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Averaging time series

Application: clustering time series 00000000

Barycentres de séries temporelles : une nouvelle approche basée sur la méthode de la signature Journées MAS (Modélisation Aléatoire et Statistique) 2022 de la Société de Mathématiques Appliquées et Industrielles

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August 29, 2022, Rouen

Joint work with M. Clausel, K. Usevich, G. Oppenheim, L. Coutin, A. Lejay

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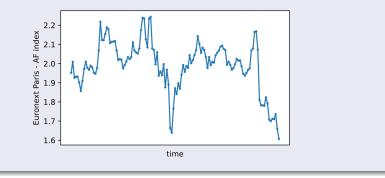
Defining signature barycenters

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#### Time series

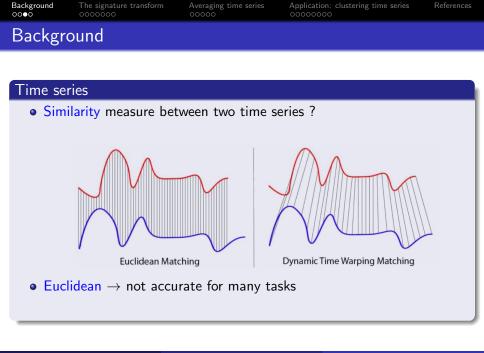


#### $\rightarrow$ sequential data appears in many contexts!

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Defining signature barycenters

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Time se	ries			
<ul> <li>Sim</li> </ul>	ilarity measure bet	ween two time s	eries ?	
	Euclidean Mate	thing	Dynamic Time Warping Matching	



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Time ser	ries			
<ul> <li>Simi</li> </ul>	ilarity measure bet	ween two time s	eries ?	
	Euclidean Mato	ching	Dynamic Time Warping Matching	
• Eucl	lidean  ightarrow not accur	rate for many ta	sks	
Oyn	amic Time Warpin	g (DTW) $ ightarrow$ rel	evant, versatile	J

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• Many useful methods in statistical learning rely on averaging

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- Many useful methods in statistical learning rely on averaging
- **Problem:** how to extend those statistical learning procedure to the time series framework

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- Many useful methods in statistical learning rely on averaging
- **Problem:** how to extend those statistical learning procedure to the time series framework

 $\rightarrow$  How to average a set of time series?

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- Many useful methods in statistical learning rely on averaging
- **Problem:** how to extend those statistical learning procedure to the time series framework

 $\rightarrow$  How to average a set of time series?

#### What has been done?

- Pairwise averaging (with eg. euclidean distance)
- Averaging method using DTW<sup>1</sup>
- Averaging methods on Lie groups

<sup>&</sup>lt;sup>1</sup>Petitjean, F., Ketterlin, A., & Gançarski, P. (2011). A global averaging method for dynamic time warping, with applications to clustering. Pattern recognition, 44(3), 678-693. [PKG11]

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The sig	nature transfo	rm		

#### Definition

• Input: a continuous path  $X:[0,1] 
ightarrow \mathbb{R}^d$ 

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#### Definition

- Input: a continuous path  $X:[0,1] \to \mathbb{R}^d$
- Signature of order *m*:

$$S^{(m)}_{[0,1]}(X) \stackrel{\mathrm{def}}{=} \int_{0 < u_1 < \cdots < u_m < 1} dX_{u_1} \otimes \cdots \otimes dX_{u_m} \in (\mathbb{R}^d)^{\otimes m}$$

with  $\otimes$  the tensor product.

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## The signature transform

#### Definition

- Input: a continuous path  $X:[0,1] 
  ightarrow \mathbb{R}^d$
- Signature of order *m*:

$$S_{[0,1]}^{(m)}(X) \stackrel{\text{def}}{=} \int_{0 < u_1 < \cdots < u_m < 1} dX_{u_1} \otimes \cdots \otimes dX_{u_m} \in (\mathbb{R}^d)^{\otimes m}$$

with  $\otimes$  the tensor product.

• Signature of X is the infinite collection of signatures of all orders:

$${f S}_{[0,1]}(X)=(1,S^{(1)}_{[0,1]}(X),S^{(2)}_{[0,1]}(X),S^{(3)}_{[0,1]}(X),\dots)$$

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Chevyrev, I., & Kormilitzin, A. (2016). A primer on the signature method in machine learning. arXiv preprint arXiv:1603.03788. [CK16]

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## The signature transform





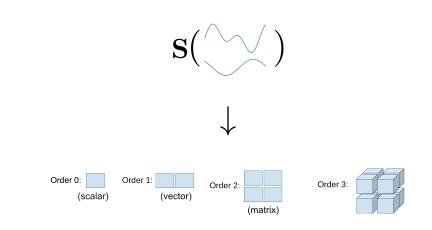
The signature transform

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## The signature transform



• Time series:  $X \in \mathbb{R}^{2 \times 100}$ 

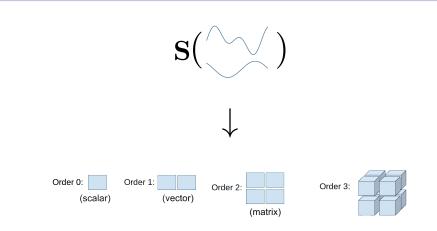
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## The signature transform



- Time series:  $X \in \mathbb{R}^{2 \times 100}$
- Signature:  $S^{(0)} \in \mathbb{R}^0$ ,  $S^{(1)} \in \mathbb{R}^2$ ,  $S^{(2)} \in \mathbb{R}^{2 \times 2}$ ,  $S^{(3)} \in \mathbb{R}^{2 \times 2 \times 2}$ , etc.

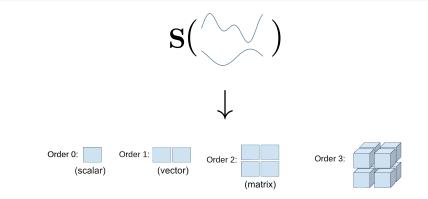
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## The signature transform



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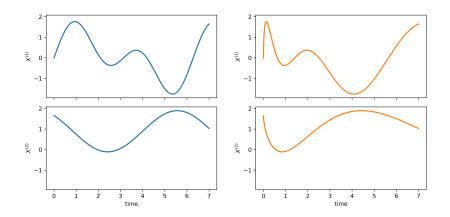
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## The signature transform



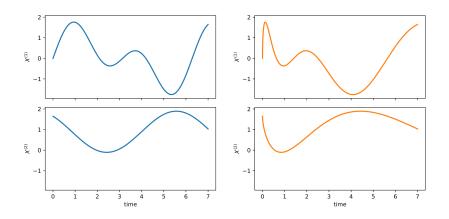
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## The signature transform



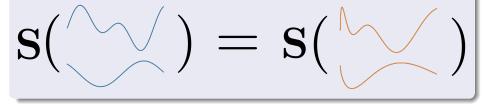
 $\rightarrow$  Same paths, but different time parametrizations!

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#### Fundamental property #1 of the signature transform

• Intrinsic characterization of the path, ignoring translation and time reparametrization: let  $\varphi$  be a reparametrisation

$$\mathbf{S}_{[a,b]}(X_{\varphi(.)}) = \mathbf{S}_{[\varphi(a),\varphi(b)]}(X)$$



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## The signature transform

### Fundamental property #2 of the signature transform

The space of signatures is a non compact Lie group under ⊗ operation<sup>1</sup>.

 $<sup>^{1}\</sup>otimes$  is an abuse of notation: it should be denoted  $\boxtimes$  as it is different from the classical tensor product  $\otimes$ .

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## The signature transform

Fundamental property #2 of the signature transform

The space of signatures is a non compact Lie group under ⊗ operation<sup>1</sup>.

ing time series

 This ⊗ operation is related to the concatenation of two paths through the so-called Chen relation: let 0 ≤ u ≤ 1

$$\mathsf{S}_{[0,1]}(X\star Y)=\mathsf{S}_{[0,u]}(X)\otimes\mathsf{S}_{[u,1]}(Y)$$

 $\mathbf{S}(\mathcal{N}) = \mathbf{S}(\mathcal{N}) \otimes \mathbf{S}(\mathcal{N})$ 

 $<sup>^{1}</sup>$   $\otimes$  is an abuse of notation: it should be denoted  $\boxtimes$  as it is different from the classical tensor product  $\otimes$ .

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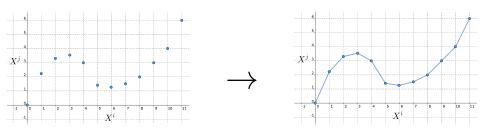
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## The signature transform

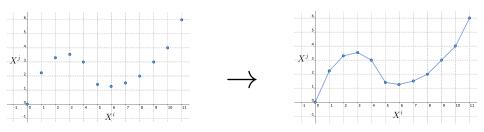


#### $\rightarrow$ linear interpolation

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## The signature transform



 $\rightarrow$  linear interpolation

 $\rightarrow$  why? easy to compute because of Chen relation

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## Averaging time series

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Motivat	ion			

### Why averaging using the signature?

• Invariance to time reparametrization (Fundamental prop. #1)

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## Why averaging using the signature?

- Invariance to time reparametrization (Fundamental prop. #1)
- Suitable for multi-dimensional structure

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#### Why averaging using the signature?

- Invariance to time reparametrization (Fundamental prop. #1)
- Suitable for multi-dimensional structure
- deal with time series of different lengths
- deal with missing values

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#### Why averaging using the signature?

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 $\rightarrow$  three averaging approaches designed

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- Suitable for multi-dimensional structure
- deal with time series of different lengths
- deal with missing values

 $\rightarrow$  three averaging approaches designed

 $\rightarrow$  all three are based on Fundamental prop. #2: signature  $\in$  Lie group

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Averaging the signature					
Approach 1: the Log Euclidean barycenter					

Let  $x_1, \ldots, x_n$  be *n* multidimensional time series Let  $X_1, \ldots, X_n$  be their linear interpolations Denote  $\mathbb{X}_i = \mathbf{S}_{[0,1]}(X_i)$ .

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Ŭ	Averaging the signature Approach 1: the Log Euclidean barycenter					

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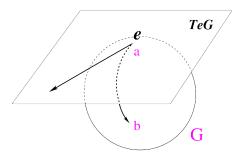


Figure: Lie Group G and its Lie algebra  $T_eG$ .



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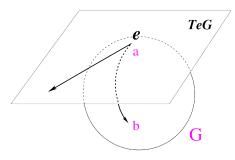
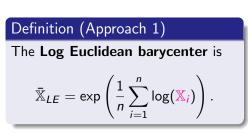


Figure: Lie Group G and its Lie algebra  $T_eG$ .



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Approach 2: the group exponential barycenter

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#### Averaging the signature Approach 2: the group exponential barycenter

#### Definition (Approach 2)

The group exponential barycenter is defined iteratively as following:

• Step 0: initialize  $\overline{\mathbb{X}}_{(0)}$ .

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#### Averaging the signature Approach 2: the group exponential barycenter

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- Step 0: initialize  $\overline{\mathbb{X}}_{(0)}$ .
- Step k:

$$\bar{\mathbb{X}}_{(k+1)} = \bar{\mathbb{X}}_{(k)} \otimes \exp\left(\frac{1}{n} \sum_{i=1}^{n} \log(\bar{\mathbb{X}}_{(k)}^{-1} \otimes \underline{\mathbb{X}}_{i})\right).$$

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#### Averaging the signature Approach 2: the group exponential barycenter

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 $\rightarrow$  Good news: under mild conditions, this algorithm converges!

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# Averaging the signature

Approach 2: the group exponential barycenter

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Pennec & Arsigny (2013). Exponential barycenters of the canonical Cartan connection and invariant means on Lie groups. [PA13, Algorithm 1 & Corollary 5]

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Approach	3: optimization on pat	th space		

#### $\rightarrow$ reconstruction of X given **S**(X): not easy!

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 $x_1, \ldots, x_n$  be *D*-dimensional.  $X_1, \ldots, X_n$  their linear interpolations.

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 Approach 3: optimization on path space

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#### Definition (Approach 3)

The barycenter is the path  $\bar{X} \in \mathbb{R}^{D imes L}$  such that

$$ar{X} = \operatorname*{arg\,min}_X \sum_{i=1}^n d(\mathbf{S}(X), \mathbf{S}(X_i))$$

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 Approach 3: optimization on path space

 $\rightarrow$  reconstruction of X given **S**(X): not easy!

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$$ar{X} = rgmin_X \sum_{i=1}^n d(\mathbf{S}(X), \mathbf{S}(X_i))$$

- Distance d: euclidean, signature distance.
- Optimization: gradient descent.

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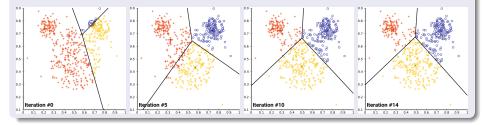
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# K-means clustering

#### • **Goal:** cluster *n* observations $(x_i)_{i=1,...,n}$ into *K* groups.

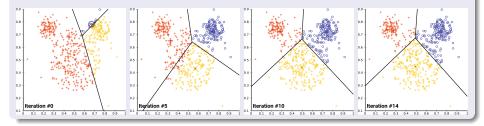
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K-mean	s clustering			
• Goa	al: cluster <i>n</i> observ	vations $(x_i)_{i=1,,i}$	n into K groups.	



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#### K-means clustering

- **Goal:** cluster *n* observations  $(x_i)_{i=1,...,n}$  into *K* groups.
- Two parameters to choose:
  - similarity measure
  - averaging method



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#### Framework

- Dataset: PenDigits<sup>1</sup>
- 11000 bidimensional time series of length 8.

data.shape = (11000, 8, 2)



 $^{1}$ Bagnall et al. 2018. The UEA multivariate time series classification archive.

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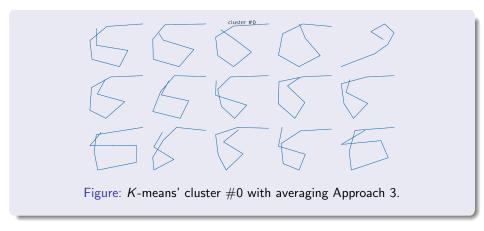
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# Application



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# Application: results

Table: K-means parameters used for benchmark. Pink indicates the use of the signature transform.

Averaging method	Similarity measure
Euclidean barycenter	euclidean
DTW Barycenter Averaging <sup>1</sup>	DTW
Approach 1: log-euclidean	euclidean
Approach 2: group exponential barycenter	euclidean
Approach 3: path space optimization	euclidean

<sup>&</sup>lt;sup>1</sup>Petitjean, F., Ketterlin, A., & Gançarski, P. (2011). A global averaging method for dynamic time warping, with applications to clustering. Pattern recognition, 44(3), 678-693. [PKG11]

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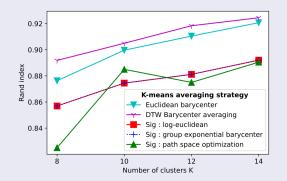
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## Application: results

Averaging method	Similarity measure
Euclidean barycenter	euclidean
DTW Barycenter Averaging	DTW
Approach 1: log-euclidean	euclidean
Approach 2: group exponential barycenter	euclidean
Approach 3: path space optimization	euclidean

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# Conclusion and next steps

# Regarding the clustering of PenDigits

Performances are not state-of-the-art.

• Combine the signature with other clustering algorithms: e.g. Hierarchical clustering, DBSCAN.

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# Conclusion and next steps

#### Regarding the clustering of PenDigits

Performances are not state-of-the-art.

- Combine the signature with other clustering algorithms: e.g. Hierarchical clustering, DBSCAN.
- Use different datasets with various shapes: high-dimensional, long time series (reverse engineering).

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# Conclusion and next steps

# Regarding the clustering of PenDigits

Performances are not state-of-the-art.

- Combine the signature with other clustering algorithms: e.g. Hierarchical clustering, DBSCAN.
- Use different datasets with various shapes: high-dimensional, long time series (reverse engineering).
- Try other similarity measures, more appropriate for the signature.

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# Conclusion and next steps

# Regarding the clustering of PenDigits

Performances are not state-of-the-art.

- Combine the signature with other clustering algorithms: e.g. Hierarchical clustering, DBSCAN.
- Use different datasets with various shapes: high-dimensional, long time series (reverse engineering).
- Try other similarity measures, more appropriate for the signature.

#### Regarding the averaging approaches

- Extend other methods to the time series framework.
- How to represent a barycenter?

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# Thank you!

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- [PA13] Xavier Pennec and Vincent Arsigny. Exponential Barycenters of the Canonical Cartan Connection and Invariant Means on Lie Groups, page 123–166. Springer Berlin Heidelberg, 2013.
- [PKG11] François Petitjean, Alain Ketterlin, and Pierre Gançarski. A global averaging method for dynamic time warping, with applications to clustering. *Pattern Recognition*, 44(3):678–693, Mar 2011.