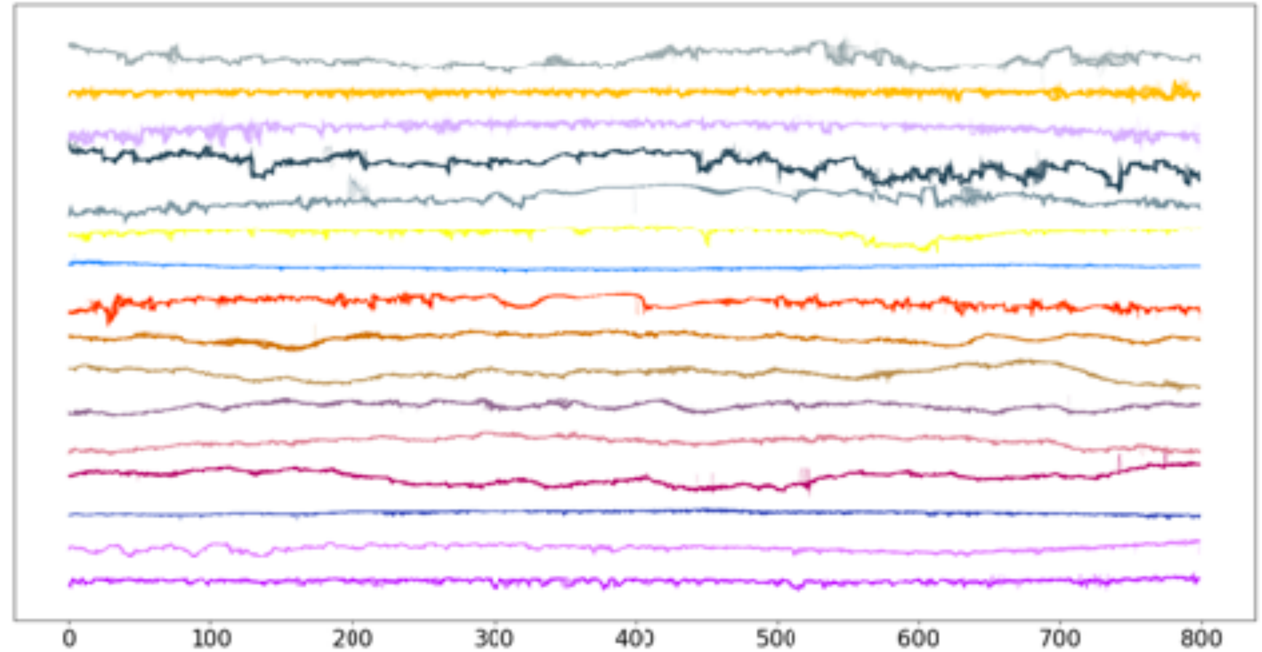
$$\mathcal{PI}_{P_i}(S) = \iint_{P_i} \rho_S(u,v)\, du\, dv.$$

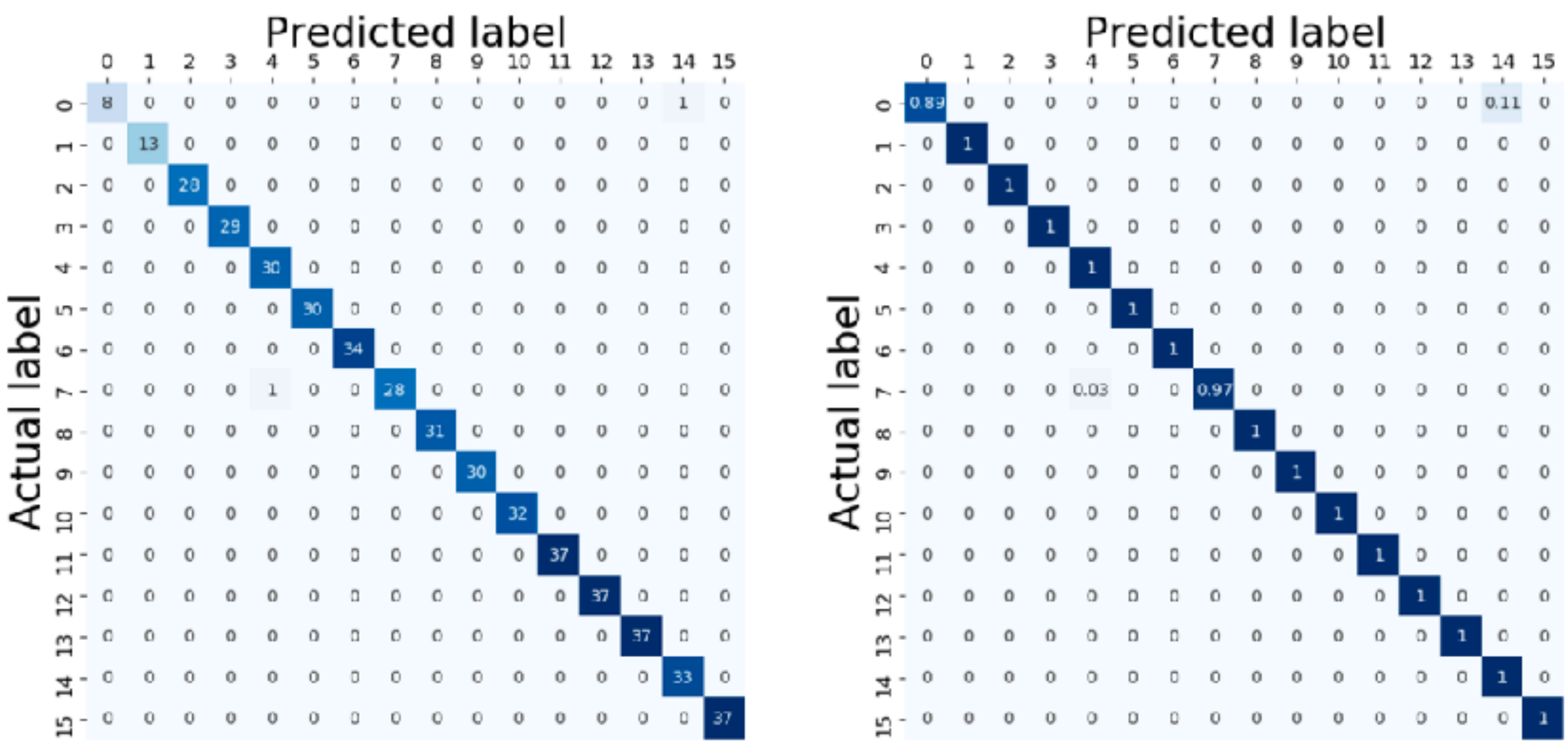


Persistence image

Rough surfaces clustering

16 families of composites

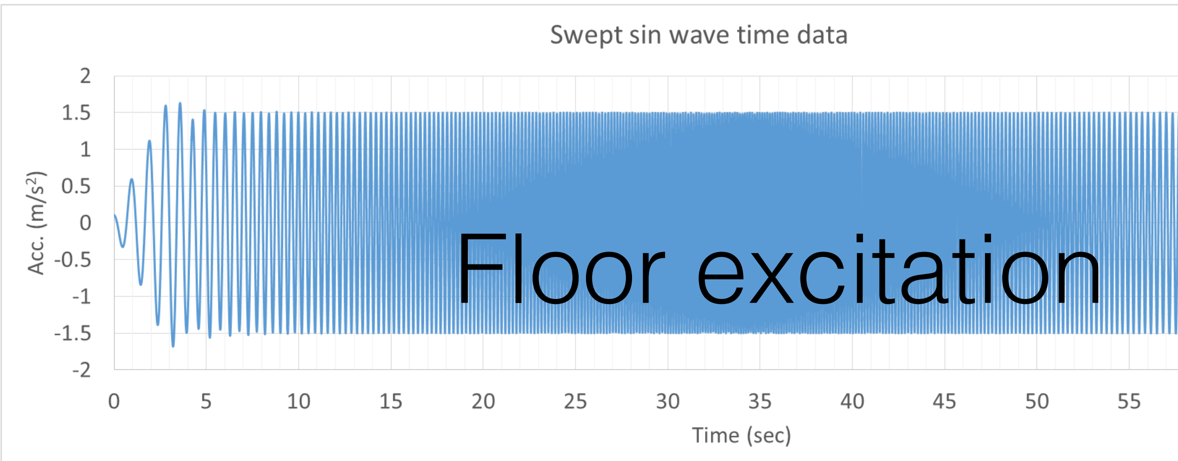


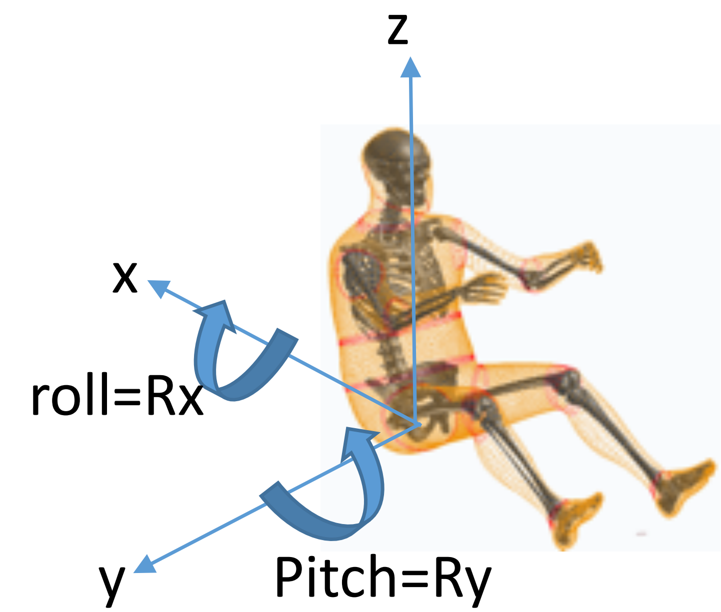


(a) Original

(b) Normalized

Human models





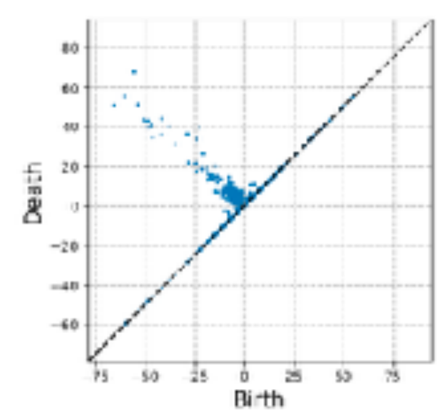
DIGITAL HUMAN LAB

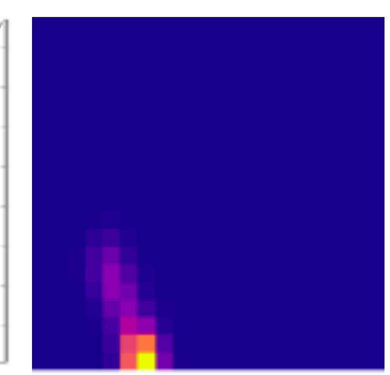
Tense, relax, …?

Data

TDA

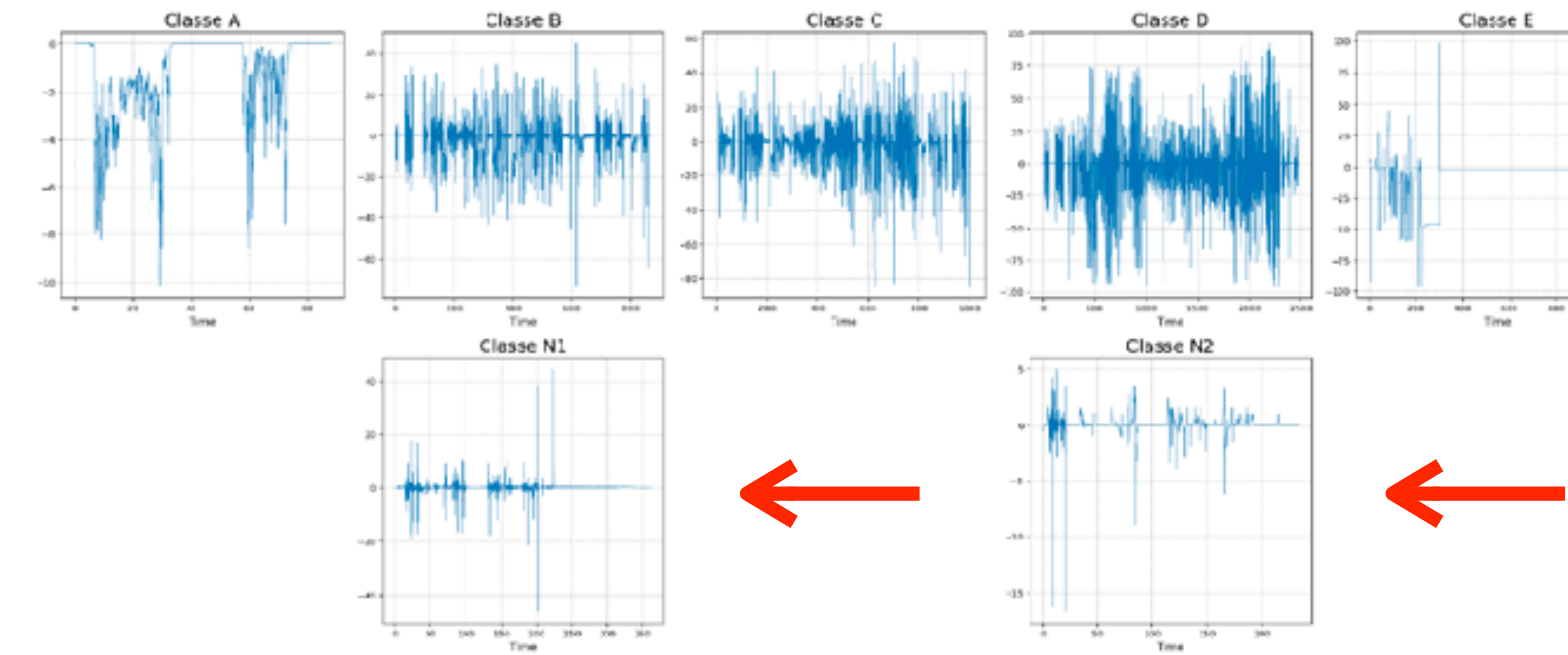
Barcode > Persistence diagram > persistence image > Behavioral classification



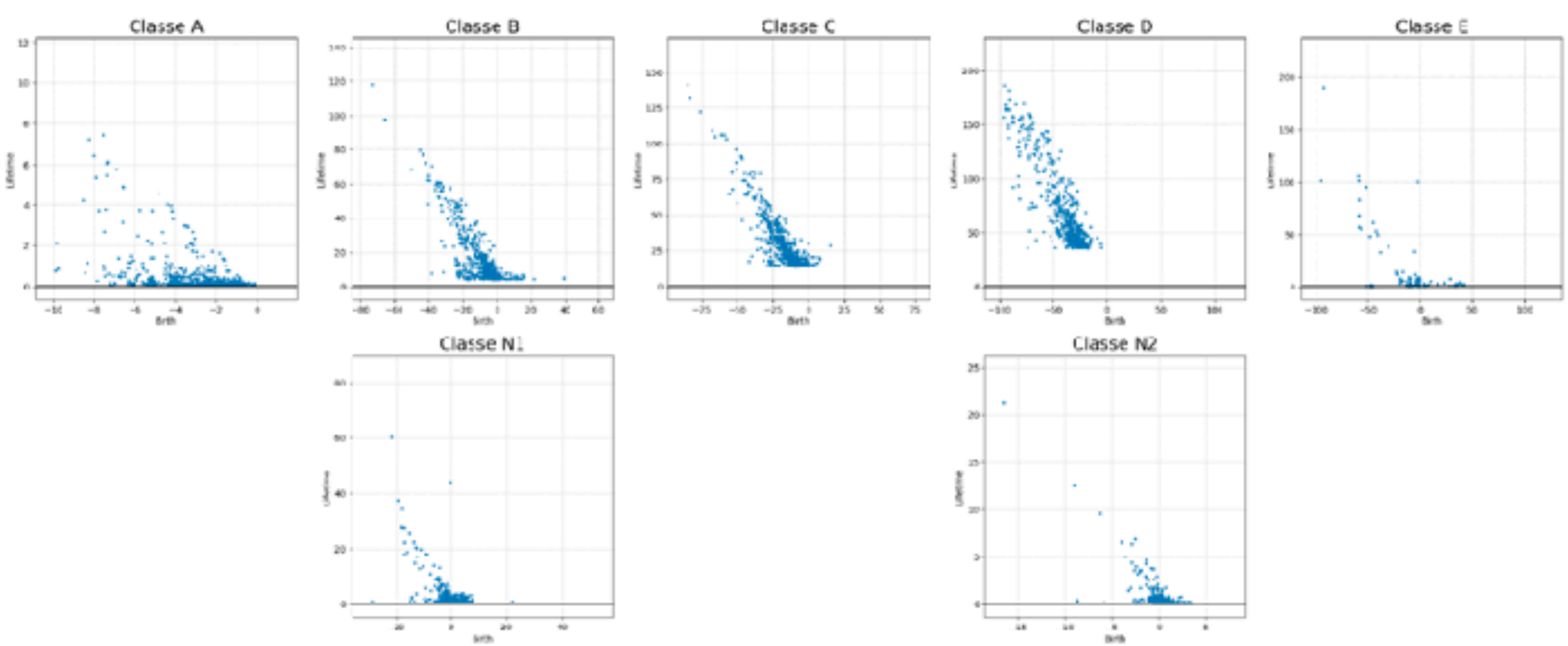


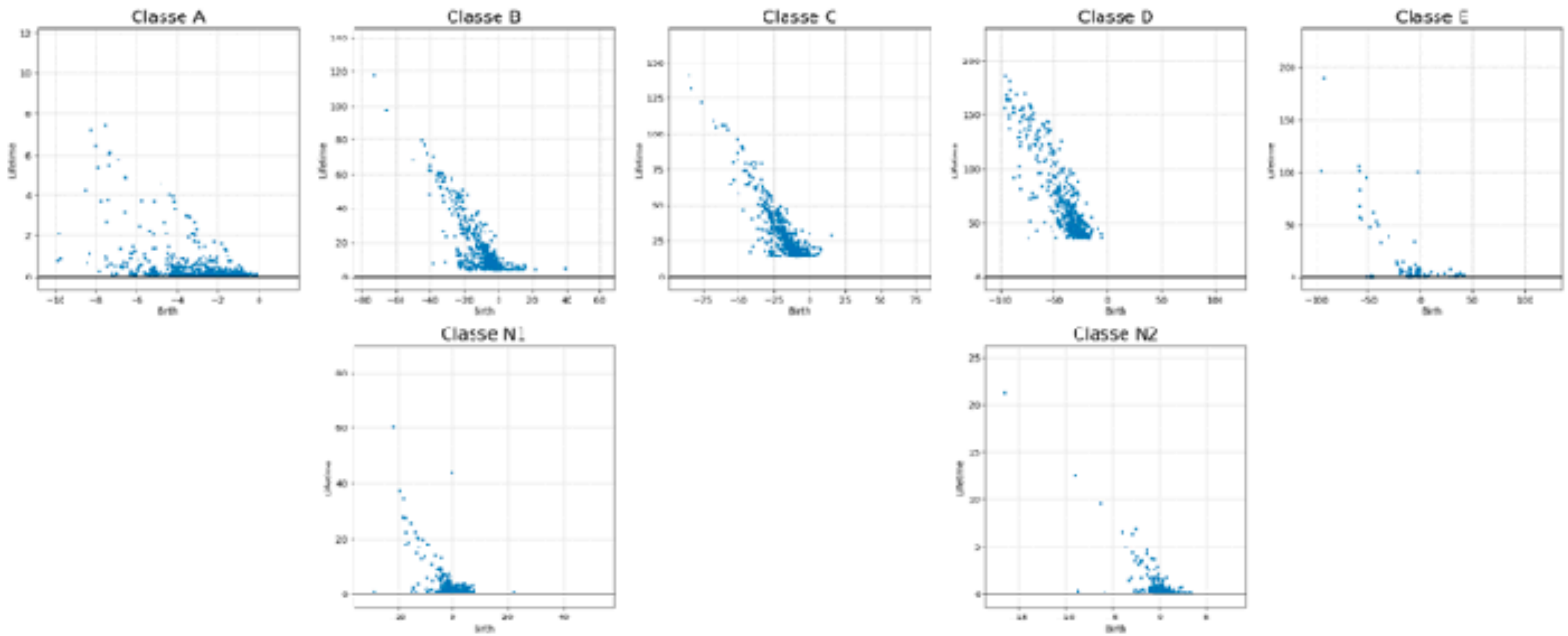
Obtained accuracy > 96%

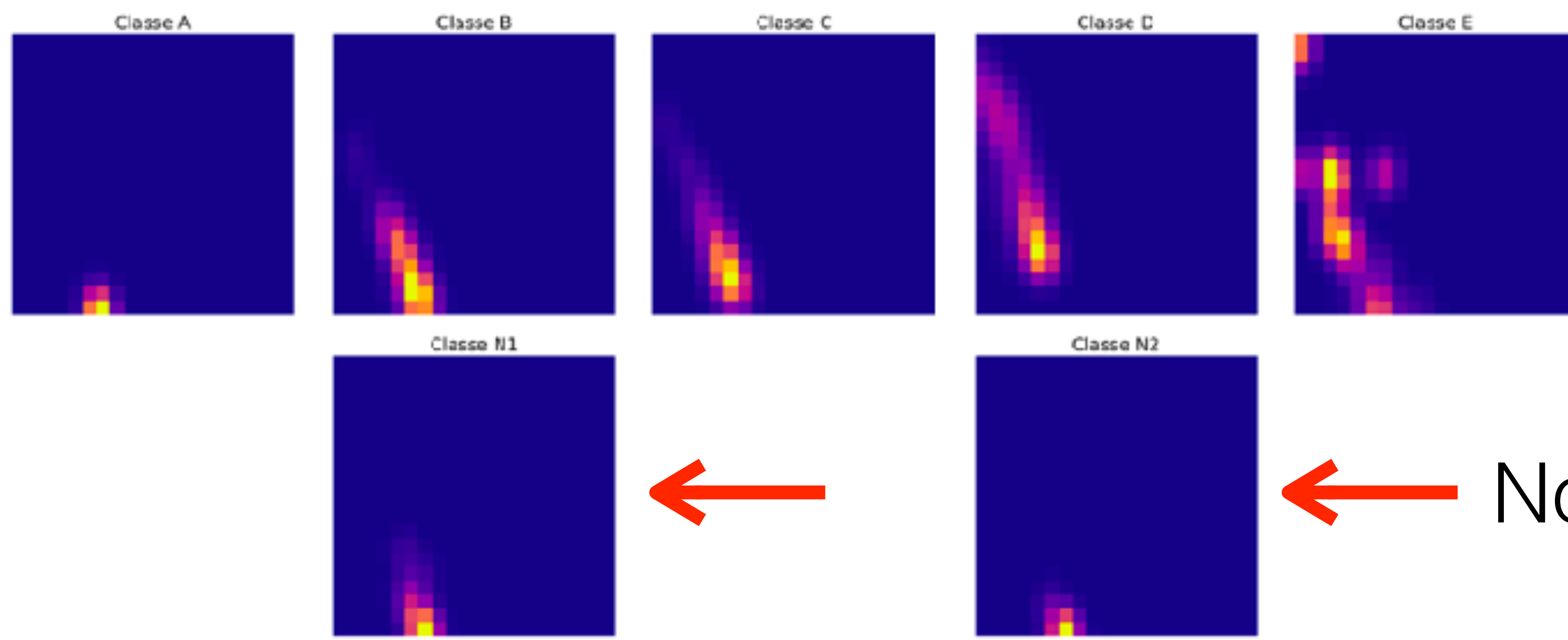
Fault identification



Nominal

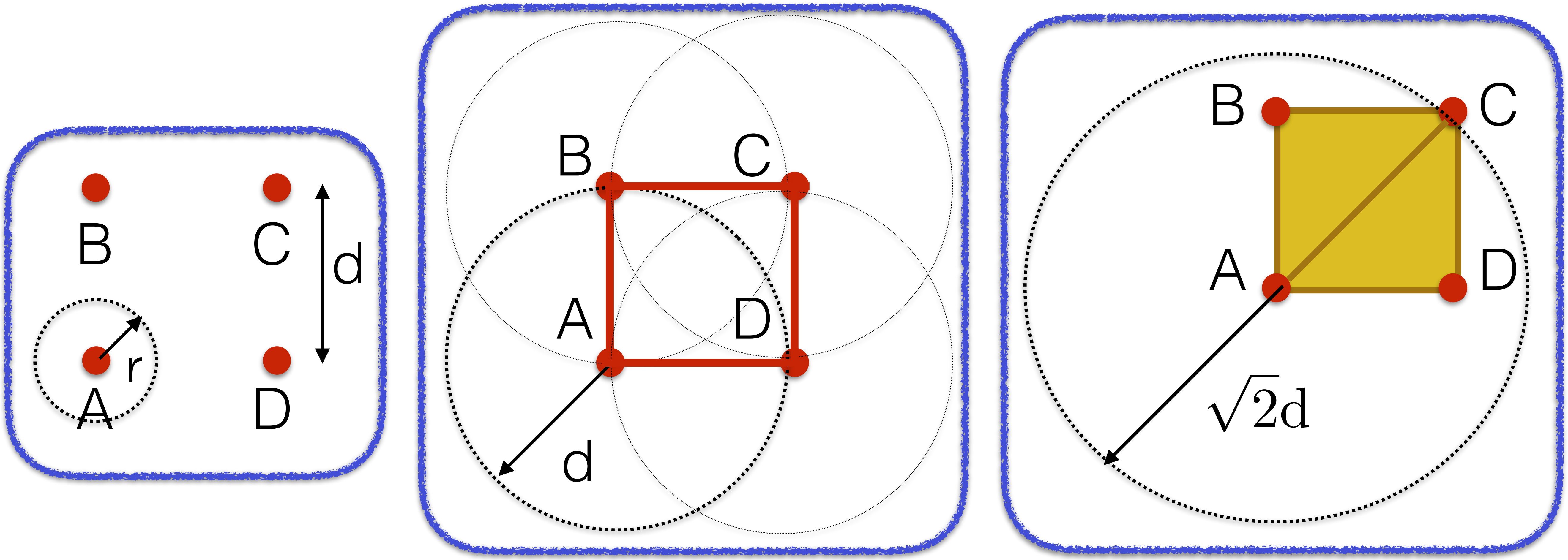



Classe A
Classe B
Classe C
Classe D
Classe E
Classe N1
Classe N2

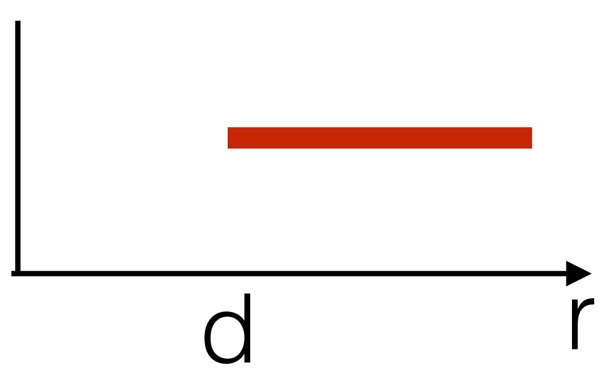

Classe A
Classe B
Classe C
Classe D
Classe E
Classe N1
Classe N2

Nominal

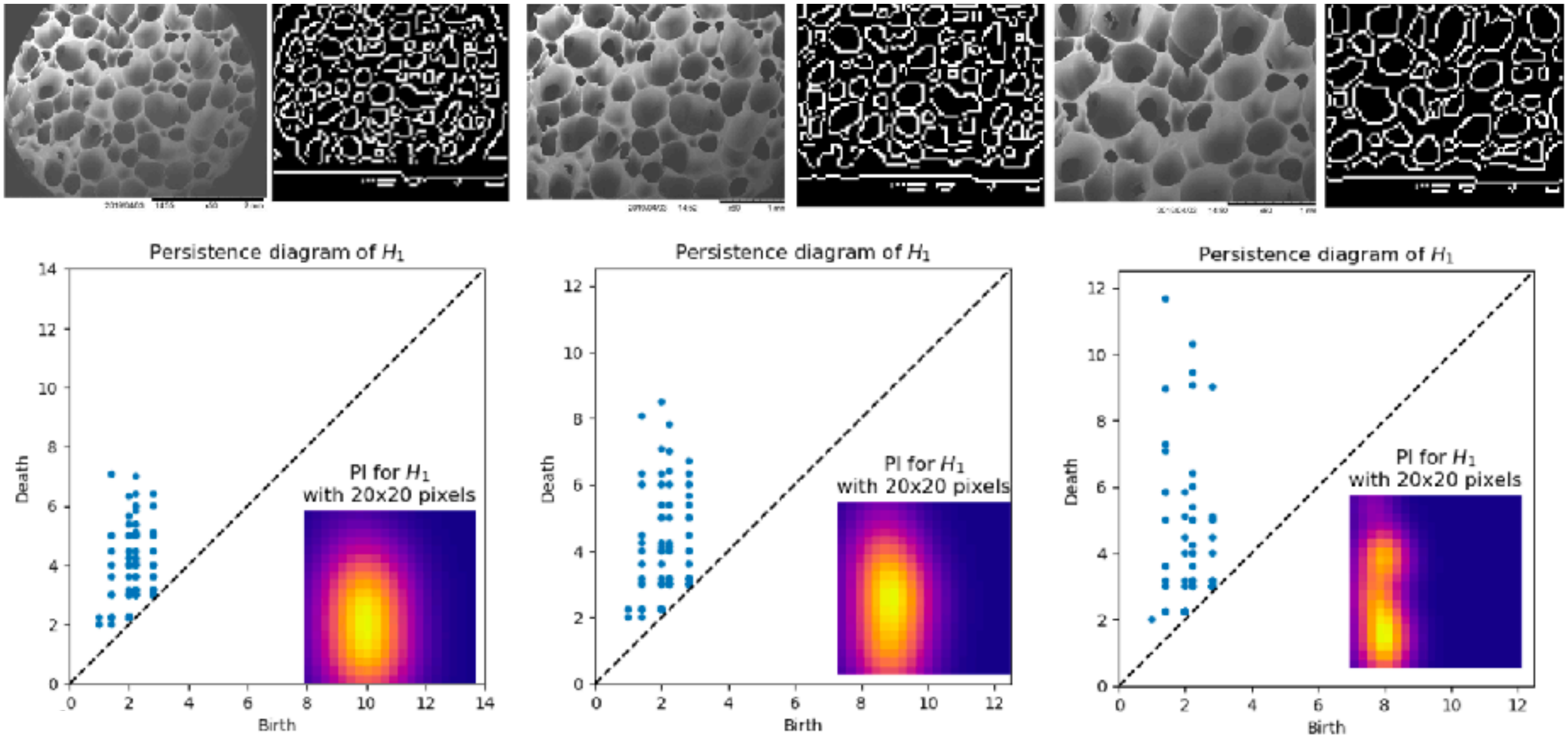
Topological Data Analysis: Images



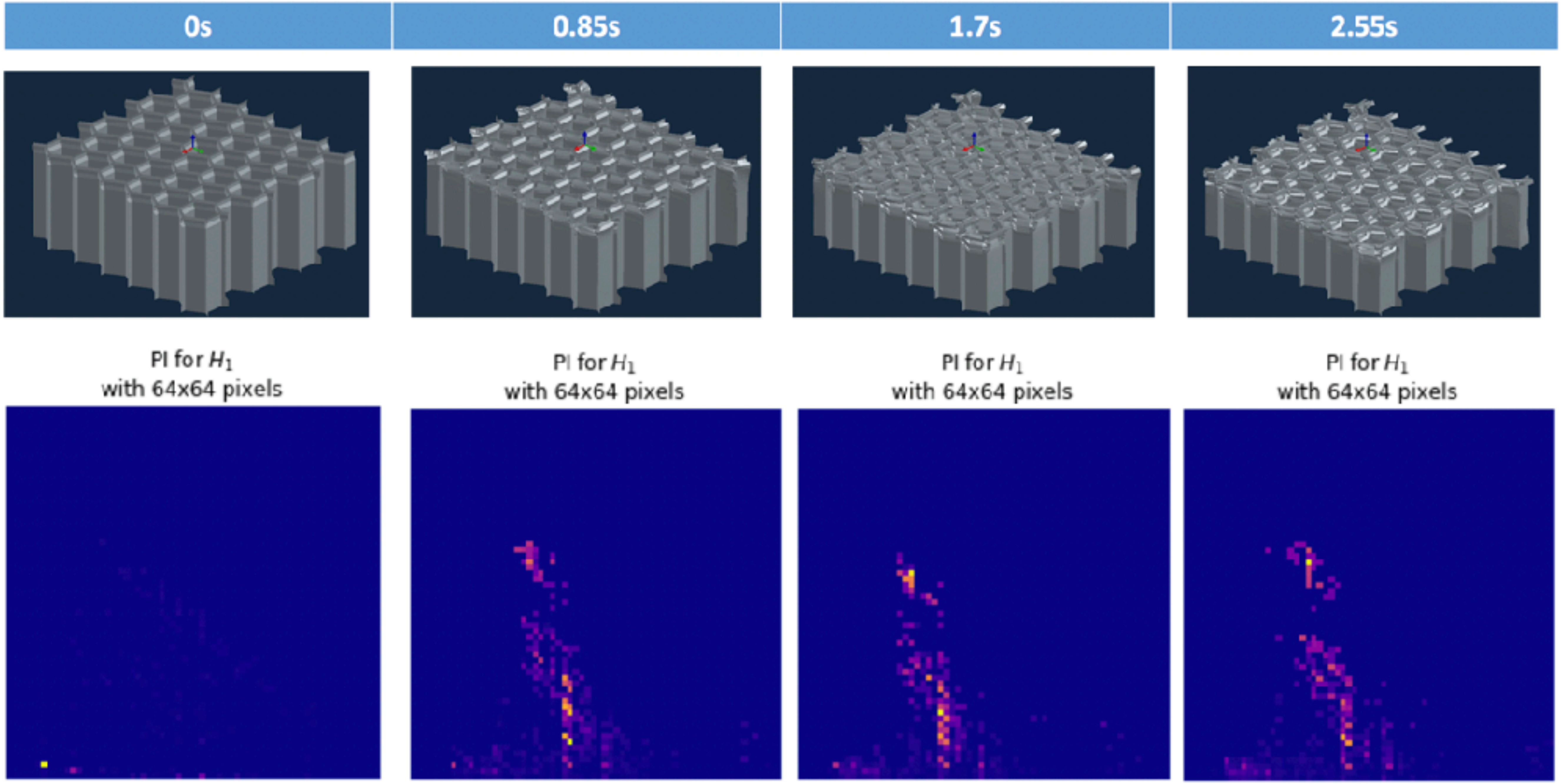
Barcode



Persistence diagram,
Lifetime diagram
&
Peristence images

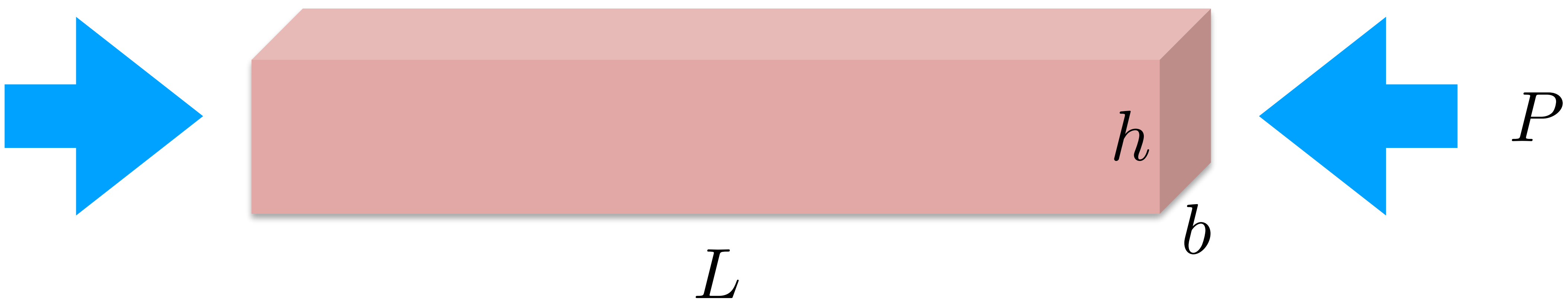


Persistence diagram of H_1
Death
Birth
PI for H_1
with 20x20 pixels
Persistence diagram of H_1
Death
Birth
PI for H_1
with 20x20 pixels
Persistence diagram of H_1
Death
Birth
PI for H_1
with 20x20 pixels


0s
0.85s
1.7s
2.55s
PI for H_1 with 64x64 pixels
PI for H_1 with 64x64 pixels
PI for H_1 with 64x64 pixels
PI for H_1 with 64x64 pixels

Extracting Knowledge

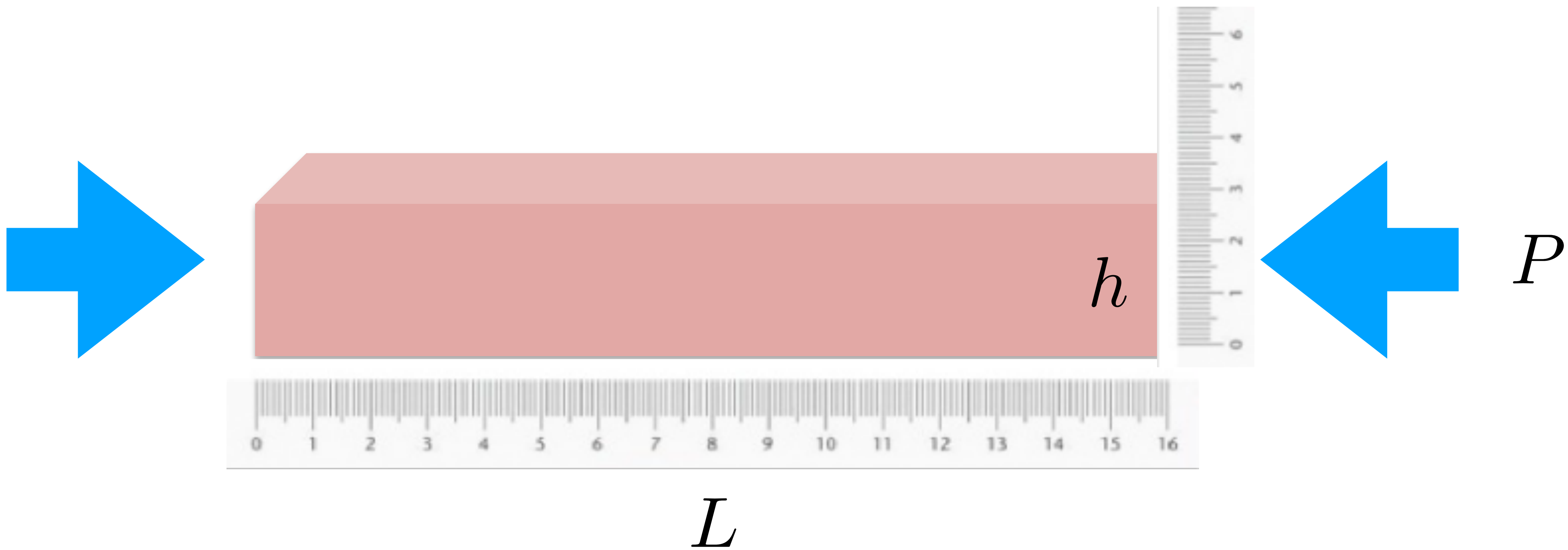
Euler buckling



Euler critical load $P \propto \frac{bh^3}{L^2}$

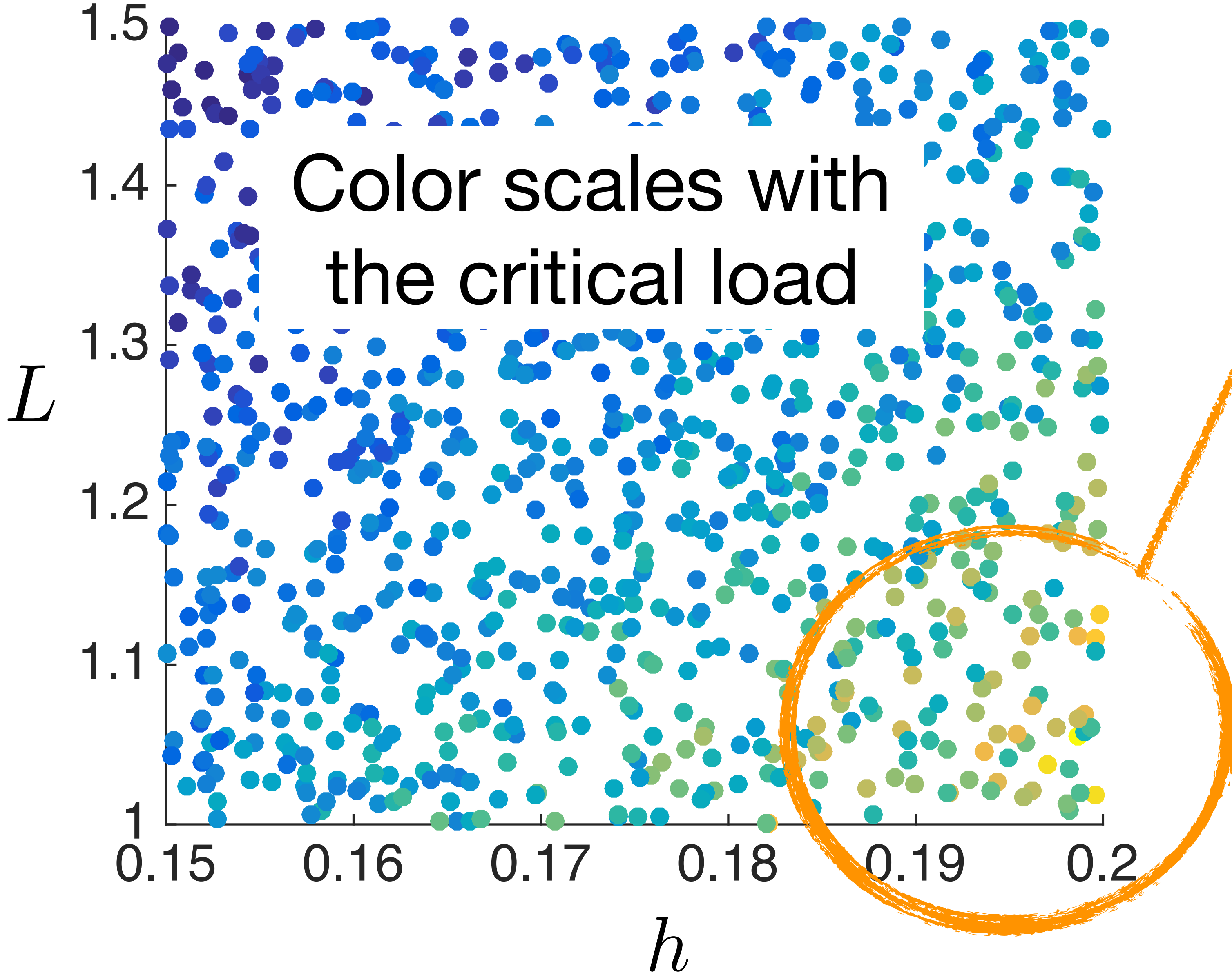
Identifying hidden variables

b, h & L are randomly changed for generating data
but imagine
we have only access to h and L (or only both are measurable)



There are may critical loads for the same h and L: all those corresponding to different values of the width « b »

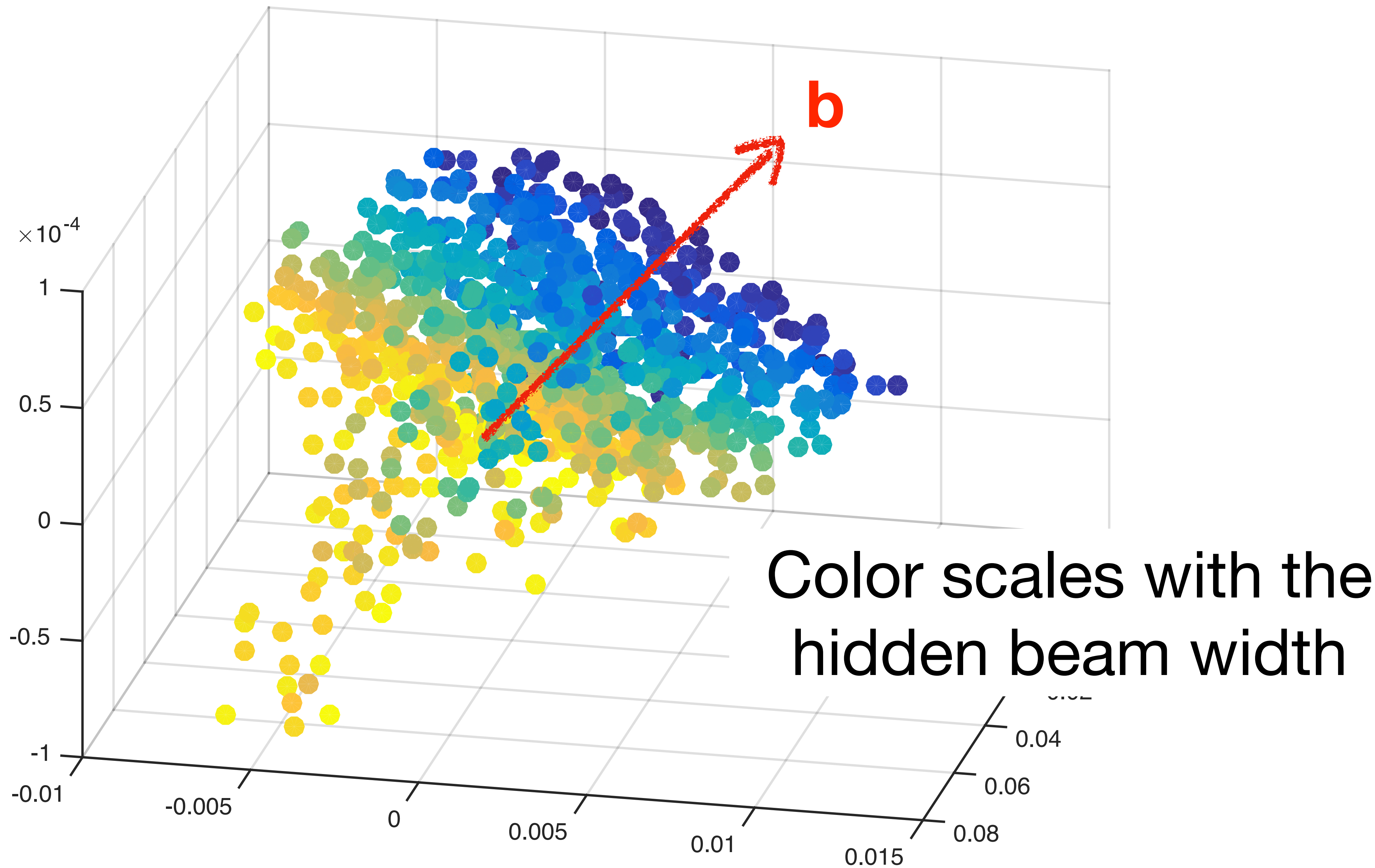
Consequence: Apparent fluctuations



Fluctuations are usually interpreted as noise

Noise or it reveals hidden internal variables operating within a deterministic physics ?

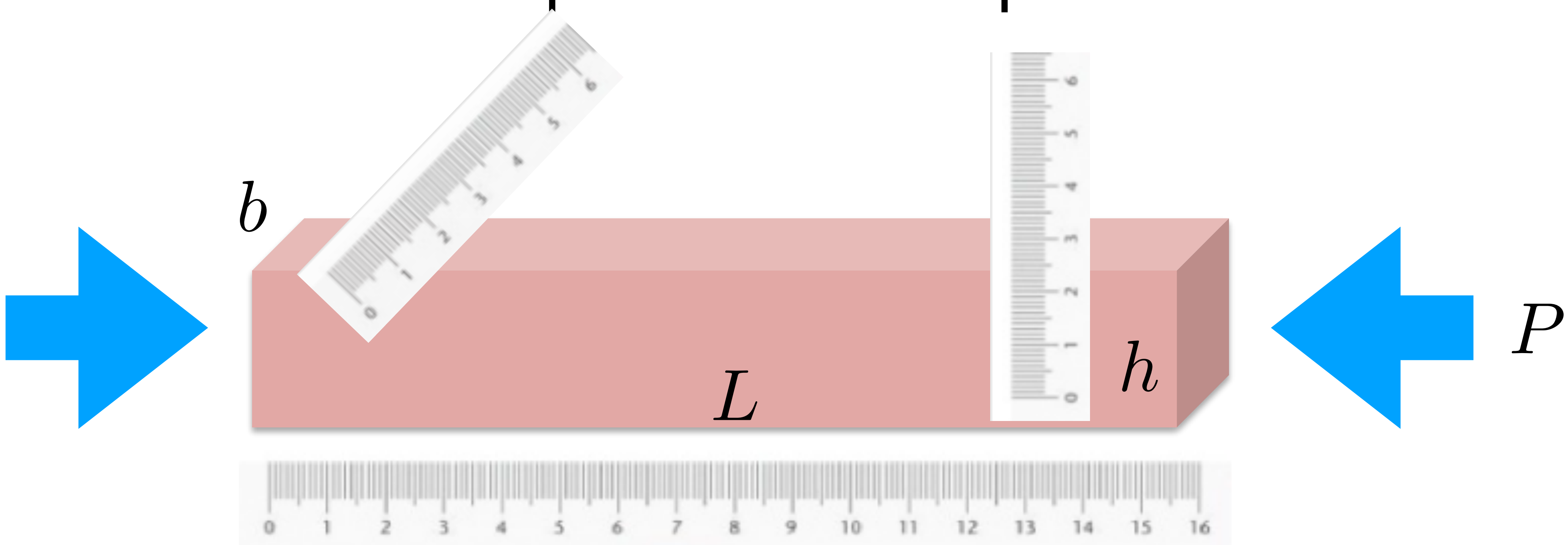
3D embedding by Manifold Learning - kPCA



the existence of the beam width « b » in the critical load expression is DISCOVERED

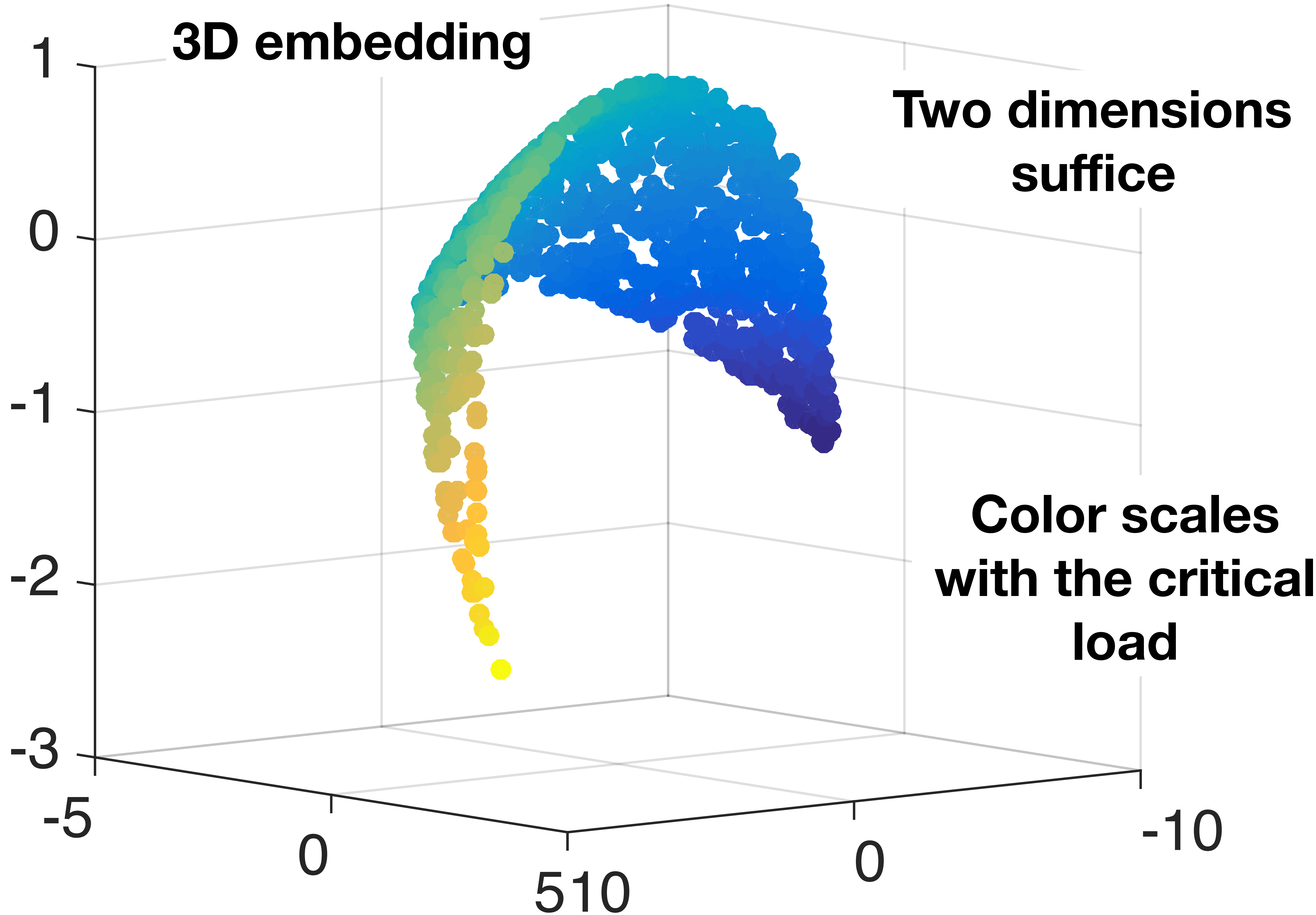
Discarding useless parameters

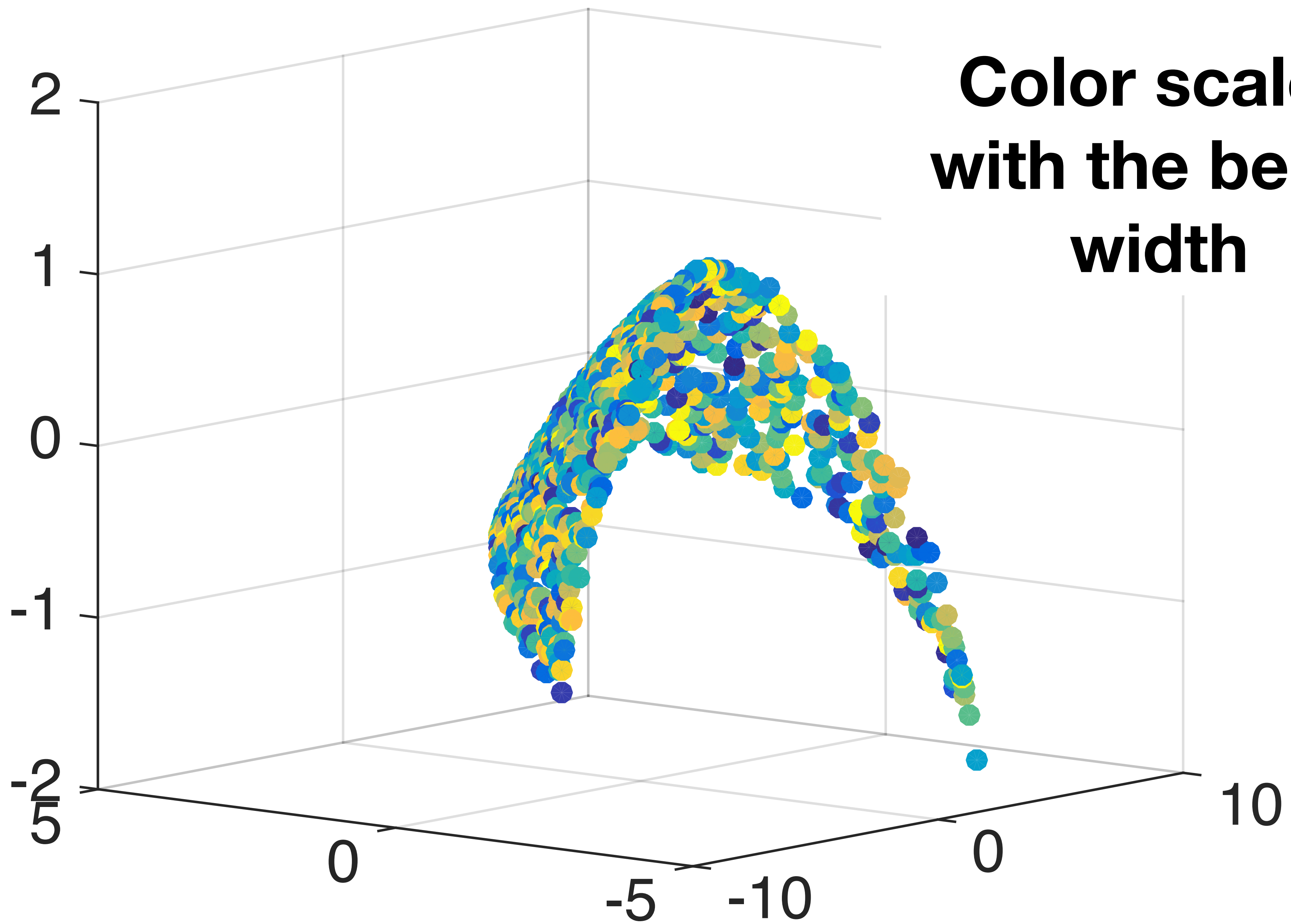
Imagine an ***hypothetical*** physics in which the critical load does not depend on the beam width, **BUT** we measure it and consider it when trying to look for the critical load parametric dependence



Hypothetical critical load $P \propto \dfrac{h^3}{L^2}$

however we look for $P(b, h, L)$

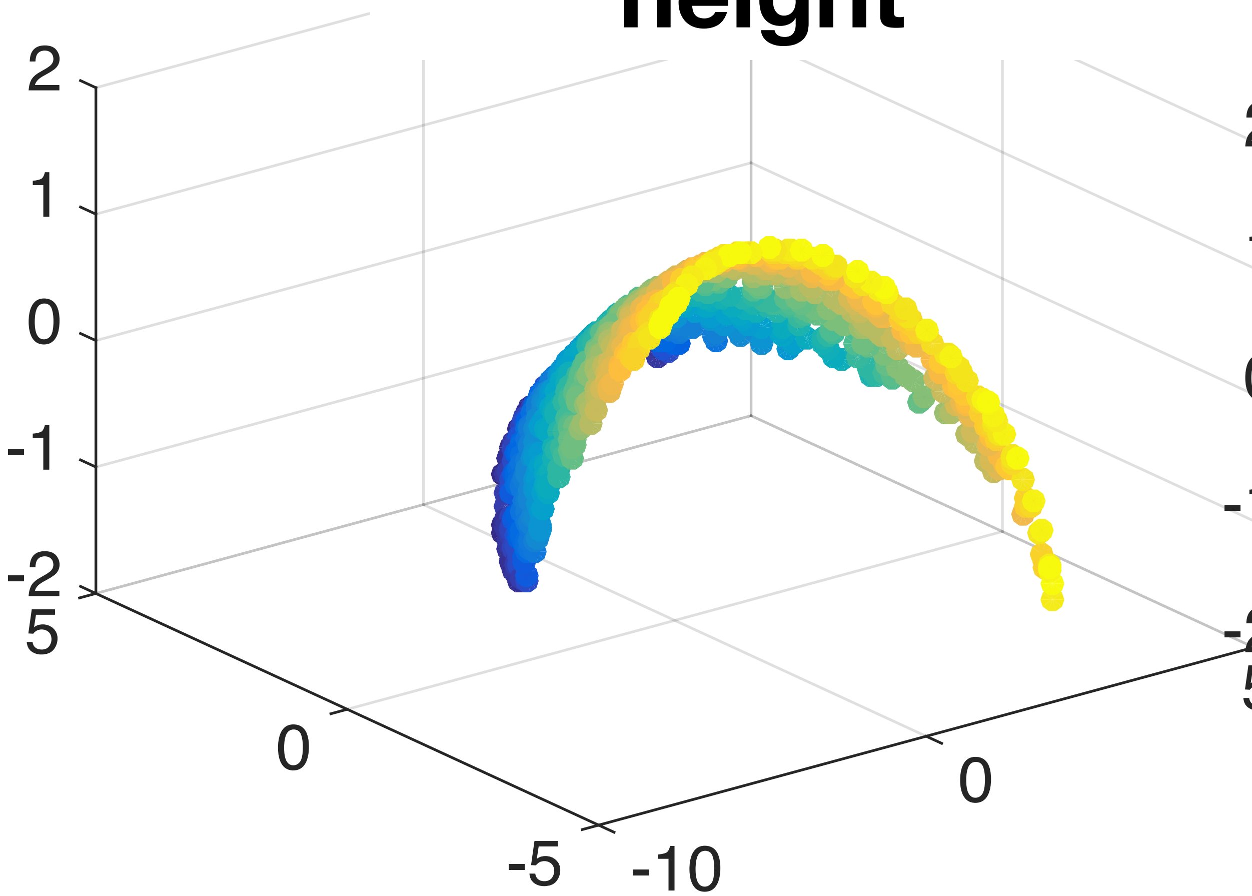

3D embedding
Two dimensions suffice
Color scales with the critical load
1
0
-1
-2
-3
-5
0
510
0
-10



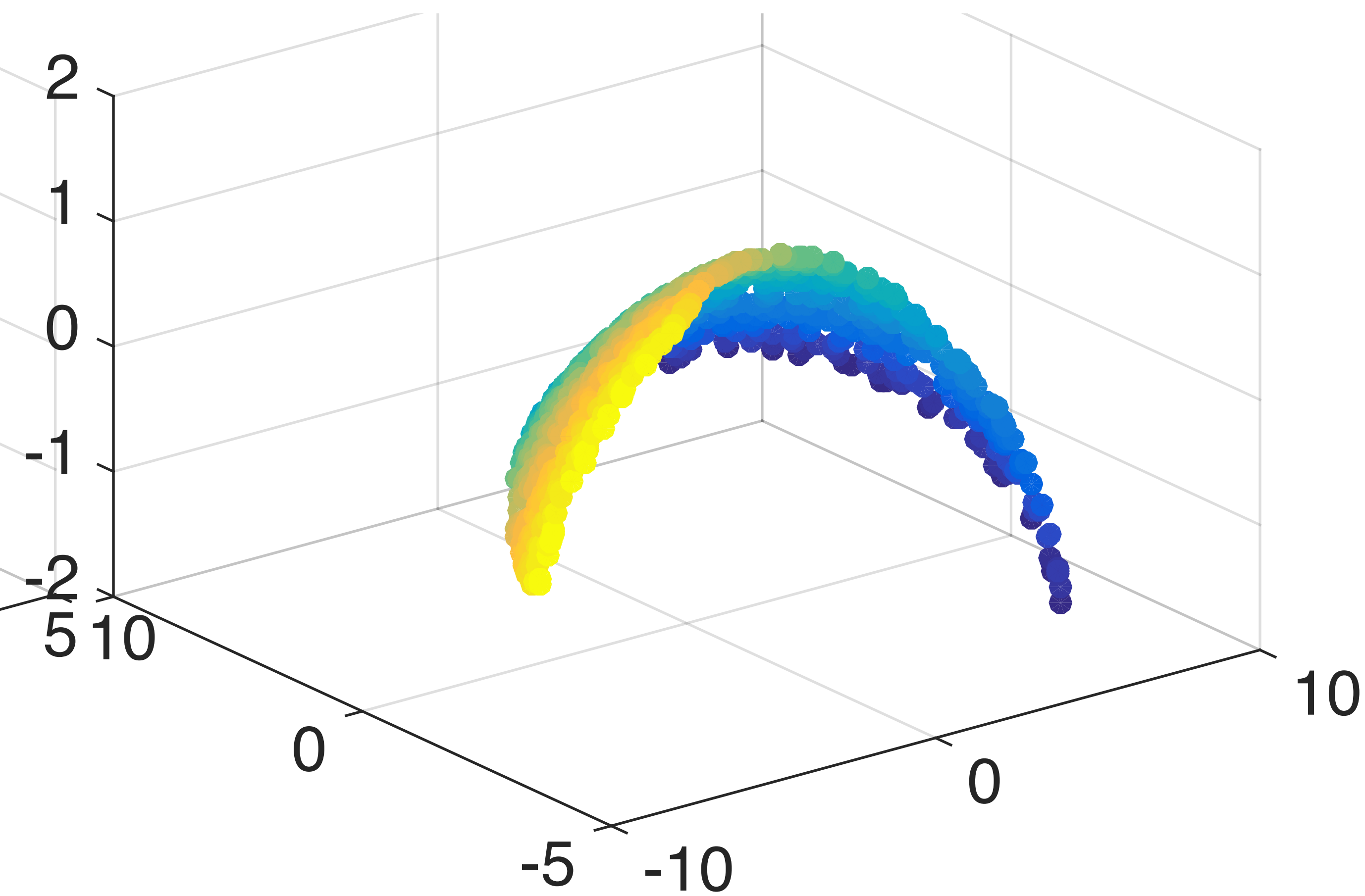
Color scales with the beam width

the beam width seems useless

Color scales with the beam height



Color scales with the beam length



both parameters seem useful

Discovering combined parameters

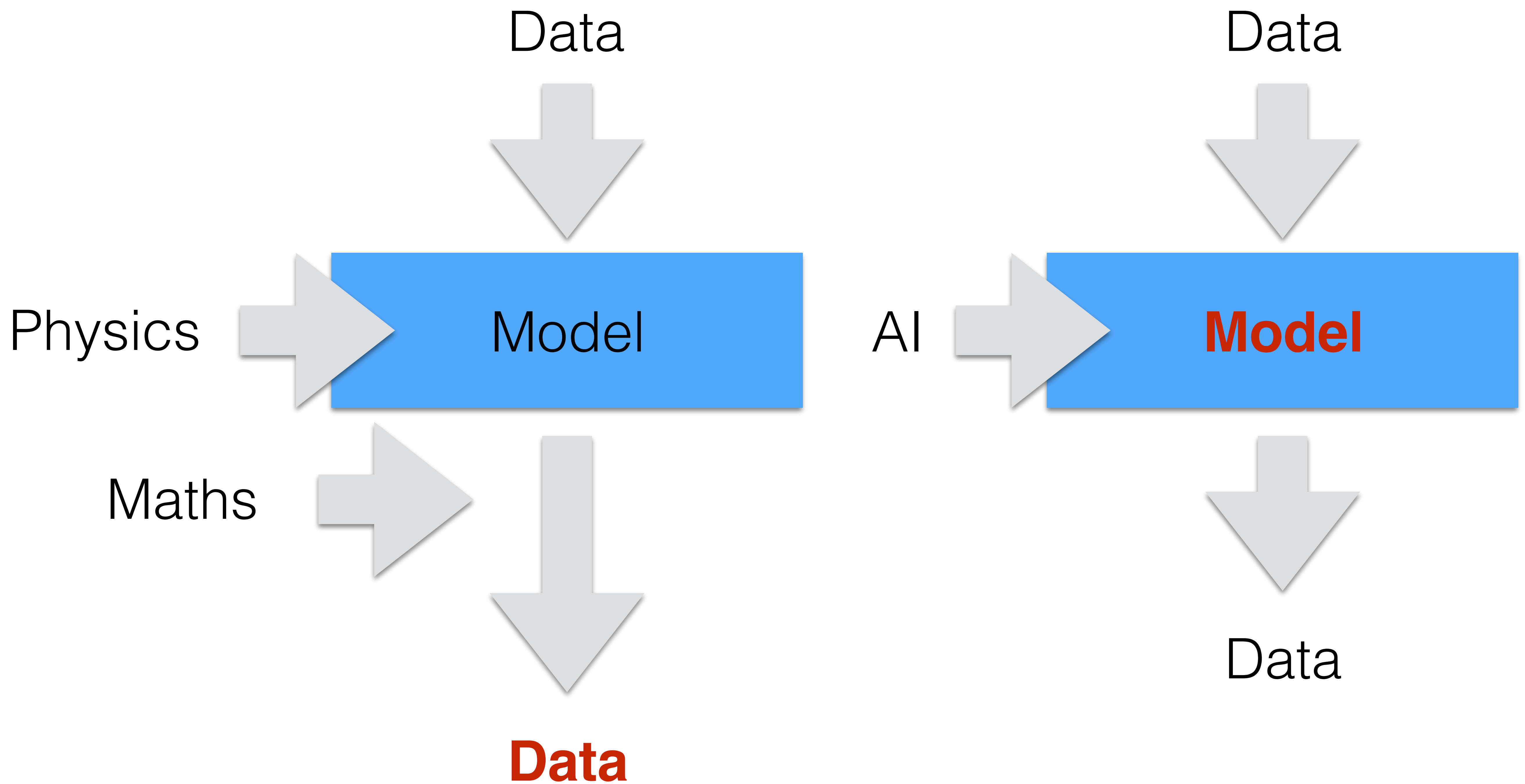
$$P_{trial} = \alpha b^{\beta} h^{\eta} L^{\lambda}$$

… using a Newton strategy

$$\begin{cases} \alpha \approx 1 \\ \beta \approx 1 \\ \eta \approx 3 \\ \lambda \approx -2 \end{cases}$$

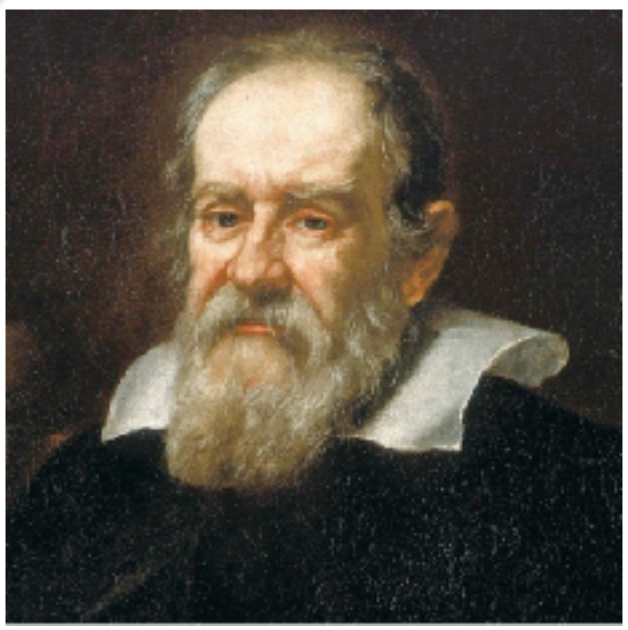
Euler's buckling is (data-driven) discovered

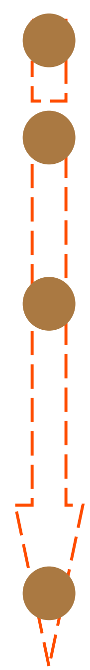
MODELLING REDUCED DATA



A bit of history

Quality (?)
Quantity (?)
Extrapolation (?)



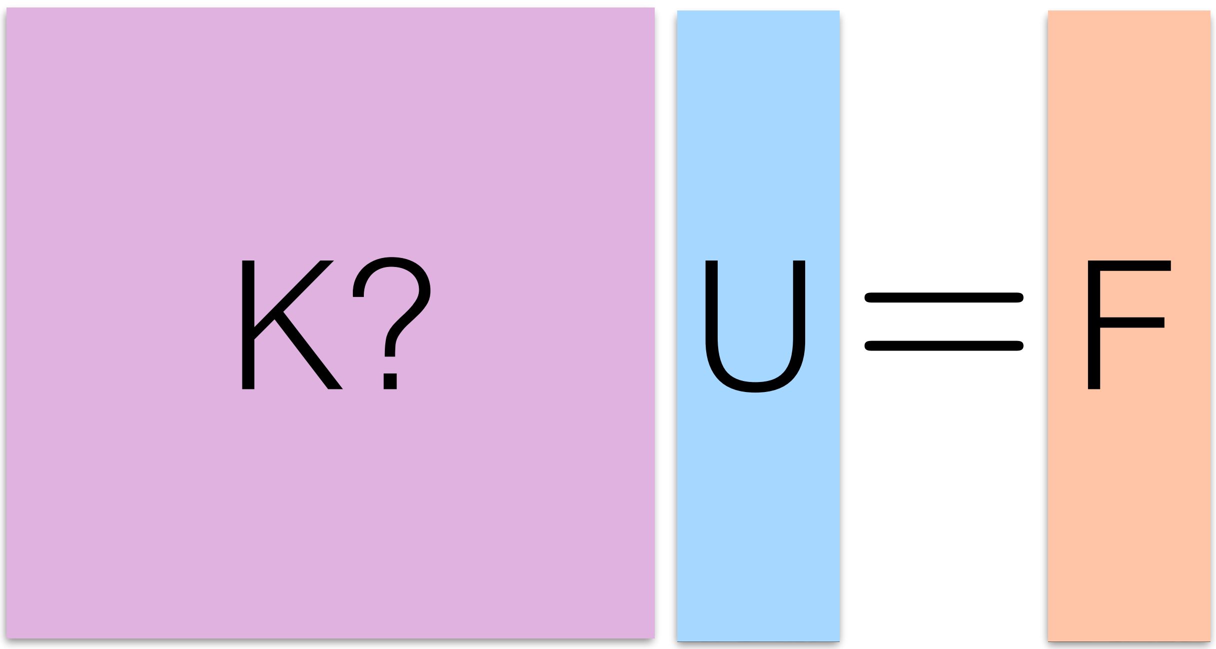


$$\begin{cases} t=1, \; v=10, \; \Delta x=5 \\ t=2, \; v=20, \; \Delta x=15 \\ t=3, \; v=30, \; \Delta x=25 \\ t=4, \; v=40, \; \Delta x=35 \\ \quad \dots \end{cases}$$

$$5/15 = 1/3$$
$$15/25 = 3/5$$
$$25/35 = 5/7$$

$$5/15 = 1/3$$
$$15/25 = 3/5$$
$$25/35 = 5/7$$

$$F_g = m\frac{d^2x}{dt^2}$$


K?
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Advanced Regressions

- **Multi-Local Sparse PGD**-Based NL Regression
- ***Code2Vect*** for heterogeneous / scarce data
- **Reduced Incremental Dynamic Mode Decomposition**
- **Thermodynamically Consistent ML**
- **Physically Informed Neural Networks**:
  combining tensor-flow and tensor formats

Data-Driven modeling:
Ensuring thermodynamic consistency in DMD

$$\dot{\boldsymbol{z}}_t = \boldsymbol{L}(\boldsymbol{z}_t)\nabla E(\boldsymbol{z}_t) + \boldsymbol{M}\nabla S(\boldsymbol{z}_t), \quad \boldsymbol{z}(0) = \boldsymbol{z}_0$$

Poisson matrix: reversibility

Friction matrix: irreversibility

with

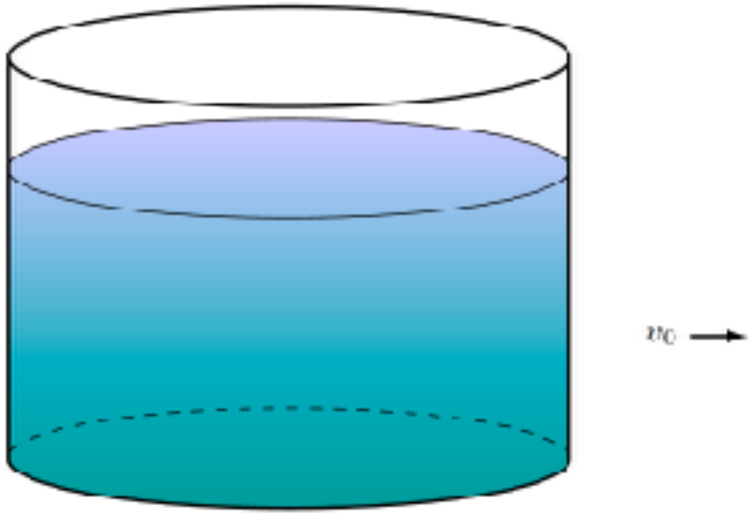
$$\boldsymbol{L}(\boldsymbol{z}) \cdot \nabla S(\boldsymbol{z}) = \boldsymbol{0},$$
$$\boldsymbol{M}(\boldsymbol{z}) \cdot \nabla E(\boldsymbol{z}) = \boldsymbol{0}.$$

$$\frac{\boldsymbol{z}_{n+1} - \boldsymbol{z}_n}{\Delta t} = \mathsf{L}(\boldsymbol{z}_{n+1}, \boldsymbol{z}_n)\mathsf{DE}(\boldsymbol{z}_{n+1}, \boldsymbol{z}_n) + \mathsf{M}(\boldsymbol{z}_{n+1}, \boldsymbol{z}_n)\mathsf{DS}(\boldsymbol{z}_{n+1}, \boldsymbol{z}_n)$$

$$\boldsymbol{\mu} = \{\mathsf{L}, \mathsf{M}, \mathsf{DE}, \mathsf{DS}\} = \arg\min_{\boldsymbol{\mu}*} ||\boldsymbol{z}(\boldsymbol{\mu}) - \boldsymbol{z}^{\mathtt{meas}}||$$

with

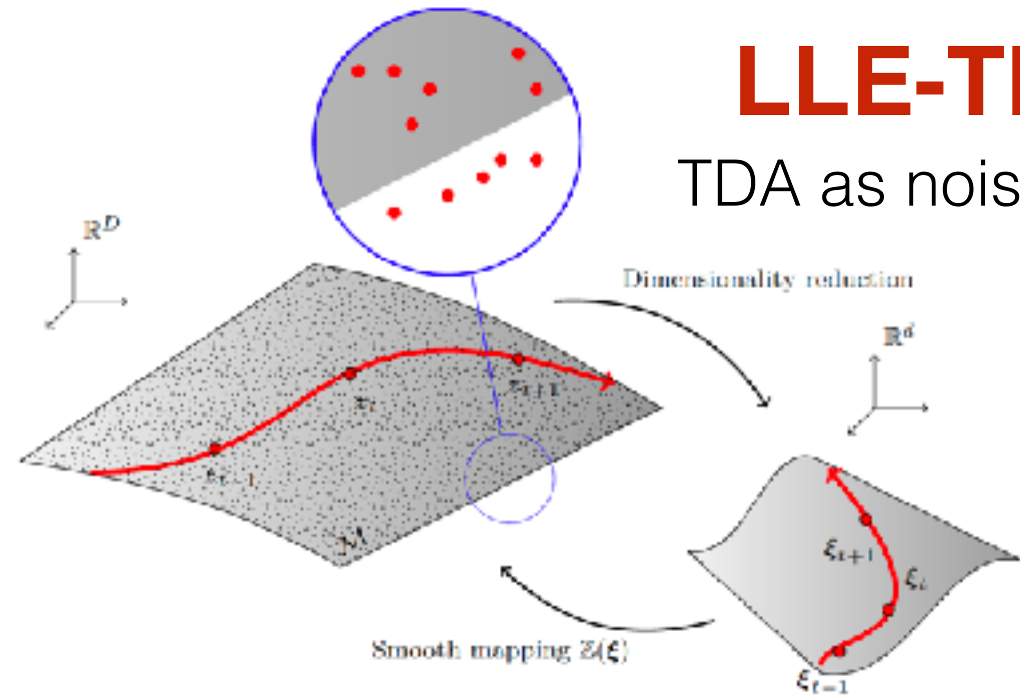
$$\mathsf{DE} = \boldsymbol{A}\boldsymbol{z}$$
$$\mathsf{DS} = \boldsymbol{B}\boldsymbol{z}$$

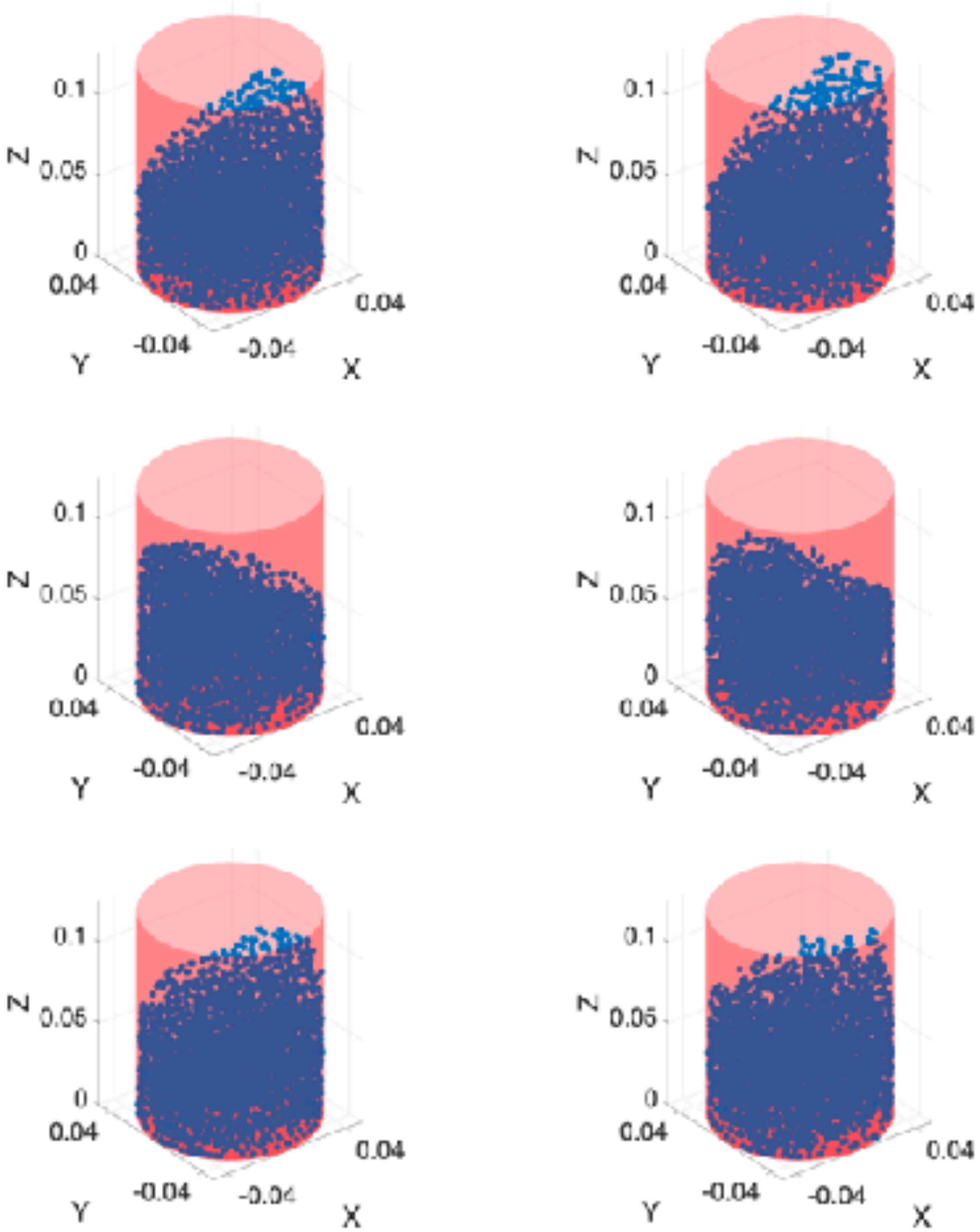


$$\dot{\boldsymbol{z}}_t = \boldsymbol{L}(\boldsymbol{z}_t)\nabla E(\boldsymbol{z}_t) + \boldsymbol{M}\nabla S(\boldsymbol{z}_t), \quad \boldsymbol{z}(0) = \boldsymbol{z}_0$$

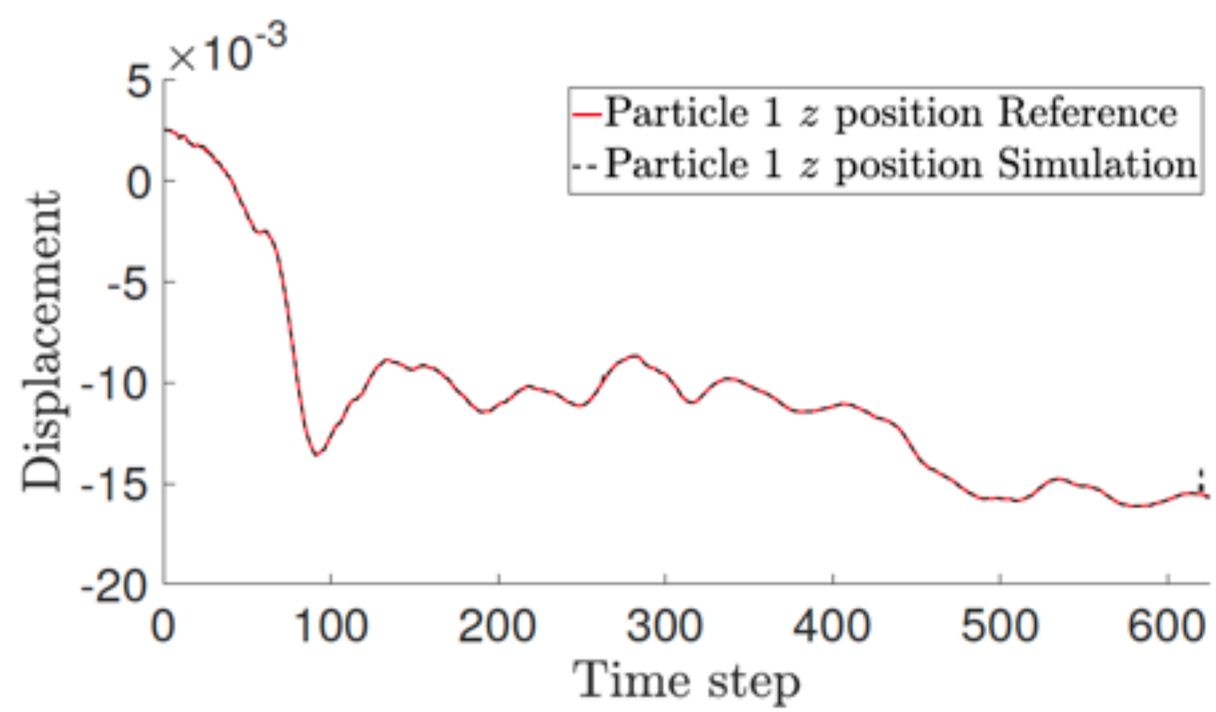
LLE-TDA

TDA as noise filter





$$\{\mathrm{M}(\boldsymbol{\xi}_t), \boldsymbol{A}(\boldsymbol{\xi}_t), \boldsymbol{B}(\boldsymbol{\xi}_t)\}$$



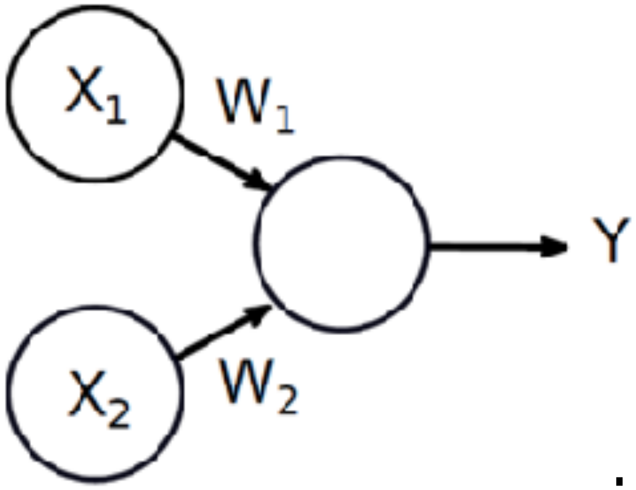
Physically sound, self-learning digital twins for sloshing fluids

B. Moya, I. Alfaro, D. González, F. Chinesta, E. Cueto

Universidad Zaragoza

unizar.es

Deep Learnig



$$Y = W_1 X_1 + W_2 X_2$$

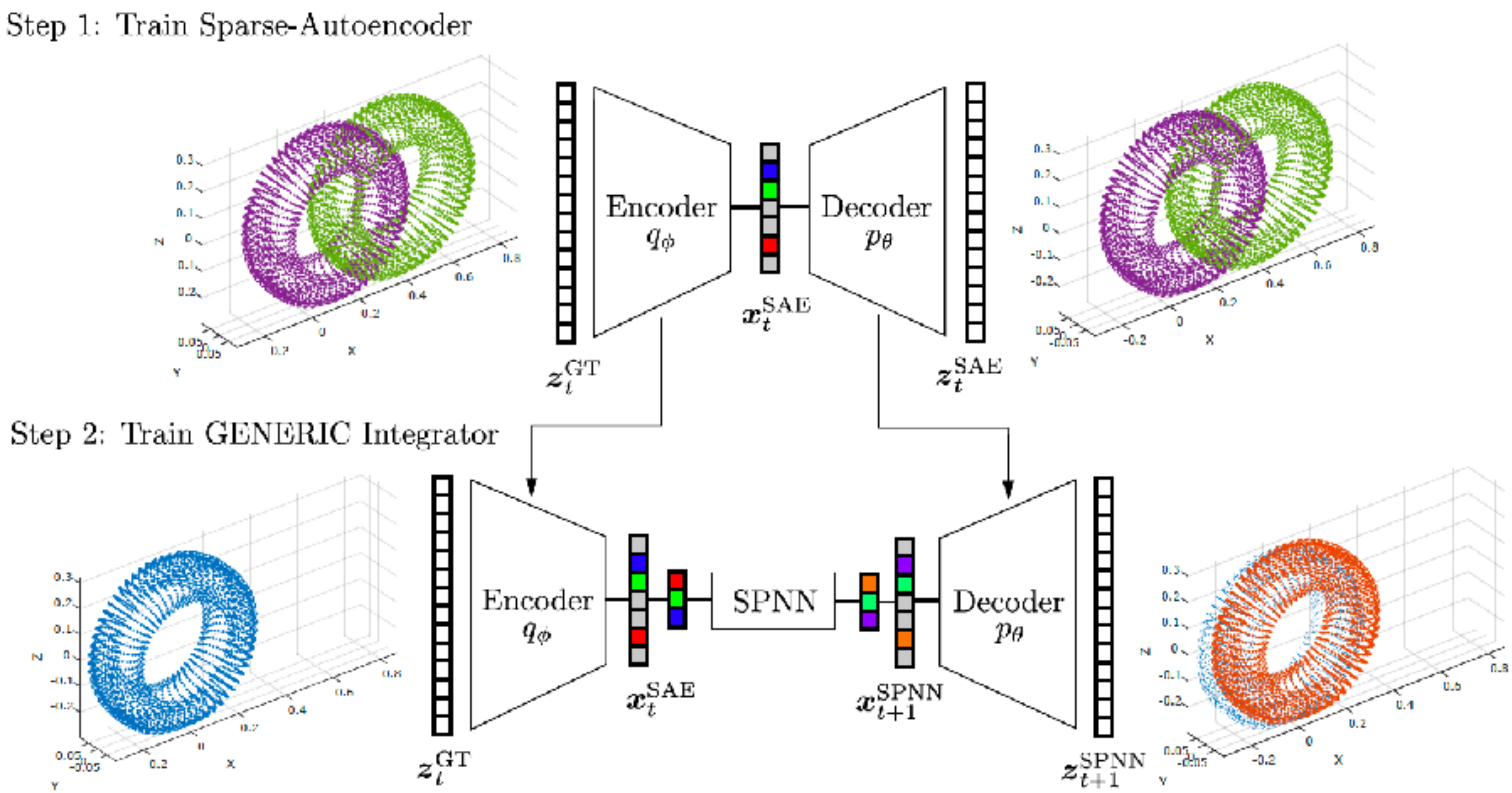
with N inputs $$Y = \sum_{i=1}^{N} W_i X_i$$

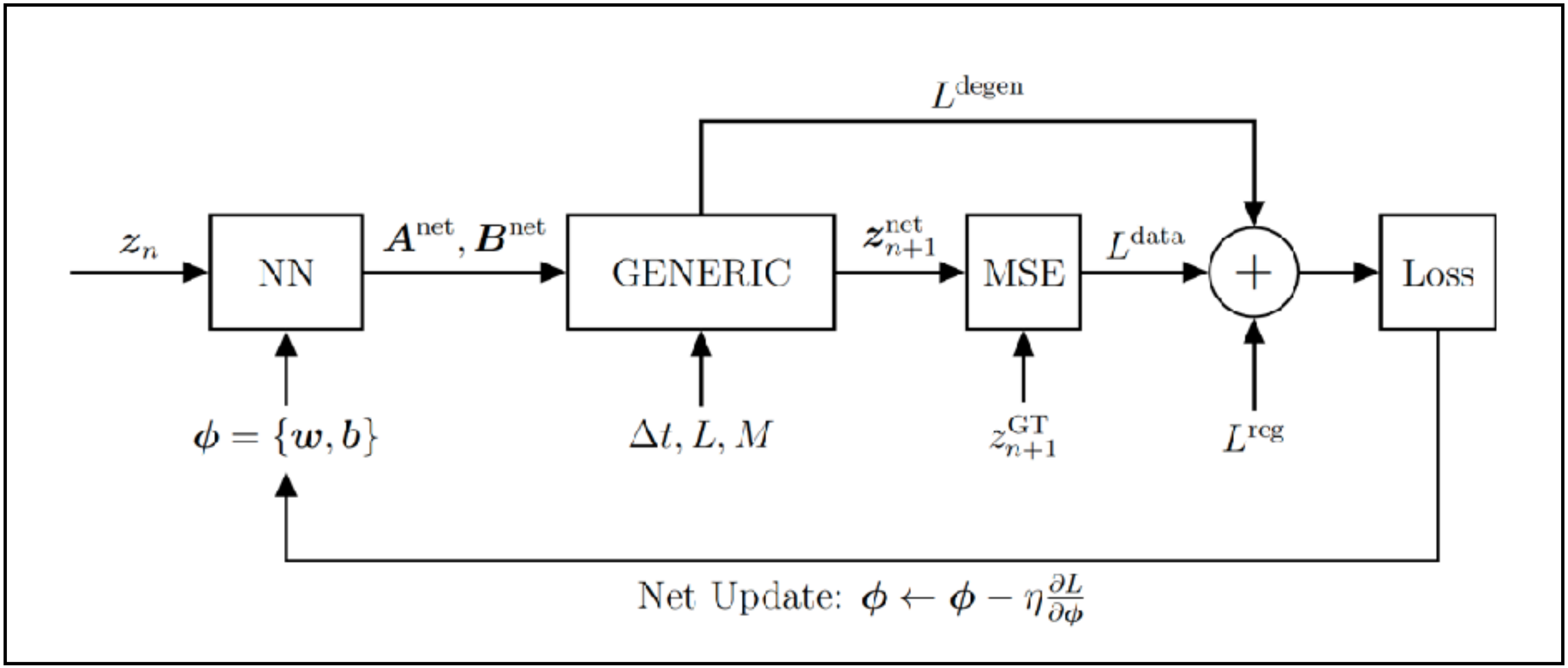
$$\varepsilon(\mathbf{W}) = \sum_{k=1}^{\mathrm{P}} \left(Y^k - \mathbf{W}^T \mathbf{X}^k\right)^2$$

$$\left.\begin{array}{l} \mathbb{Y}^T = \left(Y^1 \ Y^2 \ \cdots \ Y^{\mathrm{P}}\right) \\ \mathbb{X} = \left(\mathbf{X}^1 \ \mathbf{X}^2 \ \ldots \mathbf{X}^{\mathrm{P}}\right) \end{array}\right\} \quad \varepsilon(\mathbf{W}) = \frac{1}{2}\left(\mathbb{Y}^T - \mathbf{W}^T \mathbb{X}\right)^2$$

Nonlinear: $\varepsilon(\mathbf{W}) = \frac{1}{2}\left(\mathbb{Y}^T - \sigma\left(\mathbf{W}^T \mathbb{X}\right)\right)^2$

Structure-Preserving NN





z_n
NN
$\boldsymbol{A}^{\text{net}}, \boldsymbol{B}^{\text{net}}$
GENERIC
$\boldsymbol{z}_{n+1}^{\text{net}}$
MSE
L^{data}
L^{degen}
$+$
Loss
$\boldsymbol{\phi} = \{\boldsymbol{w}, \boldsymbol{b}\}$
$\Delta t, L, M$
z_{n+1}^{GT}
L^{reg}
Net Update: $\boldsymbol{\phi} \leftarrow \boldsymbol{\phi} - \eta \frac{\partial L}{\partial \boldsymbol{\phi}}$

Visco-Hyper-Elasticity as a Data-Driven correction

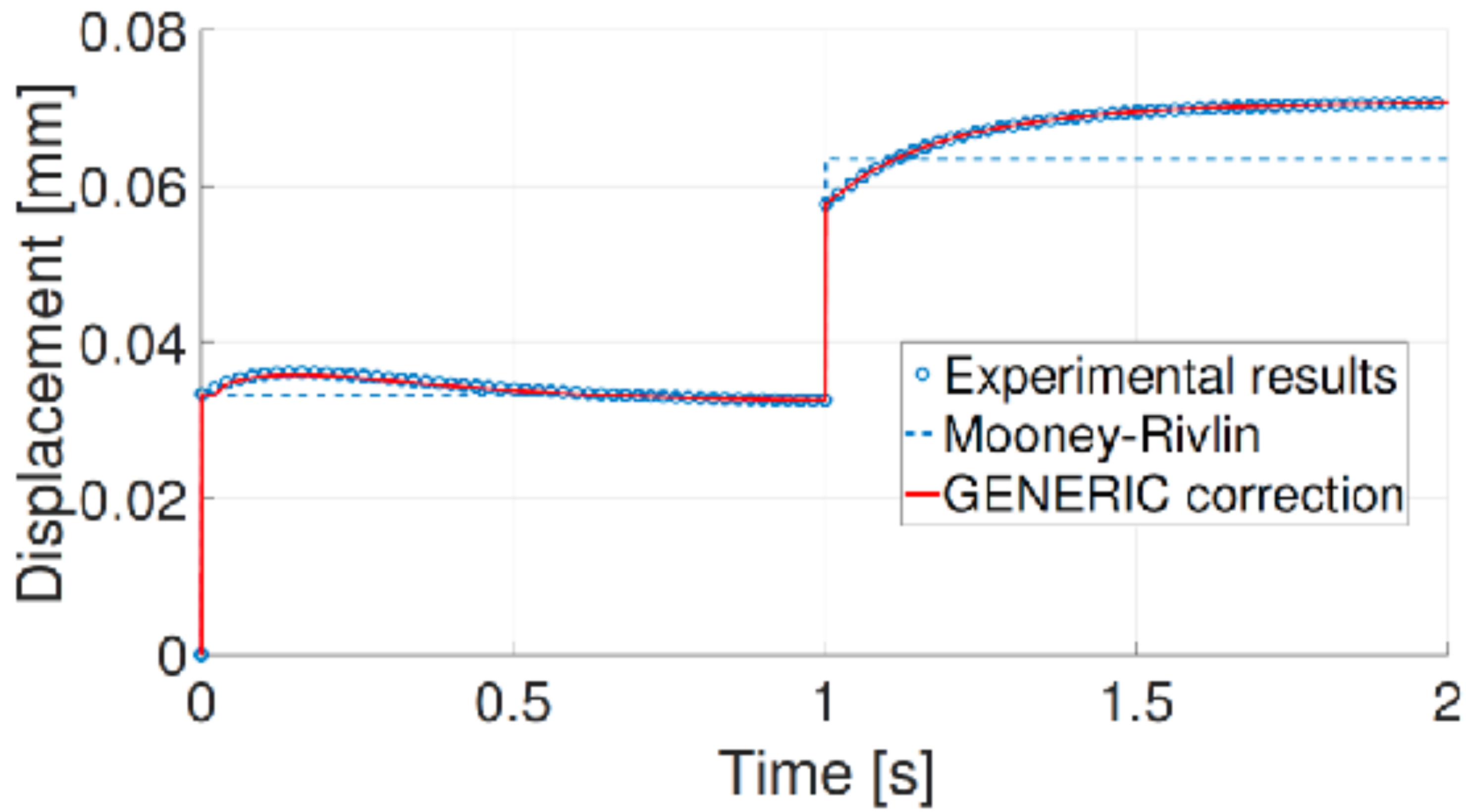
thermodynamically consistent of a purely-hyper-elasticity

$$\dot{\boldsymbol{z}}^{\text{exp}} = \boldsymbol{L}^{\text{model}}(\nabla E^{\text{model}} + \nabla E^{\text{corr}}) + (\boldsymbol{M}^{\text{model}} + \boldsymbol{M}^{\text{corr}})(\nabla S^{\text{model}} + \nabla S^{\text{corr}})$$

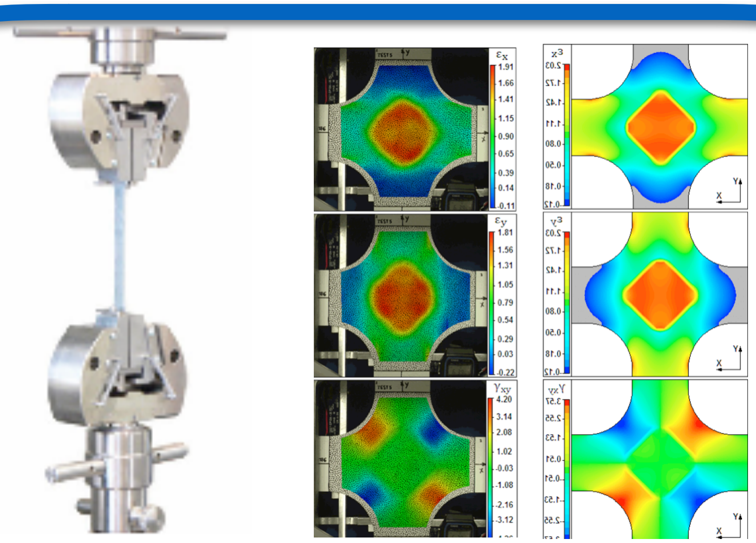
$$\dot{\boldsymbol{z}}^{\text{exp}} = \boldsymbol{L}^{\text{model}}(\nabla E^{\text{model}} + \nabla E^{\text{corr}}) + \boldsymbol{M}^{\text{corr}} \nabla S^{\text{corr}}.$$

$$\frac{\boldsymbol{z}_{n+1}^{\text{exp}} - \boldsymbol{z}_n^{\text{exp}}}{\Delta t} = \mathsf{L}\ \mathsf{DE}(\boldsymbol{z}_{n+1}^{\text{exp}}) + \mathsf{M}(\boldsymbol{z}_{n+1}^{\text{exp}})\mathsf{DS}(\boldsymbol{z}_{n+1}^{\text{exp}})$$

$$\boldsymbol{\mu}^* = \{\mathsf{M}, \mathsf{DE}, \mathsf{DS}\} = \arg\min_{\boldsymbol{\mu}} ||\boldsymbol{z}(\boldsymbol{\mu}) - \boldsymbol{z}^{\texttt{meas}}||$$



Plasticity correction

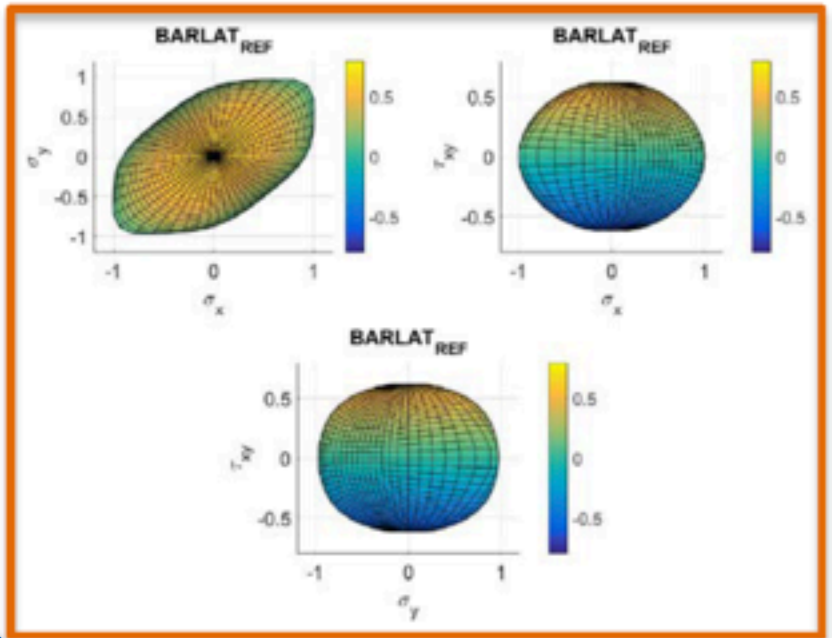


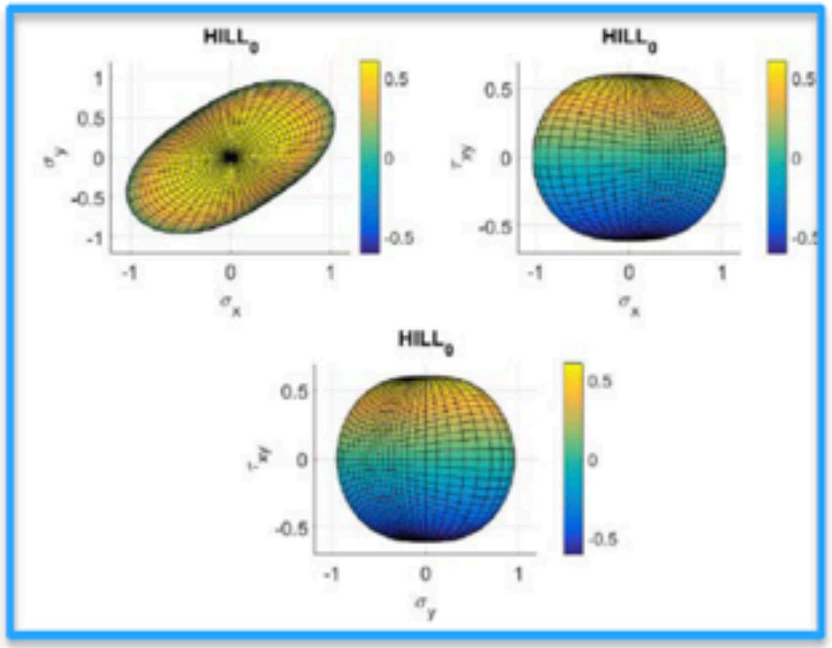
Reality = First order model + Deviation model

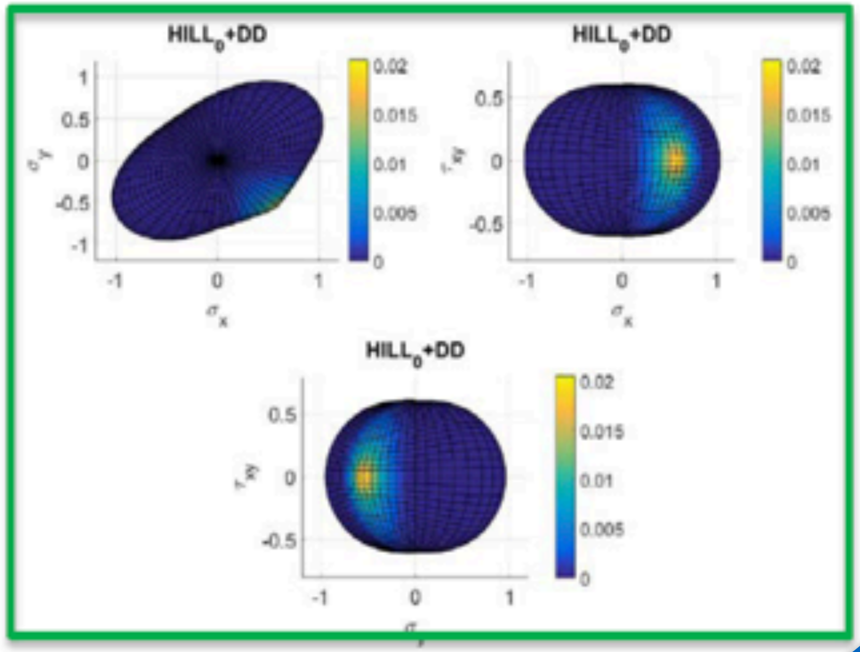
Reality e.g. **Barlat Yld2004-18p**

First order model e.g. **Quadratic Hill**

Deviation model **Perturbation Model**







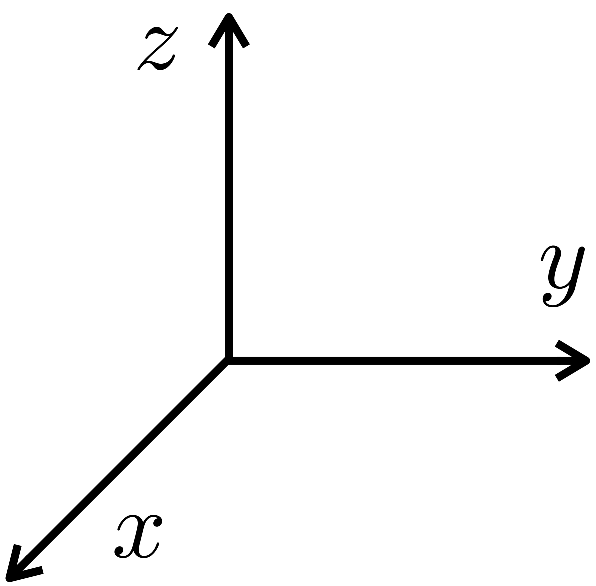
MODEL ORDER REDUCTION

Separation of Variables - PGD

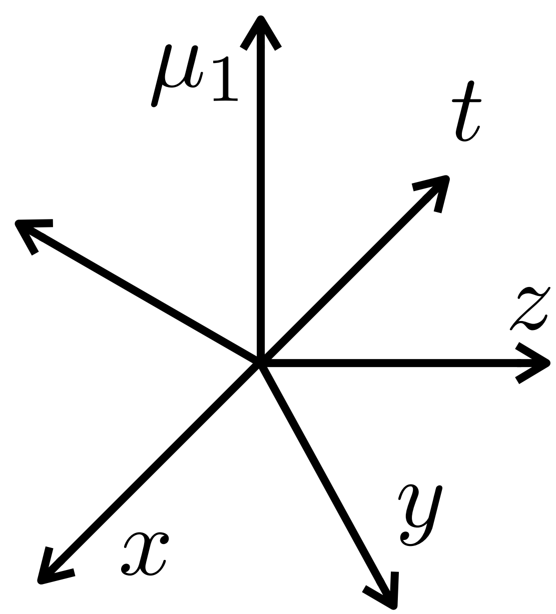
$$(x, t) \rightarrow \sum X_i(x) T_i(t)$$

$$(x, y, z) \rightarrow \sum X_i(x) Y_i(y) Z_i(z)$$

$u(x, y, z, t; \mu_1, \mu_2, ...)$



$u(x, y, z, t, \mu_1, \mu_2, \cdots)$



Separation of variables

$$\sum_i \prod_j$$

$$(\mathbf{x}, t, \mu_1, \mu_2, \cdots) \rightarrow \sum X_i(\mathbf{x}) T_i(t) \prod_j M_i^j(\mu_j)$$

Real-Time Physics

Proper Generalized Decomposition

First key idea: Parameters become coordinates

$$u(x, t, p_1, \cdots, p_N)$$

BUT **D** nodes in **N** dimensions $\longrightarrow N^D$ dof

Curse of Dimensionality = Combinatorial Explosion

Second key idea: Separation of variables

$$u(x, t, p_1, \cdots, p_N) \approx \sum_{i=1}^{M} X_i(x) T_i(t) \Pi_i^1(p_1) \cdots \Pi_i^N(p_N)$$

Multidimensional solution from a sequence of low-dimensional problems

BUT the solver becomes too intrusive

Non-intrusive constructor: sPGD

P parameters requires of order of P runs

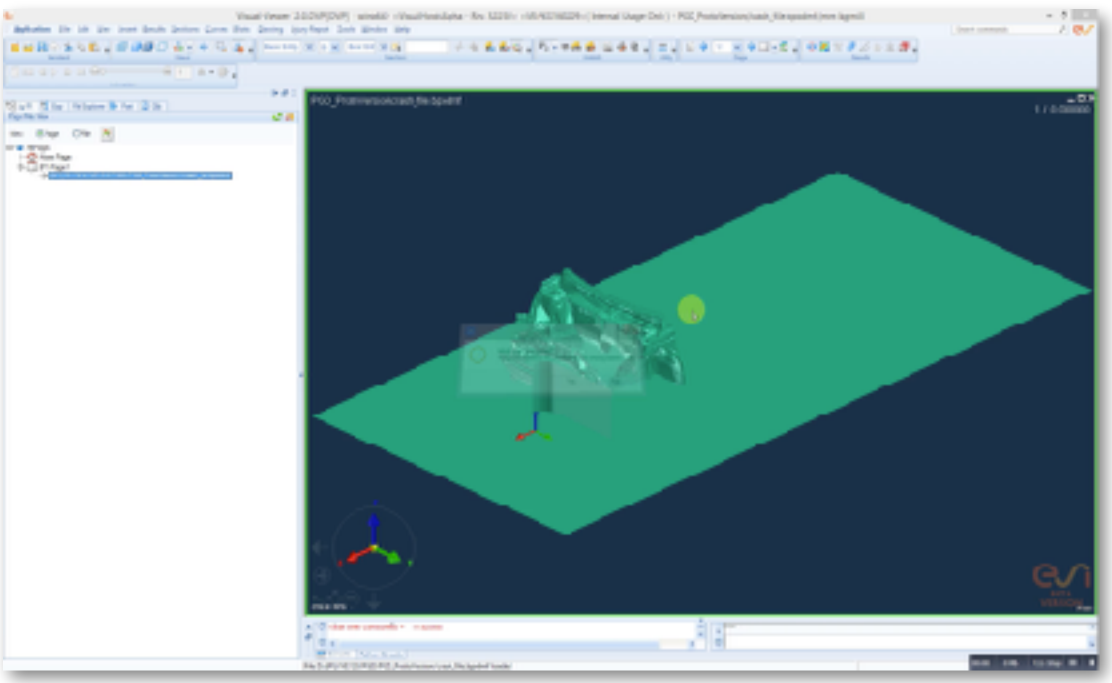
Error estimation

Technical aspects:

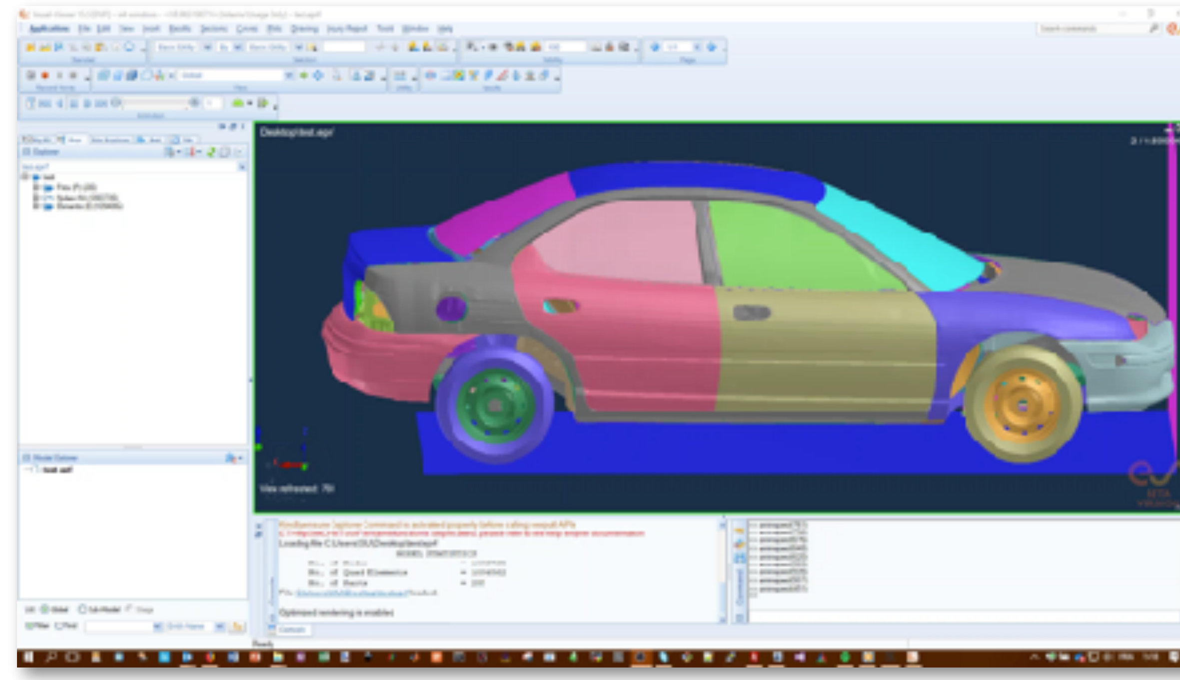
separation of variables, hierarchical adaptivity, sparse sensing and kriging

Examples

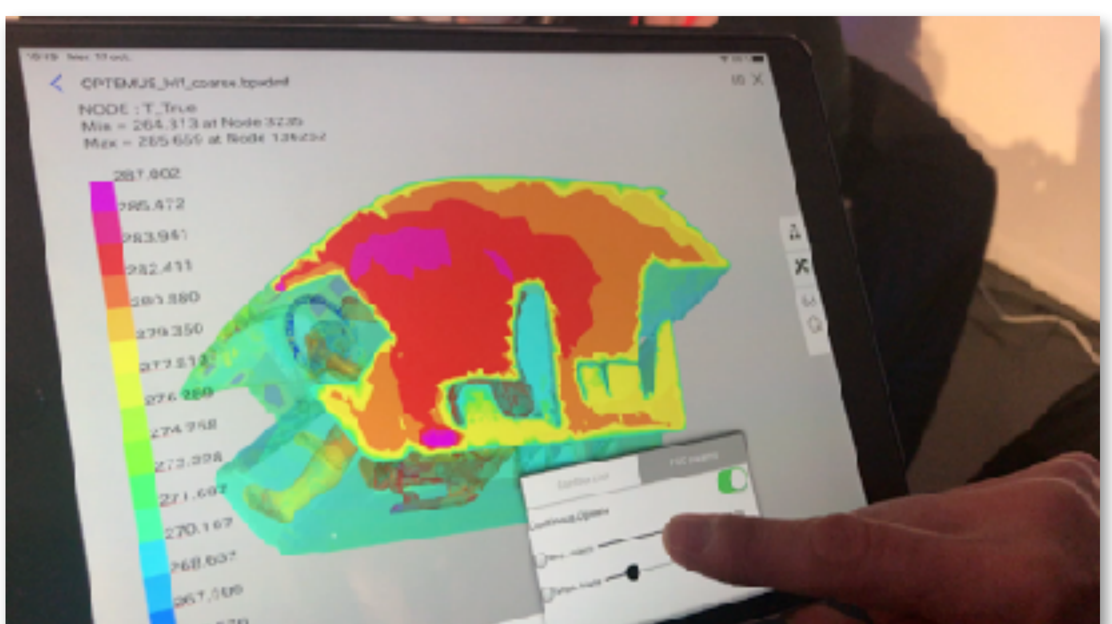
Crash



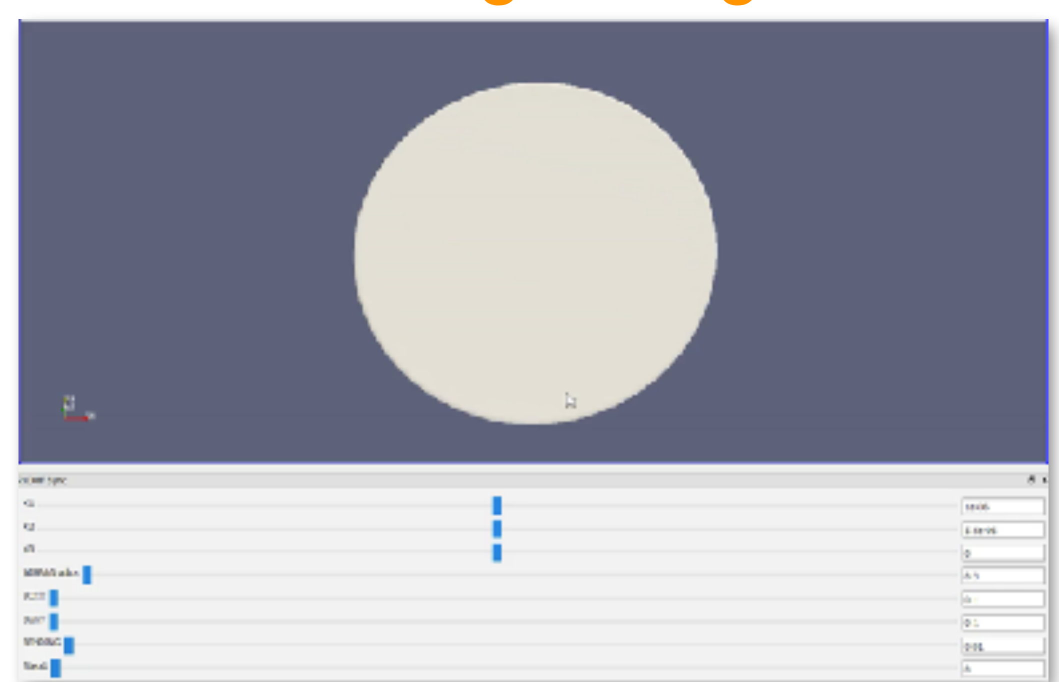
Crash



Thermal comfort



Airbag folding



Augmented reality