Signature Reconstruction from Randomized Signatures

Signatures and Rough Paths @ICMS

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Mathematics of Random Systems

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Signatures

Let $X : [0, T] \to \mathbb{R}^d$ be a Lipschitz continuous path. Set for each $n \in \mathbb{N}$:

$$\Delta^n_{[s,t]} := \{s \le r_1 \le \dots \le r_n \le t\} \quad \text{for } 0 \le s < t \le T\,,$$
$$\mathcal{W}_n := \{w = (w_1, \dots, w_n) \mid w_1, \dots, w_n \in \{1, \dots, d\}\}.$$

For any word $w \in \mathcal{W}_n$ its associated iterated integral is denoted by:

$$\int_{\Delta^n_{[s,t]}} dX^w_r := \int_s^t \int_s^{r_n} \cdots \int_s^{r_3} \int_s^{r_2} dX^{w_1}_{r_1} \dots dX^{w_n}_{r_n}\,.$$

Let $e_1, \dots, e_d$ denote the canonical basis vectors on $\mathbb{R}^d$, and set $e_w := e_{w_1} \otimes \cdots \otimes e_{w_n}$ for each $w = (w_1, \dots, w_n) \in \mathcal{W}_n$. Then the collection of n'th order iterated integrals can be written as

$$\int_{\Delta^n_{[s,t]}} dX_{r_1} \otimes \cdots \otimes dX_{r_n} := \sum_{w \in \mathcal{W}_n} \int_{\Delta^n_{[s,t]}} dX^w_r e_w \in (\mathbb{R}^d)^{\otimes n}.$$

Signatures

Definition (Signature)

The **signature** *at time T of the path $X : [0,T] \to \mathbb{R}^d$ is the map $S(X) : \Delta^2_{[0,T]} \to T((\mathbb{R}^d))$, defined by*

$$S(X)_{s,t} = \left(1, \int_s^t dX_{r_1}, \int_{\Delta^2_{[s,t]}} dX_{r_1} \otimes dX_{r_2}, \int_{\Delta^3_{[s,t]}} dX_{r_1} \otimes dX_{r_2} \otimes dX_{r_3}, \dots\right)$$
$$= 1 + \sum_{n=1}^{\infty} \int_{\Delta^n_{[s,t]}} dX_{r_1} \otimes \cdots \otimes dX_{r_n},$$

which takes value in the extended tensor algebra

$$T((\mathbb{R}^d)) := \left\{ (x_0, x_1, x_2, \dots) = \sum_{n=0}^{\infty} x_n \;\middle|\; \forall n \in \mathbb{N}_0 : \; x_n \in \left(\mathbb{R}^d\right)^{\otimes n} \right\}.$$

Randomized signature

CDE: Let $V_1, \ldots, V_d : \mathbb{R}^N \to \mathbb{R}^N$ be smooth vector fields. Consider for any initial value $y \in \mathbb{R}^N$, the controlled differential equation (CDE):

$$Y_t = y + \sum_{i=1}^{d} \int_0^t V_i(Y_s) dX_s^i \quad \text{for } t \in [0, T].$$

Denote by $Y^y : [0, T] \to \mathbb{R}^N$ the solution associated to this initial value.

Randomized signature: Let $\sigma : \mathbb{R} \to \mathbb{R}$ be a (real analytic) activation function, let $A_1, \ldots, A_d$ be random $N \times N$-matrices, let $D_1, \ldots, D_d$ be random diagonal $N \times N$-matrices.

- **No-depth case:** $V_i(y) = \sigma(A_i y + b_i)$ for $y \in \mathbb{R}^N$
- **Depth case:** $V_i(y) = \sigma(A_i \sigma(D_i y))$ for $y \in \mathbb{R}^N$

Randomized signature

Why randomized signatures?

- Foundations of reservoir computing;
- Mixing of higher order signature terms in each coordinate;
- Extending randomized signatures to Lie groups allows us to have solutions on compact manifolds;
- Numerical stability, etc.

Iterated vector fields

Let $C^\infty(\mathbb{R}^N) := \{g : \mathbb{R}^N \to \mathbb{R} \mid g \text{ is smooth}\}$.

Let $V : \mathbb{R}^N \to \mathbb{R}^N$ be a smooth vector field. Then for any $g \in C^\infty(\mathbb{R}^N)$, we write

$$Vg(x) = \underbrace{(\nabla g(x))^T}_{1\times N} \underbrace{V(x)}_{N\times 1} \quad \text{for all } x \in \mathbb{R}^N, \quad \text{such that } Vg \in C^\infty(\mathbb{R}^N).$$

This gives a **derivation** $\mathcal{D}_V : C^\infty(\mathbb{R}^N) \to C^\infty(\mathbb{R}^N)$, defined by $g \mapsto Vg$.

Recall: The map $V \mapsto \mathcal{D}_V$, provides a bijective correspondence between the space of vector fields on $\mathbb{R}^N$ and the space of derivations on $\mathbb{R}^N$.

Iterated vector fields

Let $V_1, \dots, V_d : \mathbb{R}^N \to \mathbb{R}^N$ be d vector fields. For any $g \in C^\infty(\mathbb{R}^N)$, write $V_1 g, \dots, V_d g \in C^\infty(\mathbb{R}^N)$, as usual.

Definition (Iterated vector field)

For any word $w = (w_1, \dots, w_n)$, we can iteratively apply the vector fields to one another, by setting:

$$V_w g := V_{w_1} \cdots V_{w_n} g \in C^\infty(\mathbb{R}^N).$$

In this case, $V_w : C^\infty(\mathbb{R}^N) \to C^\infty(\mathbb{R}^N)$ is precisely the composition of derivations $\mathcal{D}_{V_{w_1}} \circ \cdots \circ \mathcal{D}_{V_{w_n}}$, and it is a linear differential operator on $C^\infty(\mathbb{R}^N)$ of order n.

Iterated vector fields

Let $V_1, \ldots, V_d : \mathbb{R}^N \to \mathbb{R}^N$ be smooth vector fields. Consider for any initial value $y \in \mathbb{R}^N$, the controlled differential equation

$$Y_t = y + \sum_{i=1}^{d} \int_0^t V_i(Y_s) dX_s^i \quad \text{for } t \in [0, T].$$

Denote by $Y^y : [0, T] \to \mathbb{R}^N$ the solution associated to this initial value.

Theorem (Taylor expansion)

For every $g \in C^\infty(\mathbb{R}^N)$, we have the Taylor expansion:

$$g(Y_t) = g(y) + \sum_{m=1}^{\infty} \sum_{w \in \mathcal{W}_m} V_w g(y) \int_{\Delta^m_{[0,t]}} dX_r^w \quad \textit{for every } t \in [0, T].$$

Signature reconstruction on $\mathbb{R}^N$

Question:
Given randomized signatures across different initial values, $(Y^y)_{y\in\mathbb{R}^N}$, can we reconstruct the components of the signature $S(X)$ utilising the Taylor expansion from before?

Answer:
Yes, up to a certain order depending on the dimension of the hidden space $\mathbb{R}^N$, for randomized signatures with depth (under an appropriate choice of activation function).

$\rightarrow$ Also works for any other CDEs whose iterated vector fields satisfy certain linear independence properties.

Signature reconstruction on $\mathbb{R}^N$

The following result is inspired by a conjecture from [E. Akyildirim, M. Gambara, J. Teichmann & S. Zhou, 2022].

Theorem (Signature reconstruction on $\mathbb{R}^N$)

Fix some $N, L \in \mathbb{N}$, let $V_1, \dots, V_d : \mathbb{R}^N \to \mathbb{R}^N$ be smooth vector fields, and suppose that for all fixed $m \leq L$, the associated tree-like vector fields $\{V_\tau \mid \tau \in \mathbb{T}_w,\ w \in \mathcal{W}_m\}$ are linearly independent. Consider for each $y \in \mathbb{R}^N$, the CDE:

$$Y_t^y = y + \sum_{i=1}^{d} \int_0^t V_i(Y_s) dX_s^i \quad \text{for every } t \in [0, T], \tag{1}$$

with solution $Y^y : [0, T] \to \mathbb{R}^N$. Then the signature components of $S(X)$ up to order L can be uniquely reconstructed from the collection of solutions $(Y^y)_{y \in \mathbb{R}^N}$.

Signature reconstruction on $\mathbb{R}^N$

Proof overview: Fix $N, L \in \mathbb{N}$. Consider for $\eta \in \mathbb{R}^N$, $r \in \mathbb{R}$, the modified differential equation

$$Y_t^{\eta,r} = \eta + \sum_{i=1}^{d} \int_0^t rV_i(Y_s^{\eta,r})dX_s^i,$$

such that $Y^{\eta,r} = rY^{\frac{\eta}{r}}$ when $r \neq 0$ and $Y^{\eta,0} \equiv \eta$. Then for the vector fields $\tilde{V}_i(x) = rV_i(x)$, Taylor expansion yields for any $g \in C^\infty(\mathbb{R}^N)$:

$$g(Y_t^{\eta,r}) = g(\eta) + \sum_{k=1}^{\infty} r^k \sum_{w \in \mathcal{W}_k} V_w g(\eta) \int_{\Delta_{[0,t]}^k} dX_r^w.$$

Taking the m'th derivative w.r.t. r and evaluating in $r = 0$ then gives

$$\frac{d^m}{dr^m} g(Y_t^{\eta,r})|_{r=0} = \sum_{w \in \mathcal{W}_m} V_w g(\eta) \int_{\Delta_{[0,t]}^m} dX_r^w.$$

Proof overview (continued): The equation:

$$\frac{d^m}{dr^m} g(Y_t^{\eta,r})|_{r=0} = \sum_{w \in \mathcal{W}_m} V_w g(\eta) \int_{\Delta_{[0,t]}^m} dX_r^w,$$

can be considered as a linear equation system if we consider it across different initial values $\eta \in \mathbb{R}^N$.

- If the iterated vector fields $\{V_w \mid w \in \mathcal{W}_m\}$ are linearly independent, then the equation system can be uniquely solved w.r.t. the m'th order iterated integrals of X.
- Linear independence of tree-like vector fields for all $m \leq L$, is a way of ensuring this holds up to order L.

□

Tree-like vector fields

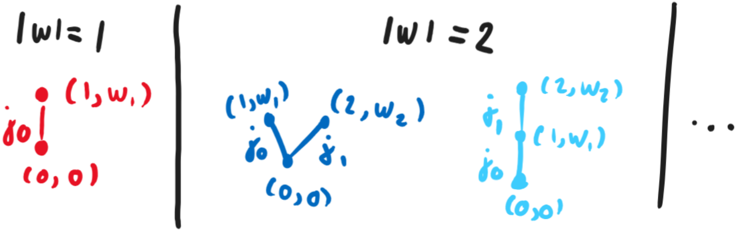
Challenge: The iterated vector fields $\{V_w \mid w \in \mathcal{W}_m\}$ quickly spiral out of control:

$$
\begin{aligned}
V_{w_1} g(x) &= (\nabla g(x))^T V_{w_1}(x) = \sum_{j_0=1}^{N} \frac{\partial}{\partial x_{j_0}} g(x) \pi_{j_0}(V_{w_1}(x)); \\
V_{w_1 w_2} g(x) &= (\nabla V_{w_1} g(x))^T V_{w_2}(x) \\
&= \sum_{j_0, j_1 = 1}^{N} \frac{\partial^2}{\partial x_{j_1} \partial x_{j_0}} g(x) \pi_{j_0}(V_{w_1}(x)) \pi_{j_1}(V_{w_2}(x)) \\
&\quad + \frac{\partial}{\partial x_{j_0}} g(x) \frac{\partial}{\partial x_{j_1}} \pi_{j_0}(V_{w_1}(x)) \pi_{j_1}(V_{w_2}(x)); \\
V_{w_1 w_2 w_3} g(x) &= \dots
\end{aligned}
$$

Tree-like vector fields

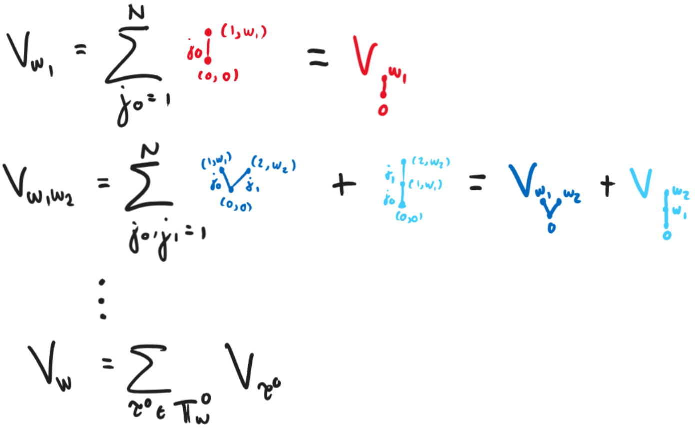
We can represent terms of V_w as labelled recursive trees with:

- Vertex 0 keeping track of the derivative operator (applied to g);
- Vertex $1, \dots, m$ keeping track of the vector fields $V_{w_1}, \dots, V_{w_m}$;
- Edges (v_1, v_2) with $v_1 < v_2$ are associated a direction j, such that:
  - The derivative in direction j is taken w.r.t. vertex v_1;
  - The projection in direction j is taken w.r.t. vertex v_2.



Tree-like vector fields

So now we can write:



$\rightarrow$ Showing $\{V_\tau \mid \tau \in \mathbb{T}_w,\ w \in \mathcal{W}_m\}$ are linearly independent is then enough to get $\{V_w \mid w \in \mathcal{W}_m\}$ linearly independent.

Randomized signature with depth

Result

Let $L - 1 \leq N$, and let $V_1, \ldots, V_d : \mathbb{R}^N \to \mathbb{R}^N$ be given by

$$V_i(x) = \sigma(A_i \sigma(D_i x)) \quad \text{for } x \in \mathbb{R}^N.$$

If $\sigma = \exp$ (or σ is a more generic real analytic function), then $\{V_\tau \mid \tau \in \mathbb{T}_w,\ w \in \mathcal{W}_m\}$ is linearly independent for all $1 \leq m \leq L$.

- → We can reconstruct signature components up to order $N+1$ from randomized signature with depth.
- → As N increases linearly, number of iterated integrals reconstructed increases exponentially!

Randomized signature with depth

Idea: Showing tree-like linear independence, boils down to being able to 'uniquely identify which (labelled) tree a term V_τ came from' (*ignoring scalars*).

Depth vs. no-depth:

- *No-depth*: $\partial_j \pi_k(\sigma(A_i x)) = a_{kj}(i)\sigma'(\pi_k(A_i x))$, i.e., only the incoming edge has 'structural importance'.
- *Depth*: $\partial_j \pi_k(\sigma(A_i \sigma(D_i x))) = a_{kj}(i)\sigma'(d_j(i)x)\sigma'(\pi_k(A_i\sigma(D_i x)))$, i.e., both in- and outgoing edges have 'structural importance'.

Dimensional dependence

Q: Is dimensional dependence always required?

Example: $N = 1, L = 3, d = 3$. Let $V_1, V_2, V_3 : \mathbb{R} \to \mathbb{R}$. Then the 3rd order iterated vector fields have the form:

$$V_{w_1 w_2 w_3} = \left(V_{w_1} \cdot V_{w_2} \cdot d^2 V_{w_3} + V_{w_1} \cdot dV_{w_2} \cdot dV_{w_3}\right) \cdot \partial_x + \left(V_{w_1} \cdot V_{w_2} \cdot 2dV_{w_3} + V_{w_1} \cdot dV_{w_2} \cdot V_{w_3}\right) \cdot \partial_x^2 + V_{w_1} \cdot V_{w_2} \cdot V_{w_3} \cdot \partial_x^3.$$

A solution to the equation $\sum_{w \in \mathcal{W}_3} c_w V_w = 0$ is e.g., obtained by setting:

$$c_{123} = c_{312} = c_{231} = +1 \quad \text{and} \quad c_{132} = c_{213} = c_{321} = -1, \qquad c_w = 0 \quad \text{otherwise}$$

→ Verify that this solution solves the equations in ∂_x, ∂_x^2 and ∂_x^3, simultaneously.

Dimensional dependence

Example (continued): Set

$$c_{123} = c_{312} = c_{231} = +1 \quad \text{and} \quad c_{132} = c_{213} = c_{321} = -1.$$

The equation in ∂_x becomes:

$$\begin{aligned}
& V_1 \cdot V_2 \cdot d^2 V_3 + V_1 \cdot dV_2 \cdot dV_3 && (c_{123} = +1) \\
+ \quad & V_3 \cdot V_1 \cdot d^2 V_2 + V_3 \cdot dV_1 \cdot dV_2 && (c_{312} = +1) \\
+ \quad & V_2 \cdot V_3 \cdot d^2 V_1 + V_2 \cdot dV_3 \cdot dV_1 && (c_{231} = +1) \\
- \quad & \left(V_1 \cdot V_3 \cdot d^2 V_2 + V_1 \cdot dV_3 \cdot dV_2 \right) && (c_{132} = -1) \\
- \quad & \left(V_2 \cdot V_1 \cdot d^2 V_3 + V_2 \cdot dV_1 \cdot dV_3 \right) && (c_{213} = -1) \\
- \quad & \left(V_3 \cdot V_2 \cdot d^2 V_1 + V_3 \cdot dV_2 \cdot dV_1 \right) && (c_{321} = -1) \\
= \quad & 0
\end{aligned}$$

The equations in ∂_x^2 and ∂_x^3 are similarly solved.

In summary

What did we show?

1. Given randomized signature with **depth** on $\mathbb{R}^N$ considered across different initial values, the associated signature components of $S(X)$ can be reconstructed for all $L \leq N + 1$.
   $\rightarrow$ Not sharp: depends on d.
2. The proof relies on an important claim of **linear independence** between iterated vector fields, which is required to uniquely solve the linear equation systems induced by the Taylor expansion.
3. Linear independence between iterated vector fields, is easier studied by decomposing into **tree-like vector fields** and checking linear independence of those.

In summary

Thank you for listening!

Main references

1. Akyildirim, Gambara, Teichmann, Zhou (2022). *Applications of Signature Methods to Market Anomaly Detection*.
2. Baudoin, Zhang (2012). *Taylor expansion for the solution of a stochastic differential equation driven by fractional brownian motions.*
3. Cuchiero, Gonon, Grigoryeva, Ortega, Teichmann (2021). *Discrete-time signatures and randomness in reservoir computing*.
4. Cuchiero, Gonon, Grigoryeva, Ortega, Teichmann (2021). *Expressive power of randomized signature*.
5. G., Muca Cirone, Teichmann (2025). *Signature Reconstruction from Randomized Signatures*.
6. Gubinelli (2019). *Ramification of rough paths*.
7. McLachlan, Modin, Munthe-Kaas, Verdier (2017). *Butcher series: A story of rooted trees and numerical methods for evolution equations*.