Bayesian Verification of Chemical Reaction Networks

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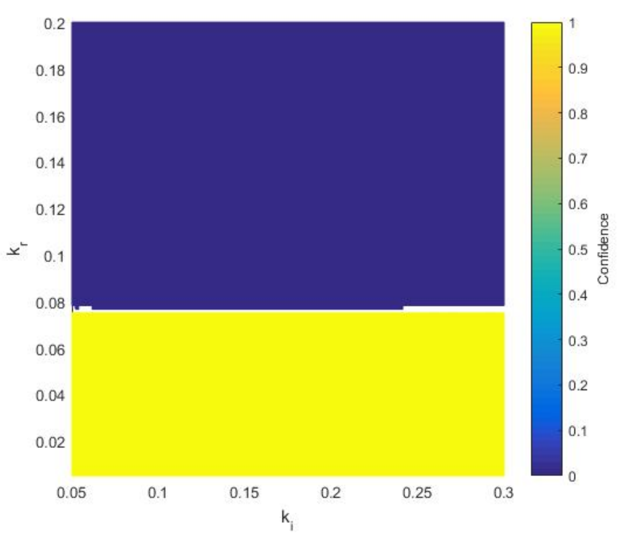
Introduction

- We wish to verify that an underlying biological system satisfies a given property using formal verification techniques.
- The problem with using formal verification techniques is that *fully known* models are required, and when modelling biological systems, many systems are not fully known.
- To overcome this issue, our framework integrates **Bayesian inference** and **formal verification**, and proves to be more data efficient than classical Statistical Model Checking (SMC).

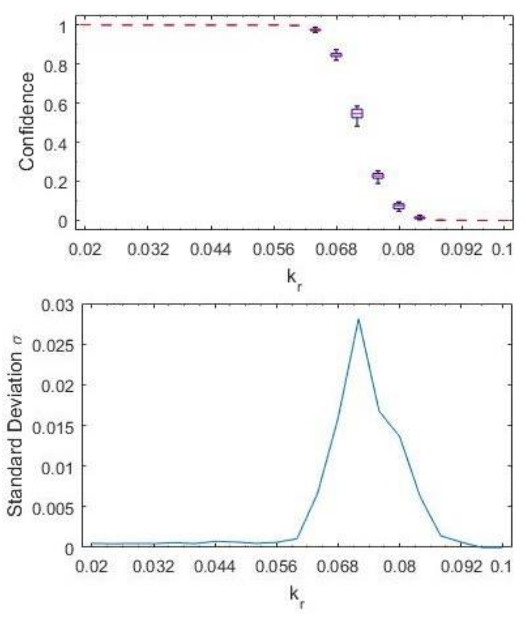
Case Study 1: SIR Model

$$S + I \xrightarrow{k_i} 2I, \; I \xrightarrow{k_r} R, \; \theta = (k_i, k_r)$$

Property to be verified: $\phi = P_{<0.1}[(I > 0)U^{[0,50]}(I = 0)]$



Parameter synthesis region [1]



Confidence calculation & STD

Case Study 2: Signalling in Prokaryotic Cells

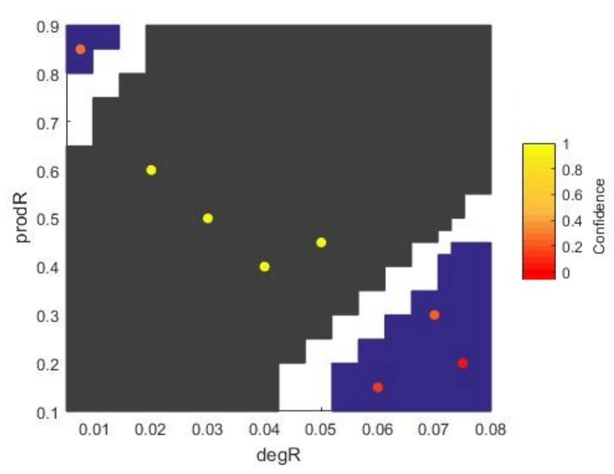
Signalling system contains 9 reactions, resulting in 9 parameters:

$$\theta = (k_1, k_2, k_3, \delta_H, \delta_{H_p}, \delta_R, \delta_{R_p}, \alpha_R, \alpha_H)$$

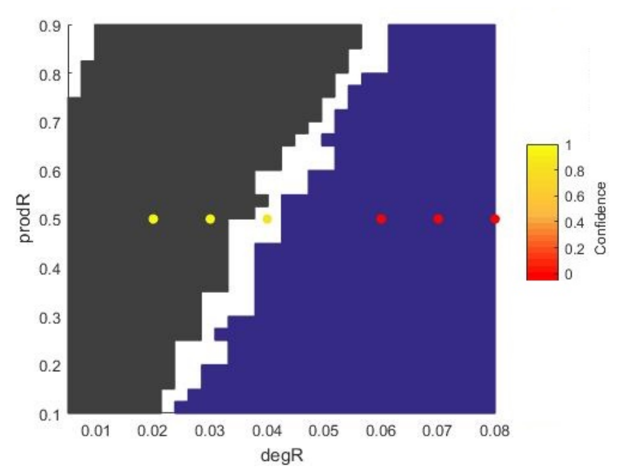
Case I: $\delta_{R_p} = \delta_R$.

Case II: $\delta_{R_p} = 2\delta_R$.

Property to be verified, $\phi = R_{\geq 7}[C^{[\leq 9]}]$

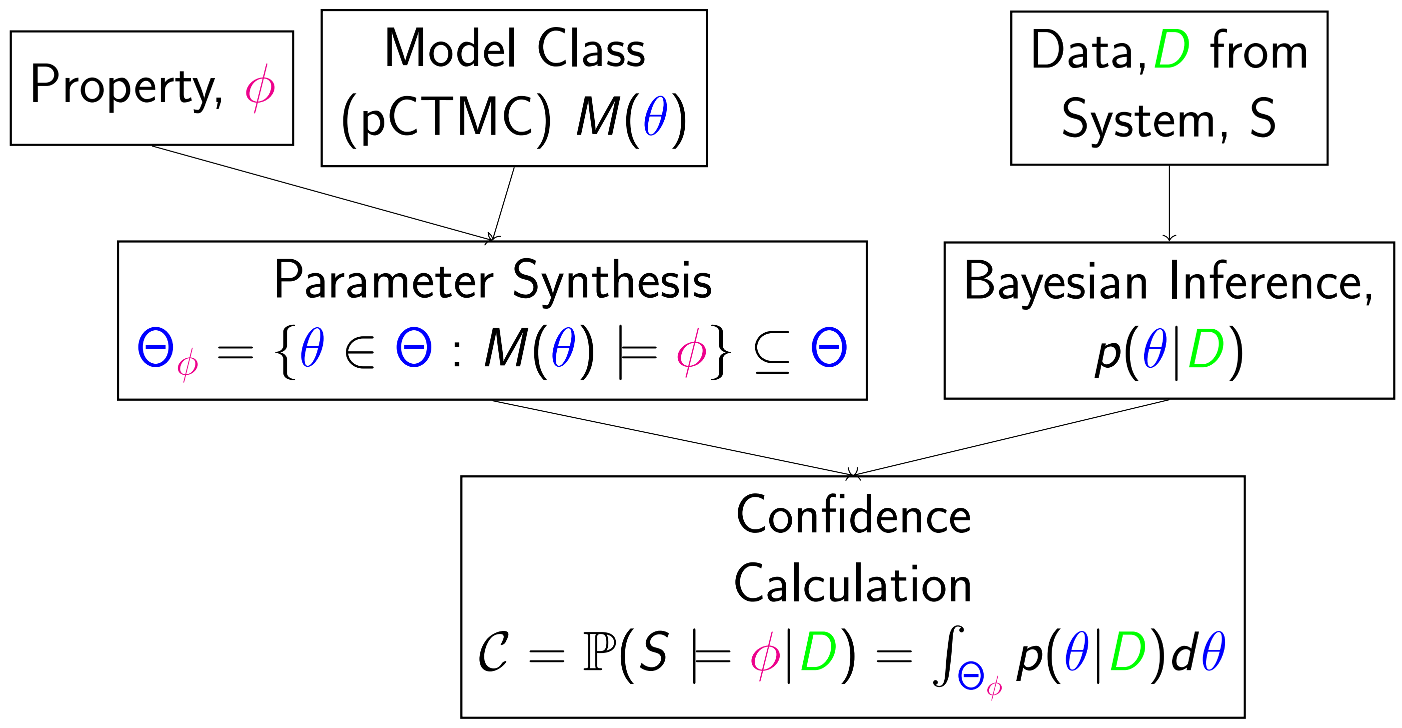


Parameter Synthesis region and sampled points for Case I: $\delta_{R_p} = \delta_R$.



Parameter Synthesis region and sampled points for Case II: $\delta_{R_p} = 2\delta_R$.

Framework

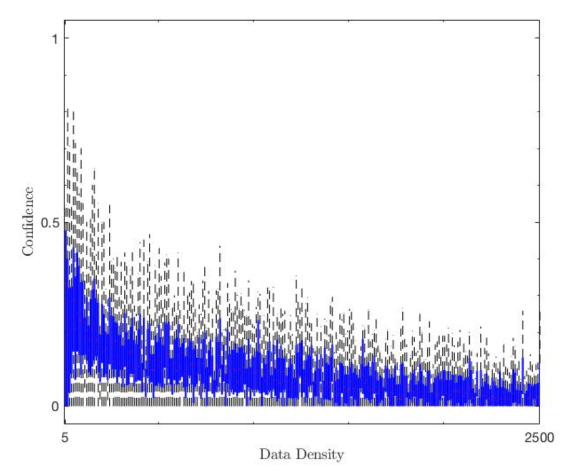


Bayesian Verification Methodology [2]

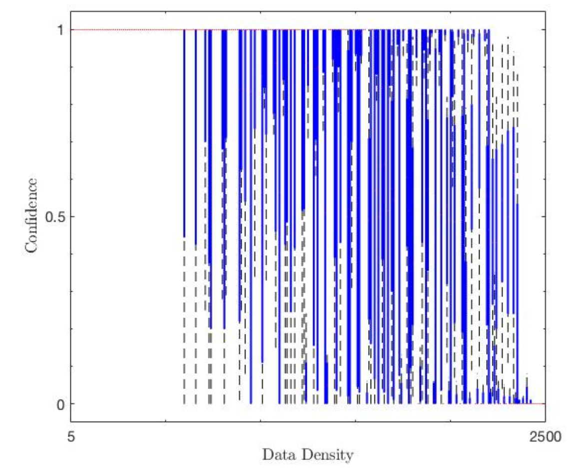
Results

- We can verify the property with a lesser amount of data than SMC whilst simultaneously learning the model.

Case 1: SIR Model

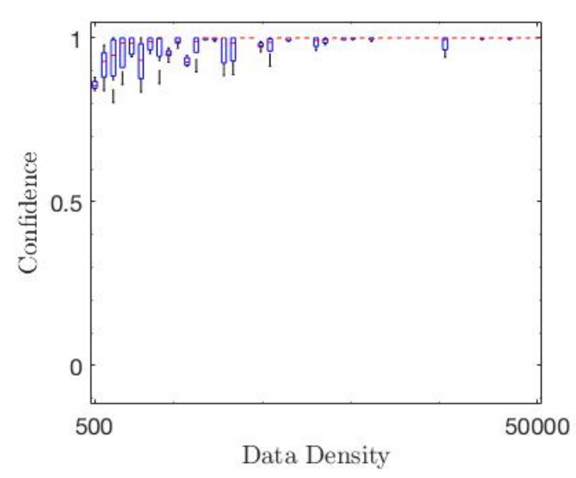


Confidence calculation using Hamiltonian Monte Carlo

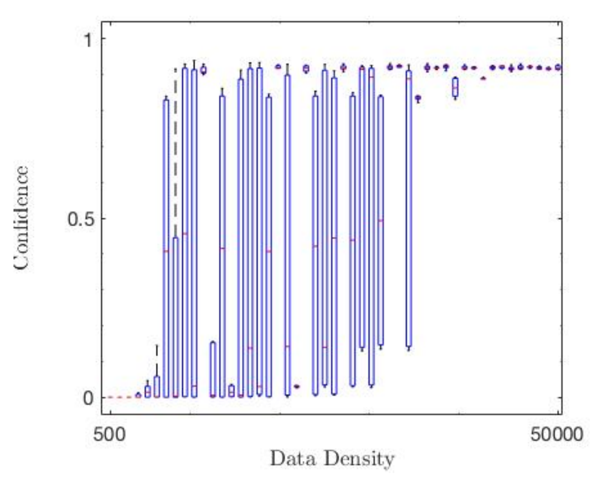


Confidence values using SMC

Case 2: Signalling Model



Confidence calculation using slice sampling



Confidence values using SMC

Future Work

- Working with partially observed data to emulate real data.
- Working with different classes of models such as LNAs and infinite state spaces.
- Compare with more advanced SMC methods.

[1] M. Ceska, P. Pilar, N. Paoletti, L. Brim, and M. Z. Kwiatkowska, "PRISM-PSY: precise gpu-accelerated parameter synthesis for stochastic systems," in *Tools and Algorithms for the Construction and Analysis of Systems - 22nd International Conference, TACAS 2016,ETAPS 2016, Eindhoven, The Netherlands, April 2-8, 2016, Proceedings*, pp. 367–384, 2016.

[2] E. Polgreen, V. B. Wijesuriya, S. Haesaert, and A. Abate, "Data-efficient Bayesian verification of parametric Markov chains," in *Quantitative Evaluation of Systems - 13th International Conference, QEST 2016, Quebec City, QC, Canada, August 23-25, 2016, Proceedings*, pp. 35–51, 2016.

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