Splitting methods in Approximate Bayesian Computation for partially observed diffusion processes

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Outline

1. Jansen and Rit Neural Mass Model (JR-NMM)

2. Structure-Preserving Approximate Bayesian Computation (ABC)

3. ABC Results on Simulated Data and Real EEG Data Application

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Jansen and Rit Neural Mass Model (JR-NMM)

Neural Mass Models

Provide a mathematical framework for studying neural brain activity

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- Model whole populations of neurons with average properties
- Reproduce EEG (Electroencephalography) rhythms
- Applied in neurological disorders (epilepsy, schizophrenia, etc.)

Structure-Preserving ABC for the JR-NMM from EEG Data



Figure: Sample path for $\hat{\theta}$ from the JR-NMM versus an EEG segment

The Original Jansen and Rit Neural Mass Model (JR-NMM)¹

Original JR-NMM

- $\begin{aligned} \dot{x}_0(t) &= x_3(t) & \text{Pyramidal cells (Main population)} \\ \dot{x}_1(t) &= x_4(t) & \text{Excitatory interneurons (Subpopulation 1)} \\ \dot{x}_2(t) &= x_5(t) & \text{Inhibitory interneurons (Subpopulation 2)} \\ \dot{x}_3(t) &= Aa \cdot \text{Sigm}(x_1(t) x_2(t)) 2a \cdot x_3(t) a^2 \cdot x_0(t) \\ \dot{x}_4(t) &= Aa \cdot [p(t) + \frac{4}{5}C \cdot \text{Sigm}(C \cdot x_0(t))] 2a \cdot x_4(t) a^2 \cdot x_1(t) \\ \dot{x}_5(t) &= \frac{1}{4}CBb \cdot \text{Sigm}(\frac{1}{4}C \cdot x_0(t)) 2b \cdot x_5(t) b^2 \cdot x_2(t) \end{aligned}$
- Related to the **EEG**-signal: $y(t) = x_1(t) x_2(t)$
- ▶ 8 biologically motivated **parameters**: $A, B, a, b, \nu_{max}, r, v_0, C$
- ▶ **Nonlinear** sigmoid function: Sigm $(x) := \frac{\nu_{max}}{1 + e^{r(v_0 x)}}$

Excitatory (stochastic) input from neighbouring columns: p(t) ¹B.H. Jansen and V.G. Rit. "Electroencephalogram and visual evoked potential generation in a mathematical model of coupled cortical columns." In: Biological cybernetics, 73(4):357-366 (1995)

How can we study the model/problem?

Mathematical level

Dynamical and structural properties

Numerical level

Efficient and structure-preserving simulation

Statistical level Parameter estimation

Reformulate the ODE with random input as an SDE

The Stochastic Jansen and Rit Neural Mass Model²

Stochastic JR-NMM

$$dX_{0}(t) = X_{3}(t) dt$$

$$dX_{1}(t) = X_{4}(t) dt$$

$$dX_{2}(t) = X_{5}(t) dt$$

$$dX_{3}(t) = \{Aa \cdot \text{Sigm}(X_{1}(t) - X_{2}(t)) - 2a \cdot X_{3}(t) - a^{2} \cdot X_{0}(t)\} dt + \sigma_{3} dW_{3}(t)$$

$$dX_{4}(t) = \{Aa \cdot [\mu + \frac{4}{5}C \cdot \text{Sigm}(C \cdot X_{0}(t))] - 2a \cdot X_{4}(t) - a^{2} \cdot X_{1}(t)\} dt + \sigma_{4} dW_{4}(t)$$

$$dX_{5}(t) = \{\frac{1}{4}CBb\text{Sigm}(\frac{1}{4}C \cdot X_{0}(t)) - 2b \cdot X_{5}(t) - b^{2} \cdot X_{2}(t)\} dt + \sigma_{5} dW_{5}(t)$$

- ▶ $(\Omega, \mathcal{F}, \mathbb{P})$ with filtration $\{\mathcal{F}_t\}_{t \geq 0}$ satisfying the usual conditions
- ▶ Independent and \mathcal{F}_t -adapted Wiener processes: $W_i(t)$, i = 3, 4, 5
- Diffusion components: $\sigma_i > 0$, i = 3, 4, 5
- Globally Lipschitz drift and diffusion imply existence of a unique *F_t*-adapted strong solution

²M. Ableidinger, E. Buckwar, and H. Hinterleitner.

"A Stochastic Version of the Jansen and Rit Neural Mass Model: Analysis and Numerics."

In: Journal of Mathematical Neuroscience 7(8) (2017)

The Stochastic Jansen and Rit Neural Mass Model

Stochastic JR-NMM

$$dX_{0}(t) = X_{3}(t) dt$$

$$dX_{1}(t) = X_{4}(t) dt$$

$$dX_{2}(t) = X_{5}(t) dt$$

$$dX_{3}(t) = \{Aa \cdot \text{Sigm}(X_{1}(t) - X_{2}(t)) - 2a \cdot X_{3}(t) - a^{2} \cdot X_{0}(t)\} dt + \sigma_{3} dW_{3}(t)$$

$$dX_{4}(t) = \{Aa \cdot [\mu + \frac{4}{5}C \cdot \text{Sigm}(C \cdot X_{0}(t))] - 2a \cdot X_{4}(t) - a^{2} \cdot X_{1}(t)\} dt + \sigma_{4} dW_{4}(t)$$

$$dX_{5}(t) = \{\frac{1}{4}CBb\text{Sigm}(\frac{1}{4}C \cdot X_{0}(t)) - 2b \cdot X_{5}(t) - b^{2} \cdot X_{2}(t)\} dt + \sigma_{5} dW_{5}(t)$$

Parameters of interest: $\theta = (C, \mu)$

 Parameter C (α-rhythmic value, original JR-NMM literature: 135) Internal connectivity

2. Parameter μ (not studied in the literature) Deterministic external input

Setting for Parameter Inference

1. The model: 6-dim solution process of the stochastic JR-NMM

$$\mathbf{X} = (X_0(t), ..., X_5(t))^T, \quad t \in [0, T]$$

2. Available data: EEG-related 1-dim output process

$$Y_{\theta}(t)=X_1(t)-X_2(t),\quad t\in[0,\,T]$$

 \implies Inference for partially observed stochastic processes 3. *Goal*: Statistical inference on the parameters

$$\theta = (C, \mu)$$

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from **EEG** time series **data** y

 4. Statistical issue: intractable likelihood ⇒ Likelihood-free inference

Structure-Preserving Approximate Bayesian Computation (ABC)

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(Likelihood-free) Approximate Bayesian Computation - ABC^3

Bayesian Computation



Approximate Bayesian Computation

$$\pi(heta|y) pprox \pi_{d,\epsilon,s}(heta|y) = \pi(\ heta \mid d(s(y),s(y_ heta)) < \epsilon \)$$

Structure-preserving ABC for the stochastic JR-NMM

$$\pi(\theta|y) pprox \pi_{d,\epsilon,s,\hat{y}_{ heta}}(\theta|y) = \pi(|\theta|| d(s(y),s(\hat{y}_{ heta})) < \epsilon|)$$

1. New interpretation of s: Incorporate SDE dynamics and structure

<u>2. Reliable numerics to simulate \hat{y}_{θ} : Efficient and structure-preserving ³M.A. Beaumont, W. Zhang, D.J. Balding</u> "Approximate Bayesian computation in population genetics." Genetics, 162(4):2025-2035 (2002)

JR-NMM: Hamiltonian Stochastic Differential Equation



Theorem (Structural property - Ergodicity)

Let $Y_{\theta} = (Y_{\theta}(t))_{t \geq 0}$ be the output process of the stochastic JR-NMM.

- 1. The process Y_{θ} has a unique invariant meausure $\eta_{Y_{\theta}}$ on \mathbb{R} .
- 2. Y_{θ} converges exponentially fast towards its stationary regime $\eta_{Y_{\theta}}$.

Choice of the Numerical Data Generation Scheme \hat{y}_{θ} in ABC

$$\pi(heta|y) pprox \pi_{d,\epsilon,s,\hat{y}_{ heta}}(heta|y) = \pi(| heta||d(s(y),s(\hat{y}_{ heta})) < \epsilon|)$$

Challenge:



 \implies No exact simulation scheme available

Approach:

 \implies Numerical splitting (Efficient and preserves the structure $\eta_{Y_{\theta}}$)

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A little detour: The idea of splitting methods

Illustration with simple deterministic ODEs

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The very basic idea of splitting methods

Consider deterministic ODEs

$$\dot{y} = f(y), \quad y(0) = y_0, t \in [0, T].$$
 (1)

Step 1 consists of rearranging the function f as a sum

$$f(y) = f^{[1]}(y) + f^{[2]}(y),$$

to obtain subequations

$$\dot{y}^{[1]} = f^{[1]}(y^{[1]}) \text{ and } \dot{y}^{[2]} = f^{[2]}(y^{[2]}).$$

Step 2 consists of solving each of the subequations analytically, yielding the explicit flows

$$arphi_t^{[1]}(y_0^{[1]})$$
 and $arphi_t^{[2]}(y_0^{[2]})$

Step 3 consists of choosing how to compose the flows to obtain a numerical method producing the iterates $y_n \approx y(t_n)$ along the grid on [0, T] for the original equation (1):

the Lie-Trotter composition yields

$$y_{n+1} = \left(\varphi_{\Delta t}^{[1]} \circ \varphi_{\Delta t}^{[2]}\right)(y_n)$$

the Strang composition yields

$$y_{n+1} = \left(\varphi_{\Delta t/2}^{[1]} \circ \varphi_{\Delta}^{[2]} \circ \varphi_{\Delta t/2}^{[1]}\right) \left(y_n\right)$$

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Most simple example ever

Consider a linear system of ODEs

 $\dot{y} = Ay$, $y(0) = y_0$, $t \in [0, T]$ with solution $y(t) = \exp(At)y_0$. (2) **Step 1** consists of rewriting the matrix A as $A = A^{[1]} + A^{[2]}$ to obtain subequations

$$\dot{y}^{[1]} = A^{[1]} y^{[1]}$$
 and $\dot{y}^{[2]} = A^{[2]} y^{[2]}$.

 $\label{eq:step2} \begin{array}{l} \mbox{Step 2 consists of solving each of the subequations analytically, yielding the explicit flows} \end{array}$

$$\varphi_t^{[1]}(y_0^{[1]}) = \exp(A^{[1]}t)y_0^{[1]}$$
 and $\varphi_t^{[2]}(y_0^{[2]}) = \exp(A^{[2]}t)y_0^{[2]}$

Step 3 consists of choosing how to compose the flows to obtain a numerical method producing the iterates $y_n \approx y(t_n)$ along the grid on [0, T] for the original equation (1):

the Lie-Trotter composition yields

$$y_{n+1} = \left(\varphi_{\Delta t}^{[1]} \circ \varphi_{\Delta t}^{[2]}\right)(y_n) = \exp(A^{[1]}\Delta t) \cdot \exp(A^{[2]}\Delta t) y_n = \exp(A^{[1]}\Delta t + A^{[2]}\Delta t) y_n,$$

the Strang composition yields

$$\begin{aligned} y_{n+1} &= \left(\varphi_{\Delta t/2}^{[1]} \circ \varphi_{\Delta}^{[2]} \circ \varphi_{\Delta t/2}^{[1]}\right)(y_n) = \exp(A^{[1]}\Delta t/2) \cdot \exp(A^{[2]}\Delta t) \cdot \exp(A^{[1]}\Delta t/2) y_n \\ &= \exp(A^{[1]}\Delta t/2 + A^{[2]}\Delta t + A^{[1]}\Delta t/2) y_n \,, \end{aligned}$$

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Preserving structure, Literature

Splitting methods are one way to go in Geometric Numerical Integration of ODEs. Properties/structure/geometries to be preserved include

- Invariants, such as first integrals,
- Hamiltonian structures
- Symplecticity
- Energy bounds
- Geometric structures

Small sample of literature:

- E.Hairer, C.Lubich, G.Wanner: Geometric Numerical Integration
- ▶ J. M. Sanz-Serna & M. P. Calvo: Numerical Hamiltonian Problems
- R. Glowinski, S.Osher, W.Yin (Eds.): Splitting Methods in Communication, Imaging, Science, and Engineering, 2016
- R.Quispel, R.McLachlan, Splitting Methods, Acta Numerica, 2002

Splitting in the Stochastic case

Preserving structure, Literature on Splitting in the stochastic case

Properties/structure/geometries to be preserved include

- Invariants, such as first integrals,
- Hamiltonian structures
- Symplecticity
- Energy bounds, usually in expectation
- Geometric structures
- Ergodicity
- Invariant measures

Early references:

T. Misawa: A Lie algebraic approach to numerical integration of stochastic differential equations. SIAM J. Sci. Comput., 23(3):866-890, 2001.
T. Misawa: Numerical integration of stochastic differential equations by composition methods. RIMS Kokyuroku 1180, 166-190 (2000).

Other authors include: T. Shardlow, B. Leimkuhler, M. Tretyakov, G. Milstein, D. Cohen, J. Hong, T. Lyons, N. Victoir, C.E. Brehier, L. Goudenege, T. Yamada ...

Splitting in the stochastic case

Consider the *n*-dimensional SDE system with an *m*-dimensional Wiener process

$$dY(t) = F(t, Y(t)) dt + G(t, Y(t)) dW(t), \quad Y(0) = y_0, \quad t \in [0, T],$$

Step 1 consists of rearranging the drift and diffusion functions into sums

$$F(t,Y(t)) = \sum_{l=1}^{d} F^{[l]}(t,Y(t)), \quad G(t,Y(t)) = \sum_{l=1}^{d} G^{[l]}(t,Y(t)), \quad d \in \mathbb{N},$$

to obtain subequations

$$dY^{[l]}(t) = F^{[l]}(t, Y^{[l]}(t)) dt + G^{[l]}(t, Y^{[l]}(t)) dW(t), \quad l \in \{1, ..., d\},$$

Step 2 consists of analytically solving the subequations to obtain explicit flows.

Step 3 consists of choosing composition schemes of the flows, as before.

▶ Note that for multiplicative noise Itô SDEs, it may be convenient to transform to the Stratonovich version.

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Examples of splittings for Step 1 and 2 for SDEs

The Kubo oscillator, a 2-dim. Stratonovich SDE system with a 1-dim. Wiener process $(W(t))_{t\geq 0}$, parameters α , $\sigma > 0$ of the form

$$d\begin{pmatrix} X(t)\\ Y(t) \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & -\alpha\\ \alpha & 0 \end{pmatrix}}_{=:A} \begin{pmatrix} X(t)\\ Y(t) \end{pmatrix} dt + \underbrace{\begin{pmatrix} 0 & -\sigma\\ \sigma & 0 \end{pmatrix}}_{=:\Sigma} \begin{pmatrix} X(t)\\ Y(t) \end{pmatrix} \circ dW(t), \quad \begin{pmatrix} X(0)\\ Y(0) \end{pmatrix} = \begin{pmatrix} X_0\\ Y_0 \end{pmatrix}$$

Step 1: Setting $Z(t) = (X(t), Y(t))^{\intercal}$, subsystems are

$$dZ^{[1]}(t) = AZ^{[1]}(t)dt$$
 and $dZ^{[2]}(t) = \Sigma Z^{[2]}(t) \circ dW(t)$.

Step 2 consists of solving each of the subequations analytically, yielding the explicit flows

$$arphi_t^{[1]}(Z[1]_0) = \exp(At)Z_0^{[1]} \quad ext{and} \quad arphi_t^{[2]}(Z_0^{[2]}) = \exp(\Sigma W(t))Z_0^{[2]}$$

We have

$$\exp(At) = \begin{pmatrix} \cos(\alpha t) & -\sin(\alpha t) \\ \sin(\alpha t) & \cos(\alpha t) \end{pmatrix} \exp(\Sigma W(t)) = \begin{pmatrix} \cos(\sigma W(t)) & -\sin(\sigma W(t)) \\ \sin(\sigma W(t)) & \cos(\sigma W(t)) \end{pmatrix}$$
$$\exp(At + \Sigma W(t)) = \begin{pmatrix} \cos(\alpha t + \sigma W(t)) & -\sin(\alpha t + \sigma W(t)) \\ \sin(\alpha t + \sigma W(t)) & \cos(\alpha t + \sigma W(t)) \end{pmatrix}$$

The matrices A and Σ commute, so the solution of the Kubo oscillator is $Z(t) = \exp(At + \Sigma W(t))Z_0$, also the splitting methods will compute the exact solution, thus the Kubo oscillator corresponds to the *most simple example ever* in the stochastic case.

Back to: Structure-Preserving Approximate Bayesian Computation (ABC)

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Efficient and Structure-Preserving Numerical Splitting

$$\underbrace{\frac{dQ(t) = \nabla_P H(Q, P) dt}{dP(t) = [-\nabla_Q H(Q, P)]}}_{Hamiltonian} - \underbrace{2\Gamma P}_{\substack{linear \\ damping}} + \underbrace{G(\theta, Q)}_{\substack{nonlinear \\ displacement}} \right] dt + \underbrace{\Sigma}_{\substack{diffusion \\ matrix}} dW(t)$$

1. Subsystem a: linear SDE

$$\begin{pmatrix} dQ \\ dP \end{pmatrix} = \begin{pmatrix} \nabla_P H(Q, P) \\ -\nabla_Q H(Q, P) - 2\Gamma P \end{pmatrix} dt + \begin{pmatrix} 0_3 \\ \Sigma dW(t) \end{pmatrix}$$

2. Subsystem b: non-linear ODE

$$\begin{pmatrix} dQ\\ dP \end{pmatrix} = \begin{pmatrix} 0_3\\ G(\theta, Q) \end{pmatrix} dt$$

Strang splitting in a discretized regime with equidistant time steps Δt :

$$\hat{\mathbf{X}} = X^{b}_{\Delta t/2} \circ X^{a}_{\Delta t} \circ X^{b}_{\Delta t/2}, \quad \hat{\mathbf{Y}}_{\theta} = \hat{X}_{1} - \hat{X}_{2}$$

Efficient and Structure-Preserving Numerical Splitting



Figure: Invariant densities for $\theta = (C = 150, \mu = 220)$ and different $\Delta t = -9$ and

A new Interpretation of Summaries s in ABC

$$\pi(\theta|y) \approx \pi_{d,\epsilon,s,\hat{y}_{\theta}}(\theta|y) = \pi(\theta \mid d(s(y),s(\hat{y}_{\theta})) < \epsilon)$$

Challenge:



Figure: 2 sample paths for $\theta = (C = 135, \mu = 220)$

 \implies How to account for the variability in the data for identical θ ? Approach:

 \implies Transform the data from time to frequency domain

Spectral Density (Periodogram)

Stationary stochastic process: $\mathbf{Y}_{\theta} = (Y_{\theta}(t))_{t \geq 0}$

• Autocovariance function: $Cov(Y_{\theta}(t), Y_{\theta}(s)) = r_{\theta}(\tau = t - s)$

$$S_{\mathbf{Y}_{\theta}}(\omega = 2\pi f) = \int_{-\infty}^{\infty} r_{\theta}(\tau) e^{-i\omega\tau} d\tau, \quad \omega \in [-\pi, \pi]$$

Definition (Periodogram)

$$s(y) = \hat{S}_y(\omega) = rac{1}{J} \left| \sum_{j=1}^J y_j e^{-i\omega j} \right|^2$$

▶ Time domain: Discrete data y = (y₁, ..., y_J), J ∈ N
 ▶ Frequency domain: *R*-function spectrum (Fast Fourier Transform)

Simulated Data and Periodogram Estimates



Figure: 2 sample paths for $\theta = (C = 135, \mu = 220)$



Figure: 2 (smoothed) periodograms for $\theta = (C = 135, \mu = 220)$ (日) (日) (日) (日) (日) (日) (日) (日)

The Splitting Scheme Preserves the Periodogram



Figure: Periodogram estimates for $\theta = (C = 150, \mu = 220)$ and different Δt

Structure-Preserving ABC-Algorithm

ABC for the stochastic JR-NMM

Input: Observed datasets (EEG segments) $y = (y_1, ..., y_M)$, $M \in \mathbb{N}$

- Precompute the periodograms $s(y) = (\hat{S}_{y_1}, ..., \hat{S}_{y_M}) = (s_1, ..., s_M)$
- Choose prior distribution $\pi(\theta)$ and tolerance ϵ

for i=1:N do Parallel simulation on the HPC (High Performance Cluster) Radon1

- Draw θ_i from the prior $\pi(\theta)$
- Simulate new data \hat{y}_{θ_i} using the numerical splitting approach
- Compute the periodogram $s(\hat{y}_{\theta_i}) = \hat{s}_{\theta_i}$
- ► Calculate $D_i(s(y), \hat{s}_{\theta_i}) = \text{median}(d(s_1, \hat{s}_{\theta_i}), ..., d(s_M, \hat{s}_{\theta_i}))$
- Store samples (D_i, θ_i)

end for

If $D_i < \epsilon$, keep θ_i as a sample of the posterior $\pi_{d,\epsilon,s,\hat{y}_{\theta}}(\theta|y)$

Output: Samples $\theta_1, ..., \theta_n$ from the approximated posterior $\pi_{d,\epsilon,s,\hat{y}_{\theta}}(\theta|y)$

ABC Results on Simulated Data and Real EEG Data Application

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ABC for the JR-NMM: Simulated Data

α -rhythmic behaviour:

- Original JR-NMM literature: C = 135
- \blacktriangleright Newly introduced in the SDE-version (not yet investigated): μ



Figure: Sample path for $\theta = (C = 135, \mu = 220)$

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Structure-Preserving ABC: Results for Simulated Data



Figure: Marginal ABC posterior densities

- Prior distributions: $\pi(C) = U(105, 165), \ \pi(\mu) = U(130, 310)$
- Number of simulated synthetic datasets: N = 10⁶
- ▶ Data generation: time step $\Delta t = 2 \cdot 10^{-3}$, time horizon T = 200
- Tolerance: $\epsilon = 0.5^{\text{th}}$ percentile
- Observed datasets (independent repeated experiments): M = 30

Structure-Preserving ABC: Results for Simulated Data



Figure: Marginal ABC posterior densities

	С	μ
ABC Posterior Mean	$\int_{D} C \cdot \pi_{ABC}(C y) \ dC = 134.966 = \hat{C}$	$\int_{D} \mu \cdot \pi_{ABC}(\mu \mathbf{y}) \ d\mu = 219.79$
Relative Error	$\frac{\hat{C}-C}{C} = -0.025$ %	$\frac{\hat{\mu}-\mu}{\mu} = -0.095 \%$

Structure-Preserving ABC: Results for Simulated Data



Figure: Marginal ABC posterior densities

	С	μ
Credible Probability CP	$CP = \int_{Cl} \pi_{ABC}(C y) \ dC = 0.997$	$CP = \int\limits_{Cl} \pi_{ABC}(\mu y) \ d\mu = 0.95$
Credible Interval <i>CI</i>	CI = [133, 137]	<i>Cl</i> = [205, 235]

ABC for the JR-NMM: Real EEG α -rhythmic Data⁴



Figure: α -rhythmic EEG segment: sampling rate 173.61 hz

⁴R. Andrzejak, K. Lehnertz, F. Mormann, C. Rieke, P. David, C. Elger. "Indications of nonlinear deterministic and finite-dimensional structures in time series of brain electrical activity: Dependence on recording region and brain state." Physical Review E, 64(6), 8 (2001)

Structure-Preserving ABC: Results for EEG Data



Figure: Marginal ABC posterior densities

- ▶ Prior distributions: $\pi(C) = U(85, 185), \pi(\mu) = U(70, 370)$
- Expected values: C = 135, $\mu = 220$
- Number of simulated synthetic datasets: $N = 10^6$
- **•** Data generation: time step $\Delta t = 2 \cdot 10^{-3}$, time horizon T = 23.6
- **•** Tolerance: $\epsilon = 0.5^{\text{th}}$ percentile
- ► Observed EEG segments of same type: $M = 5_{0}$, $A = 5_{0}$, A =

Structure-Preserving ABC: Results for EEG Data



Figure: Marginal ABC posterior densities

	С	μ
ABC Posterior Mean	$\int_{D} C \cdot \pi_{ABC}(C y) \ dC = 134.383 = \hat{C}$	$\int_{D} \mu \cdot \pi_{ABC}(\mu y) \ d\mu = 224.57$

 $\hat{\theta} = (\hat{C}, \hat{\mu}) = (134.383, 224.578)$

Structure-Preserving ABC: Results for EEG Data



Figure: Sample path for $\hat{ heta} = (\hat{C}, \hat{\mu})$ versus an EEG segment

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Non-Preservative ABC: The Method of Euler-Maruyama



Figure: Marginal ABC posterior densities (simulated reference data)

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 \implies Need for structure-preserving data generation!

Thank you for your attention

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