Nonlinear dimensionality reduction for functional computer code modelling

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CEA - UPMC

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Thesis since 02/2008

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Bertrand Iooss (EDF)

Industrial context

Framework : life span of reactor vessels.

$\longrightarrow$ Several sequences of accidents can occur.

Goal = estimate their probabilities of occurrence.

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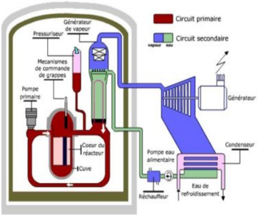

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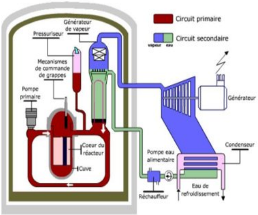

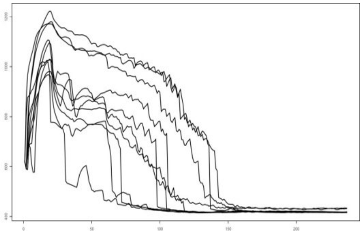

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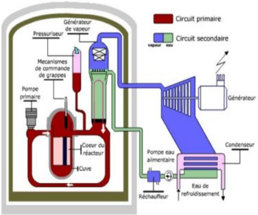

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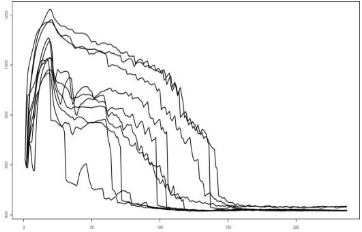

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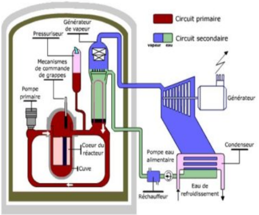

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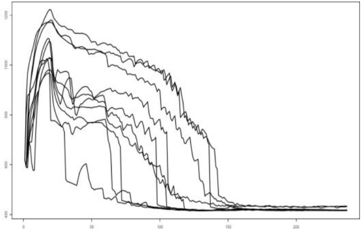

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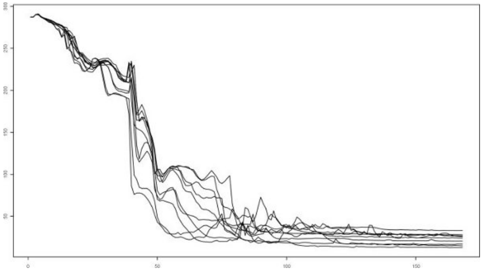
Improve the simulation stage to allow accurate computations

In my laboratory (CEA) ...

Thermal-hydraulic code CATHARE = time consuming



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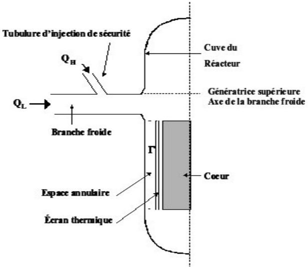

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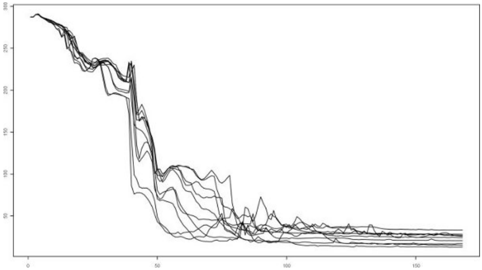

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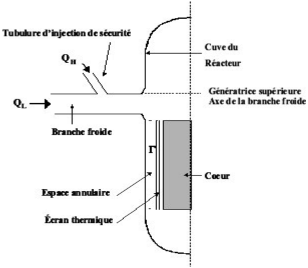

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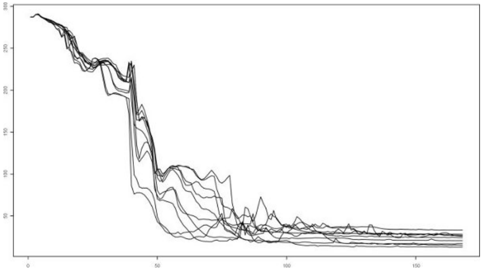

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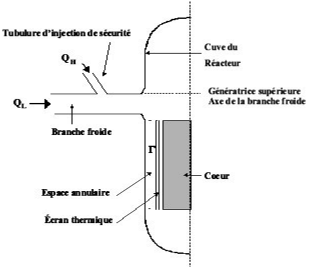

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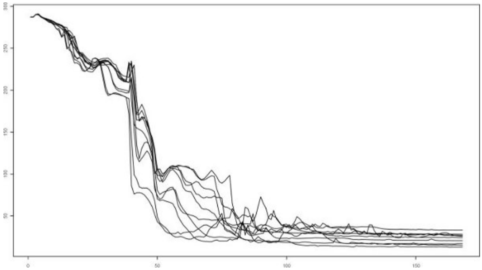

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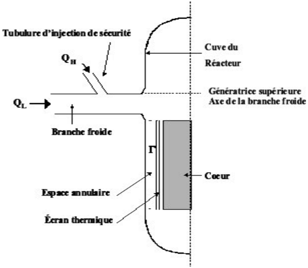

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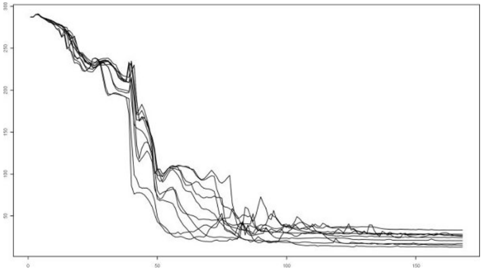

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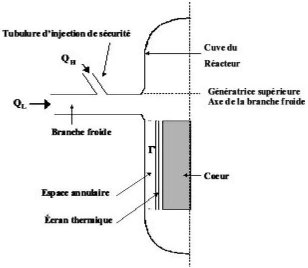

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"Speed up" *the execution of CATHARE code* = statistical modeling

Mathematical formulation

n known couples (x_i, y_i) = inputs-outputs of a very slow code :

- Inputs $x_i \in \mathbb{R}^p$ = initial state of physical system ;
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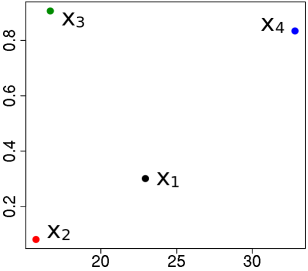

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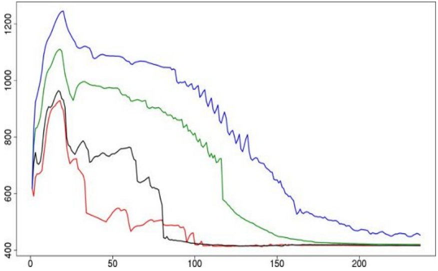

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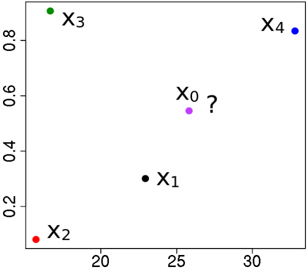

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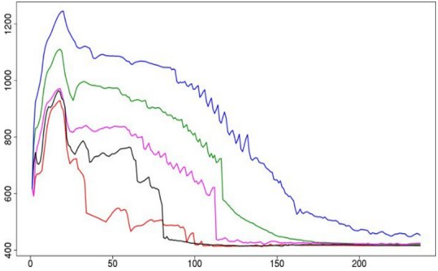

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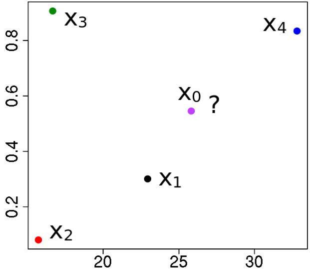

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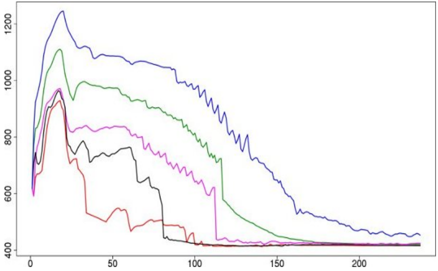

Statistical learning "regression" $\mathbb{R}^p \to \mathcal{C}([a, b], \mathbb{R})$

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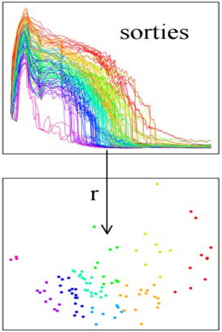

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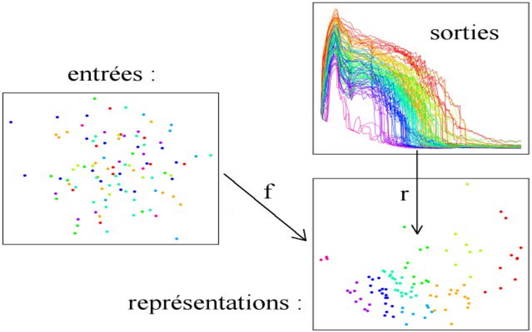

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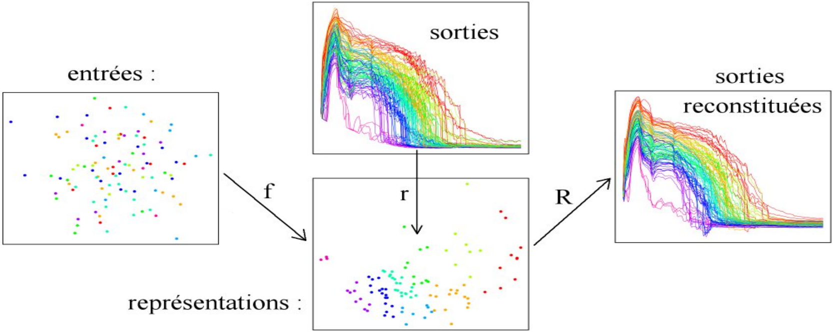

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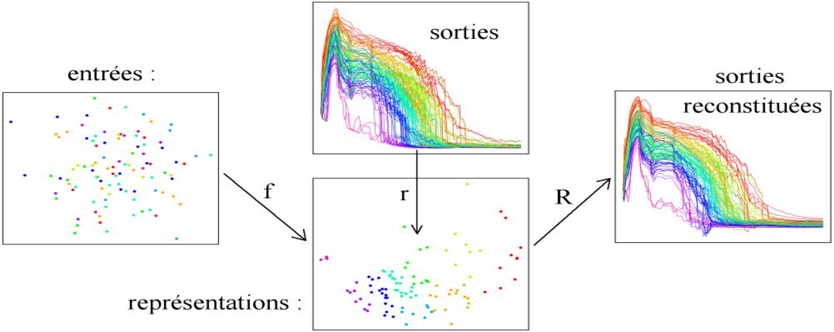

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(More or less) classical methods

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(New) goal : minimize the representation dimension d, to

- simplify the model ;
- avoid overfitting,

while keeping good performances.

1. "Stepwise" dimension reduction
   - Local PCA Manifold Learning (Zhan et al. 2008)
   - Riemannian Manifold Learning (Lin et al. 2006)

2. Applications

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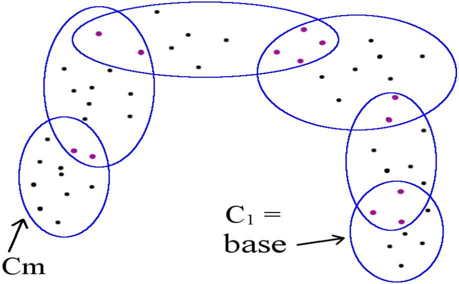

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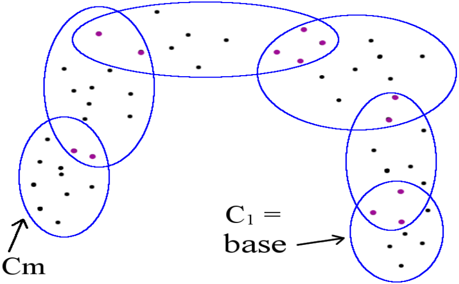

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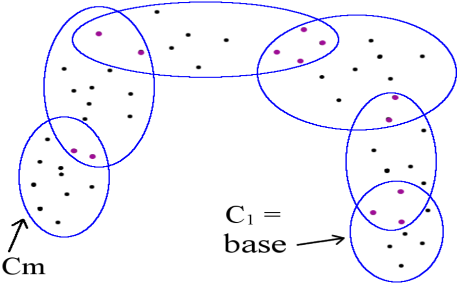

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3. Affine transformations $\rightarrow$ global z_i coordinates ; $\hookrightarrow$
   method : optimize transformation matrix on the intersection, then apply on next "cell".

Estimation of global coordinates (steps 2−3)

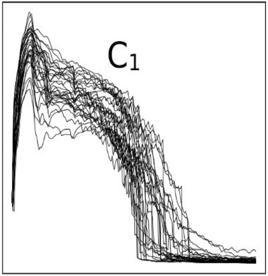
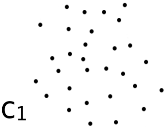


FIG.: data



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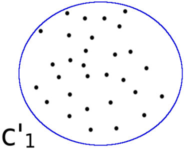

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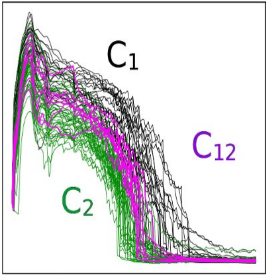

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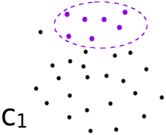

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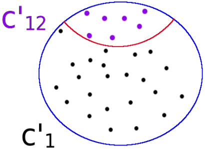

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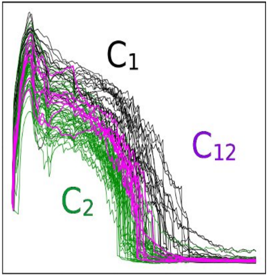

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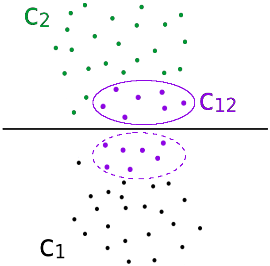

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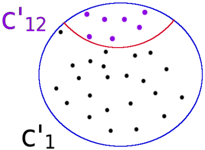

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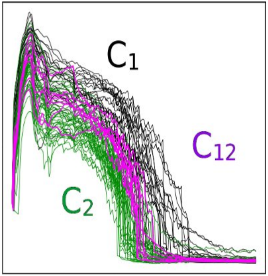

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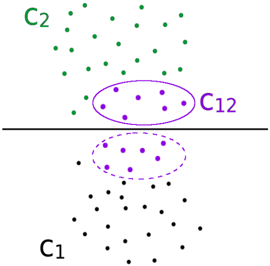

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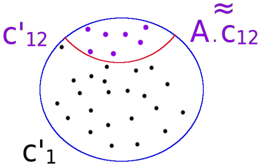

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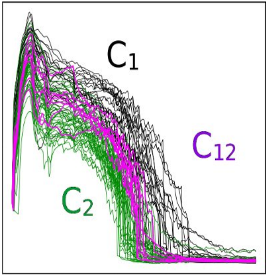

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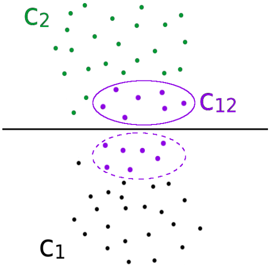

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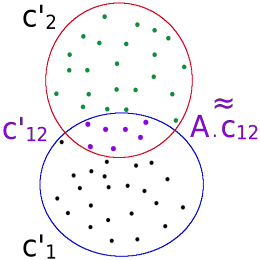

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5. A applied on the elements of $C_2 \setminus C_1 \rightarrow c_2'$;
   back to 2. with c_2' . . . etc.

Exemples

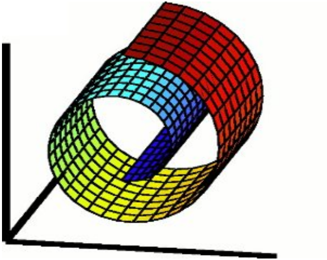


FIG.: Swissroll, 400 points 3D

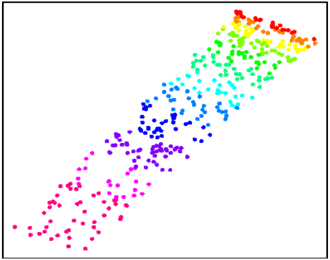


FIG.: LPcaML representation

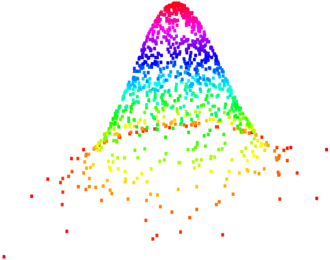
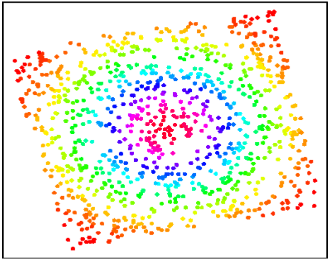


FIG.: Gaussian, 1000 points 3D



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2. Applications

Local steps

RML $\simeq$ preservation of angles *and* geodesic distances.

1. choose an origin curve y_0 among the y_i, (e.g., the mean) ;

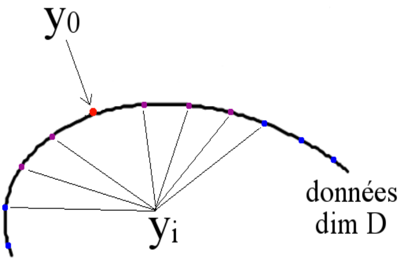

FIG.: Origin curve y_0

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1. choose an origin curve y_0 among the y_i, (e.g., the mean) ;
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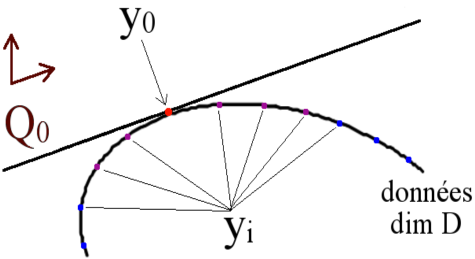

FIG.: Tangent plane at y_0 + local basis Q_0

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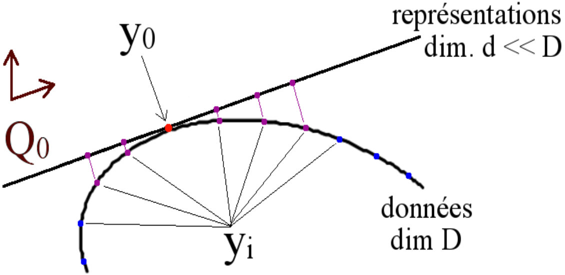

FIG.: Local coordinates z_i on the tangent plane

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4. then normalize to verify the identity $\|y - y_0\| = \|z - z_0\|$.

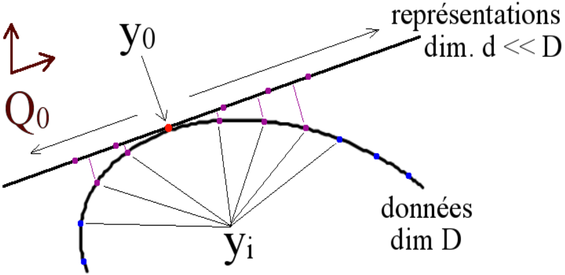

FIG.: Normalization of coordinates z_i

"far" from y_0

Step 4 : for y far from y_0 (too far for last step to be accurate),

- y_p = predecessor of y on a shortest path from y_0
- $y_{i_1}, \ldots, y_{i_d} = y_p$ neighbors with known z_i coordinates

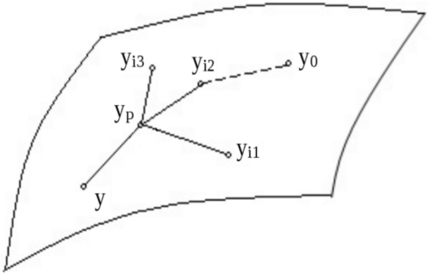

FIG.: Data y_i in dim. D

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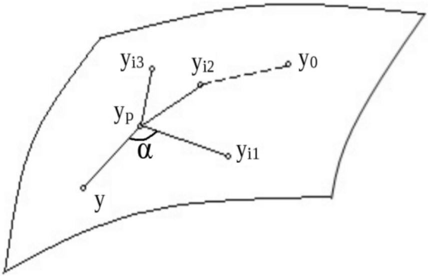
$z = r(y)$ computed by..

- ..preserving angles as much as possible : $\widehat{zz_pz_{i_j}} \simeq \widehat{yy_py_{i_j}}$;
- ..under the normalization constraint $\|y - y_p\| = \|z - z_p\|$.



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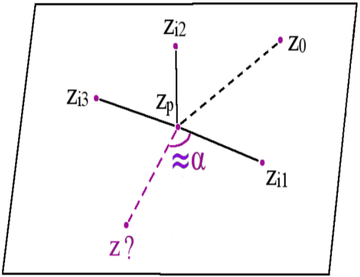

FIG.: $z_i = r(y_i)$ in dim. $d \ll D$

Examples

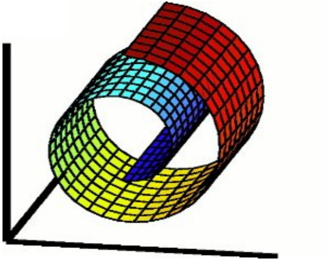

Fig.: Swissroll, 400 points 3D

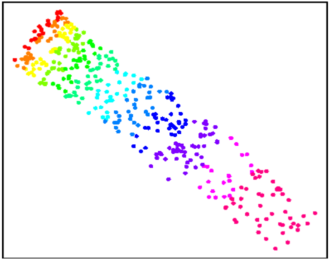

Fig.: RML representation

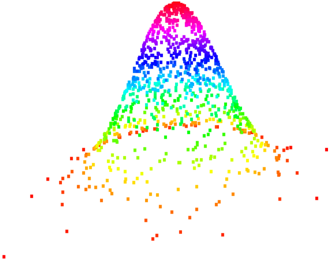

Fig.: Gaussian, 1000 points 3D

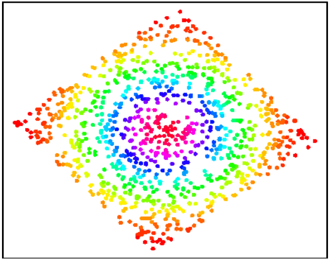

Fig.: RML Representation

About reconstruction...

Assume $z \in \mathbb{R}^d$ must be turned into a curve ($\mathbb{R}^D$).

RML :

1. local PCA around y_{i_0} where i_0 is $\arg\min_{i=1..n} \|z - z_i\|$;
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LPcaML :

1. find the most probable cell(s) from which z was generated ;
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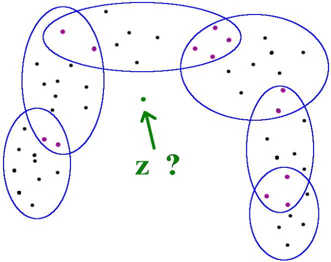
..Step 1 = supervised classification ! (Training set = (z_i, cell_i)).



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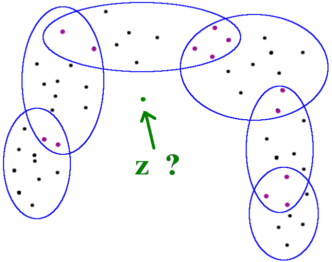

Which cell(s)/weight(s) to choose ?

Implemented : weighted average of neighbors' cells reconstructions.

Doesn't work well . . .

1. "Stepwise" dimension reduction
   - Local PCA Manifold Learning (Zhan et al. 2008)
   - Riemannian Manifold Learning (Lin et al. 2006)

2. Applications

Validation step

Data :

- training $= \{(x_i, y_i)\,,\ i = 1, \ldots, n\}\,;$
- test $= \{(x'_i, y'_i)\,,\ i = 1, \ldots, m\}\,;$

Model predictions : $\hat{y}'_i = M(x'_i)$, $i = 1, \ldots, m$.

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"Absolute" then relative measures of the pointwise error

$$MSE[j] = \frac{1}{m} \sum_{i=1}^{m} (\hat{y}_i'(j) - y_i'(j))^2\,, \quad j = 1, \dots, D \text{ (discretization)}.$$

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$$Q_2[j] = 1 - \frac{m.MSE[j]}{\sum_{i=1}^{m}(\bar{y}(j) - y'_i(j))^2} \text{ (compararison to the mean)}.$$

$-\infty < Q_2 \leq 1$: $\leq 0 \Rightarrow$ (very) bad model ;
$\simeq 1 \Rightarrow$ perfect model.

Test I - temperature curves

100 model runs,
4 dimensions on input,
168 discretization points.

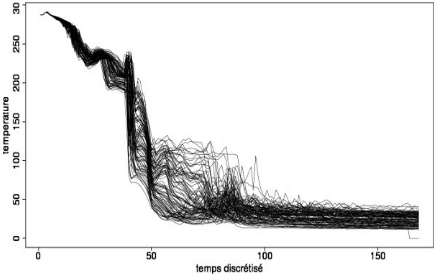

FIG.: The 100 code outputs

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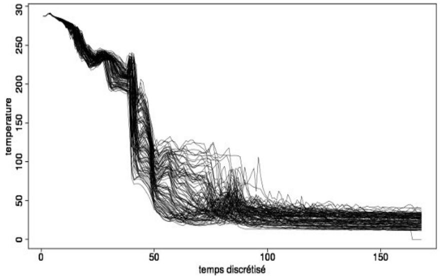
cross validation
leave-10-out :

MSE at l., Q_2 at r. ; $d = 4$



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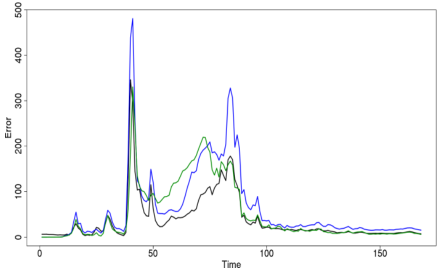


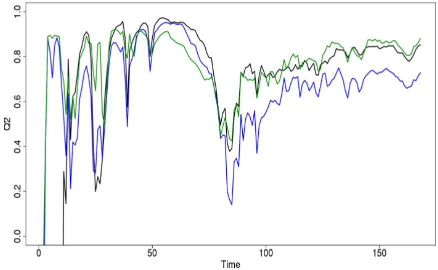


FIG.: Black : functional PCA ; blue : RML ; green : Nadaraya-Watson.

5 predicted curves

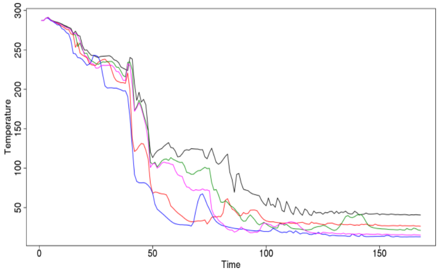


FIG.: Real curves

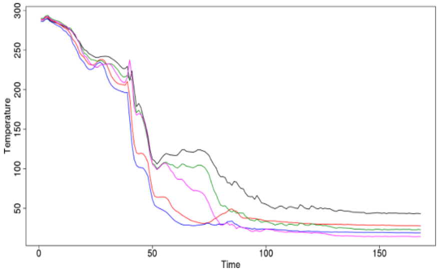
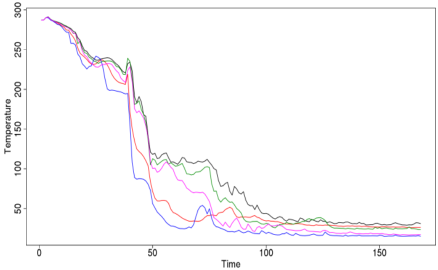


FIG.: PCA dim. red.



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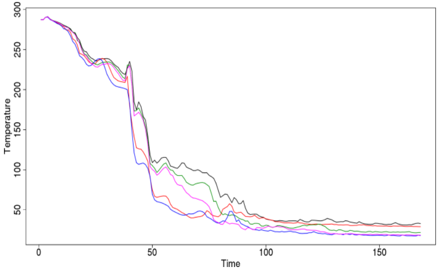
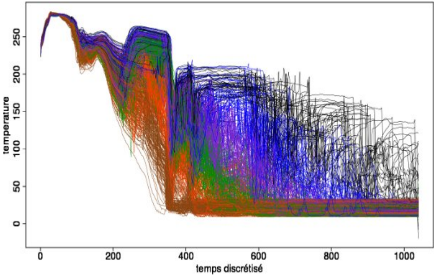


FIG.: Nadaraya-Watson

Test II - temperature curves

600 model runs,
11 dimensions on input,
414 discretization points.



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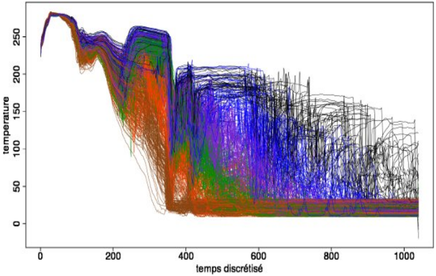

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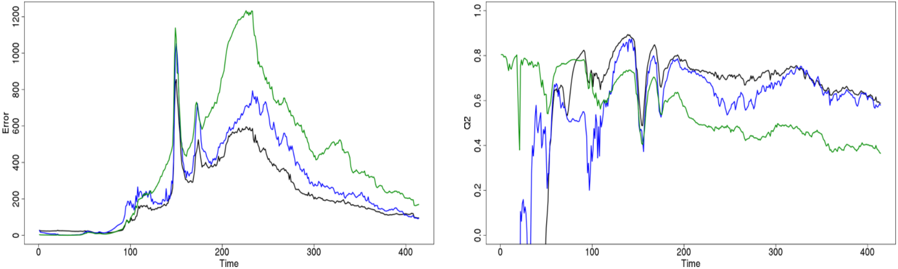

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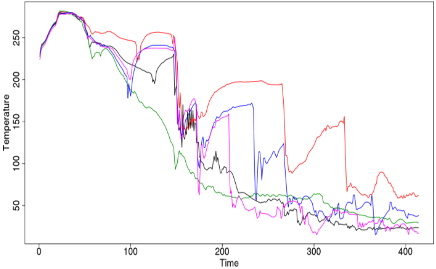

FIG.: Real curves

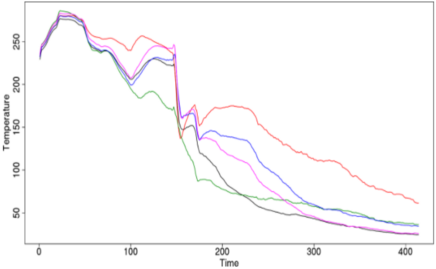

FIG.: PCA red. dim.

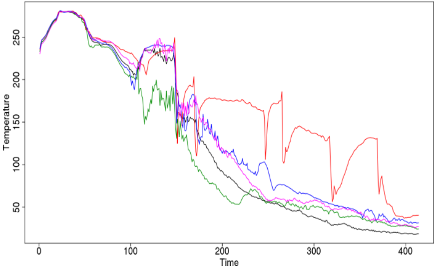

FIG.: RML red. dim.

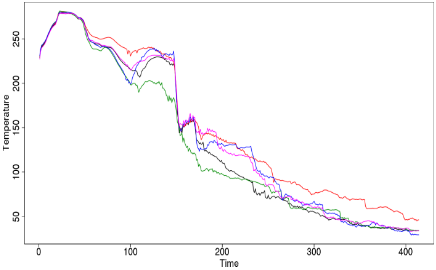

FIG.: Nadaraya-Watson

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The model is good enough regarding to the industrial context.

$\Rightarrow$ help to the projet DDVCV (life span of reactor vessels).

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Linear (PCA) and non-linear : complementary.

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. . .and some parameters which should be "optimized" automatically.

Future research : "functional" principal curves and surfaces.

Example of a principal surface in $2D$: