Generalized expected signatures

Joscha Diehl

University of Greifswald, Germany

January 24, 2023

Let $X : [0,T] \to \mathbb{R}^d$ be a smooth curve. It is well-known that, for various purposes, it is useful to consider its iterated integrals. These are conveniently indexed by words in the alphabet $\{1, \ldots, d\}$,

$$\mathbf{w_1} \cdots \mathbf{w_n} \mapsto \langle S(X)_{0,T}, \mathbf{w_1} \cdots \mathbf{w_n} \rangle := \int_{0 < s_1 < \cdots < s_n < T} dX_{s_1}^{(\mathbf{w_1})} \cdots dX_{s_n}^{(\mathbf{w_n})}$$
$$= \int_{0 < s_1 < \cdots < s_n < T} \dot{X}_{s_1}^{(\mathbf{w_1})} \cdots \dot{X}_{s_n}^{(\mathbf{w_n})} ds_1 \cdots ds_n$$

The object S(X) is Kuo-Tsai Chen's signature, which is defined as an infinite series of iterated-integrals over a path (see [10] for a collection of Chen's works including his seminal papers on integration of paths and related topic). In the last twenty-five years, Chen's signature has received much attention thanks to the seminal work by Terry Lyons (Oxford), which pioneered the development of rough path theory [8]. The latter provides an alternative integration theory for differential equations driven by rough signals such as stochastic processes. Rough paths were generalized by Massimiliano Gubinelli (Oxford) to branched rough paths, which inspired Martin Hairer's work on regularity structures (Fields Medal 2014) [6, 7].

The information contained in the signature of a path can be seen as an analogue to higher order moments of a probability measure. Considering a stream of data as a path, the signature captures significant information about the chronology of the data. This perspective on analyzing data has resulted in a vast amount of papers over the last few years applying so-called signature methods in machine learning algorithms (see [9] for an up-to-date review). More recently, the notion of iterated-sums signature was introduced [5] to deal with the discrete nature of time series.

Signature-type methods are based on rich algebraic, topological and analytic properties of iterated-integrals and sums. In this short note, we present a fragment of a larger project focusing on algebraic aspects related to the notion of expected signature. Let $X: \Omega \times [0,T] \to \mathbb{R}^d$ be a smooth *random* curve. For various applications in stochastic analysis and data science [2, 3, 4, 9], its expected signature

$$\mathbb{E}[S(X)_{0,T}] = \langle\!\langle S(X)_{0,T} \rangle\!\rangle,$$

is of value.

During my visit to NTNU in Trondheim as a TMS guest professor, my host, Kurusch Ebrahimi-Fard, another visitor, Nicolas Gilliers (Toulouse, France), and I were investigating a mathematical object that contains the expected signature, but in fact yields much more information on the stochastic process. Here, I will not report on the *reasons* this larger object appears in our research, but instead will report on its structure.

The goal is finding an algebraic framework to economically describe expressions such as the following

$$\int_{0 < s_1 < s_2 < s_3 < T} \langle \langle \dot{X}^{\mathbf{a}}_{s_1} \dot{X}^{\mathbf{c}}_{s_3} \rangle \rangle \langle \langle \dot{X}^{\mathbf{a}}_{s_2} \rangle \rangle ds_1 ds_2 ds_3.$$

Consider tuples

(v, P),

where $v = \mathbf{v_1} \cdots \mathbf{v_n}$ is a word on the alphabet $\{1, \ldots, \mathbf{d}\}$, and $P = \{P_1, \ldots, P_\ell\}$ is a set-partition of [n]. Let \mathcal{P} be the free \mathbb{R} -module over such tuples, i.e.

$$\mathcal{P} = \bigoplus_{(v,P)} \mathbb{R} \cdot (v,P).$$

Define on it the following shuffle-like operation

$$(\mathbf{v_1}\cdots\mathbf{v_m},P)\sqcup_{\mathcal{P}}(\mathbf{v_{m+1}}\cdots\mathbf{v_{m+n}},Q) := \sum_{f\in\mathsf{sh}(m,n)} (\mathbf{v_{f^{-1}(1)}}\cdots\mathbf{v_{f^{-1}(m+n)}}, f_*P \cup f_*(Q+m)).$$

Here the summation is over the set

$$sh(m,n) := \{f : [m+n] \to [m+n] \mid f \text{ is bijective and } f(1) < f(2) < \dots < f(m), \\ f(m+1) < f(m+2) < \dots < f(m+n)\}$$

and

$$Q + m := \{q + m \mid q \in Q\}$$

$$f_*(\{P_1, \dots, P_k\}) := \{f'_*(P_1), \dots, f'_*(P_k)\}$$

$$f'_*(P_i) := \{f(x) \mid x \in P_i\}.$$

Let us consider an example.

Example 1.

$$(\mathbf{a}, \{\{1\}\}) \sqcup_{\mathcal{P}} (\mathbf{bc}, \{\{1, 2\}\}) = (\mathbf{abc}, \{\{1\}, \{2, 3\}\}) + (\mathbf{bac}, \{\{2\}, \{1, 3\}\}) \\ + (\mathbf{bca}, \{\{1, 2\}, \{3\}\}),$$

or, using colors to signify the underlying set partition,

 $\mathbf{a} \sqcup_{\mathcal{P}} \mathbf{bc} = \mathbf{a} \mathbf{bc} + \mathbf{b} \mathbf{a} \mathbf{c} + \mathbf{bc} \mathbf{a}.$

It turns out that the product $\sqcup_{\mathcal{P}}$ splits into a sum,

$$x \amalg_{\mathcal{P}} y = x \succ_{\mathcal{P}} y + y \succ_{\mathcal{P}} x,$$

where,

$$(\mathbf{v_1}\cdots\mathbf{v_m},P)\succ_{\mathcal{P}}(\mathbf{v_{m+1}}\cdots\mathbf{v_{m+n}},Q) := \sum_{\substack{f\in\mathsf{sh}(m,n),\\f(m+n)=m+n}} (\mathbf{v_{f^{-1}(1)}}\cdots\mathbf{v_{f^{-1}(m+n)}}, f_*P\cup f_*(Q+m)).$$

Example 2.

$$(\mathbf{a}, \{\{1\}\}) \succ_{\mathcal{P}} (\mathbf{bc}, \{\{1, 2\}\}) = (\mathbf{abc}, \{\{1\}, \{2, 3\}\}) + (\mathbf{bac}, \{\{2\}, \{1, 3\}\})$$

or, with colors,

 $\mathbf{a} \succ_{\mathcal{P}} \mathbf{b} \mathbf{c} = \mathbf{a} \mathbf{b} \mathbf{c} + \mathbf{b} \mathbf{a} \mathbf{c}.$

Define on \mathcal{P} the following concatenation-like operation

 $(v, P) \cdot (w, Q) := (vw, P \cup (Q + \operatorname{len}(v))),$

and let Δ be the dual coproduct.

Example 3.

$$(\mathbf{a}, \{\{1\}\}) \cdot (\mathbf{bc}, \{\{1,2\}\}) = (\mathbf{abc}, \{\{1\}, \{2,3\}\})$$

or, with colors,



The following statement provides a structural understanding of the setting.

Theorem 4.

1.
$$\succ_{\mathcal{P}}$$
 is Zinbiel.

2. $(\mathcal{P}, \sqcup_{\mathcal{P}}, \Delta)$ is a bialgebra.

For details and on Zinbiel algebras, we refer the reader to [1].



$$\Delta(\mathbf{a} \ \sqcup_{\mathcal{P}} \mathbf{bc}) = \Delta(\mathbf{a} \ \mathbf{bc} + \mathbf{b} \ \mathbf{a} \ \mathbf{c} + \mathbf{bc} \ \mathbf{a})$$

$$= \left(\mathbf{a} \ \mathbf{bc} + \mathbf{b} \ \mathbf{a} \ \mathbf{c} + \mathbf{bc} \ \mathbf{a}\right) \otimes \mathbf{e} + \mathbf{e} \otimes \left(\mathbf{a} \ \mathbf{bc} + \mathbf{b} \ \mathbf{a} \ \mathbf{c} + \mathbf{bc} \ \mathbf{a}\right)$$

$$+ \mathbf{a} \otimes \mathbf{bc} + \mathbf{bc} \otimes \mathbf{a}$$

$$\Delta(\mathbf{a}) \ \sqcup_{\mathcal{P}} \Delta(\mathbf{bc}) = \left(\mathbf{a} \otimes \mathbf{e} + \mathbf{e} \otimes \mathbf{a}\right) \ \sqcup_{\mathcal{P}} \left(\mathbf{bc} \otimes \mathbf{e} + \mathbf{e} \otimes \mathbf{bc}\right)$$

$$= \left(\mathbf{a} \ \sqcup_{\mathcal{P}} \ \mathbf{bc}\right) \otimes \mathbf{e} + \mathbf{a} \otimes \mathbf{bc} + \mathbf{bc} \otimes \mathbf{a} + \mathbf{e} \otimes \left(\mathbf{a} \ \sqcup_{\mathcal{P}} \ \mathbf{bc}\right)$$

$$= \Delta(\mathbf{a} \ \sqcup_{\mathcal{P}} \ \mathbf{bc}).$$

We are finally ready to define the promised generalization of the notion of expected signature. For $0 \le s < t \le T$ let $\mathcal{U}(X)_{s,t}$ be the linear map on \mathcal{P} defined via

$$\left(\mathcal{U}(X)_{s,t}, (v, P = \{P_1, \dots, P_\ell\})\right) := \int_{s < r_1 < \dots < r_n < t} \prod_{i=1}^\ell \langle\!\langle \prod_{j \in P_i} \dot{X}_{r_j}^{(\mathbf{v}_j)} \rangle\!\rangle dr$$

Example 6.

$$\begin{split} \left(\mathcal{U}(X)_{s,t}, \mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{de} \right) &= \left(\mathcal{U}(X)_{s,t}, (\mathbf{abcde}, \{\{1,3\}, \{2,4,5\}\}) \right) \\ &= \int_{s < r_1 < \dots < r_5 < t} \langle\!\langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_3}^{\mathbf{c}} \rangle\!\rangle \langle\!\langle \dot{X}_{r_2}^{\mathbf{b}} \dot{X}_{r_4}^{\mathbf{d}} \dot{X}_{r_5}^{\mathbf{e}} \rangle\!\rangle dr \\ &= \int_{s < r_1 < \dots < r_5 < t} \langle\!\langle \dot{X}_{r_4}^{\mathbf{d}} \dot{X}_{r_2}^{\mathbf{b}} \dot{X}_{r_5}^{\mathbf{d}} \rangle\!\langle \langle \dot{X}_{r_3}^{\mathbf{c}} \dot{X}_{r_1}^{\mathbf{a}} \rangle\!\rangle dr, \end{split}$$

where the last equality is shown just to make clear that variables commute.

Proposition 7.

- 1. $\mathcal{U}(X)_{s,t}$ is a character on \mathcal{P} .
- 2. Let $\phi : [0,T] \to [0,T]$ be a deterministic time change (i.e. an increasing diffeomorphism). Define $Y_r := X_{\phi(r)}$. Then

$$\mathcal{U}(Y)_{s,t} = \mathcal{U}(X)_{\phi(s),\phi(t)}$$

Remark 8. Note that $\mathcal{U}(X)$ does not satisfy an obvious Chen's relation. For example, for 0 < s < t,

$$\begin{aligned} \left(\mathcal{U}(X)_{0,t}, \mathbf{ab} \right) &= \int_{0 < r_1 < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle \rangle \\ &= \int_{0 < r_1 < r_2 < s} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle \rangle + \int_{s < r_1 < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < r_1 < s < r_2 < t} \langle \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < r_1 < s < r_2 < t} \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < r_1 < s < r_2 < t} \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < r_1 < s < r_2 < t} \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < s < r_1 < s < r_2 < t} \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < s < r_2 < t} \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < r_2 < t} \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < s < r_2 < t} \langle \dot{X}_{r_1}^{\mathbf{a}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < s < r_2 < t} \langle \dot{X}_{r_2}^{\mathbf{b}} \langle \dot{X}_{r_1}^{\mathbf{b}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < s < r_2 < t} \langle \dot{X}_{r_1}^{\mathbf{b}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < s < r_2 < t} \langle \dot{X}_{r_1}^{\mathbf{b}} \langle \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < s < r_2 < t} \langle \dot{X}_{r_2}^{\mathbf{b}} \langle \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < s < r_2 < t} \langle \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < s < r_2 < t} \langle \dot{X}_{r_2}^{\mathbf{b}} \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_{s < s < r_2 < t} \langle \dot{X}_{r_2}^{\mathbf{b}} \rangle + \int_$$

and the last term cannot be simplified further (that is, it cannot be "split up").

References

- M. Aguiar, Pre-Poisson Algebras, Letters in Mathematical Physics, 54 (2000), 263– 277. (document)
- H. Boedihardjo, J. Diehl, M. Mezzarobba, H. Ni, The expected signature of Brownian motion stopped on the boundary of a circle has finite radius of convergence, Bulletin of the London Mathematical Society, 53 (2021), 285–299. (document)
- [3] P. Bonnier, H. Oberhauser, Signature cumulants, ordered partitions, and independence of stochastic processes, Bernoulli, 26(4) (2020), 2727-2757 (document)
- [4] I. Chevyrev, H. Oberhauser, Signature Moments to Characterize Laws of Stochastic Processes, Journal of Machine Learning Research, 23 (2022), 1–42. (document)
- [5] J. Diehl, N. Tapia, K. Ebrahimi-Fard, Time warping invariants of multidimensional time series, Acta Applicandae Mathematicae, 170 (2020), 265–290. (document)
- [6] P. K. Friz, M. Hairer, A Course on Rough Paths With an Introduction to Regularity Structures, Springer Cham 2020. (document)
- M. Hairer, D. Kelly, Geometric versus non-geometric rough paths, Ann. inst. Henri Poincaré (B) Probab. Stat., 51, No. 1 (2015), 207–251. (document)
- [8] T. Lyons, Differential equations driven by rough signals, Revista Matemática Iberoamericana, 14(2) (1998), 215–310. (document)
- [9] T. Lyons, A. D. McLeod, Signature Methods in Machine Learning, arXiv:2206.14674. (document)
- [10] Ph. Tondeur, Collected Papers of K.-T. Chen, Contemporary Mathematicians, Birkhäuser Boston 2001. (document)