Master Thesis

Bayesian Parameter Estimation of State-Space Models with Intractable Likelihood

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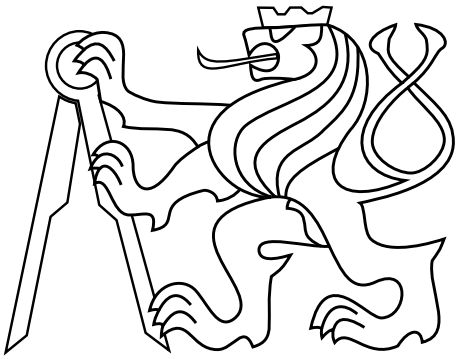

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ZADÁNÍ DIPLOMOVÉ PRÁCE

I. OSOBNÍ A STUDIJNÍ ÚDAJE

Příjmení: **Kala** Jméno: **Tomáš** Osobní číslo: **434690**

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:

Ing. Kamil Dedecius, Ph.D., ÚTIA AV ČR

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**

Ing. Kamil Dedecius, Ph.D. podpis vedoucí(ho) práce	podpis vedoucí(ho) ústavu/katedry	prof. Ing. Pavel Ripka, CSc. podpis děkana(ky)

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

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). Random samples are iteratively generated from the Markov chain transition distribution, called the proposal distribution in this context. 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). A particularly 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 in 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 in 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 samples would get assigned low weights. This has been investigated in 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 nonlinear, 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.

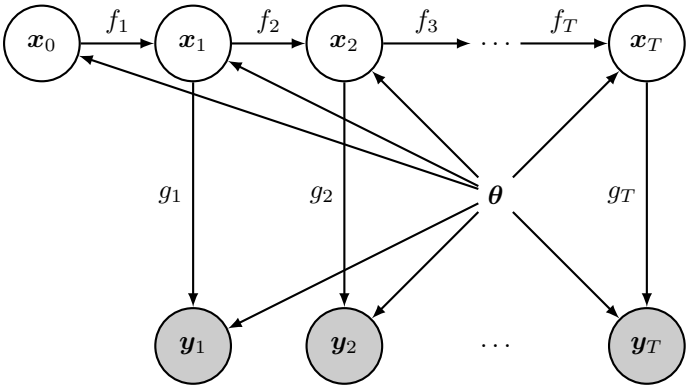

Figure 3.1: Graphical model describing the full joint distribution (3.2). The shaded nodes denote the observed variables, white nodes represent the latent variables.

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

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

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 target distribution is the parameter posterior $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T}) \propto p(\boldsymbol{y}_{1:T} \mid \boldsymbol{\theta})\pi(\boldsymbol{\theta})$. In this case, it is not necessary to evaluate the normalizing constant, since it gets cancelled out.

The algorithm further requires a proposal distribution q. Similarly to the prior π, it is problem-dependent, and must be selected carefully.

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

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,

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

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 probability density $q(\boldsymbol{x}) = \frac{q^*(\boldsymbol{x})}{Z_Q}$ such that

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

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

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 by itself is

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**

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,

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 $\boldsymbol{x}_t^{(i)} \sim f_t(\boldsymbol{x}_t \mid \boldsymbol{x}_{t-1}, \boldsymbol{\theta}), \quad i = 1, \ldots, N.$ ▷ 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**

due to resemblance of the resampling step to the non-parametric bootstrap (Efron, 1979).

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 $\widehat{z}$:

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

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

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

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).

Algorithm 5 Marginal Metropolis-Hastings

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

1: Initialize $\boldsymbol{\theta}^{(0)}$.
2: Run Algorithm 4 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 (3.15) 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 4 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 (3.15) 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: $\left\{\boldsymbol{\theta}^{(1)}, \ldots, \boldsymbol{\theta}^{(M)}\right\}$

This algorithm, called marginal Metropolis-Hastings, was introduced in 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 $p(\boldsymbol{\theta} \mid \boldsymbol{y}_{1:T})$.

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, mention some limitations of the basic formulation, and discuss how to address them using kernel functions. Section 4.3 then introduces the ABC to our state-space model framework. Finally, in Section 4.4, we describe 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 provide a likelihood estimate.

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 a 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 a 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. This is exactly the idea behind the approximate Bayesian computation methodology, and is discussed in more detail in the next section.

4.2 ABC in general

Before describing how to apply ABC in our SSM framework in Section 4.3, we first provide an overview of the method in full generality. 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.

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, and considering only values sufficiently close to the true measurement. It takes the form of

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

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

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 $\boldsymbol{u}^{(i)}$ 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 $\boldsymbol{s} : \mathbb{R}^{d_y} \to \mathbb{R}^p$ where $1 \leq p < d_y$ 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.

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 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 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 to the posterior $p^{\epsilon}(\boldsymbol{\theta} \mid \boldsymbol{y})$ is then given in terms of the accepted samples $\boldsymbol{\theta}^{(1)}, \ldots, \boldsymbol{\theta}^{(M)}$ as the empirical distribution

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

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 correct

value of ϵ is therefore the main difficulty when using ABC. Several approaches are discussed in Jasra et al. (2012); Jasra (2015), and 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 in 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 Section 4.3. Before investigating the use of ABC in SSMs, we consider one more issue in the next section, which will become particularly relevant.

Use of kernel functions TODO: Replacing the uniform kernel by a more general is similar to the importance sampling "improving" rejection sampling.

4.3 ABC in SSMs

4.4 Likelihood estimate through ABC

Chapter 5

Applications

5.1 Preliminary: the Gillespie algorithm

5.2 Lotka-Volterra model

5.3 Prokaryotic auto-regulation model

Chapter 6

Conclusion and future work

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