Approximate Bayesian Computation with Path Signatures

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Oxford Mathematics

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Introduction

Aim: To convince you that path signatures can be a useful tool when applying approximate Bayesian computation to time-series simulators of different kinds.

Approximate Bayesian Computation with Path Signatures
Dyer, J.; Cannon, P.; and Schmon, S. M.
arXiv:2106.12555 (2023)

(Just updated!)

Context & notation

Inference for dynamic, stochastic simulation models

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- Consequence: inference on $\boldsymbol{\theta}$ is tricky – many inference procedures require access to $p(\mathbf{x} \mid \boldsymbol{\theta})$ e.g. Bayes

$$\pi(\boldsymbol{\theta} \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid \boldsymbol{\theta})}{p(\mathbf{x})} \pi(\boldsymbol{\theta}) \tag{1}$$

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- Resort to simulation-based inference, such as approximate Bayesian computation (ABC): with kernel function K_ϵ, bandwidth parameter $\epsilon > 0$, and summary statistics $\mathbf{s}$ s.t. $\mathbf{s}_\mathbf{x} := \mathbf{s}(\mathbf{x})$,

$$\pi_{\mathrm{ABC},\epsilon}(\boldsymbol{\theta} \mid \mathbf{s}_\mathbf{x}) \propto \int K_\epsilon(\mathbf{s}_\mathbf{x}, \mathbf{s}_{\tilde{\mathbf{x}}})\, p(\tilde{\mathbf{x}} \mid \boldsymbol{\theta})\, \pi(\boldsymbol{\theta})\, \mathrm{d}\tilde{\mathbf{x}} \tag{2}$$

Challenge

Choosing appropriate distances/summary statistics for time-series data

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- Kernel K_ϵ typically uses some distance $\mathcal{D}$ internally, e.g.

$$K_\epsilon(\mathbf{s_x}, \mathbf{s_{\tilde{x}}}) \propto \mathbb{I}\left[\mathcal{D}(\mathbf{s_x}, \mathbf{s_{\tilde{x}}}) \leq \epsilon\right], \qquad \text{(Uniform kernel)}$$

$$K_\epsilon(\mathbf{s_x}, \mathbf{s_{\tilde{x}}}) \propto \exp\left\{-\mathcal{D}(\mathbf{s_x}, \mathbf{s_{\tilde{x}}})/\epsilon\right\} \qquad \text{(Gaussian kernel)}$$

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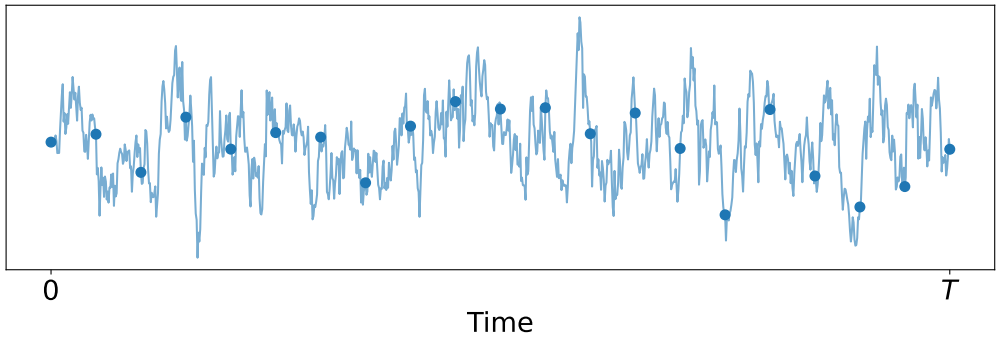

Figure: Univariate time-series

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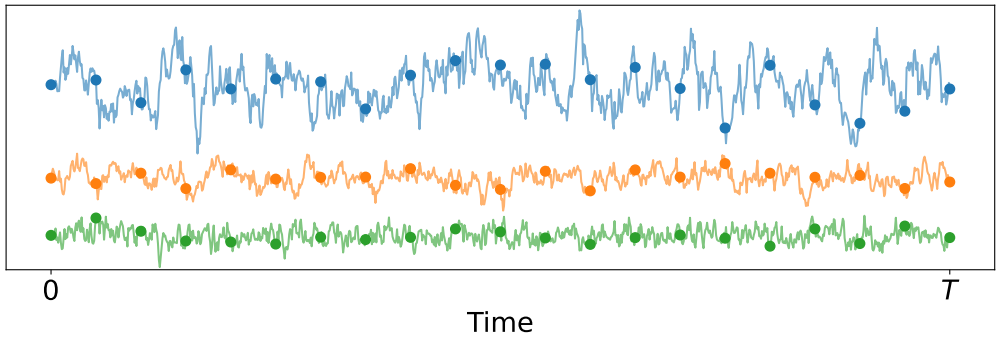

Figure: Multivariate time-series

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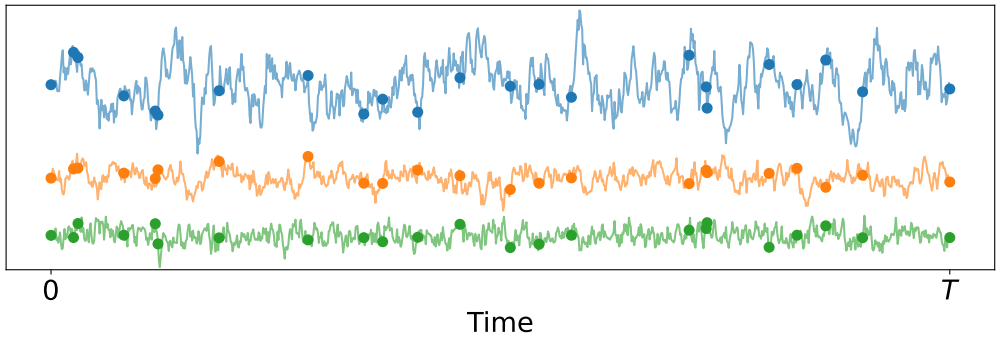

Figure: Irregularly sampled, multivariate time-series

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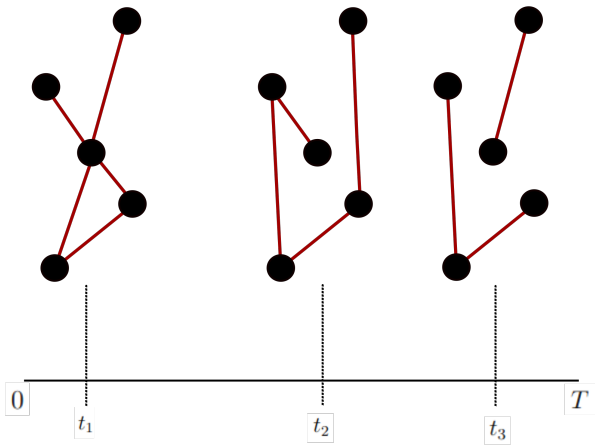

Figure: Irregularly spaced, non-Euclidean time-series

Existing approaches to choosing distance/summary statistics

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Prototypical approach: Euclidean distance between hand-crafted summary statistics $\mathbf{s}$.

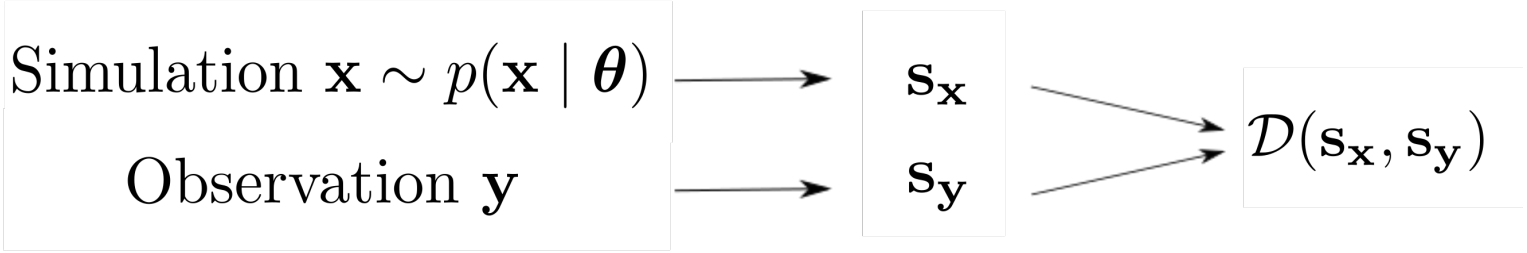


Figure: Schematic of manual method for defining "distance".

Ad-hoc derivation of hand-crafted summary statistics can be time-consuming, expensive, risky...

Existing approaches to choosing distance/summary statistics

Semi-automatic ABC (Fearnhead and Prangle, 2012)

- Use $\mathbf{s_x} = \mathbb{E}_\pi[\boldsymbol{\theta} \mid \mathbf{x}]$ in ABC$\rightarrow$ minimises quadratic loss between "true" parameters $\boldsymbol{\theta}^*$ and

$$\hat{\boldsymbol{\theta}}_{\mathrm{ABC}} = \mathbb{E}_{\pi_{\mathrm{ABC},\epsilon}}[\boldsymbol{\theta} \mid \mathbf{s_y}]$$

- Estimate $\mathbf{s_x}$ by learning nonlinear map from $\mathbf{x}_i$ to $\boldsymbol{\theta}_i$, where $(\mathbf{x}_i, \boldsymbol{\theta}_i)_{i=1}^n \sim p(\mathbf{x} \mid \boldsymbol{\theta})\pi(\boldsymbol{\theta})$ is simulated training data. Then use

$$\mathcal{D}(\mathbf{s_x}, \mathbf{s_y}) = \|\mathbf{s_x} - \mathbf{s_y}\|_2$$

- Drawback: need to define suitable space of functions over which to search. What function space is appropriate/useful for time-series of different kinds?

Existing approaches to choosing distance/summary statistics

K2-ABC: ABC with kernel embeddings (Park et al., 2016)

- Compare empirical distribution of simulator and real data via **MMD**
- For sufficiently expressive kernel $k(X, \cdot)$, e.g. RBF, kernel mean embedding encodes all information of the distribution

$$\mu_X := \mathbb{E}[k(X, \cdot)], \qquad \hat{\mu}_X = \frac{1}{n}\sum_{i=1}^{n} k(\mathbf{x}_i, \cdot), \qquad \mathcal{D}(\mathbf{x}, \mathbf{y}) = \mathrm{MMD}^2.$$

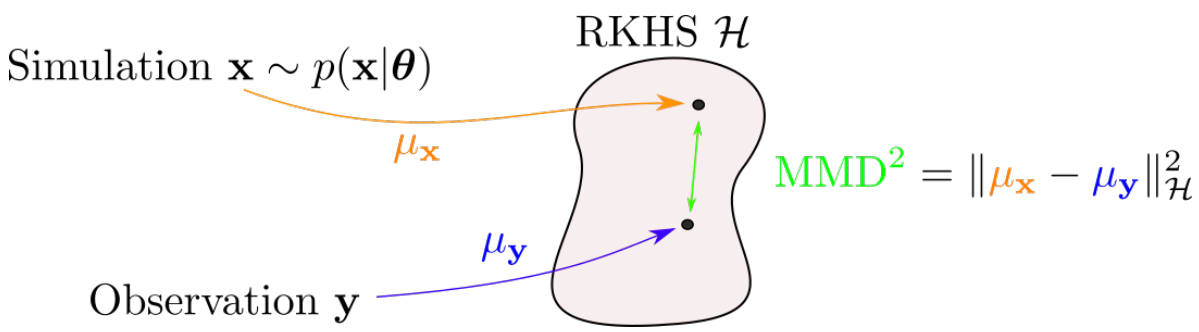


Figure: Schematic of MMD. Treats the $\mathbf{x}_i$ in $\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_n)$ as exchangeable.

Existing approaches to choosing distance/summary statistics

ABC with the Wasserstein distance (Bernton et al., 2019)

Compare simulated and real time-series, $\mathbf{x}$ and $\mathbf{y}$, via the **Wasserstein distance**:

$$\mathcal{D}(\mathbf{x}, \mathbf{y}) = W_p(\mathbf{x}, \mathbf{y}) := \min_{\sigma \in \mathcal{S}_n} \sum_{i=1}^{n} \rho(\mathbf{x}_i, \mathbf{y}_{\sigma(i)})^p,$$

$$\rho(\mathbf{x}_t, \mathbf{y}_s) = \|\mathbf{x}_t - \mathbf{y}_s\| + \lambda|t - s|$$

- $\mathcal{S}_n$: set of permutations of $1, \ldots, n$
- λ: hyperparameter balancing "vertical" and "horizontal" transport

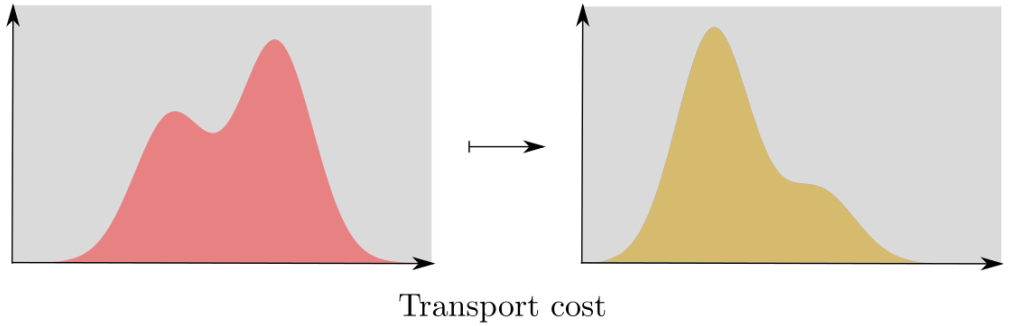


Figure: Schematic of Wasserstein distance. Sort of accounts for dependencies.

Existing approaches to choosing distance/summary statistics

Other approaches in this vein...

- ABC with the Kullback-Liebler divergence (Jiang, 2018)
- ABC with the energy statistic (Nguyen et al., 2020)
- ...

See Drovandi and Frazier (2022) for a recent review and comparison of all of the above.

These approaches are primarily designed for independent – rather than time-series-like – data. How can we deal with time-series?

Our contribution: ABC with path signatures

We propose (semi-)automatic approaches to ABC for time-series models of different kinds using **path signatures**.

Remainder of this talk:

- Overview of path signatures & properties
- Our proposed signature-based methods & some theoretical properties
- Experimental results
- Summary & conclusion

Let $h : [0, T] \to \mathcal{H}$ be a path in Hilbert space $\mathcal{H}$ with bounded variation:

$$\|h\|_{1-\mathrm{var}} := \sup_{\zeta(0,T)} \sum_{i=1}^{n-1} \|h_{t_{i+1}} - h_{t_i}\|_{\mathcal{H}} < \infty.$$

The signature map sends h to an infinite collection of tensors of increasing order:

$$\mathrm{Sig} : h \mapsto (1, S_1(h), S_2(h), \dots) \in \prod_{m \geq 0} \mathcal{H}^{\otimes m}$$

where

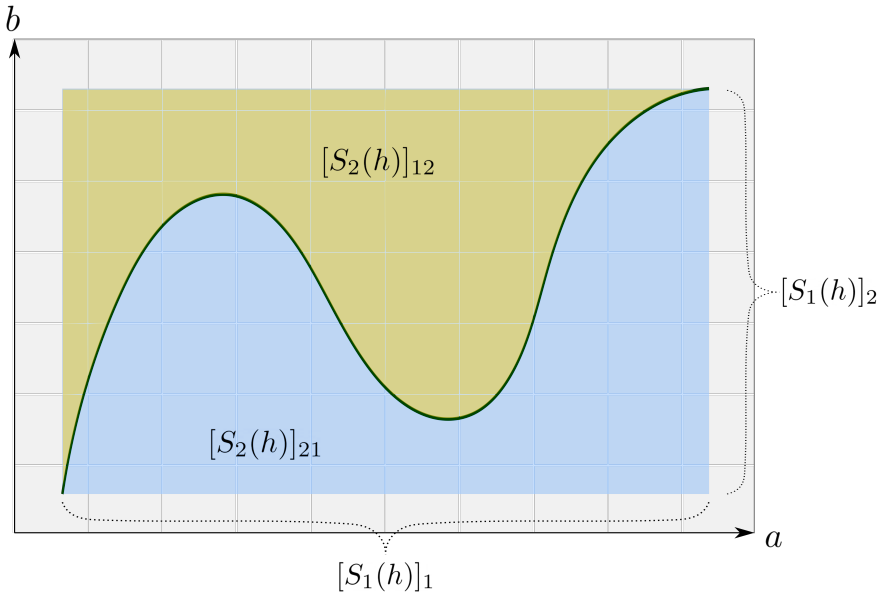
$$S_m(h) = \int_{t_m=0}^{T} \cdots \int_{t_1=0}^{t_2} \mathrm{d}h_{t_1} \otimes \cdots \otimes \mathrm{d}h_{t_m} \tag{3}$$

Path signatures

Example 2.3, Király and Oberhauser (2019)

Consider $h_t = (a_t, b_t) \in \mathbb{R}^2$.

$$S_1(h) = \begin{bmatrix} \int_0^T \mathrm{d}a_t \\ \int_0^T \mathrm{d}b_t \end{bmatrix} \quad \text{and} \quad S_2(h) = \begin{bmatrix} \int_0^T \int_0^{t_2} \mathrm{d}a_{t_1} \mathrm{d}a_{t_2} & \int_0^T \int_0^{t_2} \mathrm{d}a_{t_1} \mathrm{d}b_{t_2} \\ \int_0^T \int_0^{t_2} \mathrm{d}b_{t_1} \mathrm{d}a_{t_2} & \int_0^T \int_0^{t_2} \mathrm{d}b_{t_1} \mathrm{d}b_{t_2} \end{bmatrix}.$$



Path signatures

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$$\mathrm{d}Y_t = A(Y_t) \circ \mathrm{d}B_t, \quad Y_0 = y$$

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Lyons's *rough path theory* (see e.g. Lyons et al., 2002, 2007; Friz and Hairer, 2020) built around the closely related notion of a multiplicative functional.

Path signatures

Key properties

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Uniqueness: For injective paths h, g with common origin, $\mathrm{Sig}(h) = \mathrm{Sig}(g)$ iff $h = g$. (Enforcing these conditions always possible.)

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Universal nonlinearity: Linear functionals on signatures are dense in the space of continuous, real-valued functions on compact sets of paths.

Kernelisation: The *signature kernel* for bounded variation paths $h, g : [0, T] \to \mathcal{H}$ is

$$k(h, g) = \langle \mathrm{Sig}(h), \mathrm{Sig}(g) \rangle := \sum_{m \geq 0} \langle S_m(h), S_m(g) \rangle_{\mathcal{H}^{\otimes m}} .$$

Király and Oberhauser (2019): $k(h, g)$ can be evaluated using only inner products on points in the path. Király and Oberhauser (2019) and Salvi et al. (2020) provide efficient methods for evaluating k.

Path signatures

From sequences in data space to paths in Hilbert space

Real scenario: observe sequence $\mathbf{x} = (\mathbf{x}_1, \ldots, \mathbf{x}_n) \in \mathcal{X}^n$ at times $0 = t_1 < \cdots < t_n = T$. How to map to path in $\mathcal{H}$?

1. **Embed data in a Hilbert space**: Through canonical feature map for kernel $\kappa : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ with corresponding RKHS $\mathcal{H}$.
2. **Obtain a $\mathcal{H}$-valued path**: Through interpolation (e.g. linear).

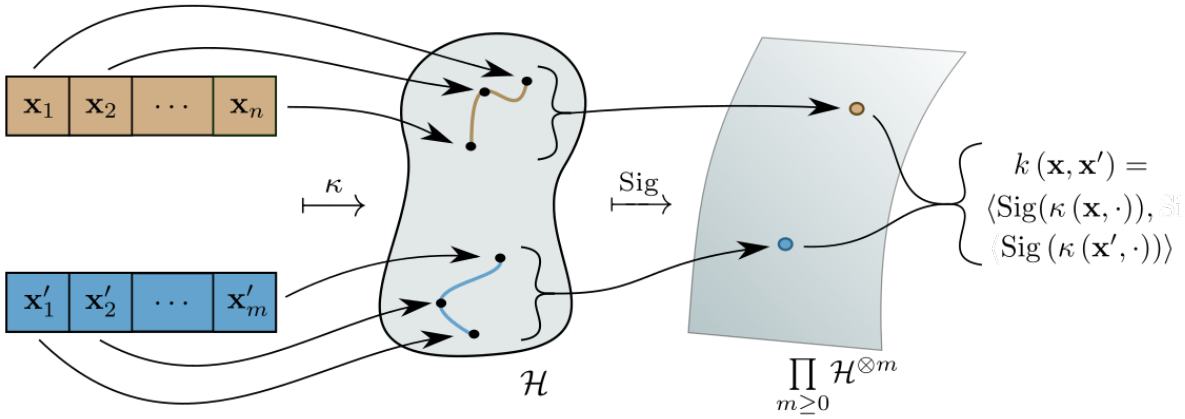

Figure: Embedding sequences with the signature kernel (Dyer et al., 2022).

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Distance computation can be kernelised with signature kernel k:

$$\mathcal{D}(\mathbf{x}, \mathbf{y}) := \|\mathrm{Sig}(\mathbf{x}) - \mathrm{Sig}(\mathbf{y})\|^2 = k(\mathbf{x}, \mathbf{x}) + k(\mathbf{y}, \mathbf{y}) - 2k(\mathbf{x}, \mathbf{y}) \tag{4}$$

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Convergence of Signature ABC posterior

Let $\mathcal{X} = \mathbb{R}^m$, $\mathbf{x}, \mathbf{y} \in \mathcal{X}^n$ be length-n sequences in $\mathcal{X}$. Under the regularity conditions on $p(\mathbf{x} \mid \boldsymbol{\theta})$ assumed in Bernton et al. (2019), and with $\mathcal{D}$ as in Equation (4) + some additional benign conditions on κ, the ABC posterior

$$\pi_{\mathrm{ABC},\epsilon}(\boldsymbol{\theta} \mid \mathrm{Sig}(\mathbf{y})) \to \pi(\boldsymbol{\theta} \mid \mathbf{y}) \quad \text{as} \quad \epsilon \to 0.$$

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Behaviour as $n \to \infty$ for fixed ϵ

For a continuous-time process observed over fixed time interval $[0, T]$,

$$\pi_{\mathrm{ABC},\epsilon}(\boldsymbol{\theta} \mid \mathrm{Sig}(\mathbf{y})) \rightharpoonup \pi_{\mathrm{ABC},\epsilon}(\boldsymbol{\theta} \mid \mathrm{Sig}(h)) \quad \text{as} \quad n \to \infty.$$

Exploit "universal nonlinearity" of Sig to perform **semi-automatic** ABC for time-series simulators.

What space of functions to optimise over? Linear functionals on signatures – signature kernel is universal for sequences (Király and Oberhauser, 2019).

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E.g. kernel ridge regression with signature kernel k, s.t.

$$\hat{\boldsymbol{\theta}}(\mathbf{x}) := \left(\sum_{r=1}^{R} a_{1,r} k(\mathbf{x}, \mathbf{x}^{(r)}), \ldots, \sum_{r=1}^{R} a_{d,r} k(\mathbf{x}, \mathbf{x}^{(r)}) \right)'$$

and

$$\mathcal{D}(\mathbf{x}, \mathbf{y}) = \|\hat{\boldsymbol{\theta}}(\mathbf{x}) - \hat{\boldsymbol{\theta}}(\mathbf{y})\|_2$$

Experimental results

Ricker model (Wood, 2010)

$$\log N_{t+1} = \log r + \log N_t - N_t + \sigma\epsilon_t, \quad \epsilon_t \sim \mathcal{N}(0,1)$$
$$\mathbf{y}_t \sim \mathrm{Po}\left(\phi N_t\right).$$

Aim: approximate posterior for $\boldsymbol{\theta} = (\log r, \phi, \sigma)$ with pseudo-data $\mathbf{y} \sim p(\mathbf{y} \mid \boldsymbol{\theta}^*)$, $\boldsymbol{\theta}^* = (4, 10, 0.3)$ and priors

$$\log r \sim \mathcal{U}(3,8), \qquad \phi \sim \mathcal{U}(0,20), \qquad \sigma \sim \mathcal{U}(0,0.6).$$

Experimental results

Ricker model (Wood, 2010)

$$\text{“Delay”} : (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n) \mapsto ((\mathbf{x}_1, \mathbf{x}_2), (\mathbf{x}_2, \mathbf{x}_3), \ldots, (\mathbf{x}_{n-1}, \mathbf{x}_n))$$

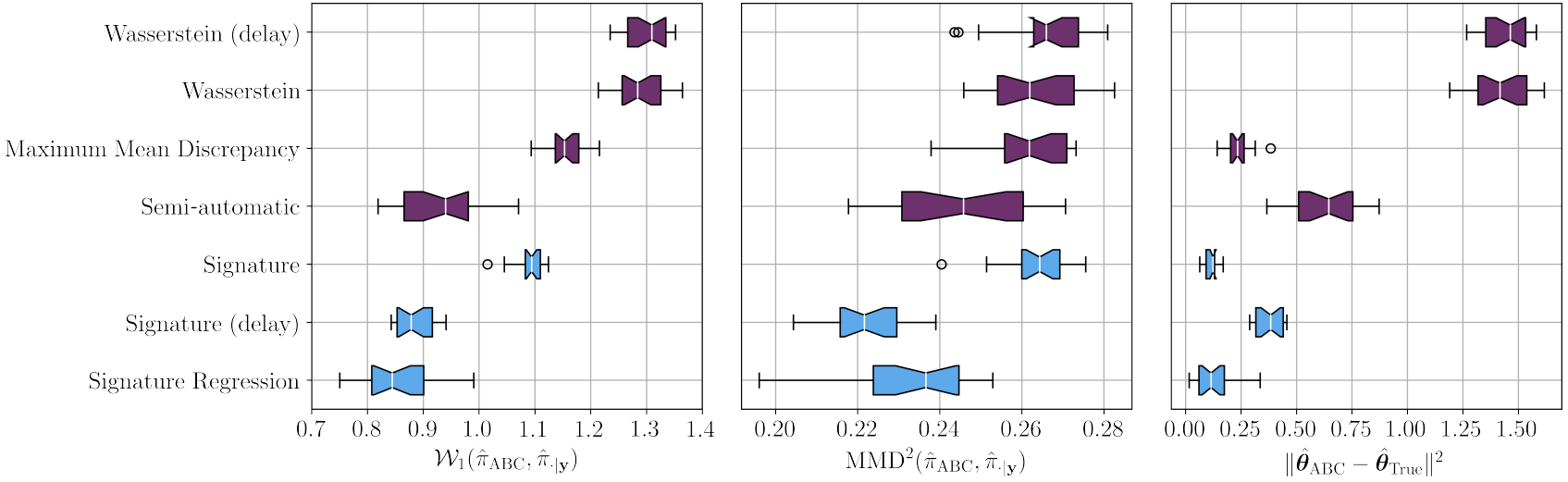

Figure: (Ricker model) Wasserstein distance (**left**) and MMD (**middle**) between ABC and ground-truth posteriors. **Right**: Euclidean distances between ABC and ground truth posterior means.

Experimental results

Results for multivariate, irregularly spaced sequences of variable length: Kypraios (2007)

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- Stochastic model of infections by and recovery from virus in population, determine by parameters β and γ
- Event-based simulation: events occur with time-dependent rate in discrete population over time interval $[0, T]$
- Output: multivariate time-series $\mathbf{y}$ of variable length and with irregularly spaced observations counting number of infected and susceptible individuals at each time
- Posterior available in closed form for Gamma priors on β and γ
- Perform inference on $\boldsymbol{\theta} = (\beta, \gamma)$ given pseudo-true data $\mathbf{y}$

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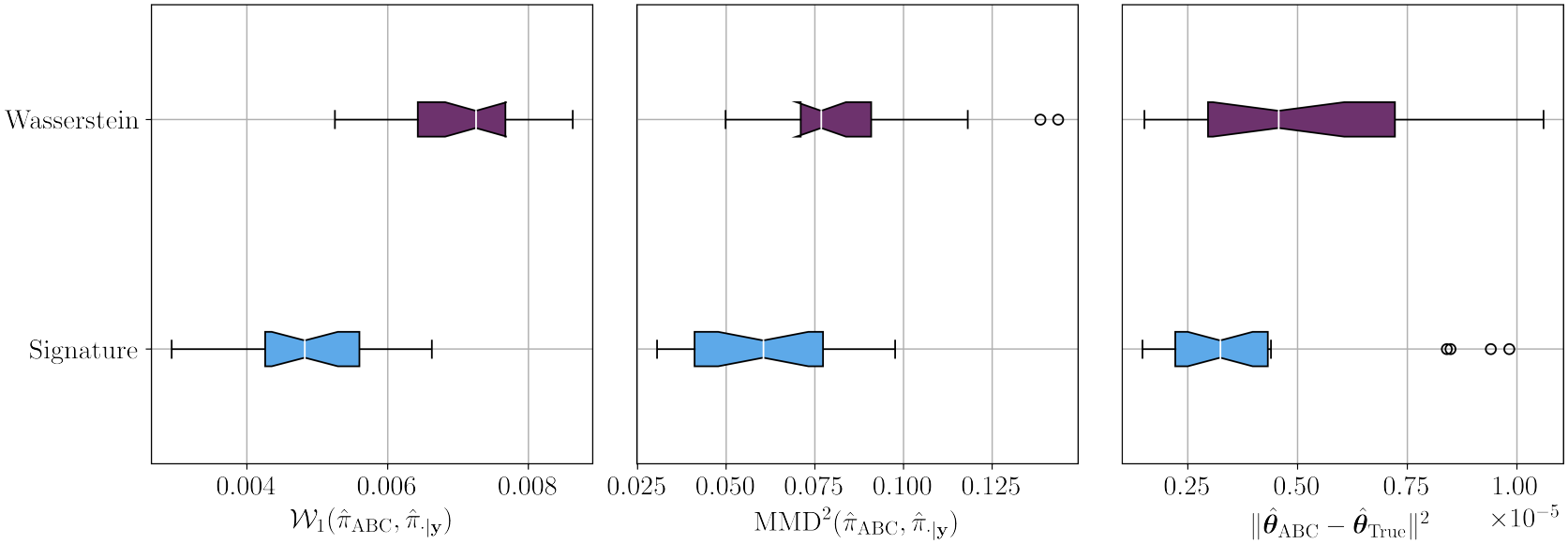

Figure: (Generalised stochastic epidemic model) **Left**: Wasserstein distance between ABC and ground-truth posteriors. **Middle**: MMD between ABC and ground-truth posteriors. **Right**: Euclidean distances between ABC and ground truth posterior means.

Kernelisation lets us operate on sequences of arbitrary objects. Example: **graphs** (e.g. simulating social networks).

Signature/Signature Regression ABC performs the following steps implicitly:

1. Send observations to RKHS $\mathcal{H}$ of graph kernel κ (e.g. Weisfeiler-Lehman)
2. Compute signature kernel for these $\mathcal{H}$-valued, piecewise-linear paths

Experimental results

Results for dynamic graph model: Zhang et al. (2017)

Model:

- If an edge absent at time $t-1$, they appear (resp. remain absent) with probability φ (resp. $1-\varphi$);
- If edge present at time $t-1$, they disappear (resp. remain present) with probability τ (resp. $1-\tau$).

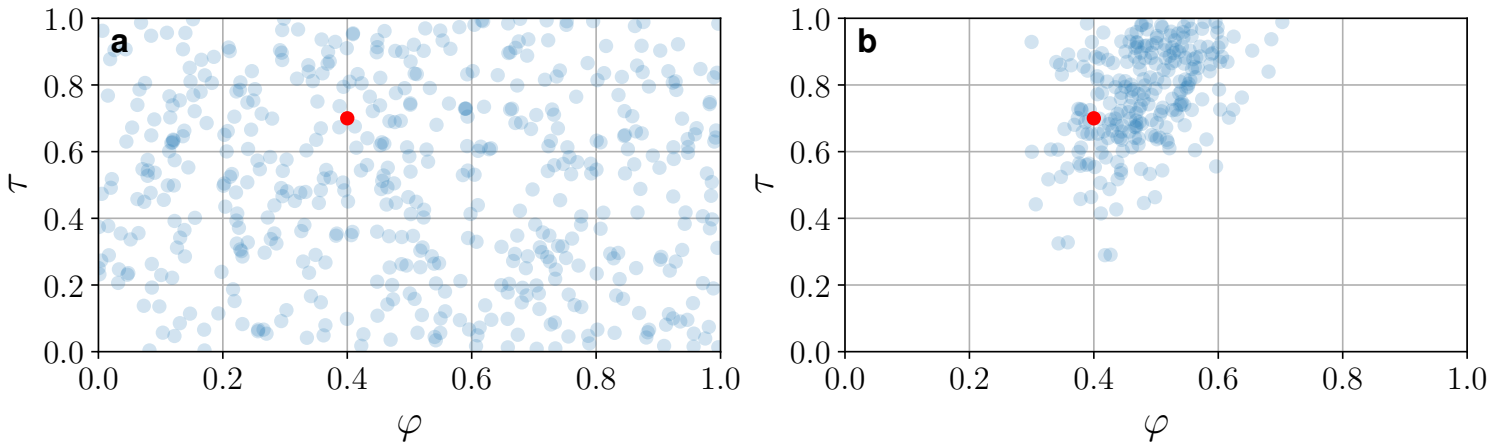

Figure: **a**: Prior. **b**: Signature ABC posterior. **Red point**: true parameters.

Computational complexity & cost

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Complexity:

- Signature kernel: $\mathcal{O}(n^2)$
- MMD: $\mathcal{O}(n^2)$
- Wasserstein: $\mathcal{O}(n^3)$ in multivariate settings with Hungarian algorithm

Observed cost: signature methods generally more expensive in our experiments (with some exceptions)

- Possible to reduce cost with e.g. GPUs, truncated signature kernels etc.
- Possible improvements to implementation

Summary & conclusion

- ABC for dynamic, stochastic simulation models can be challenging: difficult to construct summary statistics or distance measure
- Argued for the use of path signatures in ABC for generic time-series simulators
- Demonstrated empirical performance on a range of dynamic, stochastic simulation models

Thank you!

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