Simulation-based inference of dynamical systems with model uncertainty

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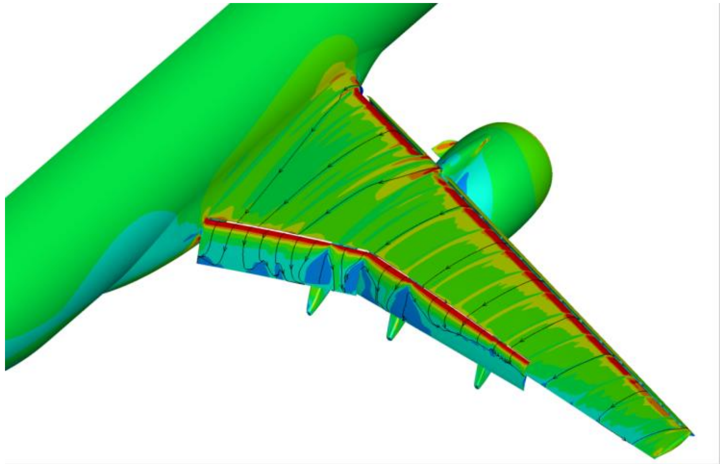
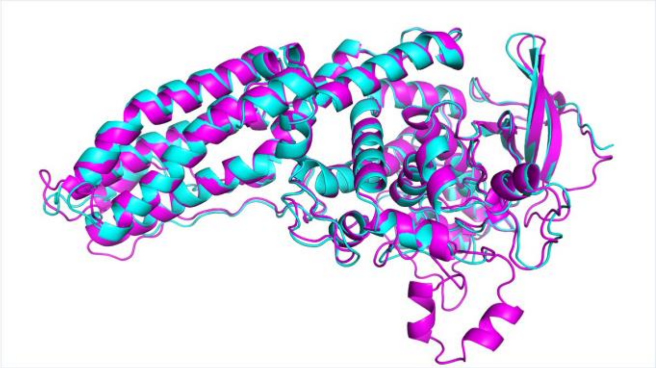
Motivation

- Dynamical systems arise in various fields and applications
  - Fluid flow
  - Financial markets
  - Biological systems
- Dynamics models are important tools for studying such systems
  - Forecasting, control, etc…
- When estimating dynamics models, accounting for model uncertainty can lead to several benefits
  - Improved generalization and accuracy
- Unfortunately, including model uncertainty also adds complexity
  - Posterior is costly to evaluate
  - Posterior is challenging to sample from



https://hiliftpw.larc.nasa.gov/index.html



https://www.technologyreview.com/2020/11/30/1012712/deepmind-protein-folding-ai-solved-biology-science-drugs-disease/

Simulation-based inference

- Simulation-based inference are a group of methods that draw samples from a *surrogate* distribution using simulations
- A simulator is a computer model that generates a stochastic realization of the model outputs

- **Question:** Can these methods be used to improve sampling in terms of speed and efficiency?

- **Objective:** Compare a filtering-based approach to two simulation-based approaches for likelihood estimation on an example problem

Outline

1. Filtering-based approach
2. Simulation-based inference
3. Results
4. Conclusions and future work

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Introduction

Filtering-based approach

Simulation-based inference

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Probabilistic formulation

The inclusion of process noise accounts for model uncertainty

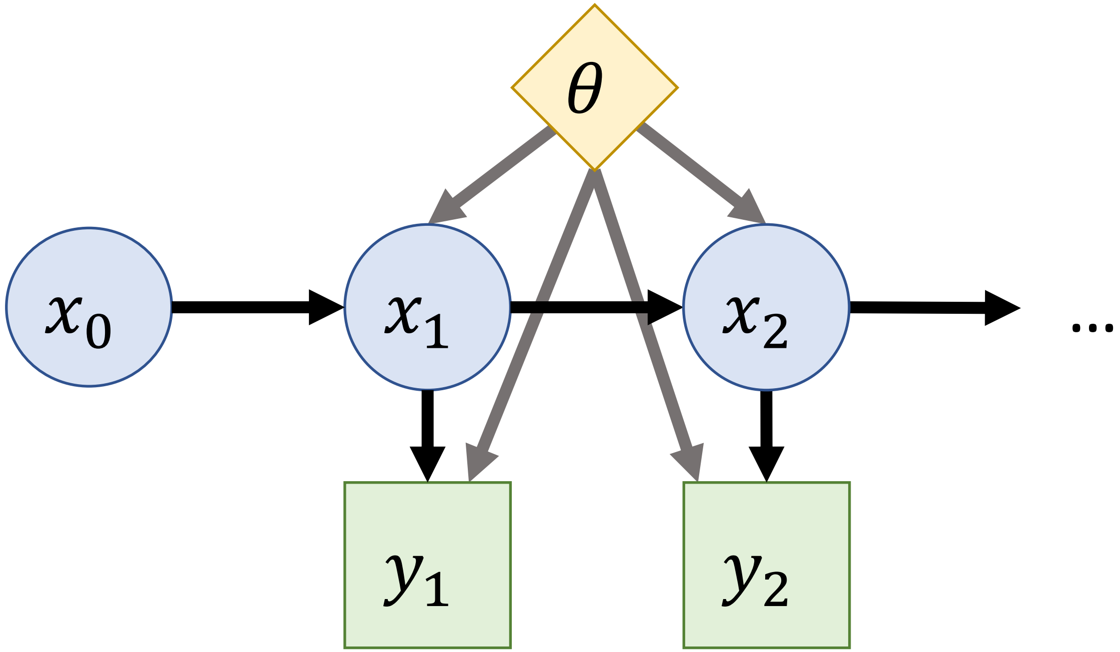
$$X_k \in \mathbb{R}^{d_x}, \qquad Y_k \in \mathbb{R}^{d_y}, \qquad \theta = (\theta_\Psi, \theta_h, \theta_\Sigma, \theta_\Gamma) \in \mathbb{R}^{d_\theta}$$

$$X_k = \Psi(X_{k-1}, \theta_\Psi) + \xi_{k-1}; \quad \xi_{k-1} \sim \mathcal{N}\big(0, \Sigma(\theta_\Sigma)\big)$$

$$Y_k = h(X_k, \theta_h) + \eta_k; \qquad \eta_k \sim \mathcal{N}\big(0, \Gamma(\theta_\Gamma)\big)$$

The process noise term ξ_k accounts for model error

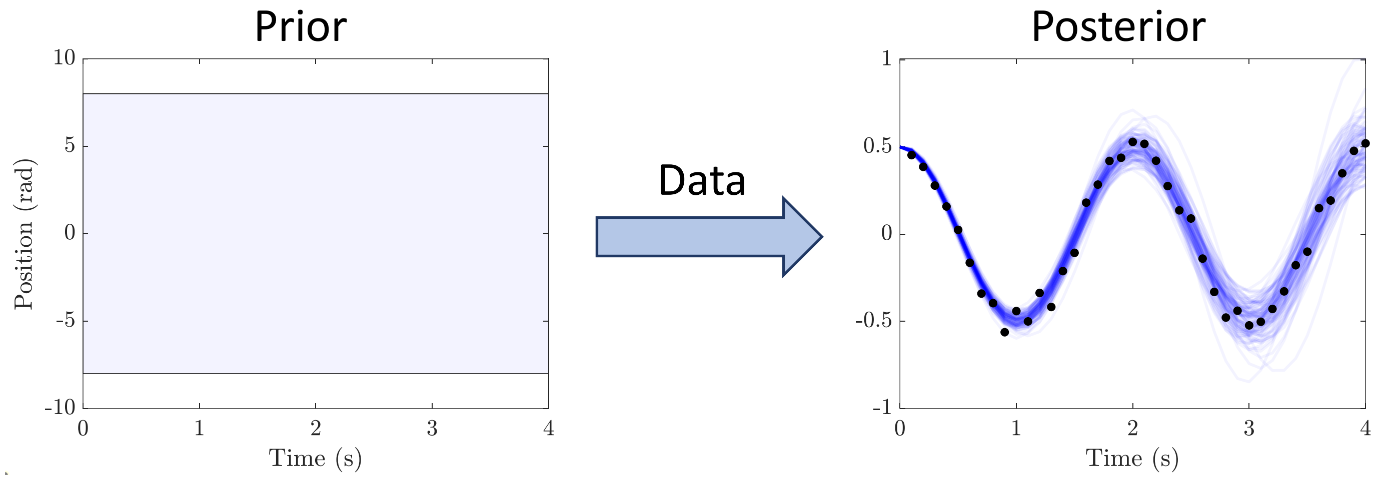
- Parameter error
- Integration error
- Insufficient model expressiveness



1. Parameter Uncertainty
2. Model Uncertainty
3. Measurement Uncertainty

Bayesian inference

- Goal: compute $p(\theta|\mathcal{Y}_T)$ where $\mathcal{Y}_T = (y_1, y_2, \dots, y_T)$
- Bayes' rule: $p(\theta|\mathcal{Y}_T) = \dfrac{\mathcal{L}(\theta; \mathcal{Y}_T)p(\theta)}{p(\mathcal{Y}_T)}$



- Due to uncertainty in the states, we can only access the joint likelihood: $\mathcal{L}(\theta;\ \mathcal{X}_T, \mathcal{Y}_T)$
- To get the marginal likelihood, we must evaluate the integral

$$\mathcal{L}(\theta;\ \mathcal{Y}_T) = \int \mathcal{L}(\theta;\ \mathcal{X}_T, \mathcal{Y}_T)\, d\mathcal{X}_T$$

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Bayesian system identification algorithm

MCMC

for $i = 1, \dots, M$

Propose sample θ

<u>Evaluate posterior:</u> $\pi(\theta|\mathcal{Y}_T) = \pi(\theta)\prod_{k=1}^{T}\mathcal{L}_k(\theta;\mathcal{Y}_k)$

Bayesian filtering

for $k = 1, \dots, T$

Predict: $\pi(\mathbf{x}_{k+1}|\mathcal{Y}_k,\theta) = \int \pi(\mathbf{x}_{k+1}|\mathbf{x}_k,\theta)\pi(\mathbf{x}_k|\mathcal{Y}_k,\theta)\mathrm{d}\mathbf{x}_k$

Marginalize: $\mathcal{L}_{k+1}(\theta;\mathcal{Y}_{k+1}) = \int \pi(\mathbf{y}_{k+1}|\mathbf{x}_{k+1},\theta)\pi(\mathbf{x}_{k+1}|\mathcal{Y}_k,\theta)\mathrm{d}\mathbf{x}_{k+1}$

Update: $\pi(\mathbf{x}_{k+1}|\mathcal{Y}_{k+1},\theta) = \dfrac{\pi(\mathbf{y}_{k+1}|\mathbf{x}_{k+1},\theta)\pi(\mathbf{x}_{k+1}|\mathcal{Y}_k,\theta)}{\pi(\mathbf{y}_{k+1}|\mathcal{Y}_k,\theta)}$

end for

Accept θ with Metropolis-Hastings probability; otherwise reject

end for

Särkkä, S. (2013). *Bayesian filtering and smoothing* (No. 3). Cambridge University Press.

The computational expense of filtering can quickly become limiting

The computational cost is on the order

$$\mathcal{O}\left(T\left(d_x^3 + d_y^3 + d_xF\right)\right)$$

where F is the cost of one timestep of forward model/simulator

Goal: Replace the filter with a simulation-based surrogate likelihood to significantly reduce the computational cost

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Bayesian synthetic likelihood (BSL)

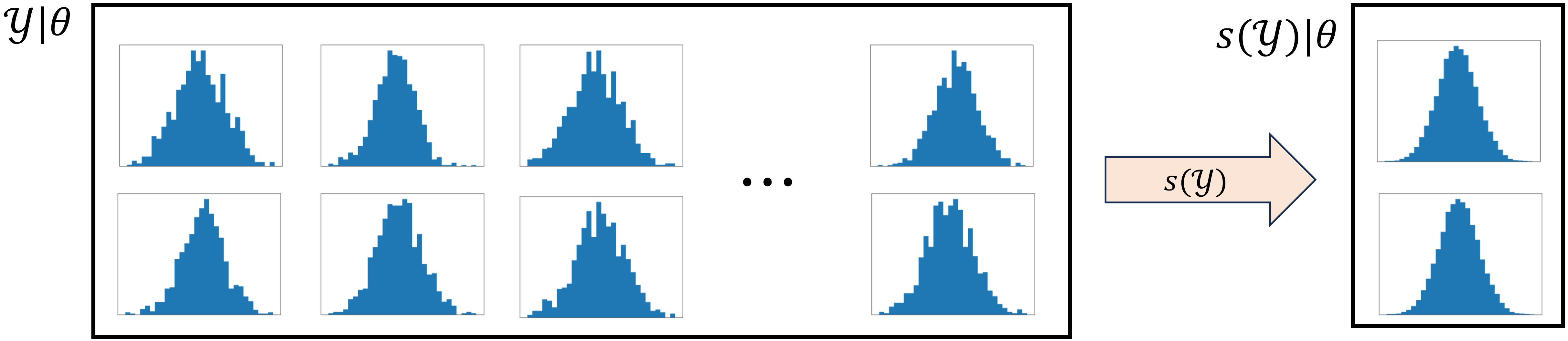
Wood, Simon N. "Statistical inference for noisy nonlinear ecological dynamic systems." *Nature* 466.7310 (2010): 1102-1104.

- The likelihood is non-Gaussian

$$p(\theta|\mathcal{Y}) \propto p(\mathcal{Y}|\theta)p(\theta)$$

- Assume we can map the data to a collection of summary statistics that are approximately Gaussian
  - E.g., coefficients of polynomial regression
- Replace the non-Gaussian likelihood with the Gaussian *synthetic likelihood* $p(s(\mathcal{Y})|\theta)$

$$p(\theta|\mathcal{Y}) \approx p(\theta|s(\mathcal{Y})) \propto p(s(\mathcal{Y})|\theta)p(\theta)$$



Choice of summary statistics

Maraia, Ramona, et al. "Bayesian synthetic likelihood for stochastic models with applications in mathematical finance." *Frontiers in Applied Mathematics and Statistics* 9 (2023): 1187878.

Donsker's theorem:

Guarantees asymptotic Gaussianity of the empirical cumulative distribution function (eCDF) vectors

Select a set of features $\mathcal{Y}_T = (y_1, \dots, y_T)$, $\mathrm{d}\mathcal{Y}_T = (y_2 - y_1, \dots, y_T - y_{T-1})$

Select a collection of d_{bins} bins $\mathcal{B}$

Construct eCDF vectors $s(\mathcal{Y}_T) \in \mathbb{R}^{d_{bins}}$

Bayesian synthetic likelihood (BSL)

Input:

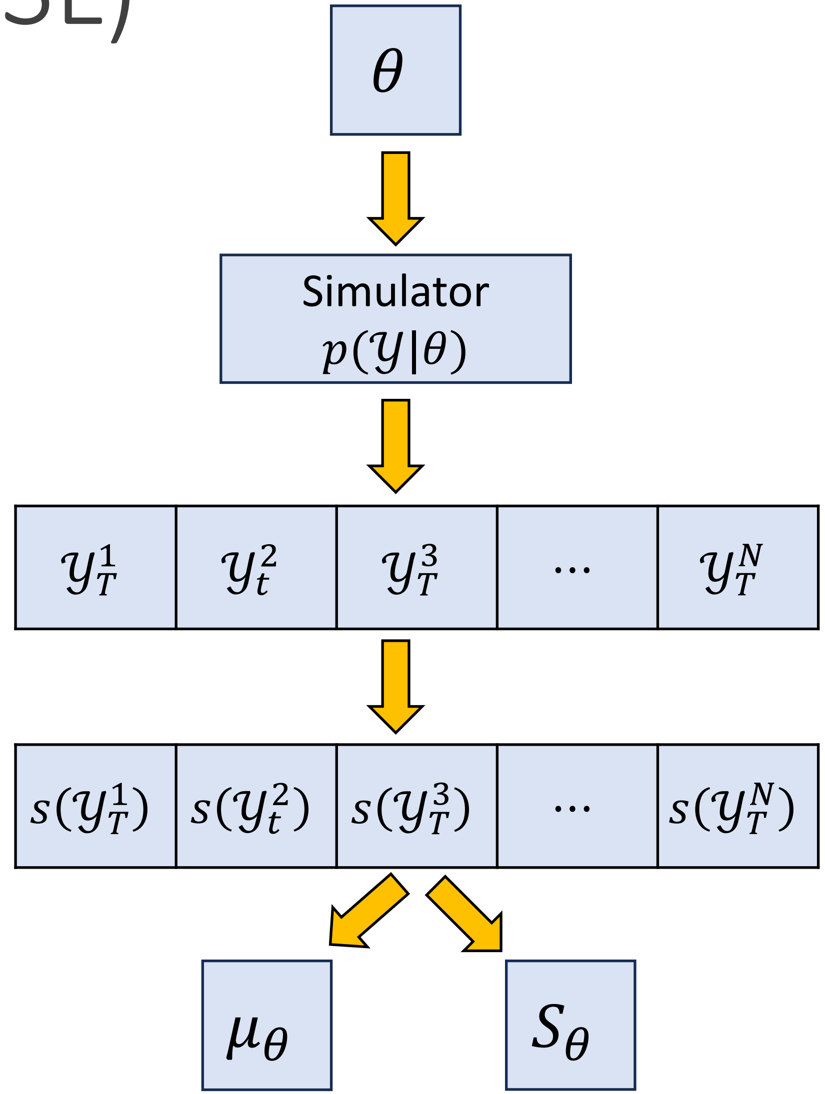
Parameter value θ

Number of simulations N

Output:

Evaluation of synthetic likelihood

1. Draw $\mathcal{Y}_T$ samples $\mathcal{Y}_T \sim p(\mathcal{Y}_T|\theta)$
2. Compute summary statistics $s(\mathcal{Y}_T)$
3. Compute empirical mean μ_θ and covariance S_θ
4. Evaluate $\mathcal{N}(\bar{\mathcal{Y}}_T; \mu_\theta, S_\theta)$



Sequential neural likelihood (SNL)

- The Gaussian assumption can be limiting in many situations
- The neural likelihood uses a neural network, e.g., a normalizing flow, to model the likelihood density

- Requires a proposal distribution to draw samples to train the network
- To achieve convergence, these samples should come from high density regions of the posterior
- SNL iteratively improves its proposal to target high density regions

Sequential neural likelihood (SNL)

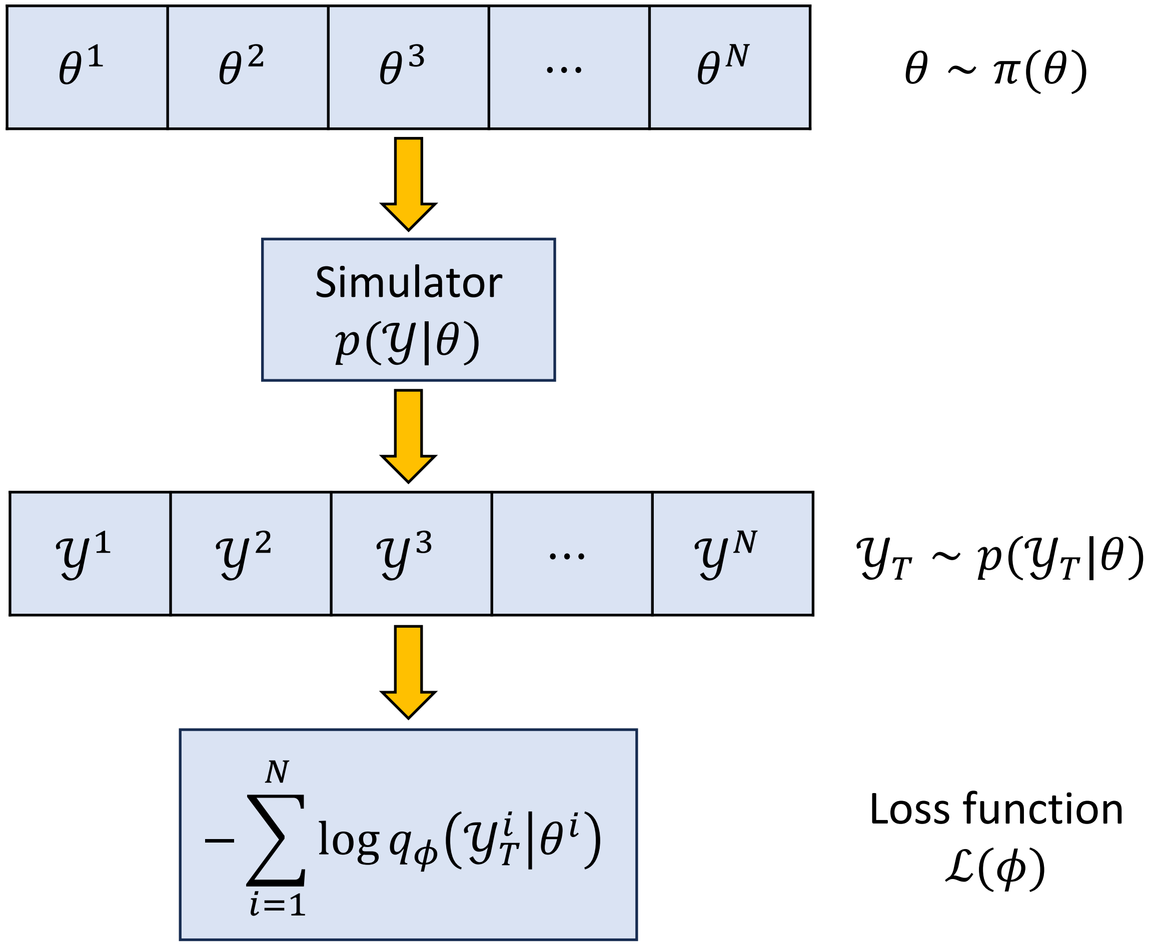
Input:

Initial proposal $\pi_0(\theta)$
Density model q_ϕ
Number of simulations N
Number of training rounds R

Output:

Density $q_\phi(\mathcal{Y}_T|\theta) \approx p(\mathcal{Y}_T|\theta)$

1. Set proposal $\pi(\theta) = \pi_0(\theta)$
   For $round = 1, \dots, R$:
2. Draw θ samples $\theta \sim \pi(\theta)$
3. Draw $\mathcal{Y}_T$ samples $\mathcal{Y}_T \sim p(\mathcal{Y}_T|\theta)$
4. Train $q_\phi(\mathcal{Y}_T|\theta) \approx p(\mathcal{Y}_T|\theta)$
   If $round < R$:
5. Set proposal $\pi(\theta) \propto q_\phi(\mathcal{Y}_T|\theta)p(\theta)$



Schematic of training round (lines 2—4)

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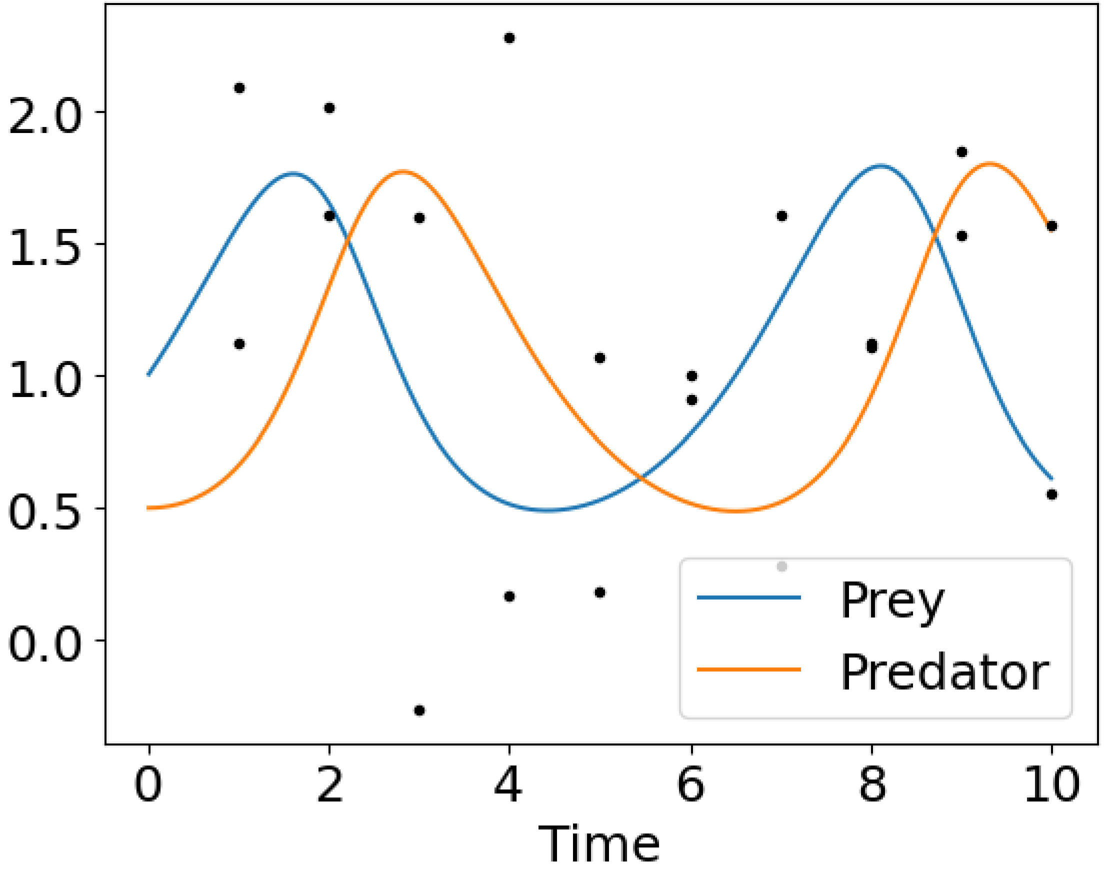
Lotka-Volterra

$$\dot{x} = \alpha x - xy$$

$$\dot{y} = \beta xy - y$$



Model setup:

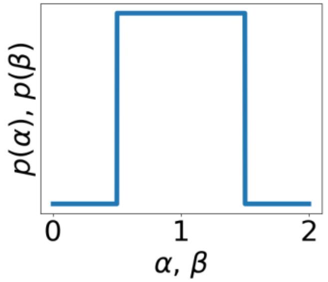
Euler-Maruyama with $\Delta t = 0.01$
Data at times $t = 1s, 2s, \ldots, 10s$
Measurement noise: $\mathcal{N}(0, 0.5^2)$

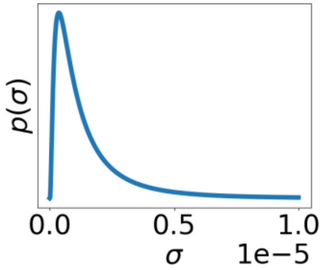
Learnable parameters:

$\theta = [\alpha, \beta, \sigma]$,
where $\Sigma = \sigma^2 I_2$

Priors:

$\alpha, \beta \sim \mathcal{U}[0.5, 1.5]$,
$\sigma \sim lognormal(10^{-6}, 1)$

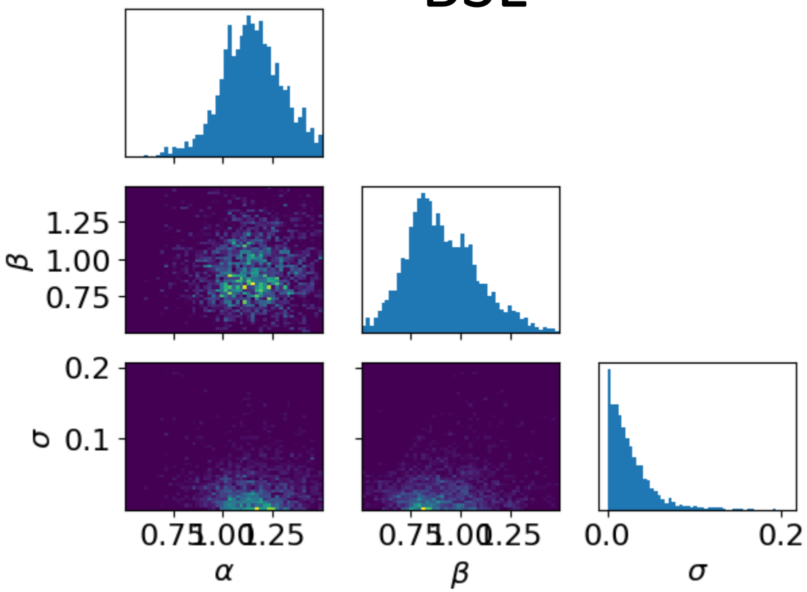




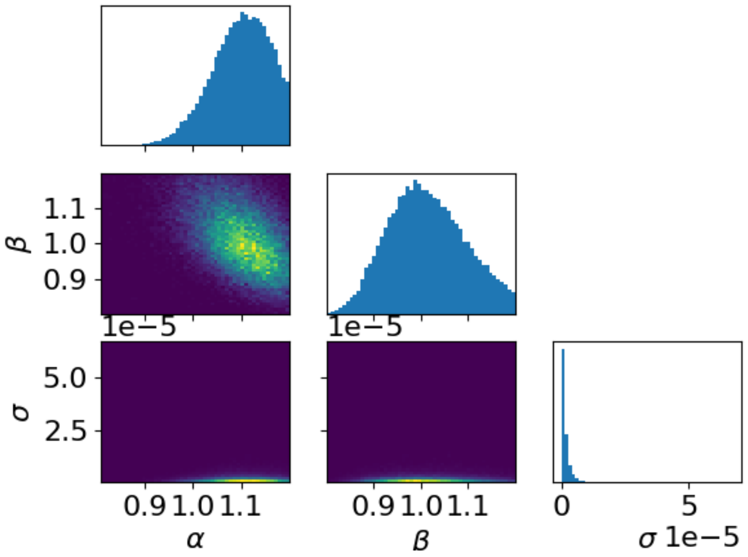
Distributions

SNL visually matches filter with better sampling

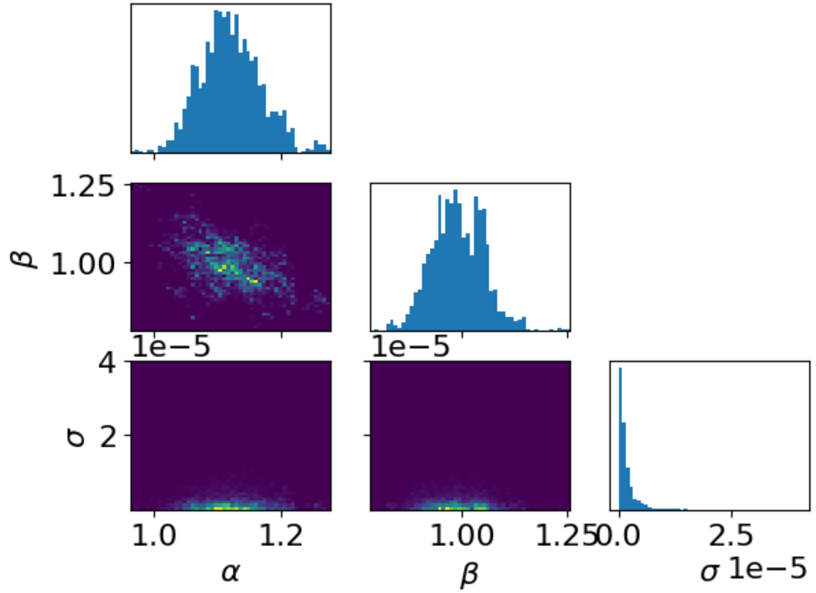
BSL



SNL



Filter

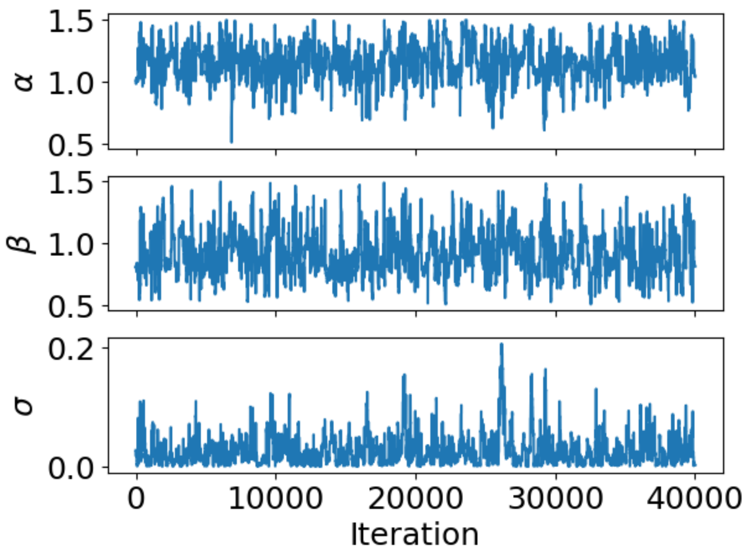


Chains and time comparison

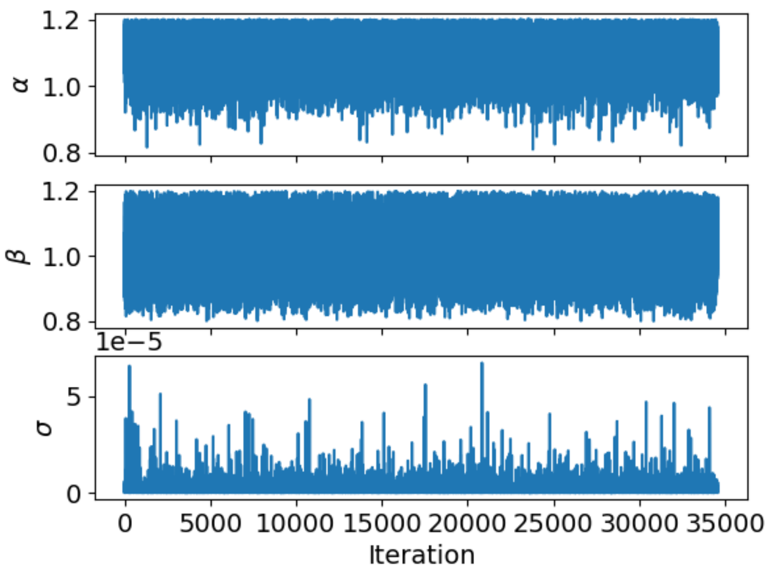
The SNL is fastest by a wide margin

Algorithm	Total time (h:mm:ss)
BSL	4:47:36
SNL	0:17:20
Filter	2:05:42

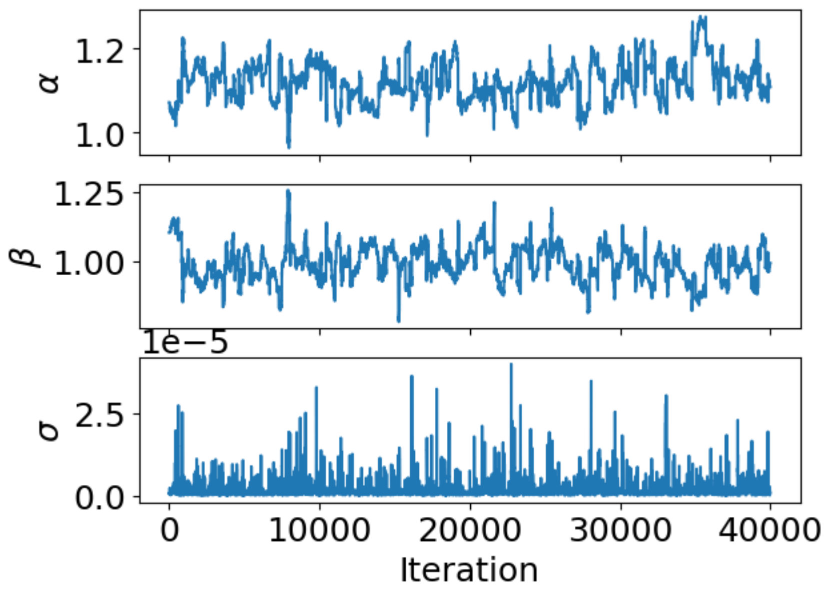
BSL



SNL

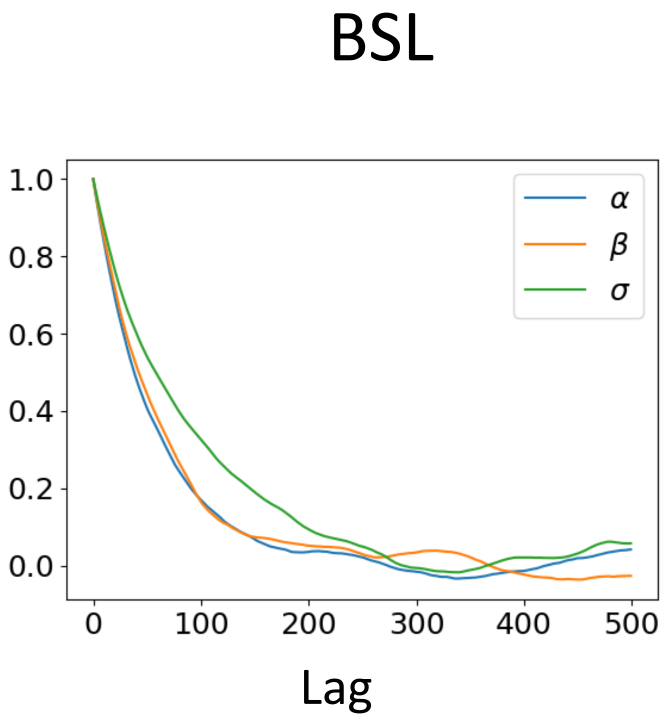


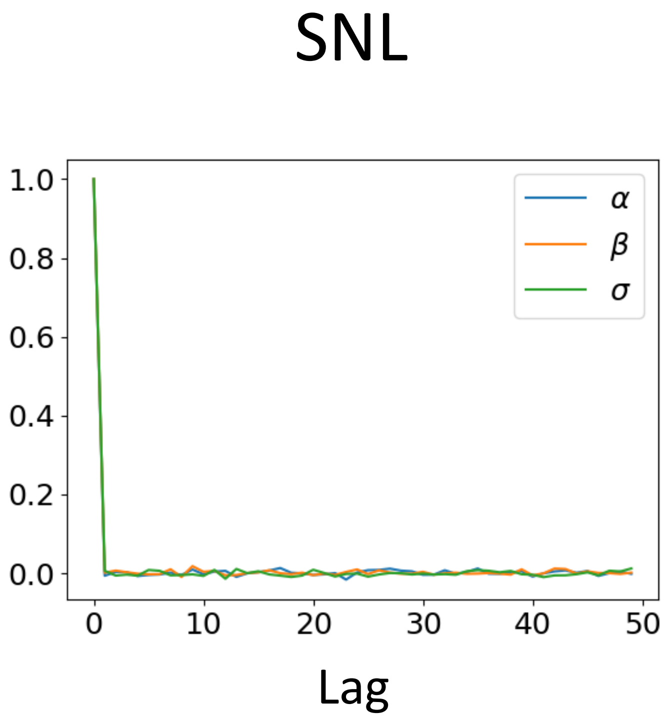
Filter

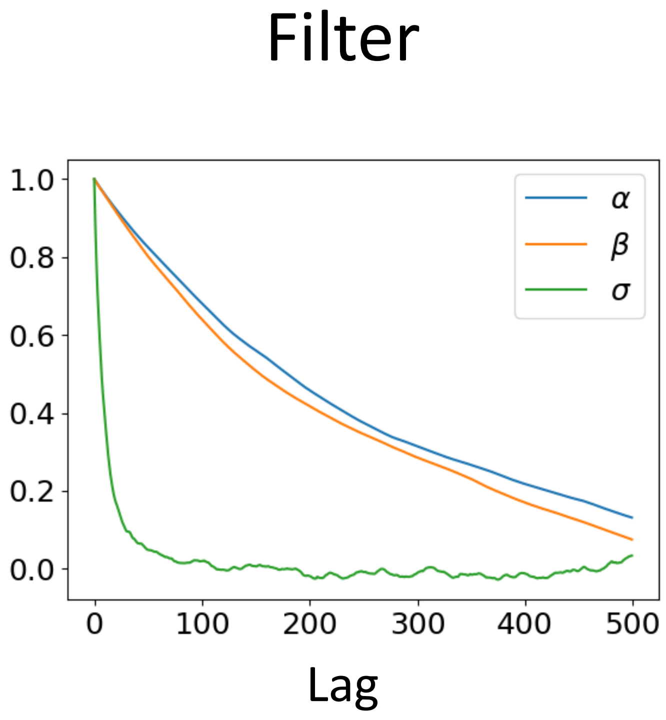


Autocorrelation plots

The SNL shows the best sample efficiency







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Conclusions

- Simulation-based methods show potential for accelerating posterior sampling in estimating dynamics models
- The SNL showed the best performance on the example problem in terms of speed and sampling efficiency
- The BSL method is potentially better-suited for high dimensions

Future work

- Investigate discrepancies in sampling efficiency between the methods
- Analyze the differences in performance of simulation-based methods when process noise is and is not included

References

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