Learning dynamical systems with particle stochastic approximation EM

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Abstract—we present the particle stochastic approximation EM (PSAEM) algorithm for learning of dynamical systems. The method builds on the EM algorithm, an iterative procedure for maximum likelihood inference in latent variable models. By combining stochastic approximation EM and particle Gibbs with ancestor sampling (PGAS), PSAEM obtains superior computational performance and convergence properties compared to plain particle-smoothing-based approximations of the EM algorithm. PSAEM can be used for plain maximum likelihood inference as well as for empirical Bayes learning of hyperparameters. Specifically, the latter point means that existing PGAS implementations easily can be extended with PSAEM to estimate hyperparameters at almost no extra computational cost. We discuss the convergence properties of the algorithm, and demonstrate it on several signal processing applications.

I. INTRODUCTION

Learning dynamical systems, or state-space models, is central to many classical signal processing problems, such as time-series modeling, filtering and control design. State-space models are also at the core of recent model developments in machine learning, such as Gaussian process state-space models [1], [2], infinite factorial dynamical models [3], [4], and stochastic recurrent neural networks [5] for example. A strategy to learn state-space models, independently suggested by [6] and [7], is the use of the Expectation Maximization (EM) [9] method. Originally proposed for maximum likelihood estimation of linear models with Gaussian noise, the strategy can be generalized to the more challenging non-linear and non-Gaussian cases, as well as the empirical Bayes setting. Many contributions have been made during the last decade, and this paper takes another step along the path towards a computational performance and convergence properties compared to the predecessors. This overall picture is also briefly summarized in Figure 1.

Throughout the paper we assume that the reader is familiar with Markov chain Monte Carlo (MCMC, [12], [13]) as well as particle filters/SMC [14], [15].

II. PROBLEM FORMULATION AND CONCEPTUAL SOLUTION

Given a batch of observations \(y_{1:T}\) we wish to learn the unknown parameters \(\theta\) as well as the unobserved states \(x_{0:T}\) of the model \(\{\}\). For the states \(x_{0:T}\) we are interested in their posterior distribution. For the parameters \(\theta\), we consider two cases: In the frequentistic, or rather Fisherian, setting we are interested in a (possibly regularized) maximum likelihood estimate \(\hat{\theta}\). In the Bayesian setting, we assign a prior distribution to the parameters, \(\theta \sim p_{\theta}(\theta)\). The prior, in turn, is assumed to be parameterized by some hyperparameter \(\eta\), which needs to be estimated\(^2\). Thus, we address both of the following two problems:

\(^1\)For notational brevity we assume that the initial density \(p(x_0)\) is fully specified and not parameterized by \(\theta\), but the extension to an unknown initial density is straightforward.

\(^2\)Hyperparameters can also be set using prior knowledge.
1) (Fisherian setting) Compute the maximum likelihood estimate of the model parameters,
\[
\hat{\theta} = \arg \max_{\theta} \log p_{\theta}(y_{1:T}),
\]
where \( p_{\theta}(y_{1:T}) = \int p_{\theta}(y_{1:T} | x_{0:T}) p_{\theta}(x_{0:T}) dx_{0:T} \) is the likelihood function. A regularization term, such as \( \|\theta\|_1 \), may also be included in the maximization criterion.\(^3\)

2) (Bayesian setting) Compute the posterior distribution of the model parameters \( p_{\hat{\eta}}(\eta | y_{1:T}) \), where the hyperparameters are estimated using empirical Bayes
\[
\hat{\eta} = \arg \max_{\eta} \log p_{\eta}(y_{1:T}),
\]
where the marginal likelihood function is \( p_{\eta}(y_{1:T}) = \int p_{\eta}(y_{1:T} | x_{0:T}) p_{\theta}(\theta) d\theta dx_{0:T} \).

These two problems are in fact strongly related, and can be seen as exactly the same problem on a more abstract level. In the interest of concreteness we will, however, distinguish between those two problems, but the computational algorithm that we will propose can be used to address both. The algorithm will compute a Monte Carlo approximation of the posterior distribution over the latent variables.

Both settings involve the computation of a maximum likelihood estimate; of the model parameters in the first case and of the hyperparameters in the second case. A conceptual solution to these problems is given by the expectation maximization (EM) algorithm. EM is a data augmentation method, meaning that it is based on the notion of a complete data, comprising the observed data as well as the latent (or missing) variables. The EM algorithm iteratively updates the (hyper-)parameters, and each iteration consists of two steps:

(E) Compute the expected value of the complete data log-likelihood for fixed (hyper-)parameters
(M) Maximize the Q-function (which will be defined below) with respect to the (hyper-)parameters

\(^3\)To avoid too complicated expressions, we do not include the regularization term. From a user’s perspective, it simply amounts to replace \( p_{\theta}(y_{1:T} | x_{0:T}) \), whenever it appears, with \( p_{\theta}(y_{1:T} | x_{0:T}) + \lambda \|\theta\|_1 \).

The observed data is always \( y_{1:T} \), and what differs between the Fisherian and the Bayesian problem is what constitutes the latent variables. For the Fisherian problem, the latent variables are \( x_{0:T} \) and we obtain, at iteration \( k \),

\[(E) \quad \text{Let } Q_k^{\text{Fish}}(\theta) := \int \log p_{\theta}(y_{1:T}, x_{0:T}) p_{k-1}(x_{0:T} | y_{1:T}) dx_{0:T}.
\]

\[(M) \quad \text{Solve } \theta_k \leftarrow \arg \max_{\theta} Q_k^{\text{Fish}}(\theta).
\]

Note that the expectation in the (E)-step is w.r.t. the smoothing distribution \( p_{k-1}(x_{0:T} | y_{1:T}) \) parameterized by the previous parameter iterate \( \theta_{k-1} \). It is well known that iterating \( \text{[2]} \) gives a monotone increase of the likelihood \( p_k(y_{1:T}) \), and \( \theta_k \) will under weak assumptions converge to a stationary point of the likelihood function as \( k \to \infty \) (e.g. \([16]\)).

For empirical Bayes we obtain similar expressions, but the latent variables are both \( x_{0:T} \) and \( \theta \). The (E)-step is as

\[(E) \quad \text{Let } Q_k^{\text{Bay}}(\eta) := \int \log p_{\eta}(y_{1:T}, x_{0:T}, \theta) p_{k-1}(\theta, x_{0:T} | y_{1:T}) d\theta dx_{0:T} = \int \log p_{\eta}(\theta) p_{k-1}(\theta | y_{1:T}) d\theta + \text{const.,}
\]

\[(M) \quad \text{Solve } \eta_k \leftarrow \arg \max_{\eta} Q_k^{\text{Bay}}(\eta),
\]

where the second line of (3) follows from the fact that in the factorization of the complete data likelihood, only the prior density \( p_{\eta}(\theta) \) depends on the hyperparameter \( \eta \). The M-step remains unchanged. In complete analogy to the Fisherian setting, \( \text{[3]} \) will also under weak assumptions converge to a stationary point of the marginal likelihood as \( k \to \infty \).

Both \( \text{[2]} \) and \( \text{[3]} \) can be implemented and iterated until convergence, as long as the integrals can be computed and the maximization problem solved. However, in most cases—specifically for the models we consider in this paper—the integrals can not be solved analytically, and the topic for the rest of this paper is essentially to design an efficient method for approximating the integrals. The solution will be based on PMCMC \([17]\), but also a stochastic approximation of the Q-function \([18]\) to ensure a computationally efficient solution with good convergence properties. Our solution will therefore be more involved than just replacing the integrals in \( \text{[2]} \) or \( \text{[3]} \) with vanilla Monte Carlo estimators (Monte Carlo EM).
A short word on notation: we will use subscripts to denote sequences of variables for which we are seeking a maximum, like $\eta_k$, and brackets for samples of variables for which we are seeking a posterior distributions, like $x_{0:T}[k]$.

III. RELATED WORK AND CONTRIBUTIONS

The use of EM for learning linear state-space models appears to have been independently suggested by, at least, [6] and [7] For linear models the state inference problem can be solved exactly using a Kalman filter, but not for nonlinear models. To this end, the extended Kalman filter has been proposed [19], [20], as well as SMC-based solutions [9], [10], [11], leading to a so-called Monte Carlo EM solution.

EM is a general strategy for latent variable models, and the standard choice in the application of EM to state-space models is to select the states as the latent variable. It is, however, shown by [21] that if considering the process noise realization (instead of the states) as latent variables, it is possible to introduce stability guarantees for the learned model at the cost of a more involved maximization problem.

This paper considers the offline (or batch) problem, but EM can also be applied for online (or streaming data) problems. For the nonlinear online problem, the combination of EM and SMC dates back to at least [22], [23], and recent contributions include [24].

Stochastic approximation EM (SAEM, [18], [25]) can be used to improve the convergence properties and reduce the computational cost, compared to Monte Carlo EM. This is particularly true when the Monte Carlo simulation is computationally involved, which is the case for SMC-based solutions. In the context of state-space models, SAEM appears to first have been proposed by [26] and [27], who suggest to combine it with a particle independent Metropolis–Hastings procedure (PIMH, [17]) to infer the latent states. The idea to combine SAEM with particle Gibbs with ancestor sampling (PGAS, [28]), which often has a much lower computational cost, was first suggested in a brief conference paper by [29] — the present article is an extension of this paper. Since its first publication, this method — which we refer to as PSAEM — has found applications in system identification [30], [31], causal inference [32], and econometrics [33], to mention a few. In this paper, we will study PSAEM more thoroughly, formulate it explicitly for empirical Bayes, present a new theoretical result, and illustrate the method’s applicability to some contemporary dynamical systems models from the machine learning literature (Gaussian process state-space models [1], [34] and infinite factorial dynamical models [4]).

IV. PARTICLE STOCHASTIC APPROXIMATION EM

We will now build up and present the contribution of this paper, the particle stochastic approximation EM (PSAEM) algorithm. The two main components are (i) an MCMC kernel for simulating the latent variables from either $p_{\theta}(x_{0:T} | y_{1:T})$ or $p_{\theta}(\theta, x_{0:T} | y_{1:T})$, and (ii) a stochastic approximation version of the EM algorithm (SAEM, [18], [25]), to update the (hyper-)parameter estimate. We will start with the former (Section IV-A) and thereafter turn to the latter (Section IV-B).

A. Sampling the latent variables using PGAS

At the core of the EM algorithm is the posterior inference of the latent variables, which is needed for the integrals in (2) or (3). For general non-linear or non-Gaussian state-space models these posterior distributions are intractable and we have to use numerical approximations. Much research has been done over the past decades on computational algorithms for this problem, and many powerful tools are available. We will focus on PMCMC [17] methods which we believe are particularly well suited for this. PMCMC is a framework for using particle filters to construct efficient high-dimensional Markov kernels, and we will specifically make use of the particle Gibbs with ancestor sampling (PGAS) [28]. PGAS has been shown to have good empirical performance in many situations (e.g., [35], [36], [4], [37]), but other versions of particle Gibbs could possibly also be employed, such as Particle Gibbs with backward simulation [38], [39] or blocked particle Gibbs [40].

To start we assume that the parameters to estimate ($\theta$ or $\eta$) are fixed at some value, and consider how $p_{\theta}(x_{0:T} | y_{1:T})$ or $p_{\theta}(\theta, x_{0:T} | y_{1:T})$ can be approximated using PGAS. Consider first the Fisherian setting. Just like any MCMC method would do, PGAS makes use of an Markov kernel on the space $X^{T+1}$ with $p_{\theta}(x_{0:T} | y_{1:T})$ as its unique stationary distribution. This kernel is then applied iteratively, and if certain ergodicity assumptions hold, this procedure will eventually produce samples from $p_{\theta}(x_{0:T} | y_{1:T})$. With PGAS this Markov kernel is constructed using a particle filter, or more precisely a conditional particle filter with ancestor sampling, given in Algorithm 1. One execution of the entire Algorithm 1 corresponds to one iteration of the Markov kernel. The conditional particle filter resembles a standard particle filter with $N - 1$ particles, with the addition that there is also a conditional particle trajectory (for convenience numbered $N$, line 2 and 8) which is specified a priori. In the resampling step (line 5), this conditional trajectory can be replicated, but never discarded. At the end, one single trajectory is extracted, which will be used as conditional trajectory in a later iteration. The ancestor sampling (line 7) assigns ancestors to the conditional trajectory, similar to resampling but ‘backwards’ in time and only for the conditional trajectory. We refer to [28] for further details. Algorithm 1 is formulated in its ‘bootstrap’ version, but a more general SMC formulation is also possible, see [28].

Formally we let Algorithm 1 define a Markov kernel $\Pi_{\theta}$ on the space of state trajectories $X^{T+1}$ given by

$$\Pi_{\theta}(x_{0:T}^\star, B) = E \left[ \mathbb{I}(x_{0:T}^\star \in B) \right]$$

where the expectation is w.r.t. the random variables used in Algorithm 1. The Markov kernel constructed by Algorithm 1 takes a state trajectory $x_{0:T}[j - 1] = x_{0:T}^\star$ in $X^{T+1}$ as input and outputs another state trajectory $x_{0:T}[j] = x_{0:T}^\star$ in $X^{T+1}$. Put differently, a sample $x_{0:T}[j] \sim \Pi_{\theta}(x_{0:T}[j - 1], \cdot)$ can be generated by executing Algorithm 1 with fixed $\theta$ and $x_{0:T}[j - 1]$ as input reference trajectory. If this is iterated, an MCMC procedure on the space $X^{T+1}$ is obtained, and the trajectories $x_{0:T}[0], x_{0:T}[1], x_{0:T}[2], \ldots$ will eventually be samples from the sought smoothing distribution $p_{\theta}(x_{0:T} | y_{1:T})$. MCMC methods like this, which uses Markov kernels based on particle filters, are called PMCMC.
Algorithm 1 Markov kernel $\Pi_\theta(x_{0:T}^i, x_{0:T}^{i-1})$

**Input:** Conditional trajectory $x_{0:T}^i$, parameter $\theta$.

**Output:** Trajectory $x_{0:T}^i$.

1: Draw $x_0^i \sim p(x_0)$,
2: Set $x_0^i \leftarrow x_0^i$,
3: Set $w_0^i \leftarrow 1$, $i = 1, \ldots , N$.
4: for $t = 1, 2, \ldots , T$ do
5: \hspace{1em} Draw $a_t^i$ with $\Pr(a_t^i = j) \propto w_{t-1}^i$ for $i = 1, \ldots , N$.
6: \hspace{1em} Draw $x_t^i \sim p_{\theta}(x_t | x_{t-1}^{a_t^i})$ for $i = 1, \ldots , N$.
7: \hspace{1em} Draw $a_t^i$ with $\Pr(a_t^i = j) \propto w_{t-1}^i p_{\theta}(x_t^i | x_{t-1}^j)$.
8: \hspace{1em} Set $x_t^N \leftarrow x_t^i$.
9: \hspace{1em} Set $w_t^i \leftarrow p_{\theta}(y_t | x_t)$ for $i = 1, \ldots , N$.
10: end for
11: Draw $I$ with $\Pr(I = i) \propto w_T^i$.
12: Set $x_T^i = x_T^I$.
13: for $t = T - 1, T - 2, \ldots , 0$ do
14: \hspace{1em} Set $I \leftarrow a_t^I$.
15: \hspace{1em} Set $x_t \leftarrow x_t^i$.
16: end for

It is far from obvious that $\Pi_\theta$ admits $p_\theta(x_{0:T} | y_{1:T})$ as its stationary distribution. However, its properties (as well as those of its older sibling presented by [17]) have been extensively studied, see for example [17], [41], [28], [42], [43]. The main results are: (i) $p_\theta(x_{0:T} | y_{1:T})$ is a stationary distribution of $\Pi_\theta$, and (ii) $\Pi_\theta$ is uniformly geometrically ergodic in $x_{0:T}$ for any $N \geq 2$ and any $\theta \in \Theta$ under upper boundedness conditions on $w_t^i$ in Algorithm 1. We summarize this PMCMC procedure to infer $p_\theta(x_{0:T} | y_{1:T})$ in Algorithm 2 (still assuming $\theta$ is fixed).

Algorithm 2 Sampling $p_\theta(x_{0:T} | y_{1:T})$ (Fisherian, fixed $\theta$)

1: Initialize $x_{0:T}[0]$ arbitrarily, e.g., by running a standard particle filter targeting $p_\theta(x_{0:T} | y_{1:T})$.
2: for $j = 1, 2, \ldots , J$ do
3: \hspace{1em} Sample $x_{0:T}[j] \sim \Pi_\theta(x_{0:T} | y_{1:T})$ (run Alg. 1 once)
4: end for

So far we have only considered the Fisherian setting, in which the latent variables only comprise the state trajectory. For the Bayesian setting we assume that $\eta$ (instead of $\theta$) is fixed, and we see from [4] that we have to compute the model parameter posterior distribution $p_\eta(\theta | y_{1:T})$. We will do this by splitting the simulation problem into two steps, one in which we sample $x_{0:T}$ conditionally on $\theta$ (and $y_{1:T}$) and one in which we sample $\theta$ conditionally on $x_{0:T}$ (and $y_{1:T}$). The first step, sampling $x_{0:T}$ conditionally on $\theta$, is equivalent to the problem discussed for the Fisherian setting, and we can use the Markov kernel $\Pi_\eta$ Algorithm 1. For the second step, sampling $\theta$ conditionally on $x_{0:T}$, exact solutions are often possible, leading to Gibbs sampling. Otherwise, methods like Hastings within-Gibbs (see, for instance, [13], Section 2.4) are possible. The particular choice depends on the actual model, and we will later illustrate it by an example. Let the Markov kernel used to simulate $\theta$ be denoted by $\Pi_{\eta,x_{0:T}}(\theta'|\cdot)$. Most of the previously referenced literature on properties for $\Pi_\eta$ covers also the setting of a joint kernel for $\theta, x_{0:T}$. The resulting MCMC procedure used in the Bayesian setting (still assuming a fixed value for $\eta$) is summarized in Algorithm 3 and converges (in the same sense as Algorithm 2) to $p_\eta(\theta, x_{0:T} | y_{1:T})$.

Algorithm 3 Sampling $p_\eta(\theta, x_{0:T} | y_{1:T})$ (Bayesian, fixed $\eta$)

1: Initialize $\theta[0]$ and $x_{0:T}[0]$ arbitrarily. For the latter e.g., by a particle filter targeting $p_{\eta|0}(x_{0:T} | y_{1:T})$.
2: for $j = 1, 2, \ldots , J$ do
3: \hspace{1em} Sample $x_{0:T}[j] \sim \Pi_{\eta,x_{0:T}}(x_{0:T} | y_{1:T})$ (run Alg. 1 once).
4: \hspace{1em} Sample $\theta[j] \sim \Pi_{\eta|x_{0:T}}(\theta | x_{0:T}[j-1], \cdot)$ (run Alg. 1 once).
5: end for

B. Combining PGAS and EM

We have so far assumed that the (hyper-)parameters are fixe. The objective in this paper is, however, to learn those, and we will for this purpose use a stochastic approximation version of the EM algorithm.

1) A naive solution using EM and PMCMC: The problem with the preliminary EM solutions outlined in (2) and (3), respectively, is the analytically intractable integrals in their $Q$-functions. A first idea would be to replace the integrals with sums over $J$ Monte Carlo samples. For the Fisherian setting, this means replacing the (E)-step of (2) with a simulation (Si) step as follows:

(Si) \[ \text{Draw } x_{0:T}[j] \sim p_{\theta_{k-1}}(x_{0:T} | y_{1:T}) \text{ and let } \hat{Q}^\text{EM}_{k-1}(\theta) := \frac{1}{J} \sum_{j=1}^J \log p_{\theta_{k-1}}(y_{1:T}, x_{0:T}[j]). \]

(M) Solve $\theta_k \leftarrow \arg \max_{\theta} \hat{Q}^\text{EM}_{k-1}(\theta)$.

Note that this is our initial EM scheme (2), but with the analytically intractable integral over $\log p_\eta(y_{1:T}, x_{0:T})$ approximated by a sum. This algorithm is commonly referred to as Monte Carlo EM [45] or, if $J = 1$, stochastic EM [46]. To draw the samples in the (Si)-step we can use PGAS from Section V-A, which would give Algorithm 4.

Algorithm 4 Monte Carlo EM for the Fisherian problem

1: Initialize $\theta_0$.
2: for $k = 1, 2, \ldots , J$ do
3: \hspace{1em} Run Alg. 3 with $\theta_{k-1}$ ‘until convergence’, get $\{x_{0:T}[j]|y_{1:T}\}$.
4: \hspace{1em} Solve $\theta_k \leftarrow \arg \max_{\theta} \frac{1}{J} \sum_{j=1}^J \log p_\theta(y_{1:T}, x_{0:T}[j]).$
5: end for

A similar algorithm could be devised for the Bayesian setting. Even though Algorithm 4 might look promising, there are two issues with this solution:

(i) To guarantee that Algorithm 2 has converged to its stationary distribution, we cannot bound its number of iterations at line 3.

(ii) For the sum in line 4 to converge to the integral it approximates, we must let $J \rightarrow \infty$.

Indeed, these two issues are related. We basically need to allow $J \rightarrow \infty$ to ensure convergence, whilst the convergence of the EM iteration happens as $k \rightarrow \infty$. This is not desirable since it, intuitively, gives a computational complexity of $\infty \times \infty$; see further [47]. Existing methods based on various types of particle smoothing for approximating the integral with respect to $p_\eta(x_{0:T} | y_{1:T})$, for instance [10], [11], suffer from the same issues. Indeed, these methods are (SMC-based) instances of Monte Carlo EM.

We will now first address issue (ii) with stochastic approximation EM, and thereafter handle issue (i) by ‘entangling’ the convergence of Algorithm 2 ($J \rightarrow \infty$) with the convergence of the EM algorithm ($k \rightarrow \infty$).
2) **SAEM: Handling sample approximations within EM:** Stochastic approximation, as introduced by \([48]\), is an averaging procedure to solve a (deterministic) equation which can only be evaluated through noisy (stochastic) observations. In stochastic approximation a step length \(\gamma_k \in [0, 1]\) is used, which has to fulfill
\[
\sum_{k=1}^{\infty} \gamma_k = \infty, \quad \sum_{k=1}^{\infty} \gamma_k^2 < \infty, \quad \gamma_1 = 1.
\]

Following \([18]\), the SAEM algorithm can be introduced by making a stochastic approximation of the \(Q\)-function. In SAEM, we transform Monte Carlo EM \([5]\) by introducing a stochastic approximation (SA)-step. For simplicity we only use one sample \((J = 1)\) in the simulation (Si)-step, but in practice it can be favorable to use a small batch of samples.

For iteration \(k\) this becomes
(Si) Draw \(x_{0:T}[k] \sim p_{0-k-1}(x_{0:T} | y_{1:T})\).

(\text{SA}) Let \(Q_k^{\text{Fish}}(\theta) \leftarrow (1 - \gamma_k)Q_k^{\text{Fish}}(\theta) + \gamma_k \log p_\theta(y_{1:T}, x_{0:T}[k])\),

(M) Solve \(\theta_k \leftarrow \arg \max_\theta Q_k^{\text{Fish}}(\theta)\). \hspace{1cm} (7)

To intuitively understand the stochastic approximation, let us first ignore the (M)-step and assume \(\gamma_k = \frac{1}{k}\). In such a case, the (SA)-step would simply be online averaging, equivalent to \(Q_k^{\text{Fish}}(\theta) = \frac{1}{k} \sum_{\ell=1}^{k} \log p_\theta(y_{1:T}, x_{0:T}[\ell])\), where \(x_{0:T}[\ell] \sim p_\theta(x_{0:T} | y_{1:T})\), which converges to \(\int \log p_\theta(y_{1:T}, x_{0:T})p_\theta(x_{0:T} | y_{1:T})dx_{0:T}\) when \(k \rightarrow \infty\) by the law of large numbers. The introduction of the (M) step complicates the picture, but assuming that \(\theta_k\) will eventually converge to a stationary point, the influence from the transient phase will vanish as \(k \rightarrow \infty\), and the averaging argument can still be applied. In Section \(\ref{section:convergence}\) we discuss the convergence properties in detail. Before that, in Section \(\ref{section:SAEM:EM}\) we will consider the important special case of exponential family models, for which the (SA) step reduces to a convenient recursive update of sufficient statistics.

With \(\ref{section:SAEM:EM}\) in place, we can make stronger theoretical claims (even though we are using only a single sample, \(J = 1\), from \(p_{0-k-1}(x_{0:T} | y_{1:T})\), at each iteration!) thanks to the use of stochastic approximation \([18]\). However, for the problem under study it is still of limited practical use since we cannot generate samples from \(p_{0-k-1}(x_{0:T} | y_{1:T})\) by other means than using Algorithm \(\ref{section:EM}\) with an infinite number of iterations (in order to ensure that it has converged). Thus, our final step is to use the method studied by \([25]\) to combine SAEM with an MCMC procedure in a much more intricate way than \(\ref{section:EM}\).

3) **PSAEM: Combining SAEM with PGAS:** As suggested and analyzed by \([25]\), the draw from \(p_{0-k-1}(x_{0:T} | y_{1:T})\) in \(\ref{section:SAEM:EM}\) can be replaced with a draw from a Markov kernel which has \(p_{0-k-1}(x_{0:T} | y_{1:T})\) as its invariant distribution. As discussed, this is exactly what \(\Pi_\phi\) from Algorithm \(\ref{section:EM}\) is, and we can thus assemble
(Si) Draw \(x_{0:T}[k] \sim \Pi_{0-k-1}(x_{0:T}[k-1], \cdot)\) (that is, run Algorithm \(\ref{section:EM}\) once).

(\text{SA}) Let \(Q_k^{\text{Fish}}(\theta) \leftarrow (1 - \gamma_k)Q_k^{\text{Fish}}(\theta) + \gamma_k \log p_\theta(y_{1:T}, x_{0:T}[k])\).

(M) Solve \(\theta_k \leftarrow \arg \max_\theta Q_k^{\text{Fish}}(\theta)\). \hspace{1cm} (8)

Note that we do not make use of Algorithm \(\ref{section:EM}\) anymore, but only Algorithm \(\ref{section:EM}\) This means that we do not run the Markov kernel “until convergence” at each iteration, but it will (intuitively speaking) converge in parallel with the SAEM iterations indexed with \(k\). We summarize and present this as Algorithms \(\ref{section:PSAEM:EM}\) and \(\ref{section:PSAEM:EM-Bay}\).

\begin{algorithm}[h]
\caption{PSAEM for the Fisherian setting}
\begin{algorithmic}
1: Initialize \(x_{0,T}[0], \theta_0\)
2: for \(k = 1, 2, \ldots\) do
3: Run Alg. \(\ref{section:EM}\) cond. on \(x_{0:T}[k-1]\) and \(\theta_{k-1}\) to sample \(x_{0,T}[k]\)
4: \(Q_k^{\text{Fish}}(\theta) \leftarrow (1 - \gamma_k)Q_k^{\text{Fish}}(\theta) + \gamma_k \log p_\theta(y_{1:T}, x_{0:T}[k])\)
5: Solve and update parameters \(\theta_k \leftarrow \arg \max_\theta Q_k^{\text{Fish}}(\theta)\)
6: end for
\end{algorithmic}
\end{algorithm}

\begin{algorithm}[h]
\caption{PSAEM for the Bayesian setting}
\begin{algorithmic}
1: Initialize \(x_{0,T}[0], \theta[0], \eta_0\)
2: for \(k = 1, 2, \ldots\) do
3: Run Alg. \(\ref{section:EM}\) cond. on \(x_{0:T}[k-1]\) and \(\theta[k-1]\) to sample \(x_{0,T}[k]\)
4: Sample \(\theta[k] \sim \Pi_{0-k-1, x_{0:T}[k]}(\theta | k - 1, \cdot)\)
5: Update \(Q_k^{\text{Bay}}(\eta) \leftarrow (1 - \gamma_k)Q_k^{\text{Bay}}(\eta) + \gamma_k \log p_\eta(\theta[k])\)
6: Solve and update hyperparameters \(\eta_k \leftarrow \arg \max_\eta Q_k^{\text{Bay}}(\eta)\)
7: end for
\end{algorithmic}
\end{algorithm}

We have now obtained an algorithm which only relies on asymptotics as \(k \rightarrow \infty\), by ‘entangling’ the convergence of PGAS with the convergence of SAEM. As we will see in Section \(\ref{section:convergence}\) convergence can be shown under certain assumptions. We will now consider the important special case of models \(\ref{section:EM}\) in the exponential family, for which the recursively defined function \(Q_k\) reduces to a much simpler expression.

C. **PSAEM for exponential family models**

Studying Algorithm \(\ref{section:EM}\) or \(\ref{section:EM}\) one may expect the computational cost of all computations involving the \(Q\)-function to increase as \(k \rightarrow \infty\), since \(Q_k\) is defined as a sum with \(k\) terms, each a function of a past sample of \(x_{0:T}\). This is, however, not the case if the model belongs to the exponential family, which is an important special case discussed below.

When we write “the model belongs to the exponential family”, we mean that the joint distribution for the latent and observed variables, \(p_\theta(x_{0:T}, y_{1:T})\) or \(p_\eta(\theta, x_{0:T}, y_{1:T})\), belongs to the exponential family with \(\theta\) or \(\eta\) as its parameter, respectively. For the Fisherian case, this is fulfilled if both equations in \(\ref{section:EM}\) can, with some choice of \(S_x : \mathbb{X} \times \mathbb{X} \rightarrow \mathbb{R}^r, \phi_x : \mathbb{X} \rightarrow \mathbb{R}^r, \phi_y : \Theta \rightarrow \mathbb{R}^r\) (for some \(\ell\), and similarly for some \(S_y, \psi_y, \phi_y\)), be written as
\[
p_\theta(x_{1:t-1}) \propto \exp \left\{-\psi_x(\theta) + \langle S_x(x_{1:t-1}, x_t), \phi_x(\theta) \rangle \right\}, \quad (9a)
\]
\[
p_\eta(y_t | x_t) \propto \exp \left\{-\psi_y(\eta) + \langle S_y(y_t, x_t), \phi_y(\eta) \rangle \right\}. \quad (9b)
\]

Here, \(\propto\) reads “proportional (with respect to \(\theta\) to)” and \(\langle \cdot, \cdot \rangle\) is an inner product. The subscripts \((x, y)\) and \(\theta\) do not denote dependencies in this context, but are only names.

For the Bayesian case, the requirements are weaker, and it is enough that the prior distribution for \(\theta\) belongs to the exponential family,
\[
p_\eta(\theta) \propto \exp \left\{-\psi_\eta(\eta) + \langle S_\theta(\theta), \phi_\eta(\eta) \rangle \right\}. \quad (10)
\]
We will now see how the \( Q \)-function from the (SA)-step simplifies for models which can be written on one of these forms. First consider the Fisherian case. Using the Markovian structure of (4), we can write

\[
\log p_\theta(y_{1:T}, x_{0:T}) = \sum_{t=1}^{T} \log p_\theta(y_t | x_t) + \log p_\theta(x_t | x_{t-1}) + \text{const.}
\]

\[
= -\psi(\theta) + \langle S(x_{0:T}, y_{1:T}), \phi(\theta) \rangle + \text{const.} \tag{11}
\]

where

\[
\psi(\theta) = T \{ \psi_x(\theta) + \psi_y(\theta) \},
\]

\[
S(x_{0:T}, y_{1:T}) = \sum_{t=1}^{T} \left( S_x(x_{t-1}, x_t) \right),
\]

\[
\phi(\theta) = \left( \phi_x(\theta), \phi_y(\theta) \right).
\]

Here we have used the fact that the initial distribution \( p(x_0) \) is independent of \( \theta \) (for notational simplicity). It follows that

\[
Q^\text{Fish}_k(\theta) = -\psi(\theta) + \langle S_k, \phi(\theta) \rangle + \text{constant}, \tag{12a}
\]

where

\[
S_k = (1 - \gamma_k)S_{k-1} + \gamma_k S(x_{0:T}[k], y_{1:T}). \tag{12b}
\]

Note that this is a non-recursive definition of \( Q^\text{Fish}_k(\theta) \), but instead recursive in \( S_k \). From an algorithmic point of view, this means that we can compute and store \( S_k \) as (12b), and solve the maximization problem for (12a) instead of the more intricate and computationally challenging (8). In fact, the maximizing argument to (12a) can be expressed on closed form in many cases.

Analogously the Bayesian case is obtained as,

\[
Q^\text{Bay}_k(\eta) = -\psi_\eta(\eta) + \langle S_k, \phi_\eta(\eta) \rangle + \text{constant}, \tag{13a}
\]

where

\[
S_k = (1 - \gamma_k)S_{k-1} + \gamma_k S_\theta(\theta[k]). \tag{13b}
\]

We summarize in Algorithms 7 and 8.

**Algorithm 7** PSAEM for exponential family models, Fisherian

1: Initialize \( x_{0:T}[0] \) and \( \theta_0 \)
2: for \( k = 1, 2, \ldots \) do
3: Run Algorithm 1 conditional on \( x_{0:T}[k-1] \) and \( \theta[k-1] \) to sample \( x_{0:T}[k] \)
4: Update sufficient statistics \( S_k \) according to (12b)
5: Solve and update parameters \( \theta_k \leftarrow \arg \max \phi(\theta) \) using (12a)
6: end for

**Algorithm 8** PSAEM for exponential family models, Bayesian

1: Initialize \( x_{0:T}[0] \), \( \theta(0) \) and \( \eta_0 \)
2: for \( k = 1, 2, \ldots \) do
3: Run Algorithm 1 conditional on \( x_{0:T}[k-1] \) and \( \theta[k-1] \) to sample \( x_{0:T}[k] \)
4: Sample \( \theta[k] \sim \Pi_{\eta_{k-1}, x_{0:T}[k]}(\theta[k-1], \cdot) \)
5: Update sufficient statistics \( S_k \) according to (13b)
6: Solve and update hyperparameters \( \eta_k \leftarrow \arg \max \eta \phi(\eta) \) using (13a)
7: end for

V. CONVERGENCE

The convergence of SAEM and its extensions, including MCMC-based implementations, has received a lot of attention \([18, 25, 49, 27]\). In Section V-A we present a basic convergence result for PSAEM. This is essentially an application of \([25\text{ Theorem } 1]\), however, we also add a missing piece regarding the continuity of the PGAS Markov kernel. This will under certain (strong) assumptions on \( X \) and the model \([11]\) imply convergence of PSAEM as \( k \to \infty \) (with finite \( N \geq 2 \) fixed in Algorithm 1). Some of these conditions could possibly be weakened by using the algorithmic modifications proposed by \([27]\), but we do not pursue this further here. We will also, in Section V-B discuss some practical considerations regarding the choice of \( N \) and \( \gamma_k \).

In the presentation below we write \( ||f||_\infty = \sup_x |f(x)| \) for the supremum norm of function \( f \) and \( \Pi f(x) = \int \Pi(x, dx') f(x') \) for the Markov kernel \( \Pi \) acting on \( f \).

A. Theoretical results

We will for brevity present this section in the Fisherian setting. By considering \( \{x_{0:T}, \theta \} \) as the latent variables instead of \( x_{0:T} \), the results are applicable also to the Bayesian setting.

Convergence of the SAEM algorithm has only been established for models in the exponential family. In addition to the requirements on the step size sequence in (6), the essence of the assumptions used by \([25]\) are:

(A1) The parameter space \( \Theta \) is an open subset of \( \mathbb{R}^p \). The model belongs to the exponential family, and the log-likelihood function and its components \( \phi, \psi \) and \( S \) are sufficiently smooth, differentiable and integrable.

(A2) A unique solution to the maximization problem in the (M)-step exists, and that mapping from \( S_k \) to \( \theta_k \) is sufficiently differentiable.

(A3) \( X \) is compact and \( S \) is continuous on \( X \).

(A4) The Markov kernel \( \Pi_\theta \) for sampling \( x_{0:T} \) is uniformly ergodic uniformly in \( \theta \). Furthermore, \( \Pi_\theta \) is Lipschitz continuous w.r.t. \( \theta \) uniformly in \( x_{0:T} \).

**Remark:** For more precise statements of the actual assumptions under which we prove convergence of PSAEM, see Appendix A.

Under such assumptions \([25]\) show that SAEM converges, up to a stationary point of the likelihood surface. Assumption (A1)-(A3) define the class of models \([11]\) for which convergence is proven. The compactness assumption on \( X \) is strong, and ensures that \( S_k \) cannot diverge, but is not strictly necessary. The more general case is, however, far from trivial, see \([18\text{ Section } 5], [49] \) and \([27]\). Assumption (A4) puts requirements (uniform ergodicity and Lipschitz continuity) on the MCMC kernel that is used, which is PGAS in our case. Uniform ergodicity has been shown for PGAS under a boundedness assumption on the weights of the conditional particle filter \([28\text{ Theorem } 3]\). In Appendix A we extend this result to hold uniformly in \( \theta \) under assumption (A5), stated below. What has not previously been shown, though, is Lipschitz continuity of the PGAS Markov kernel. This property is establish below under the following additional assumption.
(A5) There exists constants $L_1, L_2 < \infty$, $\delta_1, \delta_2 > 0$ and $\kappa_1, \kappa_2 < \infty$, independent of $x_{t-1}, x_t, \theta$, such that, for all $x_{t-1}, x_t \in X$ and all $t = 1, \ldots, T$,

a) Lipschitz continuity of transition and likelihood densities: For all $\theta, \tilde{\theta} \in \Theta$,

$$|p_\theta(x_t | x_{t-1}) - p_\tilde{\theta}(x_t | x_{t-1})| \leq L_1 \|\theta - \tilde{\theta}\|,$$

$$|p_\theta(y_t | x_t) - p_\tilde{\theta}(y_t | x_t)| \leq L_2 \|\theta - \tilde{\theta}\|.$$ 

b) Strong mixing: For all $\theta \in \Theta$, $\delta_1 \leq p_\theta(x_t | x_{t-1}) \leq \kappa_1$ and $\delta_2 \leq p_\theta(y_t | x_t) \leq \kappa_2$.

Remark: The lower bound on the state transition and likelihood functions in (A5), commonly referred to as the strong mixing condition, are indeed strong but have traditionally been used for establishing many theoretical results on SMC, see for instance [50]. Furthermore, this assumption essentially boils down to compactness of $X$, which is assumed in (A3) already. The strong mixing condition has been weakened for some results [51, 52], and could possibly be extended further.

Theorem 1 (Lipschitz continuity of PGAS). Assume (A1) and (A5) and let $\Pi_\theta$ denote the PGAS Markov kernel [4]. Then there exists a constant $C < \infty$ such that for any bounded function $f : X^{T+1} \to \mathbb{R}$, it holds that for all $\theta, \tilde{\theta} \in \Theta$,

$$\|\Pi_\theta f - \Pi_{\tilde{\theta}} f\|_{\infty} \leq C\|f\|_{\infty} \|\theta - \tilde{\theta}\|.$$

Proof. See Appendix B.

We may now piece all results together into the main theorem of this section, which establishes the convergence of PSAEM.

Theorem 2 (Convergence of PSAEM). Assume (A1), (A5); see precise statements in Appendix A. Additionally, assume (A3) and let $\theta_k$ be computed by Algorithm 1. Then, with probability 1, $\lim_{k \to \infty} d(\theta_k, \mathcal{L}) = 0$, where $d(\theta, \mathcal{L})$ denotes the distance from $\theta$ to the set $\mathcal{L} = \{\theta \in \Theta : \frac{\partial}{\partial \theta} p(\cdot | y_{1:T}) = 0\}$.

Proof. The proof, together with precise statements of the assumptions, is given in Appendix A. The big picture is that Theorem 1 (together with existing ergodicity results) implies (A3), and therefore Theorem 2 follows from 25, Theorem 1.

B. Practical considerations

Even though Theorem 2 gives a reassuring theoretical foundation for using PSAEM, it does not give any practical advice on some of the (few) tuning parameters available: the choice of step length $\{\gamma_k\}_{k=1}^\infty$ and the number of particles $N$ in Algorithm 1.

A common choice for step length is $\gamma_k = k^{-\alpha}$, and the requirements (6) are fulfilled for any $\alpha \in \left(\frac{1}{2}, 1\right]$. In our experience, it is often advisable to choose $\alpha < 1$, perhaps $\alpha = 0.7$, not to constrain the steps too much. Even though not necessary, the initial convergence speed can sometimes be improved by setting some initial step lengths to constant 1, before starting the sequence of decreasing step lengths.

For $N$, we have to make a balance between a well mixing Markov kernel (large $N$) and the computational load (small $N$). Let $K$ denote the number of iterations of PSAEM, and assume that the computational budget available is such that the product $KN$ is limited. In such a situation, the general advice would be to take $N$ ‘small’ and $K$ ‘large’. However, if $N$ is too small, the Markov kernel will not mix well, affecting the convergence speed. To monitor the mixing, the overlap between two consecutive state trajectories $x_{0:T}[k \pm 1]$ and $x_{0:T}[k]$ could be computed, and if it exceeds a certain threshold, say 90%, a warning could be raised that the mixing is not sufficient and $N$ should be increased.

VI. Experiments and applications

We will in this section first (Section VI-A) illustrate the behavior of PSAEM on a small toy example (where the maximum likelihood estimate can be found exactly), and study the advantage over a standard Monte Carlo EM implementation for the same problem. We will thereafter turn to three different applications, namely parameter estimation in a non-linear state-space model (the Fisherian setting, Section VI-B), and hyperparameter estimation (Bayesian setting) in infinite factorial dynamical models (Section VI-C) and Gaussian process state-space models (Section VI-D), respectively. Full details for all examples are found in Appendix C.

A. Linear Gaussian state-space model

We consider $T = 300$ data points from the model

$$x_{t+1} = \theta x_t + w_t, \quad w_t \sim \mathcal{N}(0, 1), \quad (14a)$$

$$y_t = x_t + e_t, \quad e_t \sim \mathcal{N}(0, 0.3), \quad (14b)$$

with $\theta \in (-1, 1)$. We apply PSAEM and four alternative methods. A close relative to PSAEM, namely PIMH-SAEM (using particle independent Metropolis–Hastings instead of PGAS; [27, 53]), is applied. We also use two different Monte Carlo EM solutions [5], one using the forward filter backward simulator (FFBSi) smoother [10, 54] and one using the particle-based rapid incremental (PaRIS) smoother [55]. Compared to FFBSi, the PaRIS smoother has the computational advantage that it approximates not the entire distribution $p_{\theta_k}(x_{0:T} | y_{1:T})$, but only $p_{\theta_k}(x_t, x_{t+1} | y_{1:T})$, which in fact is sufficient for the Fisherian problem. In fact, PaRIS is an online smoothing algorithm so it can also be combined with online-EM as proposed by [24]. The online-EM method solves indeed also the (challenging) online problem, and is included in the comparison. We iterate each method 1 000 times, and study the convergence to the true maximum likelihood estimate (which is available exactly in this toy model). For the online-EM algorithm we loop over the $T = 300$ data points 1 000 times (note that this method makes one parameter update per single time step). All methods are applied with different numbers of particles $N$.

In Figure 4 the evolution of the absolute error is shown as a function of computational time on the same standard desktop computer with comparable implementations, averaged over 200 realizations of each algorithm. Note that PSAEM

This is similar to the method proposed by [11], but it uses a more efficient smoother.
pumped into an upper water tank, from which it flows through only the pump voltage. A physically motivated discrete-time
the problem is to predict the water level in the lower tank given
[56]. A training and a test data set of input-output data samples
for a cascaded water tank system, using the data presented by
B. Cascaded water tanks
scaling properties of PGAS compared to PIMH.

and PIMH-SAEM converge as \( k \to \infty \) (for fixed \( N \)), whereas Monte Carlo EM has a non-vanishing bias which only decreases as \( N \to \infty \). In other words, \( k \to \infty \) is not sufficient for convergence in Monte Carlo EM. Comparing
PSAEM and PIMH-SAEM, the latter requires a significantly larger number of particles than PSAEM, and has therefore
a higher computational cost. This difference is likely to be even more pronounced for larger values of \( T \), due to superior
scaling properties of PGAS compared to PIMH.

B. Cascaded water tanks

We consider the benchmark problem of learning a model for a cascaded water tank system, using the data presented by[58]. A training and a test data set of input-output data samples
\( \{u_t, y_t\} \), each with \( T = 1024 \) data points, are provided. The data is recorded from an experimental setup where water
is pumped into an upper water tank, from which it flows through a small opening into a lower water tank, and from there through another small opening into a basin. During the data
collection, the tanks occasionally overflowed, and the excess water from the upper tank partially flowed into the lower
tank. Only the pump voltage (input) and the water level in the lower tank (output) is measured each \( T_u = 4 \) second, and the problem is to predict the water level in the lower tank given
only the pump voltage. A physically motivated discrete-time
nonlinear state-space model (partly adopted from [52]) is
\[
\begin{align*}
x_{t+1}^{\text{u}} &= 10 \times x_{t}^{\text{u}} + T_u(-k_1 \sqrt{10 \times x_{t}^{\text{u}}} - k_2 \{10 \times x_{t}^R\} + k_3 u_t) + w_{t}^{\text{u}} \\
x_{t+1}^R &= 10 \times x_{t}^R + T_u(k_1 \sqrt{10 \times x_{t}^{\text{u}}} + k_2 \{10 \times x_{t}^R\} - k_3 \sqrt{10 \times x_{t}^{\text{u}}} \\
&\quad - k_4 \{10 \times x_{t}^R\} + k_6 \{x_{t}^R(10 \times x_{t}^{\text{u}} - 10)\} + w_{t}^R) \\
y_t &= 10 \times x_{t}^R + \epsilon_t,
\end{align*}
\]

(a) Besides faster convergence (in terms of computational time), PSAEM does not suffer from the bias present in Monte Carlo EM. The bias is caused by the finite number of samples in the integral [5], and the bias vanishes only as \( N \to \infty \), in contrast to PSAEM for which \( k \to \infty \) is enough.

(b) The optimal \( N \) for PSAEM in this problem appears to be in the range 10–100; smaller \( N \) causes poor mixing and slower convergence; larger \( N \) increases computational cost without improving mixing. PIMH-SAEM with \( N = 100 \) struggles because of poor mixing, whereas \( N = 1000 \) mixes better at a higher computational cost.

(c) The convergence of online-EM with the PaRIS smoother is theoretically not fully understood, but appears for \( N = 3 \) to suffer from a similar bias as Monte Carlo EM. For this example it appears to converge with larger \( N \), however at a significantly higher computational cost than PSAEM.

**Table I:** The cascaded water tank setup and modeling results. We initialize the 9 unknown parameters with an ad-hoc educated guess (top row), and then optimize them with PSAEM (middle row). We also include the best performing result previously published (last row). The figure of merit is root-mean-squared error for simulation on the test data.

where the states \( x_{t}^{\text{u}} \in \mathbb{R} \) and \( x_{t}^R \in \mathbb{R} \) are the water levels plus the inflow in the upper and lower tank, respectively. The parameters \( k_1, k_2, k_3, k_4, k_5 \) represent unknown physical quantities, such as tank and hole diameters, flow constants, pump efficiency, etc. Each tank has height 10 (in the scale of the sensor), and \( k_6 \) and 10\&\ldots) is motivated by the overflow
events. The initial level of the upper water tank is modeled as
\( x_{0}^u \sim N(\xi_0, \sqrt{1}), \) with \( \xi_0 \) unknown. Furthermore, \( w_{t}^u, \) \( w_{t}^R \) \( u_t \) and \( \epsilon_t \) are assumed to be zero mean white Gaussian noise with unknown variances \( \sigma_w^2 \) and \( \sigma_e^2 \), respectively. All in all, the unknown parameters are
\( \theta = \{k_1, k_2, k_3, k_4, k_5, \sigma_w^2, \sigma_e^2, \xi_0\} \).

The model belongs to the exponential family, and we can thus apply PSAEM as presented in Algorithm [7] to find a maximum likelihood estimate of \( \theta \). We initialize \( \theta \) randomly around physically reasonable values, and run PSAEM for 50 iterations with \( N = 100 \) (taking a few seconds on a standard desktop computer). The obtained results are reported in Table I together with the best performing result previously published (to the best of our knowledge). Many previously published methods use a more data-driven approach, but the relatively small amount of data makes the encoding of physical knowledge important, as done here by [15] and PSAEM.

\[\text{Figure 2: Estimation of } \theta \text{ in } \{14\} \text{ with five different methods; the proposed PSAEM, PIMH-SAEM (similar to PSAEM, but with a PIMH Markov kernel instead of PGAS), two Monte Carlo EM implementations (using the FFBSi and PaRIS smoother, respectively) and online-EM with the PaRIS smoother. The methods are run with various number of particles } N, \text{ cf. the discussion on } \{V\text{-B} \} \text{ Their average evolution of the absolute error } |\theta_{t} - \theta_{\text{ML}}| (\text{over 200 runs}), \text{ where } \theta_{\text{ML}} \text{ is the exact maximum likelihood estimate, is shown as a function of the wall clock time. All methods are run for } 1000 \text{ iterations, and there is a linear relationship between } k \text{ and computational time for all methods.} \]
Algorithm 9 PSAEM for infinite factorial dynamical models: the cocktail party example

1: for \( k = 0 \) to \( K \) do
2: \( \) Update the state dimensionality (number of speakers) \( M_k \) using slice sampling.
3: \( \) Sample a state trajectory using PGAS.
4: \( \) Gibbs update of the transition probabilities \( \{b^m\}_{m=1}^{M_k} \) for each speaker.
5: \( S_k \leftarrow (1 - \gamma_k)S_{k-1} + \gamma_k S_k \{b^m\}_{m=1}^{M_k} \), with \( S \) being sufficient statistics for the Beta distribution.
6: \( \eta_k \leftarrow \arg \max_\eta \mathbb{E}_{\theta_k} \mathbb{E}_{\phi_k} \left( \eta \right) = \arg \max_\eta \left( S_k, \phi(\eta) \right) - \psi(\eta) \).
7: Gibbs update of noise variance parameters.
8: end for

C. Hyperparameters in infinite factorial dynamical models

The infinite factorial dynamical model (iFDM, [3]) is a Bayesian non-parametric model for separation of aggregated time-series into independent sources. By using a Markov Indian buffet process, the number of sources (dimensionality of the hidden state) does not have to be upper bounded a priori. Each source is modeled as a (discrete or continuous) Indian buffet process, the number of sources (dimensionality of the state-space model) does not have to be upper bounded a priori. Due to the large number of hyperparameters in this Bayesian setting, and we solve the inference problem, i.e., performing the actual source separation, PGAS has proven useful [4]. There is, however, a multitude of hyperparameters in this Bayesian setting, and we demonstrate how the procedure by [4] easily can be extended with PSAEM to automatically estimate hyperparameters on-the-fly, reducing the need for extensive manual tuning.

We will consider the cocktail party problem originating from [3], to which iFDM has been applied [4] Section 4. The voices of 15 different speakers are aggregated into a \( T = 1085 \) long sequence, together with some noise, and the problem is to jointly infer (i) the number of speakers (dimension of \( x_t \)), (ii) when each speaker is talking (the trajectory \( x_t \)) and (iii) the dynamics of each speaker (how prone s/he is to talk). Each speaker is modeled as a Markov chain with two states, ‘talking’ or ‘quiet’, and the posterior distribution over its transition probabilities is inferred individually for each speaker. The Beta distribution is used as prior for these probabilities, and the hyperparameters for the Beta distribution are manually chosen by [3]. We outline in Algorithm 9 how the inference procedure can be extended with PSAEM (new lines are marked with blue). In addition to the lessened burden of manual hyperparameter tuning, we can also report slightly improved results: With the hyperparameters automatically found by PSAEM, the average number of switches between ‘talking’ and ‘quiet’ in posterior samples is closer to ground truth (84 instead of 86, ground truth: 62) and the average value of the complete data likelihood of the posterior samples increases. Of course, PSAEM could be applied also to other hyperparameters in the problem, following the very same pattern. Posterior samples of \( x_t \) are shown in Figure 3.

D. Hyperparameter estimation in Gaussian process state-space models

Gaussian process state-space models are a combination of the state-space model and the Gaussian process (GP) model as

\[
x_{t+1} = f(x_t) + \epsilon_t, \quad f \sim \mathcal{GP}(m_{\theta}^f, K_{\theta}^f), \quad \epsilon_t \sim \mathcal{N}(0, \Sigma_{\theta}^\epsilon),
\]

\[
y_t = g(x_t) + \epsilon_t, \quad g \sim \mathcal{GP}(m_{\theta}^g, K_{\theta}^g), \quad \epsilon_t \sim \mathcal{N}(0, \Sigma_{\theta}^\epsilon),
\]

Fig. 3: The cocktail problem, introduced by [3], [4], amounts to inferring the number of speakers (columns) and their periods of talking and being quiet (yellow and blue, respectively) from an aggregated observation (not shown) during a time sequence (y-axis). The middle panel is a sample from the solution by [4], and the right panel a sample after we have extended that solution with PSAEM to automatically estimate some hyperparameters. Both solutions infer the correct number of speakers (15), but the solution with PSAEM is slightly less prone to switch between quiet and talking (closer to the ground truth, left). However, the main advantage of PSAEM, not present in the plot itself, is the lessened need for manual tuning of hyperparameters at almost no extra computational cost.

Algorithm 10 PSAEM for hyperparameter estimation in Gaussian process state-space models

1: \( \) Initialize \( x_{1:T}[0], \theta[0], \eta_0 \).
2: \( \) for \( k = 0 \) to \( K \) do
3: \( \) Sample \( x_{0:T}[k] | \theta_{k-1}, \eta_{k-1} \) using Algorithm 9.
4: \( \) Sample \( \theta_k | \eta_{k-1}, x_{0:T}[k] \) with a closed-form expression.
5: \( \) Update \( \eta_k \leftarrow \arg \max_\eta \mathbb{E}_{\theta_k} \mathbb{E}_{\phi_k} \left( \eta \right) = \arg \max_\eta \left( S_k, \phi(\eta) \right) - \psi(\eta) \).
6: \( \) Solve \( \eta_k \leftarrow \arg \max_\eta Q_k^{\text{Bay}}(\eta), \)
7: end for

or variations thereof. As in any state-space model, only \( y_{1:T} \) is observed and not \( x_{0:T} \), and standard GP regression methods [59] can therefore not be used to learn the posterior \( p_{\theta}(y | y_{1:T}) \). Consequently, learning of the GP hyperparameters \( \eta \)—usually done via empirical Bayes \( \hat{\eta} = \arg \max_\eta p_{\theta}(\hat{\eta} | y_{1:T}) \)—is not straightforward either.

Despite the computational challenges, it has been argued that the model is versatile and powerful by its combination of the dynamic state-space model and the nonparametric and probabilistic GP, and has for this reason achieved attention in the machine learning literature. One proposed solution is to use PGAS for learning the model [34], [60], [61], and we extended that solution with PSAEM to also include estimation of the hyperparameters at almost no extra computational cost.

We consider the solution proposed by [34], in which the nonparametric GP is approximated with a reduced-rank representation with a finite parameter set \( \theta \). We introduce PSAEM for this solution in Algorithm 10 (new lines in blue). Since the computational burden in practice is dominated by running the conditional particle filter, the inclusion of PSAEM adds very little extra computational cost. An example of estimation of the length scale in a Gaussian process state-space model is shown in Figure 4 where the space of \( x_t \) is one-dimensional.
and \( g(x) = x \) is considered known, but the noise level is significant with \( \sigma_n^f = \sigma_n^g = 1 \).

VII. Conclusions

We have presented PSAEM for learning nonlinear state-space models, both in a maximum likelihood and an empirical Bayes setting. We have also summarized the available theoretical results, and added a missing piece about convergence. Besides maximum likelihood parameter estimation, we believe PSAEM has a great potential also for models where PGAS is currently used and automatic estimation of hyperparameters via PSAEM can be achieved with only a small modification to existing implementations.

APPENDIX A

Proof of Theorem 2 Convergence of PSAEM

We first list the assumptions behind Theorem 2 in more detail. First, assumption (A1) is explicitly:

- \( \Theta \) is an open set. The model belongs to the exponential family \((\Pi_0)\), where \( \phi \) and \( \psi \) are twice differentiable on \( \Theta \) and \( S \) is a Borel function in \( x_{0:T} \) taking its values in an open subset \( S \) of \( \mathbb{R}^k \). The convex hull of \( S(\mathbb{R}^m \times (T+1)) \) is included in \( S \). Furthermore, for all \( \theta \in \Theta \), we require, for all \( \theta \leq \theta_{0:T} \), where \( \rho_0 \leq \rho_0(\theta_{0:T} \mid y_{1:T})d\theta_{0:T} < \infty \) and \( \int S(x_{0:T} \mid y_{1:T})p_0(x_{0:T} \mid y_{1:T})d\theta_{0:T} \) is continuously differentiable w.r.t. \( \theta \).

- The log-likelihood function \( \log p_0(y_{1:T}) \) is continuously differentiable once and \( \ell \) times differentiable in \( \Theta \). Furthermore, \( \theta_0 \) \( \int p_0(x_{0:T}, y_{1:T})d\theta_{0:T} = \int \theta_0 p_0(x_{0:T} \mid y_{1:T})d\theta_{0:T} \).

This assumption corresponds to assumptions (M1), (M2), (M3) and (M4) of \((\Pi_0)\). Furthermore, \( \ell \) times differentiability of the log-likelihood function corresponds to part of their assumption (SAEM2).

Our assumption (A2), which corresponds to (M5) and the remaining part of (SAEM2) of \((\Pi_0)\), is more explicitly:

- A unique solution to the maximization problem in the (M)-step exists, and that mapping from \( S_k \) to \( \theta_k \) is continuously differentiable once and \( \ell \) times differentiable.

Our assumption (A3) is:

- \( X \) is compact and \( S \) is continuous on \( X \).

Since \( S \) is a continuous function on a compact subset of \( \mathbb{R}^m \), it is also bounded. This corresponds to (SAEM3)’1, (SAEM3)’4). Furthermore, since \( S \) is continuous and \( X \) is compact, the image \( S(X) \) is also compact, and so is its convex hull. It follows that the sequence \( \{S_k\}_{k \geq 1} \) takes its values in a compact subset of \( S \), which is \((\Pi_0) \) (C).

Finally, since our design choice \((\Pi_0)\) corresponds to (SAEM1), the only missing pieces in order to apply (SAEM) Theorem 1 are (SAEM3)’2-3, which have to do with Lipschitz continuity and uniform ergodicity of the PGAS kernel; see our (A4).

Consider first ergodicity. We require uniform ergodicity, uniformly in \( \theta \) (SAEM3)’3). Specifically, for any bounded function \( f : X_{T+1} \rightarrow \mathbb{R} \), let \( \tilde{f}_\theta(x_{0:T}) = f(x_{0:T}) - \int f(x_{0:T})p_\theta(x_{0:T} \mid y_{0:T})dx_{0:T} \). Then, we require,

\[
\sup_{\theta \in \Theta} \|\Pi_\theta^jf_\theta\|_\infty \leq M \rho_j \|f\|_\infty
\]

for all \( j \geq 0 \) and for constants \( M < \infty \) and \( \rho \in \{0, 1\} \) independent of \( \theta \).

It follows from [42, Theorem 1] that the PGAS Markov kernel \( \Pi_\theta \) satisfies a global Doeblin condition and that it is uniformly ergodic, such that,

\[
\|\Pi_\theta^jf_\theta\|_\infty \leq \rho_j^j \|f\|_\infty
\]

for \( j \geq 0 \) and where

\[
\rho_\theta = 1 - \prod_{t=0}^{T} \frac{N - 1}{2B_{T}^\theta + N - 2}
\]

and where the terms \( B_{T}^\theta \) are defined in [42, Eq. 10]. It remains to prove that these terms are bounded uniformly in \( \theta \). However, under the strong mixing assumption (A5), we have from the proof of [42, Proposition 5] that \( B_{T}^\theta \leq (\kappa_1\kappa_2)/(\delta_1\delta_2) \). This proves the first part of our (A4), which is the same as (SAEM3)’3).

The final ingredient is the Lipschitz continuity of the Markov kernel, corresponding to (SAEM3)’2). This corresponds to our Theorem 1 (proven in Appendix B). A slight difference between our Theorem 1 and (SAEM3)’2), however, is that the latter assumes that the Markov transition kernel admits a density with respect to Lebesgue measure and that this density function is Lipschitz continuous. Our continuity result is instead expressed in terms of total variation distance. The condition (SAEM3)’2) is used by (SAEM) to prove their Lemma 2, see (SAEM) p. 129. Thus, to complete the picture we provide a lemma which replaces (SAEM) Lemma 2. The result—which extends the continuity of the PGAS Markov kernel to the \( k \)-fold kernel—is a special case of [49, Proposition B.2], but for completeness we repeat the proof here.

Lemma 1. Assume that the conditions of Theorem 1 hold. Then, there exists a constant \( D \leq \infty \) such that for any \( k \geq 0 \) and any bounded function \( f \),

\[
\|\Pi_{\theta}^bf - \Pi_{\bar{\theta}}^bf\|_\infty \leq D \|f\|_\infty \|\theta - \bar{\theta}\|.
\]

Proof. Define \( \tilde{f}_\theta(x_{0:T}) = f(x_{0:T}) - \int f(x_{0:T})p_\theta(x_{0:T} \mid y_{0:T})dx_{0:T} \). Since \( \tilde{f}_\theta \) differs from \( f \) by a constant (depending on \( \theta \)) we can write,

\[
\|\Pi_{\theta}^bf - \Pi_{\bar{\theta}}^bf\|_\infty = \|\Pi_{\theta}^bf - \Pi_{\theta}^bf\|_\infty \leq \sum_{j=1}^{k} \|\Pi_{\theta}^{j-1}(\Pi_{\bar{\theta}} - \Pi_{\bar{\theta}})\Pi_{\theta}^{j-1}f_\theta\|_\infty.
\]
We have,
\[
\|\Pi_\theta^{k-j}(\Pi_\theta - \Pi_{\tilde{\theta}})^j \bar{f}_\theta\|_\infty = \sup_{x_{0:T}} \left| \int \Pi_\theta^{k-j}(x_{0:T}, dx_{0:T}) (\Pi_\theta - \Pi_{\tilde{\theta}})^j \bar{f}_\theta(x_{0:T}) \right|
\]
\[
\leq \sup_{x_{0:T}} \left| \int \Pi_{\tilde{\theta}}^{k-j}(x_{0:T}, dx_{0:T}) (\Pi_\theta - \Pi_{\tilde{\theta}})^j \bar{f}_\theta(x_{0:T}) \right|
\]
\[
\leq \sup_{x_{0:T}} \int \Pi_{\tilde{\theta}}^{k-j}(x_{0:T}, dx_{0:T}) (\Pi_\theta - \Pi_{\tilde{\theta}})^j \bar{f}_\theta(x_{0:T})\| (\Pi_\theta - \Pi_{\tilde{\theta}})^j \bar{f}_\theta\|_\infty
\]
\[
= \| (\Pi_\theta - \Pi_{\tilde{\theta}})^j \bar{f}_\theta\|_\infty.
\]

Now, consider the function \( \Pi_\theta^{j} \bar{f}_\theta(x_{0:T}) \) for some \( \ell \geq 0 \). Recall that \( \bar{f}_\theta \) is centered around the posterior expectation of \( f \) with respect to \( \rho_\theta(x_{0:T} | y_{1:T}) \), which is the limiting distribution of \( \Pi_{\tilde{\theta}} \). Thus, by uniform ergodicity of \( \Pi_{\tilde{\theta}} \) uniformly in \( \theta \),
\[
\sup_{\theta} \| \Pi_\theta^{j} \bar{f}_\theta\|_\infty \leq M \rho^j \| f \|_\infty,
\]
for some constants \( M < \infty \) and \( \rho < 1 \). Consequently, the function \( \Pi_\theta^{j} \bar{f}_\theta(x_{0:T}) \) satisfies the conditions of Theorem 1, and thus
\[
\| (\Pi_\theta - \Pi_{\tilde{\theta}})^j \bar{f}_\theta\|_\infty \leq CM \rho^j \| \theta - \tilde{\theta} \|.
\]

Plugging this into the expressions above completes the proof.

From this, the results of Lemma 2 in [25] follows for our assumptions, and hence also Theorem 1 of [25] and, ultimately, Theorem 2 of this article.

**Appendix B**

**Proof of Theorem 1**

This appendix contains a proof of Theorem 1. It is based on the construction of a coupling between the Markov kernels \( \Pi_\theta \) and \( \Pi_{\tilde{\theta}} \). A similar technique has previously been used by [41] to prove uniform ergodicity of the Particle Gibbs kernel. An explicit coupling of conditional particle filters is used by [62] to construct (practical) algorithms for, among other things, likelihood estimation and unbiased estimates of smoothing functionals.

We first review some basic properties of couplings and total variation. Let \( P \) and \( Q \) be two probability measures with densities \( p \) and \( q \), respectively, with respect to some reference measure \( \lambda \). Let \( C \) be the set of couplings of \( P \) and \( Q \), that is, joint probability measures with marginals \( P \) and \( Q \). We can then write the total variation distance between \( P \) and \( Q \) in the following equivalent ways:
\[
\| P - Q \|_{TV} = \frac{1}{2} \sup_{\| f \|_1 \leq 1} | P f - Q f | \tag{17a}
\]
\[
= \lambda(\max(p - q, 0)) \tag{17b}
\]
\[
= 1 - \lambda(\min(p, q)) \tag{17c}
\]
\[
= \inf_{\xi \in C} \int \int 1(x \neq y)\xi(dx, dy). \tag{17d}
\]

Note also that it is possible to explicitly construct a coupling attaining the infimum in (17d): let \( \alpha = \lambda(\min(p, q)) \), \( \nu(dx) = \alpha^{-1} \min(p(x), q(x)) \lambda(dx) \), and
\[
\xi(dx, dy) = \alpha\nu(dx)\delta_x(dy) + (1 - \alpha)^{-1}(P(dx) - \alpha\nu(dx))(Q(dy) - \alpha\nu(dy)). \tag{18}
\]

A coupling \( \xi \) which attains the infimum, or equivalently which maximizes the probability of \( X \) and \( Y \) being identical when \( (X, Y) \sim \xi \), is referred to as a **maximal coupling**. Finally, for a coupling \( \xi \), the quantity \( \int \int 1(x = y)\xi(dx, dy) \)—that is, the probability that \( X \) and \( Y \) are identical under \( \xi \)—is referred to as the **coupling probability** under \( \xi \).

Now, to prove the Lipschitz continuity of the PGAS Markov kernel as stated in Theorem 1, we will construct a coupling \( \xi_{\theta, \tilde{\theta}}(x'_{0:T}, dx_{0:T}, dx'_{0:T}) \) of the Markov kernels \( \Pi_\theta(x'_{0:T}, dx_{0:T}) \) and \( \Pi_{\tilde{\theta}}(x'_{0:T}, dx'_{0:T}) \). This coupling is defined via Algorithm 1, which takes \( x'_{0:T} \) as input and produces \( x_{0:T} \) and \( \tilde{x}_{0:T} \) as outputs, such that the marginal distributions of the output trajectories are \( \Pi_\theta(x_{0:T}, dx_{0:T}) \) and \( \Pi_{\tilde{\theta}}(x_{0:T}, d\tilde{x}_{0:T}) \), respectively. For ease of notation in Algorithm 1, we write \( M[P, Q] \) for any maximal coupling (for instance the one given by (18)) of some distributions \( P \) and \( Q \). For brevity, we also write \( M[p_i]_{i=1}^N \) for a maximal coupling between the two discrete distributions on \{1, 2, ..., \} with probabilities \( P(\{i\}) = p_i / \sum_{i=1}^N p_i \) and \( Q(\{i\}) = q_i / \sum_{i=1}^N q_i \).

Note that for any bounded function \( f \),
Algorithm 11 Coupled conditional particle filters with ancestor sampling defining $\xi_{0,\bar{0}}$.

**Input:** Conditional trajectory $x_{0:T}$, parameters $\theta$ and $\bar{\theta}$.

**Output:** Trajectories $x_{0:T}^n$ and $\tilde{x}_{0:T}$.

1. Draw $\tilde{x}_0 \sim p(x_0)$ and set $x_0 = \tilde{x}_0$, $i = 1, \ldots, N - 1$.
2. Set $x_0^n \leftarrow x_0$ and $\tilde{x}_0^n \leftarrow x_0$.
3. Set $w_0^n \leftarrow 1$ and $\tilde{w}_0^n \leftarrow 1$, $i = 1, \ldots, N$.
4. for $t = 1, 2, \ldots, T$ do
5. for $i = 1, \ldots, N - 1$, draw $$(a_i^n, \tilde{a}_i^n) \sim M \{w_{t-1,i}^N \}_{i=1}^N, \{\tilde{w}_{t-1,i}^N \}_{i=1}^N$$.
6. for $i = 1, \ldots, N - 1$, draw $$(x_i^n, \tilde{x}_i^n) \sim M \{p_{\theta}(\cdot | x_{t-1}^i), p_{\tilde{\theta}}(\cdot | \tilde{x}_{t-1}^i) \}.$$ 
7. Draw $$(a_i^n, \tilde{a}_i^n) \sim M \{w_{t-1,i}^N p_{\theta}(x_{t-1}^i | x_{t-1}^i), \{\tilde{w}_{t-1,i}^N p_{\tilde{\theta}}(\tilde{x}_{t-1}^i | \tilde{x}_{t-1}^i) \}_{i=1}^N$$.
8. Set $x_t^n \leftarrow x_t^n$ and $\tilde{x}_t^n \leftarrow x_t^n$.
9. Set $w_t^n \leftarrow p_{\theta}(y_t | x_t^n)$ and $\tilde{w}_t^n \leftarrow p_{\tilde{\theta}}(y_t | \tilde{x}_t^n)$ for $i = 1, N$.
10. end for
11. Draw $(J, \tilde{J}) \sim M \{w_{t-1,i}^N \}_{i=1}^N, \{\tilde{w}_{t-1,i}^N \}_{i=1}^N$.
12. Set $x_t^J = x_t^J$ and $x_t^{\tilde{J}} = \tilde{x}_t^{\tilde{J}}$.
13. for $t = T - 1, T - 2, \ldots, 0$ do
14. Set $J \leftarrow a_{t+1}^J$ and $\tilde{J} \leftarrow \tilde{a}_{t+1}^J$.
15. Set $x_t^J \leftarrow x_t^J$ and $\tilde{x}_t^J \leftarrow \tilde{x}_t^J$.
16. end for

$$||\Pi_{\theta'}f - \Pi_{\bar{\theta}}f|| \leq ||f|| \sup_{x_{0:T}} \sup_{0 < \gamma < 1} ||\Pi_{\theta}g(x_{0:T}) - \Pi_{\bar{\theta}}g(x_{0:T})||_1$$

$$\leq 2||f|| \sup_{x_{0:T}} \int \int 1(x_{0:T} = x_{0:T})\xi_{\theta,\bar{\theta}}(x_{0:T}) dx_{0:T} dx_{0:T} X_{0:T}$$

$$= 2||f|| \sup_{x_{0:T}} \left(1 - \int \int 1(x_{0:T} = x_{0:T})\xi_{\theta,\bar{\theta}}(x_{0:T}) dx_{0:T} dx_{0:T} X_{0:T} \right)$$

where we have used (17a) and (17d) for the first and second lines, respectively. Hence, it is sufficient to show that

$$\int \int 1(x_{0:T} = x_{0:T})\xi_{\theta,\bar{\theta}}(x_{0:T}) dx_{0:T} dx_{0:T} X_{0:T} \geq 1 - C \frac{||\theta - \bar{\theta}||}{2}$$

where $C$ is the same constant as in the statement of the theorem.

Let $\alpha_{t-1}$ denote the coupling probability for the coupling at line 5 of Algorithm 11 (and thus $\alpha_T$ is the coupling probability on line 11). On the set $\{x_{1:N}^t = \tilde{x}_{1:N}^t\}$ we have by (17c)

$$\alpha_t = \frac{N}{\sum_{i=1}^N \max \{w_i^n, \tilde{w}_i^n\}} 
\geq \frac{\sum_{i=1}^N \max \{w_i^n, \tilde{w}_i^n\}}{\sum_{i=1}^N \max \{w_i^n, \tilde{w}_i^n\}} 
\geq \frac{N}{\sum_{i=1}^N \max \{w_i^n, \tilde{w}_i^n\}} 
\geq \frac{N}{\sum_{i=1}^N \max \{w_i^n, \tilde{w}_i^n\}}$$

where we have used the Lipschitz continuity of the likelihood ($\mathcal{A}_{S\mathcal{S}}$) for the penultimate inequality, and the lower bound on the likelihood ($\mathcal{A}_{S\mathcal{S}}$) for the last inequality.

Similarly, let $\tilde{\beta}_t$ denote the coupling probability for the coupling on line 7. Under assumption ($\mathcal{A}_{S\mathcal{S}}$), the product $p_\theta(y_{t-1} | x_{t-1})p_\theta(x_t | x_{t-1})$ (which constitutes the unnormalized ancestor sampling weights) is bounded by $\delta_1 \delta_2$. The product is also Lipschitz continuous in $\theta$: since $|ab - cd| = |ab - ad + ad - cd| \leq |a||b - d| + |d||a - c|$ we have

$$|p_{\theta}(y_{t-1} | x_{t-1})p_\theta(x_t | x_{t-1}) - p_{\bar{\theta}}(y_{t-1} | x_{t-1})p_{\bar{\theta}}(x_t | x_{t-1})| 
\leq (\kappa_1 L_2 + \kappa_2 L_1) ||\theta - \bar{\theta}||.$$ 

Therefore, on the set $\{x_{1:N}^t = \tilde{x}_{1:N}^t\}$, we have by a computation analogous to above,

$$\beta_t \geq 1 - \frac{\kappa_1 L_2 + \kappa_2 L_1}{\delta_1 \delta_2} ||\theta - \bar{\theta}||.$$

Finally, let $\gamma^i_t$ denote the coupling probability for the coupling at line 6 for the $i$th particle. By (17b) and (17d) we have, on the set $\{x_{1:N}^t = \tilde{x}_{1:N}^t, a_{t-1}^t = \tilde{a}_{t-1}^t\}$,

$$\gamma^i_t = 1 - \lambda \max \{p_{\theta}(\cdot | x_{t-1}^i), p_{\tilde{\theta}}(\cdot | \tilde{x}_{t-1}^i), 0\} \geq 1 - L_1 \lambda(\thicksim ||\theta - \bar{\theta}||).$$

where $\lambda$ denotes Lebesgue measure and where the inequality follows by ($\mathcal{A}_{S\mathcal{S}}$). By ($\mathcal{A}_{S\mathcal{S}}$), $\lambda(X) < \infty$. Note that the bound on $\gamma^i_t$ is independent of $i$.

Let $D = \max \{L_2, \kappa_1 L_1 + \kappa_2 L_1, L_1 \lambda(X)\}$. Consider first the case $||\theta - \bar{\theta}|| \leq D^{-1}$, by which all the bounds in (20), (21), (22) are nonnegative. Thus, if we write $P$ for probability with respect to the random variables generated by Algorithm 11, we can crudely bound (19) by

$$\mathbb{P}(\{x_{1:N}^t = \tilde{x}_{1:N}^t, a_{t-1}^t = \tilde{a}_{t-1}^t : t = 1, \ldots, T\}, J = \tilde{J})$$

$$\geq E \left[ \alpha_T \prod_{t=1}^T \left( \frac{\beta_t}{\alpha_t} \gamma^i_t \right) \right]$$

$$\geq \left( \frac{1}{1 - L_2 \frac{\delta_2}{\delta_1}} \right)^{T(N-1)+1} \left( \frac{1 - \frac{\kappa_1 L_2 + \kappa_2 L_1}{\delta_1 \delta_2} ||\theta - \bar{\theta}||}{\delta_1 \delta_2} \right)^{T(N-1)+1} \left( \frac{1 - L_1 \lambda(X)||\theta - \bar{\theta}||}{\delta_1 \delta_2} \right)^{T(N-1)+1} \left( \frac{1 - D(2T(N-1) + T + 1)||\theta - \bar{\theta}||}{\delta_1 \delta_2} \right)^{T(N-1)+1}$$

where the last line follows from Bernoulli’s inequality. However, since the probability is trivially bounded from below by 0, the bound above holds also for the case $||\theta - \bar{\theta}|| > D^{-1}$. Hence, (19) holds with $C = 2D(2T(N-1) + T + 1)$, which proves Theorem 1.

It is worth commenting on the fact that the Lipschitz constant $C$ identified above increases with $N$, which might seem counterintuitive. However, this is an artefact of the proof technique, which is based on bounding the probability of a complete coupling of all particles and ancestor weights generated by Algorithm 11 which is a much stronger requirement than coupling the output trajectories only. Indeed, we expect that the Lipschitz constant stabilizes as $N \rightarrow \infty$ as the distribution of the output trajectories then converges to the joint smoothing distribution.

**Appendix C**

**Details about experiments**

This section contains additional details regarding the experiments in Section 6.
Experiment 6.1–Linear Gaussian state-space model

The step length in PSAEM, as well as in PIMH-SAEM, is chosen as $\gamma_k = k^{-0.99}$. PSEM is implemented as a particle filter with $N$ particles and a backward simulator [54] with $N$ backward trajectories. The sufficient statistics, as derived by for instance, [2], are $\frac{1}{T} \sum_t x_t x_t^T$ and $\frac{1}{T} \sum_t x_{t-1} x_{t-1}^T$, and the maximization problem can be solved analytically.

Experiment 6.2–Casceded water tanks

The step length in PSAEM is chosen as $\gamma_k = 1$ for $k = 1, \ldots, 30$, and $\gamma_k = (k - 30)^{-0.7}$ for $k = 31, \ldots$. The initial parameter values are initialized randomly around $k_1 = k_2 = k_3 = k_4 = 0.05$, $k_5 = k_6 = 0$, $\sigma^2_k = \sigma^2_w = 0.1$, $\xi_0 = 6$, and a slight $L_2$-regularization (corresponding to a $\mathcal{N}(0, 10^3)$ prior) is used for $k_4$ to avoid problems if the state trajectory contains no overflow events in the lower tank. The sufficient statistics for a model on the form

$$
x_{t+1} = a(x_t) + \theta^T b(x_t) + w_t,
$$

where $a$ and $\sigma^2$ are unknown, are $\frac{1}{T} \sum_t (x_t - a(x_t - 1)) (x_t - a(x_t - 1))^T$, and the maximization problem can be solved analytically.

Experiment 6.3–Hyperparameter estimation in infinite factorial dynamical models

The exact setup is a replica of [4], to which we refer for details. We use $\gamma_k = k^{-0.7}$, but let the PPMC run for 500 iterations (which, by a very quick look at the trace of PGAS, appears to be a rough estimate of the burn-in period) before starting PSAEM. The initial value of $\gamma$ is the ones chosen by [4]. The sufficient statistics for $M$ number of Beta random variables $\theta_m$ is $M$, $\sum_{m=1}^M \log(\theta_m)$ and $\sum_{m=1}^M \log(1 - \theta_m)$. The maximization problem lacks an analytical solution, and an off-the-shelf numerical optimization routine (fmincon in Matlab) was applied to solve the maximization problem.

Experiment 6.4–Hyperparameter estimation in Gaussian process state-space models

The true functions in the example are

$$
x_{t+1} \sim \mathcal{N} \left( -7 \arctan \left( \frac{2}{T} \right) \cos \left( \frac{2}{T} \right) \exp \left( -\frac{|x_t|}{10} \right), 1 \right)
$$

and

$$
x_{t+1} \sim \mathcal{N} \left( -7 \sin \left( \frac{2}{T} \right), 1 \right),
$$

In the approximate GP-SSM model used, the unknown function $f$ is approximated as a finite basis function expansion, whose coefficients $\theta$ (column vector) have a certain multivariate zero mean Gaussian prior distribution with a variance depending on $\eta$ (see [34] for details). Thus, the sufficient statistics is $\theta \theta^T$, and the maximization problem to solve is

$$
\arg \max_{\theta} -\frac{1}{2} \text{Tr}(\theta \theta^T V^{-1}_n) - \frac{1}{2} \log \det(V_n)
$$

where $V_n$ follows from the choice of covariance function, see again [34], which requires a numerical approach.

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