What We Talk About

When We Talk About

Probabilistic Numerics

LAI Reading Group
18 March 2026

Rui-Yang Zhang

Why?

Why?

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- and I like numerical algorithms

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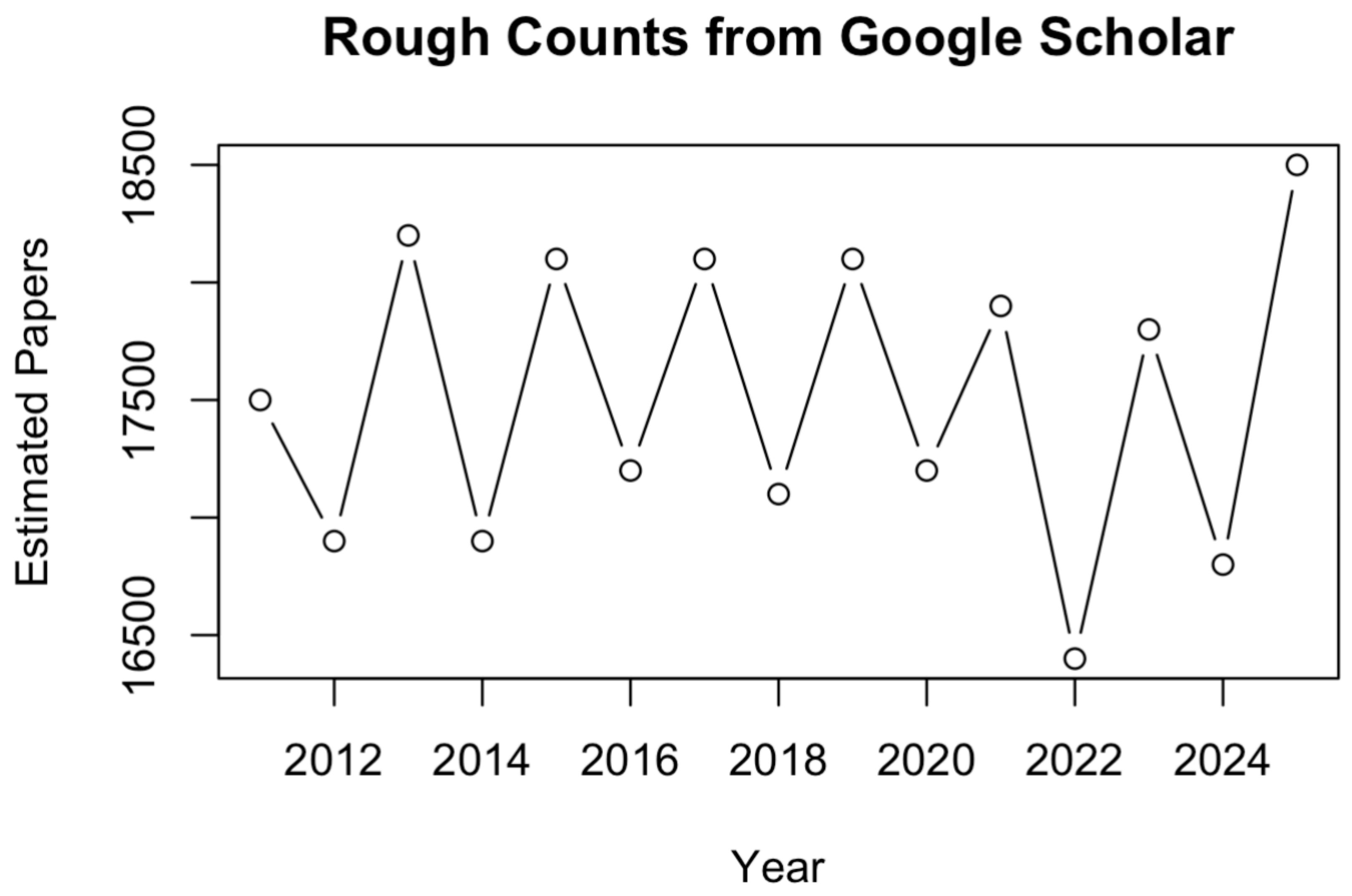

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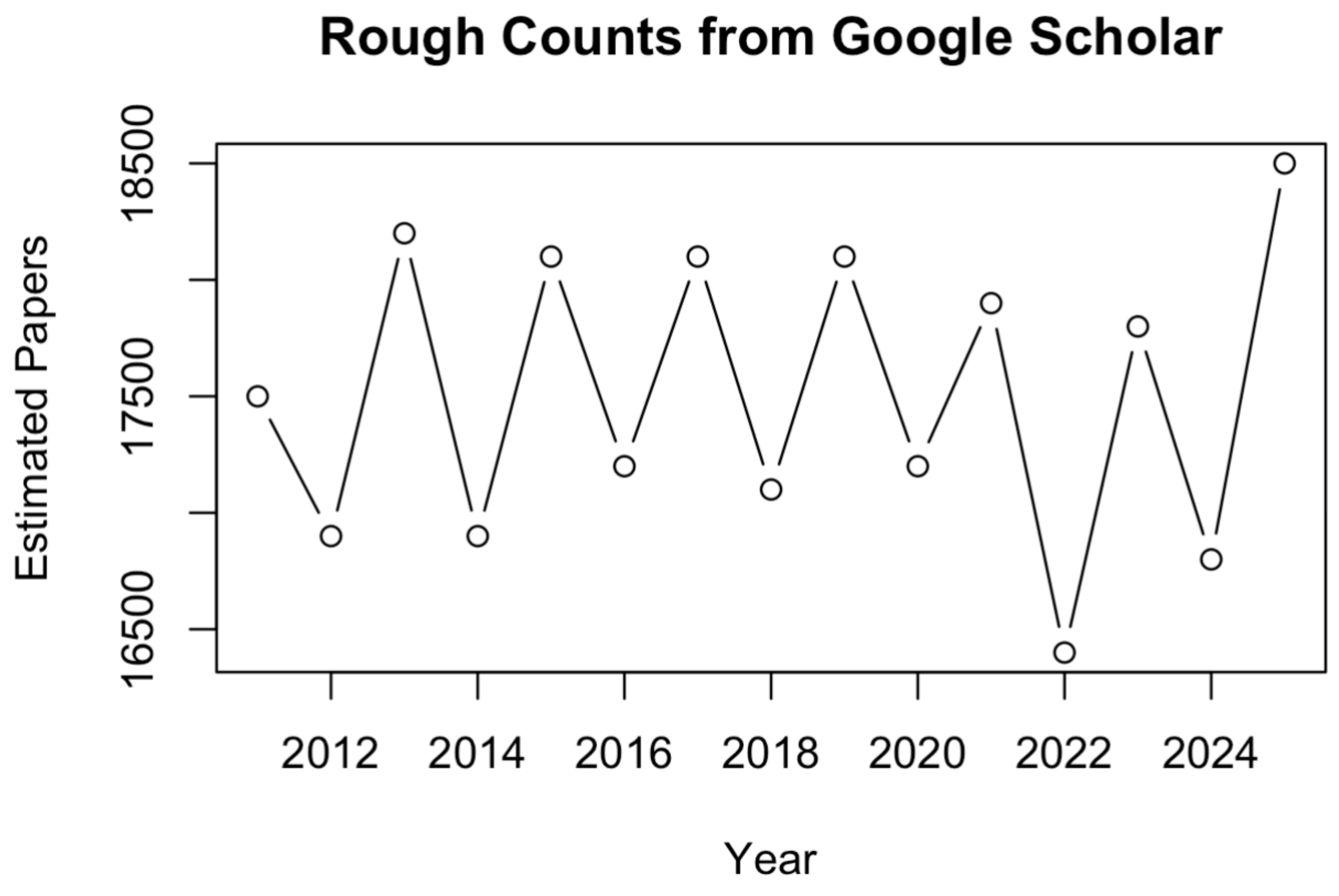

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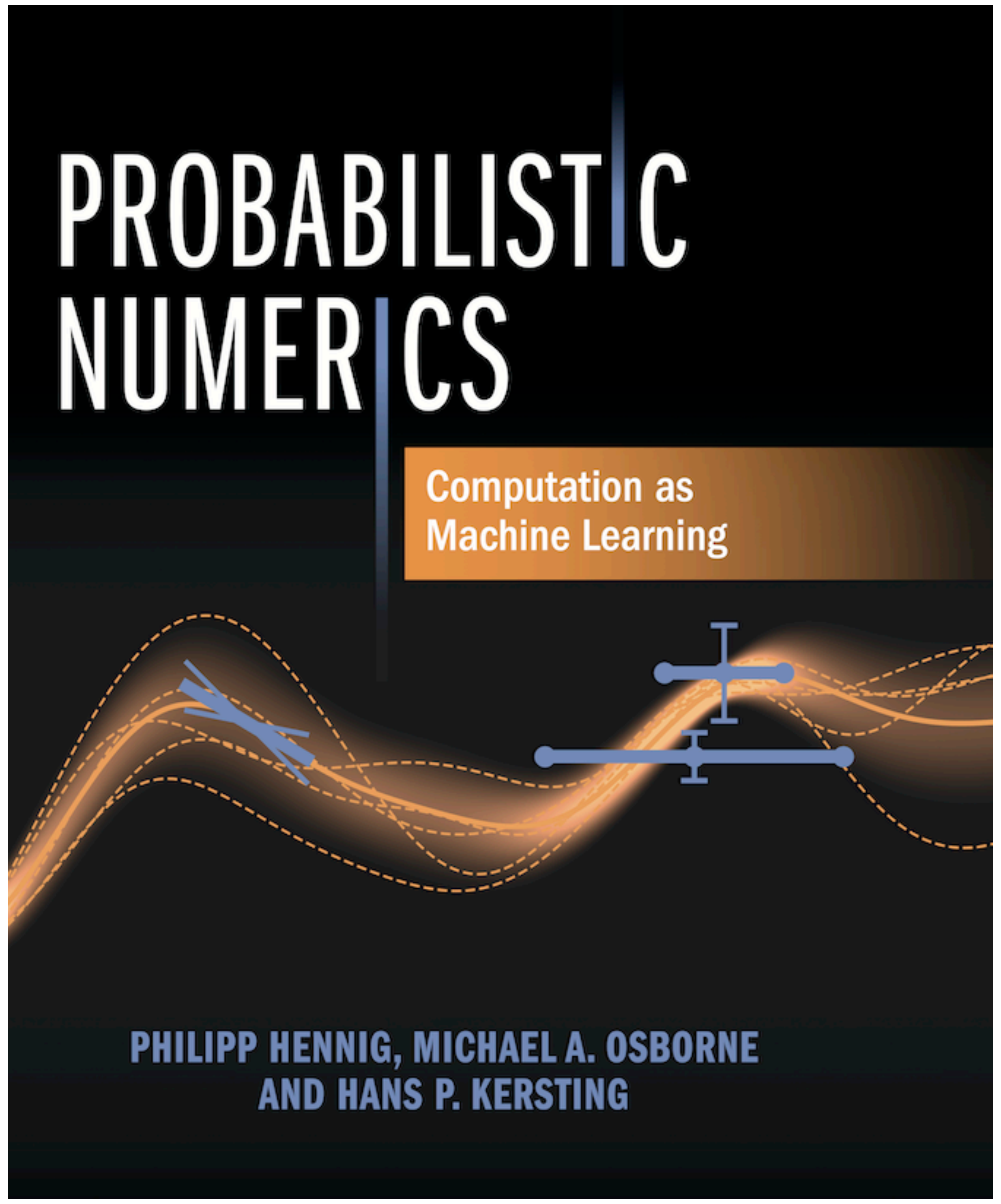

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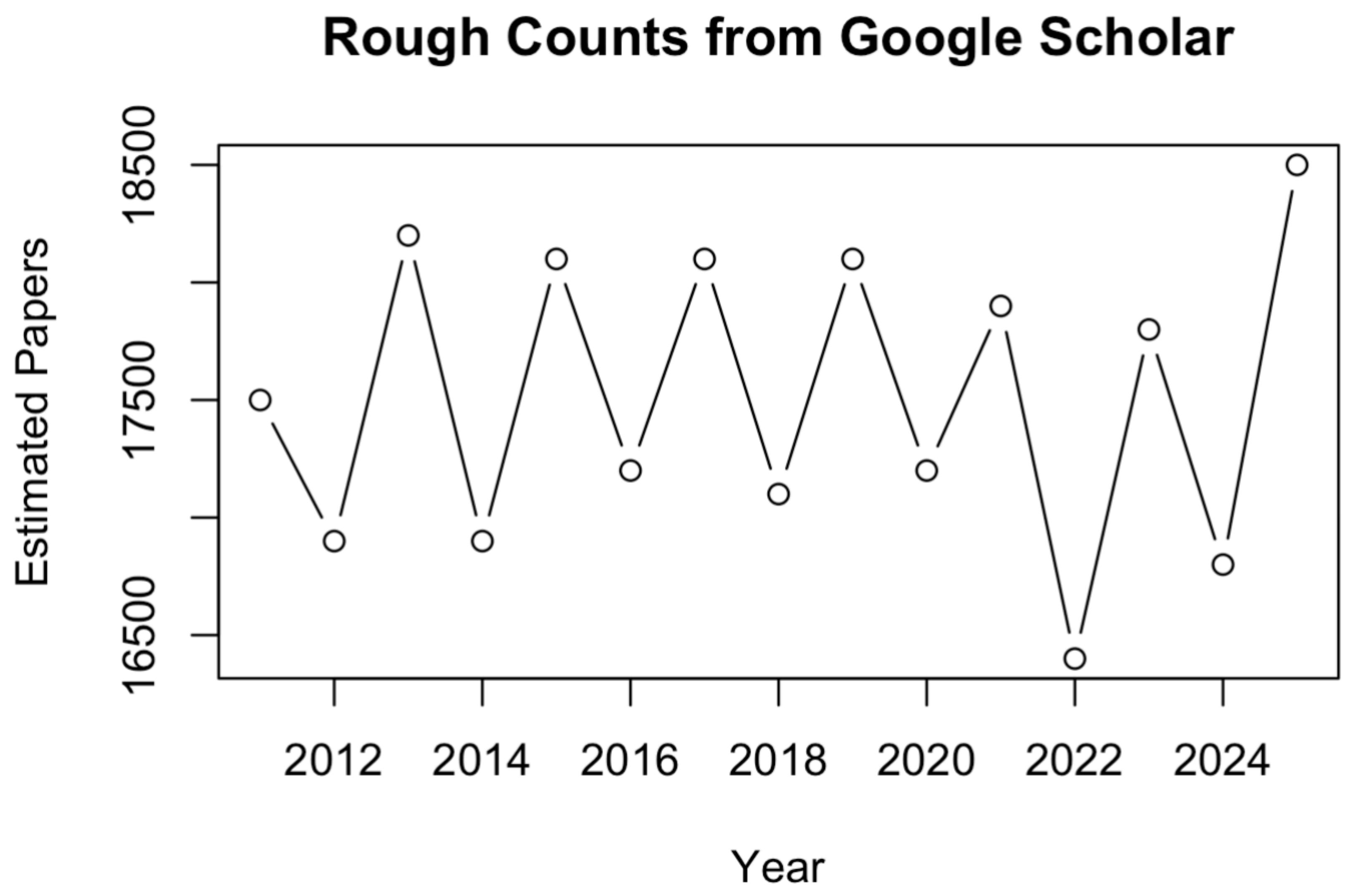

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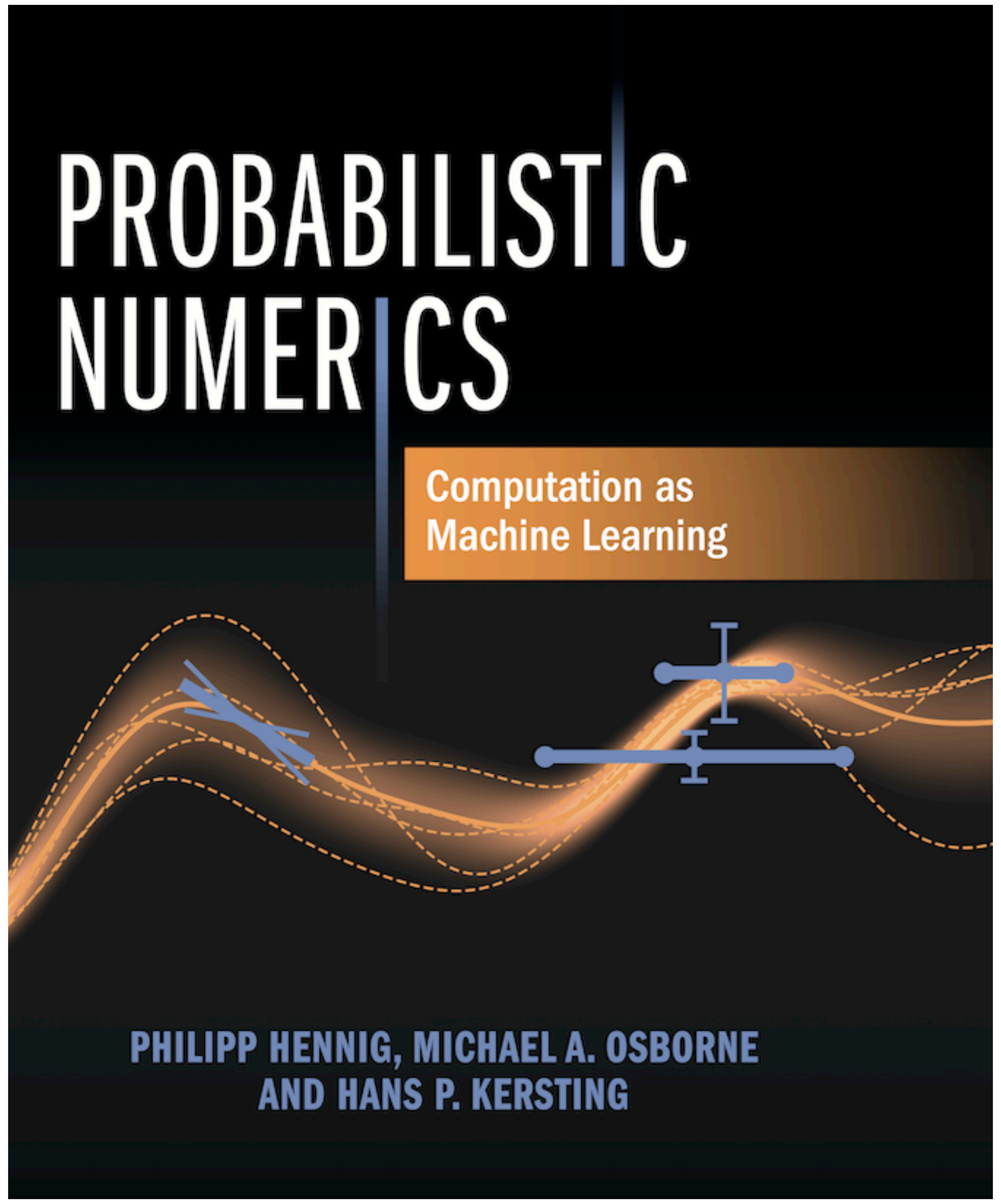

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So, what is *Probabilistic Numerics* ?

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PROCEEDINGS A

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Cite this article: Hennig P, Osborne MA, Girolami M. 2015 Probabilistic numerics and uncertainty in computations. *Proc. R. Soc. A* **471**: 20150142.
http://dx.doi.org/10.1098/rspa.2015.0142

Probabilistic numerics and uncertainty in computations

Philipp Hennig[1], Michael A. Osborne[2] and Mark Girolami[3]

[1]Department of Empirical Inference, Max Planck Institute for Intelligent Systems, Tübingen, Germany
[2]Department of Engineering Science, University of Oxford, Oxford, UK
[3]Department of Statistics, University of Warwick, Warwick, UK

Algorithms for numerical tasks, including linear algebra, integration, optimization and solving differential equations, that return uncertainties in their calculations.

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Home > Statistics and Computing > Article

A modern retrospective on probabilistic numerics

Open access | Published: 04 October 2019
Volume 29, pages 1335–1351, (2019) Cite this article

A *statistical* treatment of the errors and/or approximations that are made en route to the output of a deterministic numerical method.

ProbNum = Numerical Algorithms with Result UQ

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UQ sounds nice, but …

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    - Epistemic (Reducible) & Aleatoric (Irreducible)

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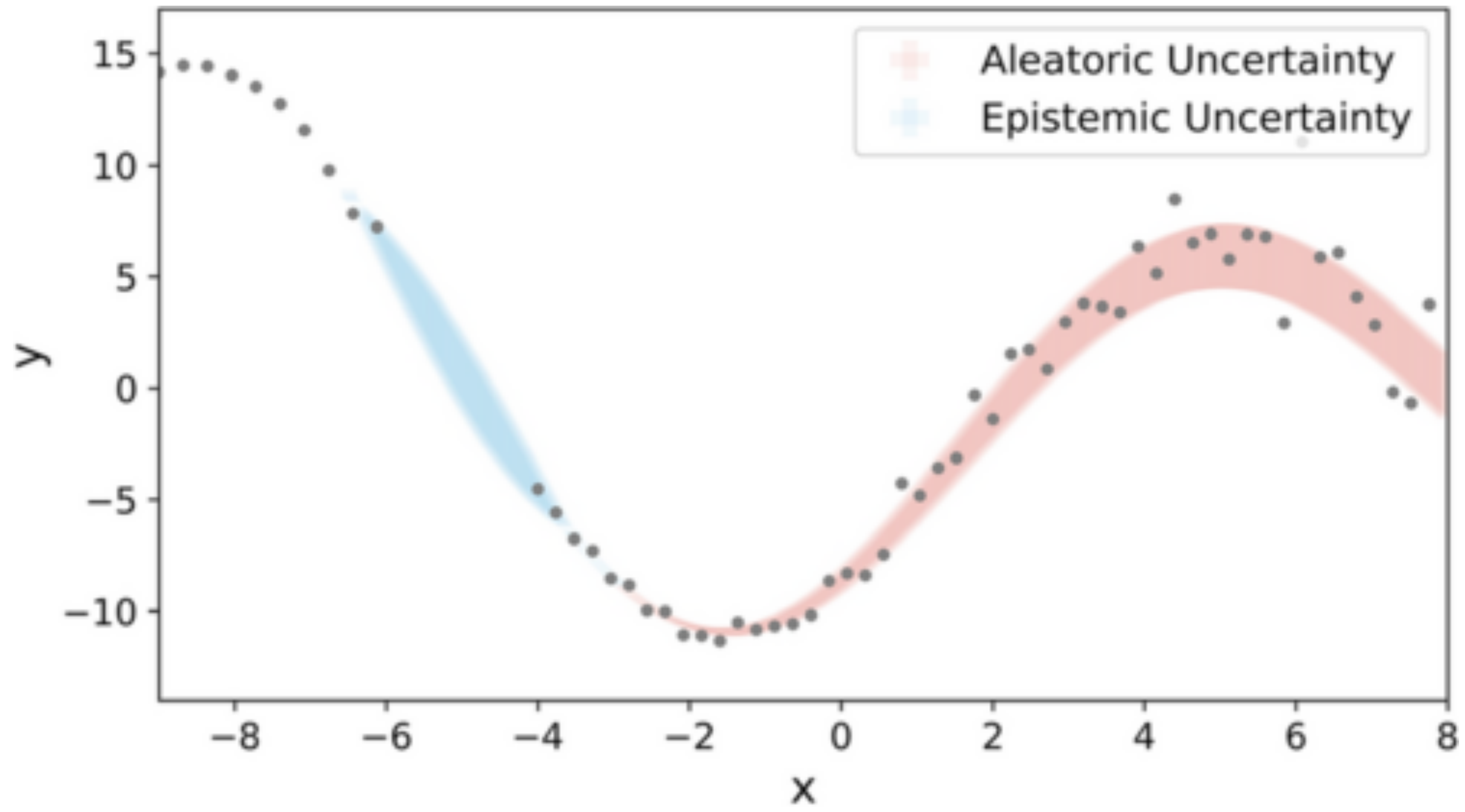

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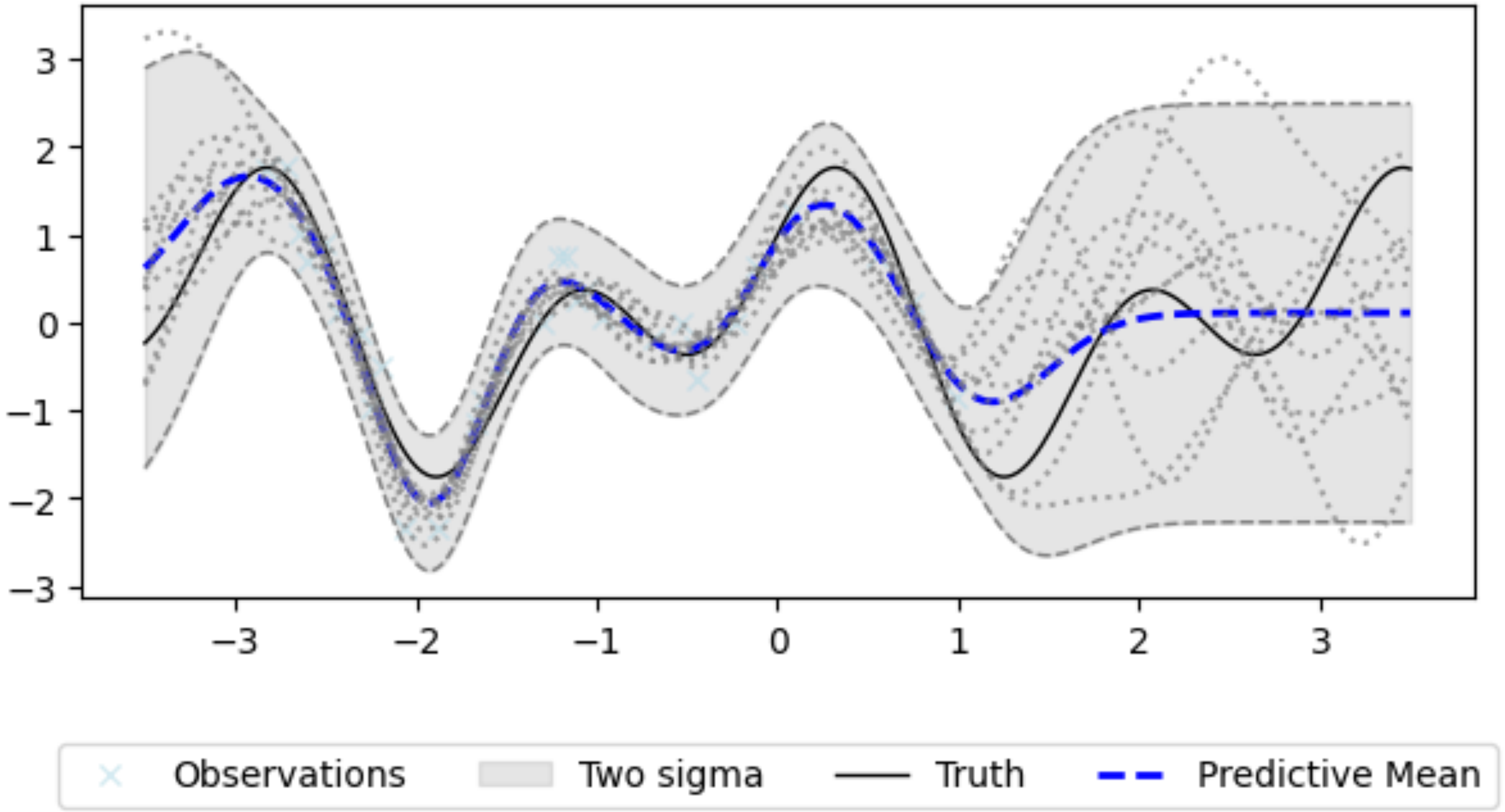

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- How much do we have to pay for these uncertainties?

Relevance of ProbNum for ML

Hennig (2023): "… (Probabilistic Numerics) never mattered more"

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Being Bayesian, Even Just a Bit, Helps

**Being Bayesian, Even Just a Bit,
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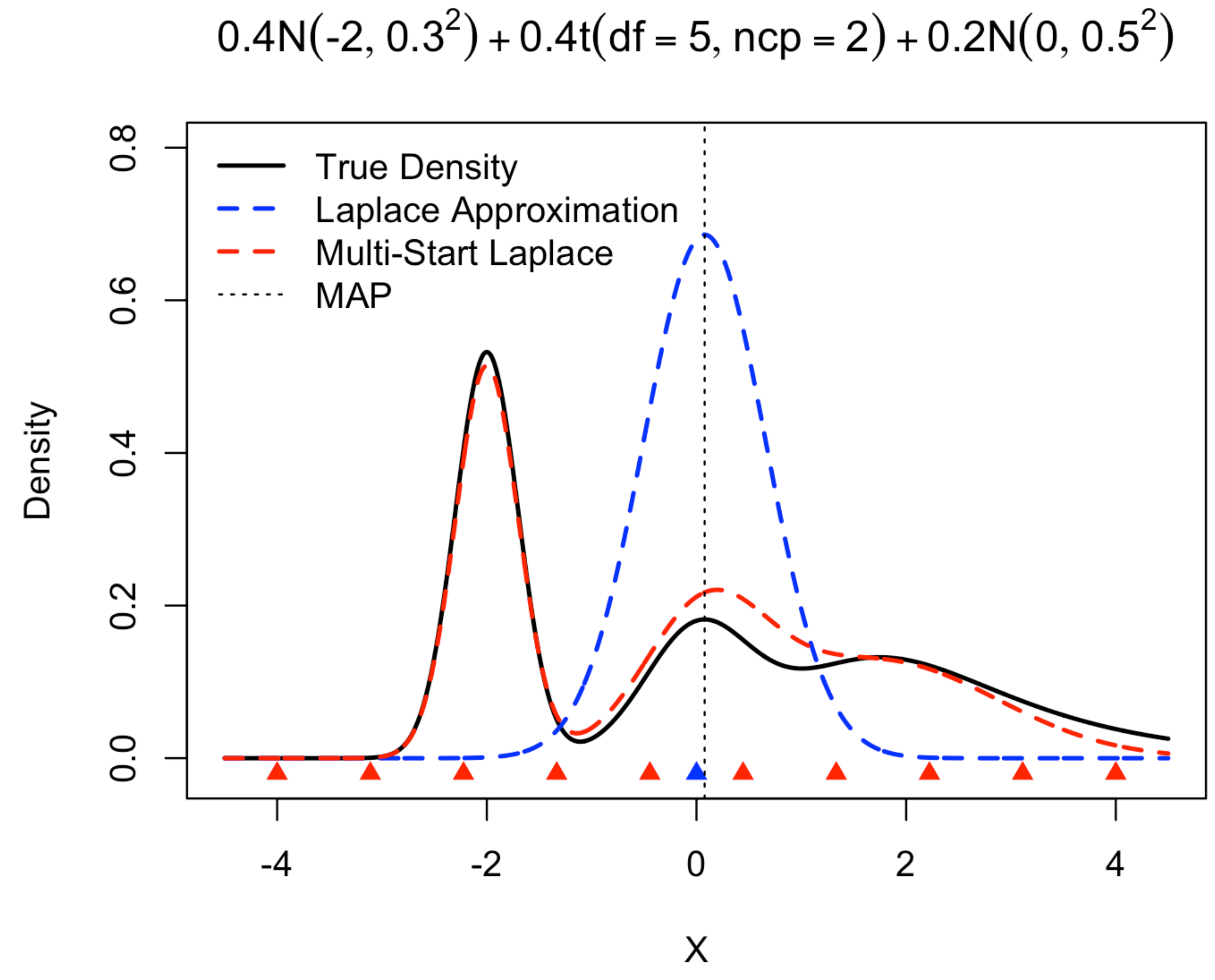

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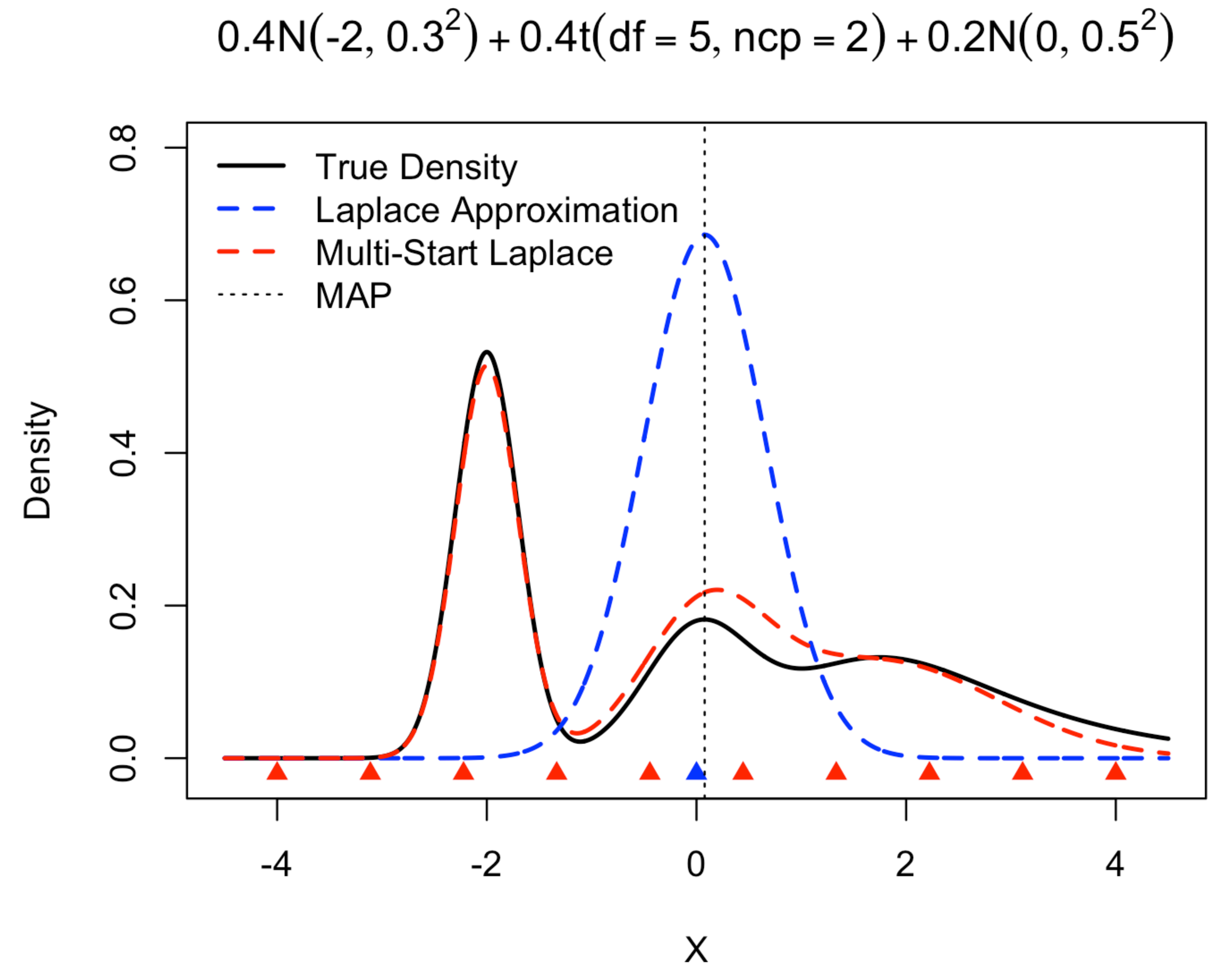

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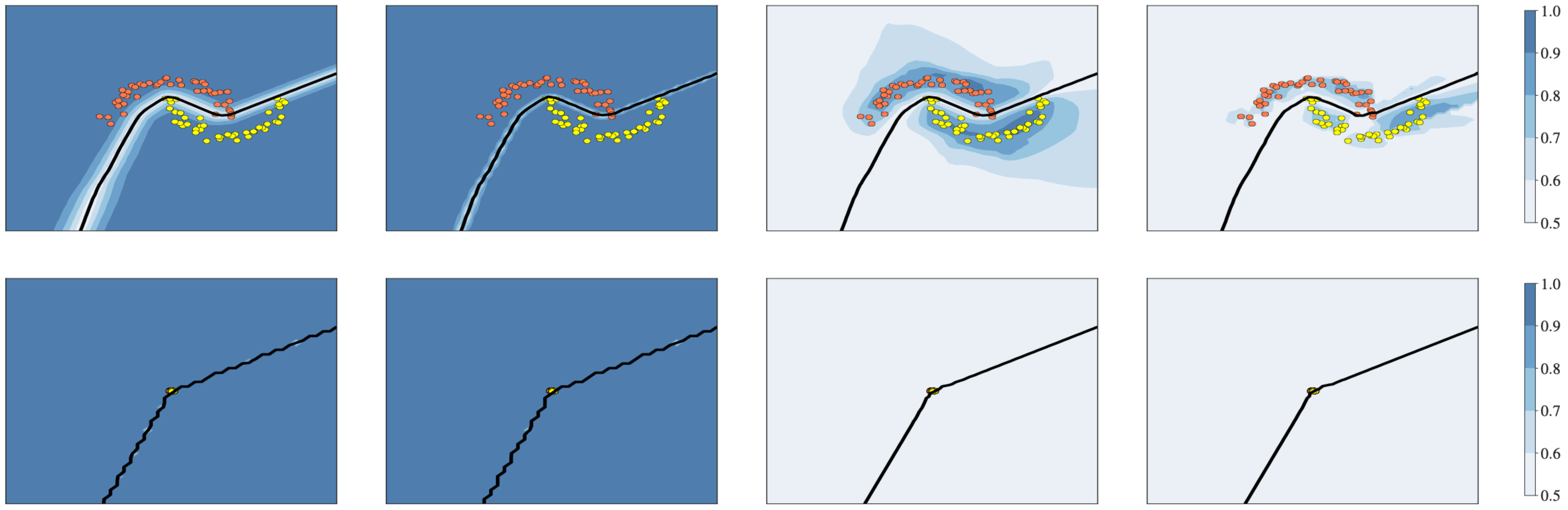
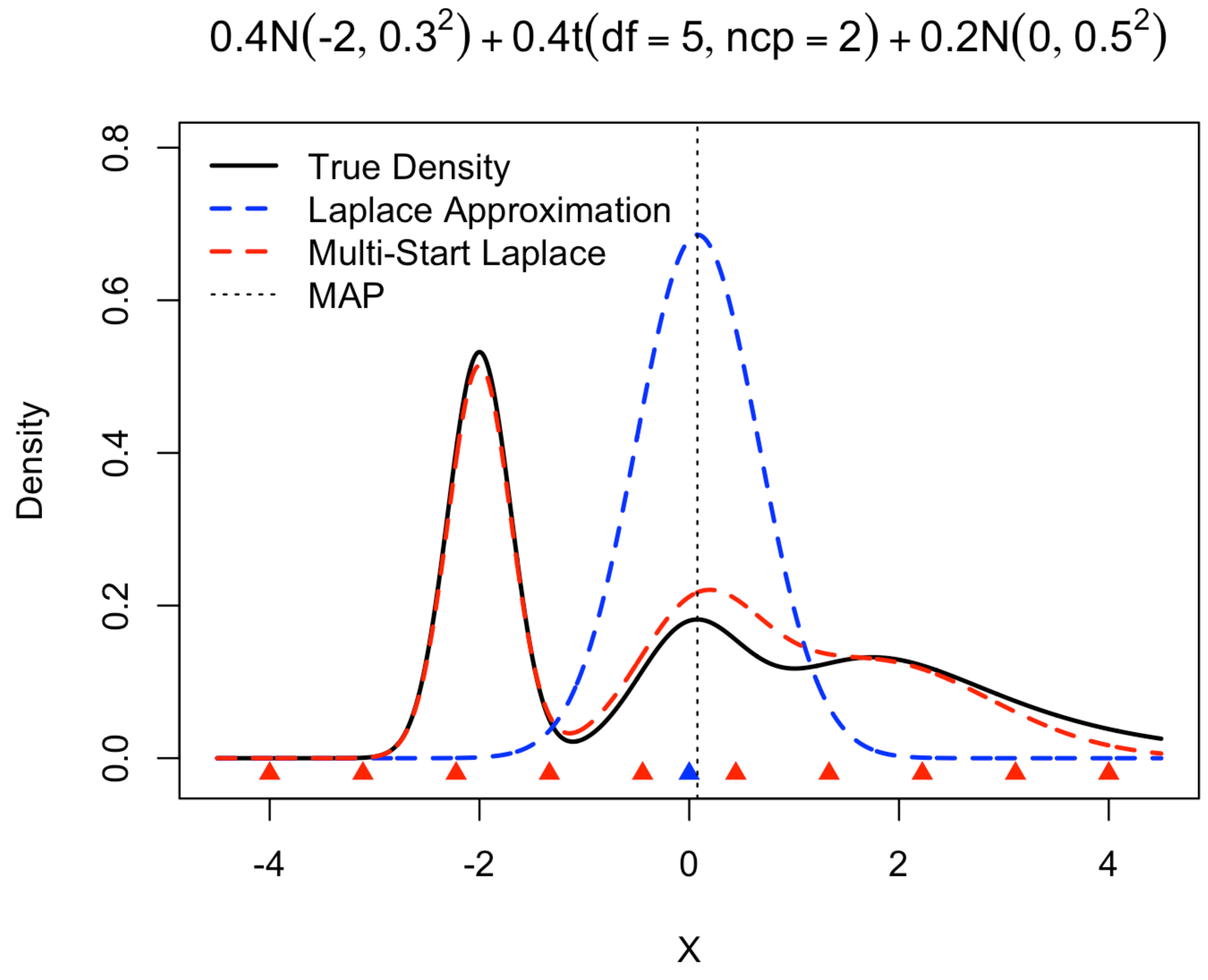


(a) MAP (b) Temp. scaling (c) Bayesian (last-layer) (d) Bayesian (all-layer)



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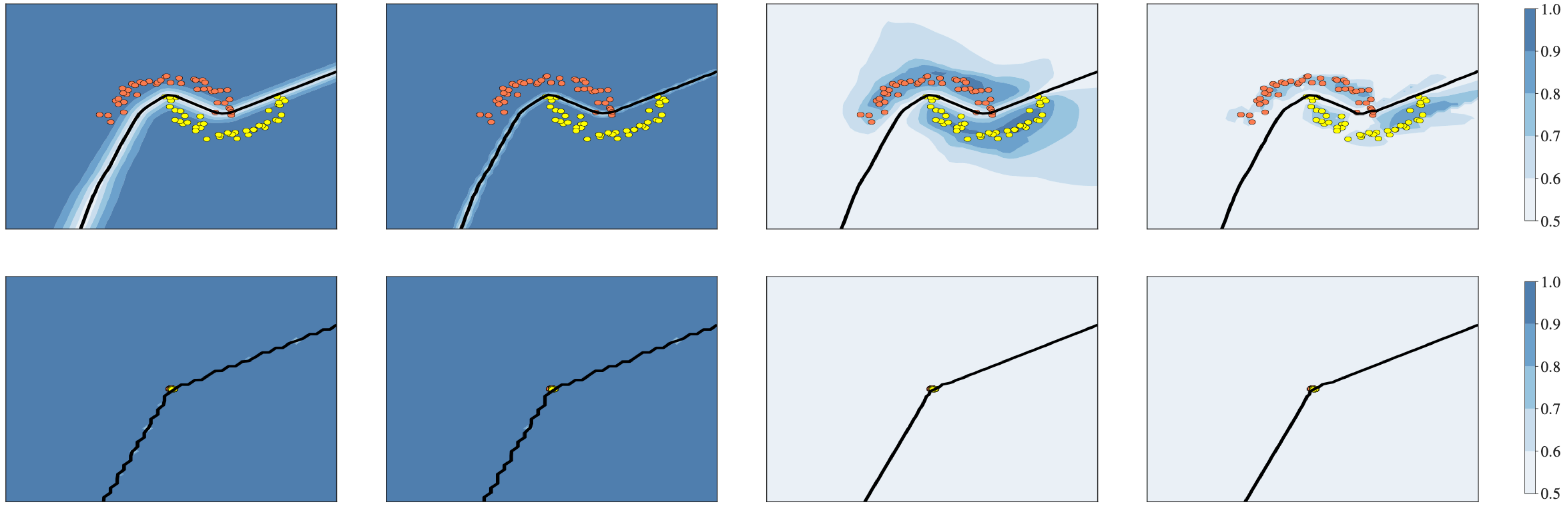

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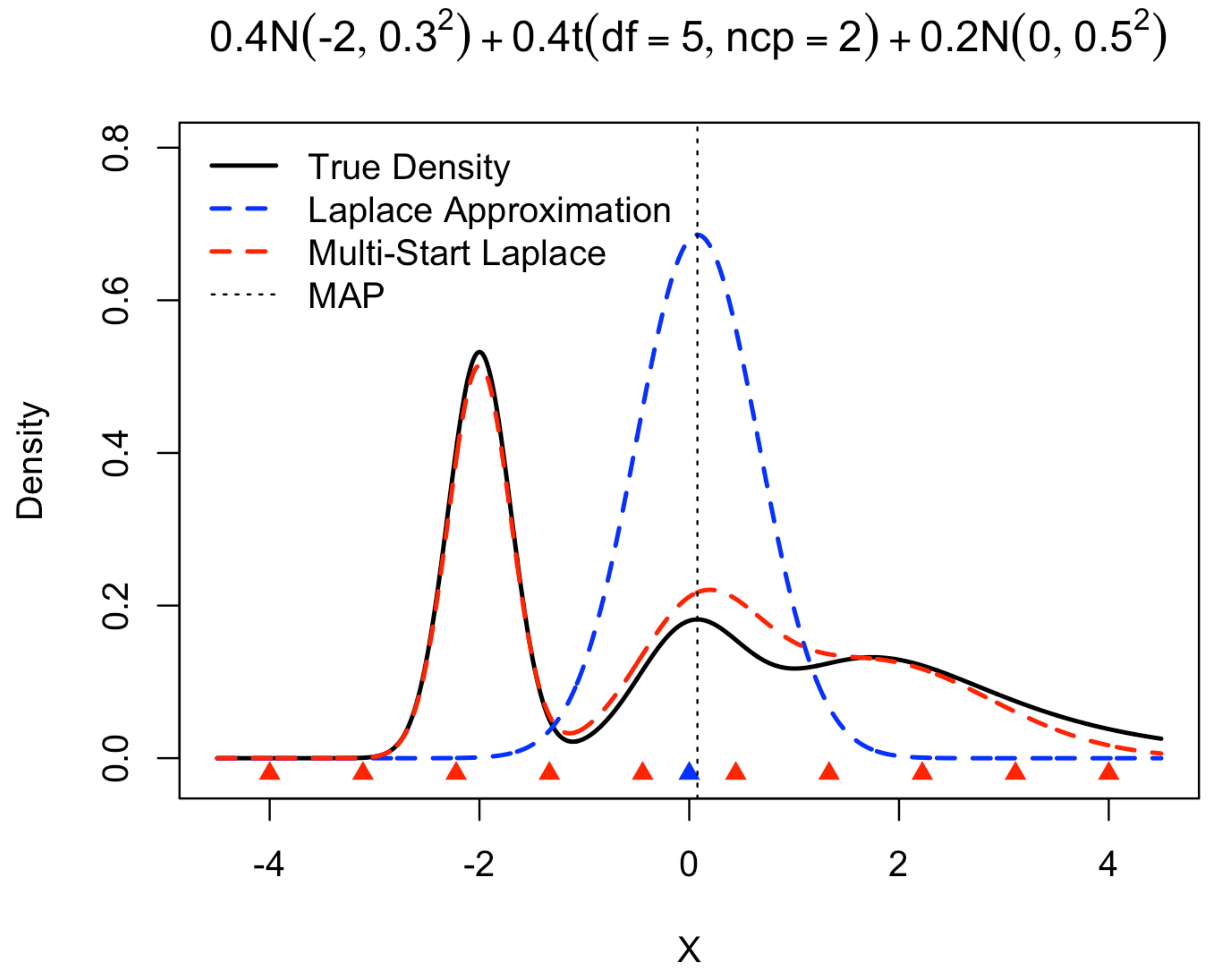

Conformal Prediction?

Smarter NN Training

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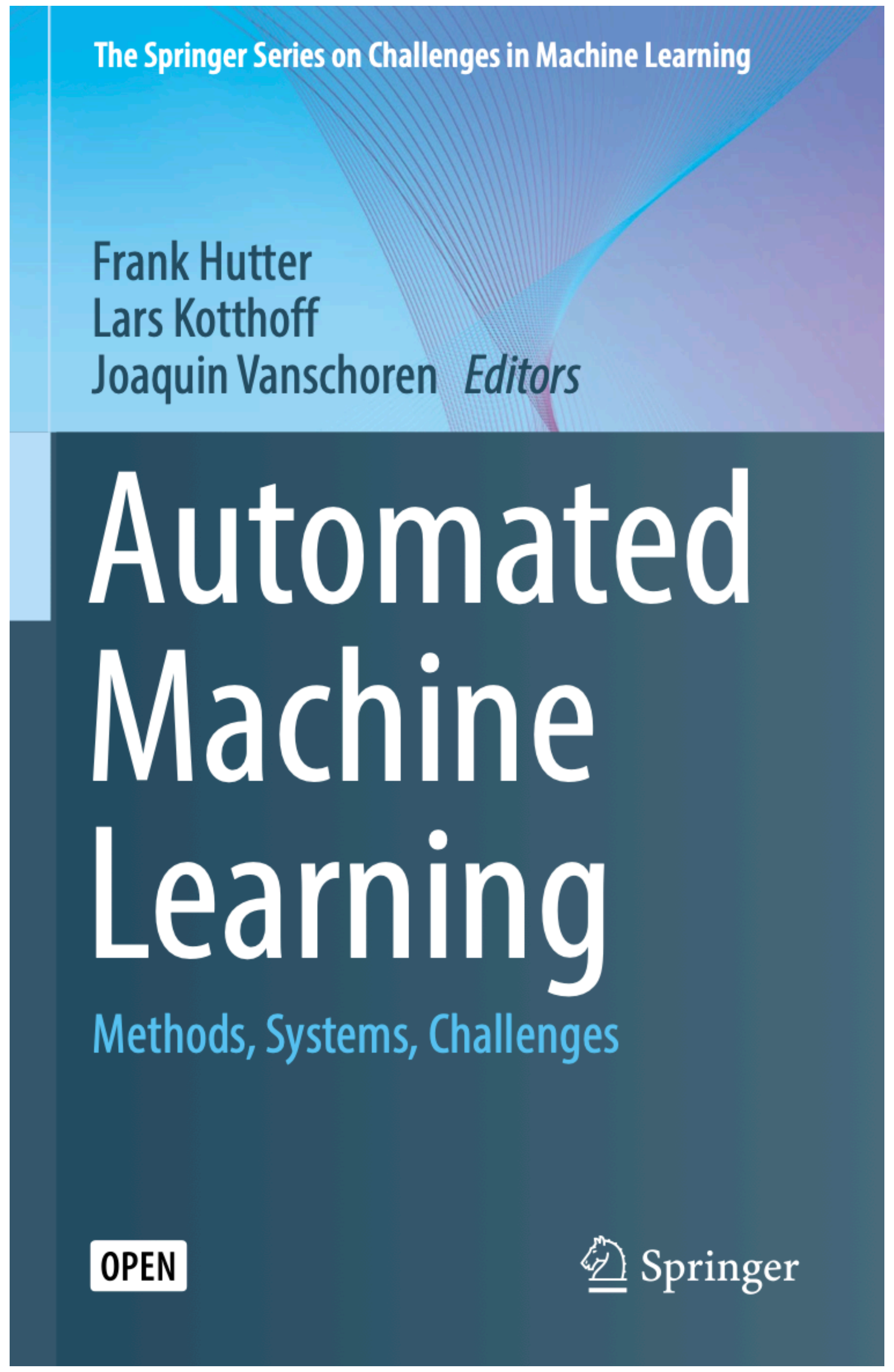

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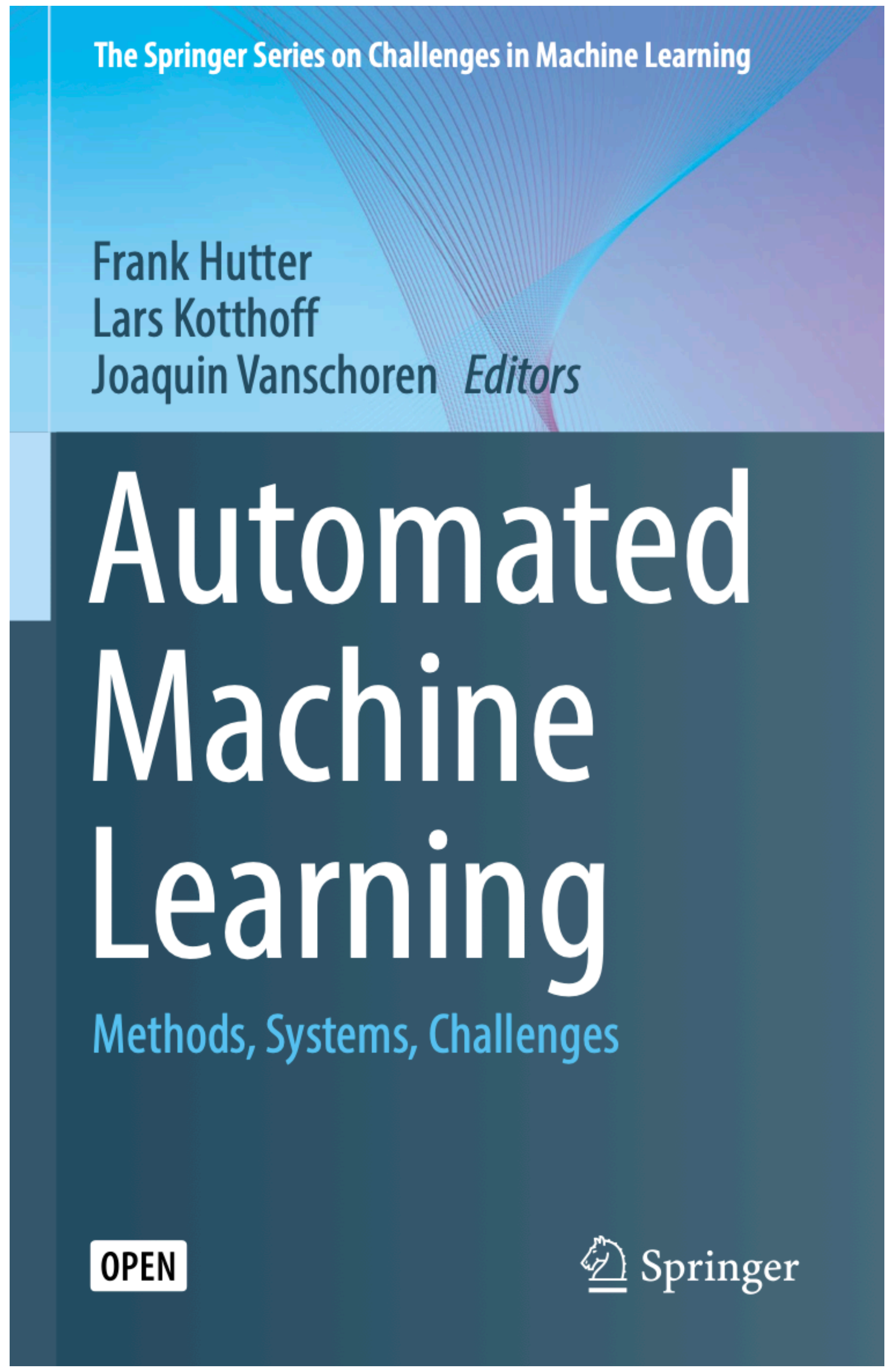
- (Are we just calling existing things ProbNum … ?)



Physics-Data Spectrum

Differential Equation Models

Neural Network Models

Physics-Driven

Data-Driven

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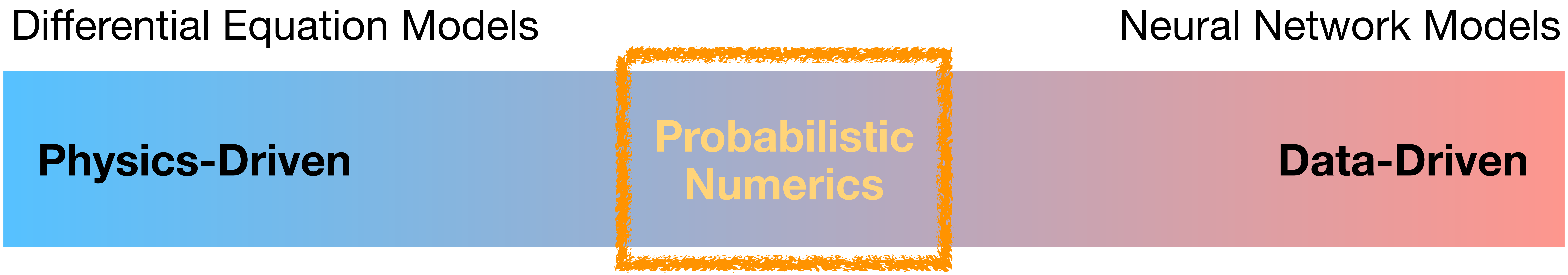

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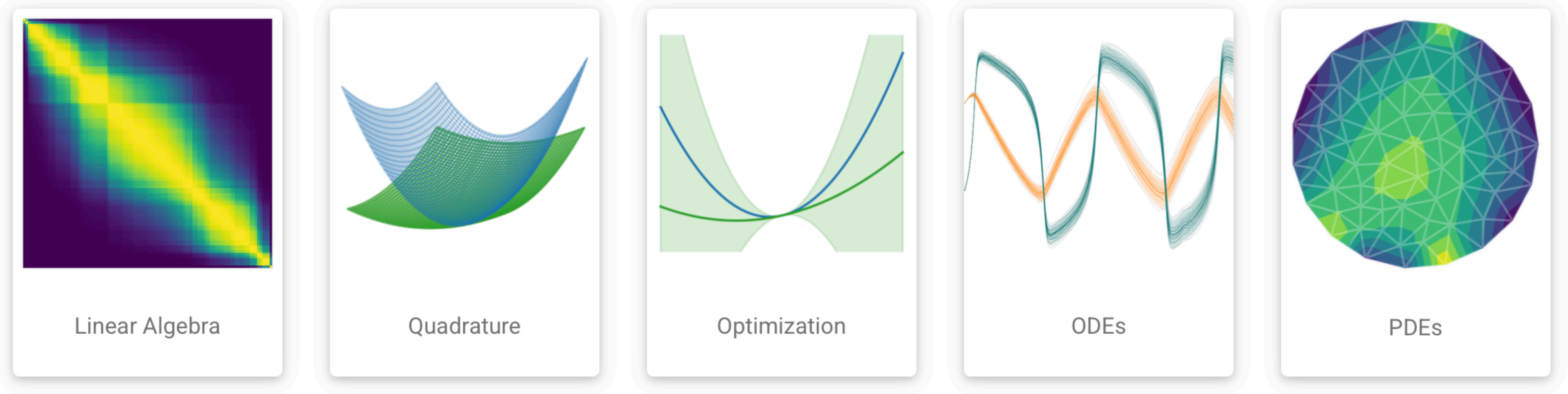

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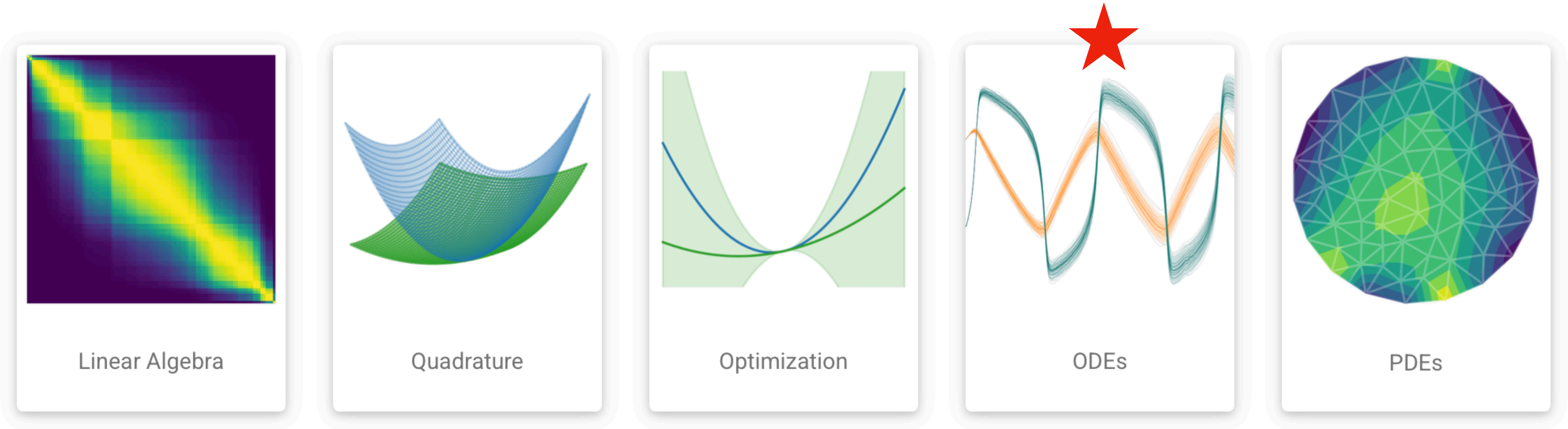

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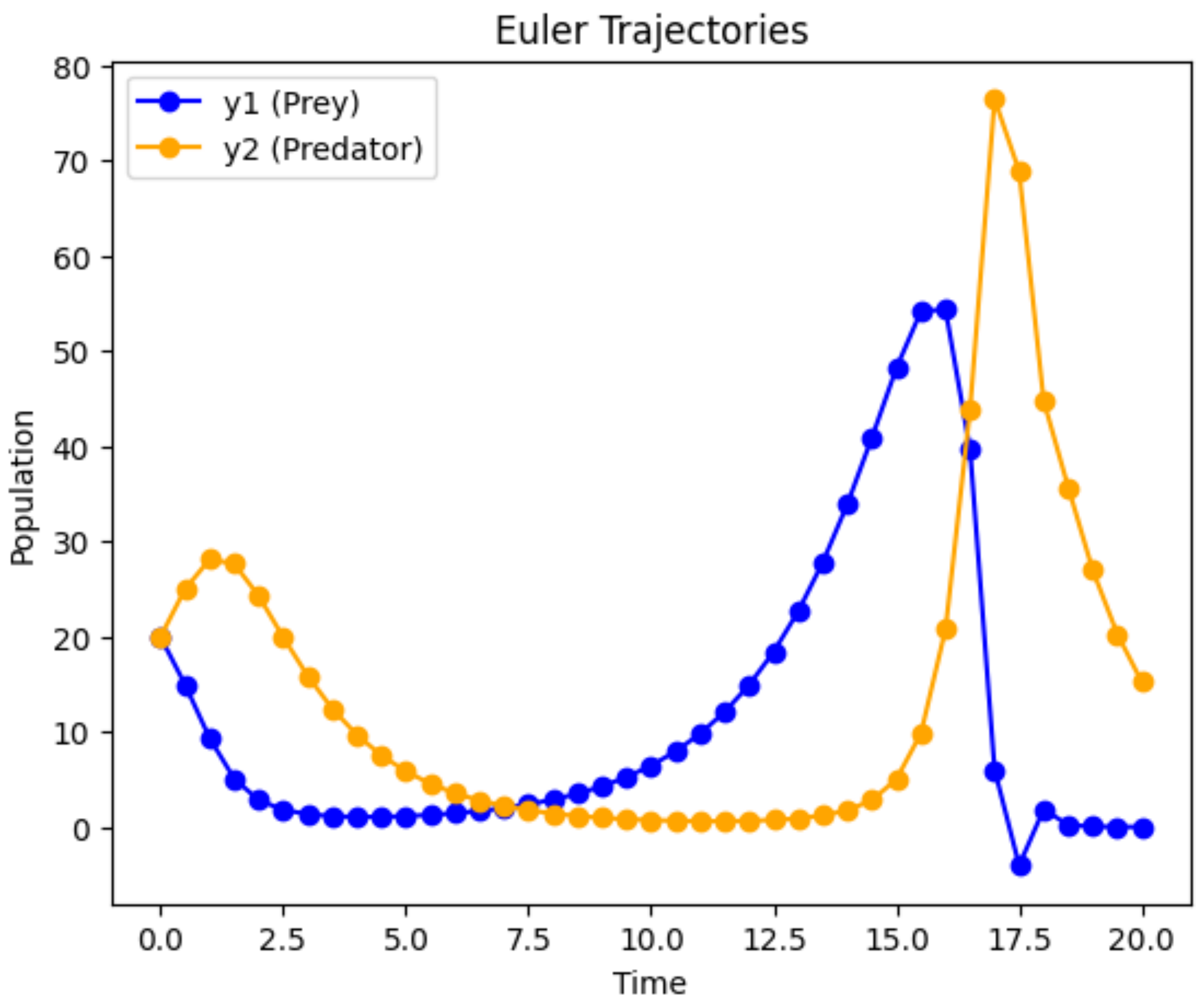
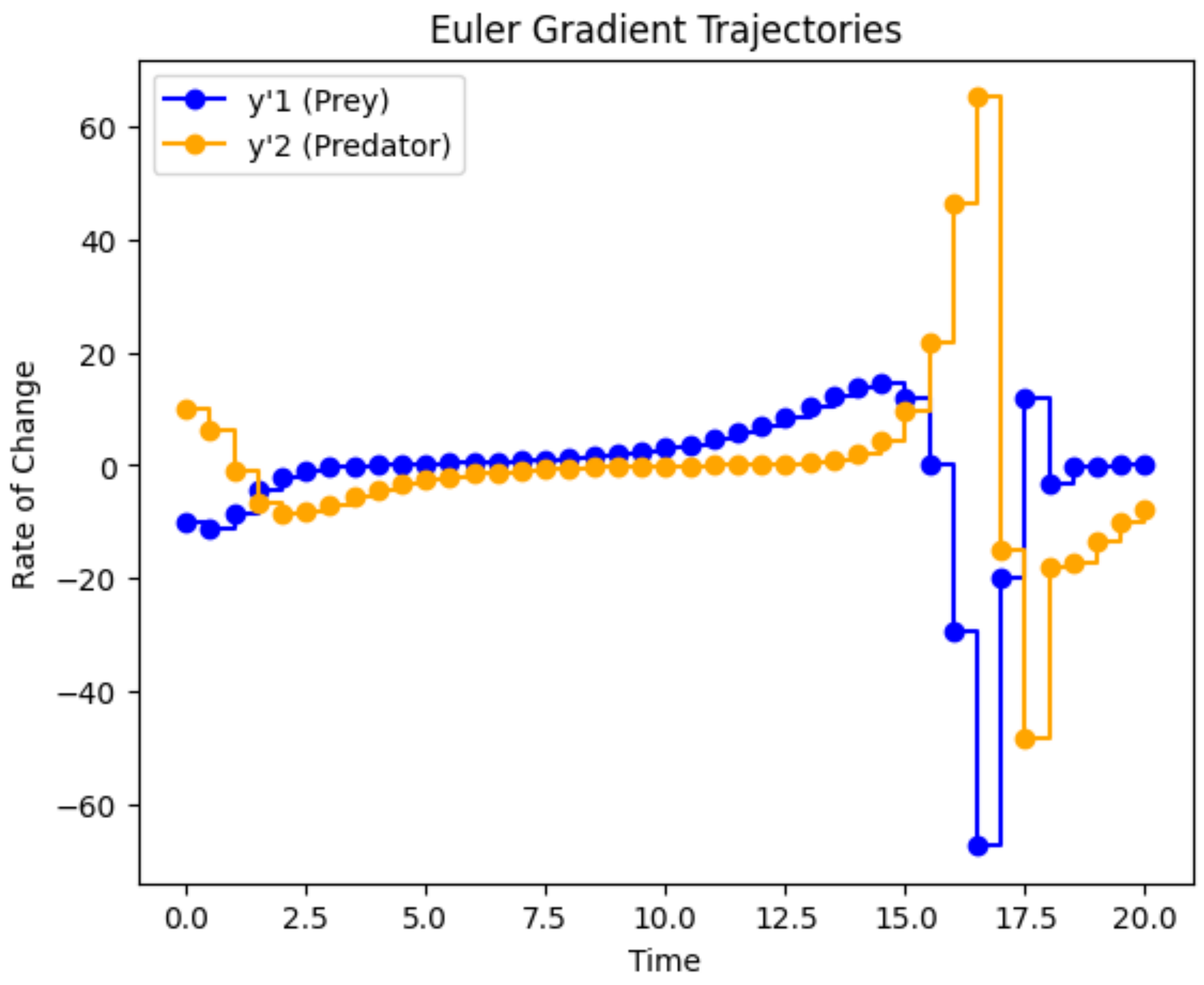
<u>Lotka-Volterra</u>

$$\begin{bmatrix} dy_1(t) \\ dy_2(t) \end{bmatrix} = \begin{bmatrix} 0.5y_1(t) - 0.05y_1(t)y_2(t) \\ -0.5y_2(t) + 0.05y_1(t)y_2(t) \end{bmatrix}$$

$$y_1(0) = y_2(0) = 20$$





Probabilistic ODE Solver

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Home > Statistics and Computing > Article

Probabilistic solutions to ordinary differential equations as nonlinear Bayesian filtering: a new perspective

Open access | Published: 18 September 2019

Volume 29, pages 1297–1315, (2019) Cite this article

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Filip Tronarp, Hans Kersting, Simo Särkkä & Philipp Hennig

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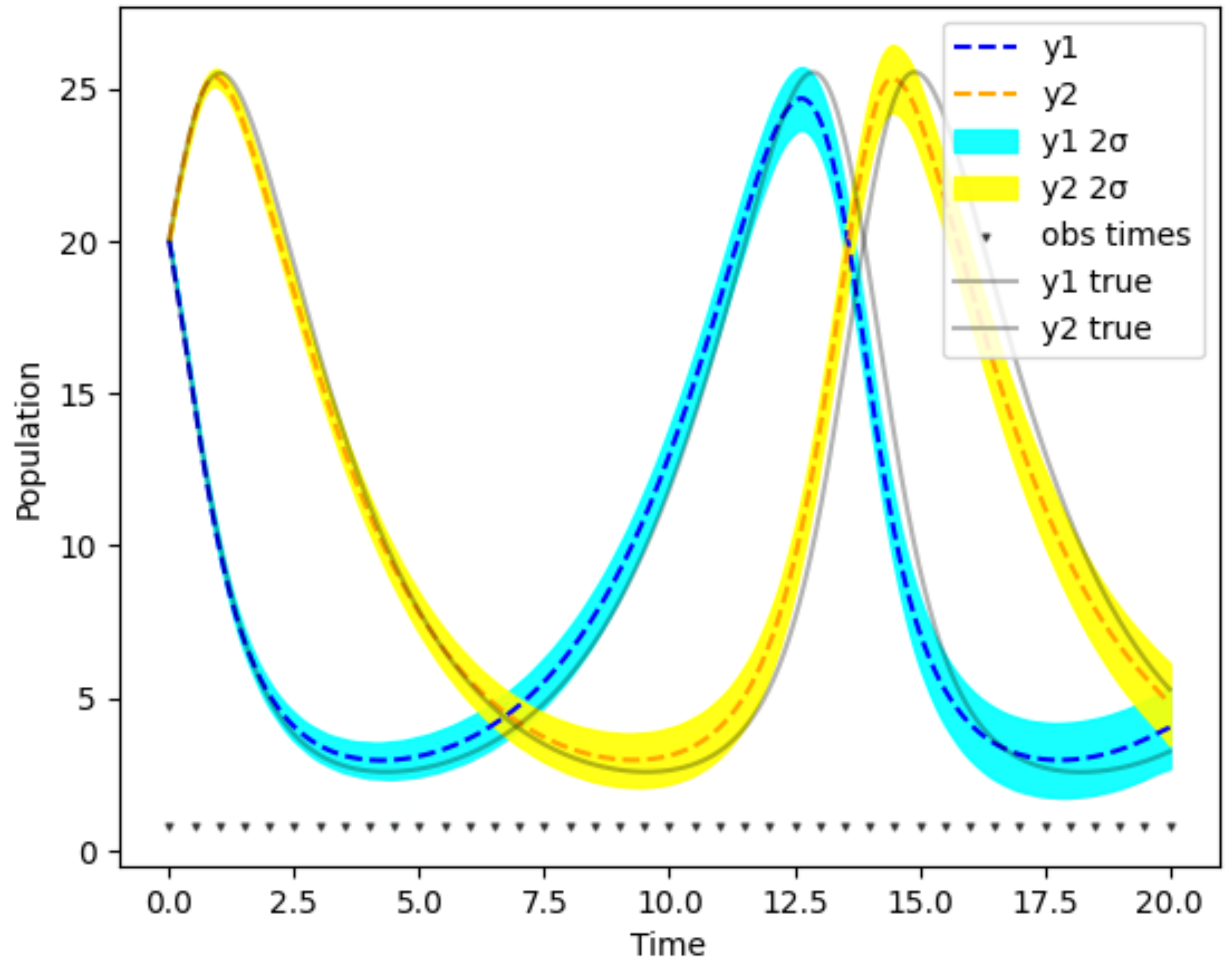

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$$d\mathbf{X}_t = d\begin{bmatrix} X_t^1 \\ X_t^2 \end{bmatrix} = F\mathbf{X}_t dt + L dW_t, \qquad \frac{d}{dt}X_t^1 = X_t^2$$

Probabilistic ODE Solver

<u>WANT</u>: Sufficiently flexible prior dynamics for $\{X_{t_k}\}_{k=0}^{N}$.

$$d\mathbf{X}_t = d\begin{bmatrix} X_t^1 \\ X_t^2 \end{bmatrix} = F\mathbf{X}_t dt + L dW_t, \qquad \frac{d}{dt}X_t^1 = X_t^2$$

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Example: Integrated Wiener Process (order-1, dim-1)

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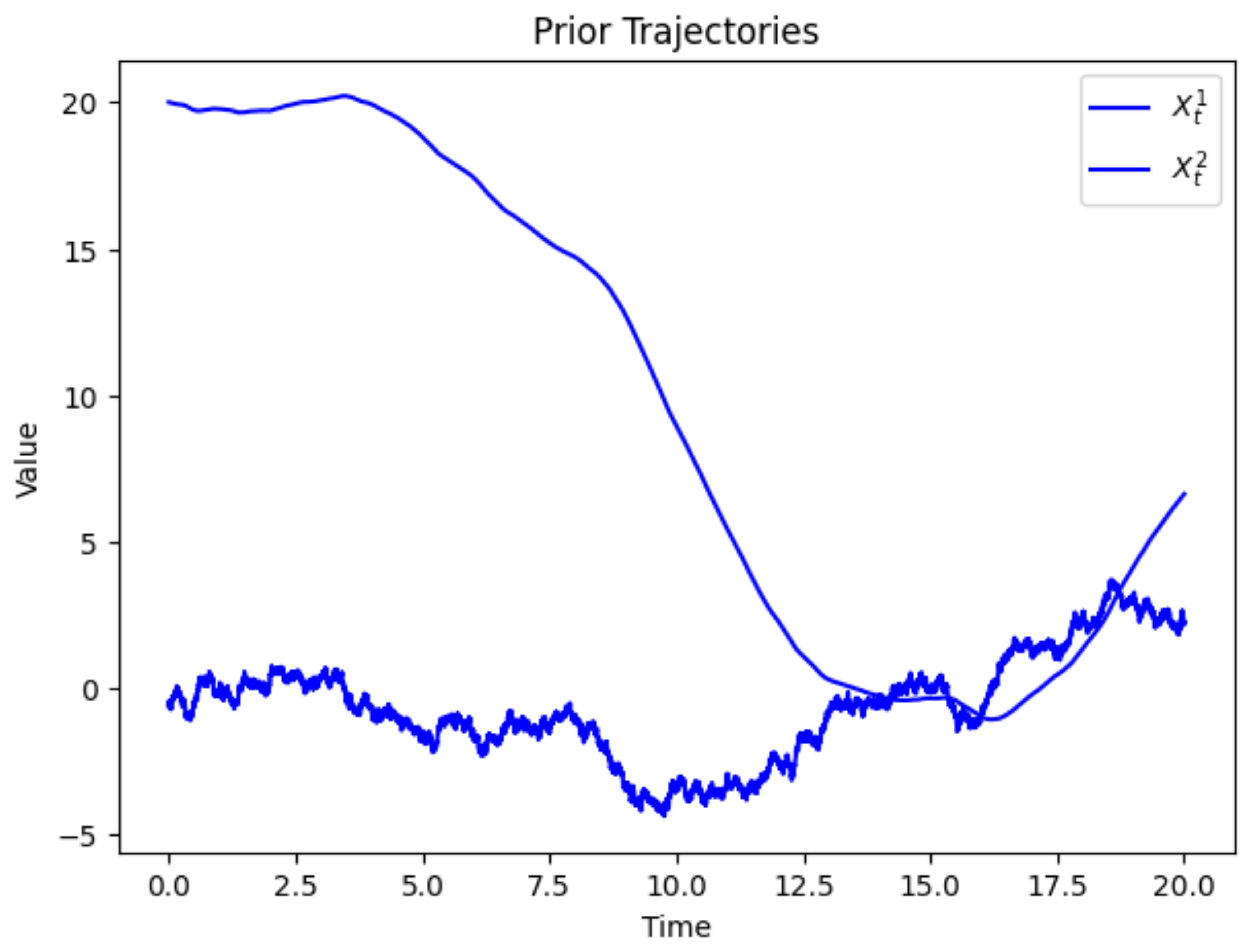

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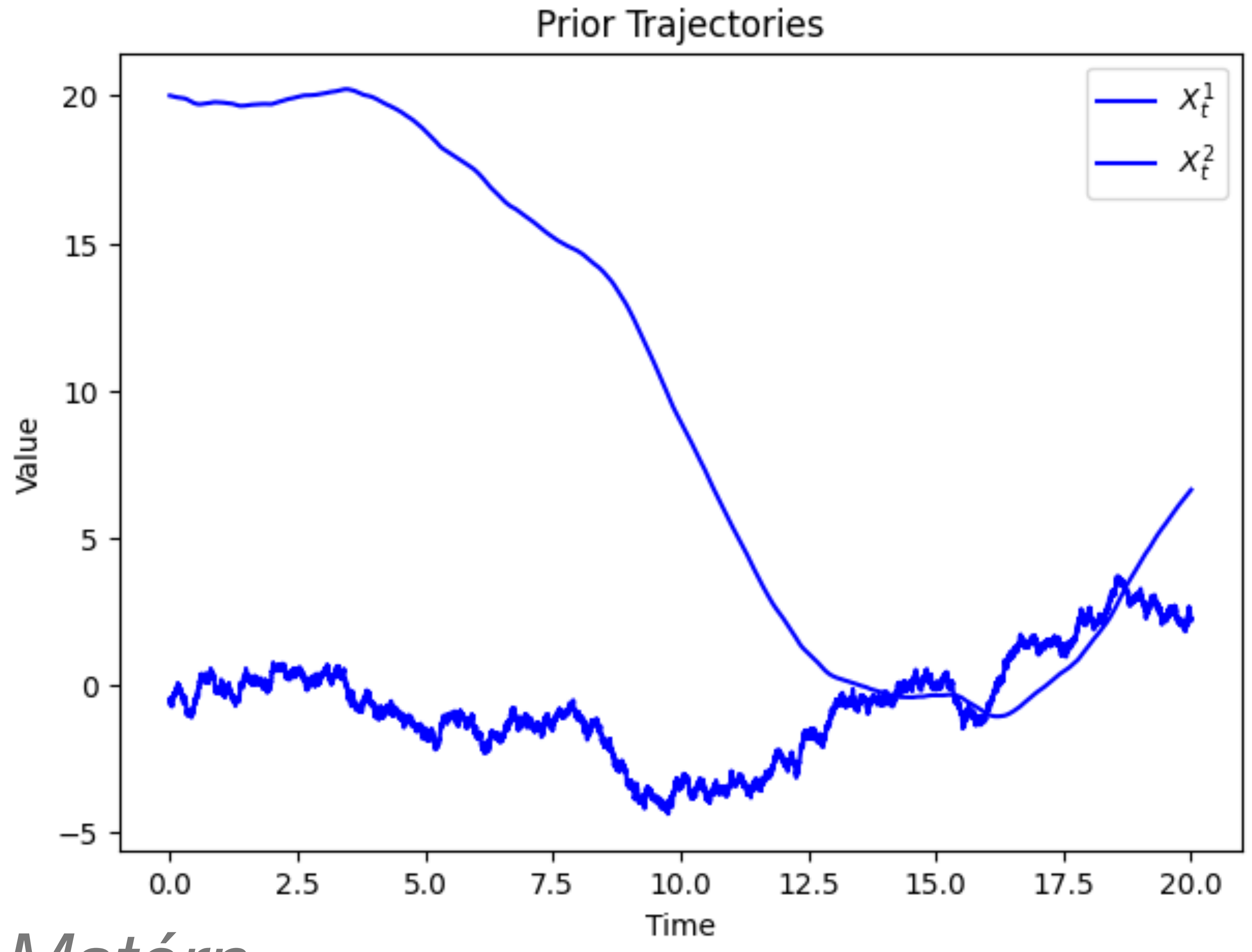

other SDE priors are also possible, e.g. Matérn

Probabilistic ODE Solver

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Enforce residuals $z_k := z_{t_k} = X^2_{t_k} - f(X^1_{t_k}, t_k) = 0$ for all N points.

<u>Notation</u>: Define $C, \dot{C}$ such that $C\mathbf{X}_t = X^1_t, \dot{C}\mathbf{X}_t = X^2_t$; so $z_k = \dot{C}\mathbf{X}_{t_k} - f(C\mathbf{X}_{t_k}, t_k) = 0$

Probabilistic ODE Solver

WANT: Standard Bayes posterior.

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Prior

$$d\mathbf{X}_t = F\mathbf{X}_t dt + L dW_t$$

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Data

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Can be phrased as a State Space Model !!

State Space Model

State Space Model

(Latent Dynamics) $A_{n+1} \mid \left(A_{0:n} = a_{0:n}, B_{0:n} = b_{0:n}\right) \sim P(\,\cdot \mid a_n)$

(Observations) $B_{n+1} \mid \left(A_{0:n+1} = a_{0:n+1}, B_{0:n} = b_{0:n}\right) \sim g(\,\cdot \mid a_{n+1})$

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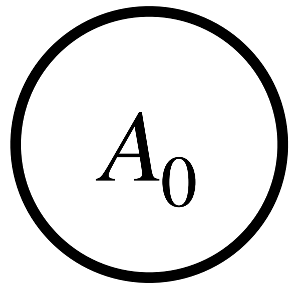

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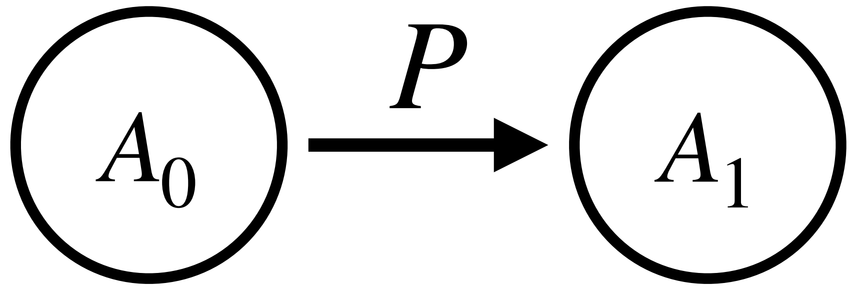

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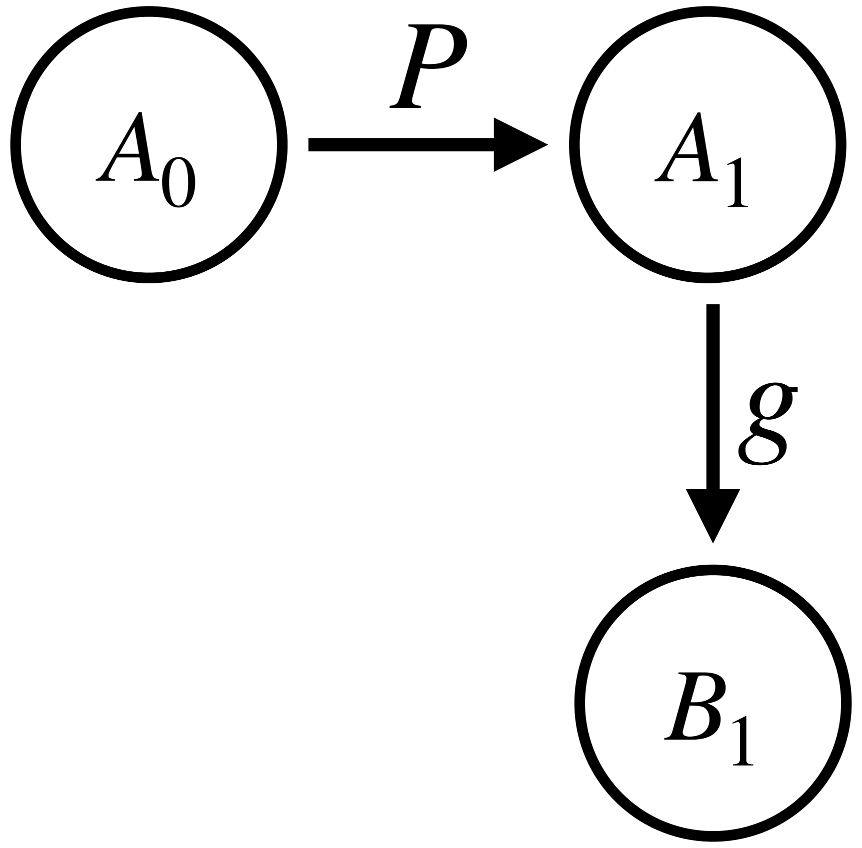

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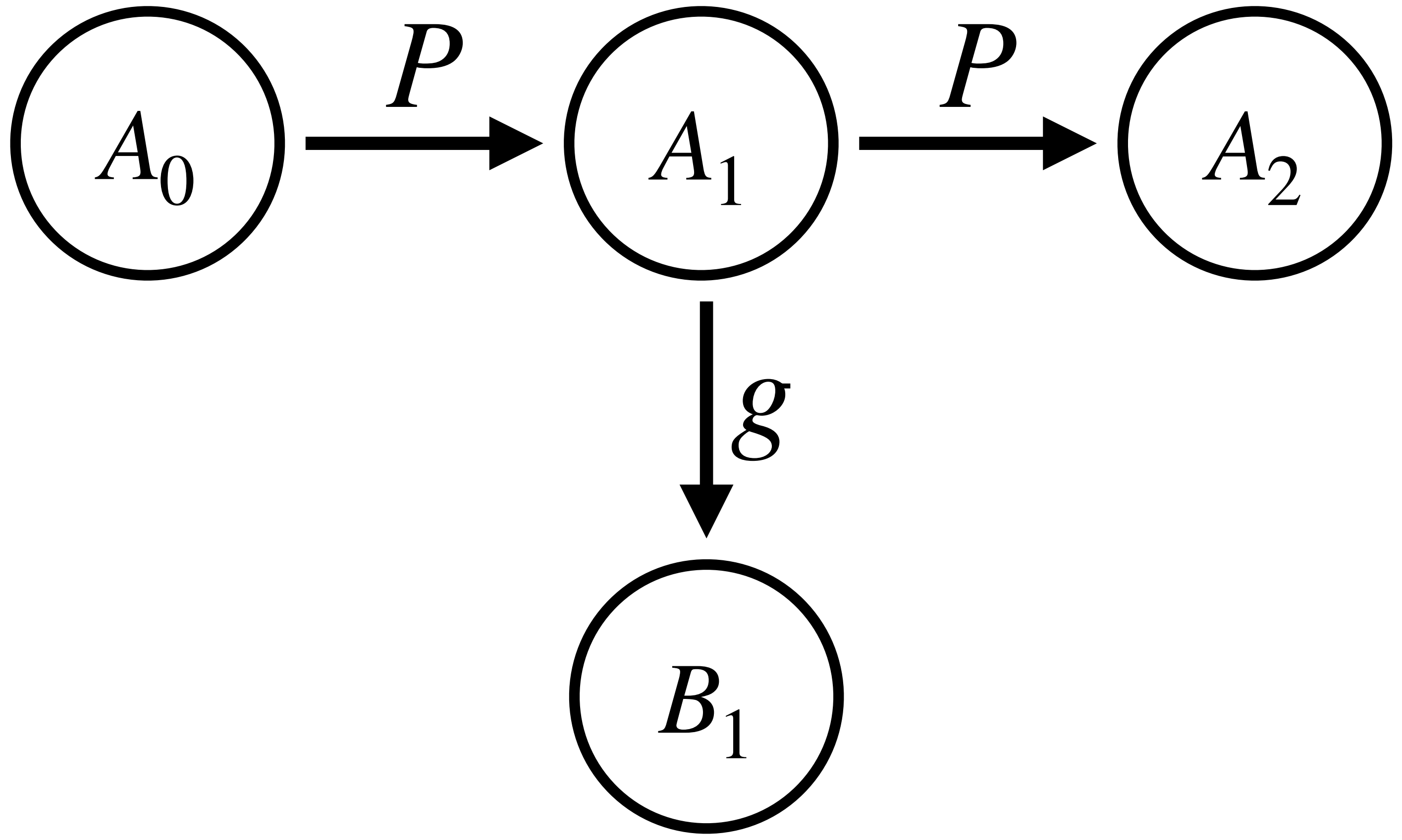

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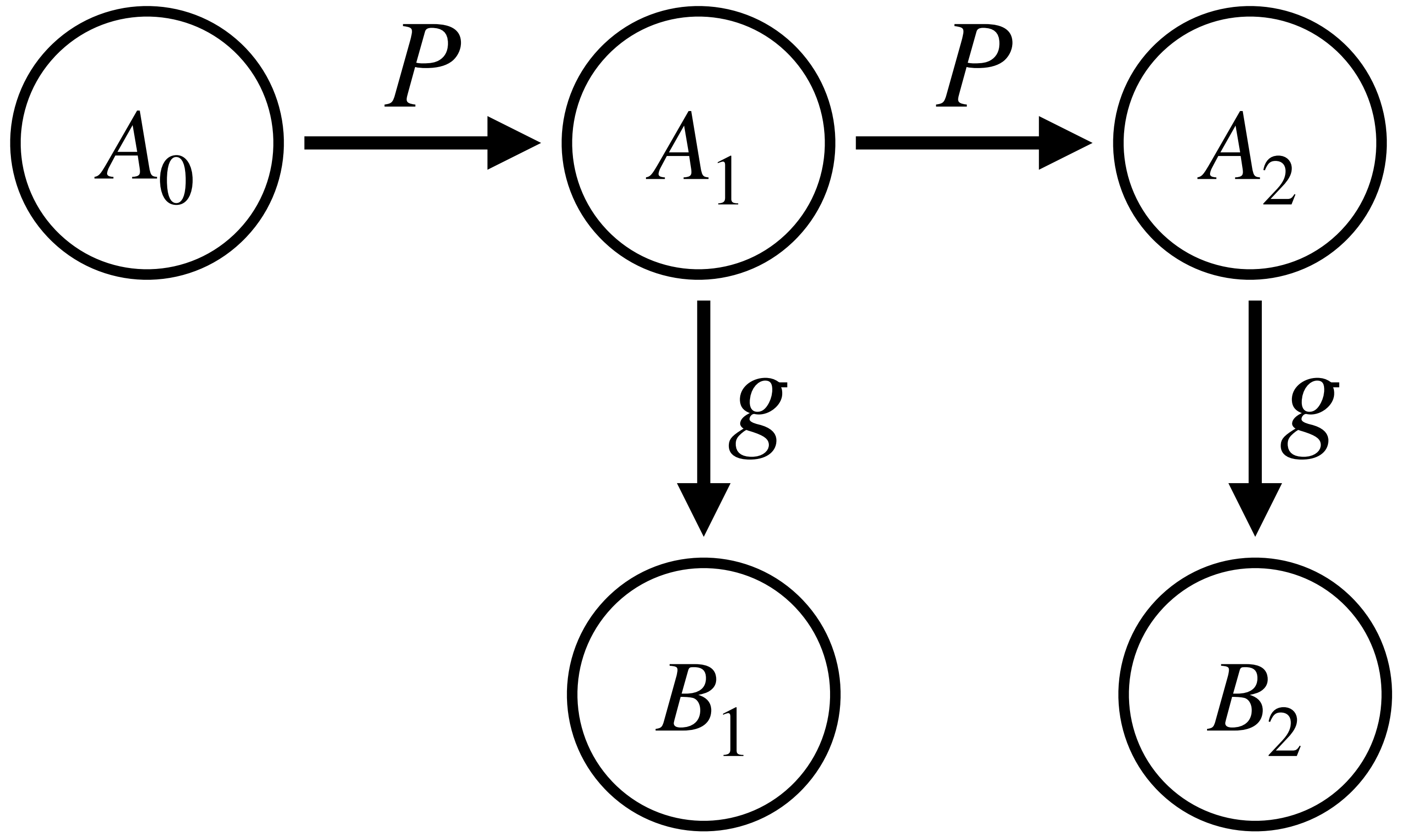

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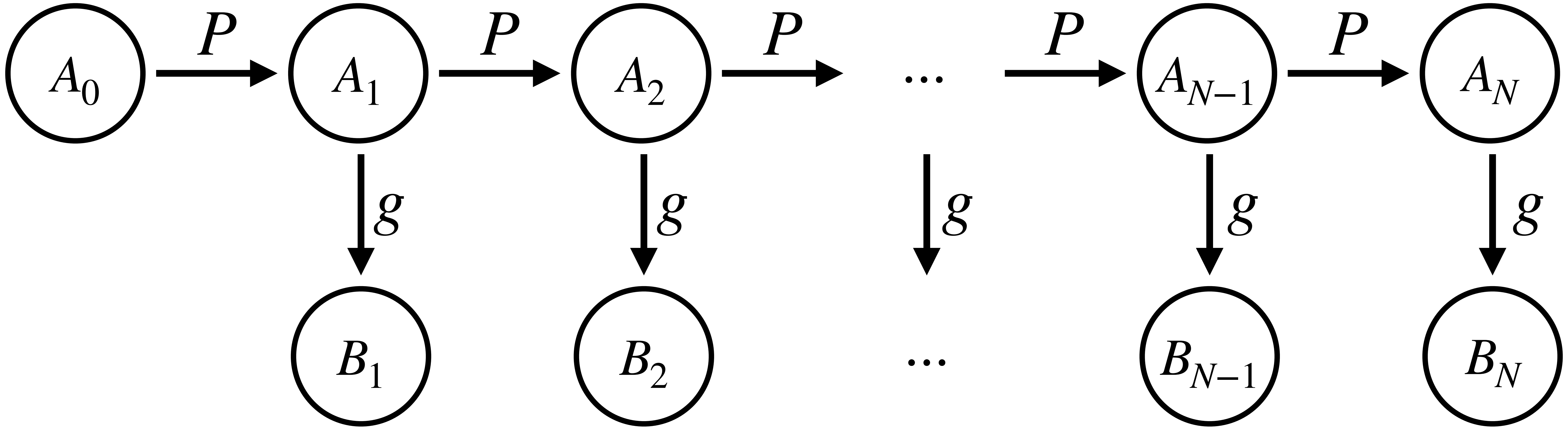

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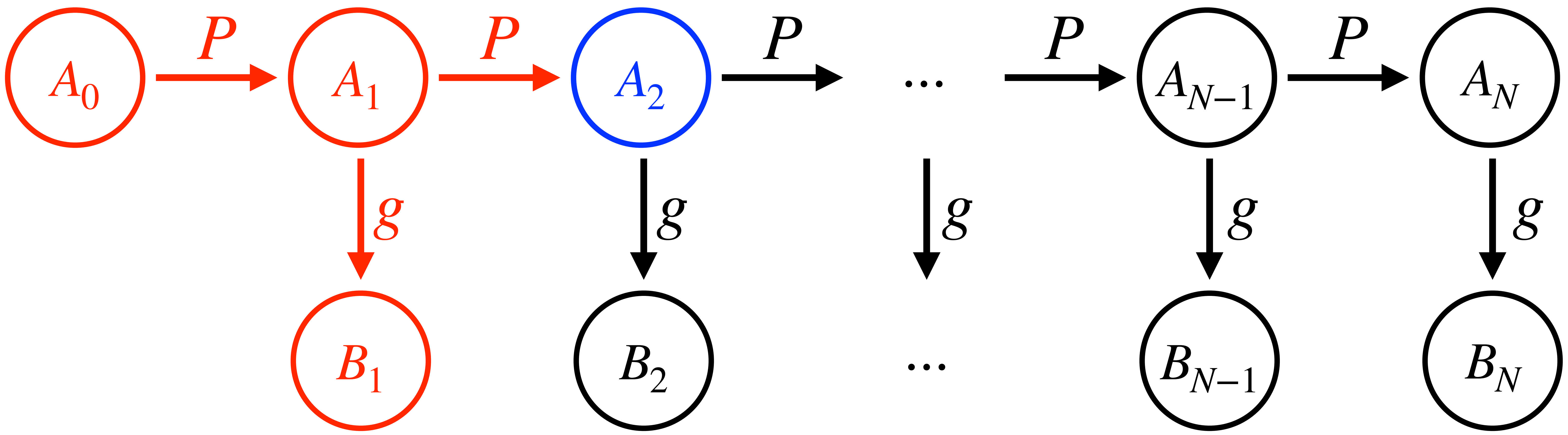

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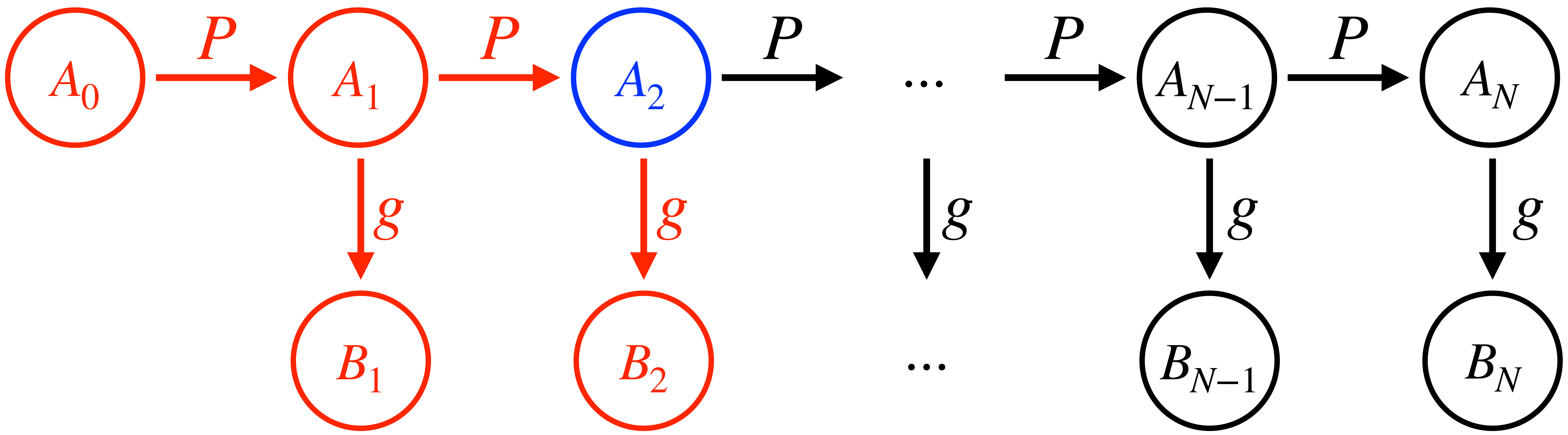

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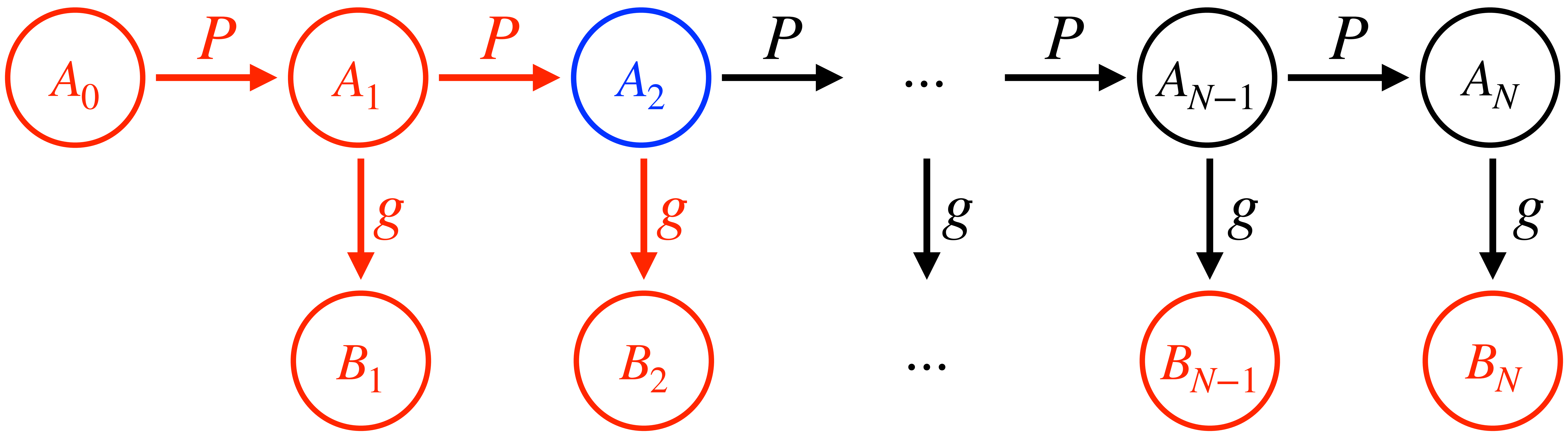

(Predicting Distribution) $p\left(A_n \mid A_{0:n-1} = a_{0:n-1}\right)$

(Filtering Distribution) $p\left(A_n \mid B_{0:n} = b_{0:n}\right)$

(Smoothing Distribution) $p\left(A_n \mid B_{0:N} = b_{0:N}\right)$

State Space Model

State Space Model

Example: Linear Gaussian Model

$$\begin{cases} A_{n+1} & = GA_n + \xi_n, \qquad \xi_n \sim N(0,Q) \\ B_{n+1} & = HA_{n+1} + \varepsilon_n, \qquad \varepsilon_n \sim N(0,R) \end{cases}$$

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- predicting distribution $A_{n+1|n} \sim N(\mu_n^P, \Sigma_n^P)$
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  - Obtain filtered state $A_{1|1} \sim N(\mu_0^P + K_1 v_1, \Sigma_0^P - K_1 S_1 K_1^T) = N(\mu_1^F, \mu_1^F)$.

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Kalman Filter!

Obtained by Gaussian algebra.

State Space Model

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  - Calculate *smoother gain* $J_{N-1} = \Sigma_{N-1|N-1} G^T (\Sigma_{N|N-1})^{-1}$.

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Example: Linear Gaussian Model

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  - Calculate *smoother covariance* $\Sigma_{N-1}^S = \Sigma_N^S + J_{N-1}(\Sigma_N^P - \Sigma_N^P) J_{N-1}^T$.

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  - Obtain smoothed state $A_{N-1|N-1} \sim N(\mu_{N-1}^S, \Sigma_{N-1}^S)$.

Example: Linear Gaussian Model

State Space Model

$$\begin{cases} A_{n+1} &= GA_n + \xi_n, \qquad \xi_n \sim N(0,Q) \\ B_{n+1} &= HA_{n+1} + \varepsilon_n, \qquad \varepsilon_n \sim N(0,R) \end{cases}$$

- Filter out all observations $B_1, B_2, \ldots, B_N$.
- Set smoothed state $A_{N|N} \sim N(\mu_N^F, \Sigma_N^F) = N(\mu_N^S, \Sigma_N^S)$.
- Going backwards
  - Calculate *smoother gain* $J_{N-1} = \Sigma_{N-1|N-1} G^T (\Sigma_{N|N-1})^{-1}$.
  - Calculate *smoother mean* $\mu_{N-1}^S = \mu_{N-1}^F + J_{N-1}(\mu_N^S - \mu_N^P)$.
  - Calculate *smoother covariance* $\Sigma_{N-1}^S = \Sigma_N^S + J_{N-1}(\Sigma_N^P - \Sigma_N^P) J_{N-1}^T$.
  - Obtain smoothed state $A_{N-1|N-1} \sim N(\mu_{N-1}^S, \Sigma_{N-1}^S)$.

RTS Smoother!

Obtained by Gaussian algebra.

Probabilistic ODE Solver

Prior

$$d\mathbf{X}_t = F\mathbf{X}_t dt + L dW_t$$

+

Data

$$\{z_k = \dot{C}\mathbf{X}_{t_k} - f(C\mathbf{X}_{t_k}, t_k) = 0\}_{k=1}^N$$

Probabilistic ODE Solver

Prior

$$dX_t = FX_t dt + LdW_t$$

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(Sometimes) Linear Gaussian Model

$$\begin{cases} \mathbf{X}_{n+1} & = G_h \mathbf{X}_n + \xi_n, \qquad \xi_n \sim N(0, Q_h) \\ Z_{n+1} & = \dot{C}\mathbf{X}_{n+1} - f(C\mathbf{X}_{n+1}, t_{n+1}) + \varepsilon_n, \qquad \varepsilon_n \sim N(0, R) \end{cases}$$

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Exact transition of Linear SDE

<u>(Sometimes) Linear Gaussian Model</u>

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Could be zero

Probabilistic ODE Solver

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(Potential) Nonlinearity Culprit!

Could be zero

Probabilistic ODE Solver

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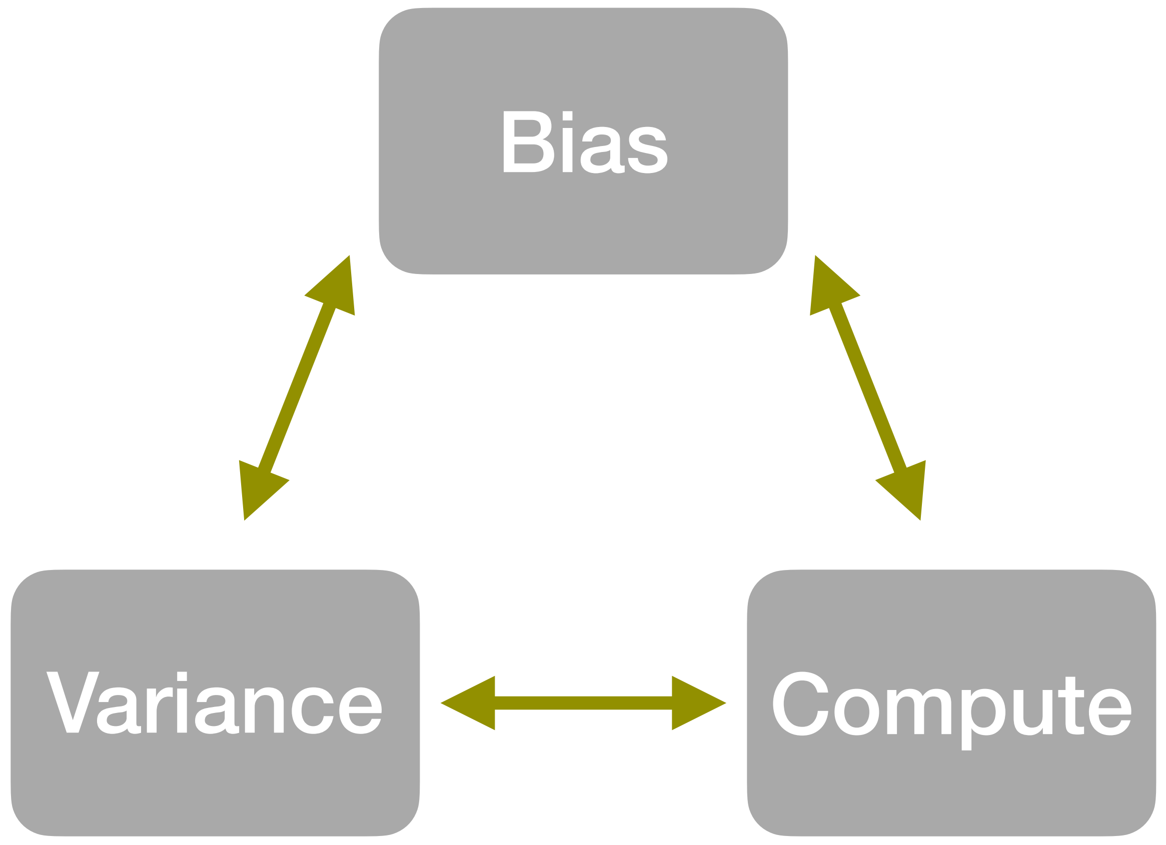

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EKF linearises by replacing nonlinearities with truncated Taylor expansion.

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[EK0] $\qquad f(C\mathbf{X}_k, t_k) \approx f(C\mu_k^P, t_k)$

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[EK0] $$f(C\mathbf{X}_k, t_k) \approx f(C\mu_k^P, t_k)$$

[EK1] $$f(C\mathbf{X}_k, t_k) \approx f(C\mu_k^P, t_k) + J_f(C\mu_k^P, t_k)C(\mathbf{X}_k - \mu_k^P)$$

J_f is the Jacobian of $y \mapsto f(y, t)$

Implementation Details

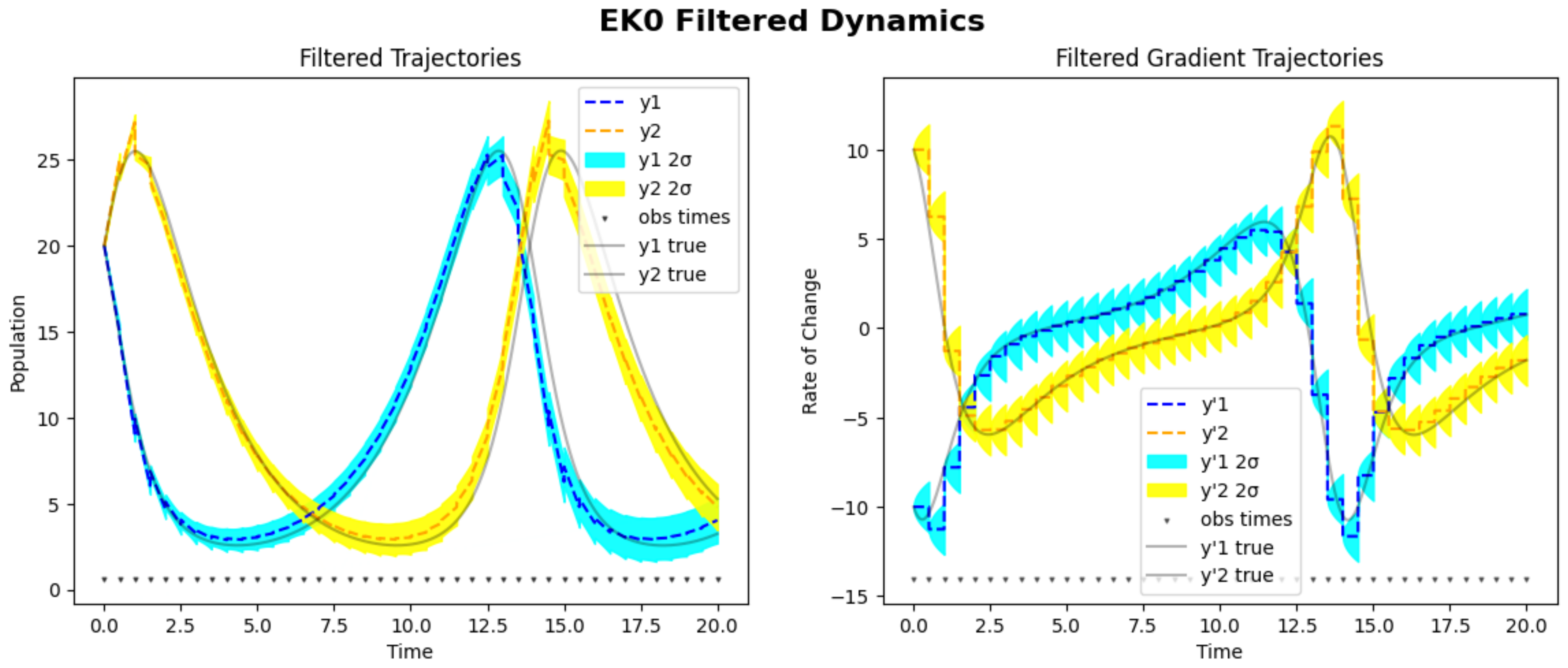
- d-Dimensional trajectories can be incorporated by expanding the matrices using Kronecker product with identity matrix I_d.
- One can include timestamps with no observations too, just propagate and not assimilate.
- When observation times are not uniform, make sure the transition matrices are re-computed.

Probabilistic ODE Solver

Lotka-Volterra

$$\begin{bmatrix} dy_1(t) \\ dy_2(t) \end{bmatrix} = \begin{bmatrix} 0.5y_1(t) - 0.05y_1(t)y_2(t) \\ -0.5y_2(t) + 0.05y_1(t)y_2(t) \end{bmatrix}$$

$$y_1(0) = y_2(0) = 20$$



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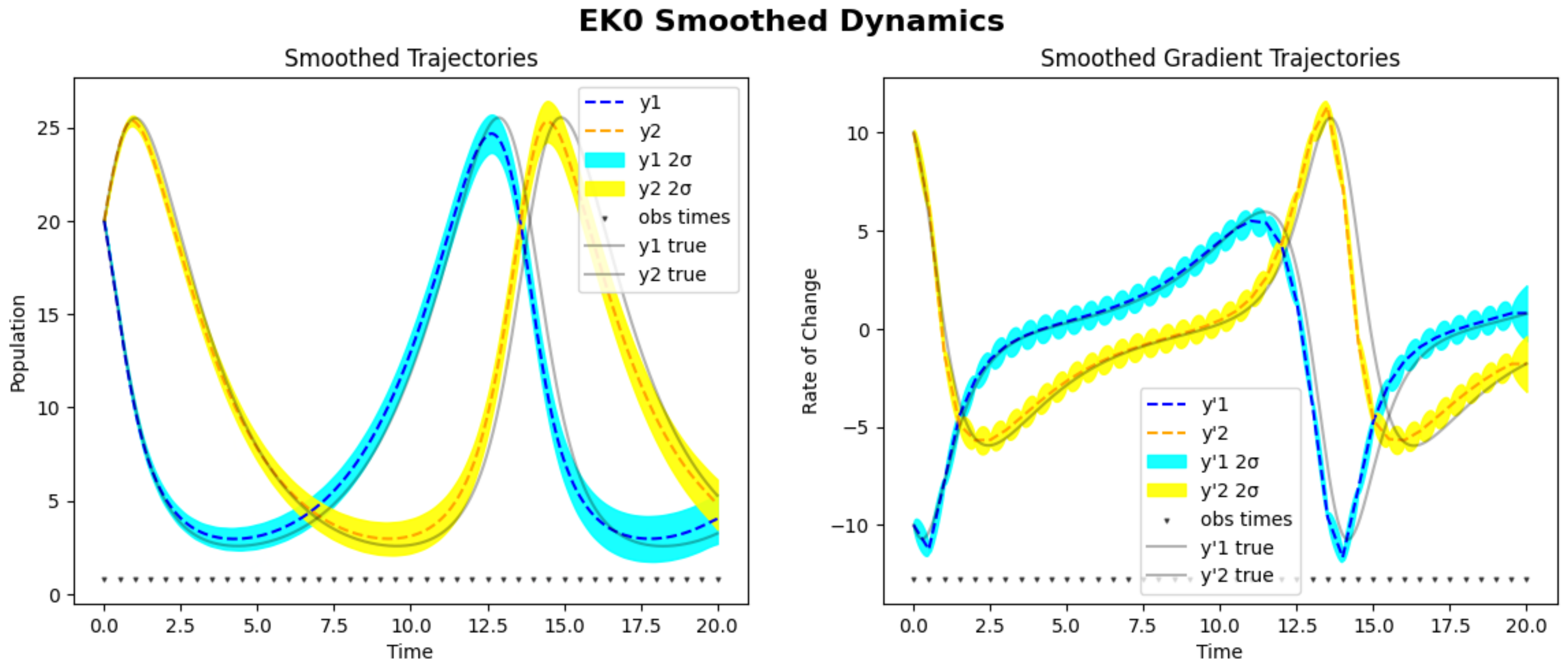

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$$y_1(0) = y_2(0) = 20$$

- What do these uncertainties mean?
  - Epistemic (Reducible) & Aleatoric (Irreducible)
- How are uncertainties represented?
  - Credible Intervals, Posterior Samples
- What can we do with these uncertainties?
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- How much do we have to pay for these uncertainties?

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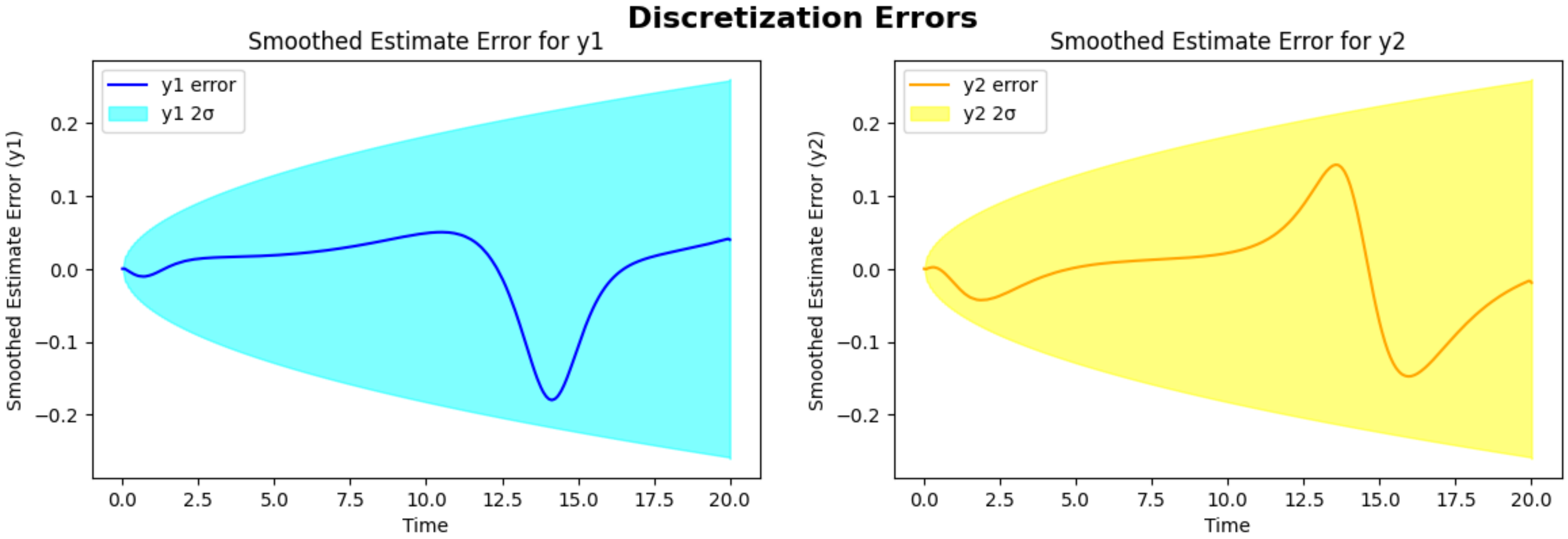

Prob

$y_1(t)y_2(t)$

$5y_1(t)y_2(t)$

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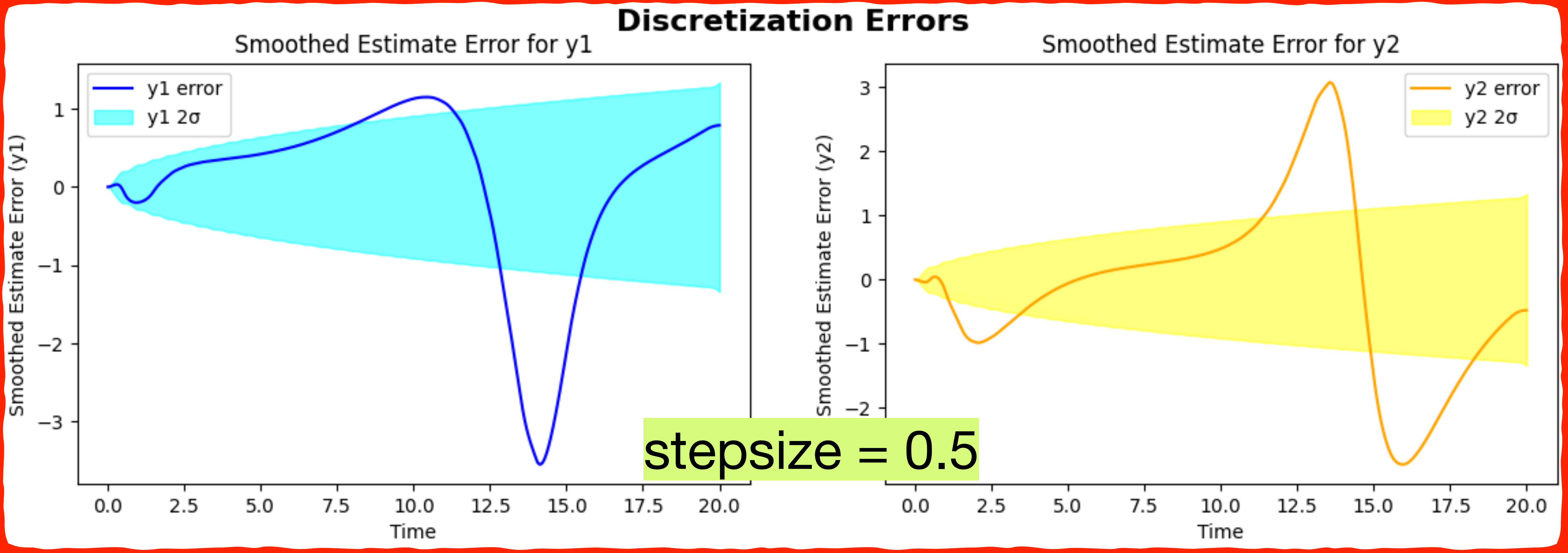
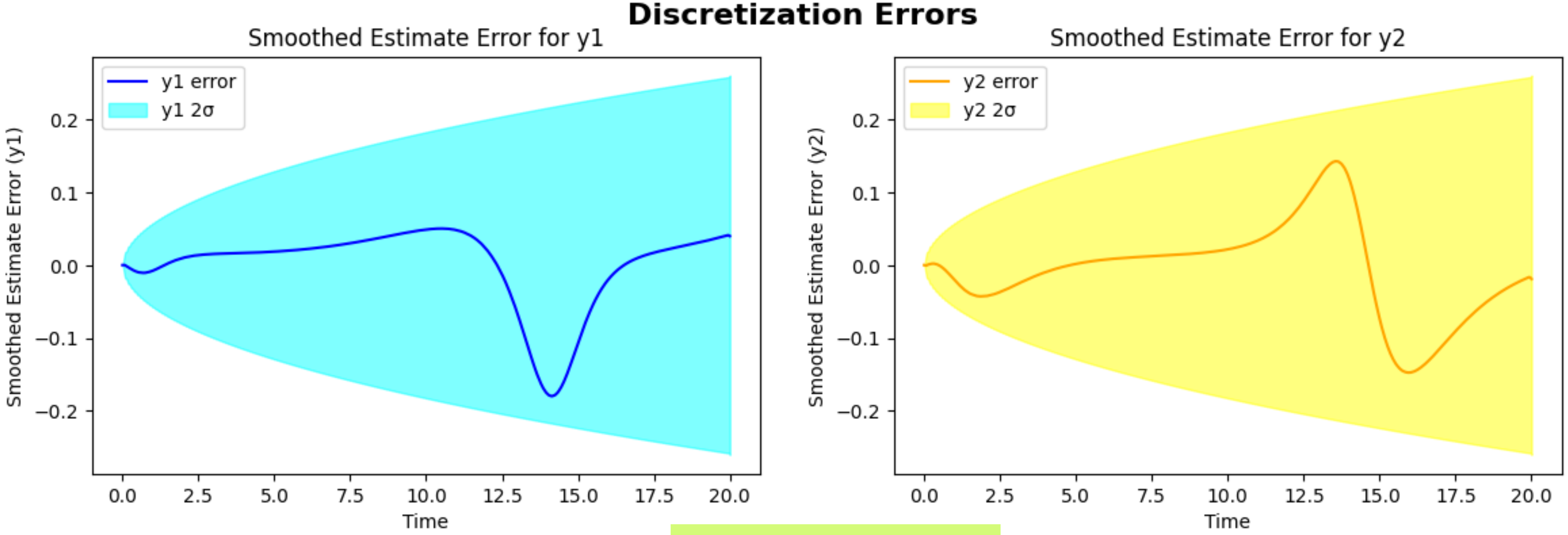
  - Epis





stepsize = 0.1

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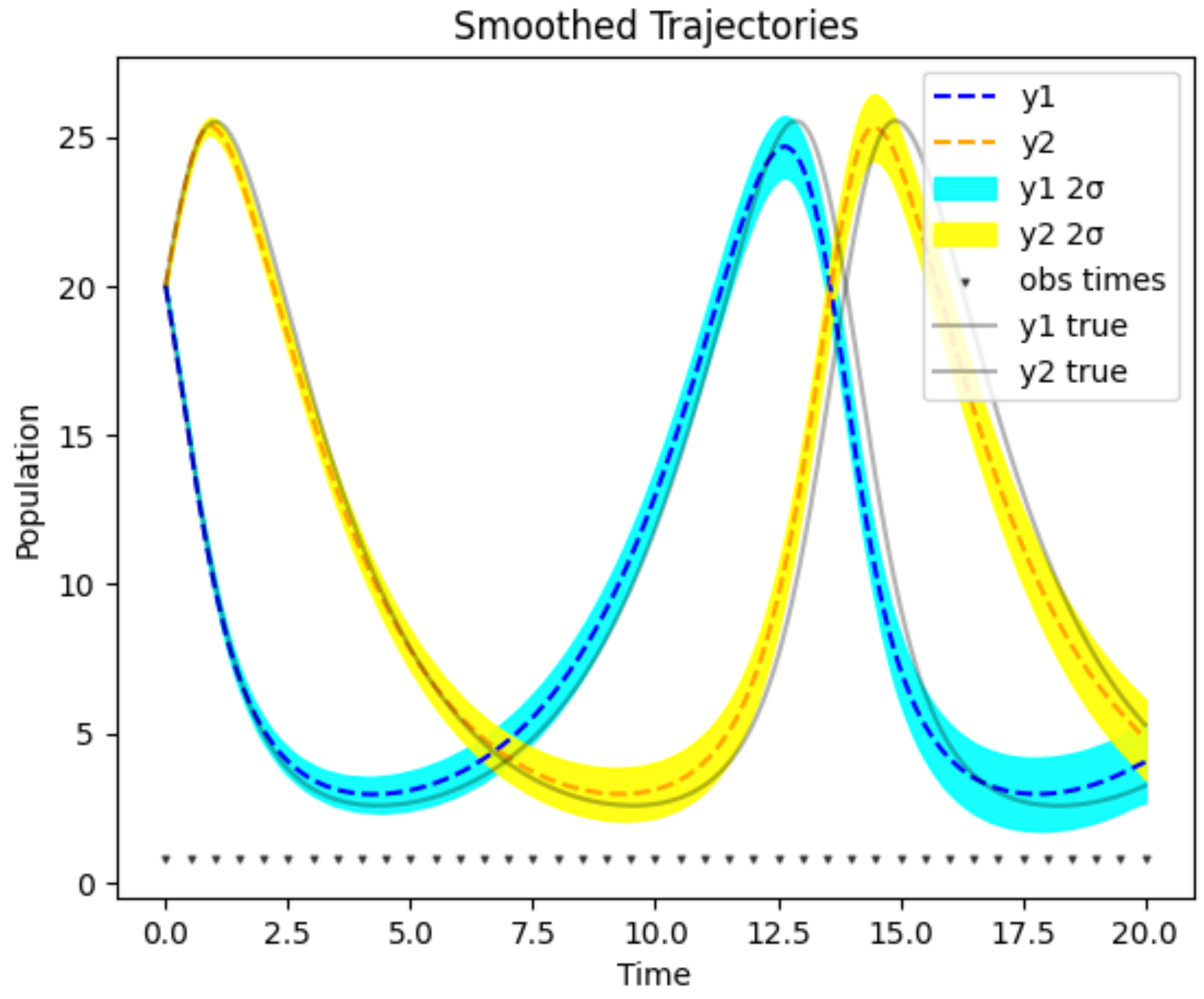

E.g. we are 95% confident that $y_1(20) \in [-0.624,\ 2.202]$

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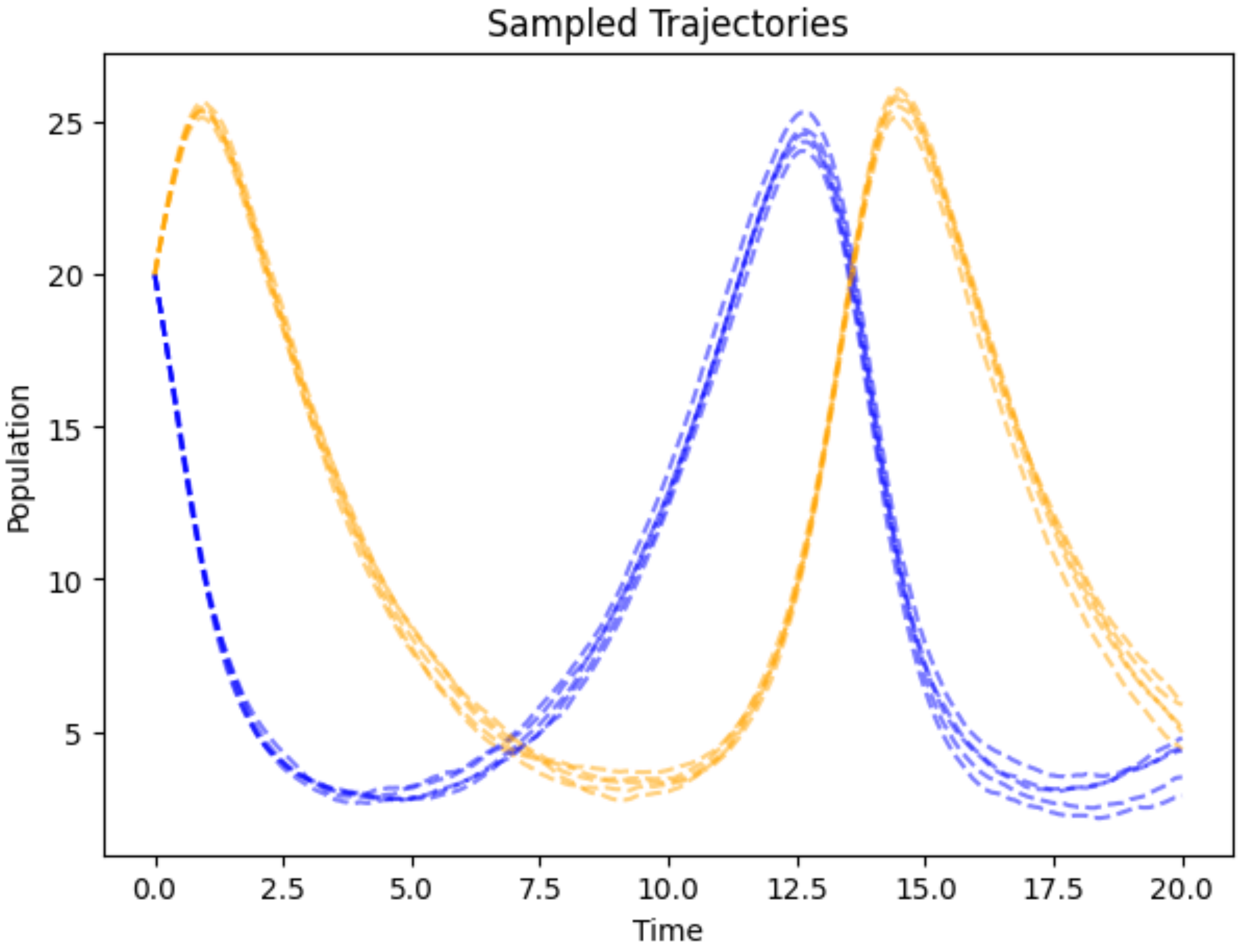

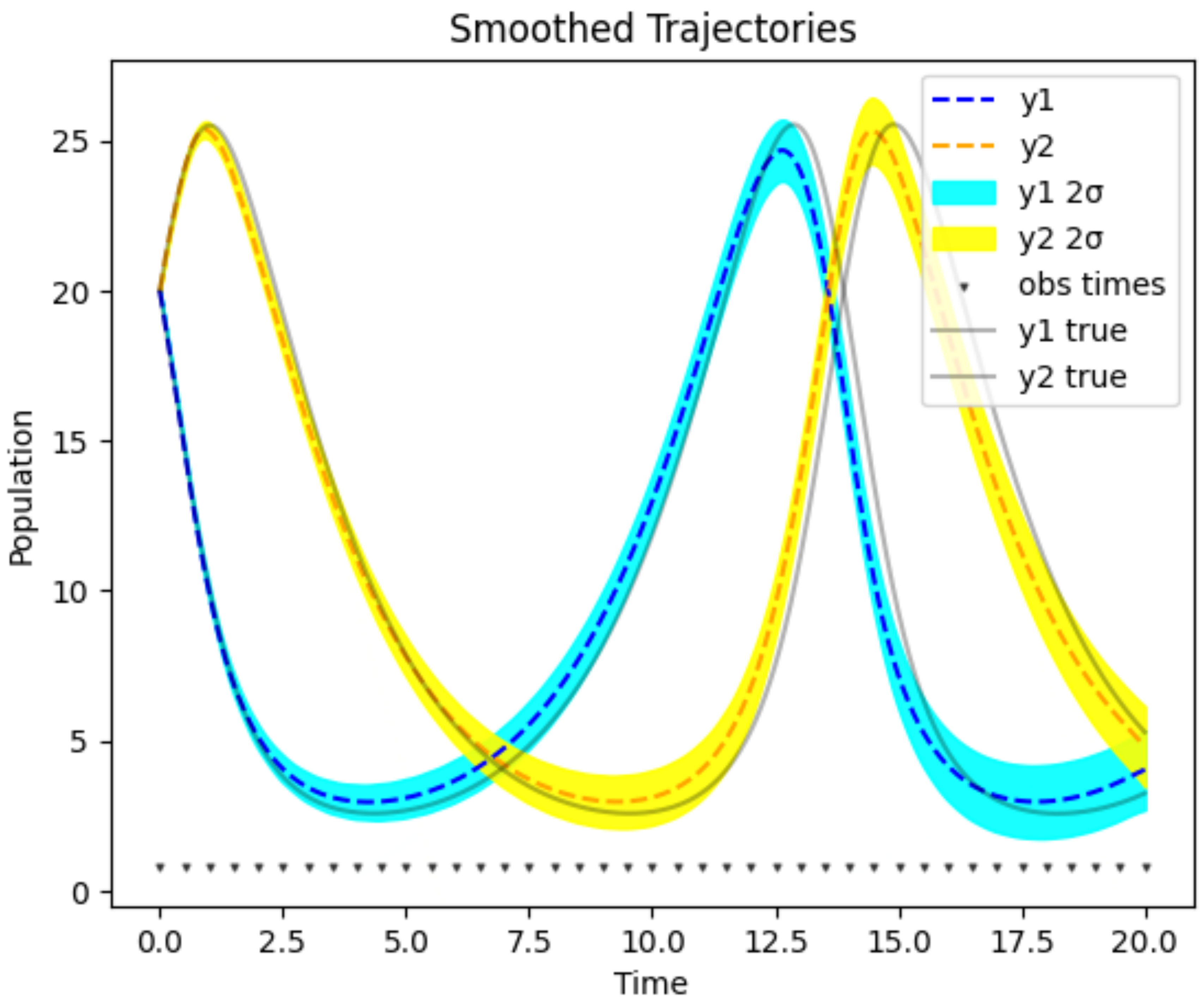

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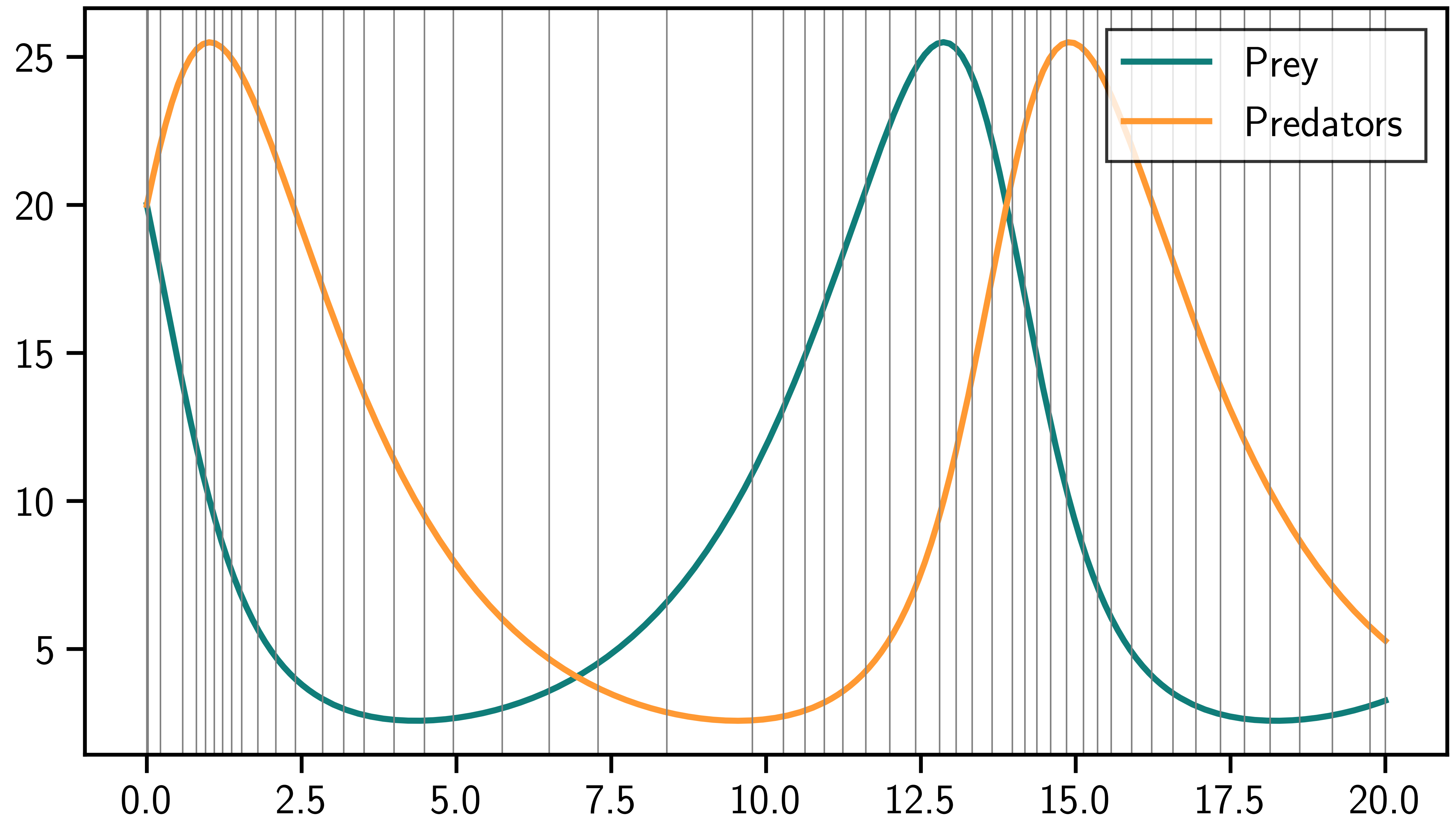

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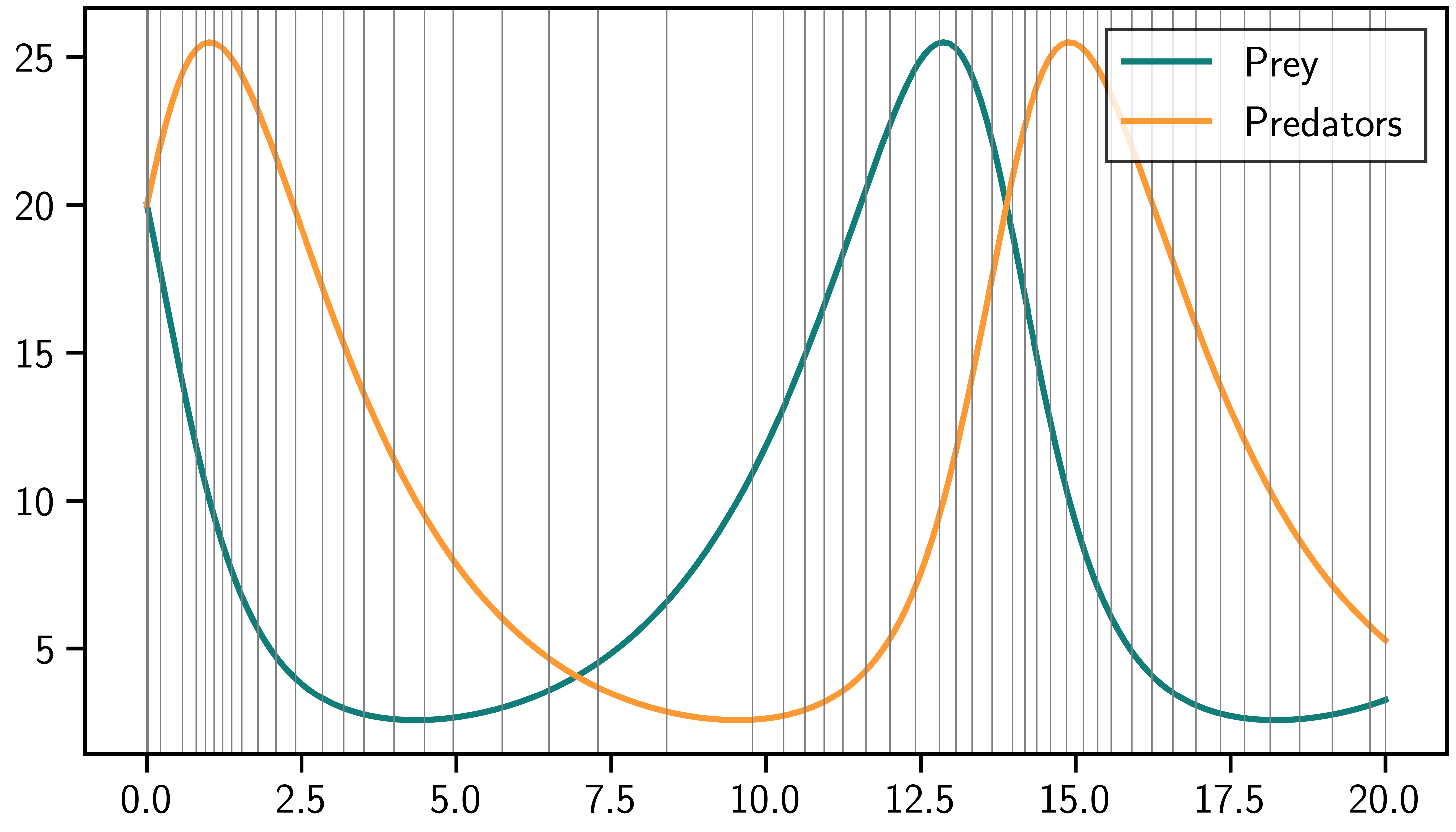

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Roughly, for the same stepsize, probabilistic solvers take 10s-X compute.

and much more time to code up …

Probabilistic ODE Solver

Remark (Relation to Bayesian quadrature). *Before introducing more ODE filters, let us briefly clarify the relation to Bayesian quadrature (BQ) – namely that the EKF0/EKS0 is a* generalisation of BQ *in the following sense: if the ODE is really just an integral (i.e. $x'(t) = g(t)$), then its solution is given by*

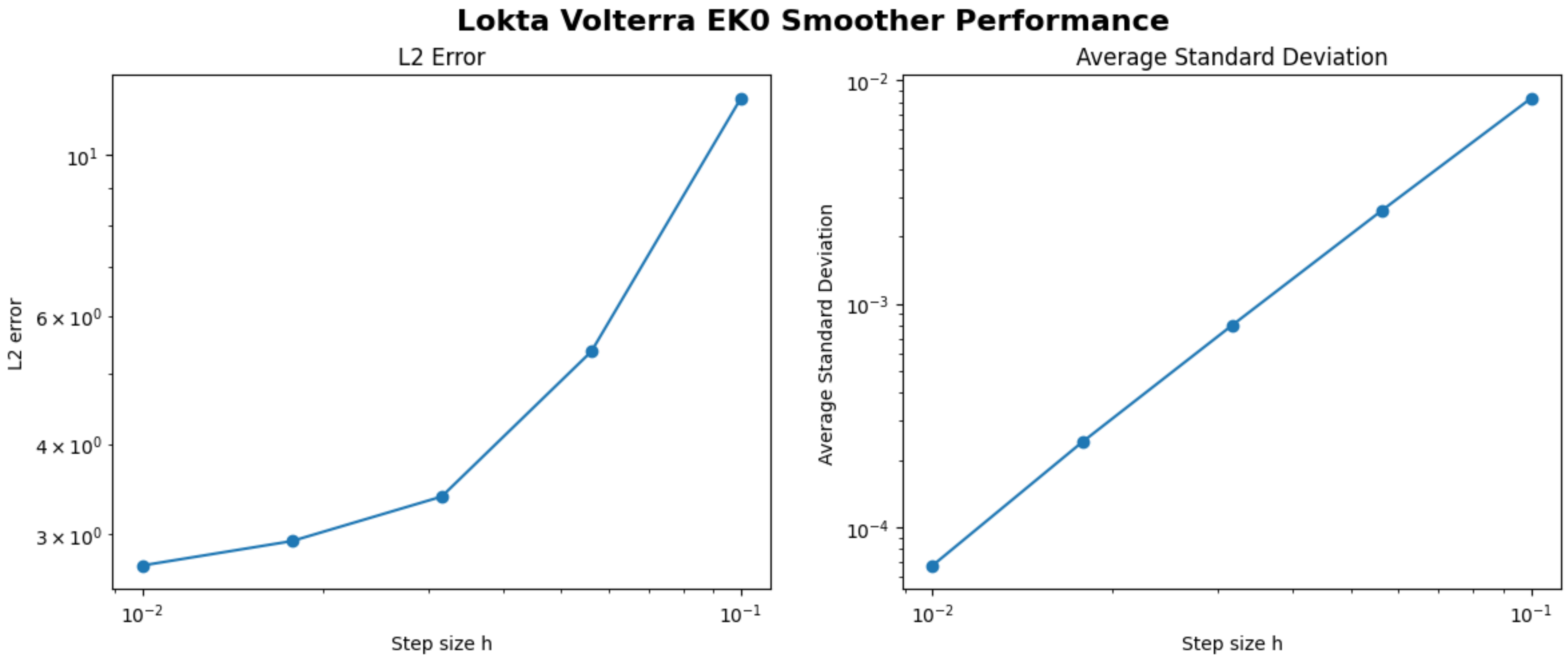
$$x(t) = x_0 + \int_0^t g(s)\,\mathrm{d}s. \tag{38.27}$$

Thus, computing $x(t)$ by approximating the integral in Eq. (38.27) with the Kalman-filter version of BQ (Algorithm 11.2 from §11.2) is equivalent to solving the ODE

$$x'(s) = g(s),\ s \in [0,t], \qquad \textit{with initial value } x(0) = x_0,$$

by the EKF0 or EKS0.[31]

Probabilistic ODE Solver



Convergence results exist too …

Alternative Probabilistic ODE Solvers

Collocation is not the only way …

Alternative Probabilistic ODE Solvers

$$\frac{d}{dt}y(t) = f(y(t), t), \qquad y(0) = y_0$$

Collocation is not the only way …

Euler's Method $$x_{n+h} = x_n + f(x_n, t_n) \cdot h, \qquad x_0 = y_0$$

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Option 1: Inject noise to drift.

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Statistical analysis of differential equations: introducing probability measures on numerical solutions

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Volume 27, pages 1065–1082, (2017) Cite this article

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Option 1: Inject noise to drift.

basically turn ODEs into SDEs

Alternative Probabilistic ODE Solvers

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Option 2: Random stepsizes

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Option 2: Random stepsizes

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Random time step probabilistic methods for uncertainty quantification in chaotic and geometric numerical integration

Published: 14 February 2020

Volume 30, pages 907–932, (2020) Cite this article

Assyr Abdulle & Giacomo Garegnani

Wait, how about combining Physics and data?

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Stay tuned for my CSML talk (23 Apr) !