Comparing Two Recent Particle Filter Implementations of Bayesian System Identification ⋆

Andreas Svensson * **Thomas B. Schön** *

* *Department of Information Technology, Uppsala University, Sweden*
(e-mail: andreas.svensson@it.uu.se, thomas.schon@it.uu.se)

Abstract: Bayesian system identification is a theoretically well-founded and currently emerging area. We describe and evaluate two recent state-of-the-art sample-based methods for Bayesian parameter inference from the statistics literature, particle Metropolis-Hastings (PMH) and SMC^2, and apply them to a non-trivial real world system identification problem with large uncertainty present. We discuss their different properties from a user perspective, and conclude that they show similar performance in practice, while PMH is significantly easier to implement than SMC^2.

Keywords: System identification, particle filters, Monte Carlo methods, Bayesian inference

1. INTRODUCTION

In this paper, we are concerned with methods for learning unknown parameters in nonlinear state space models, i.e., gray box identification. We write the state space model as

$$x_{t+1}|x_t \sim f_\theta(x_{t+1}|x_t), \tag{1a}$$
$$y_t|x_t \sim g_\theta(y_t|x_t), \tag{1b}$$

where $y_t \in \mathbb{R}^{n_y}$ is the observed output, $x_t \in \mathbb{R}^{n_x}$ is the state, and an exogenous input $u_t \in \mathbb{R}^{n_u}$ may be included in f. We let f and g denote probability densities (i.e., including stochastic noise), depending on an (unknown) parameter vector $\theta \in \mathbb{R}^{n_\theta}$, and by $\sim$ we mean distributed according to the density. We write $p_\theta(y_{1:T})$ to denote the likelihood of the model (1), and $y_{1:T} \triangleq \{y_1, \ldots, y_T\}$.

Traditionally, the system identification literature (Ljung, 1999; Söderström and Stoica, 1989) has mostly been focused on maximum likelihood (ML) *point estimates* $\widehat{\theta}_{\mathrm{ML}}$ of the unknown parameter θ,

$$\widehat{\theta}_{\mathrm{ML}} = \arg\max_\theta p_\theta(y_{1:T}) \tag{2}$$

rather than inferring its posterior *distribution* using Bayes' theorem as

$$p(\theta|y_{1:T}) \propto p_\theta(y_{1:T})p(\theta), \tag{3}$$

where $p(\theta)$ denotes the prior belief on θ. An excellent introduction to Bayesian system identification is given by Peterka (1981).

The traditional focus on the ML problem is indeed for a good reason; it is often computationally easier (and more natural) to handle a single parameter value than a full distribution. When the parameters are far from being uniquely determined by the data, however, the posterior distribution automatically gives a quantification of the amount of *uncertainty* present. Such situations may occur when, e.g., there is a model mismatch, the system was not excited enough during data collection, or the data record is very short.

The development of methods for Bayesian identification has made big advances in recent years, in particular methods based on sequential Monte Carlo (SMC) (Schön et al., 2015; Kantas et al., 2015). An important part of the advances has been published in the statistics literature, with a distinct focus on theoretical properties, such as consistency and convergence (Del Moral, 2004; Chopin, 2004). We believe these methods have a potential of being of great use also in practice. This paper compares two different state-of-the-art algorithms, and evaluate their properties from an engineering perspective.

We will focus on two popular methods, Particle Metropolis-Hastings (PMH, Andrieu et al. 2010) and SMC^2 (Chopin et al., 2013; Fulop and Li, 2013). Both methods are developed for being off-the-shelf methods for parameter learning problems, requiring nothing more than the ability to

(a) *simulate* from $f_\theta(x_{t+1}|x_t)$,

(b) *evaluate* $g_\theta(y_t|x_t)$.

The requirements (a) and (b) are fulfilled in most engineering applications. We will give a brief introduction (complete enough so the user can implement the methods on her/his own), and evaluate their performance on two examples. A more extensive introduction can be found in any of the recent tutorials by Schön et al. (2015), Kantas et al. (2015) or Dahlin and Schön (2015).

⋆ This work was supported by the Swedish Research Council (VR), project *Probabilistic modeling of dynamical systems* with contract number 621-2013-5524.

Algorithm 1 The basic (bootstrap) particle filter

1: Draw $x_0^{(i)} \sim p(x_0)$ and set $w_0^{(i)} = 1$.
2: **for** $t = 1$ **to** T **do**
3: Draw $a_{t-1}^{(i)}$ with $\mathbb{P}(a_{t-1}^{(i)} = j) \propto w_{t-1}^{(j)}$ *(resampling).*
4: Draw $x_t^{(i)} \sim f_\theta(x_t | x_{t-1}^{a_{t-1}^{(i)}})$ *(propagation).*
5: Set $w_t^{(i)} = g_\theta(y_t | x_t^{(i)})$ *(weighting).*
6: **end for**
All statements with (i) are for $i = 1, \ldots, N_x$.

2. THE PMH AND SMC^2 ALGORITHMS

We assume the reader has some familiarity with particle filters (Doucet and Johansen, 2011), and summarize the bootstrap particle filter as Algorithm 1. The particle filter is perhaps most known in the signal processing literature as a tool for state space filtering, but it can also be used as an unbiased (stochastic) estimator of $p_\theta(y_{1:T})$, i.e., the likelihood of the parameters θ. The likelihood is estimated by the weights from Algorithm 1 as

$$\widehat{p_\theta}(y_{1:T}) = \prod_{t=1}^{T} \left(\frac{1}{N_x} \sum_{i=1}^{N_x} w_t^{(i)} \right). \tag{4}$$

It can be shown (Chopin, 2004) that $\mathbb{E}[\widehat{p_\theta}(y_{1:T})] = p_\theta(y_{1:T})$.

2.1 Particle Metropolis-Hastings

The PMH algorithm (Andrieu et al., 2010) uses a Metropolis-Hastings sampler, a Markov chain Monte Carlo (MCMC) method, to sample from the posterior distribution $p(\theta|y_{1:T})$ (3).

The idea behind a Metropolis-Hastings sampler is to randomly 'walk around' in the parameter space and thus produce samples from the posterior. This is achieved as follows: While 'standing' at $\theta[k]$, propose a new parameter value θ' from a proposal $q(\theta'|\theta[k])$ (e.g., a random walk). Then, accept the proposed value, i.e. set $\theta[k+1] = \theta'$, with probability

$$\alpha = \min \left(1, \frac{\widehat{p_{\theta'}}(y_{1:T}) p(\theta')}{\widehat{p_{\theta[k]}}(y_{1:T}) p(\theta[k])} \right), \tag{5}$$

otherwise 'stay' and set $\theta[k+1] = \theta[k]$. To do this, a particle filter has to be run to evaluate (4) for each new proposed value θ'. After repeating this procedure for sufficiently many iterations, a series of samples $\{\theta[k]\}_{k=1}^K$ is obtained, consisting of (correlated) samples of the sought distribution $p(\theta|y_{1:T})$. The PMH algorithm is outlined as Algorithm 2.

There are in general two typical pitfalls with Metropolis-Hastings: It is hard to a priori tell how long the initial transient, the *burn-in period*, will be. A typical behavior is also that the chain gets 'stuck' for long periods of time, i.e., all proposals are rejected. One can intuitively understand SMC^2, which we will detail in the next section, as addressing the first issue by 'warm-starting' the chain by sequentially adding more and more data.

Algorithm 2 Particle Metropolis Hastings

Input: K (# steps), q (proposal), $\theta[0]$ initial parameter
Output: $\theta[1], \ldots, \theta[K]$ (samples from the posterior, including burn-in)
1: **for** $k = 1$ **to** K **do**
2: Draw $\theta' \sim q(\theta'|\theta[k-1])$.
3: Estimate $\widehat{p_{\theta'}}(y_{1:T})$ by a particle filter, Algorithm 1.
4: Compute α (5).
5: Draw $d \sim \mathcal{U}(d \mid 0, 1)$.
6: **if** $d < \alpha$ **then**
7: Set $\theta[k] = \theta'$ *(accept θ')*
8: **else**
9: Set $\theta[k] = \theta[k-1]$ *(reject θ')*
10: **end if**
11: **end for**

2.2 SMC^2

SMC^2 was proposed independently by Chopin et al. (2013) and Fulop and Li (2013). In SMC^2, an SMC sampler (Del Moral et al., 2006) is used instead of Metropolis-Hastings. The SMC sampler is inspired by the particle filter, but can be applied to sample from a general sequence of distributions, not necessarily originating from state space models. The SMC sampler is applied to the sequence $\{p(\theta), p(\theta|y_1), p(\theta|y_{1:2}), \ldots, p(\theta|y_{1:T})\}$, a *data-tempered* sequence, evolving from the prior to the posterior.

The SMC sampler works in a similar fashion to the particle filter, with an iteration of weighting – resampling – propagation. The particles, $\{\theta_t^{(m)}\}_{m=1}^{N_\theta}$, 'live' in θ-space. However, the weighting for particle $\theta_t^{(m)}$ should be done with respect to likelihood, so a standard particle filter has to be 'attached' to every single $\theta^{(m)}$ particle to estimate its likelihood, hence the name SMC^2. Thus, the weighting is with respect to

$$\widehat{p}_{\theta_t^{(m)}}(y_t|y_{1:t-1}) = \frac{1}{N_x} \sum_{i=1}^{N_x} w_t^{(i)}. \tag{6}$$

The resampling in the SMC sampler is identical to the particle filter, but the propagation has to be performed differently, as there is no equivalent to the function f for propagating the particles from $p(\theta|y_{1:t})$ to $p(\theta|y_{1:t+1})$. Instead PMH, Algorithm 2, is used to propagate the particles. To reduce the computational load, it is proposed by Chopin et al. (2013) to apply PMH only when some particle degeneracy criterion (e.g.the effective sample size, ESS) is fulfilled. This is summarized in Algorithm 3.

By construction, SMC^2 is an 'online algorithm' in the sense that it evolves along the time index, and if stopped prematurely at t', samples from the posterior $p(\theta|y_{1:t'})$ are obtained. Similarly, if another data point y_{T+1} is added, the algorithm does not have to start over from scratch, as opposed to the PMH. However, the computational load of SMC^2 is increasing with t, prohibiting use in online implementations with real-time requirements.

Algorithm 3 SMC^2

Input: N_θ (# θ particles), q (proposal)
Output: $\{\omega_T^{(m)}, \theta_T^{(m)}\}_{m=1}^{N_\theta}$ (samples from posterior)

1: Draw $\theta_0^{(m)} \sim p(\theta)$ and set $\omega_0^{(m)} = 1$
2: Run Step 1 of Algorithm 1 for each $\theta_0^{(m)}$
3: **for** $t = 1$ **to** T **do**
4: One iteration of the loop in Alg. 1 for each $\theta_{t-1}^{(m)}$
5: Compute $\widehat{p}_{\theta_t^{(m)}}(y_t|y_{1:t-1})$ (6)
6: Set $\omega_t^{(m)} = \omega_{t-1}^{(m)} \widehat{p}_{\theta_t^{(m)}}(y_t|y_{1:t-1})$
7: **if** ESS is too low **then**
8: Draw $b_t^{(m)}$ with $\mathbb{P}(b_t^{(m)} = n) \propto \omega_t^{(n)}$
9: Run PMH, Alg. 2, for each $\theta_{t-1}^{b_t^{(m)}}$ to obtain $\theta_t^{(m)}$
10: Set $\omega_t^{(m)} = 1$
11: **else**
12: Set $\theta_t^{(m)} = \theta_{t-1}^{(m)}$
13: **end if**
14: **end for**
All statements with (m) are for $m = 1, \ldots, N_\theta$.

3. NUMERICAL COMPARISON

In this section, we will first apply PMH and SMC^2 to a small simulated example, and then to the problem of learning parameters in a water tank model from real data. We will also discuss their different properties from a user perspective. The Matlab code for all examples can be found on the first authors homepage [1].

3.1 A simulated example

We will start the comparison by a simulated numerical example. Consider the one-dimensional state space model

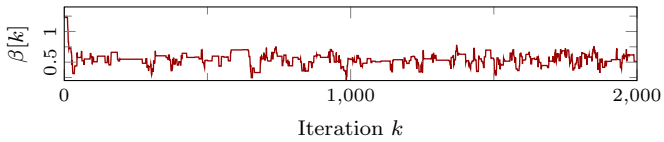
$$x_{t+1} = |x_t|^\beta + u_t + w_t, \qquad w_t \sim \mathcal{N}(0,1) \tag{7a}$$
$$y_t = x_t + e_t \qquad e_t \sim \mathcal{N}(0,1), \tag{7b}$$

where u_t is a known input signal, drawn from a Gaussian. We want to learn the parameter β, which we believe is drawn from $\mathcal{N}(0,1)$. This is thus our prior $p(\beta)$.

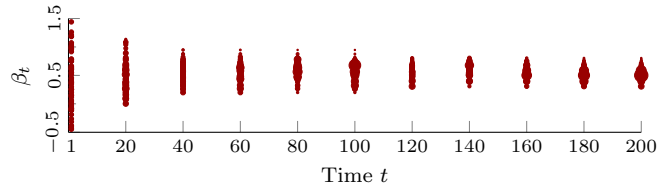
We simulate $T = 200$ data points $y_{1:T}$ from the model with $\beta = 0.4$. As the data record is relatively short in this example, we expect the posterior distribution to contain a non-negligible amount of uncertainty.

We apply the PMH algorithm to the problem, with proposal $q(\theta'|\theta)$ taken as the random walk $\theta' \sim \mathcal{N}(\theta'|\theta, 0.01)$. The trace plot for 2 000 iterations is shown in Figure 1a. Note the burn-in period; the Markov chain starts at 1.5, but moves eventually to the relevant part of the parameter space. In more complicated problems, the burn-in period is typically much longer. Also note the sequences of some hundred consecutive samples, where all proposals are rejected, a typical Metropolis-Hastings behavior.

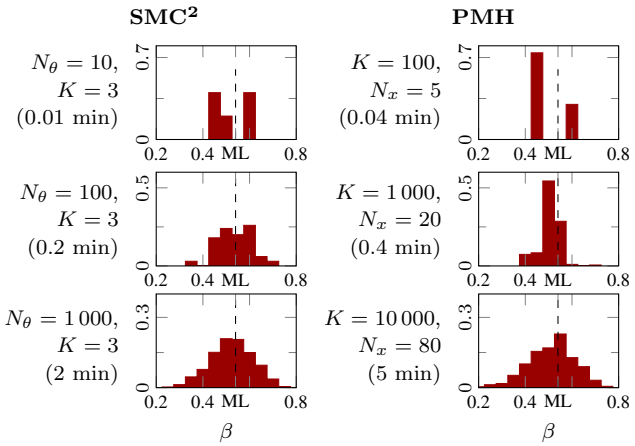
Also SMC^2 was applied to the problem. A resulting trace plot is shown as Figure 1b. To evaluate the methods, we explore three different settings (in PMH the number of iterations K and particles N_x in each particle filter, for SMC^2 the number of θ-particles N_θ and PMH step K) and plot the samples as histograms in Figure 1c. The reported time are for a standard desktop computer [2].



(a) Trace plot for 2000 iterations of the PMH.



(b) Trace plot for 50 θ-particles in the SMC^2, at certain time points. The particles are plotted with a diameter proportional to their importance weights. Note how the posterior evolves along t as more measurements are added, from a quite non-informative prior to a distribution in the region around the true value.



(c) The final samples for the simulated numerical example, for different settings of SMC^2 and PMH. A ML estimate is also indicated. Studying the samples, it is clear that the methods suffers from too few particles/iterations, except for the settings in the last row.

Fig. 1. Trace plots for PMH (a) and SMC^2 (b), and final samples (c) for Example 3.1, for different settings of the methods.

The methods only show similar results in the last row of Figure 1c, and the poor results in the first and second row are due to shortcomings of the methods when not run with sufficiently many particles/iterations. In this example, SMC^2 seems to have a slight advantage as it runs faster. For comparison, we also apply the ML method proposed by Schön et al. (2011) to the same data, and obtain the ML estimate $\widehat{\beta}_{ML} = 0.54$. Note that while the ML method only gives a point estimate of 0.54 (approximately corresponding to the peak of the posterior distribution), the full posterior also indicates the true value 0.4 to be quite likely, and also quantifies the uncertainty present.

[1] http://www.it.uu.se/katalog/andsv164

[2] Intel i7-4600 2.1 GHz CPU

3.2 A real world example

We also evaluate the methods in a real-world scenario. We use the first $T = 40$ data samples from the two water tank data presented by Wigren and Schoukens (2013), to learn a discretized version of the model with 6 unknown parameters

$$\begin{pmatrix} \dot{x}_t^{(1)} \\ \dot{x}_t^{(2)} \end{pmatrix} = \begin{pmatrix} -k_1\sqrt{x_t^{(1)}} \\ k_2\sqrt{x_t^{(1)}} - k_3\sqrt{x_t^{(2)}} \end{pmatrix} + \begin{pmatrix} k_4 u_t \\ 0 \end{pmatrix} + w_t, \quad \text{(8a)}$$

$$y_t = x_t + e_t, \quad w_t \sim \mathcal{N}(0, k_5 I_2), \quad e_t \sim \mathcal{N}(0, k_6 I_2). \quad \text{(8b)}$$

(I_2 is the 2-dimensional unit matrix, and k_5 and k_6 are scalar.) From the physical interpretation of the parameters (Wigren and Schoukens, 2013), our prior assumptions on k_1, k_2 and k_3 are a uniform distribution on $[0, 1]$, and k_4 is $\mathcal{N}(0, 1)$. As the noise parameters k_5 and k_6 are strictly positive, we formulate priors on their logarithms as $\log k_5 \sim \mathcal{N}(0, 0.1)$ and $\log k_6 \sim \mathcal{N}(-1, 0.1)$ respectively.

We run the PMH sampler for $K = 50\,000$ iterations with $N = 40$ particles, and SMC^2 with $N_\theta = 1\,000$ and $K = 30$ (requiring 12 and 27 minutes on a standard desktop computer, respectively). The samples obtained by the algorithms are plotted in Figure 2a. The results are quite similar, indicating similar ranges of possible values, but one can guess (by comparing the results for, e.g., k_3) that SMC^2 would benefit from an even bigger number N_θ.

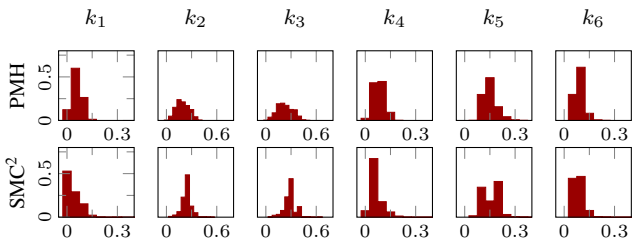
In this example, PMH seems to be the preferred option, as it requires less computational time, still not suffering from the particle degeneracy problem as SMC^2 with, e.g., k_3.

3.3 Computational load and tuning

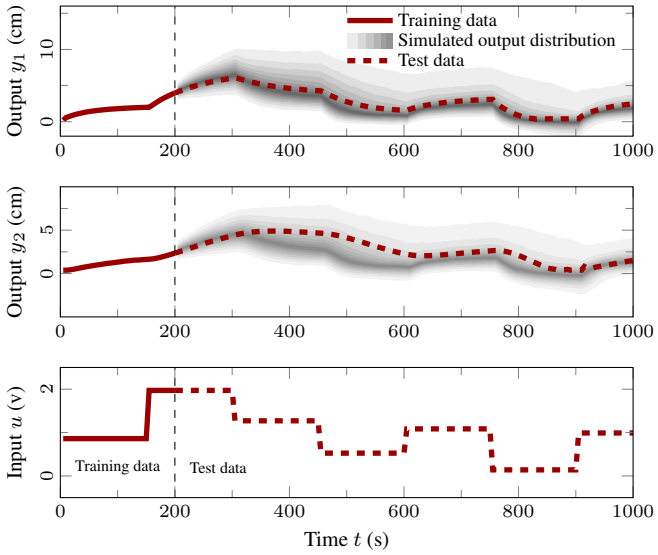
The computational load pf PMH is governed by $\mathcal{O}(KTN_x)$, i.e., proportional to the number of iterations K, the number of data points T and the number of particles N_x. The PMH is an anytime algorithm, in the sense that K does not have to be determined a priori, but can be run as long as the time permits. It has been shown that the choice of N_x in PMH affects the acceptance rate, and that N_x should be chosen $\propto T$ to keep an acceptance rate not varying with T (Chopin et al., 2013). Following this rule of thumb, the computational load of PMH becomes $\mathcal{O}(KT^2)$.

SMC^2 has the computational load $\mathcal{O}(KT^2N_xN_\theta)$. The rule of thumb for N_x for PMH also applies to the PMH within SMC^2, giving the load $\mathcal{O}(KT^3N_\theta)$. Although SMC^2 provides the user with $p(\theta|y_{1:t})$ for all t from 0 to T, it is not suited for online problems with real-time requirements, as it grows forbiddingly fast with increasing T.

The time for implementation does usually not count as a part of the computational load, but is nevertheless of big relevance in practice. Our experience from implementing the two examples is that SMC^2 is significantly harder to implement, due to the quite involved interaction between the two nested levels of SMC. PMH, on the other hand, only requires a particle filter algorithm, computation of the acceptance probability α and some storage. The implementation of PMH therefore also has the advantage of being easier to debug than SMC^2.



(a) The marginals of the posterior distributions for the six unknown parameters in the watertank model, inferred using PMH (top) and SMC^2 (bottom) from the data in (a). The data record is indeed short, but the posterior distribution provides useful information on possible ranges, much more informative than the prior $k_1 \in [0, 1]$, etc.



(b) The input-output data in the watertank data. The first 40 samples (200 s) are used as the training data, for inferring the posterior distribution of the parameters. The model learned with PMH (including the uncertainties) was here used to simulate the behavior of the tanks for another 800 s. (SMC^2 yields similar results.) The more intensive gray color, the more likely simulated output.

Fig. 2. The inferred posterior distribution of the parameters (a) are used to simulate the output in (b).

As an alternative for the user to implement the methods on her/his own, there are currently a few software packages designed for off-the-shelf use of PMH, SMC^2 and related methods available, such as LibBi [3] (Murray, 2013) and Biips [4] (Todeschini et al., 2014).

The tuning of both algorithms is indeed crucial for their performance. A perhaps subtle, but important, design choice is the proposal q inside the PMH. Suggestions on how to improve the proposal have been proposed in the literature, e.g Dahlin et al. (2015) for PMH, and Fearnhead and Taylor (2013) for SMC samplers. The number of particles, N_x and N_θ, are of course also of great importance, and a recent work on automatic adaption of N_θ in SMC^2 is presented by Chopin et al. (2015). Further, the rule of thumb $N_x \propto T$ applies, and a recent work with more extensive guidelines is Doucet et al. (2015).

[3] http://libbi.org
[4] http://alea.bordeaux.inria.fr/biips/

4. CONCLUSIONS

PMH has a clear computational advantage over SMC^2 for large T. For small T, as illustrated in the numerical examples, the methods are more comparable. In the examples, there are no clear advantage neither for PMH nor SMC^2: they both perform similarly, with a computational time of the same magnitude. SMC^2 does indeed offer more flexibility in the tuning, and might thus have a greater potential in adaption to certain problems. If all sequential posteriors $p(\theta|y_1), \ldots, p(\theta|y_{1:T})$ are of interest, SMC^2 is indeed preferable. However, as discussed, SMC^2 is considerably more challenging to implement and debug than PMH.

REFERENCES

Andrieu, C., Doucet, A., and Holenstein, R. (2010). Particle Markov chain Monte Carlo methods. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 72(3), 269–342.

Chopin, N. (2004). Central limit theorem for sequential Monte Carlo methods and its application to Bayesian inference. *Annals of Statistics*, 36(6), 2385–2411.

Chopin, N., Jacob, P.E., and Papaspiliopoulos, O. (2013). SMC^2: an efficient algorithm for sequential analysis of state space models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 75(3), 397–426.

Chopin, N., Ridgway, J., Gerber, M., and Papaspiliopoulos, O. (2015). Towards automatic calibration of the number of state particles within the SMC^2 algorithm. *arXiv preprint arXiv:1506.00570*.

Dahlin, J., Lindsten, F., and Schön, T.B. (2015). Particle Metropolis–Hastings using gradient and hessian information. *Statistics and computing*, 25(1), 81–92.

Dahlin, J. and Schön, T.B. (2015). Getting started with particle Metropolis-Hastings for inference in nonlinear models. Manuscript.

Del Moral, P. (2004). *Feynman-Kac Formulae: Genealogical and Interacting Particle Systems with Applications.* Springer, New York.

Del Moral, P., Doucet, A., and Jasra, A. (2006). Sequential Monte Carlo samplers. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 68(3), 411–436.

Doucet, A. and Johansen, A.M. (2011). A tutorial on particle filtering and smoothing: Fifteen years later. In D. Crisan and B. Rozovsky (eds.), *Nonlinear Filtering Handbook*, 656–704. Oxford University Press, Oxford.

Doucet, A., Pitt, M.K., Deligiannidis, G., and Kohn, R. (2015). Efficient implementation of Markov chain Monte Carlo when using an unbiased likelihood estimator. *Biometrika*, 102(2), 295–313.

Fearnhead, P. and Taylor, B.M. (2013). An adaptive sequential Monte Carlo sampler. *Bayesian Analysis*, 8(2), 411–438.

Fulop, A. and Li, J. (2013). Efficient learning via simulation: A marginalized resample-move approach. *Journal of Econometrics*, 176(2), 146–161.

Kantas, N., Doucet, A., Singh, S.S., Maciejowski, J.M., and Chopin, N. (2015). On particle methods for parameter estimation in state-space models. *Statistical Science*, 30(3), 328–351.

Ljung, L. (1999). *System identification: theory for the user*. Prentice Hall, Upper Saddle River, NJ, 2. ed. edition.

Murray, L.M. (2013). Bayesian state-space modelling on high-performance hardware using LibBi. *arXiv preprint arXiv:1306.3277*.

Peterka, V. (1981). Bayesian system identification. *Automatica*, 17(1), 41–53.

Schön, T.B., Lindsten, F., Dahlin, J., Wågberg, J., Naesseth, C.A., Svensson, A., and Dai, L. (2015). Sequential Monte Carlo methods for system identification. In *Proceedings of the 17th IFAC Symposium on System Identification (SYSID)*, 775–786. Beijing, China.

Schön, T.B., Wills, A., and Ninness, B. (2011). System identification of nonlinear state-space models. *Automatica*, 47(1), 39–49.

Söderström, T. and Stoica, P. (1989). *System identification*. Prentice-Hall, Inc., Hemel Hempstead, UK.

Todeschini, A., Caron, F., Fuentes, M., Legrand, P., and Del Moral, P. (2014). Biips: Software for Bayesian inference with interacting particle systems. *arXiv preprint arXiv:1412.3779*.

Wigren, T. and Schoukens, J. (2013). Three free data sets for development and benchmarking in nonlinear system identification. In *Proceedings of the 2013 European Control Conference (ECC)*, 2933–2938. Zurich, Switzerland.