

# Bayesian Parameter Synthesis of Markov Population Models.

Master Thesis

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To the complement of this thesis, I would like to describe my deep

## **Abstract**

We present frameworks for data-informed parameter synthesis of Markov population processes. Given statistics data of the population at its steady-state, the object is to synthesize a set of parameters so that a temporal property of interest is satisfied. We design Bayesian frameworks for parameter synthesis in both cases: when the closed form of the interested property is obtainable, and when only simulation is possible. The frameworks are constructed with different sampling and optimization techniques to approximate the posterior distribution. Later, we evaluate the frameworks using different population models of different size using synthetic data generated from a known true parameter. By measuring the distance between synthesized parameters and true parameters and visualize sampled parameter values with their corresponding weights, we show that our frameworks are capable of deriving a set of satisfying parameter values, as well as an estimation which is close to the true parameter.

# Chapter 1

## Introduction

In different areas of research and application, the objects are to study how the number of individuals in a closed environment develop under a certain set of assumptions. For instance

- Number of online nodes in a distributed system.
- Number of surviving individuals in an epidemic model.

Markov population models [22] are finite state-space, stochastic models that is widely used in modeling complex and dynamic systems. In a Markov population model, each state represents the number of individuals. Formally, in a Markov population model whose state space is  $S = (s_1, \dots, s_n)$ , there is a map  $f : S \rightarrow \{0, \dots, N\}$  where  $N \in \mathbf{N}^*$  is the maximum number of individuals in the system.

In a Markov population models, for example Discrete-time Markov Chain, initial and transition probabilities are known a-priori. In order to encompass unknown attributes of a system, we introduce *parametric Markov population models*. In a parametric Markov population model, each transition is a rational function of parameters. As unknown features of the system are represented by parameters, the following research questions are raised

- Given a set of data collected by observing the system, how can we know about its parameters?
- Which values of parameters instantiate a model that satisfies a certain property of interest?

Parameter synthesis is an emerging research direction on probabilistic model checking. Katoen [21] define the parameter synthesis problem for pDTMC as to find a set of parameter values, which satisfy a given reachability property. In this thesis, we combines Bayesian parameter inference and parameter synthesis, so that the result parameters (1) satisfy the property of interest, and (2) likely to produce given steady-state data. Contributions of the thesis are

- Presenting and implementing a data-informed, Bayesian frameworks on parameter synthesis of parametric Discrete-time Markov Chain with different case studies.
- Comparing the performances of optimization methods used to approximate posterior distribution in both cases: closed-form solutions are available and only simulations are possible.
- Evaluating the scalability of the frameworks with different sizes of model state-space.
- **Chapter 1** introduces motivations and goals of this research.
- **Chapter 2** presents the theoretical background on probabilistic model checking, include discrete stochastic models and their corresponding temporal logics.
- **Chapter 3** presents essential concepts on Bayesian inference, including sampling and optimization algorithms.
- **Chapter 4** reviews the state-of-the-art works of other researchers on the problem of parameter synthesis.
- **Chapter 5** present Bayesian parameter synthesis frameworks.
- **Chapter 6** describes case studies and benchmarks presented frameworks under different setups.
- **Chapter 7** conclusion and possible future works.

# Chapter 2

## Probabilistic model checking

We use Discrete-time Markov chain as the formalism to model stochastic population process. In this chapter, we present essential concepts on probabilistic model checking, including probabilistic models and properties. We also briefly present a general deterministic model checking algorithm for a specific temporal logic, namely PCTL. Due to the state space explosion, applying deterministic model checking algorithm is possible to be computationally expensive. Therefore, we also present a simulation based model checking, namely *statistical model checking* for bounded and unbounded path property. Since statistical model checking relies only on simulation of stochastic models, it is advantageous for checking models with large space size. We also introduce definitions of parametric model and parameter synthesis problems, as well as the symbolic computing approach to verify parametric models.

### 2.1 Markov models

#### 2.1.1 Discrete Time Markov chain

Markov models are stochastic models of discrete or continuous time which satisfy memoryless property.

**Definition 2.1.1** (Discrete-time memoryless property)

*Let  $X$  be a random variable of geometric distribution.  $X$  has memoryless property if and only if*

$$Pr(X = t + m | X > m) = Pr(X > m) \forall t, m \in \mathbb{N}, k \geq 1$$



Markov model can be non-deterministic (*Markov Decision Process*). However, in this thesis we consider only Markov models without non-determinism. The following definitions of discrete-time and continuous-time Markov chains follows the definitions presented by Baier [3].

**Definition 2.1.2** (Discrete Time Markov Chain)

A Discrete-time Markov chain (DTMC)  $\mathcal{M}$  is a tuple  $(S, \mathbf{P}, \iota_{init}, AP, L)$ , in which

- $S$  is a countable, non-empty set of states
- $\mathbf{P} : S \times S \rightarrow [0, 1]$  is the transition probability function such that

$$\forall s \in S : \sum_{s' \in S} \mathbf{P}(s, s') = 1$$

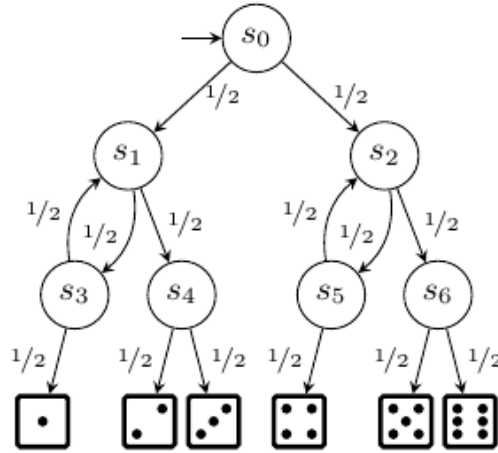
- $\iota_{init} : S \rightarrow [0, 1]$  is the initial distribution such that

$$\sum_{s \in S} \iota_{init}(s) = 1$$

- $AP$  is a set of atomic propositions.
- $L : S \rightarrow 2^{AP}$  is the labelling function on states.

**Example 2.2** (Knuth-Yao die)

Knuth-Yao die to simulate a 6-faced die by a fair coin. In this Knuth's die DTMC, there are 6 BSCCs, each of them represents an outcome of a die tossing. Image taken from [21]



**Definition 2.2.1** (Strongly Connected Component)

Let  $\mathcal{M} = (S, \mathbf{P}, \iota_{init}, AP, L)$  a DTMC. A subset  $S' \subset S$  is strongly connected if and only if for every pair  $s_1, s_2 \in S'$  there is a path between  $s_1$  and  $s_2$  which consists of only of state in  $S'$ . If there exist no  $S'' \subseteq S$ , such that  $S \subset S''$  and  $S''$  is strongly connected, then  $S'$  is a Strongly Connected Component, or SCC in short.

**Definition 2.2.2** (Bottom Strongly Connected Component)

Let  $\mathcal{M} = (S, \mathbf{P}, \iota_{init}, AP, L)$  a DTMC and  $S' \in S$  a Strongly Connected Component.  $S'$  is also a Bottom Strongly Connected Component, or BSCC for short, if and only if there exist no state  $s \in S$  that is reachable from any state in  $S'$ . If  $|S'| = 1$  then  $S'$  is a trivial BSCC. We denote  $BSCC(\mathcal{M}) \in S$  is the set of all BSCCs of  $\mathcal{M}$ .

Intuitively, BSCCs are absorbing; once a path in a DTMC reaches a state in a BSCC, it visits all states in the BSCC infinitely often. It is proven by [3] that any run on a DTMC  $\mathcal{M}$  ends in  $BSCC(\mathcal{M})$  almost surely.

**Theorem 1** (Long-run theorem)

Let  $\mathcal{M} = (S, \mathbf{P}, \iota_{init}, AP, L)$  a DTMC.

$$Pr(\Diamond BSCC(\mathcal{M})) = 1$$

In this thesis we concern the *steady-state distribution* of a DTMC.

**Definition 2.2.3** (Steady-state distribution)

Let  $\mathcal{M} = (S, \mathbf{P}, \iota_{init}, AP, L)$  a DTMC and vector  $v_t$  be a transient state distribution

$$v_t = (Pr(X_t = s_1), \dots, Pr(X_t = s_N)), s_0, \dots, s_N \in S$$

A transient state distribution  $v$  of  $\mathcal{M}$  is a steady-state distribution of  $\mathcal{M}$  if and only if

$$v = vP$$

As a result from long-run theorem, if  $BSCC(\mathcal{M}) \neq \emptyset$  then there exists a steady-state distribution  $v = (Pr(X = s_1), \dots, Pr(X = s_{|S|}))$ , such that

$$\forall 1 \leq i \leq |S| : P[X = s_i] \neq 0 \Leftrightarrow s_i \in BSCC(\mathcal{M})$$

### 2.2.1 Continuous-time Markov chain

The discrete-time memoryless property can also be extended into continuous-time memoryless property. In continuous-time, memoryless property has the following form

**Definition 2.2.4** (Continuous-time memoryless property)

*Let  $X$  be a continuous random variable of exponentially distribution.  $X$  has memoryless property if and only if*

$$Pr(X > t + \delta | X > t) = Pr(X > \delta), \forall t, \delta \in \mathbb{R}_{\geq 0}$$

Based on continuous-time memory less property, we introduce the definition of *Continuous-time Markov chain* [20].

**Definition 2.2.5** (Continuous-time Markov chain)

*A Continuous-time Markov chain (CTMC)  $\mathcal{C}$  is a tuple  $(S, \mathbf{P}, \mathbf{r}, \iota_{init}, AP, L)$*

- $S$  is a countable, non-empty set of states
- $\mathbf{P} : S \times S \rightarrow [0, 1]$  is the transition probability function such that

$$\forall s \in S : \sum_{s' \in S} \mathbf{P}(s, s') = 1$$

- $\mathbf{r} : S \rightarrow \mathbb{R}_{>0}$  is the exit rate function such that

$$\forall s \in S : \sum_{s' \in S} \mathbf{P}(s, s') = 1$$

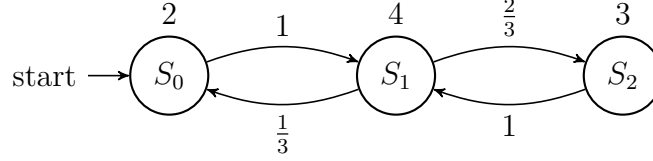
- $\iota_{init} : S \rightarrow [0, 1]$  is the initial distribution such that

$$\sum_{s \in S} \iota_{init}(s) = 1$$

- $AP$  is a set of atomic propositions
- $L : S \rightarrow 2^{AP}$  is the labelling function on states.

**Example 2.3** (CTMC)

An example of a CTMC with 3 states.



Continuous-time Markov chain has a wide range of applications, especially in bioinformatics where chemical reaction network [12] [2]. However, the frameworks in this thesis apply for discrete-time Markov models, thus we do not use continuous-time Markov chain to model systems of interest directly. Instead, we do not use Continuous-time Markov models directly. Instead, we transform CTMCs into DTMCs through uniformization [21]

**Definition 2.3.1** (CTMC Uniformization)

Let  $\mathcal{C} = (S, \mathbf{P}, \mathbf{r}, \iota_{init}, AP, L)$  be a CTMC. We define the uniformization rate  $r$  such that

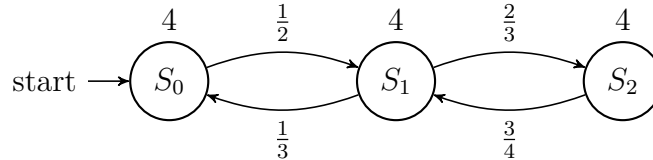
$$\forall s \in S : r \geq \mathbf{r}(s), r \in \mathbb{R}_{>0}$$

The uniformized CTMC  $\text{unif}(r, \mathcal{C}) = (S, \bar{\mathbf{P}}, \bar{\mathbf{r}}, \iota_{init}, AP, L)$  such that

$$\forall s \in S : \bar{\mathbf{r}}(s) = \begin{cases} \frac{\mathbf{r}(s)}{r} \mathbf{P}(s, s') & \text{if } s \neq s' \\ \frac{\mathbf{r}(s)}{r} \mathbf{P}(s, s') + 1 - \frac{\mathbf{r}(s)}{r} & \text{if } s = s' \end{cases}$$

**Example 2.4** (Uniformized CTMC)

We uniformize the CTMC in Example 2.3 by uniformization rate  $r = 4$ .



It has been shown by Katoen [20] that uniformization preserves the transient probability distributions. Furthermore, in this thesis we concern steady state data and state property, thus uniformizing exit rate does not affect the validity of our constructed frameworks.

## 2.5 Property specification

### 2.5.1 Probabilistic Computational Tree Logic

Model checking verifies a formalism of a system (*model*) against a property of interest. We formalize a property by a *temporal logic*, specifically *Probabilistic Computational Tree Logic* (or *PCTL*). Firstly introduced by Clarke et al. [7], PCTL is widely used in model checking of discrete-time stochastic models and supported by most probabilistic model checking tools [10], [23].

**Definition 2.5.1** (PCTL)

*The syntax of PCTL consists of state formulas and path formulas.*

- *State formulas are defined over AP*

$$\Phi ::= \text{true} \mid a \mid \Phi \mid \Phi_1 \wedge \Phi_2 \mid \Phi_1 \vee \Phi_2 \mid P_J(\phi)$$

where  $a \in AP$ ,  $\phi$  is a path formula, and  $J \subseteq [0, 1]$  is an interval.

- *Path formulas*

$$\phi ::= \bigcirc \Phi \mid \Phi_1 \mathbf{U} \Phi_2 \mid \Phi_1 \mathbf{U}^{\leq n} \Phi_2$$

where  $\Phi, \Phi_1, \Phi_2$  are state formulas, and  $n \in \mathbb{N}$ .

PCTL properties is applicable on discrete-time stochastic models such as DTMC, as the times between state transitions are uniform. In a DTMC, a PCTL state formula is verified at each state, while a PCTL path formula is verified through a trace from an execution path.

The algorithm to model check DTMC against PCTL properties is described in detail in Katoen [3]. Given a DTMC  $\mathcal{M}$  and a PCTL property  $\Phi$ , general algorithm for checking  $\mathcal{M} \models \Phi$  has complexity of polynomial to  $|\mathcal{M}|$  and linear to  $|\Phi|$  [20].

**Theorem 2** (Complexity of checking a DTMC against a PCTL formula.)  
*For finite DTMC  $\mathcal{M}$  and PCTL state-formula  $\Phi$ , the PCTL model-checking problem can be solved in time*

$$\mathcal{O}(\text{poly}(\text{size}(D) \cdot n_{\max} \cdot |\Phi|))$$

where

$$n_{\max} = \begin{cases} \max(n | (\Psi_1 \mathbf{U}^{\leq n} \Psi_2) \text{ occurs in } \Phi) \\ 1 \text{ if } \Phi \text{ contains no bounded until property} \end{cases}$$

## 2.5.2 State explosion problem

The soundness of the model checking relies heavily on how the system is modeled. In fact, the model checking is only as sound and valid as the model.

1. Which formalism is used?
2. How the system is encoded into states and transitions?

For example, we consider a distributed software system, in which a *global state* is a composition of

1. values of all variables, and
2. states of all communication channels.

It is obvious that the number of possible states grows exponentially as more variables and communication channels are added to the system.

*State-explosion problem* occurs when the size of the system state space grows exponentially as the number of state variables in the system increases [6]. As discussed before, the complexity of model checking a PCTL property against a DTMC model is polynomial to the DTMC's state-space. However, the state-explosion problem renders model checking computationally expensive. One possible way to cope with state-explosion problem and to reduce the computational cost is to use *statistical model checking*.

## 2.6 Statistical Model checking

Statistical model checking is a simulation-based approach to model check a stochastic model  $\mathcal{M}$  against a temporal property  $\Phi$ . The essential concept of probabilistic model checking is to simulate  $N$  traces from  $\mathcal{M}$ , verify if each trace satisfies  $\Phi$ , then estimate probability  $P(\mathcal{M} \models \Phi)$  by a statistical, frequentist approach.

In statistical model checking of, different methods are applied to *quantitative* and *qualitative* questions.<sup>1</sup> Given a stochastic model  $\mathcal{M}$  and a property  $\Phi$ , statistical model checking solves the following problems:

1. **Quantitative:** Estimate the probability  $p = Pr(\mathcal{M} \models \Phi)$ . In other words, it checks  $\mathcal{M}$  the property

$$P_{=?}(\Phi)$$

2. **Qualitative:** Decide if  $p = Pr(\mathcal{M} \models \Phi)$  is greater or less than a threshold  $\epsilon$ . In other words, it checks  $\mathcal{M}$  the property

$$P_J(\Phi)$$

where  $J \subseteq [0, 1]$  is an interval.

### 2.6.1 Statistical model checking of quantitative properties.

Given an approximation  $\epsilon$  and a confidential level  $\alpha$ , we estimate  $\hat{p}$  as an estimation of  $p$  such that

$$Pr(|p - \hat{p}| \leq \epsilon) \geq 1 - \alpha$$

How many simulations must be performed? As verifying a simulation trace against a reachability property  $\Phi$  is Bernoulli trial (satisfied or not satisfied), the number of simulation  $N$  can be estimated using different bounds, such as Chernoff-Hoeffding bound [5]. Let  $Sat(N)$  be number of satisfying trace

---

<sup>1</sup><https://www-verimag.imag.fr/Statistical-Model-Checking-814.html#nb3>

in  $N$  sampled traces, applying Chernoff-Hoeffding inequality gives

$$\begin{aligned} P(|\frac{Sat(N)}{N} - p| > \epsilon) &\leq 2 \exp \frac{-N\epsilon^2}{4} \\ \Leftrightarrow P(|\frac{Sat(N)}{N} - p| \leq \epsilon) &\geq 1 - 2 \exp \frac{-N\epsilon^2}{4} \end{aligned}$$

Replace  $\alpha = 2 \exp \frac{-N\epsilon^2}{4}$  and  $\hat{p} = \frac{Sat(N)}{N}$ , we have

$$\begin{aligned} P[|\hat{N} - p| \leq \epsilon] &\geq 1 - 2\alpha \\ \Leftrightarrow N &\geq 4 \frac{\log \frac{2}{\alpha}}{\epsilon^2} \end{aligned}$$

The estimation algorithm is described in detail in [1].

---

**Algorithm 1** Statistical Model Checking, Approximate Probabilistic Model Checking method.

---

```

1: procedure SMC-APMC
2:    $N \leftarrow 4 \frac{\log \frac{2}{\alpha}}{\epsilon^2}$ 
3: end procedure

```

---

## 2.6.2 Statistical model checking of qualitative properties.

Estimation of number of simulation  $N$  in this case is slightly more complicated.

---

**Algorithm 2** SPRT Statistical Model Checking

---

```

1: procedure SMC-SPRT
2: end procedure

```

---

## 2.7 Parametric model

We introduce parameters to formalize unknown attributes of the system.

**Definition 2.7.1** (Polynomial ring)

*Given a tuple  $\mathbf{x} = (x_1, \dots, x_n)$  be a tuple*



**Definition 2.7.2**

*Rational functions* Let  $\mathbf{x} = \{x_1, \dots, x_n\}$  be a variable; let  $\mathbf{Pol}[\mathbf{x}]$  be the set of all polynomial functions over  $\mathbf{x}$ . A rational function  $h(\mathbf{x})$  is defined as following.

$$h(\mathbf{x}) := \frac{f(\mathbf{x})}{g(\mathbf{x})}, f, g \in \mathbf{Pol}[\mathbf{x}], g(\mathbf{x}) \neq 0$$

We denote  $\mathbb{Q}(\mathbf{x})$  the set of all rational functions over  $\mathbf{x}$ .

**2.7.1 Parametric Discrete Time Markov chain**

With the set of rational functions formally defined, we define parametric Discrete-time Markov chain based the definition on [19].

**Definition 2.7.3** (Discrete Time Markov Chain)

A Discrete-time Markov chain (DTMC) is a tuple  $(S, \mathbf{x}, \mathbf{P}, \iota_{init}, AP, L)$  where

- $S$  is a countable, non-empty set of states
- $\mathbf{x} \in \mathbb{R}^n, n \in \mathbb{N}$  as the set of  $n$  real parameters.
- $\mathbf{P} : S \times S \rightarrow \mathbb{Q}(\mathbf{x})$  is the transition probability function such that

$$\forall s \in S : \sum_{s' \in S} \mathbf{P}(s, s') = 1$$

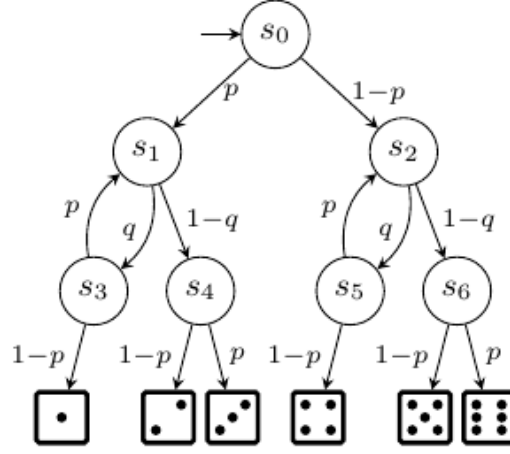
- $\iota_{init} : S \rightarrow [0, 1]$  is the initial distribution such that

$$\sum_{s \in S} \iota_{init}(s) = 1$$

- $AP$  is a set of atomic propositions
- $L : S \rightarrow 2^{AP}$  is the labelling function on states.

**Example 2.8** (Parametric Knuth-Yao die)

A Knuth-Yao die to simulate a 6-faced die by two unfair coins with probability of one side  $p$  and  $q$ . Image taken from [21].



Given a parametric Discrete-time Markov chain  $\mathcal{M}_\theta$ . A concrete assignment of parameter  $\theta$  *instantiates* a non-parametric Discrete-time Markov chain if  $f\theta$  evaluates to a real value for all  $f \in \mathbf{P}$ .

### 2.8.1 Symbolic model checking of pDTMC

Symbolic model checking is mentioned on [9].

#### Example 2.9

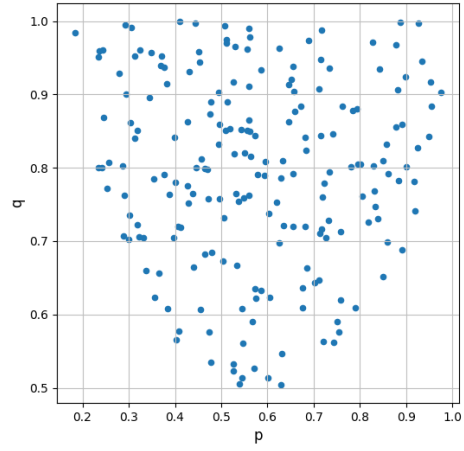
*Parametric Knuth's die* We continue the example with Knuth die model  $\mathcal{M}_p$ . Assume the

$$\begin{aligned}
 P(F \text{ "1"}) &= (p^2 * q + (-1) * p * q) / (p * q + (-1)) \\
 P(F \text{ "2"}) &= ((p)^2 * (q + (-1))) / (p * q + (-1)) \\
 P(F \text{ "3"}) &= (-1 * ((p) * (p + (-1)) * (q + (-1)))) / (p * q + (-1)) \\
 P(F \text{ "4"}) &= (-1 * (p^2 * q + (-1) * p * q)) / (p * q + (-1) * p + 1) \\
 P(F \text{ "5"}) &= (p^2 * q + (-2) * p * q + q) / (p * q + (-1) * p + 1) \\
 P(F \text{ "6"}) &= (-1 * ((p + (-1))^2 * (q + (-1)))) / (p * q + (-1) * p + 1)
 \end{aligned}$$

### 2.9.1 Parameter synthesis of pDTMC

#### Example 2.10

Given a pDTMC of Knuth die  $\mathcal{M}_{(p,q)}$ ,  $(p, q) \in [0, 1] \times [0, 1]$  and a reachability property  $\Phi = P_{\geq 0.2}[F \text{ "one"}]$ , synthesize parameter  $p$  so that  $\mathcal{M}_p \models \Phi$ . A simple Monte-Carlo search on parameter space gives the following satisfying point:



### 2.10.1 Summary

# Chapter 3

## Bayesian inference

We present essential concepts in Bayesian parameter inference and several methods to estimate posterior distribution. The methods range from posterior conjugations, in which tractability is guaranteed as we know the analytic form of both likelihood and prior distribution. Afterwards, we discuss different sampling algorithm to approximate the posterior distribution when no conjugations are available. We also present a likelihood-free method to exploit in the case that the analytical form of the likelihood is not achievable or is too complex to evaluate. The sampling algorithms presented in this chapter are the building block for the Bayesian frameworks that we present in this thesis.

### 3.1 Bayesian inference

#### 3.1.1 Bayesian formula

Let  $D_{obs}$  be observed data. In statistical inference, we assume that the observed data has a probability distribution of unknown parameter  $\theta$ , i.e  $D_{obs} \sim P(D_{obs}|\theta)$ . In frequentist approach, the estimation of  $\theta$  based on long-run property, that is, given a large enough sample size, expected value of parameter estimation  $\hat{\theta}$  is equal to  $\theta$ . Therefore, frequentist approach requires to gather a large amount of data to deliver a close estimation  $\hat{\theta}$ . The main advantage of Bayesian approach over frequentist approach is that it require less data to obtain an estimation  $\hat{\theta}$ .

In Bayesian approach, we use the information gained from previously ob-

served data (*beliefs*) to enhance the accuracy of the estimation of  $\hat{\theta}$ . The beliefs obtained from prior knowledge of model parameter  $\theta$  is represented by *prior distribution*  $\pi(\theta)$ . We have the *likelihood*  $P(D_{obs}|\theta)$  as the probability distribution over observed data, given parameter  $\theta$ . The Bayesian formula states that

$$\pi(\theta|D_{obs}) = \frac{P(D_{obs}|\theta)\pi(\theta)}{\int_{\theta} P(D_{obs}|\theta)\pi(\theta)d\theta}$$

$\int_{\theta} P(D_{obs}|\theta)\pi(\theta)d\theta$  is the *marginal distribution*.  $\pi(\theta|D_{obs})$  is the *posterior distribution*. To compute posterior distribution is the essential part of Bayesian inference, since it gives the estimation of parameter  $\theta$ .

### 3.1.2 Bayesian parameter estimation

With posterior distribution  $\pi(\theta|D)$  we estimate the parameter  $\hat{\theta}$  using Bayesian posterior mean.

$$\hat{\theta} = \mathbf{E}[\theta] = \int_{\theta} \theta \pi(\theta|D) d\theta$$

In case we have samples from posterior distribution, for example the *Trace* from Metropolis-Hastings algorithm, for example when we use MH algorithm, the discrete form of posterior mean is used:

$$\hat{\theta} = \mathbf{E}[\theta] = \sum_{\theta} \theta \pi(\theta|D)$$

**Definition 3.1.1** (Bayesian Credible Set)

Set  $C$  is a  $(1-\alpha)100\%$  credible set for the parameter  $\theta$  if the posterior probability for  $\theta$  to belong to  $C$  equals  $(1-\alpha)$ .

$$P(\theta \in C|D) = \int_C \pi(\theta|D) d\theta = 1 - \alpha$$

In this thesis, we use by default 0.95 credible set, which corresponds to  $\alpha = 0.05$

**Definition 3.1.2** (Highest Posterior Density credible set)

*Highest Posterior Density*  $(1 - \alpha)100\%$  credible set (HPD for short) is the interval with minimum length over all Bayesian  $(1 - \alpha)100\%$  Credible Set.

In this research, the HPD is calculated using algorithm from *PyMC3* library [27]. For simplicity, we assume that in all cases which we concern, HPD is computed for unimodal distribution.

---

**Algorithm 3** Compute Highest Posterior Density Interval

---

**Input:**  $S$  is samples from a distribution.

**Input:**  $0 \leq \alpha \leq 1$

**Output:** HPD interval

- 1: **procedure** COMPUTE HPD( $S$ )
  - 2:     Compute interval width  $w = |S| * \alpha$
  - 3:     Find modal (peak) of sample points.
  - 4:     Return minimal interval of size  $|S| - w$  which contains the modal.
  - 5: **end procedure**
- 

### 3.1.3 Selection of prior distribution

Theoretically, prior can be of any distribution family. However, a selection of prior distribution that is too different than the actual distribution of parameter can leads to a false propagation of beliefs and degrade inference results. It is suggested by [26] that in case of no prior knowledge exists to help the selection of prior distribution, Uniform distribution is preferable since it is less likely to propagate false beliefs to the inference.

A systematic inference to select prior distribution family and prior distribution parameter (hyperparameters) is possible with *Hierarchical Bayes Models* [1].

### 3.1.4 Estimation of posterior distribution

In posterior estimation the following factors are important:

1. Tractability: we have analytical form of posterior distribution.
2. Computationally effective: updating model parameter is of linear time to the dimension of parameter.

### Posterior conjugation

Conjugated posteriors are special cases of Bayesian inference, in which the prior and posterior distribution belongs to the same family of distribution.

We consider two conjugated posterior: Binomial-Beta and Dirichlet-Multinomial

**Lemma 3** (Binomial-Beta Conjugation)

*Binomial distribution is conjugated to beta distribution.*

*Proof.* The observed data  $D = (x_1, \dots, x_n)$  is sampled from *Binomial*( $k, \theta$ ) function

$$P(D|\theta) = \prod_{i=1}^n \binom{k}{x_i} \theta^{x_i} (1 - \theta)^{k-x_i}$$

The parameter  $\theta$  is of *Beta*( $\alpha, \beta$ ) distribution

$$\pi(\theta) = \theta^{\alpha-1} (1 - \theta)^{\beta-1}$$

We obtained:

$$\begin{aligned} \pi(\theta|D) &\sim P(D|\theta)\pi(\theta) \\ &\sim \theta^{\sum_{i=1}^n x_i} (1 - \theta)^{nk - \sum_{i=1}^n x_i} \theta^{\alpha-1} (1 - \theta)^{\beta-1} \\ &= \theta^{\alpha-1 + \sum_{i=1}^n x_i} (1 - \theta)^{\beta-1 + nk - \sum_{i=1}^n x_i} \end{aligned}$$

Thus, the posterior is *Beta*( $\alpha + \sum_{i=1}^n x_i, \beta + nk - \sum_{i=1}^n x_i$ ) □

Generalize this conjugation, we also have Multinomial-Dirichlet conjugation.

**Lemma 4** (Multinomial-Dirichlet Conjugation)

*Multinomial distribution is conjugated to Dirichlet distribution.*

*Proof.* The observed data  $D = (x_1, \dots, x_n)$  is sampled from *Multinomial*( $n; \theta_1, \dots, \theta_n$ ) function

$$P(x_1, \dots, x_n | N, \theta_1, \dots, \theta_n) = \frac{n!}{x_1! \dots x_n!} \prod_{i=1}^n \theta_i^{x_i}$$

The parameter  $(\theta_1, \dots, \theta_n)$  is *Dirichlet*( $\alpha_1, \dots, \alpha_n$ )

$$\pi(\theta_1, \dots, \theta_n) = \frac{1}{\mathbf{B}(\alpha_1, \dots, \alpha_n)} \prod_{i=1}^n \theta_i^{\alpha_i-1}$$

We obtain

$$\begin{aligned}
\pi(\theta_1, \dots, \theta_n | D) &\sim P(D | \theta) \pi(\theta) \\
&\sim \prod_{i=1}^n \theta_i^{x_i} \prod_{i=1}^n \theta_i^{\alpha_i - 1} \\
&\sim \prod_{i=1}^n \theta_i^{\alpha_i - 1 + \sum_{i=1}^n x_i}
\end{aligned}$$

Thus, the posterior is *Dirichlet*( $\alpha_1 + x_1, \dots, \alpha_n + x_n$ ) □

More detailed description in these cases can be found in [29] and [4]. We summarize the necessary results in the following table:

Likelihood	Prior	Posterior parameters
$Binomial(n, k)$	$Beta(\alpha, \beta)$	$\alpha' = \alpha + \sum_{i=1}^n x_i$ $\beta' = \beta + nk - \sum_{i=1}^n x_i$
$Multinomial(n; \theta_1, \dots, \theta_n)$	$Dirichlet(\alpha_1, \dots, \alpha_n)$	$\alpha'_i = \alpha_i + x_i, 1 \leq i \leq n$

However, posterior conjugation is applicable to a subset of prior and likelihood functions. In Bayesian inference, it is usual that the posterior distribution has no analytical form or its analytical form is difficult to directly sample from. In these cases, we can use several different sampling and optimization methods to approximate the posterior distribution. In the following section we discuss different approaches for posterior distribution approximation:

- Markov chain Monte-Carlo.
- Sequential Monte-Carlo.
- Approximate Bayesian Computation.

### Markov chain Monte-Carlo

In case the posterior distribution has no analytical form or its analytical form is difficult to sample from directly, we use *Metropolis-Hastings* algorithm (*MH* in short).



Metropolis-Hastings algorithm is a *Monte Carlo Markov Chain* algorithm. In its essential, Metropolis-Hastings algorithm draws sample from an unknown distribution. Using the MH algorithm, we can estimate the parameter by posterior mean, without knowing the analytical form of posterior distribution itself.

---

**Algorithm 4** Metropolis-Hastings Algorithm

---

**Input:**

- $D$  is the observation data

**Output:** *Trace* is the set of accepted sampling point.

```

1: procedure METROPOLIS-HASTINGS( $D$ , maxIteration)
2:   Select a proposal distribution  $\pi(\theta)$ 
3:   Draw a random initial point  $\theta$ 
4:   Init empty trace Trace
5:   while maxIteration not reached do
6:      $L \leftarrow P(D|\theta)$ 
7:     Draw a point  $\theta'$  from the proposal distribution.
8:      $L' \leftarrow P(D|\theta')$ 
9:     if  $\ln(L') - \ln(L) > 0$  then
10:      Add  $\theta'$  to Trace
11:       $\theta = \theta'$ 
12:   else
13:     Draw a random number  $x$  from Uniform(0,1)
14:     if  $x \leq \xi$ , ( $\xi$  very small, e.g  $10^{-8}$ ) then
15:       Add  $\theta'$  to Trace (avoiding local maxima)
16:        $\theta = \theta'$ 
17:     end if
18:   end if
19: end while
20: end procedure

```

---

The likelihood function can be implemented as log-likelihood to avoid underflow error. Proposal distribution defines how do we proceed to the next parameter value on the parameter space; it can be of any distribution family.

There are two advantages of using Markov Chain Monte Carlo in Bayesian

inference:

1. Parameter transition only needs the computation of likelihood function. Therefore, Monte Carlo Markov Chain can be used in general Bayesian inference, in which we are not guaranteed to have an analytical form of posterior.
2. Specifically in Metropolis-Hastings algorithm, marginal distribution is cancelled out, thus make Metropolis-Hastings a computationally efficient algorithm.

However, MH algorithm also has a drawback; its convergence becomes slower as the dimension of parameter  $\theta$  increases.

### **Sequential Monte-Carlo**

Sequential Monte-Carlo method is firstly proposed by [11]. Instead of having one particle moving in its parameter space, Sequential Monte-Carlo estimates by using  $N$  particles moving independently. Therefore Sequential Monte-Carlo method has a significant advantage of easily parallelizable.

here [8]

---

**Algorithm 5** Sequential Monte-Carlo Algorithm

---

**Input:**

- $D$  is the observation data

**Output:**  $Trace$  is the set of accepted sampling point.

```
1: procedure METROPOLIS-HASTINGS( $D$ , maxIteration)
2:   Select a proposal distribution  $\pi(\theta)$ 
3:   Draw a random initial point  $\theta$ 
4:   Init empty trace  $Trace$ 
5:   while maxIteration not reached do
6:      $L \leftarrow P(D|\theta)$ 
7:     Draw a point  $\theta'$  from the proposal distribution.
8:      $L' \leftarrow P(D|\theta')$ 
9:     if  $\ln(L') - \ln(L) > 0$  then
10:      Add  $\theta'$  to  $Trace$ 
11:       $\theta = \theta'$ 
12:   else
13:     Draw a random number  $x$  from  $Uniform(0, 1)$ 
14:     if  $x \leq \xi$ , ( $\xi$  very small, e.g  $10^{-8}$ ) then
15:       Add  $\theta'$  to  $Trace$  (avoiding local maxima)
16:        $\theta = \theta'$ 
17:     end if
18:   end if
19: end while
20: end procedure
```

---

Selection of kernel function for SMC is mentioned in [28].

### Approximate Bayesian Computation

The methods mentioned before is used with an assumption that the likelihood  $P(D_{obs}|\theta)$  has an analytical form; the analytical can be evaluated without introducing computational burden. However there are situations in which the likelihood has no analytical form, or the analytical form is expensive to be evaluated. In such cases, a class of different methods, dubbed *likelihood-free* methods, are used. Likelihood-free methods in Bayesian inference means that instead of compute the likelihood  $P(D|\theta)$ , we estimate it or replace it

by other measures. Approximate Bayesian Computation is a widely used likelihood-free method for approximating posterior distribution. Instead of estimating the likelihood  $P(D|\theta)$  directly, we sample a observable data set  $\hat{D}$  and define a distance measure  $\delta(D, \hat{D})$ . Approximate Bayesian Computation accepts a set of tuples  $(\hat{\theta}, \hat{D})$ , each satisfies that  $\delta(D_{obs}, D_{sim}) < \epsilon, \epsilon \in \mathbf{R}_{\leq 0}$ .

---

**Algorithm 6** Approximate Bayesian Computation

---

**Input:**

- $D_{obs}$ : observed data for Bayesian inference or its summary statistic  $S_{obs}$
- $\theta = (\theta_1, \dots, \theta_k)$ :  $k$ -dimensional model parameter.
- $\pi(\theta)$ : prior distribution on  $\theta$ .
- $N$ : number of particles (parameter samples).
- $\epsilon$ : absolute error threshold.

**Output:**

- $(\theta_1, \dots, \theta_N)$ :  $N$  sampled particles.
- $(\omega_1, \dots, \omega_N)$ : corresponding weights of sampled particles.

```

1: procedure APPROXIMATE-BAYESIAN-COMPUTATION( $D, \theta, \pi(\theta), N, \epsilon$ )
2:    $t := 0$ 
3:   while  $t \leq N$  do
4:     end while
5: end procedure

```

---

## 3.2 Summary

We present a set of optimization and approximation methods which are essentials to Bayesian Inference. In the following chapter we propose a data-driven approach for parameter synthesis combining Approximate Bayesian computation, Sequential Monte Carlo, and Statistical Model Checking.

# Chapter 4

## Related works

[18] [26]

[25] [24]

Polgreen et al [26] presents a method for bayesian inference of pMC parameters in [14]

[23]

The definition and model checking of DTMC and pMC is studied by [3], [17], and [21].

Bayesian inference of pMC parameters is studied in [26] and . In , the authors developed methods to synthesize parameters to satisfy a given set of PCTL properties. In [18], the authors presented methods to perform model checking of biological system using Bayesian statistic. The authors in [18] uses a Bayesian hypothesis test, where  $H_0$  is the null hypothesis that the model satisfies a PCTL  $P$ , and alternative hypothesis  $H_1$  is that the system does not satisfies  $P$ . Similar approach to the parameter estimation in this project is described by [16].

In this project, we use bee colony model semantics from [15]. The methods and implementation in this project is designed to extend the results of [15] and its tool *DiPS*

storm drawback: it does not support

In [24] the author introduces the same approach but it is to use on CSL properties and CTMC.

## Chapter 5

# Bayesian frameworks for parameter synthesis.

We present frameworks for data-informed parameter synthesis of pDTMC. The frameworks are designed to synthesize a set of parameter values so that for each value, the instantiated model satisfies the interested property, as

Given a pDTMC model  $\mathcal{M}_\theta$ , a PCTL property  $\Phi$ , and observed data  $D_{obs}$ , the frameworks synthesize a set of  $N$  parameters  $(\theta_1, \dots, \theta_N)$  such that

$$\forall i \in [1, N] : \mathcal{M}_{\theta_i} \models \Phi$$

each

## 5.1 General framework for parameter synthesis

---

**Algorithm 7** Markov chain Monte-Carlo with rational functions

---

**Input:**

- $\mathcal{M}_\theta$ : parametric Discrete-Time Markov chain of parameter  $\theta$
- $\Phi$ : bounded reachability property of interest.

**Output:**

- $(\theta_1, \dots, \theta_{N_{MH}})$ :  $N_{MH}$  sampled particles.
- $(w_1, \dots, w_{N_{MH}})$ : corresponding weights of sampled particles.

1: **procedure** RF-MCMC

2: **end procedure**

---

### 5.1.1 Model checking of parametric models

First way to

---

**Algorithm 8** Markov chain Monte-Carlo with rational functions

---

**Input:**

- $\mathcal{M}_\theta$ : parametric Discrete-Time Markov chain of parameter  $\theta$
- $\Phi$ : bounded reachability property of interest.

**Output:**

- $(\theta_1, \dots, \theta_{N_{MH}})$ :  $N_{MH}$  sampled particles.
- $(w_1, \dots, w_{N_{MH}})$ : corresponding weights of sampled particles.

1: **procedure** RF-MCMC

2: **end procedure**

---

---

**Algorithm 9** Markov chain Monte-Carlo with rational functions

---

**Input:**

- $\mathcal{M}_\theta$ : parametric Discrete-Time Markov chain of parameter  $\theta$
- $\Phi$ : bounded reachability property of interest.

**Output:**

- $(\theta_1, \dots, \theta_{N_{MH}})$ :  $N_{MH}$  sampled particles.
- $(w_1, \dots, w_{N_{MH}})$ : corresponding weights of sampled particles.

1: **procedure** RF-MCMC

2: **end procedure**

---

*Rational functions* are functions of model parameter that represent the probability of finally globally reach each terminal state. The function is delivered by PRISM model checker thanks to its capability of symbolic model checking [KNP11].

However, it is not always possible to deduct rational functions from a given model, due to the technical limitation (time, memory) and the limitation of PRISM itself. In our conducted experiment, PRISM is capable of deliver rational functions up to a population of 15 bees. For a population of more bees, we use the second approach, *DTMC sampling*.

DTMC sampling has advantages over rational function. First, it is less computationally expensive to evaluate a parametric DTMC thanks to its simpler symbolic expression. Second, DTMC sampling is *parallelizable*; sampling can be done with as many processor cores as possible. The second advantage makes DTMC sampling *scalable*, compare to the rational function evaluation approach, which is not scallable due to its nature of deep recursion.

## 5.2 Bayesian parameter synthesis with rational functions



As we have analytical form for both target property and likelihood function, we can propose a Markov chain Monte-Carlo algorithm. In this case we use Metropolis-Hastings algorithm, with rational function evaluation and model checking is performed before the calculation of acceptance rate.

---

**Algorithm 10** Markov chain Monte-Carlo with rational functions

---

**Input:**

- $\mathcal{M}_\theta$ : parametric Discrete-Time Markov chain of parameter  $\theta$
- $\Phi$ : bounded reachability property of interest.
- $\pi(\theta)$ : prior distribution on  $\theta$ .
- $N_{MH}$ : length of particle trace.
- $Q(\theta^t|\theta^{t-1})$ : transition kernel.
- $D_{obs}$ : observed data.
- $P(D_{obs}|\theta)$ : likelihood function.

**Output:**

- $(\theta_1, \dots, \theta_{N_{MH}})$ :  $N_{MH}$  sampled particles.
- $(w_1, \dots, w_{N_{MH}})$ : corresponding weights of sampled particles.

```

1: procedure RF-MCMC
2:    $sat \leftarrow False$ 
3:   while  $sat = False$  do
4:     Draw  $\theta_{cand}$  from  $\pi(\theta)$ 
5:     Evaluate  $val \leftarrow RF_\Phi(\theta)$ 
6:     if  $val$  satisfies the boundary of  $\Phi$  then
7:        $sat \leftarrow True$ 
8:     end if
9:   end while
10:   $\theta_1 \leftarrow \theta_{cand}$ 
11:   $w_1 \leftarrow \ln(P(D_{obs}|\theta_{cand}))$ 

```

---

We can also use Sequential Monte-Carlo sampling method.

---

```

12:    $i \leftarrow 2$ 
13:   while  $i \leq N_{MH}$  do
14:      $sat \leftarrow False$ 
15:     while  $sat = False$  do
16:       Draw  $\theta_{cand}$  from  $Q(\theta'|\theta_{i-1})$ 
17:       Evaluate  $val \leftarrow RF_{\Phi}(\theta)$ 
18:       if  $val$  satisfies the boundary of  $\Phi$  then
19:          $sat \leftarrow True$ 
20:       end if
21:     end while
22:     if  $\ln(P(D_{obs}|\theta_{cand})) - \ln(P(D_{obs}|\theta_{i-1})) > 0$  then
23:        $\theta_i \leftarrow \theta_{cand}$ 
24:        $w_i \leftarrow \ln(P(D_{obs}|\theta_{cand}))$ 
25:        $i \leftarrow i + 1$ 
26:     else
27:       Draw a random number  $u$  from  $Uniform(0, 1)$ 
28:       if  $u \leq \xi$ , ( $\xi$  small, e.g  $10^{-2}$ ) then
29:          $\theta_i \leftarrow \theta_{cand}$ 
30:          $w_i \leftarrow \ln(P(D_{obs}|\theta_{cand}))$ 
31:          $i \leftarrow i + 1$ 
32:       end if
33:     end if
34:   end while
35:   Return  $(\theta_1, \dots, \theta_{N_{MH}}), (w_1, \dots, w_{N_{MH}})$ 
36: end procedure

```

---

---

**Algorithm 11** Sequential Monte-Carlo with rational functions

---

**Input:**

- $\mathcal{M}_\theta$ : parametric Discrete-Time Markov chain of parameter  $\theta$
- $\Phi$ : bounded reachability property of interest.
- $\pi(\theta)$ : prior distribution on  $\theta$ .
- $N$ : number of particles in the Sequential Monte-Carlo trace.
- $M$ : number of perturbation kernels
- $F_t(\theta^t|\theta_1^{t-1}, \dots, \theta_N^{t-1}), 1 \leq t \leq M$ : perturbation kernels
- $N_{MH}$ : number of particles in each Metropolis-Hastings step.
- $Q_t(\theta^t|\theta^{t-1}), 1 \leq t \leq N_{MH}$ : transition kernel for Metropolis-Hastings step.
- $D_{obs}$ : observed data for Bayesian inference or its summary statistic  $S_{obs}$
- $P(D_{obs}|\theta)$ : likelihood function.

**Output:**

- $(\theta_1, \dots, \theta_N)$ :  $N$  sampled particles.
- $(w_1, \dots, w_N)$ : corresponding weights of sampled particles.

```
1: procedure RF-SMC
2:    $i \leftarrow 1$ 
3:   while  $i \leq N$  do                                      $\triangleright$  SMC initialization
4:     Draw  $\theta$  from  $\pi(\theta)$ 
5:      $\theta_i \leftarrow \theta$ 
6:      $w_i \leftarrow P(D_{obs}|\theta_i)$ 
7:      $i \leftarrow i + 1$ 
8:   end while
```

---

---

```

9:    $t \leftarrow 1$ 
10:  while  $t \leq M$  do
11:       $i \leftarrow 1$  ▷ SMC correction step
12:      while  $i \leq N$  do
13:           $w'_i \leftarrow \frac{w_i}{\sum_{i=1}^N w_i}$ 
14:      end while
15:      Sample with replacement  $(\theta'_1, \dots, \theta'_N)$  ▷ SMC selection step
16:      from  $(\theta_1, \dots, \theta_N)$  with probabilities  $(w'_1, \dots, w'_N)$ 
17:       $(\theta_1, \dots, \theta_N) \leftarrow (\theta'_1, \dots, \theta'_N)$ 
18:       $i \leftarrow 1$ 
19:      while  $i \leq N$  do ▷ SMC pertubation step
20:          Draw  $\hat{\theta}_i^t$  from  $F_t(\theta^t | \theta_1^{t-1}, \dots, \theta_N^{t-1}), 1 \leq t \leq M$ 
21:           $(\theta_1^*, \dots, \theta_{N_{MH}}^*), (w_1^*, \dots, w_{N_{MH}}^*) \leftarrow RF - MCMC(\hat{\theta}_i^t)$ 
22:           $\theta_i \leftarrow \theta_{N_{MH}}^*$ 
23:           $w_i \leftarrow w_{N_{MH}}^*$ 
24:      end while
25:  end while
26:  Return  $(\theta_1, \dots, \theta_N), (w_1, \dots, w_N)$ 
27: end procedure

```

---

## 5.3 Bayesian frameworks with simulation

Without the availability of analytical form of observational and interested properties, we face the following obstacles:

- **Absence of likelihood functions:** As the rational functions for properties are not available, we do not have the analytical form of likelihood. The absence of likelihood suggests to exploit *likelihood-free methods*. In this framework we use *Approximate Bayesian Computation* in combination with *Sequential Monte-Carlo method*.
- **Absence of rational function for verification of bounded reachability property:** the satisfaction of an instantiated model to a bounded path property cannot be computed. In the case that the number of states is too large, we use *Statistical Model Checking*.

For this case we present Statistical Model Checking, Approximate Bayesian Computation - Sequential Monte-Carlo method *SMC-ABC-SMC* framework.

---

**Algorithm 12** Sequential Monte-Carlo with Approximate Bayesian Computation and Statistical Model Checking

---

**Input:**

- $\mathcal{M}_\theta$ : parametric Discrete-Time Markov chain of parameter  $\theta$
- $\Phi$ : bounded reachability property of interest.
- $\pi(\theta)$ : prior distribution on  $\theta$ .
- $N$ : number of particles in the Sequential Monte-Carlo trace.
- $M$ : number of perturbation kernels
- $F_t(\theta^t | \theta_1^{t-1}, \dots, \theta_N^{t-1}), 1 \leq t \leq M$
- $N_{MH}$ : number of particles in each Metropolis-Hastings step.
- $Q_t(\theta^t | \theta^{t-1}), 1 \leq t \leq N_{MH}$ : transition kernel for Metropolis-Hastings step.
- $D_{obs}$ : observed data for Bayesian inference or its summary statistic  $S_{obs}$
- $\epsilon$ : threshold for Approximate Bayesian Computation.
- $\delta, \alpha$ : indifference and  $\alpha$ -level for Statistical Model Checking using SPRT method.

**Output:**

- $(\theta_1, \dots, \theta_N)$ :  $N$  sampled particles.
- $(w_1, \dots, w_N)$ : corresponding weights of sampled particles.

```

1: procedure SMC-ABC-SMC
2:    $i \leftarrow 1$ 
3:   while  $i \leq N$  do                                      $\triangleright$  SMC initialization
4:     Draw  $\theta$  from  $\pi(\theta)$ 
5:      $\theta_i \leftarrow \theta$ 
6:      $w_i \leftarrow 1$ 
7:   end while

```

---

---

```

8:    $t \leftarrow 1$ 
9:   while  $t \leq M$  do
10:      $i \leftarrow 1$  ▷ SMC correction step
11:     while  $i \leq N$  do
12:        $w'_i \leftarrow \frac{w_i}{\sum_{i=1}^N w_i}$ 
13:     end while
14:     Sample with replacement  $(\theta'_1, \dots, \theta'_N)$  ▷ SMC selection step
15:     from  $(\theta_1, \dots, \theta_N)$  with probabilities  $(w'_1, \dots, w'_N)$ 
16:      $(\theta_1, \dots, \theta_N) \leftarrow (\theta'_1, \dots, \theta'_N)$ 
17:      $i \leftarrow 1$ 
18:     while  $i \leq N$  do ▷ SMC perturbation step
19:        $rejected \leftarrow True$ 
20:       while  $rejected == True$  do
21:          $sat \leftarrow False$ 
22:         while  $sat = False$  do
23:           Draw  $\hat{\theta}_i^t$  from  $F_t(\theta^t | \theta_1^{t-1}, \dots, \theta_N^{t-1}), 1 \leq t \leq M$ 
24:           Do SPRT SMC on  $\mathcal{M}_{\hat{\theta}^t}$  and  $\Phi$ 
25:           if  $\mathcal{M}_{\hat{\theta}^t} \models \Phi$  then
26:              $sat \leftarrow True$ 
27:           end if
28:         end while
29:          $D_{sim} \leftarrow Simulate(\mathcal{M}_{\hat{\theta}^t})$ 
30:          $d = Distance(D_{sim}, D_{obs})$ 
31:         if  $d < \epsilon$  then
32:            $rejected \leftarrow False$ 
33:            $\theta_i \leftarrow \hat{\theta}^t$ 
34:            $w_i \leftarrow d$ 
35:         end if
36:       end while
37:     end while
38:   end while
39:   Return  $(\theta_1, \dots, \theta_N), (w_1, \dots, w_N)$ 
40: end procedure

```

---

## 5.4 Selection of perturbation kernel

Selection of perturbation kernel is mentioned in [13]. In this thesis, we use component-wise uniform kernel:



# Chapter 6

## Case studies

To evaluate the effectiveness of the presented frameworks, we use three case studies. In each case study, we benchmark the frameworks using the following steps:

1. Describe the system of interest.
2. Construct state-space and parametric transitions function for pDTMC models.
3. Apply the frameworks in different setups (rational functions available, simulation-based) using synthetic data from known model parameters.
4. Visualize the parameter synthesis and inference result.
5. Measure runtime among different state-space to evaluate the frameworks' scalability.

Three case studies include firstly a simple and standard case study *zeroconf*. The second case study comes from the experiments of the Department of Biology at the University of Konstanz on the defensive behaviour of bee colonies[15]. Third case study is an epidemics model; it is introduced in order to show the expansion of the model state-space as the system has more states to be encoded.

### 6.1 Zeroconf

Zero-configuration protocol (*zeroconf* for short) is a protocol used in IPv4 network to allocate newly attached device an unique IP address without any

intervention from network operators.

### **6.1.1 Model and properties**

From the pseudocode of Zeroconf protocol

### **6.1.2 Evaluation**

### **6.1.3 Summary**

## **6.2 Bees colony**

### **6.2.1 System description**

We study the collective behavior of a bee colony. Each bee in a colony possibly stings after observing a threat in the surrounding environment, and warn other bees by releasing a special substance, pheromone. By sensing the pheromone released in the environment, other bees in the colony may also sting. However, since stinging leads to the termination of an individual bee, it reduces the total defense capability as well. With parametric Discrete-time Markov chain as the model, we study how the actions of a single bee change with regarding to the colony size of and pheromone amount.

### **6.2.2 Model and properties**

Assume that each bee in a colony decides its next action (to sting or not to sting) based only on the current state of the environment, and the number of bees who sting or not sting can be modeled as a Markov process. To reduce the complexity of the model, we make another assumption that the states of the bees colony are observed after uniform time duration, hence the model is of discrete-time. There are 3 assumptions on the system:

1. Each bee release an unit amount of pheromone immediately after stinging.
2. A bee dies after stinging and releasing pheromone. In the other words, no bee can sting more than once.

3. Stinging behaviour only depends on the concentration of pheromone in the environment.

Under these assumption, a bee colony can be viewed as a set of agents (bees) interact with each other in a closed environment with the appearance of a factor *pheromone*. Afterward, the agent has probability to commit an action, namely *sting*. The agent is eliminated from environment after stinging. Assume that we have a colony of  $n$  bees initially. As aforementioned, an individual bee is terminated after it stings. Thus, at the end of experiment, the number of bees is  $n' \in \{0, 1, \dots, n\}$ . We model the bee colony with a DTMC  $\mathcal{M} = (S, \mathbf{P}, S_{init}, AP, L)$ , such that

- $|S_{init}| = 1$
- There exists  $n + 1$  tSCCs which encode the population at the end of the experiment.

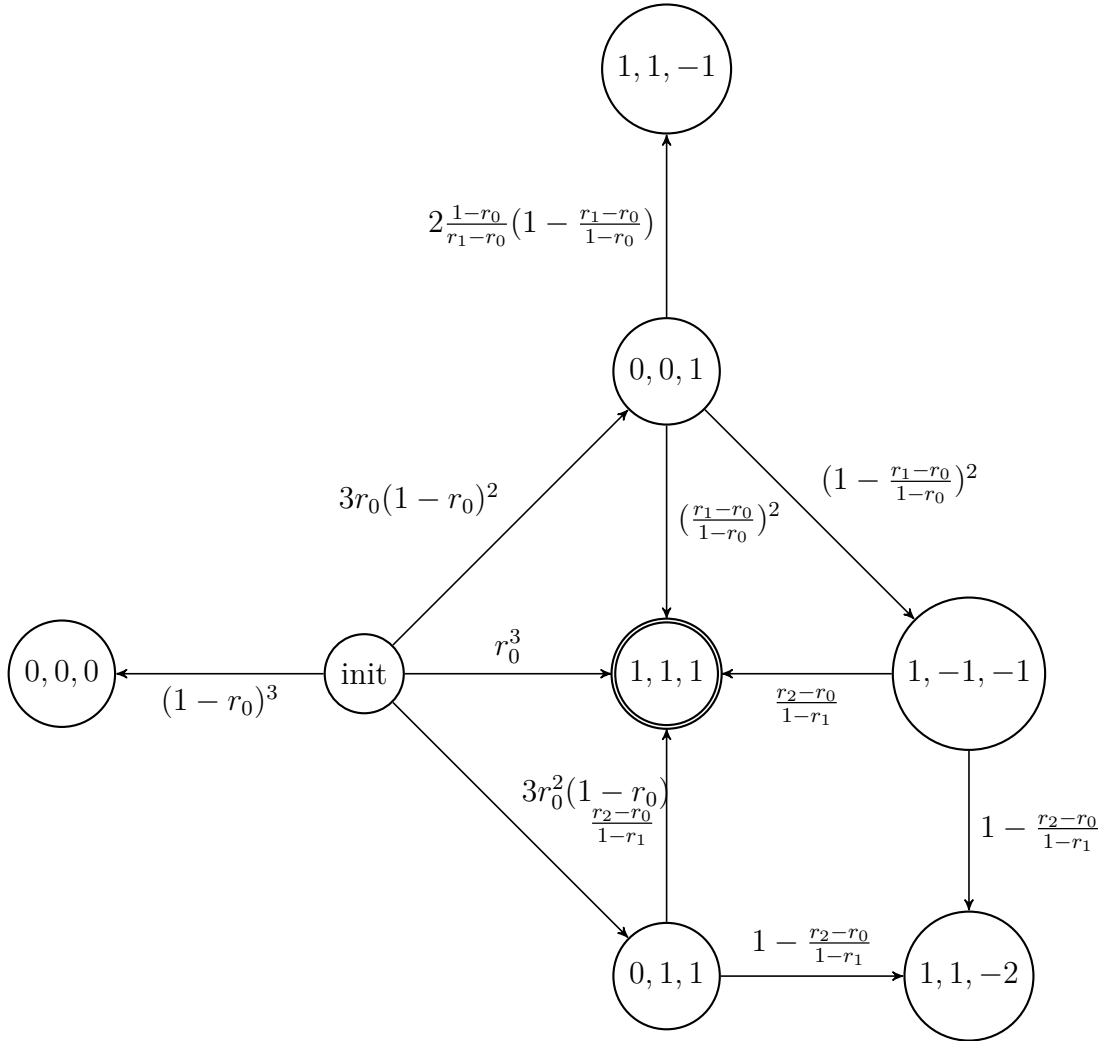


Figure 6.1: Synchronous model of 3 bees, multiparameters

Semantics of Markov population models for bees colony are developed by [15].

### 6.2.3 Evaluation

### 6.2.4 Conclusion

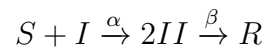
## 6.3 SIR model

### 6.3.1 System

*SIR* model is a population model, which is widely used in modeling epidemics. In a *SIR* model, each individual is of one among three types:

- *Susceptible* ( $S$ )
- *Infected* ( $S$ )
- *Recovered* ( $S$ )

*SIR* system is a stochastic system modeled by reactions between  $S$ ,  $I$  and  $R$ . In this thesis we use only 2 reactions.



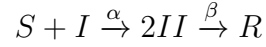
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**Algorithm 13** Generate SIR CTMC from reactions.

---

**Input:**

- $(S_0, I_0, R_0)$ : initial population.
- Reactions of rate  $\alpha, \beta$



**Output:**

- CTMC  $\mathcal{C}$

```
1: procedure SIR-EXPLORE-STATESPACE
2:   if  $i = 0$  then
3:     end if
4:   if  $(s > 0) \wedge (i > 0)$  then
5:     Sir-Explore-Statespace
6:   end if
7:   if  $(i > 0)$  then
8:     Sir-Explore-Statespace
9:   end if
10: end procedure
11: procedure SIR-EXPLORE-STATESPACE
12:   if  $i = 0$  then
13:     end if
14:   if  $(s > 0) \wedge (i > 0)$  then
15:     Sir-Explore-Statespace
16:   end if
17:   if  $(i > 0)$  then
18:     Sir-Explore-Statespace
19:   end if
20: end procedure
```

---

### 6.3.2 Model and properties

**Theorem 5**

*Acyclicity A CTMC  $\mathcal{C}$  constructed by Algorithm 13 using reactions ?? is*

*acyclic.*

**Proof:** For any arbitrary transition in  $\mathcal{C}$

1.  $|S|$  is monotonically decreasing, as there exists no reaction which produces  $S$ .
2.  $|R|$  is monotonically increasing, as there exists no reaction which consumes  $R$ .
3. If  $P((s, i, r), (s', i', r')) \neq 0$ , then  $i \neq i'$ . That is because all reactions change  $i$ .

As  $|S| + |I| + |R| = S_0 + I_0 + R_0$  and  $S_0, R_0, I_0$  are constants, if there exists a path fragment

$$(s^t, i^t, r^t) \rightarrow \dots \rightarrow (s^{t+k}, i^{t+k}, r^{t+k})$$

such that  $(s^t, i^t, r^t) = (s^{t+k}, i^{t+k}, r^{t+k})$  then  $k = 0$ , because all reactions change  $i$  (if  $P((s, i, r), (s', i', r')) \neq 0$ , then  $i \neq i'$ ).  $\square$

### Corollary 5.1

*A CTMC constructed by Algorithm 13 using reactions ?? has BSCCs and the BSCCs are trivial.*

### Example 6.4

*Example of an SIR CTMC model with initial population  $(S_0, I_0, R_0) = (3, 1, 0)$*

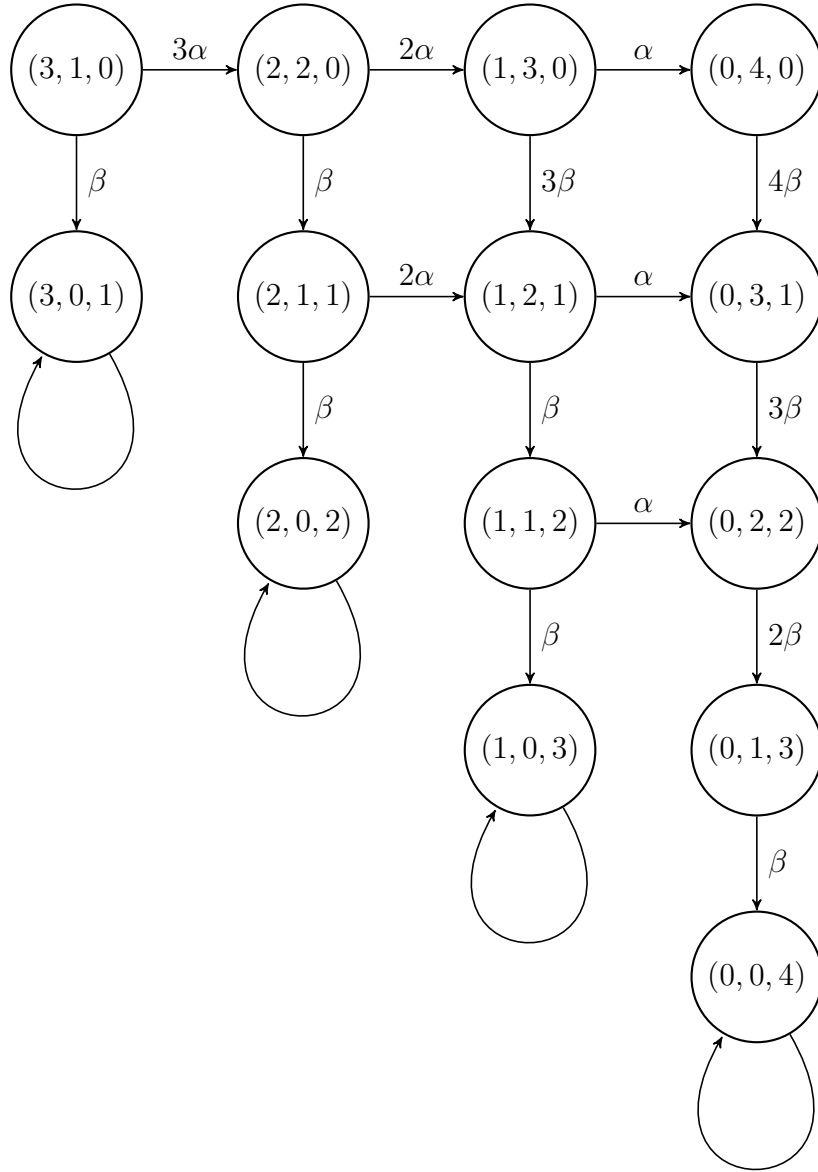


Figure 6.2:  $SIR(3, 1, 0)$  CTMC model with parameters  $(\alpha, \beta)$

**Example 6.5**

Uniformize the chain with uniformization rate  $(3\alpha + 4\beta)$ , we derive the following uniformized DTMC:



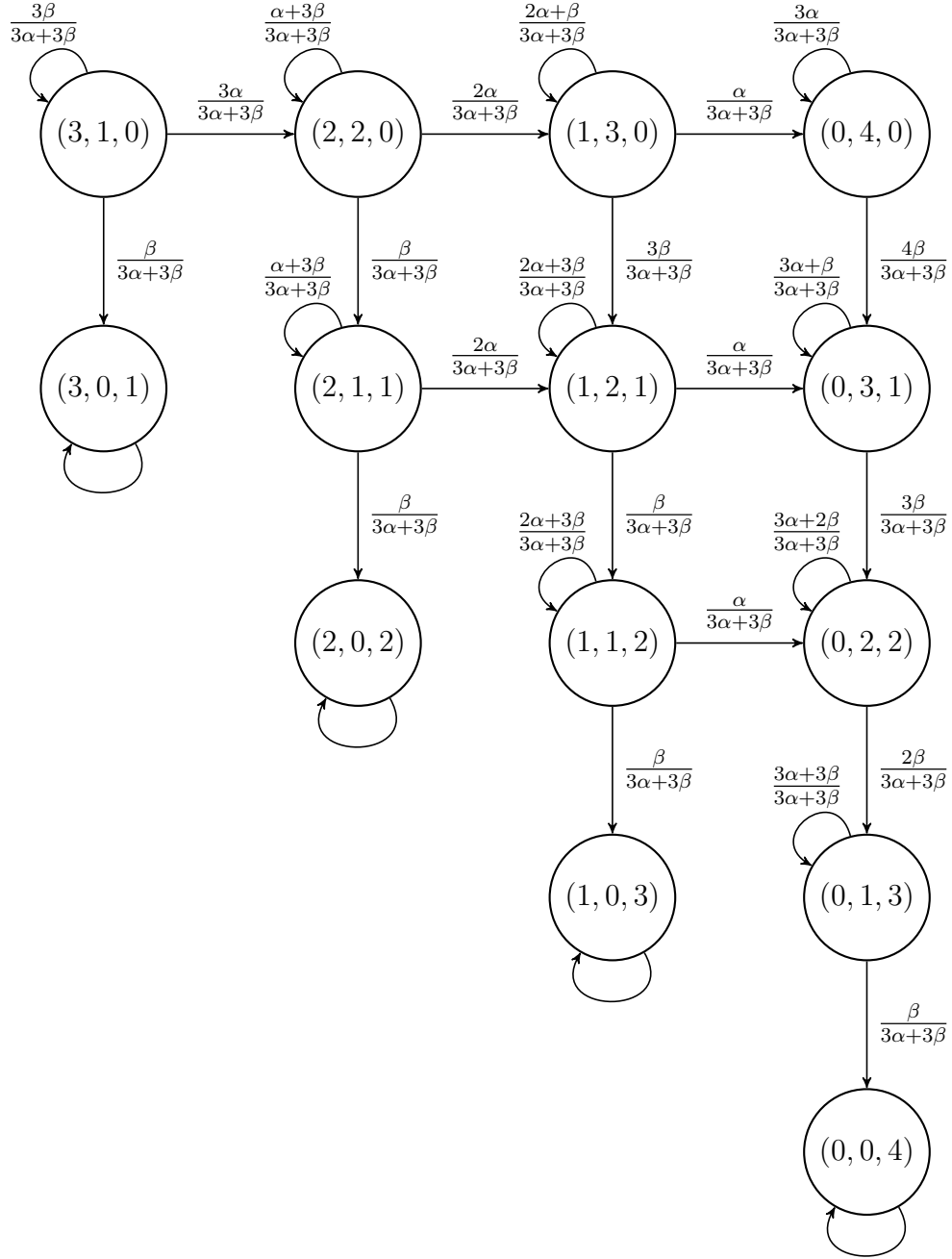


Figure 6.3:  $SIR(3,1,0)$  Uniformized DTMC model with parameters  $(\alpha, \beta)$  and uniformization rate  $(3\alpha + 4\beta)$

### 6.5.1 Evaluation

#### True parameters and synthetic data

#### Parameter synthesis result

We evaluate different frameworks on different size of initial population

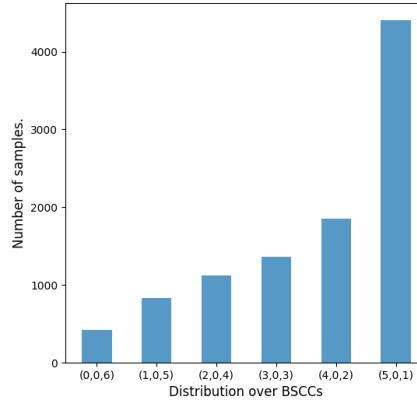
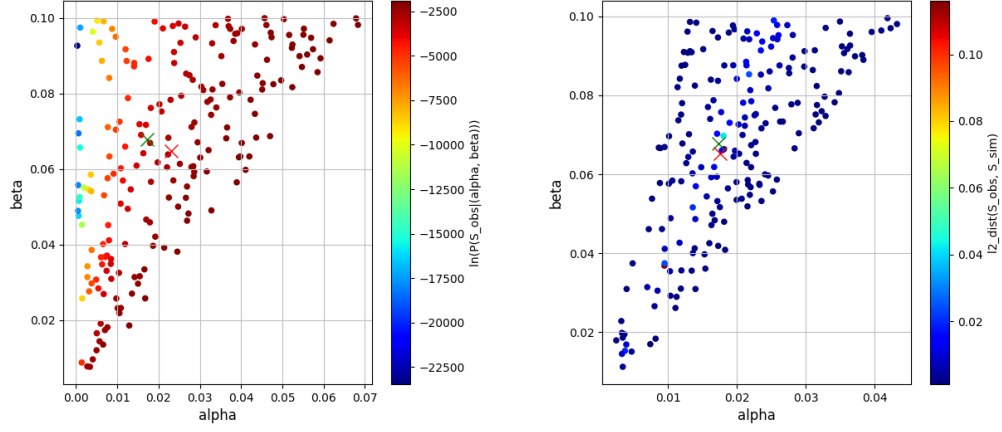


Figure 6.4: Synthetic data  $y_{obs}$  using selected true parameter.

<b>SIR(5,1,0)</b>	Rational function SMC	Statistical model checking ABC-SMC
True parameter	(0.01724649, 0.06778604)	
Number of states	27	
Number of BSCCs	6	
Target property	$P_{\geq 0.25}[!(i > 2)U^{<6}(i = 0)]$	
Synthetic data	(421, 834, 1126, 1362, 1851, 4406)	
Inferred parameter point	(0.02307652, 0.06481155)	(0.01758384, 0.06535699)
L2 distance to true parameter	0.006544985909916083	0.005519695496673707
Run time (hh:mm:ss)	1:07:36.442146	3:05:22.61795

Table 6.1: SIR(5,1,0) parameter estimation results.



(a) Sampled particles using Rational Functions SMC      (b) Sampled particles using Statistical Model Checking ABC-SMC

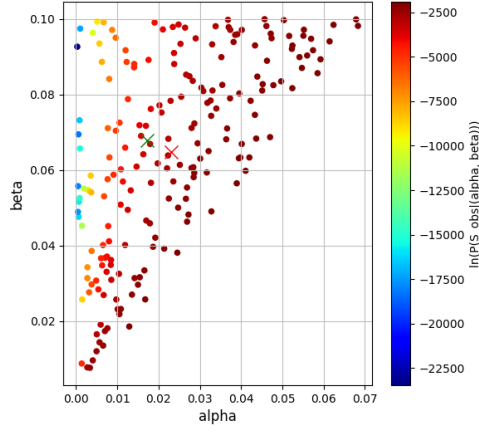
<b>SIR(10,1,0)</b>	Rational function SMC	Statistical model checking ABC-SMC
True parameter	(0.01724649, 0.06778604)	
Number of states	27	
Number of BSCCs	6	
Target property	$P_{\geq 0.25}[\neg(i > 2)U^{<6}(i = 0)]$	
Synthetic data	(421, 834, 1126, 1362, 1851, 4406)	
Inferred parameter point	(0.02307652, 0.06481155)	(0.01758384, 0.06535699)
L2 distance to true parameter	0.006544985909916083	0.005519695496673707
Run time (hh:mm:ss)	1:07:36.442146	3:05:22.61795

Table 6.2: SIR(5,1,0) parameter estimation results.

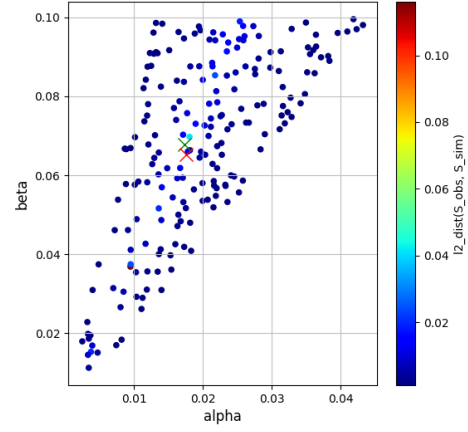
## Parameter synthesis with uncertainty

### 6.5.2 Discussion

This experiment shows good results.



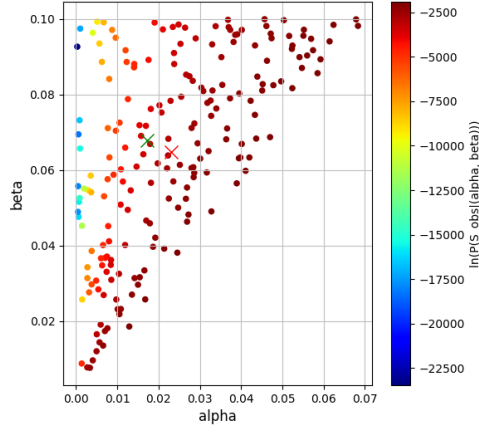
(a) Sampled particles using Rational Functions SMC



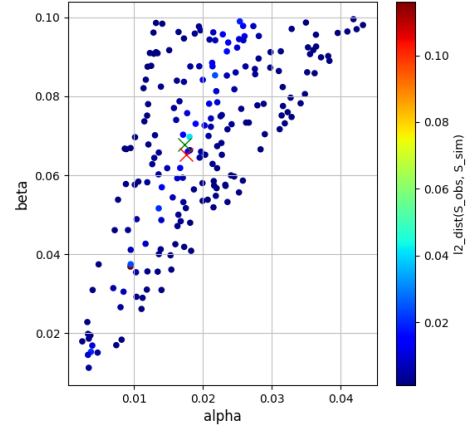
(b) Sampled particles using Statistical Model Checking ABC-SMC

<b>SIR(15,1,0)</b>	Rational function SMC	Statistical model checking ABC-SMC
True parameter	(0.01724649, 0.06778604)	
Number of states	27	
Number of BSCCs	6	
Target property	$P_{\geq 0.25}[\neg(i > 2)U^{<6}(i = 0)]$	
Synthetic data	(421, 834, 1126, 1362, 1851, 4406)	
Inferred parameter point	(0.02307652, 0.06481155)	(0.01758384, 0.06535699)
L2 distance to true parameter	0.006544985909916083	0.005519695496673707
Run time (hh:mm:ss)	1:07:36.442146	3:05:22.61795

Table 6.3: SIR(5,1,0) parameter estimation results.



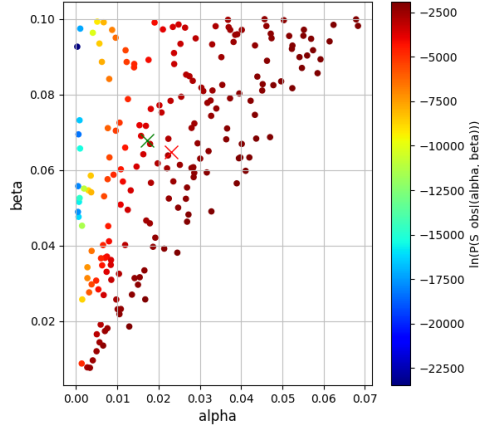
(a) Sampled particles using Rational Functions SMC



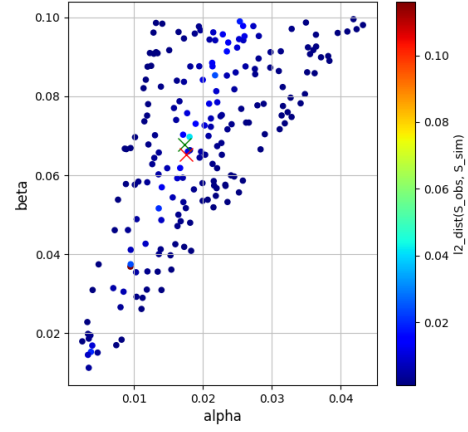
(b) Sampled particles using Statistical Model Checking ABC-SMC

<b>SIR(10,1,0)</b> , BSCC merged	Rational function SMC	Statistical model checking ABC-SMC
True parameter	(0.01724649, 0.06778604)	
Number of states	27	
Number of BSCCs	6	
Target property	$P_{\geq 0.25}[\neg(i > 2)U^{<6}(i = 0)]$	
Synthetic data	(421, 834, 1126, 1362, 1851, 4406)	
Inferred parameter point	(0.02307652, 0.06481155)	(0.01758384, 0.06535699)
L2 distance to true parameter	0.006544985909916083	0.005519695496673707
Run time (hh:mm:ss)	1:07:36.442146	3:05:22.61795

Table 6.4: SIR(5,1,0) parameter estimation results.



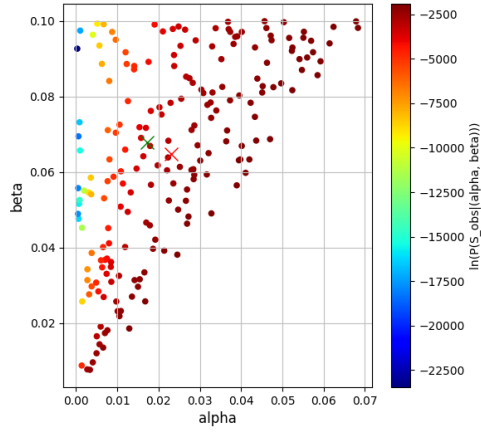
(a) Sampled particles using Rational Functions SMC



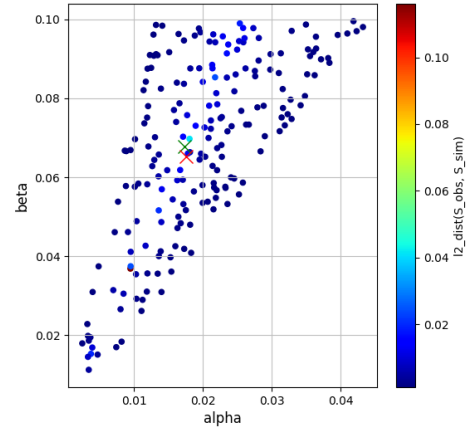
(b) Sampled particles using Statistical Model Checking ABC-SMC

<b>SIR(10,1,0)</b> , BSCC merged	Rational function SMC	Statistical model checking ABC-SMC
True parameter	(0.01724649, 0.06778604)	
Number of states	27	
Number of BSCCs	6	
Target property	$P_{\geq 0.25}[\neg(i > 2)U^{<6}(i = 0)]$	
Synthetic data	(421, 834, 1126, 1362, 1851, 4406)	
Inferred parameter point	(0.02307652, 0.06481155)	(0.01758384, 0.06535699)
L2 distance to true parameter	0.006544985909916083	0.005519695496673707
Run time (hh:mm:ss)	1:07:36.442146	3:05:22.61795

Table 6.5: SIR(5,1,0) parameter estimation results.



(a) Sampled particles using Rational Functions SMC



(b) Sampled particles using Statistical Model Checking ABC-SMC

# Chapter 7

## Conclusion

### 7.1 Summary

In this thesis we shows the possibility to infer the parameters of

### 7.2 Future works



# Bibliography

- [1] Greg M Allenby, Peter E Rossi, and RE McCulloch. “Hierarchical Bayes Models: A Practitioners Guide. Grover R, Vriens M, eds”. In: *SSRN Electron J* (2005).
- [2] David F Anderson and Thomas G Kurtz. “Continuous time Markov chain models for chemical reaction networks”. In: *Design and analysis of biomolecular circuits*. Springer, 2011, pp. 3–42.
- [3] Christel Baier and Joost-Pieter Katoen. *Principles of model checking*. MIT press, 2008.
- [4] Michael Baron. *Probability and statistics for computer scientists*. CRC Press, 2019.
- [5] Herman Chernoff. “A career in statistics”. In: *Past, Present, and Future of Statistical Science* 29 (2014).
- [6] Edmund M Clarke et al. “Model checking and the state explosion problem”. In: *LASER Summer School on Software Engineering*. Springer. 2011, pp. 1–30.
- [7] Edmund M. Clarke, E Allen Emerson, and A Prasad Sistla. “Automatic verification of finite-state concurrent systems using temporal logic specifications”. In: *ACM Transactions on Programming Languages and Systems (TOPLAS)* 8.2 (1986), pp. 244–263.
- [8] Remi Daviet. “Inference with Hamiltonian Sequential Monte Carlo Simulators”. In: *arXiv preprint arXiv:1812.07978* (2018).
- [9] Conrado Daws. “Symbolic and parametric model checking of discrete-time Markov chains”. In: *International Colloquium on Theoretical Aspects of Computing*. Springer. 2004, pp. 280–294.

- [10] Christian Dehnert et al. “A storm is coming: A modern probabilistic model checker”. In: *International Conference on Computer Aided Verification*. Springer. 2017, pp. 592–600.
- [11] Pierre Del Moral, Arnaud Doucet, and Ajay Jasra. “Sequential monte carlo samplers”. In: *Journal of the Royal Statistical Society: Series B (Statistical Methodology)* 68.3 (2006), pp. 411–436.
- [12] Martin Feinberg. “Chemical oscillations, multiple equilibria, and reaction network structure”. In: *Dynamics and modelling of reactive systems*. Elsevier, 1980, pp. 59–130.
- [13] Sarah Filippi et al. “On optimality of kernels for approximate Bayesian computation using sequential Monte Carlo”. In: *Statistical applications in genetics and molecular biology* 12.1 (2013), pp. 87–107.
- [14] Sofie Haesaert, Alessandro Abate, and Paul MJ Van den Hof. “Data-driven and model-based verification: A bayesian identification approach”. In: *2015 54th IEEE Conference on Decision and Control (CDC)*. IEEE. 2015, pp. 6830–6835.
- [15] Matej Hajnal et al. “Data-Informed Parameter Synthesis for Population Markov Chains”. In: *International Workshop on Hybrid Systems Biology*. Springer. 2019, pp. 147–164.
- [16] Faraz Hussain et al. “Automated parameter estimation for biological models using Bayesian statistical model checking”. In: *BMC bioinformatics* 16.S17 (2015), S8.
- [17] Lisa Hutschenreiter, Christel Baier, and Joachim Klein. “Parametric Markov chains: PCTL complexity and fraction-free Gaussian elimination”. In: *arXiv preprint arXiv:1709.02093* (2017).
- [18] Sumit K Jha et al. “A bayesian approach to model checking biological systems”. In: *International conference on computational methods in systems biology*. Springer. 2009, pp. 218–234.
- [19] Sebastian Junges et al. “Parameter synthesis for Markov models”. In: *arXiv preprint arXiv:1903.07993* (2019).
- [20] Joost-Pieter Katoen. “Model Checking Meets Probability: A Gentle Introduction.” In: *Engineering dependable software systems* 34 (2013), pp. 177–205.

- [21] Joost-Pieter Katoen. “The probabilistic model checking landscape”. In: *Proceedings of the 31st Annual ACM/IEEE Symposium on Logic in Computer Science*. 2016, pp. 31–45.
- [22] John FC Kingman. “Markov population processes”. In: *Journal of Applied Probability* (1969), pp. 1–18.
- [23] Marta Kwiatkowska, Gethin Norman, and David Parker. “PRISM 4.0: Verification of probabilistic real-time systems”. In: *International conference on computer aided verification*. Springer. 2011, pp. 585–591.
- [24] Gareth W Molyneux and Alessandro Abate. “ABC(SMC)<sup>2</sup>: Simultaneous Inference and Model Checking of Chemical Reaction Networks”. In: *International Conference on Computational Methods in Systems Biology*. Springer. 2020, pp. 255–279.
- [25] Gareth W Molyneux, Viraj B Wijesuriya, and Alessandro Abate. “Bayesian verification of chemical reaction networks”. In: *International Symposium on Formal Methods*. Springer. 2019, pp. 461–479.
- [26] Elizabeth Polgreen et al. “Data-efficient Bayesian verification of parametric Markov chains”. In: *International Conference on Quantitative Evaluation of Systems*. Springer. 2016, pp. 35–51.
- [27] John Salvatier, Thomas V Wiecki, and Christopher Fonnesbeck. “PyMC3: Python probabilistic programming framework”. In: *ascl* (2016), ascl–1610.
- [28] Daniel Silk, Saran Filippi, and Michael PH Stumpf. “Optimizing threshold-schedules for approximate Bayesian computation sequential Monte Carlo samplers: applications to molecular systems”. In: *arXiv preprint arXiv:1210.3296* (2012).
- [29] Stephen Tu. “The dirichlet-multinomial and dirichlet-categorical models for bayesian inference”. In: *Computer Science Division, UC Berkeley* (2014).