## A generalized signature method for multivariate time series classification

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SORBONNE UNIVERSITE

## Joint work with



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## Time series classification



Automated medical diagnosis from sensor data

## Time series classification



Characters recognition

## Common feature

The predictor is a path $X:[a, b] \rightarrow \mathbb{R}^{d}$.

## Data representation



A sample from the class flower

## Data representation



A sample from the class flower

## Data representation



A sample from the class flower

$x$ and $y$ coordinates

## Data representation



A sample from the class flower


Time reversed

## Data representation



A sample from the class flower

$x$ and $y$ at a different speed

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$\triangleright$ Independent of time parameterization.
$\triangleright$ Encodes geometric properties of the path.
$\triangleright$ No loss of information.

## Definition and basic properties

## Mathematical setting

- A path $X:[0,1] \rightarrow \mathbb{R}^{d}$. Notation: $X_{t}$.


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- Generalization to $\|X\|_{1 \text {-var }}<\infty$ via the Riemann-Stieltjes integral.


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- Recursively, for $\left(i_{1}, \ldots, i_{k}\right) \in\{1, \ldots, d\}^{k}$,

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S^{\left(i_{1}, \ldots, i_{k}\right)}(X)_{[0, t]}=\int_{0<t_{1}<t_{2}<\cdots<t_{k}<t} d X_{t_{1}}^{i_{1}} \ldots d X_{t_{k}}^{i_{k}} .
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- $S^{\left(i_{1}, \ldots, i_{k}\right)}(X)_{[0,1]}$ is the $k$-fold iterated integral of $X$ along $i_{1}, \ldots, i_{k}$.


## Signature

## Definition

The signature of $X$ is the sequence of real numbers

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S(X)=\left(1, S^{1}(X), \ldots, S^{d}(X), S^{(1,1)}(X), S^{(1,2)}(X), \ldots\right)
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- Tensor notation:

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X^{k}=\sum_{\left(i_{1}, \ldots, i_{k}\right) \subset\{1, \ldots, d\}^{k}} S^{\left(i_{1}, \ldots, i_{k}\right)}(X) e_{i_{1}} \otimes \cdots \otimes e_{i_{k}} .
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where

$$
T\left(\mathbb{R}^{d}\right)=1 \oplus \mathbb{R}^{d} \oplus\left(\mathbb{R}^{d}\right)^{\otimes 2} \oplus \cdots \oplus\left(\mathbb{R}^{d}\right)^{\otimes k} \oplus \cdots
$$

## Example

For $X_{t}=\left(X_{t}^{1}, X_{t}^{2}\right)$,

$$
X^{1}=\left(\begin{array}{ll}
\int_{0}^{1} d X_{t}^{1} & \int_{0}^{1} d X_{t}^{2}
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## Truncated signature

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- Dimension:

$$
s_{d}(m)=\sum_{k=0}^{m} d^{k}=\frac{d^{m+1}-1}{d-1}
$$

## Geometric interpretation



## Important example

## Linear path

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- For any $I=\left(i_{1}, \ldots, i_{k}\right)$,

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$\triangleright$ Very useful: in practice, we always deal with piecewise linear paths.
$\triangleright$ Needed: concatenation operations.

## Properties 1

Chen's identity

- $X:[a, b] \rightarrow \mathbb{R}^{d}$ and $Y:[b, c] \rightarrow \mathbb{R}^{d}$ paths.


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$\triangleright$ We can compute the signature of piecewise linear paths!
$\triangleright$ Data stream of $p$ points and truncation at $m: O\left(p d^{m}\right)$ operations.
$\triangleright$ Fast packages and libraries available in C++ and Python.

## Properties 2

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If $X$ has at least one monotone coordinate, then $S(X)$ determines $X$ uniquely up to translations and reparametrizations.
$\triangleright$ The signature characterizes paths.
$\triangleright$ Trick: add a dummy monotone component to $X$.
$\triangleright$ Important concept of augmentation.

## Properties 3

## Signature approximation

- $D$ compact subset of paths from $[0,1]$ to $\mathbb{R}^{d}$ that are not tree-like equivalent.


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$\triangleright$ Signature and linear model are happy together!
$\triangleright$ This raises many interesting statistical issues.

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$\triangleright$ Flexible tool and many choices: transformations to the path, domain of integration...
$\triangleright$ Could we find a canonical signature pipeline that would be a domain-agnostic starting point for practitioners?

A generalized signature method

## Overview

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- Goal: systematic comparison of the different variations of the signature method.
- Empirical study over 26 datasets of time series classification.
- Define a generalised signature method as a framework to capture all these variations.
- Give practitioners some simple, domain-agnostic guidelines for a first signature algorithm.


## Framework

- Input: a sequence $x \in \mathcal{S}\left(\mathbb{R}^{d}\right)$, where

$$
\mathcal{S}\left(\mathbb{R}^{d}\right)=\left\{\left(x_{1}, \ldots, x_{n}\right) \mid x_{i} \in \mathbb{R}^{d}, n \in \mathbb{N}\right\} .
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Racketsports dataset


A sample $\times$ with $d=6, n=30$

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$\triangleright$ Racketsports dataset: $q=4$
$\rightarrow$ forehand squash, backhand squash, clear badminton, smash badminton.


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$\triangleright$ For some $e, p \in \mathbb{N}$, an augmentation is a map

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Feature set

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$\triangleright$ Data-dependent transformation $\rightarrow$ make the path adapted to signatures.

## Augmentations

- Time augmentation

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\phi(x)=\left(\left(1, x_{1}\right), \ldots,\left(n, x_{n}\right)\right) \in \mathcal{S}\left(\mathbb{R}^{d+1}\right)
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Sample $\mathrm{x} \in \mathcal{S}\left(\mathbb{R}^{6}\right)$


Augmented path $\phi(\mathrm{x}) \in \mathcal{S}\left(\mathbb{R}^{7}\right)$

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Sample $\mathrm{x} \in \mathcal{S}\left(\mathbb{R}^{6}\right)$


Augmented path $\phi(\mathrm{x}) \in \mathcal{S}\left(\mathbb{R}^{7}\right)$
$\triangleright$ Sensitivity to parametrization and ensures signature uniqueness.

## Augmentations

- Lead-lag augmentation

$$
\phi(\mathrm{x})=\left(\left(x_{1}, x_{1}\right),\left(x_{2}, x_{1}\right),\left(x_{2}, x_{2}\right), \ldots,\left(x_{n}, x_{n}\right)\right) \in \mathcal{S}\left(\mathbb{R}^{2 d}\right) .
$$

## Augmentations

- Lead-lag augmentation

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Sample $x \in \mathcal{S}\left(\mathbb{R}^{6}\right)$


Augmented path $\phi(\mathrm{x}) \in \mathcal{S}\left(\mathbb{R}^{12}\right)$

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Sample $\mathrm{x} \in \mathcal{S}\left(\mathbb{R}^{6}\right)$


Augmented path $\phi(\mathrm{x}) \in \mathcal{S}\left(\mathbb{R}^{12}\right)$
$\triangleright$ Captures the quadratic variation of a process.

## Augmentations

- Basepoint augmentation

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\phi(x)=\left(\left(1, x_{1}\right), \ldots,\left(1, x_{n-1}\right),\left(1, x_{n}\right),\left(0, x_{n}\right),(0,0)\right) \in \mathcal{S}\left(\mathbb{R}^{d+1}\right)
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$$

$\triangleright$ Sensitivity to translations.

## Framework

$\triangleright$ For some $e, p \in \mathbb{N}$, an augmentation is a map

$$
=\left(\phi^{1}, \ldots, \phi^{p}\right): S\left(\mathbb{R}^{d}\right) \rightarrow S\left(\mathbb{R}^{e}\right)^{p}
$$

$\triangleright$ For some $q \in \mathbb{N}$, a window is a map

$$
W=\left(W^{1}, \ldots, W^{q}\right): \mathcal{S}\left(\mathbb{R}^{e}\right) \rightarrow \mathcal{S}\left(\mathcal{S}\left(\mathbb{R}^{e}\right)\right)^{q}
$$

## $\triangleright$ Signature or logsignature transform: $S^{m}$.

$\triangleright$ Rescaling operation $\rho$ post or $\rho$ pre.
Feature set

$$
\mathrm{y}_{i, j, k}=\left(\rho_{\text {post }} \circ S^{m} \circ \rho_{\text {pre }} \circ W^{i, j} \circ \phi^{k}\right)(x)
$$

## Windows

- Global window

$$
W(x)=(x) \in \mathcal{S}\left(\mathbb{R}^{e}\right)
$$




## Windows

- Sliding window

$$
W(\mathrm{x})=\left(\mathrm{x}_{1, \ell}, \mathrm{x}_{I+1, l+\ell}, \mathrm{x}_{2 /+1,2 /+\ell}, \ldots\right) \in \mathcal{S}\left(\mathcal{S}\left(\mathbb{R}^{e}\right)\right)
$$






## Windows

- Expanding window

$$
W(x)=\left(x_{1, \ell}, x_{1, l+\ell}, x_{1,2 l+\ell}, \ldots\right) \in \mathcal{S}\left(\mathcal{S}\left(\mathbb{R}^{e}\right)\right)
$$






## Windows

- Dyadic window

$$
W(x)=\left(W^{1}(x), \ldots, W^{q}(x)\right) \in \mathcal{S}\left(\mathcal{S}\left(\mathbb{R}^{e}\right)\right)^{q}
$$





## Framework

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$\triangleright$ Same information and logsignature less dimensional but no linear approximation property.

## Signature versus logsignature

Table 1: Typical dimensions of $S^{m}(x)$ and $\log \left(S^{m}(\mathrm{x})\right)$.

|  | $d=2$ | $d=3$ | $d=6$ |
| :---: | :---: | :---: | :---: |
| $m=1$ | $2 / 2$ | $3 / 3$ | $6 / 6$ |
| $m=2$ | $6 / 3$ | $12 / 6$ | $42 / 21$ |
| $m=5$ | $62 / 14$ | $363 / 80$ | $9330 / 1960$ |
| $m=7$ | $254 / 41$ | $3279 / 508$ | $335922 / 49685$ |

## Framework

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## Empirical study methodology

- 26 datasets: Human Activities and Postural Transitions, Speech Commands and 24 datasets from the UEA archive.


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$\rightarrow 9984$ combinations.


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|  | Window |  |  |  |
| :--- | :---: | :---: | :---: | :---: |
| Dataset | Global | Sliding | Expanding | Dyadic |
| ArticularyWordRecognition | $96.3 \%$ | $89.3 \%$ | $99.0 \%$ | $99.0 \%$ |
| AtrialFibrillation | $46.7 \%$ | $46.7 \%$ | $46.7 \%$ | $60.0 \%$ |
| BasicMotions | $100.0 \%$ | $100.0 \%$ | $100.0 \%$ | $100.0 \%$ |
| CharacterTrajectories | $93.2 \%$ | $94.6 \%$ | $96.9 \%$ | $97.1 \%$ |
| Cricket | $97.2 \%$ | $93.1 \%$ | $97.2 \%$ | $95.8 \%$ |

## Empirical study methodology

- Evaluation of one combination: compute the best accuracy accross the 4 classifiers.
- Compute the average rank over all datasets.

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| Dataset | Global | Sliding | Expanding | Dyadic |
| ArticularyWordRecognition | 3 | 4 | 1.5 | 1.5 |
| AtrialFibrillation | 3 | 3 | 3 | 1 |
| BasicMotions | 2 | 2 | 2 | 2 |
| CharacterTrajectories | 4 | 3 | 2 | 1 |
| Cricket | 1.5 | 4 | 1.5 | 3 |

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| ArticularyWordRecognition | 3 | 4 | 1.5 | 1.5 |
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| CharacterTrajectories | 4 | 3 | 2 | 1 |
| Cricket | 1.5 | 4 | 1.5 | 3 |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ |
|  |  |  |  |  |
| Average ranks | 2.83 | 3.04 | 2.17 | $\mathbf{1 . 7 3}$ |

## Empirical study methodology

- Evaluation of one combination: compute the best accuracy accross the 4 classifiers.
- Compute the average rank over all datasets.
- Use a critical differences plot, a global Friedman test, and pairwise Wilcoxon signed-rank tests at $5 \%$ with Holm's alpha correction.


## Results

$\triangleright$ Windows:


## Results

$\triangleright$ Invariance-removing augmentations:


## Results

$\triangleright$ Other augmentations:


## Results

$\triangleright$ Signature versus logsignature transform:

|  | Signature | Logsignature |
| :--- | :---: | :---: |
| Average ranks | $\mathbf{1 . 2 5}$ | 1.75 |
| p-value |  | 0.01 |

## Results

$\triangleright$ Rescalings:


## Canonical signature pipeline

$\triangleright$ Unless the problem is known to be translation or reparameterisation invariant, then use the time and basepoint augmentations.

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$\triangleright$ Unless the problem is known to be translation or reparameterisation invariant, then use the time and basepoint augmentations.
$\triangleright$ The lead-lag augmentation should be considered, but we do not recommend it in general, due to its computational cost.
$\triangleright$ Use hierarchical dyadic windows, and the signature transform; both have a depth hyperparameter that must be optimised.

## Canonical signature pipeline

$\rightarrow$ Implement this pipeline on the 30 datasets from the UEA archive and compare it to benchmark classifiers.

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- Signatures are a flexible tool.
- We are able to find a canonical signature method that represents a domain-agnostic starting point.
- The combination "signature + generic algorithm" $\approx$ state-of-the-art.
- Few computing resources and no domain-specific knowledge.
- A lot of open questions and potential applications.

Thank you!

