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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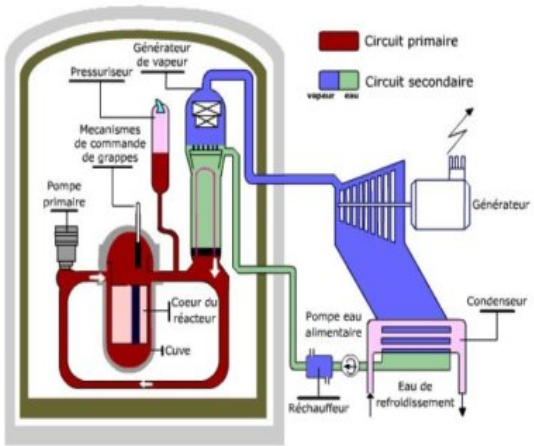
Modelling



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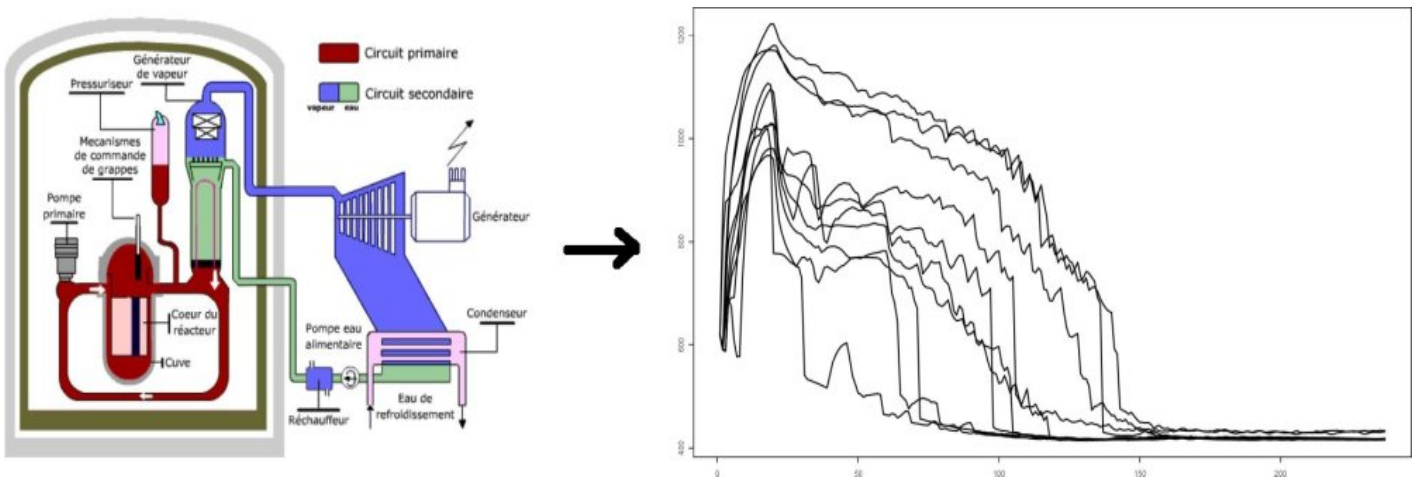

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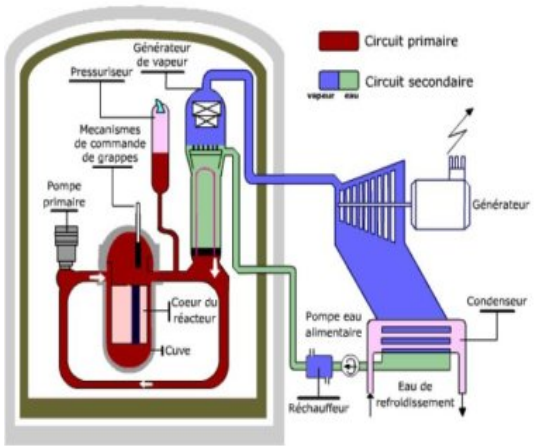

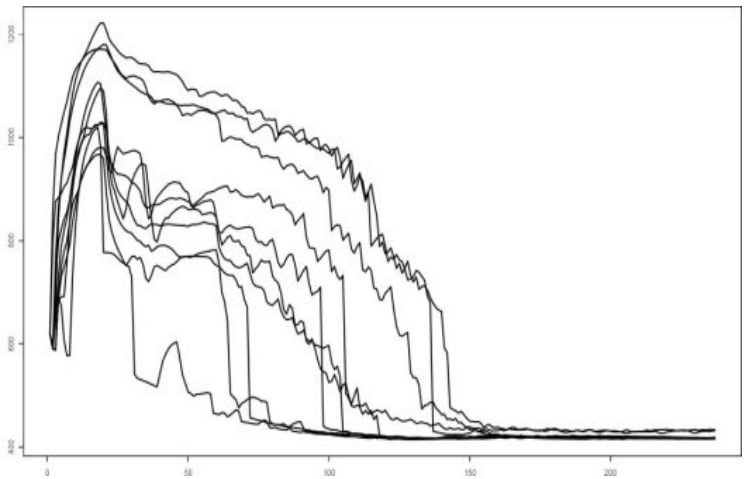

$\longrightarrow$ Sensitivity analysis, uncertainty propagation

...

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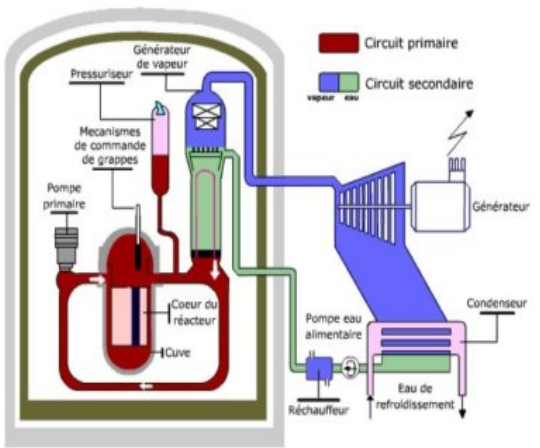
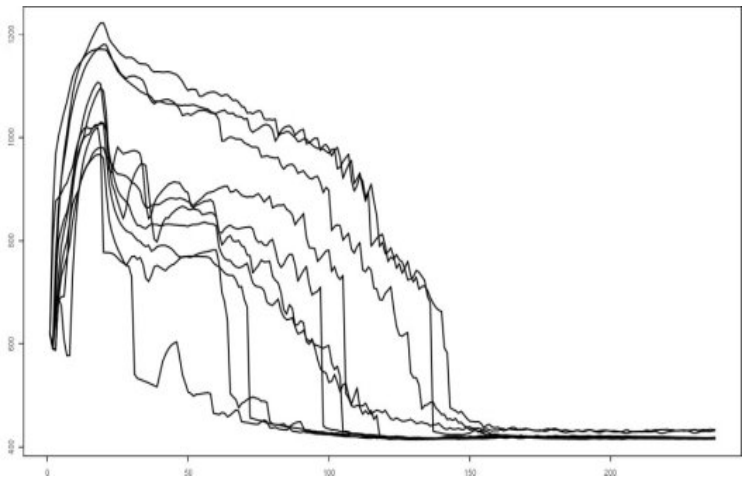




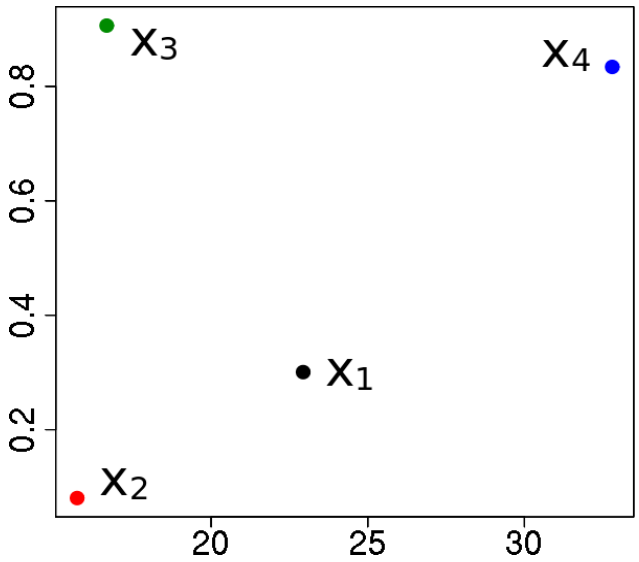
$\longrightarrow$ Sensitivity analysis, uncertainty propagation ...

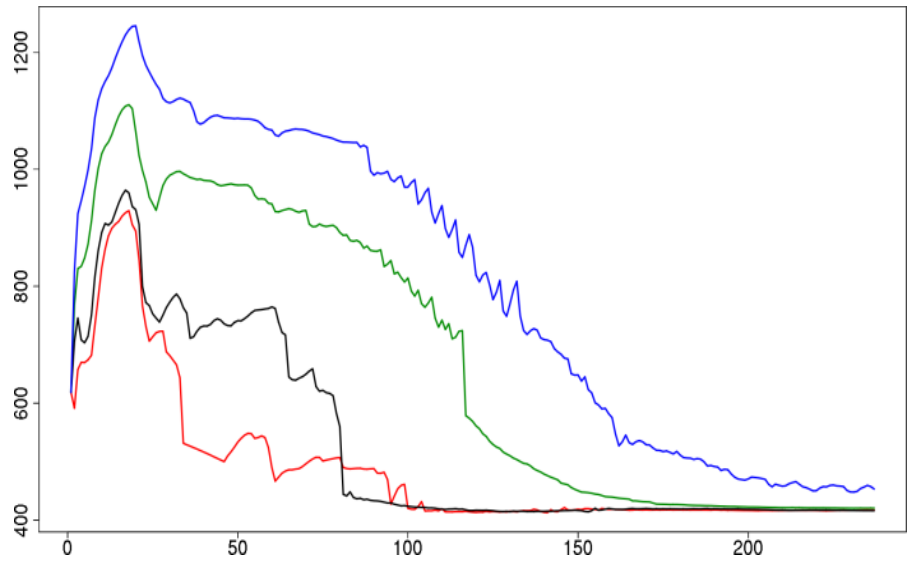
Improve the simulation stage to allow accurate computations

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 ;
- Outputs $y_i \in \mathcal{C}([a, b], \mathbb{R})$ = evolutions of parameters.





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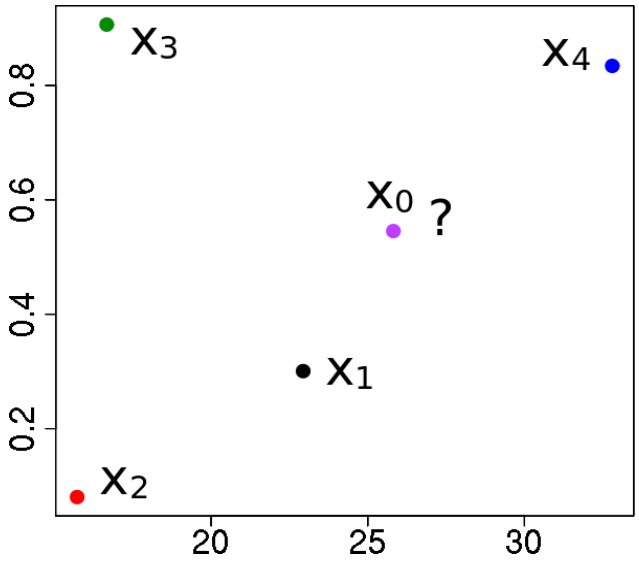
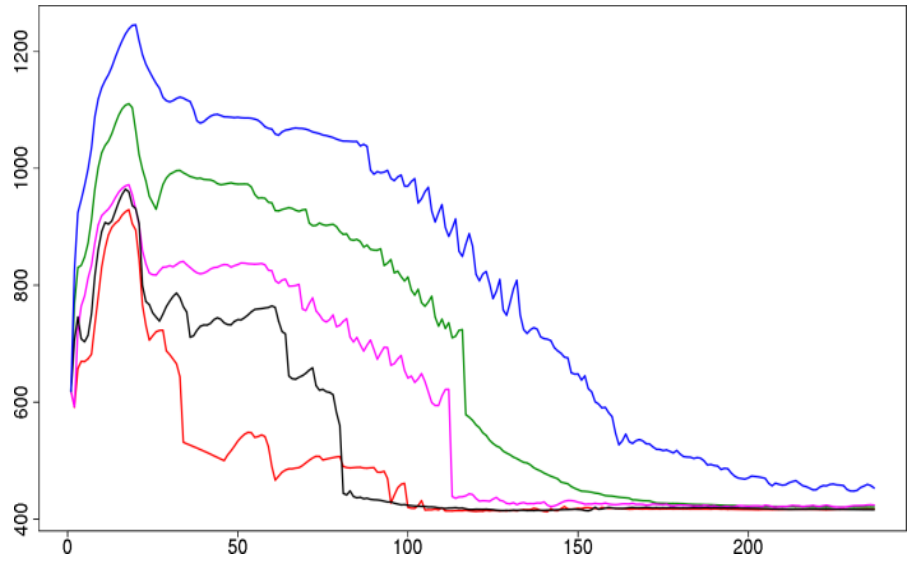
$$y^{\text{new}} \simeq \varphi(x^{\text{new}}) .$$





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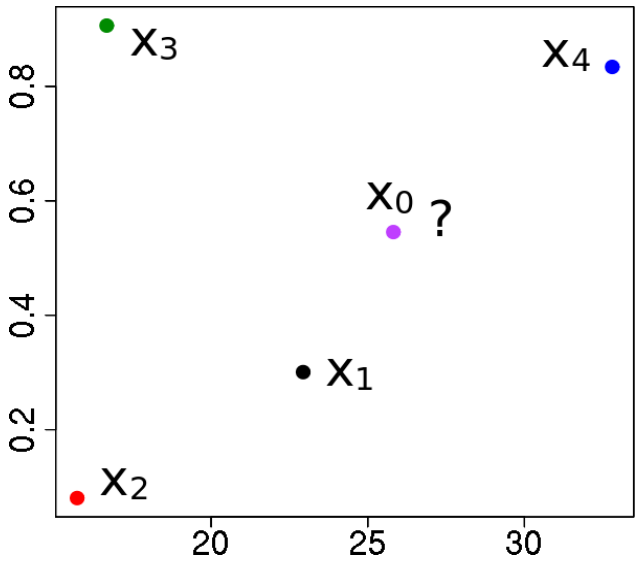

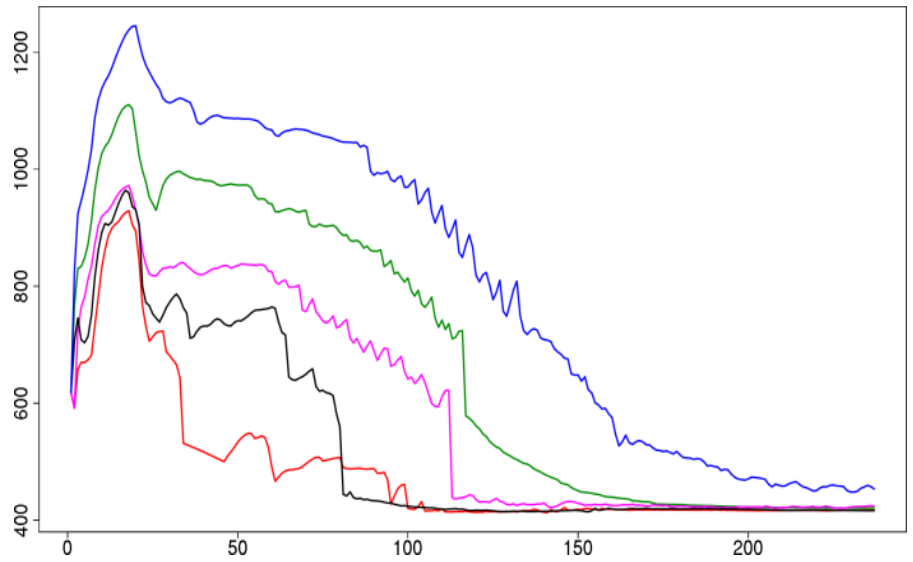

Statistical learning "regression" $\mathbb{R}^p \longrightarrow \mathcal{C}([a, b], \mathbb{R})$

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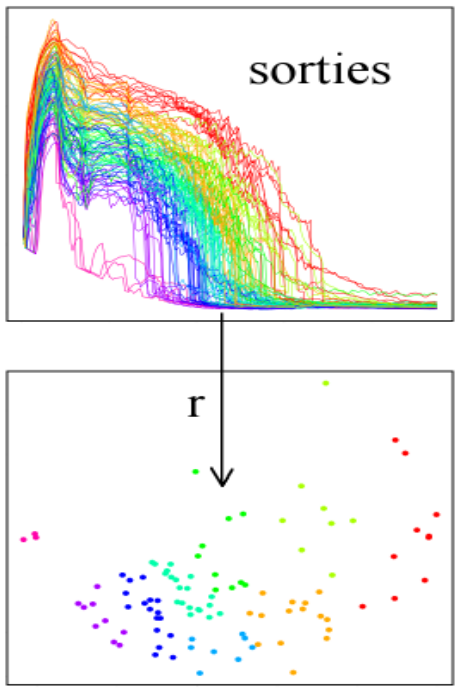

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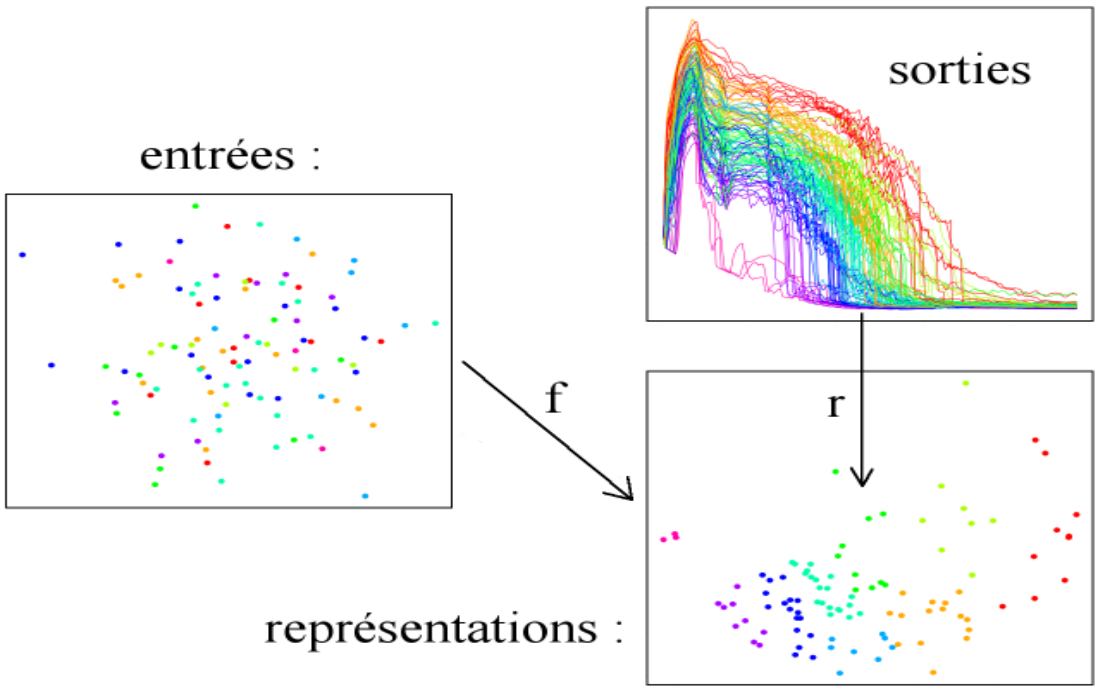

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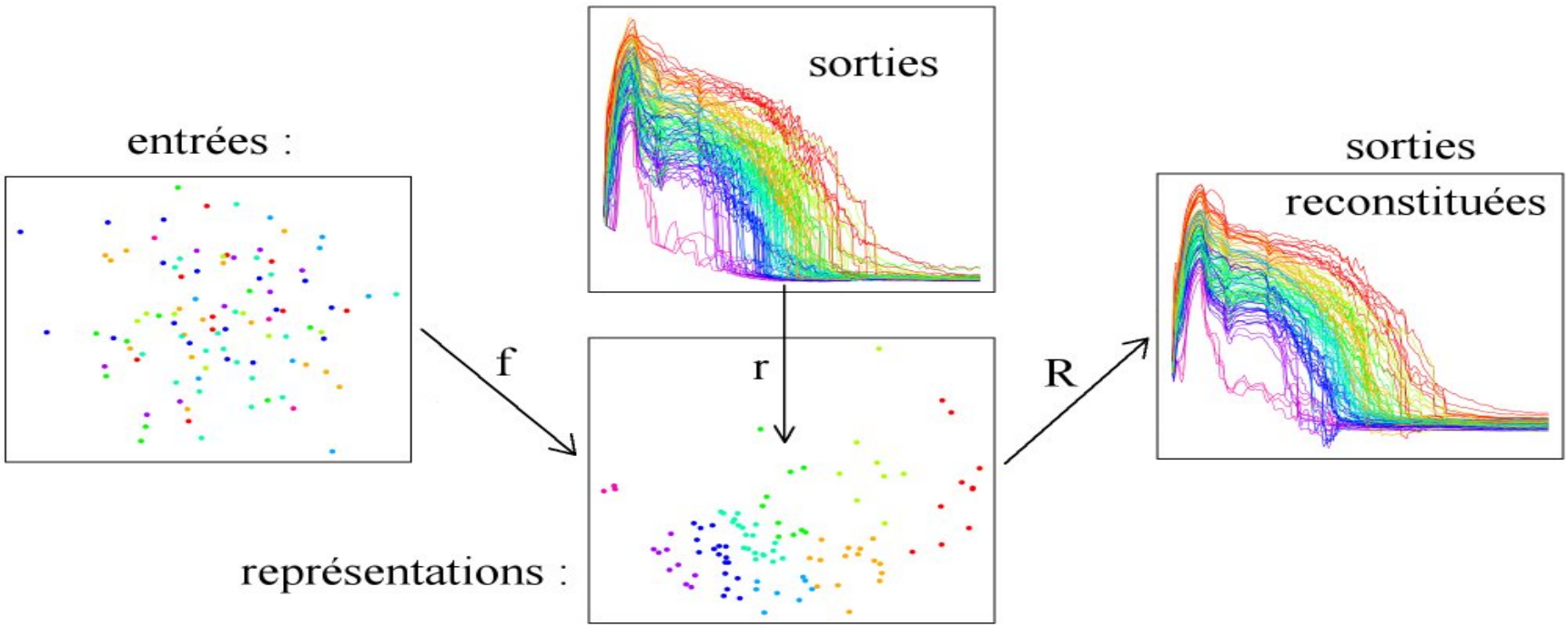

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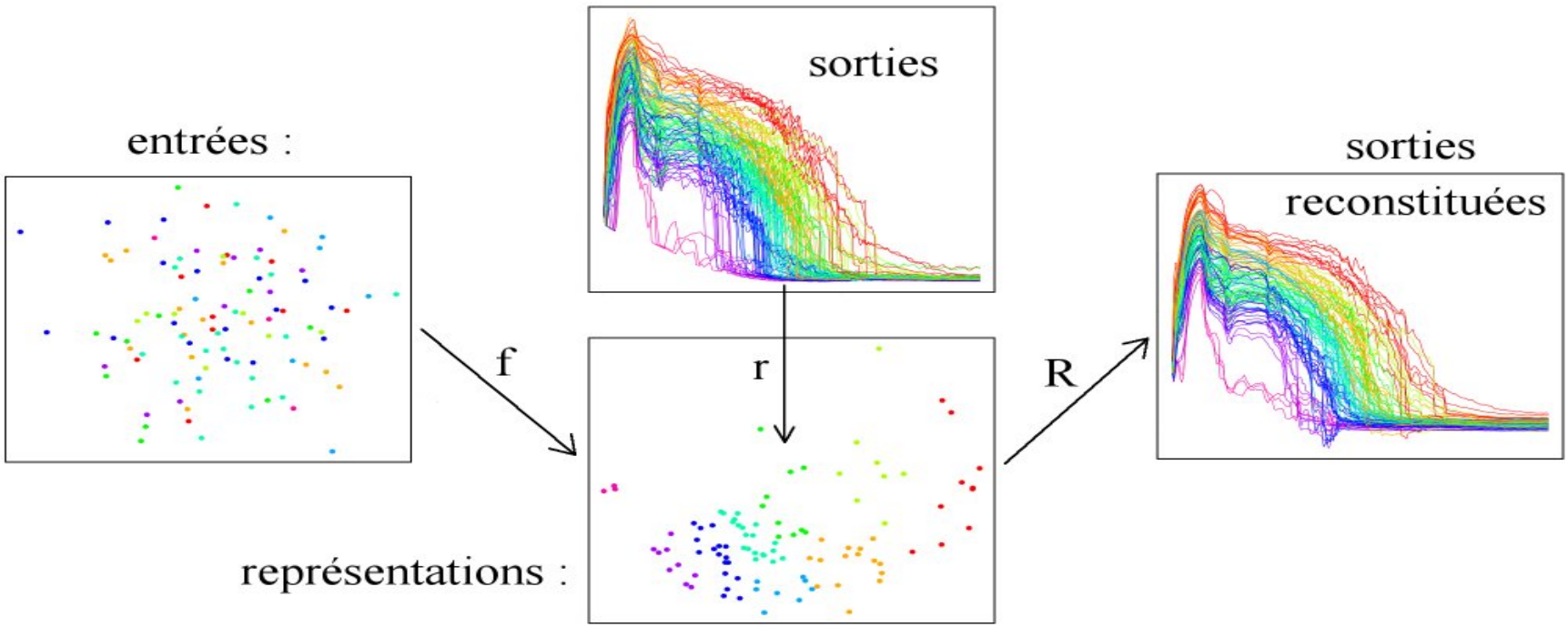

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(More or less) classical methods

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

- simplify the model ;
- avoid overfitting,

while keeping good performances.

1. Riemannian Manifold Learning

2. Applications

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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) ;

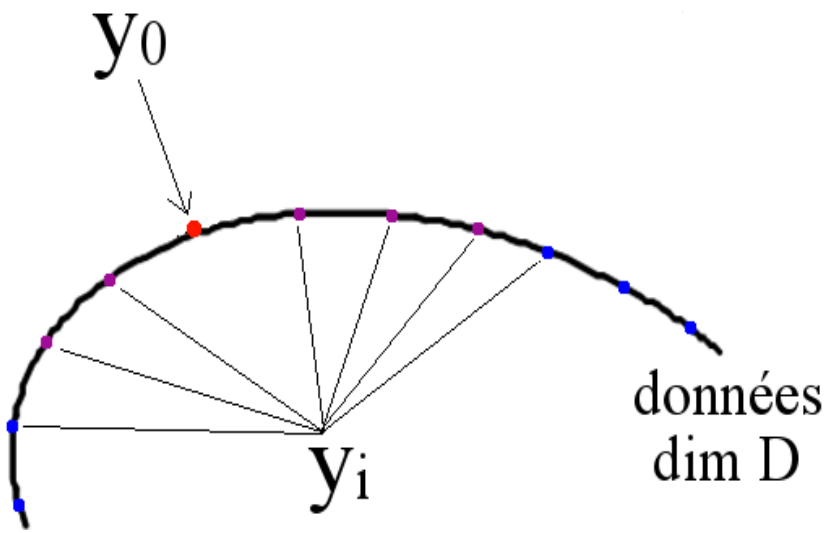

FIG.: Origin curve y_0

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1. choose an origin curve y_0 among the y_i, (e.g., the mean) ;
2. determine a local basis $Q_0 = (e_1, \ldots, e_d)$ for the tangent space at y_0 (PCA on the neighborhoods curves) ;

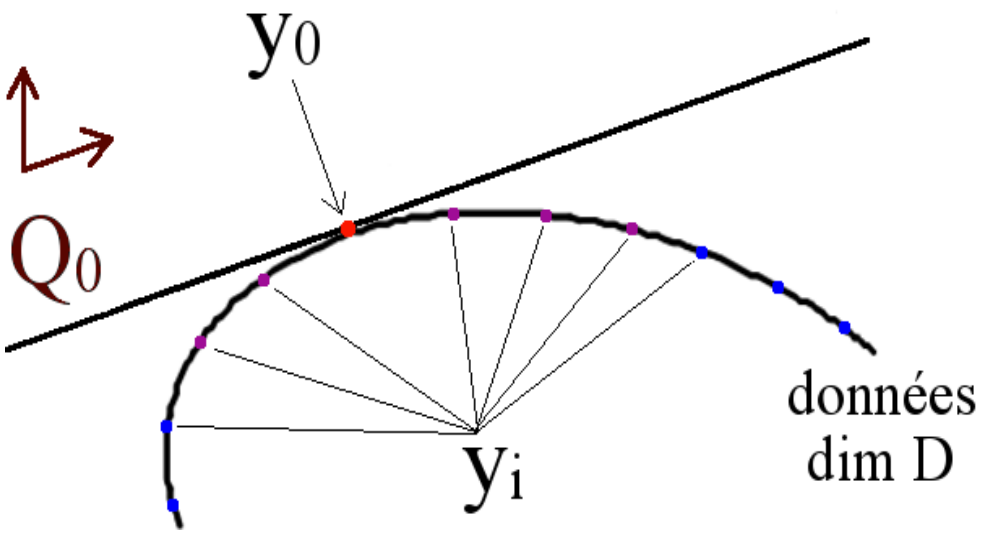

FIG.: Tangent plane at y_0 + local basis Q_0

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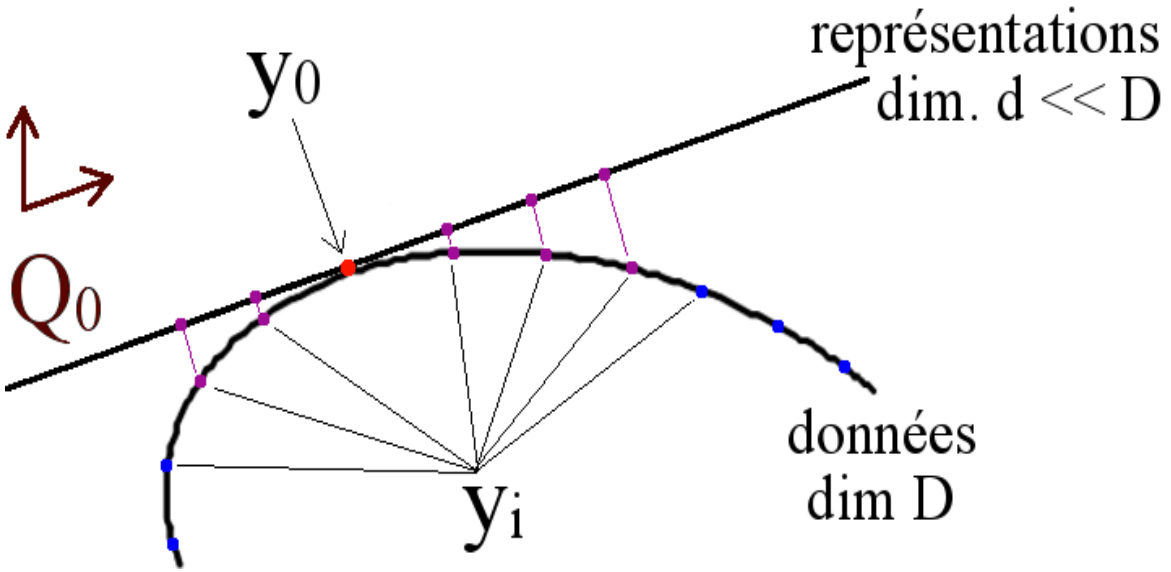

FIG.: Local coordinates z_i on the tangent plane

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4. then normalize to verify the identity $\|y - y_0\| = \|x - x_0\|$.

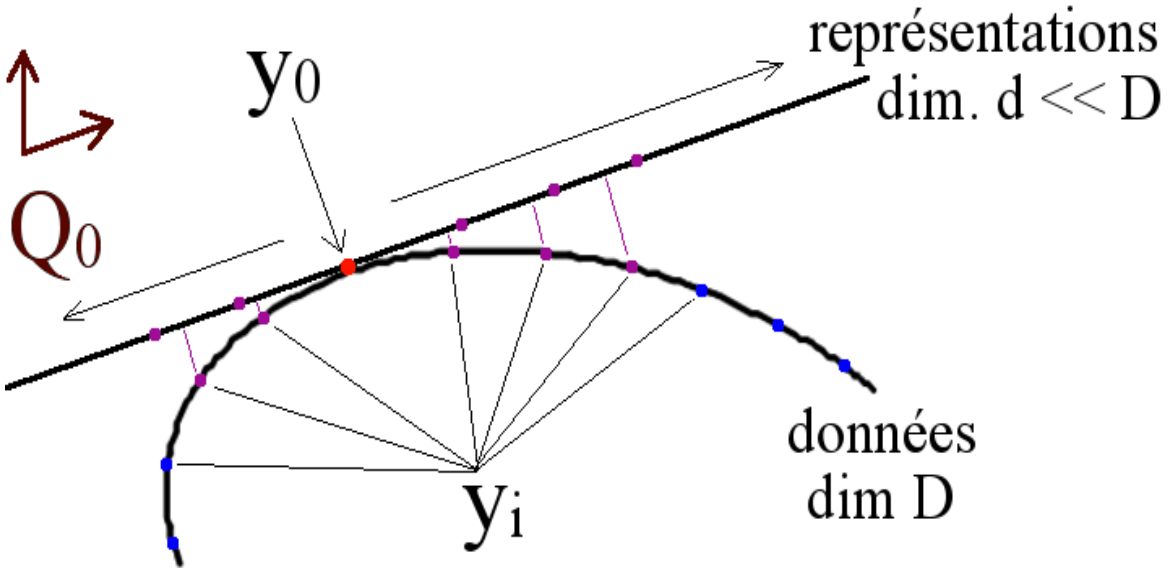
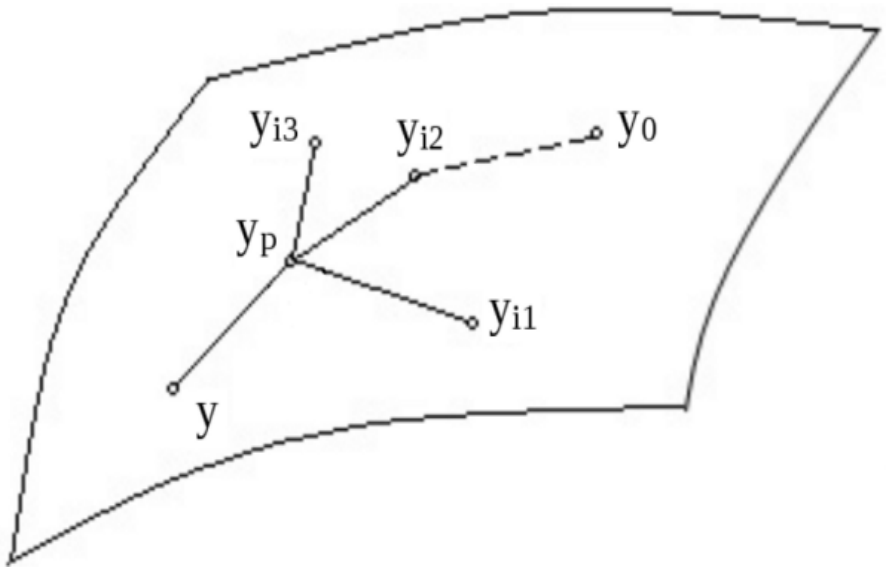


FIG.: Normalization of coordinates z_i

"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
- $y_{i_1}, \ldots, y_{i_d}$ = neighbors of y_p for which the z_i coordinates are known (breadth-first)



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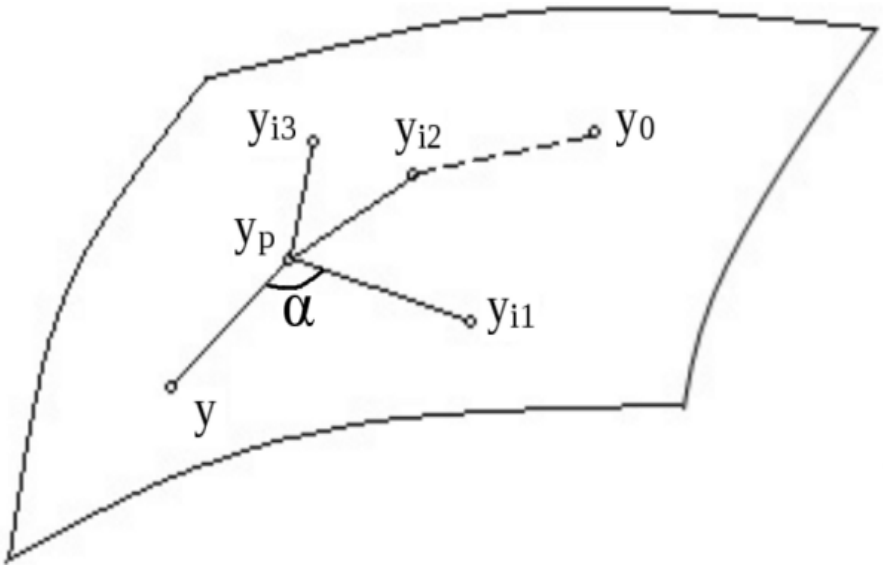
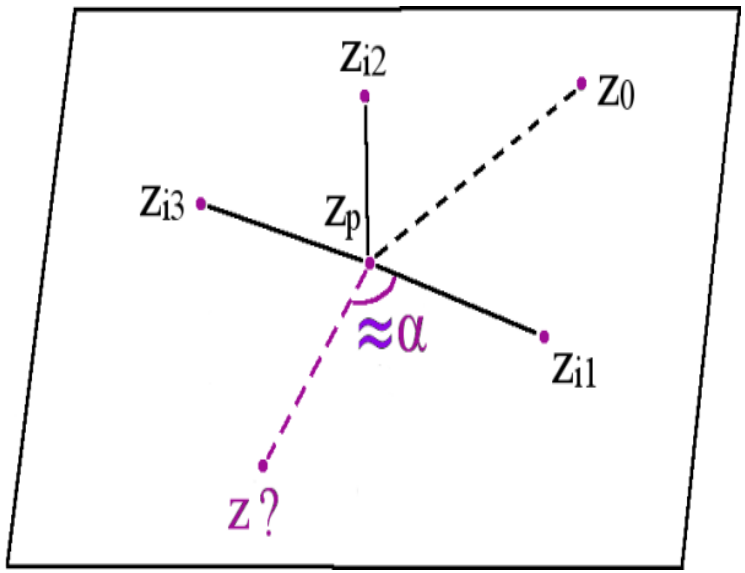
$z = r(y)$ computed by..

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





Examples

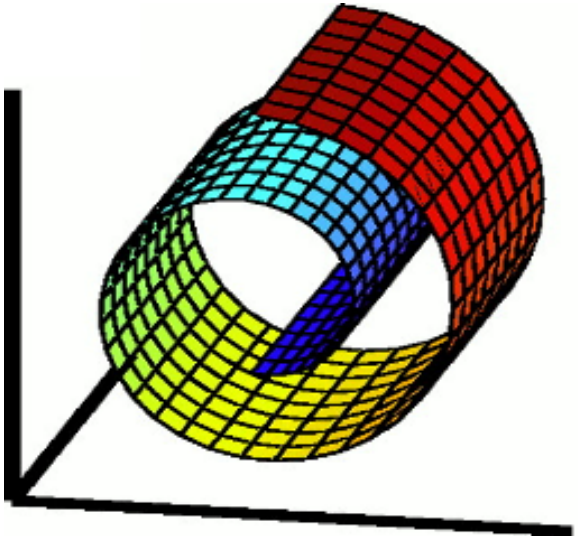


FIG.: 3D Swissroll, 400 points

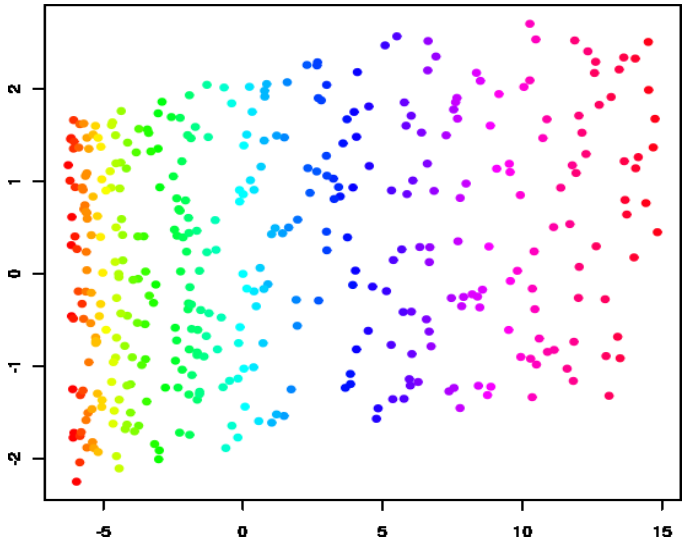


FIG.: RML Representation

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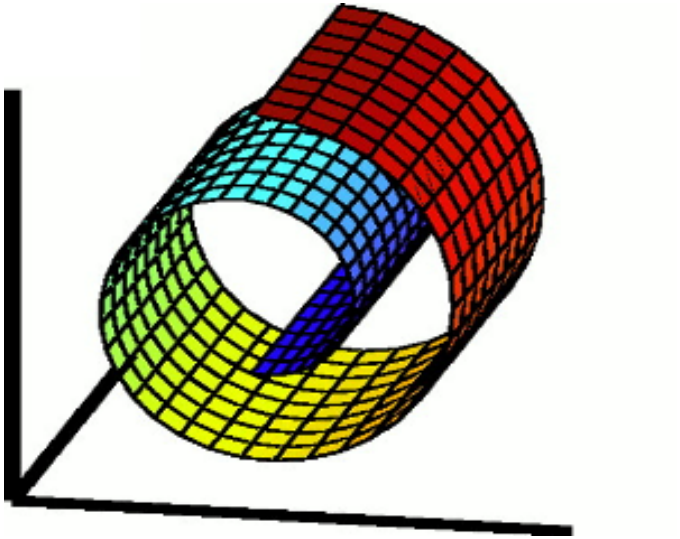

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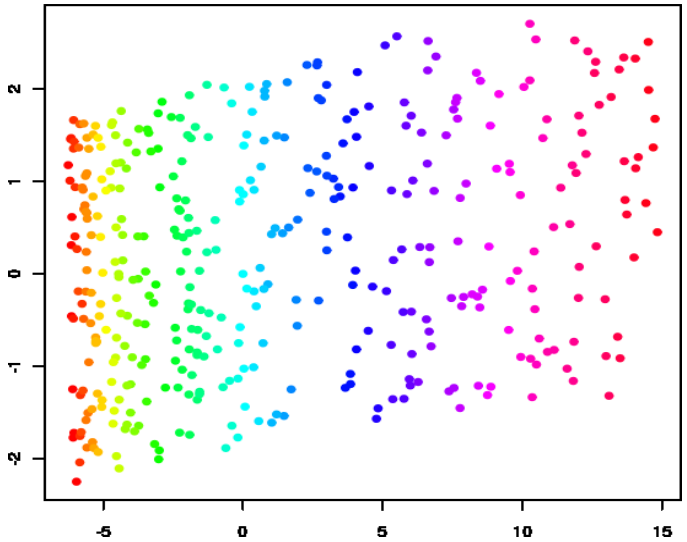

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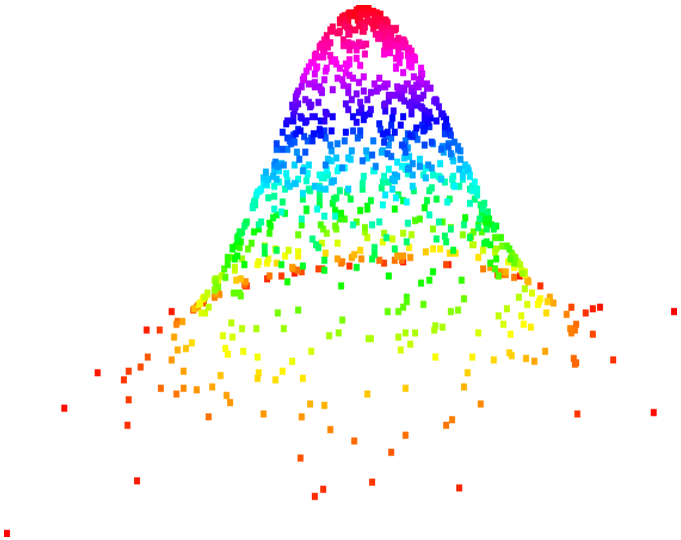
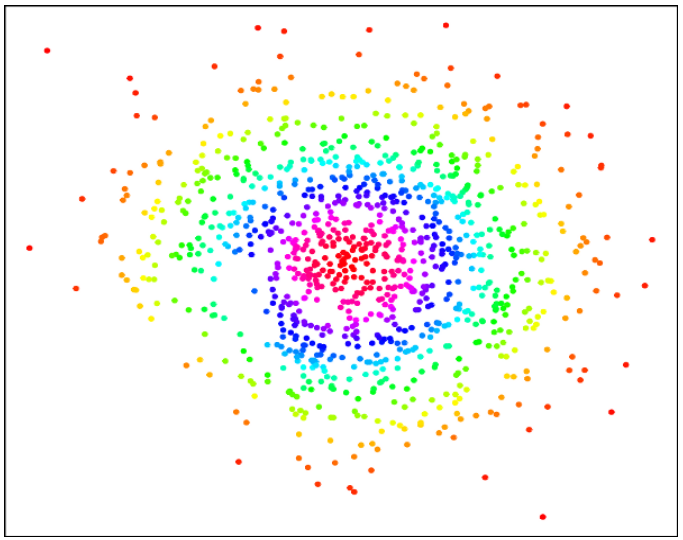


FIG.: 3D Gaussian, 1000 points



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1 Riemannian Manifold Learning

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

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

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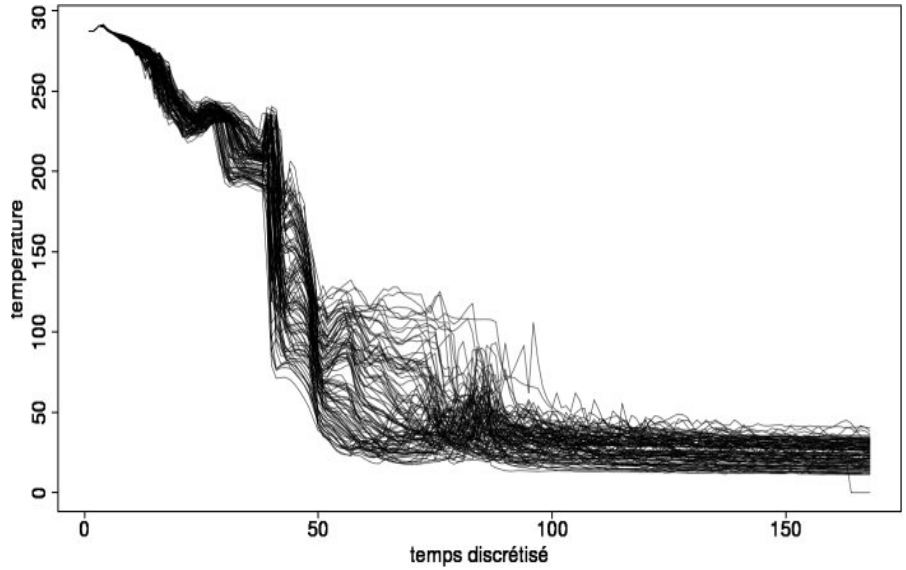
$$Q_2[j] = 1 - \frac{m.MSE[j]}{\sum_{i=1}^{m}(\bar{y}(j) - y'_i(j))^2} \text{ (compararison to the mean)}.$$

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

$\simeq 1 \Rightarrow$ perfect model.

Test I - temperature curves

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



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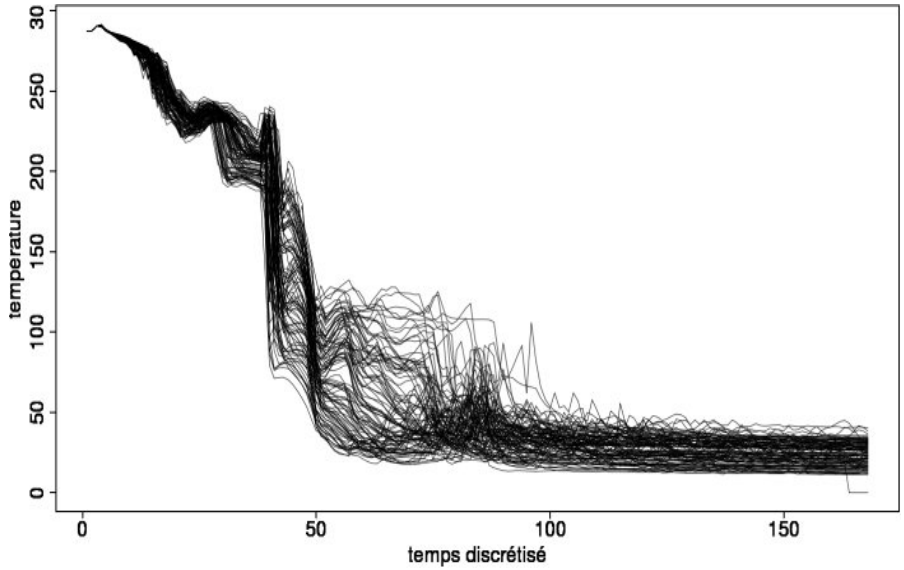
cross validation
leave-10-out :

MSE at l., Q_2 at r. ; $\boxed{d = 4}$



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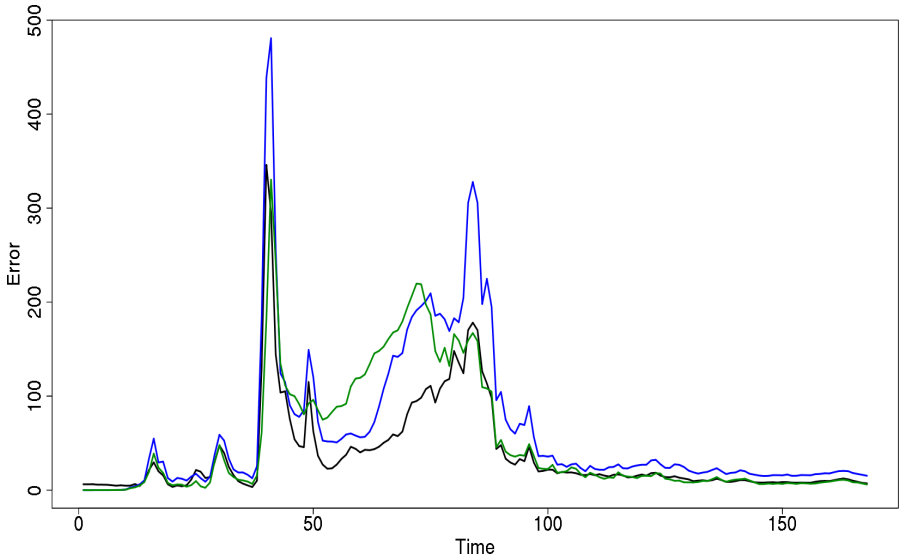

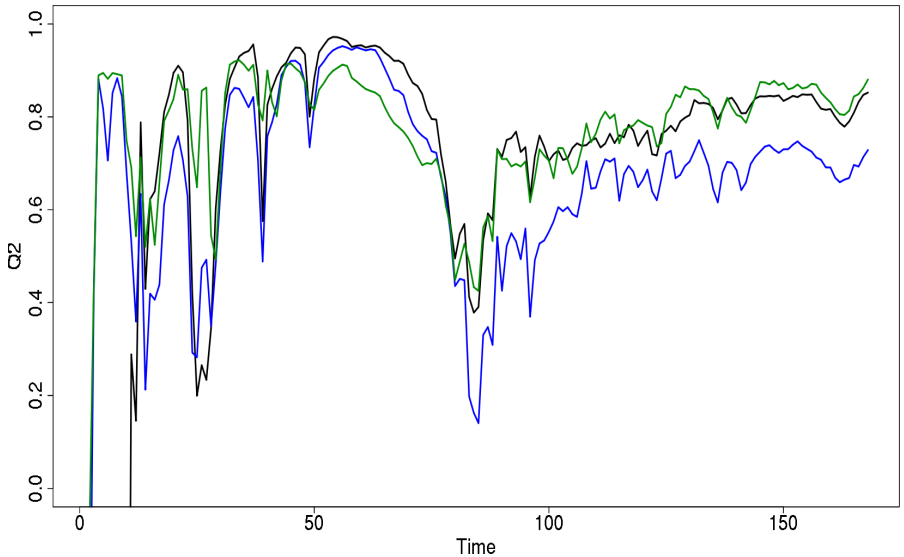

FIG.: Black : functional PCA ; blue : RML ; green : Nadaraya-Watson.

5 predicted curves

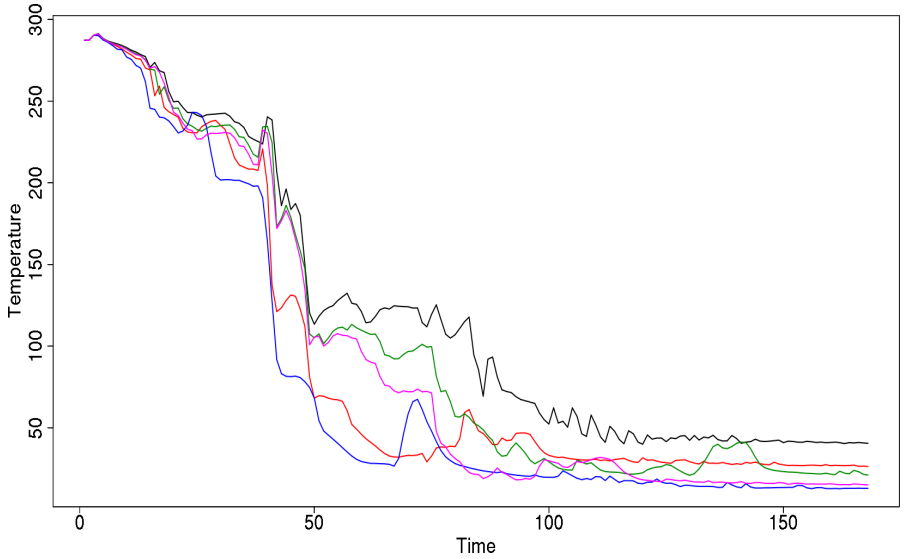

FIG.: Real curves

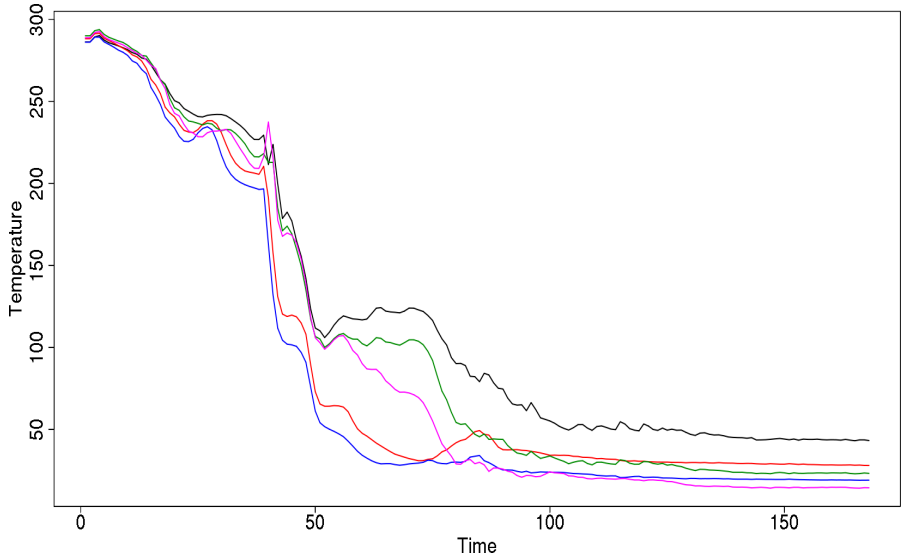

FIG.: PCA dim. red.

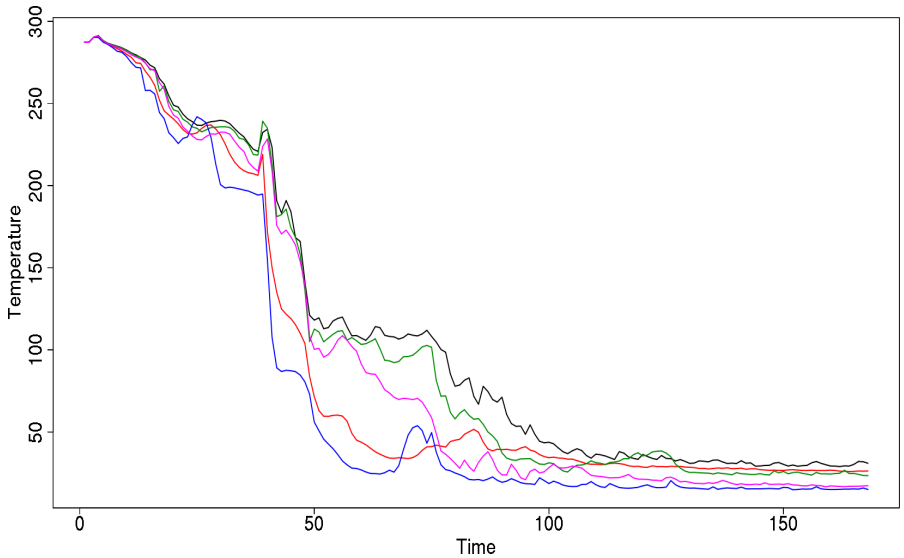

FIG.: RML dim. red.

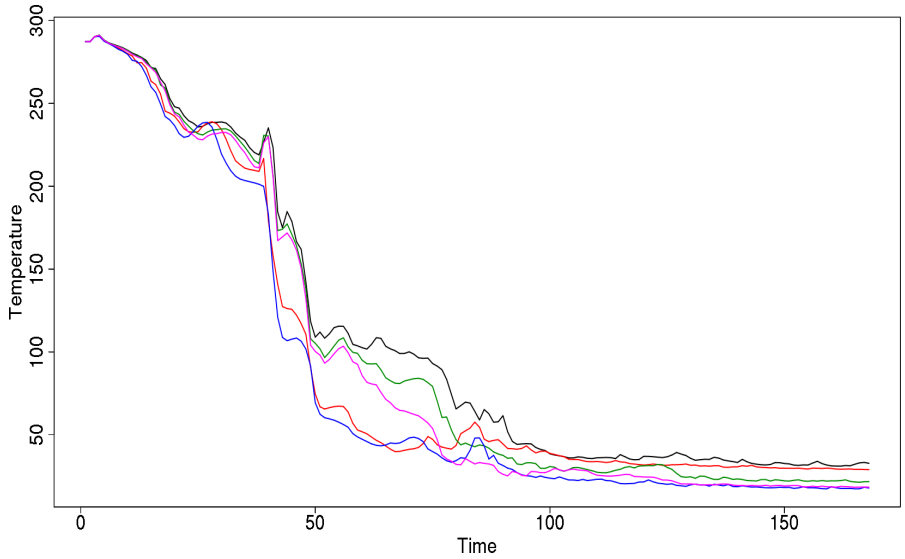

FIG.: Nadaraya-Watson

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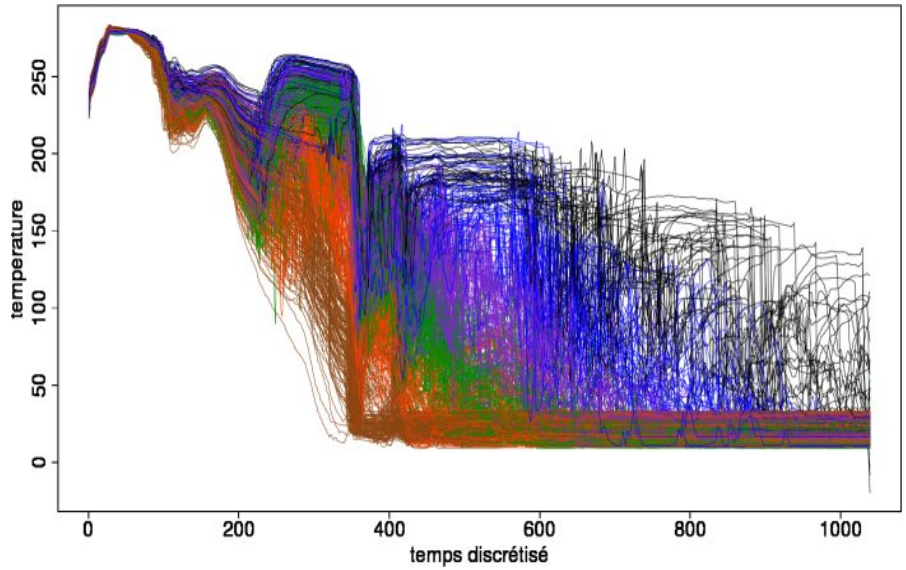

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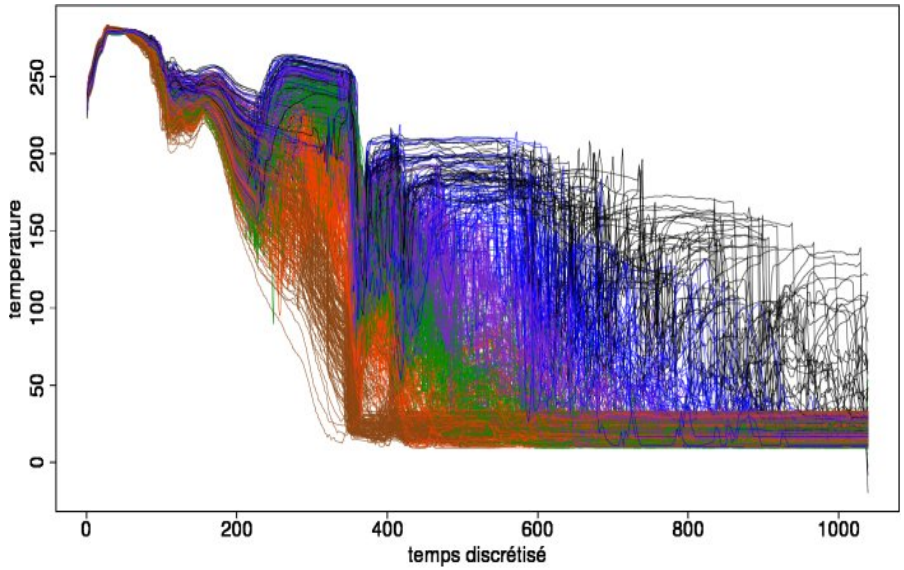
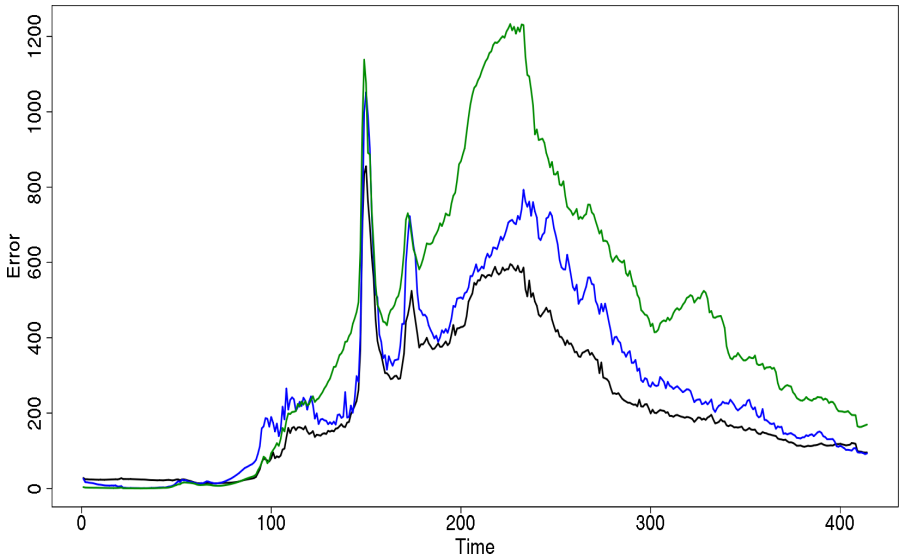


FIG.: The 600 code outputs



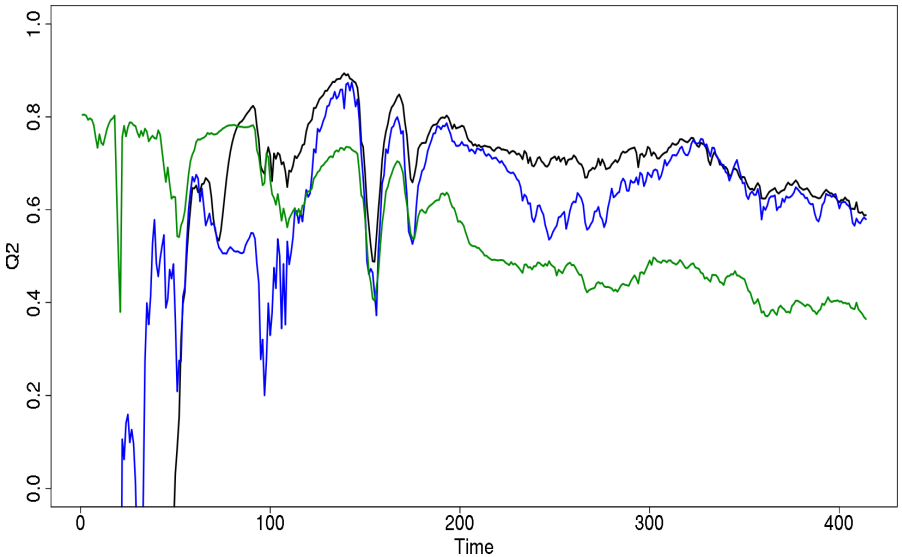


FIG.: Black : functional PCA ; blue : RML ; green : Nadaraya-Watson.

5 predicted curves

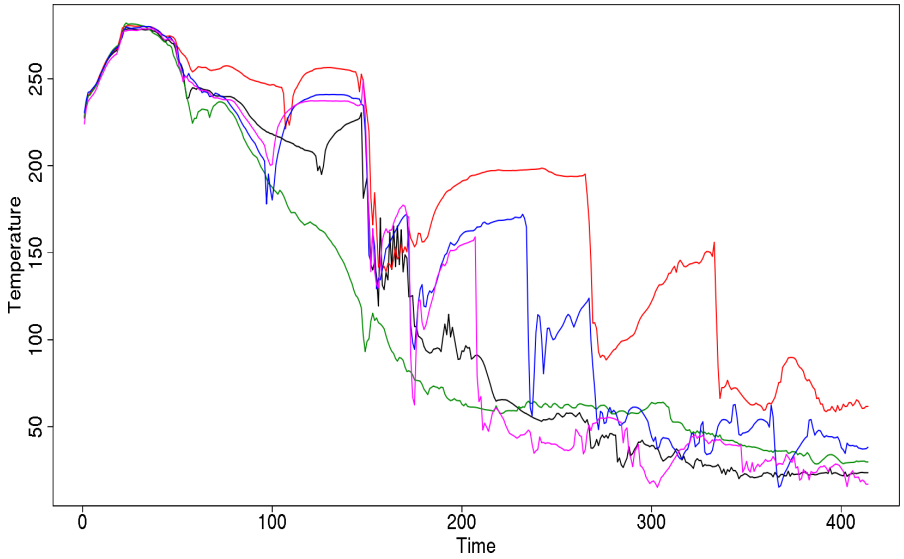


FIG.: Real curves

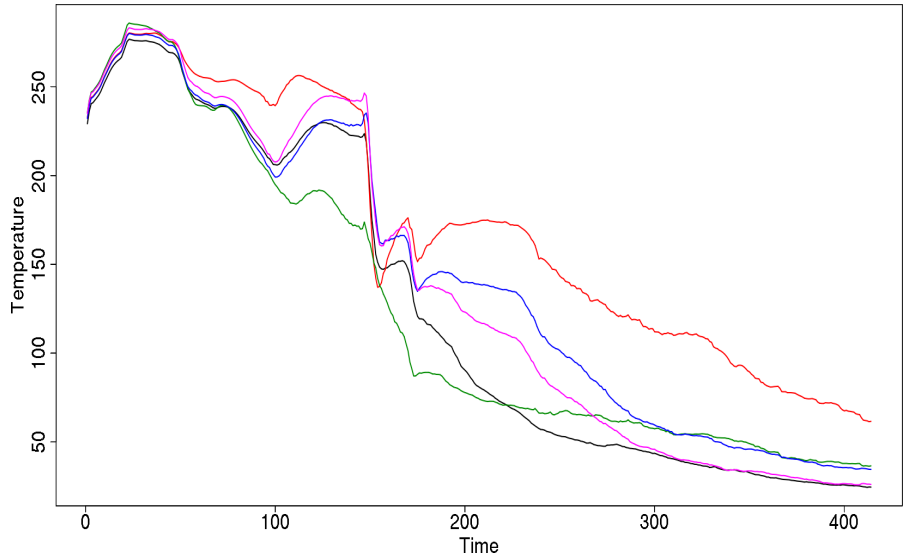


FIG.: PCA red. dim.

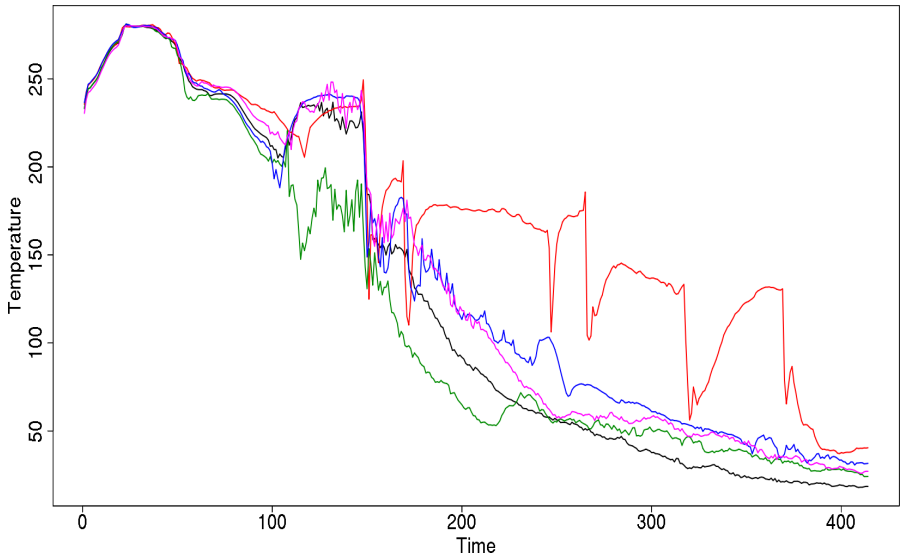


FIG.: RML red. dim.

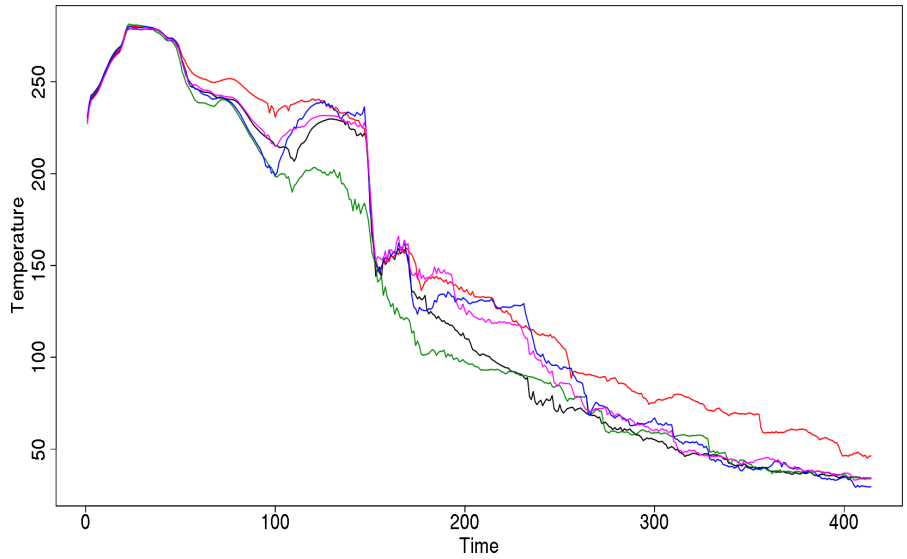


FIG.: Nadaraya-Watson

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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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Future research : "functional" principal curves and surfaces.

Example of a principal surface in $2D$: