# Signatures, trees and pdes





A rough path between mathematics and data science



Terry Lyons 4 March 2021

with many others... but particularly Cris, Patrick, James, Varun, Cris, Maud, Peter, Roly, Sam, Patricia

### A DataS<sub>1</sub>g vision



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We channel our research around developing the mathematics needed to model and understand complex streams of nonstationary multimodal data. We build prototypes that have real world value to develop this understanding. This is only possible because of significant collaboration and partnership.



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# Modelling behavior of evolving systems

### A public domain collaboration on detecting malware



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### DataSig | an EPSRC/UKRI 5-year program grant

↓ ↓ ↓ ↓ DataSig

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### Mathematics

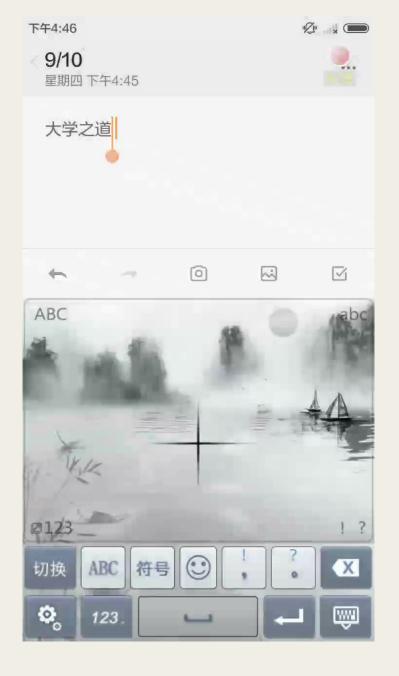
- rough path theory and signatures
- describing the interactions between complex systems from the top down
- extending the calculus of differential equations to complex contexts

#### Data science

- the notion of an unparameterized path captured by the order of events
- clean and minimal universal feature sets (expected) signature
- the notion of a neural controlled differential equation
- the notion of a pde-kernel
- a principled mathematical framework that allows further innovation

### **Embedded contexts**

• streamed data is everywhere; Chinese handwriting, hospital wards, event logs ...



### Streamed data

- a character drawn on the screen of an iPhone
- an order book
- a piece of text
- progression through hospital record
- astronomical data
- video of a person moving
- an evolving stream of emotions
- ICU data to detect sepsis
- an evolving inventory

#### Ensembles of streamed data

- the event log of processes generated by malware
- the behaviour of crowds
- the evolution of cancer cell lines

#### Key questions

- understand what you have observed
- predict the distribution of what is happening next
- identify anomalies



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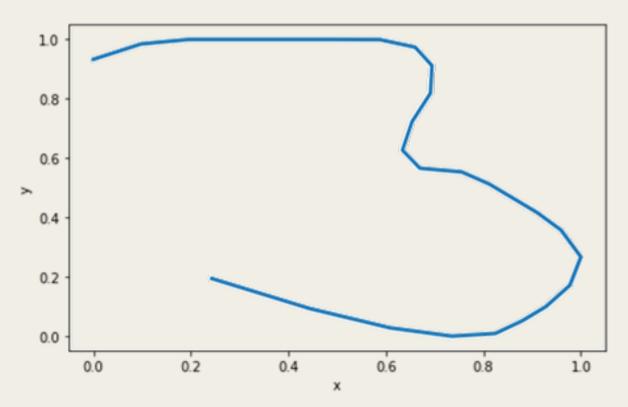
# Some maths of evolving systems

### Data science does not like symmetry



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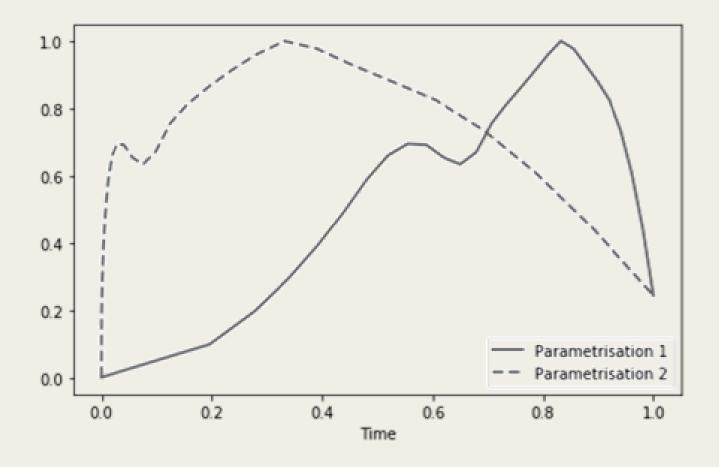
- Re-parameterisation is a huge symmetry group
- Multimodal streams modulo reparameterisation form a group
- Representing this group in the tensor algebra provides a faithful feature set and removes the symmetry
- New tools signature and log signature, new maths describing the functions on streams



### Different sampling procedures



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- The letter "3" is drawn from top to bottom
- The x coordinate of the evolving symbol sampled differently (at uneven speeds)

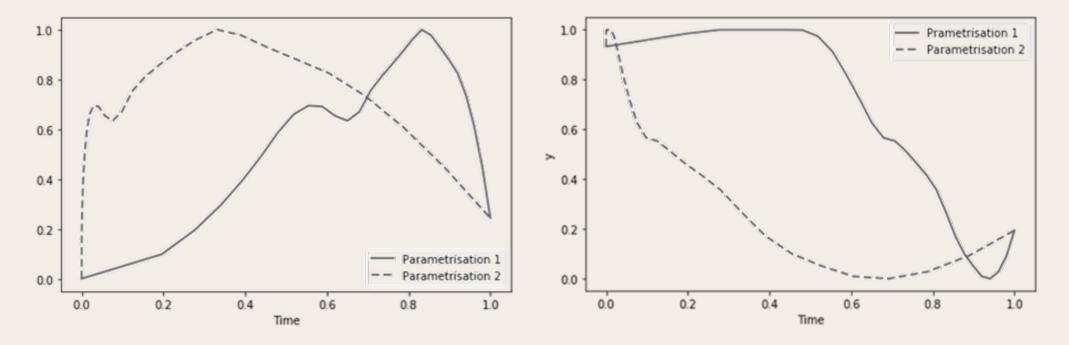
### Different sampling procedures



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The number "3" x, y coordinates – same picture drawn at two different speeds

- no consistent wavelets
- reparameterisations do not form a linear space!

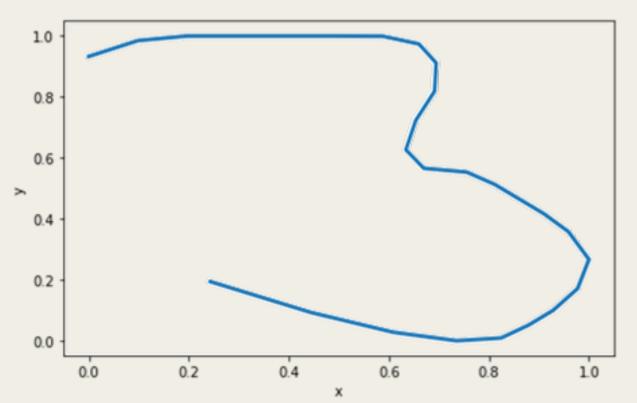


### Different sampling procedures



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- The letter "3" is drawn from top to bottom
- How does one describe the three or any path modulo the symmetry of parametrisation?



The signature of a path describes an unparameterised stream  $\gamma$ 



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Signature is a *top down* description for unparameterised paths that describes a path segment through its effects of stylised nonlinear systems

$$dS = S \otimes d\gamma$$

It filters out the infinite dimensional noise of resampling allowing prediction and classification with *much* smaller learning sets.

It gives fixed dimensional feature sets regardless of the sample points.\*

\* missing data/varying parameterisation not issues although inadequacy may be

The signature - faithful and universal features describing an unparameterised stream



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The signature of a stream  $\gamma$  over I = [s, t] defined by  $\sum_{k=0}^{\infty} S_k$ where  $S_0 = 1$  and

$$S_k(\gamma, I) \coloneqq \iint_{s < u_1 < \dots < u_k < t} d\gamma_{u_1} d\gamma_{u_2} \dots d\gamma_{u_k}$$

These "Fourier-like" features exactly describe the *unparameterised* stream (Hambly Lyons Annals Math 2010)

Projected controlled differential equations are universal models

 $< e, Y_t >$  where  $dY_u = f(Y_u)dX_u$ 

# Analysis, geometry, combinatorial Hopf/dendriform/sensor algebras



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- Signature leads to linear space of real valued functionals  $\langle e|S_I \rangle$  on streams
- Pointwise multiplication and integration of these functionals
- can usefully be described in purely algebraic language.
- The log signature is structurally important.

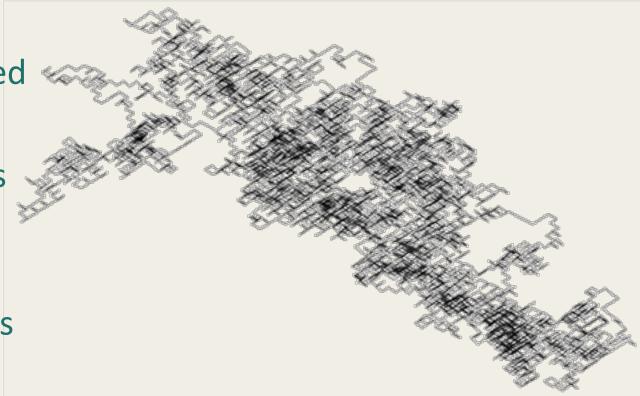


## Analysis, geometry, combinatorial Hopf/dendriform/sensor algebras



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- The *Signature* is a faithful embedding of the unparametrized stream into a vector space
- Continuous functions on streams can be well approximated by linear functionals on signatures
- The Expected Signature describes the ensemble of paths
- There is a natural pde kernel



## Analysis, geometry, combinatorial Hopf/dendriform/sensor algebras



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- Let be x, y be unparametrized paths in H and consider the bilinear form K(x, y) ≔ (S(x), S(y)). Franz J. Kiraly, Harald Oberhauser; JMLR 20(31):1-45, 2019 gave a kernel trick for the unparametrized truncated signature kernel.
- Salvi et al. then proved the Goursat pde is the kernel trick for the full kernel:

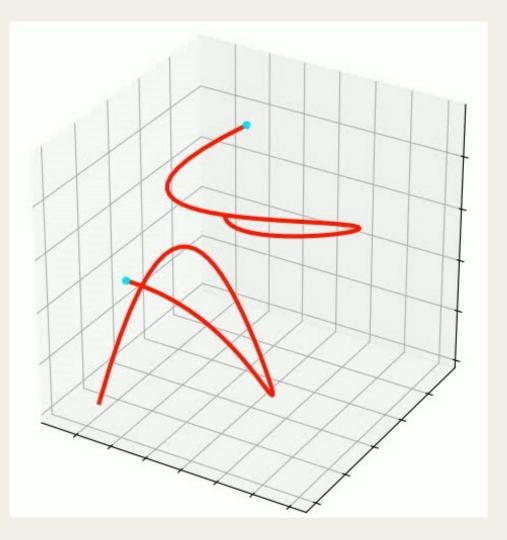
 $\frac{\partial^2 K(x|_{[u_0,u]},y|_{[v_0,v]})}{\partial u \partial v} = \langle \dot{x}, \dot{y} \rangle K(x|_{[u_0,u]},y|_{[v_0,v]})$ 

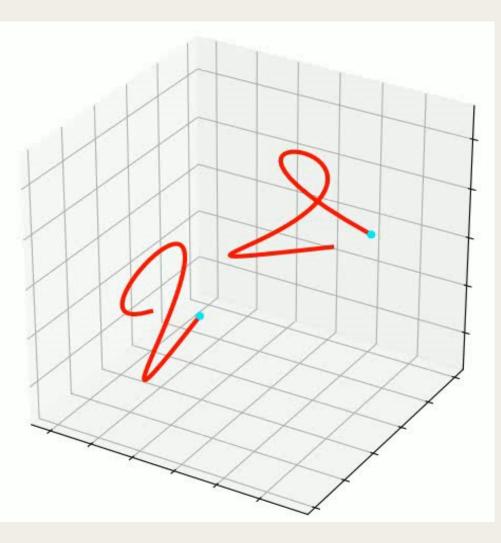


### Recovering the curves from the signature



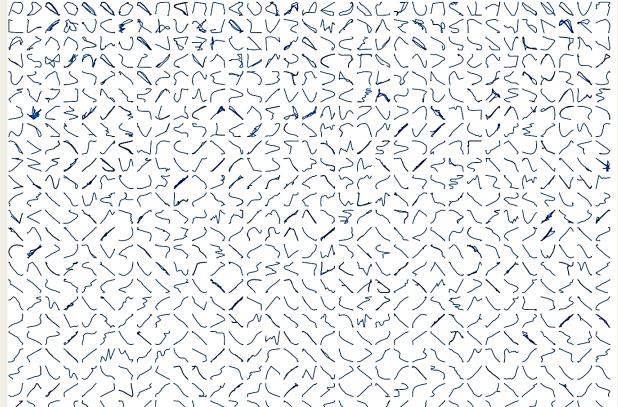
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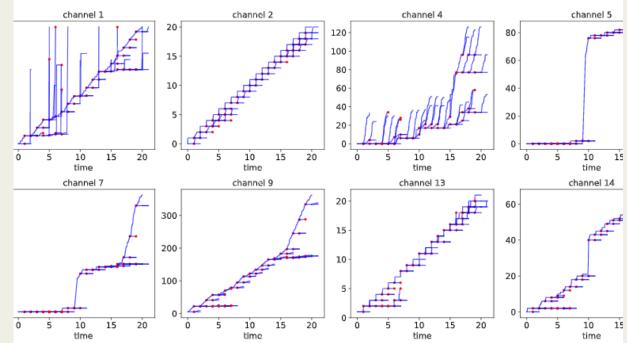




Weixin Yang, Jaiwei Chang

### Our data





I representation of selected channels of one single streaming tree. Each plot represents the evolution in time of the value of a tree, on its various branches. A red dot indicates a point where the currently-tracked process sets off a child process, causing

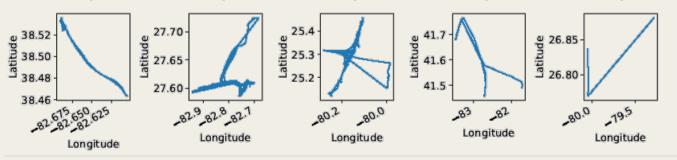
### Paths or Signatures? |Long / Short vessel



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- The vectorisation of unparametrized streams allows efficient use of many standard methods.
- Anomaly detection can be applied this to these real-world shipping trajectories example.

Vessel length 14.8m Vessel length 18.3m Vessel length 19.1m Vessel length 22.9m Vessel length 23.1m Stream length: 114.0km Stream length: 788.4km Stream length: 382.6km Stream length: 415.1km Stream length: 85.9km Number of points: 1571 Number of points: 1559 Number of points: 1536 Number of points: 1580 Number of points: 118



Vessel length 128.8m Vessel length 142.8m Vessel length 186.4m Vessel length 189.8m Vessel length 229.2m Stream length: 227.4km Stream length: 84.1km Stream length: 696.4km Stream length: 749.8km Stream length: 617.3km Number of points: 151 Number of points: 71 Number of points: 897 Number of points: 1177 Number of points: 422 23.65 23.70 26 Patitrade 23.60 23.55 Latitude Latitude 57 Latitude 57 e 25 Latitude 23.66 24 24 -84.0 -- 80.0 -82.5 -80.0 -83.5 -18 -82.5 .83 -82 282 .80 Longitude Longitude Longitude Longitude Longitude

### Vectorisation of unparamterised streams



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- signatures connect streams to the data science pipeline, but allows graduated approach
- expected signatures describe ensembles of paths
- pdes provide FAST kernels on paths and scalability

• There are also neural controlled differential equations,... www.datasig.ac.uk/papers

## **Ensembles of paths**



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 $\sqrt{2}$ 

### Process tree example: Expected signatures of clouds of paths



Developed a way to apply expected signature techniques by viewing processes as trees evolving over time eg the crop yield prediction task.

Predicting the yield of wheat crops over a region from the longitudinal measurements of climatic variables recorded across different locations of the region.

Eurostat dataset containing the total annual regional yield of wheat crops in mainland France divided in 22 administrative regions—from 2015 to 2017.

#### for i in tqdm(range(NUM\_TRIALS)):

pwES = pathwiseExpectedSignatureTransform(order=2). SpwES = SignatureTransform(order=3).fit\_transform(p X\_train, X\_test, y\_train, y\_test = train\_test\_split model = GridSearchCV(pipe, parameters, verbose=0, n model.fit(X\_train, y\_train) y\_pred = model.predict(X\_test) us\_test[i] = mean\_squared\_error(y\_pred, y\_test)

### Process tree example: Expected signatures of clouds of paths



Developed a way to apply expected signature techniques by viewing processes as trees evolving over time eg the crop yield prediction task AISTATS 2021 arxiv.org/pdf/2006.05805.pdf

The climatic measurements (temperature, soil humidity and precipitation) are extracted from the GLDAS database (Rodell et al, 2004), are recorded every 6 hours at a spatial resolution of  $0.25^{\circ} \times 0.25^{\circ}$ , and their number varies across regions.

Model	MSE	MAPE
Baseline	2.38	23.31
DeepSets	2.67	22.88
DR-RBF	.82	13.18
DR-Matern32	.82	13.18
DR-GA	.72	12.55
KES	.65	12.34
SES	.62	10.98

for i in tqdm(range(NUM\_TRIALS)):

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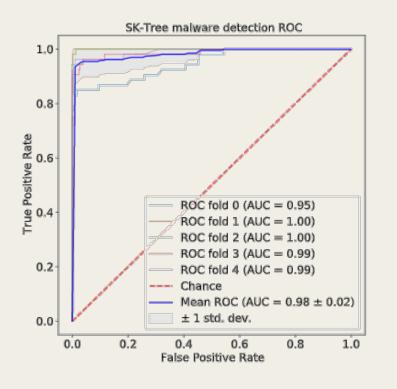
// test[i] = mean\_squared\_error(y\_pred, y\_test)

### Process tree example: Expected signatures of clouds of paths



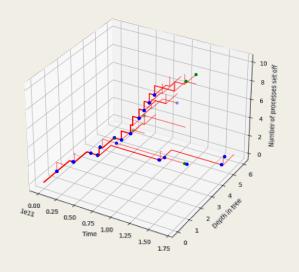
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Developed SK-tree structure to apply standardised expected signature techniques to host-based event logs, by viewing processes as trees evolving over time analysed as expected signatures through a PDE kernel.



#### 2102.07904.pdf (arxiv.org)

We demonstrate the SK-Tree to detect malicious events on a portion of the publicly available DARPA OpTC dataset, achieving an initial AUROC score of 98% for a supervised question.



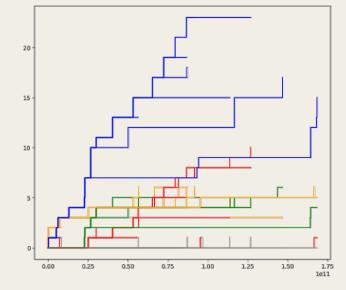


Fig. 2. ROC evaluation of the SK-Tree binary classifier on the OpTC data

### Communication



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### Landmark-based action recognition

To communicate our methodology, and aside from our papers, with their software we are constructing notebooks with introductory examples of what we can do.

People moving can easily be anonymized to landmarks. It is a static process. The moving stick people still contain information.

Peter Foster has put together a simple notebook you can run that demonstrates viable approaches to recognizing these actions that can be trained on small datasets.

https://www.datasig.ac.uk/examples