Master Thesis

Bayesian Parameter Estimation of State-Space Models with Intractable Likelihood

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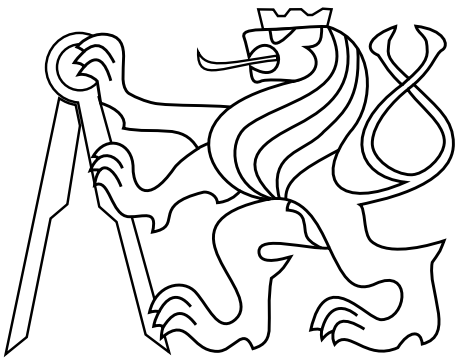
May 2019



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ZADÁNÍ DIPLOMOVÉ PRÁCE

I. OSOBNÍ A STUDIJNÍ ÚDAJE

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Fakulta/ústav: **Fakulta elektrotechnická**

Zadávající katedra/ústav: **Katedra počítačů**

Studijní program: **Otevřená informatika**

Studijní obor: **Bioinformatika**

II. ÚDAJE K DIPLOMOVÉ PRÁCI

Název diplomové práce:

Bayesovské odhadování parametrů stavových modelů při nedostupné věrohodnostní funkci

Název diplomové práce anglicky:

Bayesian parameter estimation of state-space models with intractable likelihood

Pokyny pro vypracování:

Stavové modely představují velmi populární formalismus vhodný pro popis celé řady různých náhodných procesů, od časových řad po aplikace v teorii řízení. Pokud tyto modely neobsahují statické parametry, lze pro jejich odhad použít např. Kalmanův filtr a jeho varianty, dále particle filtraci aj. Pokud ovšem statické parametry obsahují, tyto filtry zpravidla nekonvergují a nezbývá, než přikročit k optimalizačním technikám typu maximalizace věrohodnosti či particle Markov chain Monte Carlo. Další komplikace nastávají, pokud navíc není věrohodnostní funkce pro pozorovanou veličinu dostupná, nebo je nepřesná či příliš komplikovaná. Diplomová práce je specificky zaměřena poslední zmíněnou problematiku.
Specifické pokyny
1. Seznamte se s metodami pro odhadování stavových modelů pomocí kalmanovské filtrace a sekvenční Monte Carlo filtrace. Nastudujte problematiku statických parametrů a jejich odhadu.
2. Proveďte rešerši ohledně využití daných metod v oblasti bioinformatiky, například v modelování buněčných procesů.
3. Seznamte se s metodami ABC - Approximate Bayesian Computation a jejich využití ve filtraci stavových modelů.
4. Navrhněte vhodný způsob odhadování statických parametrů stavových modelů s využitím metod ABC.
5. Experimentálně (na vhodném problému z oblasti molekulární biologie) a případně teoreticky ověřte vlastnosti navržené metody, diskutujte její vlastnosti a navrhněte další možné směry výzkumu.

Seznam doporučené literatury:

1] C. C. Drovandi, A. N. Pettitt, and R. A. McCutchan, “Exact and approximate Bayesian inference for low integer-valued time series models with intractable likelihoods,” Bayesian Anal., vol. 11, no. 2, pp. 325–352, 2016.
[2] S. Martin, A. Jasra, S. S. Singh, N. Whiteley, P. Del Moral, and E. McCoy, “Approximate Bayesian Computation for Smoothing,” Stoch. Anal. Appl., vol. 32, no. 3, pp. 397–420, 2014.
[3] T. B. Schön, A. Svensson, L. Murray, and F. Lindsten, “Probabilistic learning of nonlinear dynamical systems using sequential Monte Carlo,” Mech. Syst. Signal Process., vol. 104, pp. 866–883, May 2018.
[4] C. Andrieu, A. Doucet, and R. Holenstein, “Particle Markov chain Monte Carlo methods,” J. R. Stat. Soc. Ser. B (Statistical Methodol., vol. 72, no. 3, pp. 269–342, Jun. 2010.
[5] K. Dedecius, “Adaptive kernels in approximate filtering of state-space models,” Int. J. Adapt. Control Signal Process., vol. 31, no. 6, pp. 938–952, Jun. 2017.

Jméno a pracoviště vedoucí(ho) diplomové práce:

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Jméno a pracoviště druhé(ho) vedoucí(ho) nebo konzultanta(ky) diplomové práce:

Datum zadání diplomové práce: **04.02.2019** Termín odevzdání diplomové práce: **24.05.2019**

Platnost zadání diplomové práce: **20.09.2020**

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III. PŘEVZETÍ ZADÁNÍ

Diplomant bere na vědomí, že je povinen vypracovat diplomovou práci samostatně, bez cizí pomoci, s výjimkou poskytnutých konzultací. Seznam použité literatury, jiných pramenů a jmen konzultantů je třeba uvést v diplomové práci.

. | Datum převzetí zadání

Podpis studenta

Abstract

Abstract in English

Abstrakt

Abstract in Czech

Author statement for graduate thesis:

I declare that the presented work was developed independently and that I have listed all sources of information used within it in accordance with the methodical instructions for observing the ethical principles in the preparation of university theses.

Prague, date ....

signature

Acknowledgements

I would like to thank my supervisor Kamil Dedecius for being such a positive person. It was a real pleasure to work with him, and I believe I have learned a great deal. Next, I want to thank my family for keeping me alive and well-fed. Finally, I thank my friends Lukáš and Petr for keeping me sane.

Contents

Chapter 1

Introduction

Probabilistic modelling arises in a wide variety of situations. Often, the measurements one uses to perform inference have been carried out with an unknown error. Frequently, one also does not have access to a correct model for the particular situation — the true model is either unknown, or even impossible to formulate.

In the former case, one naturally assumes a random error associated with the observations, and attempts to infer something from the data while accounting for this randomness.

In the latter case, one has no choice but to work with a given, although possibly simplified model, either because of insufficient domain knowledge, or for computational reasons. Connected with such a model is some degree of uncertainty about its parameters. It is often beneficial to think of these parameters as random variables themselves, in accordance with the Bayesian methodology (Robert, 2007). Such formulation allows to formulate one's prior beliefs about the parameter values, and then updating them upon receiving new observations.

In this thesis, we work with state-space models (SSMs) consisting of a sequence of observed random variables $\boldsymbol{y}_t$ indexed by discrete time $t = 1, \ldots, T$, which are assumed to have been generated by a latent random process $\boldsymbol{x}_t$, $t = 1, \ldots, T$. The distribution of $\boldsymbol{x}_t$ and $\boldsymbol{y}_t$ is assumed to be parameterized by a static parameter $\boldsymbol{\theta}$. Our goal is to perform posterior inference about this parameter, given the observed sequence $\{\boldsymbol{y}_t\}_{t=1}^T$. Furthermore, we assume that the likelihood function of the SSM is intractable and must be estimated. This assumption is well-grounded, as the likelihood is only available in severely restricted cases to be discussed in Chapter 3, together with a formal definition of the SSM.

Our contribution is twofold. First, we show how to apply the Approximate Bayesian Computation (ABC) methodology (Rubin et al., 1984; Pritchard et al., 1999) to obtain an estimate of the likelihood even under a misspecified model for the observed variables $\boldsymbol{y}_t$. Second, we use our results to model the genetic auto-regulation process in prokaryotes. In such a problem, the observation model is typically misspecified, as all attempts to describe such a complex system are necessarily simplified. The quote by the famous statistician George E. P. Box, *"all models are wrong, but some are useful"* (Box, 1979), comes to mind here.

The rest of the thesis is organized as follows. In Chapter 2, we review some of the related work. Discussed is the literature on Markov Chain Monte Carlo (MCMC) methods, and their use in estimating the parameters of an SSM. We state several results dealing with inference in SSMs with intractable likelihoods, as these are relevant to this thesis. Literature on ABC methods is reviewed as well, along with papers describing how these could be applied to SSMs. Finally, we discuss the application of SSMs to bioinformatics, focusing on molecular biology.

In Chapter 3, we properly define the assumed form of a state-space model. We show how one would implement a sampler to approximately infer the static parameters given a sequence of observations. We also show that in this basic form, such sampler is unusable, since it relies on the evaluation of the likelihood function, which is intractable (up to certain special cases). We then describe how this likelihood can be estimated using the particle filter (Doucet et al., 2001) without affecting the asymptotic properties of the sampler.

Chapter 4 provides a description of the ABC method, and also how it can be applied to estimate the likelihood even under a misspecified observation model. We discuss the pros and cons of such approach compared to the particle filter described in Chapter 3.

Chapter 5 provides numerical studies, where we apply the model developed in Chapter 4 to several examples and compare it with the model utilizing the particle filter. This chapter also includes the prokaryotic auto-regulation study discussed above.

Finally, Chapter 6 concludes the thesis and discusses some possible directions to be investigated in the future.

Chapter 2

Related work

In this chapter, we provide a survey of literature relevant to our work. Addressed are works on the use of Markov Chain Monte Carlo methods for approximate inference, works devoted to the use of the particle filter for state-space models likelihood estimation, and those related to Approximate Bayesian Computation methods. The chapter is concluded by a section describing the use of the state-space models in bioinformatics, focusing on problems arising in molecular biology and genetics.

2.1 Markov Chain Monte Carlo methods

Monte Carlo methods can be described as a class of algorithms relying on random sampling to produce numerical results. Typically, the expectation of some transformation of a probability distribution is of interest. This is then approximated by the empirical mean of a transformed random sample generated according to this distribution. Often, the probability distribution of interest is too complex to sample exactly. Assuming that the probability density function of this distribution can be evaluated (at least up to a normalizing constant), Monte Carlo methods are able to output a random sample approximately distributed according to the true distribution. *Markov Chain* Monte Carlo (MCMC) methods employ a Markov chain designed so that its limiting distribution is the target. At least asymptotically, the samples are indeed distributed according to the desired distribution.

An attractive property of MCMC, as opposed to plain Monte Carlo, is that the transition distribution of such chain need not resemble the target distribution even closely, and that the problem is relatively unaffected by the dimensionality. The downside is a difficulty to determine convergence — for how long should a chain be simulated in order to approximately reach the limiting distribution. In addition, one typically requires independent samples from the target distribution, which, however, the Markov chain samples are *not*. Typically, one needs to "thin" the Markov chain samples by keeping every nth one to ensure their approximate independence.

Perhaps the best known MCMC algorithm is the Metropolis algorithm (Metropolis et al., 1953), later improved by Hastings (1970). In this algorithm, random samples are iteratively generated from the Markov chain transition distribution. Each such sample is then compared with the previous one, and accepted with a certain probability ensuring that the limiting distribution is indeed the target. The go-to reference for Monte Carlo methods is Robert and Casella (2005). An appealing treatment of MCMC methods with applications towards physics and machine learning can be found in MacKay (2002).

There are of course many more MCMC algorithms. For our task, the Metropolis-Hastings algorithm is sufficient, since the main problem is in the likelihood estimation, and not in designing the best sampler possible.

2.2 Parameter inference in state-space models

We assume that the state-space model (SSM) takes the form informally stated in Chapter 1 and more formally given in Chapter 3, equation (3.1). If all the parameters of interest are changing in time, that is, the inference is about the latent process $\boldsymbol{x}_t$ given the observed sample $\boldsymbol{y}_1, \ldots, \boldsymbol{y}_T$, one arrives at the task of filtering.

If the transition distribution from state $\boldsymbol{x}_t$ to state $\boldsymbol{x}_{t+1}$ is linear in the states and corrupted by uncorrelated additive noise centered at 0, this task can be solved exactly by the Kalman filter (Kalman, 1960). The resulting filter is then optimal with respect to the mean squared error. An especially nice overview of the Kalman filter connecting it with other linear statistical models is Roweis and Ghahramani (1999).

Once the state transition becomes non-linear, as is typically the case, one can use various generalizations of the Kalman filter, such as the extended Kalman filter (EKF), which locally linearizes the transition distribution and then applies the Kalman filter to it, or the unscented Kalman filter (Julier and Uhlmann, 1997). These methods come without any optimality guarantees, though. The EKF additionally works best under a very mild non-linearity, due to its first-order approximation.

In recent years, the particle filter (Doucet et al., 2001) has become a popular alternative due to its simple implementation, appealing asymptotic properties and the fact that it allows for the transition model to be arbitrarily non-linear. Since the particle filter is used later in Chapter 3, we postpone a more detailed description there.

If, on the other hand, some of the unknown parameters are static, the task becomes more complex. Blindly applying an MCMC algorithm or any other approximation is not possible, as the likelihood function, on which such algorithms typically depend, cannot be evaluated. The paper Andrieu et al. (2010) introduced the idea of using the particle filter to obtain an estimate of the likelihood, which has been shown by Del Moral (2004) to preserve the limiting distribution of the underlying Markov chain. The resulting algorithm is called *Marginal Metropolis-Hastings*. A more recent overview can be found in the tutorial by Schön et al. (2017).

2.3 Approximate Bayesian Computation

In its original formulation, the method of Approximate Bayesian Computation (ABC) provides a way to approximate the posterior distribution $p(\theta \mid y) \propto f(y \mid \theta)p(\theta)$, assuming that the prior $p(\cdot)$ is fully known, and that the likelihood $f(\cdot \mid \theta)$ can be sampled from, but not evaluated (Rubin et al., 1984; Pritchard et al., 1999). A more recent treatment of ABC methods can be found in Marin et al. (2012).

Informally, ABC works by simulating a sample $\tilde{\theta}$ from the prior, substituting it to the likelihood, and generating pseudo-observations $\tilde{y}$. These are then compared to the real observations y, and if they are "similar enough", the sample $\tilde{\theta}$ is accepted. Otherwise, it is rejected. The posterior distribution of θ is then given in terms of the accepted samples $\tilde{\theta}$. This variant is referred to as the accept-reject ABC, for obvious reasons.

In this thesis, we apply the ABC method in place of the particle filter to allow for inference about the static parameter θ when the likelihood is not available. In addition, the use of ABC allows for a possibly misspecified observation model of the SSM, which is often the case, as one may not possess the necessary domain knowledge or computational power needed for the real model. Such a situation has been considered by Jasra (2015), although only through the use of the accept-reject variant given above.

Since accepting a sufficient number of samples may take a long time, an idea is to measure the distance between the true and pseudo-observations through a kernel function. This formulation would not reject any samples — instead, previously rejected sam-

ples would get assigned low weights. This has been investigated by Dedecius (2017), along with a proposed way to automatically tune the kernel width. How to exactly apply the ABC method to our problem is addressed in Chapter 4 in detail.

2.4 Applications to molecular biology

Finally, we review works describing how the framework of SSMs and their parameter inference can be applied in the context of bioinformatics, focusing on problems of molecular biology and genetics.

The go-to reference for stochastic modelling in biology is Wilkinson (2011). It contains a broad overview of applications of various probabilistic models to examples from molecular biology and chemistry. Included is a description of the Gillespie algorithm Gillespie (1976, 1977) used to simulate chemical reactions, which we use in Chapter 5.

A recent application of SSMs to molecular biology can be found in Golightly and J Wilkinson (2011), where the authors use the particle filter to approximate the unknown likelihoods of various biological models. We implement these examples in Chapter 5 and compare them with the ABC approximation.

The paper d'Alché Buc et al. (2007) models biological networks, such as gene regulatory networks or signalling pathways, by SSMs, and estimates their parameters. The static parameters of the model are viewed as dynamic states which, however, do not change in time. The unscented Kalman filter is then applied to estimate these "dynamic" parameters. Such approach is simple, as it does not require the use of MCMC algorithms, but comes without the appealing asymptotic properties of MCMC inference.

Wang et al. (2009), Sun et al. (2008) and Zeng et al. (2011) proceed in a similar fashion when estimating the parameters of various biochemical networks. The used models are only mildly non-linear, and so the extended Kalman filter is sufficient, again without any asymptotic guarantees of identifying the true parameters.

An interesting approach to learning the structure of a gene regulatory network from a gene expression time series can be found in Noor et al. (2012). First, the particle filter is applied to learn the hidden states of the network. Once these hidden states are known, the LASSO regression is applied to learn a sparse representation of the regulatory network, since each gene is assumed to interact only with a small number of other genes.

Chapter 3

Learning the parameters of a state-space model

This chapter describes the state-space model (SSM) formulation we are working with. In Section 3.1, we formally define the SSM and state our assumptions about the individual probability distributions.

In Section 3.2, we calculate the posterior distribution of the parameters of interest, and show that straightforward inference is not possible. Further on, we derive a sampler to approximate this distribution. By itself, this sampler is unusable, as it requires the evaluation of the intractable likelihood. Nevertheless, it is illustrative to compare it with the variant derived later.

To circumvent the likelihood evaluation, we introduce the particle filter in Section 3.3. This section gives the definition and some of the properties of the filter.

Finally, in Section 3.4 we show how to use the particle filter to estimate the likelihood, and argue that it does not affect the asymptotic properties of the sampler.

Most of this chapter is based on Andrieu et al. (2010) and Schön et al. (2017).

3.1 State-Space Model definition

The state-space model, often also called the hidden Markov model (HMM) assumes a sequence of latent states $\{\boldsymbol{x}_t\}_{t=0}^{\infty} \subseteq \mathbb{R}^{d_x}$ following a Markov chain, and a sequence of observed variables $\{\boldsymbol{y}_t\}_{t=1}^{\infty} \subseteq \mathbb{R}^{d_y}$. All involved distributions are parameterized by an unknown static parameter $\boldsymbol{\theta} \in \Theta \subset \mathbb{R}^d$.

For a fixed time $T \geq 1$, we use the shorthands $\boldsymbol{x}_{0:T} = \{\boldsymbol{x}_t\}_{t=0}^{T}$ and $\boldsymbol{y}_{1:T} = \{\boldsymbol{y}_t\}_{t=1}^{T}$ throughout the chapter.

The HMM formulation means that the joint distribution of $\boldsymbol{x}_{0:T}$ and $\boldsymbol{y}_{1:T}$ factorizes, for any $T \geq 1$, into

$$p(\boldsymbol{x}_{0:T}, \boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) = p(\boldsymbol{x}_0 \mid \boldsymbol{\theta}) \prod_{t=1}^{T} f_t(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{\theta}) g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta}), \tag{3.1}$$

where p is the prior distribution over the initial state, f_t is the transition distribution at time t and g_t is the observation model at time t.

The factorization (3.1) can be written more clearly as

$$\begin{aligned} \boldsymbol{x}_0 \mid \boldsymbol{\theta} &\sim p(\cdot \mid \boldsymbol{\theta}), \\ \boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{\theta} &\sim f_t(\cdot \mid \boldsymbol{x}_{t-1}, \boldsymbol{\theta}), \quad t = 1, \ldots, T, \\ \boldsymbol{y}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta} &\sim g_t(\cdot \mid \boldsymbol{x}_t, \boldsymbol{\theta}), \quad t = 1, \ldots, T. \end{aligned}$$

Finally, in accordance with the Bayesian approach (Robert, 2007), we introduce a prior distribution π over the unknown parameters $\boldsymbol{\theta}$ quantifying our knowledge about $\boldsymbol{\theta}$ before having observed any data. This allows us to state the full joint distribution

$$p(\boldsymbol{x}_{0:T}, \boldsymbol{y}_{1:T}, \boldsymbol{\theta}) = p(\boldsymbol{x}_{0:T}, \boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})\pi(\boldsymbol{\theta}). \tag{3.2}$$

The corresponding graphical model is depicted in Figure 3.1.

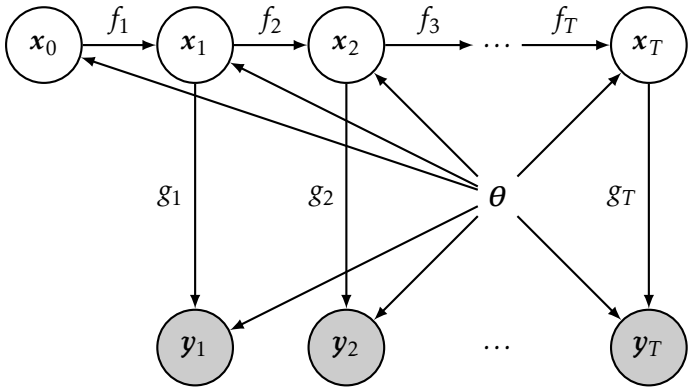

Figure 3.1: Graphical model describing the full joint distribution (3.2). The shaded nodes denote the observed variables, white nodes represent the latent variables.

3.2 Parameter inference

Given an observed sequence $\boldsymbol{y}_{1:T}$, Bayesian inference relies on the joint posterior density

$$p(\boldsymbol{\theta}, \boldsymbol{x}_{0:T} \mid \boldsymbol{y}_{1:T}) = \underbrace{p(\boldsymbol{x}_{0:T} \mid \boldsymbol{\theta}, \boldsymbol{y}_{1:T})}_{\text{State inference}} \underbrace{p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})}_{\text{Parameter inference}}. \tag{3.3}$$

Our primary interest is to perform inference about the static parameter $\boldsymbol{\theta}$. From (3.3), it is clear that to infer about the hidden states $\boldsymbol{x}_{0:T}$, one needs knowledge about $\boldsymbol{\theta}$, so even if the hidden states are of interest, inference about $\boldsymbol{\theta}$ is necessary.

Bayesian inference To perform Bayesian inference about $\boldsymbol{\theta}$, we express the posterior of $\boldsymbol{\theta}$ by applying the Bayes theorem:

$$p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T}) = \frac{p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})\pi(\boldsymbol{\theta})}{\int p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})\pi(\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta}}. \tag{3.4}$$

Evaluating the likelihood $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$ requires marginalizing over $\boldsymbol{x}_{0:T}$:

$$p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) = \int p(\boldsymbol{x}_{0:T}, \boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{x}_{0:T},$$

where $p(\boldsymbol{x}_{0:T}, \boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$ is given in (3.1). Unless the SSM is linear and Gaussian, such $d_x(T+1)$-dimensional integral is intractable (Andrieu et al., 2010).

Inference under tractable likelihood assumption For the time being, we proceed as if the likelihood was tractable. We derive a sampler for $\boldsymbol{\theta}$ and note which component cannot be evaluated due to the likelihood being present. Section 3.4 then describes the necessary changes to allow circumventing the likelihood evaluation.

Often, the interest is not in the posterior $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$ itself, but on the expectation of some function ϕ w.r.t. this distribution, i.e. on

$$\mathbb{E}_{p(\cdot|\boldsymbol{y}_{1:T})}[\phi(\boldsymbol{\theta})] = \int \phi(\boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T}) \, \mathrm{d}\boldsymbol{\theta}. \tag{3.5}$$

We construct a Metropolis-Hastings sampler (Metropolis et al., 1953; Hastings, 1970) with target distribution $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$. This gives us M samples approximately distributed according to this target, denoted $\boldsymbol{\theta}^{(m)}$, $m = 1, \ldots, M$. The expectation (3.5) is then approximated by the arithmetic mean

$$\frac{1}{M} \sum_{m=1}^{M} \phi(\boldsymbol{\theta}^{(m)}).$$

An appealing property of the Metropolis-Hastings algorithm is that such arithmetic mean almost surely converges to (3.5) as the number of samples grows (Robert and Casella, 2005), i.e.

$$\frac{1}{M} \sum_{m=1}^{M} \phi(\boldsymbol{\theta}^{(m)}) \xrightarrow[M \to \infty]{a.s} \int \phi(\boldsymbol{\theta}) p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T}) \, \mathrm{d}\boldsymbol{\theta}.$$

Finally, we note that if one is indeed interested in the distribution $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$ itself, it can be recovered by the empirical distribution

$$\widehat{p}(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T}) = \frac{1}{M} \sum_{m=1}^{M} \delta_{\boldsymbol{\theta}^{(m)}}(\boldsymbol{\theta}),$$

where δ denotes the Dirac distribution. This estimate can be additionally smoothed using kernel methods (Wand and Jones, 1994).

Metropolis-Hastings algorithm The Metropolis-Hastings algorithm is described in Algorithm 1. Although well-known, it is included for comparison with the variant employing the particle filter, introduced in Algorithm 5.

The algorithm constructs a Markov chain on the variable $\boldsymbol{\theta}$, whose transition distribution q is called the proposal distribution in this context. Starting at an initial state $\boldsymbol{\theta}_0$, candidate states $\boldsymbol{\theta}'$ are iteratively sampled according to $q(\cdot \mid \boldsymbol{\theta})$, where $\boldsymbol{\theta}$ is the current state of the chain.

We then calculate the acceptance probability α in (3.6), which considers which of the two states $\boldsymbol{\theta}$ and $\boldsymbol{\theta}'$ is more probable under the target distribution $p(\cdot \mid \boldsymbol{y}_{1:T}) \propto p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) \pi(\boldsymbol{\theta})$. Additionally, it allows the chain to "step back" and not move to the new state $\boldsymbol{\theta}'$ by comparing the probability of the two states under q, but in reverse direction. With probability α, the Markov chain then evolves into $\boldsymbol{\theta}'$; otherwise, it remains in the current state.

It can be shown (Robert and Casella, 2005) that the distribution $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$ is the limiting distribution of such Markov chain. This means that with the number of transitions going to infinity, the sampled $\boldsymbol{\theta}$ are distributed according to our target distribution $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$. To approximately reach this limiting distribution, a number of initial samples (called the burn-in period) is often discarded. In addition, one usually wants independent samples from the target distribution, which the samples from a Markov chain are *not*. In practice, only samples with a given spacing are kept to ensure their approximate independence.

Similarly to the prior π, setting the proposal q is problem-dependent, and both distributions must be selected carefully. Diagnosing converge of the sampler is a notably difficult task, and one usually resorts to graphical tools to determine whether the sampled values have stabilized. Some such plots are given in Chapter 5.

Algorithm 1 Metropolis-Hastings

Input: Number of samples M, $\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_T\}$.

1: Initialize $\boldsymbol{\theta}^{(0)}$.
2: **for** $m = 1$ **to** M **do**
3: Sample $\boldsymbol{\theta}' \sim q(\cdot \mid \boldsymbol{\theta}^{(m-1)})$.
4: Calculate the aceptance probability

$$\alpha = \min\left\{1, \frac{p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}')\pi(\boldsymbol{\theta}')}{p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}^{(m-1)})\pi(\boldsymbol{\theta}^{(m-1)})} \frac{q(\boldsymbol{\theta}^{(m-1)} \mid \boldsymbol{\theta}')}{q(\boldsymbol{\theta}' \mid \boldsymbol{\theta}^{(m-1)})}\right\}. \tag{3.6}$$

5: Sample $u \sim \mathcal{U}(0, 1)$.
6: **if** $u \leq \alpha$ **then**
7: $\boldsymbol{\theta}^{(m)} \leftarrow \boldsymbol{\theta}'$ ▷ With probability α, accept the proposed sample.
8: **else**
9: $\boldsymbol{\theta}^{(m)} \leftarrow \boldsymbol{\theta}^{(m-1)}$ ▷ With probability $1 - \alpha$, reject the proposed sample.
10: **end if**
11: **end for**

Output: $\left\{\boldsymbol{\theta}^{(1)}, \ldots, \boldsymbol{\theta}^{(M)}\right\}$

From Algorithm 1, we see that the acceptance probability (3.6) cannot be calculated, as it depends on the intractable likelihood $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$. In Section 3.4, we give a modified variant of the Metropolis-Hastings algorithm, where the likelihood is approximated using the particle filter. The derivation of this filter is the content of the next section.

3.3 The particle filter

The particle filter (Doucet et al., 2001) is a method for approximating the filtering distribution $p(\boldsymbol{x}_t \mid \boldsymbol{y}_{1:t}, \boldsymbol{\theta})$ using a finite number of samples called particles. The algorithm is also known as sequential Monte Carlo or sequential importance sampling. The latter name sheds some light on how the method works, and it is exactly through importance sampling that the particle filter is derived.

Importance sampling Here we briefly review the basic idea behind importance sampling. For a more thorough treatment, the reader is referred to MacKay (2002) or Robert and Casella (2005).

Consider a situation where the expectation of some function ϕ w.r.t. the distribution with density p,

$$\Phi := \mathbb{E}_p[\phi(\boldsymbol{X})] = \int \phi(\boldsymbol{x}) p(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}, \tag{3.7}$$

is of interest. Assume that the integral is analytically intractable, and that one cannot generate samples from p to approximate this expectation. Assume further that the density p can be evaluated, at least up to a multiplicative constant, i.e. that it takes the form

$$p(\boldsymbol{x}) = \frac{p^*(\boldsymbol{x})}{Z},$$

where Z is an unknown normalizing constant, and p^* can be evaluated. Such situation frequently arises in Bayesian statistics, where a posterior distribution of interest $p(\boldsymbol{\theta} \mid \boldsymbol{x}) = \frac{p(\boldsymbol{x}|\boldsymbol{\theta})p(\boldsymbol{\theta})}{\int p(\boldsymbol{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{\theta}}$ is given in terms of the Bayes theorem. The normalizing constant in the denominator is often unavailable in analytic form. However, the numerator can be evaluated.

Next, we introduce a (typically simpler) distribution with density $q(\boldsymbol{x}) = \frac{q^*(\boldsymbol{x})}{Z_Q}$ s.t.

1. One can sample from q;
2. One can evaluate q^*;
3. $p(\boldsymbol{x}) > 0$ implies $q(\boldsymbol{x}) > 0$.

The expectation (3.7) can then be written as

$$\Phi = \int \phi(\boldsymbol{x}) \frac{q(\boldsymbol{x})}{q(\boldsymbol{x})} p(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \int \phi(\boldsymbol{x}) \underbrace{\frac{p(\boldsymbol{x})}{q(\boldsymbol{x})}}_{w^*(\boldsymbol{x})} q(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x} = \mathbb{E}_q[\phi(\boldsymbol{X}) w^*(\boldsymbol{X})],$$

where $w^*(\boldsymbol{x})$ are called the importance weights. By defining $w(\boldsymbol{x}) = \frac{p^*(\boldsymbol{x})}{q^*(\boldsymbol{x})}$, Φ can be approximated by

$$\Phi \approx \widehat{\Phi} := \frac{\sum_{i=1}^N \phi(\boldsymbol{x}^{(i)}) w(\boldsymbol{x}^{(i)})}{\sum_{i=1}^N w(\boldsymbol{x}^{(i)})}, \quad \boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(N)} \overset{iid}{\sim} q.$$

We note that by using w instead of w^* and normalizing by the weights sum instead of the sample size N, we bypass the evaluation of Z and Z_Q, since they cancel out. The importance weights here account for correcting the discrepancy between the distribution q and the true distribution p.

The estimator $\widehat{\Phi}$ converges to the true expectation Φ as $N \to \infty$. However, it is not necessarily unbiased (MacKay, 2002).

Sequential importance sampling (SIS) The SIS algorithm uses a set of weighted particles $\left\{\left(\boldsymbol{x}_t^{(i)}, w_t^{(i)}\right) : i = 1, \ldots, N\right\}$ to represent the filtering distribution $p(\boldsymbol{x}_t \mid \boldsymbol{y}_{1:t}, \boldsymbol{\theta})$. To simplify notation, we write $w_t^{(i)}$ instead of $w_t(\boldsymbol{x}^{(i)})$ from now on. The empirical approximation to $p(\boldsymbol{x}_t \mid \boldsymbol{y}_{1:t}, \boldsymbol{\theta})$ is then

$$\widehat{p}(\boldsymbol{x}_t \mid \boldsymbol{y}_{1:t}, \boldsymbol{\theta}) = \frac{\sum_{i=1}^N w_t^{(i)} \delta_{\boldsymbol{x}_t^{(i)}}(\boldsymbol{x}_t)}{\sum_{i=1}^N w_t^{(i)}}.$$

As the name suggests, the algorithm involves a sequential application of the importance sampling procedure with increasing time t.

Returning to the SSM (3.1), we consider the posterior distribution of a sequence of states $\boldsymbol{x}_{0:t}$ given a sequence of observations $\boldsymbol{y}_{1:t}$. By application of the Bayes theorem, we obtain the following recursive formula:

$$\begin{aligned} p(\boldsymbol{x}_{0:t} \mid \boldsymbol{y}_{1:t}) &\propto p(\boldsymbol{y}_t \mid \boldsymbol{x}_{0:t}, \boldsymbol{y}_{1:t-1}) p(\boldsymbol{x}_{0:t} \mid \boldsymbol{y}_{1:t-1}) \\ &= g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t) p(\boldsymbol{x}_t \mid \boldsymbol{x}_{0:t-1}, \boldsymbol{y}_{1:t-1}) p(\boldsymbol{x}_{0:t-1} \mid \boldsymbol{y}_{1:t-1}) \\ &= g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t) f_t(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}) p(\boldsymbol{x}_{0:t-1} \mid \boldsymbol{y}_{1:t-1}), \end{aligned}$$

where the equalities follow from the hidden Markov model independence assumptions. For better clarity, we suppress the static parameter $\boldsymbol{\theta}$ from the conditioning.

For the target $p(\boldsymbol{x}_{0:t} \mid \boldsymbol{y}_{1:t})$, we introduce an importance sampling distribution $q(\boldsymbol{x}_{0:t} \mid \boldsymbol{y}_{1:t})$ and sample $\boldsymbol{x}_{0:t}^{(i)}$ from it. The importance weights are (up to normalization) given by

$$\begin{aligned} w_t^{(i)} &\propto \frac{p(\boldsymbol{x}_{0:t}(i) \mid \boldsymbol{y}_{1:t})}{q(\boldsymbol{x}_{0:t}^{(i)} \mid \boldsymbol{y}_{1:t})} \\ &\propto \frac{g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t^{(i)}) f_t(\boldsymbol{x}_t^{(i)} \mid \boldsymbol{x}_{t-1}^{(i)}) p(\boldsymbol{x}_{0:t-1}^{(i)} \mid \boldsymbol{y}_{1:t-1})}{q(\boldsymbol{x}_{0:t}^{(i)} \mid \boldsymbol{y}_{1:t})}. \end{aligned} \tag{3.8}$$

By definition of the conditional probability and the hidden Markov model assumptions, we can write the importance sampling distribution as

$$q(\boldsymbol{x}_{0:t} \mid \boldsymbol{y}_{1:t}) = q(\boldsymbol{x}_t \mid \boldsymbol{x}_{0:t-1}, \boldsymbol{y}_{1:t}) q(\boldsymbol{x}_{0:t-1} \mid \boldsymbol{y}_{1:t-1}).$$

By substituting into (3.8), we obtain the following recursion:

$$\begin{aligned} w_t^{(i)} &\propto \frac{g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t^{(i)}) f_t(\boldsymbol{x}_t^{(i)} \mid \boldsymbol{x}_{t-1}^{(i)})}{q(\boldsymbol{x}_t^{(i)} \mid \boldsymbol{x}_{0:t-1}^{(i)}, \boldsymbol{y}_{1:t})} \frac{p(\boldsymbol{x}_{0:t-1}^{(i)} \mid \boldsymbol{y}_{1:t-1})}{q(\boldsymbol{x}_{0:t-1}^{(i)} \mid \boldsymbol{y}_{1:t-1})} \\ &\propto \frac{g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t^{(i)}) f_t(\boldsymbol{x}_t^{(i)} \mid \boldsymbol{x}_{t-1}^{(i)})}{q(\boldsymbol{x}_t^{(i)} \mid \boldsymbol{x}_{0:t-1}^{(i)}, \boldsymbol{y}_{1:t})} w_{t-1}^{(i)}. \end{aligned} \tag{3.9}$$

So updating the ith weight when transitioning from time $t-1$ to t is a relatively simple task involving only multiplication by the first fraction in (3.9).

The sequential importance sampling algorithm is summarized in Algorithm 2. This

Algorithm 2 Sequential Importance Sampling

Input: Number of particles N, current parameter value $\boldsymbol{\theta}$, $\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_T\}$.

1: Sample $\boldsymbol{x}_0^{(i)} \sim p(\cdot \mid \boldsymbol{\theta}), \quad i = 1, \ldots, N.$ ▷ Initialize N particles.
2: $w_0^{(i)} \leftarrow \frac{1}{N}, \quad i = 1, \ldots, N.$ ▷ Initialize uniform weights.
3: **for** $t = 1$ **to** T **do**
4: Sample $\boldsymbol{x}_t^{(i)} \sim q(\cdot \mid \boldsymbol{x}_{0:t-1}^{(i)}, \boldsymbol{y}_{1:t}, \boldsymbol{\theta}), \quad i = 1, \ldots, N.$ ▷ Sample N new particles.
5: Set $w_t^{(i)} \propto \frac{g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t^{(i)}, \boldsymbol{\theta}) f_t(\boldsymbol{x}_t^{(i)} \mid \boldsymbol{x}_{t-1}^{(i)}, \boldsymbol{\theta})}{q(\boldsymbol{x}_t^{(i)} \mid \boldsymbol{x}_{0:t-1}^{(i)}, \boldsymbol{y}_{1:t}, \boldsymbol{\theta})} w_{t-1}^{(i)}, \quad i = 1, \ldots, N.$ ▷ Update the weights as per (3.9).
6: **end for**

by itself is almost the particle filter. There are still two issues to be addressed, though. First, the problem of weight degeneracy discussed in the next paragraph. Second, the choice of the importance sampling distribution q addressed later.

Resampling A serious problem preventing the use of the SIS algorithm is that the weights degenerate over time. In each time step, the variance of the weights reduces (Doucet et al., 2001). This means that the (normalized) weights always converge to a situation where a single weight is 1 and the others are 0.

To alleviate this, the following resampling step is introduced.

Algorithm 3 Multinomial resampling

Input: Importance weights $w_t^{(1)}, \ldots, w_t^{(N)}$, particles $\boldsymbol{x}_t^{(1)}, \ldots, \boldsymbol{x}_t^{(N)}$.

1: $\widetilde{w}_t^{(i)} \leftarrow \frac{w_t^{(i)}}{\sum_{j=1}^N w_t^{(j)}}, \quad i = 1, \ldots, N.$ ▷ Normalize the weights.
2: Sample a_i s.t. $\mathbb{P}(a_i = j) = \widetilde{w}_t^{(j)}, \quad i, j = 1, \ldots, N.$ ▷ Sample indices with replacement.
3: $w_t^{(a_i)} \leftarrow \frac{1}{N}, \quad i = 1, \ldots, N.$ ▷ Reset weights.

Output: Resampled particles $\boldsymbol{x}_t^{(a_1)}, \ldots, \boldsymbol{x}_t^{(a_N)}$ and weights $w_t^{(a_1)}, \ldots, w_t^{(a_N)}$.

The normalized importance weights are interpreted as a probability vector of a categorical distribution. The particles are then resampled (sampled with replacement) according to this distribution. This effectively selects a population of "strong individuals" for the next time step.

Algorithm 3 is known as multinomial resampling. There are other, more sophisticated, approaches, such as stratified resampling (Douc and Cappe, 2005), which come at the cost of increased complexity.

The particle filter The remaining step is the choice of the importance sampling distribution q. Obviously, the more similar this distribution is to the target p, the closer approximation we obtain.

The particle filter arises when the transition distribution f_t is chosen as the importance distribution, that is, when

$$q(\boldsymbol{x}_t \mid \boldsymbol{x}_{0:t-1}, \boldsymbol{y}_{1:t}, \boldsymbol{\theta}) = f_t(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{\theta}).$$

The importance weights (3.9) then simplify into

$$w_t^{(i)} \propto g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t^{(i)}) w_{t-1}^{(i)}. \tag{3.10}$$

The particle filter is summarized in Algorithm 4. The algorithm is called *bootstrap* particle filter, due to resemblance of the resampling step to the non-parametric bootstrap (Efron, 1979). By being defined in terms of importance sampling, the algorithm inherits the appealing asymptotic properties.

Algorithm 4 Bootstrap particle filter

Input: Number of particles N, current parameter value $\boldsymbol{\theta}$, $\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_T\}$.

1: Sample $\boldsymbol{x}_0^{(i)} \sim p(\cdot \mid \boldsymbol{\theta}), \quad i = 1, \ldots, N.$ ▷ Initialize N particles.
2: $w_0^{(i)} \leftarrow \frac{1}{N}, \quad i = 1, \ldots, N.$ ▷ Initialize uniform weights.
3: **for** $t = 1$ **to** T **do**
4: Sample $\boldsymbol{x}_t^{(i)} \sim f_t(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}^{(i)}, \boldsymbol{\theta}), \quad i = 1, \ldots, N.$ ▷ Sample N new particles.
5: Set $w_t^{(i)} \propto g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t^{(i)}, \boldsymbol{\theta}) w_{t-1}^{(i)}, \quad i = 1, \ldots, N.$ ▷ Update the weights as per (3.10).
6: Resample $\boldsymbol{x}_t^{(i)}$ and reset $w_t^{(i)}$ using Algorithm 3, $\quad i = 1, \ldots, N.$
7: **end for**

3.4 Using the particle filter to estimate the likelihood

As mentioned in Section 3.3, the particle filter is typically used to approximate the filtering distribution $p(\boldsymbol{x}_t \mid \boldsymbol{y}_{1:t}, \boldsymbol{\theta})$. This will be utilized to provide a tractable approximation to the likelihood $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$ such that the limiting distribution of the Metropolis-Hastings Markov chain remains unaffected. This section describes how it is done, and gives the resulting variant of the sampler

Likelihood estimate in general Suppose that we are in possession of an estimator $\widehat{z}$ of the likelihood $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$. As such, it necessarily depends on $\boldsymbol{y}_{1:T}$ and $\boldsymbol{\theta}$. Since we aim to use the particle filter to calculate $\widehat{z}$, the estimator also depends on the importance weights calculated using random samples $\boldsymbol{x}_t^{(i)}$. This makes the estimator a random variable with some distribution denoted $\psi(z \mid \boldsymbol{\theta}, \boldsymbol{y}_{1:T})$. It is not necessary to have this distribution available, as it is later shown to cancel out in the Metropolis-Hastings acceptance ratio.

We now return to our model (3.4) and introduce $\widehat{z}$ as an auxiliary variable, along with our variable of interest $\boldsymbol{\theta}$. This changes the target distribution from $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$ to

$$\psi(\boldsymbol{\theta}, z \mid \boldsymbol{y}_{1:T}) = p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T}) \psi(z \mid \boldsymbol{\theta}, \boldsymbol{y}_{1:T}) = \frac{p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) \pi(\boldsymbol{\theta})}{p(\boldsymbol{y}_{1:T})} \psi(z \mid \boldsymbol{\theta}, \boldsymbol{y}_{1:T}). \tag{3.11}$$

In theory, we could now construct a Metropolis-Hastings algorithm with $\psi(\boldsymbol{\theta}, z \mid \boldsymbol{y}_{1:T})$ as the target, instead of $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$ as was the case in Algorithm 1. However, this would not solve our problem, since calculating the acceptance ratio still requires the calculation of the likelihood $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$, as (3.11) makes clear.

Instead, we define a new target distribution over $(\boldsymbol{\theta}, \widehat{z})$ by replacing the likelihood in (3.11) by its estimate $\widehat{z}$:

$$\pi(\boldsymbol{\theta}, z \mid \boldsymbol{y}_{1:T}) := \frac{z\pi(\boldsymbol{\theta})}{p(\boldsymbol{y}_{1:T})} \psi(z \mid \boldsymbol{\theta}, \boldsymbol{y}_{1:T}). \tag{3.12}$$

There are of course some conditions imposed on $\pi(\boldsymbol{\theta}, z \mid \boldsymbol{y}_{1:T})$ for it to be useful:

1. $\pi(\boldsymbol{\theta}, z \mid \boldsymbol{y}_{1:T})$ must be non-negative for all $(\boldsymbol{\theta}, z)$;
2. $\pi(\boldsymbol{\theta}, z \mid \boldsymbol{y}_{1:T})$ must integrate to 1;
3. the marginal distribution of $\pi(\boldsymbol{\theta}, z \mid \boldsymbol{y}_{1:T})$ for $\boldsymbol{\theta}$ must be the original target $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$.

The first two conditions simply state that π is a valid probability distribution. The third condition ensures that by constructing a Metropolis-Hastings algorithm with π as the target, the original target distribution is preserved once the auxiliary variables are marginalized out. All three conditions are satisfied if $\widehat{z}$ is a non-negative unbiased estimator of the likelihood $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$. This is shown as follows.

1. Non-negativity of π follows from the assumed non-negativity of the estimator $\widehat{z}$ and validity of the distributions in (3.12).

2, 3. Assume that $\widehat{z}$ is an unbiased estimate of $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$, i.e. that $\mathbb{E}_\psi[\widehat{z}] = p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$. Consider now the marginal of π for $\boldsymbol{\theta}$:

$$\begin{aligned} \int \pi(\boldsymbol{\theta}, z \mid \boldsymbol{y}_{1:T}) \, \mathrm{d}z &= \frac{\pi(\boldsymbol{\theta})}{p(\boldsymbol{y}_{1:T})} \int z\psi(z \mid \boldsymbol{\theta}, \boldsymbol{y}_{1:T}) \, \mathrm{d}z \\ &= \frac{\pi(\boldsymbol{\theta})}{p(\boldsymbol{y}_{1:T})} \mathbb{E}_\psi[\widehat{z}] \\ &= \frac{\pi(\boldsymbol{\theta})}{p(\boldsymbol{y}_{1:T})} p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) \\ &= p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T}), \end{aligned} \tag{3.13}$$

the original target distribution. This satisfies condition 3. For condition 2, we simply integrate (3.13) w.r.t. $\boldsymbol{\theta}$, which results in unity due to $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$ being a valid probability distribution.

Acceptance ratio computation Given the new target distribution π, we can now construct a Metropolis-Hastings algorithm on the joint space of $(\boldsymbol{\theta}, z)$.

This means that the proposed samples are now given as $(\boldsymbol{\theta}', z') \sim \psi(\cdot, \cdot \mid \boldsymbol{y}_{1:T})$. In practice, this is done by first sampling $\boldsymbol{\theta}' \sim q(\cdot \mid \boldsymbol{\theta}^{(m-1)})$, and then $\widehat{z}' \sim \psi(\cdot \mid \boldsymbol{\theta}', \boldsymbol{y}_{1:T})$. The acceptance ratio can now be computed as

$$\begin{aligned} \alpha &= \min\left\{1, \frac{\pi(\boldsymbol{\theta}', z' \mid \boldsymbol{y}_{1:T})}{\pi(\boldsymbol{\theta}^{(m-1)}, z^{(m-1)} \mid \boldsymbol{y}_{1:T})} \frac{q(\boldsymbol{\theta}^{(m-1)} \mid \boldsymbol{\theta}')\psi(z^{(m-1)} \mid \boldsymbol{\theta}^{(m-1)}, \boldsymbol{y}_{1:T})}{q(\boldsymbol{\theta}' \mid \boldsymbol{\theta}^{(m-1)})\psi(z' \mid \boldsymbol{\theta}', \boldsymbol{y}_{1:T})}\right\} \\ &= \min\left\{1, \frac{z'\pi(\boldsymbol{\theta}')\psi(z' \mid \boldsymbol{\theta}', \boldsymbol{y}_{1:T})}{z^{(m-1)}\pi(\boldsymbol{\theta}^{(m-1)})\psi(z^{(m-1)} \mid \boldsymbol{\theta}^{(m-1)}, \boldsymbol{y}_{1:T})} \frac{q(\boldsymbol{\theta}^{(m-1)} \mid \boldsymbol{\theta}')\psi(z^{(m-1)} \mid \boldsymbol{\theta}^{(m-1)}, \boldsymbol{y}_{1:T})}{q(\boldsymbol{\theta}' \mid \boldsymbol{\theta}^{(m-1)})\psi(z' \mid \boldsymbol{\theta}', \boldsymbol{y}_{1:T})}\right\} \\ &= \min\left\{1, \frac{z'\pi(\boldsymbol{\theta}')}{z^{(m-1)}\pi(\boldsymbol{\theta}^{(m-1)})} \frac{q(\boldsymbol{\theta}^{(m-1)} \mid \boldsymbol{\theta}')}{q(\boldsymbol{\theta}' \mid \boldsymbol{\theta}^{(m-1)})}\right\}. \end{aligned}$$

Since (3.13) shows that the marginal of π for $\boldsymbol{\theta}$ is the original target $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$, all we need to do is to discard the sampled $\widehat{z}^{(m)}$ and keep only $\boldsymbol{\theta}^{(m)}$ when running Metropolis-Hastings on the joint space of $(\boldsymbol{\theta}, z)$.

Calculating the estimate using the particle filter Finally, we describe how exactly is the particle filter used as an estimator of $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$.

First, we decompose the likelihood into a product of simpler distributions, which are then marginalized over the corresponding hidden state:

$$\begin{aligned} p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) &= \prod_{t=1}^{T} p(\boldsymbol{y}_t \mid \boldsymbol{y}_{1:t-1}, \boldsymbol{\theta}) \\ &= \prod_{t=1}^{T} \int p(\boldsymbol{y}_t, \boldsymbol{x}_t \mid \boldsymbol{y}_{1:t-1}, \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{x}_t \\ &= \prod_{t=1}^{T} \int p(\boldsymbol{y}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta}) p(\boldsymbol{x}_t \mid \boldsymbol{y}_{1:t-1}, \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{x}_t. \end{aligned} \tag{3.14}$$

Using the particles $\left\{\boldsymbol{x}_t^{(i)}\right\}_{i=1}^{N}$, we plug in the empirical approximation to $p(\boldsymbol{x}_t \mid \boldsymbol{y}_{1:t-1}, \boldsymbol{\theta})$, $\widehat{p}(\boldsymbol{x}_t \mid \boldsymbol{y}_{1:t-1}, \boldsymbol{\theta}) = \frac{1}{N} \sum_{i=1}^{N} \delta_{\boldsymbol{x}_t^{(i)}}(\boldsymbol{x}_t)$, into (3.14), obtaining

$$\begin{aligned} p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) &\approx \prod_{t=1}^{T} \int p(\boldsymbol{y}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta}) \left[\frac{1}{N} \sum_{i=1}^{N} \delta_{\boldsymbol{x}_t^{(i)}}(\boldsymbol{x}_t) \right] \mathrm{d}\boldsymbol{x}_t \\ &= \prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} \int p(\boldsymbol{y}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta}) \delta_{\boldsymbol{x}_t^{(i)}}(\boldsymbol{x}_t) \, \mathrm{d}\boldsymbol{x}_t \\ &= \prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} p(\boldsymbol{y}_t \mid \boldsymbol{x}_t^{(i)}, \boldsymbol{\theta}) \end{aligned}$$

due to linearity of the integral and properties of the Dirac distribution.

In $p(\boldsymbol{y}_t \mid \boldsymbol{x}_t^{(i)}, \boldsymbol{\theta})$, we recognize the particle filter weights $w_t^{(i)}$ defined in (3.10). This allows us to finally define the likelihood estimate as

$$\widehat{z} := \prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} w_t^{(i)}. \tag{3.15}$$

This estimator is obviously non-negative due to construction of the weights. The proof that it is also unbiased (and therefore also integrates to unity) is more involved, and the reader is referred to Del Moral (2004) for the original proof.

Finally, we describe the resulting variant of the Metropolis-Hastings algorithm employing the likelihood estimate (3.15).

This algorithm, called marginal Metropolis-Hastings, was introduced by Andrieu et al. (2010). Compared to Algorithm 1, all components of this algorithm can be evaluated. Due to construction of the estimator $\widehat{z}$, the marginal of the limiting distribution of Algorithm 5 is the original target $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$.

Algorithm 5 Marginal Metropolis-Hastings

Input: Number of samples M, $\{y_1, \ldots, y_T\}$.

1: Initialize $\theta^{(0)}$.
2: Run Algorithm 4 with $\theta^{(0)}$ to obtain the weights $w_{0,t}^{(i)}, \quad t = 1, \ldots, T, \ i = 1, \ldots, N$.
3: Calculate $\widehat{z}^{(0)}$ according to (3.15) using $w_{0,t}^{(i)}$.
4: **for** $m = 1$ **to** M **do**
5: Sample $\theta' \sim q(\cdot \mid \theta^{(m-1)})$.
6: Run Algorithm 4 with θ' to obtain the weights $w_{m,t}^{(i)}, \quad t = 1, \ldots, T, \ i = 1, \ldots, N$.
7: Calculate $\widehat{z}'$ according to (3.15) using $w_{m,t}^{(i)}$.
8: Calculate the aceptance probability

$$\alpha = \min\left\{1, \frac{\widehat{z}'\pi(\theta')}{\widehat{z}^{(m-1)}\pi(\theta^{(m-1)})} \frac{q(\theta^{(m-1)} \mid \theta')}{q(\theta' \mid \theta^{(m-1)})}\right\}.$$

9: Sample $u \sim \mathcal{U}(0, 1)$.
10: **if** $u \leq \alpha$ **then**
11: $\left(\theta^{(m)}, \widehat{z}^{(m)}\right) \leftarrow (\theta', \widehat{z}')$ ▷ With probability α, accept the proposed sample.
12: **else**
13: $\left(\theta^{(m)}, \widehat{z}^{(m)}\right) \leftarrow \left(\theta^{(m-1)}, \widehat{z}^{(m-1)}\right)$ ▷ With probability $1 - \alpha$, reject the proposed sample.
14: **end if**
15: **end for**

Output: $\left\{\theta^{(1)}, \ldots, \theta^{(M)}\right\}$

Chapter 4

Approximate Bayesian Computation

This chapter discusses the methodology of Approximate Bayesian Computation (ABC). We first motivate the use of ABC methods in our problem in Section 4.1. Then, in Section 4.2, we describe the method in general and discuss some limitations. Section 4.3 then introduces the ABC to our state-space model framework, and addresses some potential issues through kernel functions. Finally, in Section 4.4, we summarize how exactly is the ABC method used in our model, and provide an alternative variant of the Metropolis-Hastings algorithm which relies on ABC instead of the particle filter to estimate the likelihood.

4.1 Motivation

In the previous chapter, we have derived a way to bypass the likelihood function evaluation when calculating the Metropolis-Hastings acceptance ratio. The method relies on the particle filter to calculate a set of weights $w_t^{(i)} \propto g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t^{(i)}, \boldsymbol{\theta})$, where g_t is the observation model defined in (3.1). These weights are then used to estimate the likelihood $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$, as given in (3.15). However, calculating the weights in such way requires full knowledge of this observation model.

In practice, one may not have access to a correct observation model in the form of a probability density g_t. Instead, only a model of the process which generates an observation $\boldsymbol{y}_t$ from the latent state $\boldsymbol{x}_t$ may be available. This generative process may take the form of a differential equation, chemical reaction, simulation, etc. One is then in possession of a mean to generate an observation, but not to evaluate how probable it is. By attempting to fit an arbitrary probability distribution to this generative model, an error is necessarily introduced. The particle filter weights might then not reflect reality, and would lead to incorrect results when using such misspecified model for g_t.

Instead, we can utilize our knowledge of the generative process $\boldsymbol{x}_t \mapsto \boldsymbol{y}_t$ to simulate a number of pseudo-observations $\boldsymbol{u}_t$, and use them to approximate the likelihood $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$. Then, we need not evaluate g_t, and so inference can proceed even without knowing the observation model density. This is exactly the idea behind the approximate Bayesian computation methodology, and is discussed in more detail in the next section.

Unfortunately, such approximation comes with a price. In Chapter 3, it has been shown that using the particle filter does not introduce any approximation error, since the likelihood estimate is unbiased, and leaves the limiting distribution of the Metropolis-Hastings Markov chain intact. This is not the case when applying ABC methods, and is addressed in Section 4.3.

4.2 ABC in general

Before describing how to apply ABC in our SSM framework in Section 4.3, we first review the method in general. Since the SSM framework does not require as general variant, we do not give a detailed treatment, and instead refer the reader to some of the literature mentioned below. This section should mostly give an idea of what exactly does ABC attempt to accomplish. Later on, we spend more time discussing the parts relevant to our problem.

One thing to note is that ABC has traditionally been applied to estimate the posterior $p(\boldsymbol{\theta} \mid \boldsymbol{y})$ for some parameter $\boldsymbol{\theta}$ and observation $\boldsymbol{y}$. The method is considered with this in mind, and in Section 4.3, we describe how use it to estimate the likelihood instead.

Approximate Bayesian Computation The methodology of ABC dates back to Rubin et al. (1984), where a procedure using simulated psedudo-observations to approximate the posterior distribution was first described. Lately, ABC methods have gained popularity in modelling biological processes (Pritchard et al., 1999). A more recent review can be found in Marin et al. (2012).

In its classical formulation, ABC provides a way to approximate an intractable posterior $p(\boldsymbol{\theta} \mid \boldsymbol{y}) \propto p(\boldsymbol{y} \mid \boldsymbol{\theta})\pi(\boldsymbol{\theta})$ by introducing an auxiliary variable $\boldsymbol{u}$. The posterior approximation is then constructed by integrating over this variable (Jasra et al., 2012), and considering only values sufficiently close to the true measurement. It takes the form of

$$p(\boldsymbol{\theta} \mid \boldsymbol{y}) \approx p^{\epsilon}(\boldsymbol{\theta} \mid \boldsymbol{y}) = \frac{\int \mathbb{I}_{\mathcal{A}_{\epsilon,\boldsymbol{y}}}(\boldsymbol{u}) p(\boldsymbol{u} \mid \boldsymbol{\theta}) \pi(\boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{u}}{\int_{\mathcal{A}_{\epsilon,\boldsymbol{y}}} \mathrm{d}\boldsymbol{u}}, \tag{4.1}$$

where $\mathbb{I}_{\mathcal{A}_{\epsilon,\boldsymbol{y}}}$ is the indicator function of a set $\mathcal{A}_{\epsilon,\boldsymbol{y}} = \left\{\boldsymbol{u} \in \mathbb{R}^{d_y} : \rho(\boldsymbol{u},\boldsymbol{y}) \leq \epsilon\right\}$ and $\rho : \mathbb{R}^{d_y} \times \mathbb{R}^{d_y} \to \mathbb{R}$ is a metric, typically the Euclidean distance.

The motivation behind (4.1) is that such integral can be approximated by randomly sampling from the likelihood $p(\cdot \mid \boldsymbol{\theta})$ without needing to evaluate it. This way, the likelihood can exist only conceptually, and we are able to simulate samples $\boldsymbol{u}$ from a model reflecting some real-world process, without considering the underlying probability density.

The hyper-parameter $\epsilon \geq 0$ controls how far can the auxiliary variable $\boldsymbol{u}$ be from the true measurement $\boldsymbol{y}$ for them to be considered similar. Clearly, if we set $\epsilon = 0$, the integral becomes $p(\boldsymbol{y} \mid \boldsymbol{\theta})\pi(\boldsymbol{\theta})$, and we recover the true posterior. In general, the smaller ϵ, the better approximation is obtained, though at the cost of increased computational complexity, discussed in the next paragraph.

To avoid the curse of dimensionality, a summary statistic $\boldsymbol{s} : \mathbb{R}^{d_y} \to \mathbb{R}^p$, $1 \leq p < d_y$ is often introduced. Instead of comparing $\rho(\boldsymbol{u},\boldsymbol{y}) \leq \epsilon$, one then compares $\rho(\boldsymbol{s}(\boldsymbol{u}),\boldsymbol{s}(\boldsymbol{y})) \leq \epsilon$ (assuming that the metric has been redefined to $\rho : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$).

It can be shown that if $\boldsymbol{s}$ is a sufficient statistic for the parameter $\boldsymbol{\theta}$, the probability density $p^{\epsilon}(\boldsymbol{\theta} \mid \boldsymbol{y})$ converges to $p(\boldsymbol{\theta} \mid \boldsymbol{y})$ as $\epsilon \to 0$ (Jasra, 2015). However, it is typically impossible to find such statistic outside of the exponential family of distributions. Otherwise, using a statistic that is not sufficient introduces an additional approximation error.

Basic version of the ABC simulation We now give a basic variant of a sampling-based approximation to $p^{\epsilon}(\boldsymbol{\theta} \mid \boldsymbol{y})$. In the spirit of (4.1), the algorithm performs rejection sampling by comparing whether a sampled $\boldsymbol{u}$ is in $\mathcal{A}_{\epsilon,\boldsymbol{y}}$ or not. After describing the algorithm, we discuss some limitations of this basic approach.

The algorithm iteratively samples parameters $\boldsymbol{\theta}'$ from the prior, plugs them into the likelihood $p(\cdot \mid \boldsymbol{\theta}')$, and simulates pseudo-observations $\boldsymbol{u}$. These are then compared to

Algorithm 6 ABC Rejection Algorithm

Input: Number of samples M, observation $\boldsymbol{y}$, metric ρ, maximum distance ϵ.

$i \leftarrow 1$
while $i \leq M$ **do**
  Sample $\boldsymbol{\theta}' \sim \pi(\cdot)$. ▷ Sample from the prior.
  Simulate $\boldsymbol{u}$ from $p(\cdot \mid \boldsymbol{\theta}')$. ▷ Simulate a pseudo-observation.
  if $\rho(\boldsymbol{u}, \boldsymbol{y}) \leq \epsilon$ **then**
    $\boldsymbol{\theta}^{(i)} \leftarrow \boldsymbol{\theta}'$ ▷ Accept the proposed sample.
    $i \leftarrow i + 1$
  end if
end while

Output: Accepted samples $\left\{\boldsymbol{\theta}^{(1)}, \ldots, \boldsymbol{\theta}^{(M)}\right\}$.

the true measurement $\boldsymbol{y}$ using the metric ρ. If the proposed parameter $\boldsymbol{\theta}'$ gave rise to a pseudo-observation similar enough to the true $\boldsymbol{y}$ (i.e. $\boldsymbol{u} \in \mathcal{A}_{\epsilon,\boldsymbol{y}}$), the parameter is kept under the assumption that the true data are likely under $\boldsymbol{\theta}'$. The ABC approximation is then given in terms of the accepted samples $\boldsymbol{\theta}^{(1)}, \ldots, \boldsymbol{\theta}^{(M)}$ as the empirical distribution

$$p(\boldsymbol{\theta} \mid \boldsymbol{y}) \approx \frac{1}{M} \sum_{i=1}^{M} \delta_{\boldsymbol{\theta}^{(i)}}(\boldsymbol{\theta}).$$

Setting a low value of ϵ increases the approximation accuracy, at the cost of increased rejection rate. On the other hand, setting ϵ too large causes the algorithm to accept more often, but leads to simulating pseudo-measurements dissimilar to $\boldsymbol{y}$ and, in turn, incorrect $\boldsymbol{\theta}^{(i)}$. Setting a suitable value of ϵ is therefore the main difficulty when using ABC. Several approaches are discussed by Jasra et al. (2012); Jasra (2015). One particular way (Dedecius, 2017) is used in Section 4.3 in the context of SSMs.

There are many improvement to the basic ABC of Algorithm 6, discussed for instance by Marin et al. (2012). In particular, more sophisticated sampling approaches relying again on MCMC are described. This is not an issue relevant to the SSM framework, as the samples are generated in a different fashion, given in the next section.

4.3 ABC in SSMs

Next, we describe how exactly is the ABC methodology applied in the context of SSMs.

Section 4.2 states that the typical use case of ABC arises in cases where we have knowledge about the data-generating process, but are unable to evaluate the probability of such data. In the context of SSMs, this translates into knowing how the observed values $\boldsymbol{y}_t$ have been generated from the latent states $\boldsymbol{x}_t$, but being unable to evaluate the density $g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta})$. This prevents us from calculating the importance weights w_t through the particle filter, which relies on the availability of g_t.

The papers Toni et al. (2009) and Jasra et al. (2012) describe how a filter could be constructed using the ABC approximation. Additionally, Jasra (2015) applies this filter in the context of SSMs. We first discuss the construction of this filter. Afterwards, we address a particular limitation of this approach through kernel functions.

Filter construction through ABC In SSMs, the observations $\boldsymbol{y}_t$ are typically low-dimensional, often scalar quantities. It is then not necessary to consider any summary statistics.

Jasra et al. (2012) consider a modification of the particle filter (Algorithm 4) which simulates pseudo-observations according to the observation model, and calculates the

importance weights based on their closeness to the true measurements. The pseudocode is given in Algorithm 7.

Algorithm 7 ABC-based filter

Input: Number of particles N, current parameter value $\boldsymbol{\theta}$, maximum distance ϵ, $\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_T\}$.

1: Sample $\boldsymbol{x}_0^{(i)} \sim p(\cdot \mid \boldsymbol{\theta}), \quad i = 1, \ldots, N.$ ▷ Initialize N particles.
2: $w_0^{(i)} \leftarrow \frac{1}{N}, \quad i = 1, \ldots, N.$ ▷ Initialize uniform weights.
3: **for** $t = 1$ **to** T **do**
4: Sample $\boldsymbol{x}_t^{(i)} \sim f_t(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}^{(i)}, \boldsymbol{\theta}), \quad i = 1, \ldots, N.$ ▷ Sample N new particles.
5: Simulate $\boldsymbol{u}_t^{(i)}$ from $g_t(\cdot \mid \boldsymbol{x}_t^{(i)}), \quad i = 1, \ldots, N.$ ▷ Simulate N pseudo-observations.
6: Set $w_t^{(i)} \propto \mathbb{I}_{\mathcal{A}_{\epsilon, \boldsymbol{y}_t}}(\boldsymbol{u}_t^{(i)}) w_{t-1}^{(i)}, \quad i = 1, \ldots, N.$
7: Resample $\boldsymbol{x}_t^{(i)}$ and reset $w_t^{(i)}$ using Algorithm 3, $\quad i = 1, \ldots, N.$
8: **end for**

The algorithm proceeds similarly to Algorithm 4 except for the way the weights are computed. Instead of evaluating the unavailable density g_t at the true observation $\boldsymbol{y}_t$, a pseudo-observation $\boldsymbol{u}_t$ is simulated. The weight is then set to a non-zero value if $\boldsymbol{u}_t \in \mathcal{A}_{\epsilon, \boldsymbol{y}_t}$, and 0 otherwise. It may seem that the weights for the same particle i necessarily collapse to 0 after a number of time steps due to the recursive multiplication in step 6. However, step 7 resets the weights uniformly after resampling, so such collapse does not occur.

Analogously to Section 3.4, the weights are then used to approximate the likelihood $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$. According to Jasra (2015), the estimate is given by

$$\widehat{z} = \prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} \frac{w_t^{(i)}}{\int_{\mathcal{A}_{\epsilon, \boldsymbol{y}_t}} \mathrm{d}\boldsymbol{u}}. \tag{4.2}$$

The integral in the denominator essentially normalizes the weights $w_t^{(i)}$ to be equal to the probability density of $\mathcal{U}(\boldsymbol{y}_t; \epsilon)$, the uniform distribution in a sphere centered at $\boldsymbol{y}_t$ with radius ϵ given in terms of the metric ρ.

Bias The use of this ABC filter introduces bias to the parameter inference. Recall that in Section 3.4, we required $\widehat{z}$ to be an unbiased estimator of $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$. This was the case when the weights were calculated according to $w_t^{(i)} \propto g_t(\boldsymbol{y}_t \mid \boldsymbol{x}_t) w_{t-1}^{(i)}$. This unbiasedness is not preserved here, since $\widehat{z}$ estimates

$$\begin{aligned} p^{\epsilon}(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) &= \int p^{\epsilon}(\boldsymbol{x}_{0:T}, \boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{x}_{0:T} \\ &= \int p(\boldsymbol{x}_0 \mid \boldsymbol{\theta}) \prod_{t=1}^{T} f_t(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{\theta}) g_t^{\epsilon}(\boldsymbol{y}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{x}_{0:T}, \end{aligned}$$

(compare the inside of the integral with (3.1)), as noted by Jasra (2015). Here the approximate observation density is given by the ABC form

$$g_t^{\epsilon}(\boldsymbol{y}_t \mid \boldsymbol{x}_t, \boldsymbol{\theta}) = \frac{\int \mathbb{I}_{\mathcal{A}_{\epsilon, \boldsymbol{y}_t}}(\boldsymbol{u}) g_t(\boldsymbol{u} \mid \boldsymbol{x}_t, \boldsymbol{\theta}) \, \mathrm{d}\boldsymbol{u}}{\int_{\mathcal{A}_{\epsilon, \boldsymbol{y}_t}} \mathrm{d}\boldsymbol{u}},$$

similarly to (4.1). This essentially means that by plugging (4.2) into the Metropolis-Hastings acceptance ratio, the limiting distribution of the underlying Markov chain becomes $p^{\epsilon}(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T}) \propto p^{\epsilon}(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta}) \pi(\boldsymbol{\theta})$, instead of the correct $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$. In general, this bias cannot be dealt with, and is a price to pay for using the incorrect observation model.

An interesting way to address this deficiency has been proposed by Fearnhead and Prangle and by Wilkinson (2013). The authors note that one uses data $\boldsymbol{y}_{1:T}$ assumed to have been generated according to (3.1), $p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$, but fitting the ABC approximation $p^{\epsilon}(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})$. In an attempt to bring the data closer the model being really fitted, the authors use a sequence of perturbed observations $\boldsymbol{z}_t = \boldsymbol{y}_t + \boldsymbol{v}$, $\boldsymbol{v} \sim \mathcal{U}(\mathbf{0}; \epsilon)$ which denotes the uniform distribution in a sphere given by ρ, with radius ϵ and centered at the origin. It is proved that if $\boldsymbol{\theta}$ is estimated according to maximum likelihood, the estimate is consistent when using the perturbed sequence $\boldsymbol{z}_{1:T}$. This approach is called the Noisy ABC.

Use of kernel functions A limitation of Algorithm 6 and Algorithm 7 lies in the use of the indicator function $\mathbb{I}_{\mathcal{A}_{\epsilon,\boldsymbol{y}}}$. There are two problems:

1. A practical one; it may happen that no samples are accepted, and the output is null in case of Algorithm 6, or too many weights become zero in case of Algorithm 7, and the filter collapses.

2. A more fundamental one, the simulated pseudo-observations $\boldsymbol{u}_t$ are all assigned equal weights, regardless of how far they lie from the true measurement $\boldsymbol{y}_t$. Intuitively, a pseudo-observation closer to the true $\boldsymbol{y}_t$ should be assigned a higher weight than one which is further away.

Both issues can be mitigated by considering a general kernel function in place of the indicator $\mathbb{I}_{\mathcal{A}_{\epsilon,\boldsymbol{y}}}$. Let a kernel of width ϵ centered at $\boldsymbol{y}$ and evaluated at $\boldsymbol{u}$ be denoted by $\kappa(\boldsymbol{u}; \boldsymbol{y}, \epsilon)$. In machine learning, kernel functions are often taken *proportional* to some symmetric probability density function (Hastie et al., 2001). However, as we aim to replace the indicator function $\mathbb{I}_{\mathcal{A}_{\epsilon,\boldsymbol{y}}}$ by such kernel, we require the kernel to be properly normalized (integrate to unity), to mirror the normalization in (4.2).

With such kernel function, we can then write $w_t^{(i)} \propto \kappa(\boldsymbol{u}_t; \boldsymbol{y}_t, \epsilon) w_{t-1}^{(i)}$. The likelihood estimate (4.2) then becomes

$$\widehat{z} = \prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} w_t^{(i)} \tag{4.3}$$

due to the kernel having been normalized. This way, the weights are no longer uniformly set, but instead reflect the distance of $\boldsymbol{u}_t$ from $\boldsymbol{y}_t$. There is also no risk of the filter collapsing due to majority of the weights becoming zero.

Introducing the kernel function to the weights computation is in principle similar to using importance sampling rather than simple rejection sampling (MacKay, 2002). Instead of accepting/rejecting the generated samples based on whether they match some criterion, they are all accepted, and weighted according to *how well* they match it.

With the kernel functions in mind, we describe a procedure for automatic tuning of the kernel width ϵ, which has been ignored thus far. The adopted method has been derived in a one-dimensional setting, i.e. $\boldsymbol{u}, \boldsymbol{y} \in \mathbb{R}$. We thus denote $\boldsymbol{y}$ by y and $\boldsymbol{u}$ by u, them being scalar quantities. When considering multivariate observations, the kernels are applied coordinate-wise (assuming independence between the components of $\boldsymbol{y}$ or $\boldsymbol{u}$, respectively).

Before describing the kernel tuning procedure, we give several examples of commonly used kernel functions and comment on their usage. The kernels are shown in Figure 4.1.

1. **Gaussian kernel** The Gaussian kernel takes the form

$$\kappa(u; y, \epsilon) = \frac{1}{\sqrt{2\pi\epsilon^2}} \exp\left\{-\frac{(u-y)^2}{2\epsilon^2}\right\}.$$

   It is one of the most-commonly used kernel functions.

2. **Cauchy kernel** The Cauchy kernel takes the form

$$\kappa(u; y, \epsilon) = \frac{1}{\pi\epsilon\left[1 + \left(\frac{u-y}{\epsilon}\right)^2\right]}.$$

As opposed to the Gaussian distribution, the Cauchy distribution has heavier tails, and so it is suitable for situations with potential distant observations. This kernel typically assigns non-trivial probability even to distant pseudo-observations, and so the filter does not collapse even under outliers.

3. **Uniform kernel** The uniform kernel takes the form

$$\kappa(u; y, \epsilon) = \begin{cases} \frac{1}{2\epsilon}, & y - \epsilon < u < y + \epsilon; \\ 0, & \text{otherwise.} \end{cases}$$

Using this kernel, we recover the standard ABC which accepts u if $u \in \mathcal{A}_{\epsilon,y} = \left\{u : \left|u - y\right| < \epsilon\right\}$. If we are in a situation with multivariate observations $\boldsymbol{y}_t$ and apply the uniform kernel coordinate-wise, the set of accepted samples coincides with the standard ABC using $\rho(\boldsymbol{u}, \boldsymbol{y}) = \max_{i=1}^{d_y} \left|u_i - y_i\right|$, the L_∞ distance.

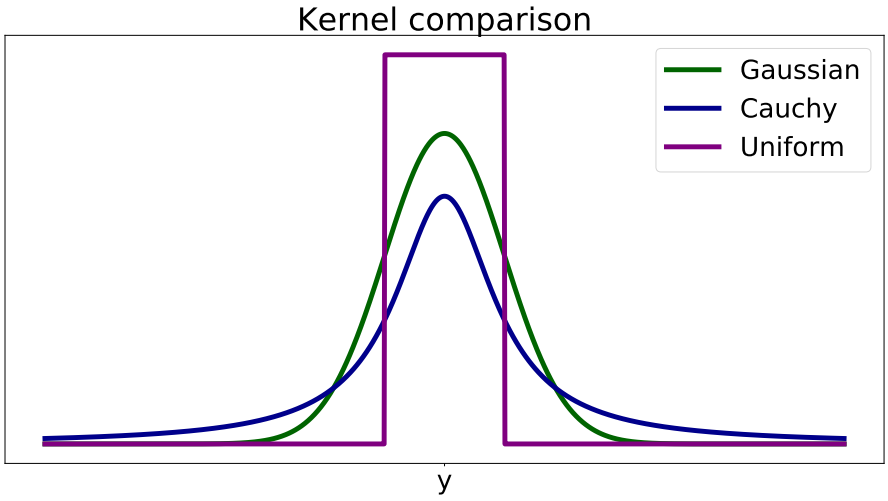

Figure 4.1: The Gaussian, Cauchy and uniform kernel functions centered at $y = 0$ with width $\epsilon = 3$.

The Noisy ABC procedure described above is then naturally generalized by perturbing the observations by samples from a given kernel, instead of the uniform distribution in a ball.

Kernel width tuning In this paragraph, we address the issue of tuning the kernel width ϵ. Since the previous section has shown that the indicator function $\mathbb{I}_{\mathcal{A}_{\epsilon,y}}$ is recovered by a particular kernel, the method also applies to the standard ABC formulation.

A careful setting of ϵ is necessary. When the kernel width is too low, most of the N generated pseudo-observations are assigned with low probabilities, and the importance weights are close to zero. On the other hand, when the width is too high, even outlying pseudo-observations are assigned a non-trivial probability and shift the filter to incorrect values. In addition, the kernel becomes flat and close to the uniform variant. A manual

setting of ϵ is thus a non-obvious task without any guidelines in the data. Additionally, the width should somehow reflect the filter evolution over time, since all observations $\boldsymbol{y}_t$ are different and may require different kernel widths.

In this thesis, we adopt a procedure described by Dedecius (2017), which is briefly reviewed below. More details can be found in the original paper.

The method is based on the idea that the true observation model g_t should cover a given number of generated pseudo-observations $\boldsymbol{u}_t^{(i)}, i = 1,\dots,N$ by a $100p\%$ high probability region (p-HPR), where $p \in (0,1)$ is a given constant. If this is true, the pseudo-observations can be expected to describe the distribution g_t sufficiently-well. As this distribution is not known, it is approximated by the kernel κ evaluated at $\boldsymbol{u}_t^{(i)}, i = 1,\dots,N$.

As given in (4.3), the kernel is evaluated at each pseudo-observation $\boldsymbol{u}_t^{(i)}, i = 1,\dots,N$ while centered at $\boldsymbol{y}_t$. We then need to tune the width at time t, denoted ϵ_t, so that a given fraction $\frac{\alpha}{N}$ of the pseudo-observations is covered by the p-HPR of the kernel. For the procedure to work, the kernel function κ must be invariant under translation and scaling, i.e. belong to the location-scale family of distributions. Many popular kernels, including the three discussed above, belong to this family.

The tuning procedure involves two steps:

1. Identify $u_t^{[\alpha]}$, the αth closest pseudo-observation to y_t.

2. Center the kernel κ at y_t and set the width ϵ_t so that

$$\left| \int_{y_t}^{u_t^{[\alpha]}} \kappa(u_t; y_t, \epsilon_t)\, \mathrm{d}u_t \right| = \frac{p}{2}, \tag{4.4}$$

   meaning that $u_t^{[\alpha]}$ lies at the boundary of the p-HPR of $\kappa(\cdot; y_t, \epsilon_t)$.

These two steps are visualized in Figure 4.2. In case of multidimensional $\boldsymbol{y}_t$ and $\boldsymbol{u}_t$, this procedure is performed coordinate-wise.

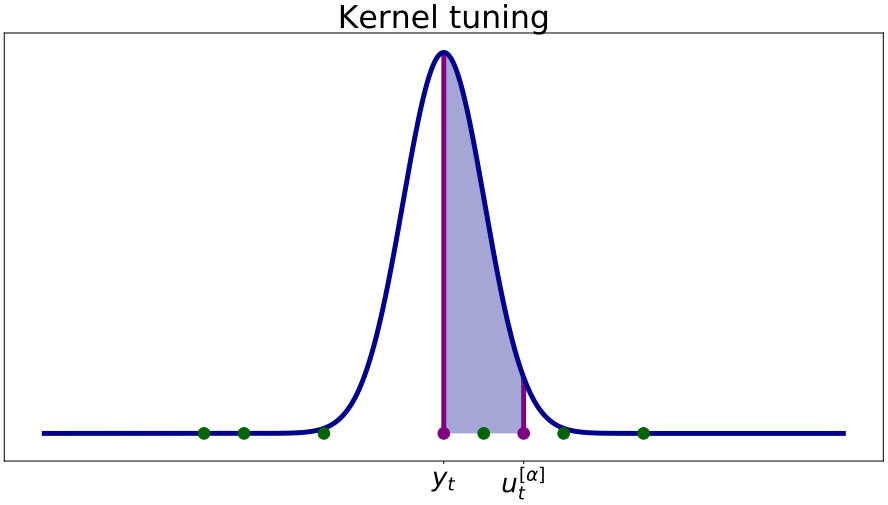

Figure 4.2: Visualization of the kernel tuning procedure. In this picture, $\alpha = 2$, $p = 0.95$, and the kernel is Gaussian. Plotted is the kernel along with a number of pseudo-observations $u_t^{(i)}$ and the true measurement y_t. Equation (4.4) states that the shaded area has volume $\frac{p}{2} = 0.475$.

The meaning of equation (4.4) is that $u_t^{[\alpha]}$ is either the $\frac{1-p}{2}$-quantile or the $\frac{1+p}{2}$-quantile of $\kappa(\cdot; y_t, \epsilon_t)$, depending on whether $u_t^{[\alpha]} \leq y_t$ or $u_t^{[\alpha]} \geq y_t$. If we restrict ourselves to symmetric kernels, we may get rid of this case division by exploiting kernel symmetry.

Let F denote the cumulative distribution function of the kernel $\kappa(\cdot; 0, 1)$ centered at 0 with width $\epsilon = 1$. Let its quantile function be denoted by F^{-1}. From κ belonging to the location-scale family, we get that the quantile function of a general kernel $\kappa(\cdot; y_t, \epsilon_t)$ is

$$Q(\beta) = y_t + \epsilon_t F^{-1}(\beta), \quad \beta \in (0, 1). \tag{4.5}$$

As (4.4) and the assumed kernel symmetry require $\left|u_t^{[\alpha]}\right|$ to be the $\frac{1+p}{2}$-quantile of $\kappa(\cdot; y_t, \epsilon_t)$, we can substitute $u_t^{[\alpha]}$ for $Q(\beta)$ in (4.5) and solve for ϵ_t, obtaining

$$\epsilon_t = \frac{\left|u_t^{[\alpha]} - y_t\right|}{F^{-1}(\frac{1+p}{2})}, \tag{4.6}$$

where the absolute value comes from the kernel being symmetric, so it is irrelevant whether we consider pseudo-observations lower or greater than the true observation y_t. The quantile function F^{-1} is uniquely associated with each kernel, and the only free parameters are α and p.

4.4 Likelihood estimate through ABC

To conclude this chapter, we summarize the entire inference about $\boldsymbol{\theta}$ in the model (3.1) when ABC is used to estimate the likelihood, as given in Equation 4.3.

First, we give the ABC-based filter utilizing the kernel weight tuning described above. This is summarized in Algorithm 8. The algorithm is simply a modification of Algo-

Algorithm 8 ABC-based filter with automatic kernel tuning

Input: Number of particles N, current parameter value $\boldsymbol{\theta}$, HPR p, number of covered pseudo-observations α, $\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_T\}$.

1: Sample $\boldsymbol{x}_0^{(i)} \sim p(\cdot \mid \boldsymbol{\theta}), \quad i = 1, \ldots, N.$ ▷ Initialize N particles.
2: $w_0^{(i)} \leftarrow \frac{1}{N}, \quad i = 1, \ldots, N.$ ▷ Initialize uniform weights.
3: **for** $t = 1$ **to** T **do**
4: Sample $\boldsymbol{x}_t^{(i)} \sim f_t(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}^{(i)}, \boldsymbol{\theta}), \quad i = 1, \ldots, N.$ ▷ Sample N new particles.
5: Simulate $\boldsymbol{u}_t^{(i)}$ from $g_t(\cdot \mid \boldsymbol{x}_t^{(i)}), \quad i = 1, \ldots, N.$ ▷ Simulate N pseudo-observations.
6: Identify $\boldsymbol{u}_t^{[\alpha]}$. ▷ Find the αth closest pseudo-observation to $\boldsymbol{y}_t$.
7: $\epsilon_t \leftarrow \frac{\left|u_t^{[\alpha]} - y_t\right|}{F^{-1}(\frac{1+p}{2})}$ ▷ Set the kernel width at time t according to (4.6).
8: Set $w_t^{(i)} \propto \kappa(\boldsymbol{u}_t^{(i)}; \boldsymbol{y}_t, \epsilon_t) w_{t-1}^{(i)}, \quad i = 1, \ldots, N.$
9: Resample $\boldsymbol{x}_t^{(i)}$ and reset $w_t^{(i)}$ using Algorithm 3, $\quad i = 1, \ldots, N.$
10: **end for**

rithm 7 utilizing a kernel function instead of the indicator and accounting for an automatic tuning of the kernel widths.

Next, we describe a variant of the Metropolis-Hastings algorithm utilizing this adaptive filter to estimate the likelihood. This is shown in Algorithm 9. The only difference from Algorithm 5 is the use of the ABC filter (Algorithm 8) to estimate the likelihood according to (4.3).

Algorithm 9 Marginal Metropolis-Hastings with ABC filter

Input: Number of samples M, $\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_T\}$.

1: Initialize $\boldsymbol{\theta}^{(0)}$.
2: Run Algorithm 8 with $\boldsymbol{\theta}^{(0)}$ to obtain the weights $w_{0,t}^{(i)}, \quad t = 1, \ldots, T,\ i = 1, \ldots, N$.
3: Calculate $\widehat{z}^{(0)}$ according to (4.3) using $w_{0,t}^{(i)}$.
4: **for** $m = 1$ **to** M **do**
5: Sample $\boldsymbol{\theta}' \sim q(\cdot \mid \boldsymbol{\theta}^{(m-1)})$.
6: Run Algorithm 8 with $\boldsymbol{\theta}'$ to obtain the weights $w_{m,t}^{(i)}, \quad t = 1, \ldots, T,\ i = 1, \ldots, N$.
7: Calculate $\widehat{z}'$ according to (4.3) using $w_{m,t}^{(i)}$.
8: Calculate the aceptance probability

$$\alpha = \min\left\{1, \frac{\widehat{z}'\pi(\boldsymbol{\theta}')}{\widehat{z}^{(m-1)}\pi(\boldsymbol{\theta}^{(m-1)})} \frac{q(\boldsymbol{\theta}^{(m-1)} \mid \boldsymbol{\theta}')}{q(\boldsymbol{\theta}' \mid \boldsymbol{\theta}^{(m-1)})}\right\}.$$

9: Sample $u \sim \mathcal{U}(0, 1)$.
10: **if** $u \leq \alpha$ **then**
11: $\left(\boldsymbol{\theta}^{(m)}, \widehat{z}^{(m)}\right) \leftarrow (\boldsymbol{\theta}', \widehat{z}')$ ▷ With probability α, accept the proposed sample.
12: **else**
13: $\left(\boldsymbol{\theta}^{(m)}, \widehat{z}^{(m)}\right) \leftarrow \left(\boldsymbol{\theta}^{(m-1)}, \widehat{z}^{(m-1)}\right)$ ▷ With probability $1 - \alpha$, reject the proposed sample.
14: **end if**
15: **end for**

Output: $\left\{\boldsymbol{\theta}^{(1)}, \ldots, \boldsymbol{\theta}^{(M)}\right\}$

Chapter 5

Applications

In this chapter, we apply the models developed earlier to two selected problems. The first problem is the Lotka-Volterra model described in Section 5.2, the second is a simple model for auto-regulation in prokaryotes considered in Section 5.3. The particle filter-based approach is compared with the one depending on ABC methods in various settings and model misspecifications.

Both problems require simulating reactions in order to propagate the system states through time. This is done with the help of the Gillespie algorithm, which is first described in Section 5.1.

5.1 Preliminary: the Gillespie algorithm

The Gillespie algorithm (Gillespie, 1976, 1977) is used to simulate a stochastic process describing the time evolution of a system of reactions. The discussion given here follows Wilkinson (2011).

Time evolution of a reaction system Consider a system consisting of u species $\mathcal{X}_1, \ldots, \mathcal{X}_u$ and v reactions $\mathcal{R}_1, \ldots, \mathcal{R}_v$. The species can describe literal animal species, as is the case in the Lotka-Volterra model in Section 5.2, or individual molecule types, as in Section 5.3. The reactions describe the interactions between these species through time.

Let the number of molecules (or individuals, in case of animal species) of the species $\mathcal{X}_i$ at time t be denoted by $X_{i,t}$, and let $\boldsymbol{X}_t = (X_{1,t}, \ldots, X_{u,t})^T$. Additionally, let the number of reactions of type $\mathcal{R}_i$ which occurred in a time window $(0, t]$ be denoted by $R_{i,t}$, and let $\boldsymbol{R}_t = (R_{1,t}, \ldots, R_{v,t})^T$. The evolution of the system from time 0 to time t is described by the equation

$$\boldsymbol{X}_t - \boldsymbol{X}_0 = \mathbb{S}\boldsymbol{R}_t, \tag{5.1}$$

where $\mathbb{S} \in \mathbb{R}^{u \times v}$ is called the stoichiometry matrix of the system, and describes the difference in the number of molecules of each species after each reaction occurs. To gain insight into the meaning of $\mathbb{S}$, it is instructive to write it as

$$\mathbb{S} = \mathbb{P}_{\text{post}} - \mathbb{P}_{\text{pre}},$$

where the element (i, j) of $\mathbb{P}_{\text{pre}}$ denotes the number of molecules of $\mathcal{X}_i$ before a reaction of type $\mathcal{R}_j$ takes place, and the element (i, j) of $\mathbb{P}_{\text{post}}$ describes the same quantity *after* it takes place. Equation (5.1) can then be written as

$$\boldsymbol{X}_t = \boldsymbol{X}_0 + \left(\mathbb{P}_{\text{post}} - \mathbb{P}_{\text{pre}}\right)\boldsymbol{R}_t,$$

and describes the net gain in the number of molecules of each species, given their initial numbers, and accounting for their increase/decrease when a number of reactions of each type occurs.

In addition, each reaction $\mathcal{R}_i$ has a stochastic rate constant c_i and a rate law (also called the hazard function) $h_i(\boldsymbol{X}_t, c_i)$ associated with it. The interpretation of the hazard function is such that $h_i(\boldsymbol{X}_t, c_i)\mathrm{d}t$ is the probability of a reaction of type $\mathcal{R}_i$ occurring in a time interval $(t, t+\mathrm{d}t]$, conditionally on the system being in state $\boldsymbol{X}_t$. Such a situation is described by an exponential distribution – the time to the event of a reaction of type $\mathcal{R}_i$ occurring, assuming no other reaction is taking place, is distributed according to $\mathcal{E}xp(h_i(\boldsymbol{X}_t, c_i))$. This is however a convenient simplification, since multiple reactions are typically occurring at the same time.

The Gillespie algorithm In a system with v reactions and their hazard functions $h_i(\boldsymbol{X}_t, c_i)$, the hazard of *some* reaction occurring is

$$h_0(\boldsymbol{X}_t, \boldsymbol{c}) = \sum_{i=0}^{v} h_i(\boldsymbol{X}_t, c_i),$$

where $\boldsymbol{c} = (c_1, \ldots, c_v)^T$. The time to the next reaction is then distributed according to $\mathcal{E}xp(h_0(\boldsymbol{X}_t, \boldsymbol{c}))$. The particular reaction type is a random variable with a categorical distribution $\mathcal{C}at(\widetilde{h}_1(\boldsymbol{X}_t, c_1), \ldots, \widetilde{h}_v(\boldsymbol{X}_t, c_v))$, where $\widetilde{h}_i(\boldsymbol{X}_t, c_i) = \dfrac{h_i(\boldsymbol{X}_t, c_i)}{h_0(\boldsymbol{X}_t, \boldsymbol{c})}$.

With the above in mind, the Gillespie algorithm can now be formulated, and is given in Algorithm 10. Its purpose is to simulate the state evolution (5.1) for a given time horizon T while accounting for the randomness in the time until a reaction of a particular type takes place. For the purpose of this algorithm, denote the columns of the stoichiometry matrix $\mathbb{S}$ by $\boldsymbol{S}^i$, $\quad i = 1, \ldots, v$. The algorithm us usually the bottleneck of most

Algorithm 10 Gillespie algorithm

Input: Time horizon T, rate constants $\boldsymbol{c} = (c_1, \ldots, c_v)$, initial molecule numbers $\boldsymbol{X}_0$.

1: $t \leftarrow 0$
2: $\boldsymbol{X}_t \leftarrow \boldsymbol{X}_0$
3: **while** $t \leq T$ **do**
4: Calculate $h_i(\boldsymbol{X}_t, c_i), \quad i = 1, \ldots, v.$
5: $h_0(\boldsymbol{X}_t, \boldsymbol{c}) \leftarrow \sum_{i=1}^{v} h_i(\boldsymbol{X}_t, c_i)$
6: Calculate $\widetilde{h}_i(\boldsymbol{X}_t, c_i) = \dfrac{h_i(\boldsymbol{X}_t, c_i)}{h_0(\boldsymbol{X}_t, \boldsymbol{c})}, \quad i = 1, \ldots, v.$
7: Sample $\mathrm{d}t \sim \mathcal{E}xp(h_0(\boldsymbol{X}_t, \boldsymbol{c}))$. ▷ Simulate the time to the next reaction.
8: Sample $i \sim \mathcal{C}at(\widetilde{h}_1(\boldsymbol{X}_t, c_1), \ldots, \widetilde{h}_v(\boldsymbol{X}_t, c_v))$. ▷ Simulate the reaction type.
9: $\boldsymbol{X}_{t+\mathrm{d}t} \leftarrow \boldsymbol{X}_t + \boldsymbol{S}^i$ ▷ Update the state according to the reaction i.
10: $t \leftarrow t + \mathrm{d}t$
11: **end while**

Output: Final state $\boldsymbol{X}_t$, final time t.

simulations, and must be implemented carefully; otherwise, the simulation becomes unacceptably slow. The final time t is at the output as well, since it may exceed the horizon T. If the algorithm is run consecutively during a simulation, the interest is to follow the previous run by starting at its final time t.

5.2 Lotka-Volterra model

5.3 Prokaryotic auto-regulation model

Chapter 6

Conclusion and future work

TODO: Multivariate kernels and their width tuning.

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