Higher-order iterated sums signatures

WIAS

Leibniz Association

Nikolas Tapia
joint with J. Diehl (Greifswald) and K. Ebrahimi-Fard (NTNU)

FG6

Introduction

Consider a time series

$$x = (x_0, x_1, \ldots, x_N) \in \mathbb{R}^N.$$

The goal is to extract *features* out of x, that are invariant to *time warping*.

Example

We measure the heartbeat in a patient's ECG. This is modelled as

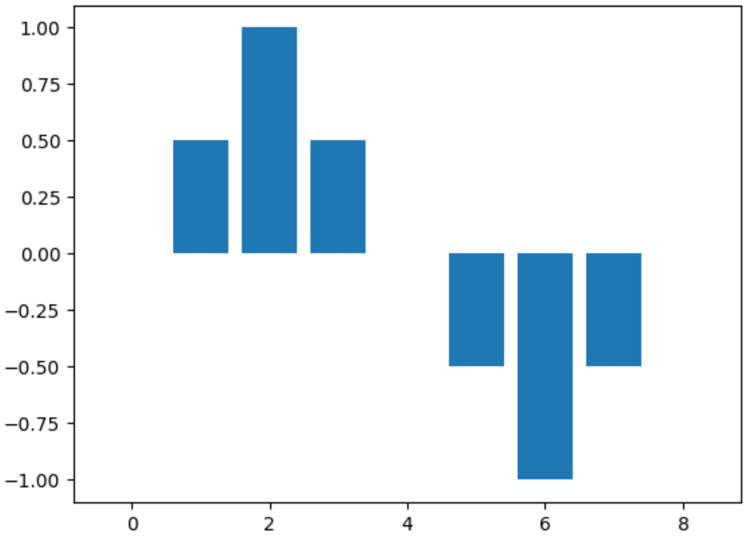
$$y_j^{(k)} = x_{h^{(k)}(j)} + \xi_j^{(k)}, \quad j = 1, \ldots, M; \;\; k = 1, \ldots, K$$

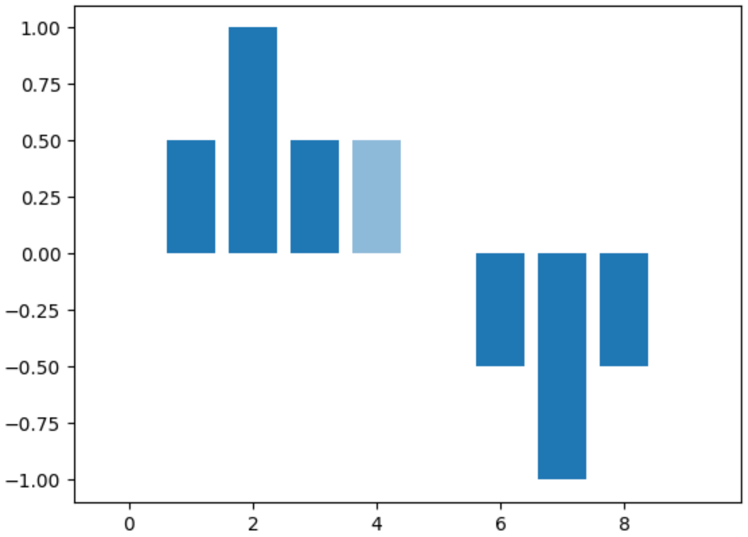
where $M \geq N$ and $h^{(k)}\colon \{1, \ldots, M\} \longrightarrow \{1, \ldots, N\}$ is a (unknown) surjective non-decreasing time change.

Some invariants

Definition

A functional $F : \mathbb{R}^{\mathbb{N}} \longrightarrow \mathbb{R}$ is said to be invariant to *standing still* (or stuttering) if $F \circ \tau_n = F$ for all $n \geq 0$. Here $\tau_n : \mathbb{R}^{\mathbb{N}} \longrightarrow \mathbb{R}^{\mathbb{N}}$ is the operator that acts by repeating the value at time n.





Some invariants

It's not hard to see that the total increment

$$x_N - x_0 = \sum_j (x_j - x_{j-1})$$

as well as

$$\sum_{j<k} (x_j - x_{j-1})(x_k - x_{k-1}), \quad \sum_j (x_j - x_{j-1})^2, \quad \sum_{j \le k} (x_j - x_{j-1})(x_k - x_{k-1})$$

are all features invariant to time warping.

Questions

1. Are all invariants some kind of iterated sum?
2. The last three expressions are linearly dependent since summing the first two gives the third. How to store only linearly independent information?

Quasisymmetric functions

Definition

A formal series $Q \in \mathbb{R}\langle Y_1, Y_2, \ldots \rangle$ is a *quasisymmetric function* if for all indices $i_1 < i_2 < \cdots < i_n$, $j_1 < j_2 < \cdots < j_n$ and integers $\alpha_1, \ldots, \alpha_n \geq 1$ the coefficient of the monomials $(Y_{i_1})^{\alpha_1} \cdots (Y_{i_n})^{\alpha_n}$ and $(Y_{j_1})^{\alpha_1} \cdots (Y_{j_n})^{\alpha_n}$ in Q are equal.

Theorem (Diehl, Ebrahimi-Fard, T. 2019)

Let F be a polynomial functional invariant to standing still and space translations. Then F is realized as a quasisymmetric function on the increments of x.

This answers Question 1.

Monomial basis

Different linear bases are known. Malvenuto and Reutenauer (1995) introduced the *monomial quasisymmetric functions*

$$M_{(\alpha_1,\ldots,\alpha_m)} := \sum_{i_1<\cdots<i_m} (Y_{i_1})^{\alpha_1}\cdots(Y_{i_m})^{\alpha_m}$$

indexed by *compositions* of integers.

Definition

A composition of the integer n is a tuple $(\alpha_1,\ldots,\alpha_m)$ of positive integers such that

$$\alpha_1+\cdots+\alpha_m = n.$$

We call $\ell(\alpha) := m$ the length of the composition and $|\alpha| = n$ its weight.
The collection of all compositions of n is denoted by $\mathcal{C}(n)$.

This answers Question 2.

Quasi-shuffle algebras

The monomial quasisymmetric functions actually form a monomial basis for QSym.

The product is described by *contractions*.

Example

$$M_{(1)}M_{(1)} = 2\sum_{j<k} Y_j Y_k + \sum_j Y_j^2 = 2M_{(1,1)} + M_{(2)}.$$

Example

$$M_{(1)}M_{(3,7)} = M_{(1,3,7)} + M_{(3,1,7)} + M_{(3,7,1)} + M_{(4,7)} + M_{(3,8)}.$$

This is an example of a *quasi-shuffle algebra*.

Quasi-shuffle algebras (cont.)

Definition (Gaines 1994; Hoffman 2000)

Let $\mathfrak{A}$ be an alphabet having a *semigroup* structure $[--] : \mathfrak{A} \times \mathfrak{A} \to \mathfrak{A}$.
On the tensor algebra $T(\mathfrak{A})$ define the *quasi-shuffle product* $*$ recursively by $e * u := u =: u * e$ and

$$ua * vb := (u * vb)a + (ua * v)b + (u * v)[ab]$$

for $u, v \in T(\mathfrak{A})$ and $a, b \in \mathfrak{A}$.

Example

Take $\mathfrak{A} = (\mathbb{N}_+, +)$. Then $\mathbf{1} * \mathbf{1} = 2 \cdot \mathbf{11} + \mathbf{2}$ and

$$\mathbf{1} * \mathbf{37} = \mathbf{137} + \mathbf{317} + \mathbf{371} + \mathbf{47} + \mathbf{38}.$$

Theorem (Hoffman, 2000)

Let $\delta : T(\mathfrak{A}) \to T(\mathfrak{A}) \otimes T(\mathfrak{A})$ be the deconcatenation coproduct. Then, $(T(\mathfrak{A}), *, \delta, |\cdot|)$ is a graded, connected, commutative and non-cocommutative Hopf algebra.

Iterated-sums signature

Notation

We set $A = \{\mathbf{1}, \dots, \boldsymbol{d}\}$ and $\mathfrak{A}$ is the free commutative semigroup over A. For $a = [\boldsymbol{i}_1 \cdots \boldsymbol{i}_\ell] = [\mathbf{1}^{k_1} \cdots \boldsymbol{d}^{k_d}] \in \mathfrak{A}$, let $\Delta x_j^a = \Delta x_j^{\boldsymbol{i}_1} \cdots \Delta x_j^{\boldsymbol{i}_\ell} = (\Delta x_j^{\mathbf{1}})^{k_1} \cdots (\Delta x_j^{\boldsymbol{d}})^{k_d}$.

Definition (Diehl, Ebrahimi-Fard, T. 2019)

For $a_1, \dots, a_p \in \mathfrak{A}$,

$$\langle \mathrm{ISS}(x)_{n,m}, a_1 \cdots a_p \rangle := \sum_{j=n+1}^{m} \langle \mathrm{ISS}(x)_{n,j-1}, a_1 \cdots a_{p-1} \rangle \Delta x_j^{a_p}.$$

Example

$$\langle \mathrm{ISS}(x)_{0,N}, [\mathbf{11}] \rangle = \sum_{j=0}^{N} (\Delta x_j^{\mathbf{1}})^2, \quad \langle \mathrm{ISS}(x)_{0,N}, \mathbf{1}[\mathbf{12}] \rangle = \sum_{1 \le j < k \le N} \Delta x_j^{\mathbf{1}} \Delta x_k^{\mathbf{1}} \Delta x_k^{\mathbf{2}}.$$

Iterated-sums signature (cont.)

We have the factorization

$$\begin{aligned}\mathrm{ISS}(x)_{0,N} &= \varepsilon + \sum_{a\in\mathfrak{A}}\left(\sum_{j=1}^{N}\Delta x_j^{a}\right)a + \sum_{a_1,a_2\in\mathfrak{A}}\left(\sum_{j_1<j_2}\Delta x_{j_1}^{a_1}\Delta x_{j_2}^{a_2}\right)a_1a_2 + \cdots\\ &= \left(\varepsilon + \sum_{a\in\mathfrak{A}}\Delta x_1^{a}a\right)\left(\varepsilon + \sum_{a\in\mathfrak{A}}\Delta x_2^{a}a\right)\cdots\left(\varepsilon + \sum_{a\in\mathfrak{A}}\Delta x_N^{a}a\right)\\ &= \overrightarrow{\prod_{1\le j\le N}}\left(\varepsilon + \sum_{a\in\mathfrak{A}}\Delta x_j^{a}\,a\right)\end{aligned}$$

Compare with

$$S(X)_{0,1} = \overrightarrow{\prod_{1\le j\le N}}\exp_{\otimes}(\Delta x_j) = \overrightarrow{\prod_{1\le j\le N}}\left(\varepsilon + \sum_{\boldsymbol{i}\in A}\Delta x_j^{\boldsymbol{i}}e_{\boldsymbol{i}} + \frac{1}{2}\sum_{\boldsymbol{i}_1,\boldsymbol{i}_2\in A}\Delta x_j^{\boldsymbol{i}_1}\Delta x_j^{\boldsymbol{i}_2}e_{\boldsymbol{i}_1\boldsymbol{i}_2} + \cdots\right) + \cdots$$

Quasi-shuffle algebras (cont.)

Proposition (Diehl, Ebrahimi-Fard, T. 2019)

The Poincaré–Hilbert series of $T(\mathfrak{A})$ *is*

$$H(t) := \sum_{n\geq 0} t^n \dim T(\mathfrak{A})_n = \frac{(1-t)^d}{2(1-t)^d - 1}$$
$$= 1 + dt + \frac{d(3d+1)}{2}t^2 + \frac{d(13d^2+9d+2)}{6}t^3 + O(t^4)$$

Compare with

$$\sum_{n\geq 0} t^n \dim T(A)_n = \frac{1}{1-td} = 1 + dt + d^2t^2 + d^3t^3 + O(t^4).$$

Iterated-sums signature (cont.)

Theorem (Diehl, Ebrahimi-Fard, T. 2019)

For each $n \leq m$, $\mathrm{ISS}(x)_{n,m}$ is a quasi-shuffle character, i.e.

$$\langle \mathrm{ISS}(x)_{n,m}, u * v\rangle = \langle \mathrm{ISS}(x)_{n,m}, u\rangle\langle \mathrm{ISS}(x)_{n,m}, v\rangle$$

for all $u, v \in T(\mathfrak{A})$.

Theorem (Chen's property; Diehl, Ebrahimi-Fard, T. 2019)

For all $n \leq p \leq m$ we have

$$\mathrm{ISS}(x)_{n,p} \otimes \mathrm{ISS}(x)_{p,m} = \mathrm{ISS}(x)_{n,m}$$

Remark

In this case Chow's theorem fails!

$$\log_{\otimes} \mathrm{ISS}(x)_{0,N} = \sum_{j=1}^{N} \Delta x_j^1 \mathbf{1} + \cdots + \sum_{j=1}^{N} \left(\Delta x_j^1\right)^2 \left([\mathbf{11}] - \tfrac{1}{2}\mathbf{11}\right) + \cdots$$

Hoffman's isomorphism

Definition (Hoffman, 2000)

Let $a_1, \dots, a_n \in \mathfrak{A}$. Given $I = (i_1, \dots, i_p) \in C(n)$ define

$$I[a_1 \dots a_n] = [a_1 \cdots a_{i_1}][a_{i_1+1} \cdots a_{i_1+i_2}] \cdots [a_{i_1+\dots+i_{p-1}} \cdots a_n] \in T(\mathfrak{A})$$

Theorem (Hoffman, 2000)

The linear map $\Phi_{\mathrm{H}} : (T(\mathfrak{A}), ⊔⊔, \delta) \to (T(\mathfrak{A}), *, \delta)$ *defined by*

$$\Phi_{\mathrm{H}}(a_1 \cdots a_n) := \sum_{I \in C(n)} \frac{1}{i_1! \cdots i_p!} I[a_1 \cdots a_n]$$

is an isomorphism of Hopf algebras.
Its inverse is given by

$$\Phi_{\mathrm{H}}^{-1}(a_1 \cdots a_n) = \sum_{I \in C(n)} \frac{(-1)^{n-p}}{i_1 \cdots i_p} I[a_1 \cdots a_n].$$

Hoffman's isomorphism (cont.)

Theorem (Diehl, Ebrahimi-Fard, T. 2019)

Let x be a time series and consider the (infinite dimensional) path $(X^a : a \in \mathfrak{A})$ where, for $a = [\mathbf{1}^{k_1} \cdots \mathbf{d}^{k_d}] \in \mathfrak{A}$ the path X^a is the piecewise linear interpolation of the path

$$n \mapsto \sum_{j=1}^{n} \Delta x_j^a = \sum_{j=1}^{n} (\Delta x_j^{\mathbf{1}})^{k_1} \cdots (\Delta x_j^{\mathbf{d}})^{k_d}.$$

Then

$$\langle S(X)_{0,N}, u \rangle = \langle \mathrm{ISS}(x)_{0,N}, \Phi_{\mathrm{H}}(u) \rangle$$

for all $u \in T(\mathfrak{A})$.

Higher-order iterated sums signature

Definition (Diehl, Ebrahimi-Fard, T. 2020+)

Let $1 \leq p \leq \infty$,

$$\mathrm{ISS}^{(p)}(x)_{n,m} := \overrightarrow{\prod_{n<j\leq m}} \left\{ \varepsilon + \sum_{r=1}^{p} \frac{1}{r!} \left(\sum_{a\in\mathfrak{A}} \Delta x_j^a a \right)^{\otimes r} \right\}.$$

Remark

If $1 < p < \infty$, $\mathrm{ISS}^{(p)}(x)$ is not a character for neither $*$ nor $⧢$. Indeed, e.g. $p = 2$,

$$\langle \mathrm{ISS}^{(2)}(x)_{n,m}, \boldsymbol{i} \rangle = \sum_j \Delta x_j^{\boldsymbol{i}},$$

$$\langle \mathrm{ISS}^{(2)}(x)_{n,m}, \boldsymbol{ij} \rangle = \sum_{k_1<k_2} \Delta x_{k_1}^{\boldsymbol{i}} \Delta x_{k_2}^{\boldsymbol{j}} + \frac{1}{2} \sum_k \Delta x_k^{\boldsymbol{i}} \Delta x_k^{\boldsymbol{j}} = \langle \mathrm{ISS}(x)_{n,m}, \boldsymbol{ij} + \tfrac{1}{2}[\boldsymbol{ij}] \rangle.$$

So,

$$\langle \mathrm{ISS}^{(2)}(x)_{n,m}, \boldsymbol{ij} + \boldsymbol{ji} \rangle = \langle \mathrm{ISS}^{(2)}_{n,m}, \boldsymbol{i} \rangle \langle \mathrm{ISS}^{(2)}_{n,m}, \boldsymbol{j} \rangle.$$

Higher-order iterated sums signature (cont.)

Remark (cont.)

$$\langle \mathrm{ISS}^{(2)}(x)_{n,m}, \boldsymbol{i}_1\boldsymbol{i}_2\boldsymbol{i}_3\rangle = \sum_{k_1<k_2<k_3} \Delta x^{i_1}_{k_1}\Delta x^{i_2}_{k_2}\Delta x^{i_3}_{k_3} + \frac{1}{2}\sum_{k_1<k_2}(\Delta x^{i_1}_{k_1}\Delta^{i_2}_{k_1}\Delta x^{i_3}_{k_2} + \Delta x^{i_1}_{k_1}\Delta x^{i_2}_{k_2}\Delta x^{i_3}_{k_2})$$
$$= \langle \mathrm{ISS}(x)_{n,m}, \boldsymbol{i}_1\boldsymbol{i}_2\boldsymbol{i}_3 + \tfrac{1}{2}[\boldsymbol{i}_1\boldsymbol{i}_2]\boldsymbol{i}_3 + \tfrac{1}{2}\boldsymbol{i}_1[\boldsymbol{i}_2\boldsymbol{i}_3]\rangle.$$

So,

$$\langle \mathrm{ISS}^{(2)}(x)_{n,m}, \boldsymbol{i}_1\rangle\langle \mathrm{ISS}^{(2)}(x)_{n,m}, \boldsymbol{i}_2\boldsymbol{i}_3\rangle = \langle \mathrm{ISS}^{(2)}(x)_{n,m}, \boldsymbol{i}_1\boldsymbol{i}_2\boldsymbol{i}_3 + \boldsymbol{i}_2\boldsymbol{i}_1\boldsymbol{i}_3 + \boldsymbol{i}_2\boldsymbol{i}_3\boldsymbol{i}_1 - [\boldsymbol{i}_1\boldsymbol{i}_2]\boldsymbol{i}_3\rangle.$$

Theorem (Diehl, Ebrahimi-Fard, T. 2020+)

We have

$$\langle \mathrm{ISS}^{(p)}(x)_{n,m}, a_1\cdots a_\ell\rangle = \sum_{I\in C_p(\ell)} \frac{1}{i_1!\cdots i_k!}\langle \mathrm{ISS}(x)_{n,m}, I[a_1\cdots a_\ell]\rangle.$$

Hoffmann–Ihara construction

Any invertible formal power series $f(t) = c_1 t + c_2 t^2 + \cdots$ induces a linear *automorphism* on $T(\mathfrak{A})$ by

$$\Phi_f(a_1 \cdots a_n) := \sum_{I \in C(n)} c_{i_1} \cdots c_{i_p} I[a_1 \cdots a_n]$$

with inverse $\Phi_f^{-1} = \Phi_{f^{-1}}$.

Remark

Therefore $\Phi_{\mathrm{H}} = \Phi_{\exp(t)-1}$, $\Phi_{\mathrm{H}}^{-1} = \Phi_{\log(1+t)}$ and $\Phi_p := \Phi_{t+\frac{1}{2}t^2+\cdots+\frac{1}{p!}t^p}$.

Theorem (Diehl, Ebrahimi-Fard, T. 2020+)

We have

$$\langle \mathrm{ISS}^{(p)}(x)_{n,m}, a_1 \cdots a_\ell \rangle = \langle \mathrm{ISS}(x)_{n,m}, \Phi_p(a_1 \cdots a_\ell) \rangle.$$

Twisted quasi-shuffles

Definition (Diehl, Ebrahimi-Fard, T. 2020+)

For $1 \leq p \leq \infty$ and $u, v \in T(\mathfrak{A})$,

$$u \diamond_p v := \Phi_p^{-1}(\Phi_p(u) * \Phi_p(v)).$$

Remark

$\diamond_1 = *$ and $\diamond_\infty = ⧢$.

Theorem

The triple $H_p := (T(\mathfrak{A}), \diamond_p, \delta)$ is a commutative, non-cocommutative, graded and connected Hopf algebra. Moreover, $\Phi_p \colon H_p \to H$ is a Hopf isomorphism.

Corollary (Diehl, Ebrahimi-Fard, T. 2020+)

The iterated-sums signature of order p is a character over H_p.

Definition (Diehl, Ebrahimi-Fard, T. 2020+)

Given $f(t) = c_1 t + c_2 t^2 + \cdots \in t\mathbb{R}[[t]]$,

$$\langle \mathrm{ISS}^{(f)}(x)_{n,m}, w\rangle := \langle \mathrm{ISS}(x)_{n,m}, \Phi_f(w)\rangle$$

As before we define $u \diamond_f v = \Phi_f^{-1}(\Phi_f(u) * \Phi_f(v))$.

Theorem (Foissy, Thibon, Patras 2016)

The triple $H_f := (T(\mathfrak{A}), \diamond_f, \delta)$ is a Hopf algebra, and $\Phi_f : H_f \longrightarrow H$ is a Hopf algebra isomorphism.

Remark

Foissy (2017) characterized *all* possible products on $T(\mathfrak{A})$ compatible with δ. They are given in terms of B_∞-algebras, of which semigroups are a special case.

Higher-order iterated sums signature (cont.)

Corollary (Diehl, Ebrahimi-Fard, T. 2020+)

The higher-order iterated sums signature associated to f is a character over H_f.

The series f also induces a map on tensor space by

$$f_{\otimes}(z) = \sum_{k=1}^{\infty} c_k z^{\otimes k}.$$

Proposition (Diehl, Ebrahimi-Fard, T. 2020+)

We have

$$\mathrm{ISS}^{(f)}(x)_{n,m} = \overrightarrow{\prod_{n<j\leq m}} \left\{ \varepsilon + f_{\otimes}\left(\sum_{a \in \mathfrak{A}} \Delta x_j^a a \right) \right\}.$$

Thanks for your attention

Questions