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Sequential Monte Carlo opens up for nonlinear system identification

Thomas Schön

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Joint work with

Local team:

- Fredrik Lindsten
- Johan Dahlin
- Johan Wågberg
- Christian A. Naesseth
- Andreas Svensson
- Liang Dai

Nonlinear system identification

A state space model (SSM) consists of a Markov process $\{x_t\}_{t\geq 1}$ that is indirectly observed via a measurement process $\{y_t\}_{t\geq 1}$,

$$\begin{aligned} x_{t+1} \mid x_t &\sim f_{\theta,t}(x_{t+1} \mid x_t, u_t), \\ y_t \mid x_t &\sim g_{\theta,t}(y_t \mid x_t, u_t), \\ x_1 &\sim \mu_\theta(x_1), \\ (\theta &\sim \pi(\theta)). \end{aligned} \qquad \begin{aligned} x_{t+1} &= a_\theta(x_t, u_t) + v_{\theta,t}, \\ y_t &= c_\theta(x_t, u_t) + e_{\theta,t}, \\ x_1 &\sim \mu_\theta(x_1), \\ (\theta &\sim \pi(\theta)). \end{aligned}$$

We observe

$$y_{1:T} \triangleq \{y_1, \dots, y_T\}, \quad \text{and possibly } u_{1:T} \triangleq \{u_1, \dots, u_T\}.$$

(leaving the latent variables $x_{1:T}$ unobserved).

Identification problem: Find θ based on $y_{1:T}$ (and $u_{1:T}$).

Two commonly used problem formulations

Maximum likelihood (ML) formulation – model the unknown parameters as a deterministic variable and solve

$$\widehat{\theta}_{\mathsf{ML}} = \arg\max_{\theta \in \Theta} p_{\theta}(y_{1:T}).$$

Bayesian formulation – model the unknown parameters as a random variable $\theta \sim \pi(\theta)$ and compute

$$p(\theta \mid y_{1:T}) = \frac{p_{\theta}(y_{1:T})\pi(\theta)}{p(y_{1:T})},$$

where $p_{\theta}(y_{1:T}) = p(y_{1:T} \mid \theta)$.

Central object – the likelihood

The central object in both formulations is the likelihood

$$p_\theta(y_{1:T}) = \prod_{t=1}^{T} p_\theta(y_t \mid y_{1:t-1}).$$

The likelihood is computed by marginalizing the joint density $p_\theta(x_{1:T}, y_{1:T})$ w.r.t. the state sequence $x_{1:T}$

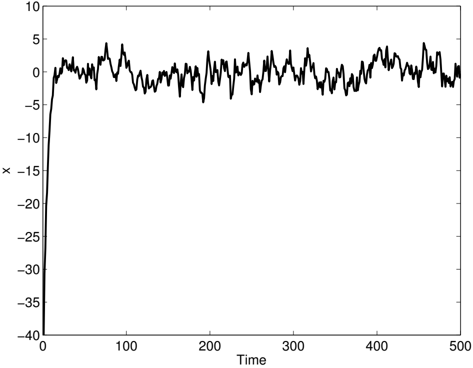
$$p_\theta(y_{1:T}) = \int p_\theta(x_{1:T}, y_{1:T}) \mathrm{d}x_{1:T} = \prod_{t=1}^{T} \int g_\theta(y_t \mid x_t) p_\theta(x_t \mid y_{1:t-1}) \mathrm{d}x_t.$$

Key challenge: How to deal with the latent states.

Our solution: Sequential Monte Carlo (SMC) including particle filters/smoothers.

Micro: MCMC – AR(1) example (I/II)

One realisation from $x[k+1] = 0.8x[k] + v[k]$ where $v[k] \sim \mathcal{N}(0,1)$. Initialise in $x[0] = -40$.

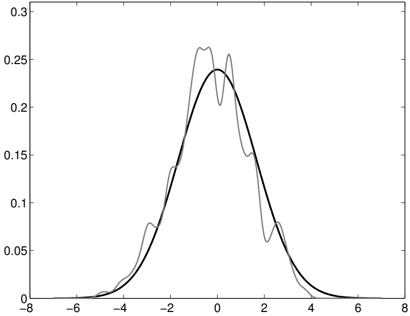


This will eventually generate samples from the following **stationary distribution**:

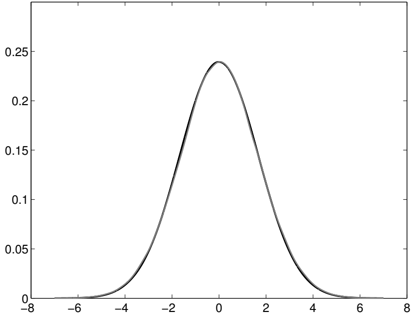
$$\pi^{\mathsf{s}}(x) = \mathcal{N}\left(x \,\middle|\, 0, \frac{1}{1-0.8^2}\right)$$

as $t \to \infty$.

Micro: MCMC – AR(1) example (II/II)



$1\,000$ samples



$100\,000$ samples

The true stationary distribution is showed in black and the empirical histogram obtained by simulating the Markov chain $x[k+1] = 0.8x[k] + v[k]$ is plotted in gray.

The initial $1\,000$ samples are discarded (burn-in).

Micro: MCMC

In the example, the Markov chain was fully specified and the stationary distribution could be expressed in closed form.

Not possible in the situations we are interested in, **but** we can (since 2010) find a Markov chain that has the target distribution (e.g. $p(\theta \mid y_{1:T})$) as its stationary distribution.

Two constructive ways of doing this are:

1. Metropolis Hastings (MH) algorithm
2. Gibbs sampling

Markov chain Monte Carlo (MCMC) methods allow us to generate samples from a **target distribution** by simulating a Markov chain which has the target distribution as its stationary distribution.

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Outline

1. Problem formulation
2. Micro – MCMC
3. Sketching identification strategies for nonlinear SSMs
   a. Marginalization
   b. Data augmentation
4. Sequential Monte Carlo (SMC)
5. Using SMC as a proposal mechanism within MCMC
6. A nontrivial example
7. The nonlinear SSM is just a special case...

Identification strategies

The two identification strategies we are concerned with are:

- **Marginalization** Deal with the states by marginalizing them out.
- **Data augmentation** Deal with the states by treating them as auxiliary variables to be estimated along with the parameters.

	Marginalization	**Data augmentation**
ML	Direct optimization	Expectation Maximization
Bayesian	Metropolis Hastings	Gibbs sampling

Identification strategy – marginalization

Deal with the states by marginalizing them out.

1. Direct optimization work directly with the optimization problem

$$\widehat{\theta}_{\mathsf{ML}} = \arg\max_{\theta \in \Theta} \prod_{t=1}^{T} \int g_\theta(y_t \mid x_t) p_\theta(x_t \mid y_{1:t-1}) \mathrm{d}x_t.$$

Cannot be solved in closed form, use iterative numerical methods

$$\theta_{k+1} = \theta_k + \alpha_k s_k.$$

The search direction is typically computed according to

$$s_k = H_k g_k, \qquad g_k = \nabla_\theta p_\theta(y_{1:T})\big|_{\theta=\theta_k}.$$

SMC used to approximate the cost function and its derivative(s).

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Identification strategy – marginalization

2. Metropolis Hastings (MH) is an MCMC method that produce a sequence of random variables $\{\theta[m]\}_{m\geq 1}$ by iterating

1. Propose a new sample θ'

$$\theta' \sim q(\cdot \mid \theta[m]).$$

2. Accept the new sample with probability

$$\alpha = \min\left(1, \frac{p_{\theta'}(y_{1:T})\pi(\theta')}{p_{\theta[m]}(y_{1:T})\pi(\theta[m])} \frac{q(\theta[m] \mid \theta')}{q(\theta' \mid \theta[m])}\right)$$

The above procedure results in a Markov chain $\{\theta[m]\}_{m\geq 1}$ with $p(\theta \mid y_T)$ as its stationary distribution!

SMC used to approximate the likelihood $p_\theta(y_{1:T})$ in the acceptance probability.

thomas.schon@it.uu.se

Identification strategy – data augmentation

Deal with the states by treating them as auxiliary variables to be estimated along with the parameters.

Intuitively: Alternate between updating θ and $x_{1:T}$.

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1. Expectation Maximization (EM)

(E) Compute a conditional expectation

$$\mathcal{Q}(\theta, \theta[k]) \triangleq \int \log p_\theta(x_{1:T}, y_{1:T}) \underbrace{p_{\theta[k]}(x_{1:T} \mid y_{1:T})} \mathrm{d}x_{1:T}.$$

(M) Maximize $\mathcal{Q}(\theta, \theta[k])$ w.r.t. θ

$$\theta[k+1] = \arg\max_\theta \ \mathcal{Q}(\theta, \theta[k]).$$

SMC is used to approximate the JSD $p_{\theta[k]}(x_{1:T} \mid y_{1:T})$.

Identification strategy – data augmentation

2. Gibbs sampling aim at compute $p(\theta, x_{1:T} \mid y_{1:T})$.

Gibbs sampling (blocked) for SSMs amounts to iterating

- Draw $\theta[m] \sim p(\theta \mid x_{1:T}[m-1], y_{1:T})$,
- Draw $x_{1:T}[m] \sim p(x_{1:T} \mid \theta[m], y_{1:T})$.

The above procedure results in a Markov chain,

$$\{\theta[m], x_{1:T}[m]\}_{m \geq 1}$$

with $p(\theta, x_{1:T} \mid y_T)$ as its stationary distribution!

SMC is used to generate a state sequence $x_{1:T}[m]$ from $p(x_{1:T} \mid \theta[m], y_{1:T})$.

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Sequential Monte Carlo (SMC)

The particle filter provides an approximation $p(x_{1:t} \mid y_{1:t})$, when the state evolves according to an SSM,

$$\begin{aligned} x_{t+1} \mid x_t &\sim f_\theta(x_{t+1} \mid x_t), \\ y_t \mid x_t &\sim g_\theta(y_t \mid x_t), \\ x_1 &\sim \mu_\theta(x_1). \end{aligned}$$

The particle filter maintains an empirical distribution made up N samples (particles) and corresponding weights

$$\widehat{p}(x_{1:t} \mid y_{1:t}) = \sum_{i=1}^{N} w_t^i \delta_{x_{1:t}^i}(x_{1:t}).$$

"Think of each particle as one simulation of the system state. Only keep the good ones."

Particle filter

··· → Weighting → Resampling → Propagation → Weighting → Resampling → ···

SMC = resampling + sequential importance sampling

1. **Resampling:** $\mathbb{P}\left(a_t^i = j\right) = \bar{w}_{t-1}^j / \sum_l \bar{w}_{t-1}^l$.
2. **Propagation:** $x_t^i \sim f_\theta(x_t \,|\, x_{1:t-1}^{a_t^i})$ and $x_{1:t}^i = \{x_{1:t-1}^{a_t^i}, x_t^i\}$.
3. **Weighting:** $\bar{w}_t^i = W_t(x_t^i) = g_\theta(y_t \,|\, x_t)$.

The **ancestor indices** $\{a_t^i\}_{i=1}^N$ are very **useful** auxiliary variables!
They make the stochasticity of the resampling step explicit.

Sequential Monte Carlo (SMC)

Let

$$\boldsymbol{x}_t \triangleq \{x_t^1, \dots, x_t^N\}, \qquad \boldsymbol{a}_t \triangleq \{a_t^1, \dots, a_t^N\}$$

denote all particles and ancestor indices generated at time t.

The SMC algorithm generats a single realization of a collection of random variables

$$\{\boldsymbol{x}_{1:T}, \boldsymbol{a}_{2:T}\} \in \mathsf{X}^{NT} \times \{1, \dots, N\}^{N(T-1)}$$

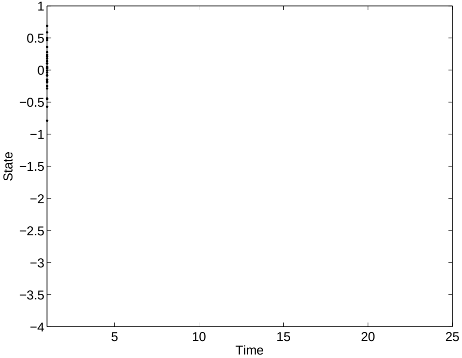
distributed according to

$$\boxed{\psi(\boldsymbol{x}_{1:T}, \boldsymbol{a}_{2:T}) \triangleq \prod_{i=1}^{N} q_1(x_1^i) \prod_{t=2}^{T} \prod_{i=1}^{N} M_t(a_t^i, x_t^i),}$$

where

$$M_t(a_t, x_t) = \frac{\bar{w}_{t-1}^{a_t}}{\sum_l \bar{w}_{t-1}^l} f_t(x_t \mid x_{1:t-1}^{a_t}).$$

The particle system degenerates (illustration)



Clearly motivates the need for **particle smoothers**.

Self-contained introduction to particle smoothing using BS and AS

Fredrik Lindsten and Thomas B. Schön, **Backward simulation methods for Monte Carlo statistical inference**, *Foundations and Trends in Machine Learning*, 6(1):1-143, 2013.

Using SMC within MCMC (PMCMC)

Particle MCMC (PMCMC) is a systematic way of combining SMC and MCMC.

Intuitively: SMC is used as a high-dimensional proposal mechanism on the space of state trajectories X^T.

A bit more precise: Construct a Markov chain with $p(\theta \mid y_{1:T})$ as its stationary distribution.

Pioneered by the work

Christophe Andrieu, Arnaud Doucet and Roman Holenstein, **Particle Markov chain Monte Carlo methods**, *Journal of the Royal Statistical Society: Series B*, 72:269-342, 2010.

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Reminder – identification strategies

	Marginalization	Data au
ML	Direct optimization	Expectation
Bayesian	Metropolis Hastings **Metropolis Hastings**	Gibbs

Iterating the two steps below will results in a Markov chain $\{\theta[m]\}_{m\geq 1}$ with $p(\theta \mid y_T)$ as its stationary distribution.

1. Propose a new sample θ' according to $\theta' \sim q(\cdot \mid \theta[m])$.
2. Accept the new sample with probability

$$\alpha = \min\left(1, \frac{p_{\theta'}(y_{1:T})\pi(\theta')}{p_{\theta[m]}(y_{1:T})\pi(\theta[m])} \frac{q(\theta[m] \mid \theta')}{q(\theta' \mid \theta[m])}\right)$$

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Using unbiased likelihood within MH

Fact (non-trivial): SMC produce an unbiased estimate of the likelihood!

$$\widehat{p}_\theta(y_{1:T}) = \widehat{p}_\theta(y_1)\prod_{t=2}^{T}\widehat{p}_\theta(y_t \mid y_{1:t-1}) = \prod_{t=1}^{T}\left(\frac{1}{N}\sum_{i=1}^{N}\bar{w}_t^i\right).$$

Intuitive idea: What about using this estimate within MH?!

The extended target distribution

Introduce an auxiliary variable

$$u = (\boldsymbol{x}_{1:T}, \boldsymbol{a}_{2:T}), \qquad u \sim \psi(u \,|\, \theta).$$

Note that,

$$p(\theta, u \,|\, y_{1:T}) = \frac{p_{\theta,u}(y_{1:T})\psi(u \,|\, \theta)p(\theta)}{p(y_{1:T})} = \frac{p_{\theta,u}(y_{1:T})\psi(u \,|\, \theta)p(\theta \,|\, y_{1:T})}{p(y_{1:T} \,|\, \theta)}.$$

Non-trivial construction: Consider the following **extended target** distribution

$$\phi(\theta, u) = \frac{\widehat{p}_{\theta,u}(y_{1:T})\psi(u \,|\, \theta)p(\theta \,|\, y_{1:T})}{p_\theta(y_{1:T})},$$

defined on $\Theta \times \mathsf{X}^{NT} \times \{1, \ldots, N\}^{N(T-1)}$.

Marginalization

Marginalize (recall strategy) out the auxiliary variables u

$$\int \phi(\theta, u)\mathrm{d}u = \frac{p(\theta \mid y_{1:T})}{p_\theta(y_{1:T})} \int \widehat{p}_{\theta,u}(y_{1:T})\psi(u \mid \theta)\mathrm{d}u.$$

What can we do about the integral?

SMC produce an unbiased estimate of $\widehat{p}_{\theta,u}(y_{1:T})$

$$\mathrm{E}_{u \mid \theta}\left[\widehat{p}_{\theta,u}(y_{1:T})\right] = \int \widehat{p}_{\theta,u}(y_{1:T})\psi(u \mid \theta)\mathrm{d}u = p_\theta(y_{1:T}),$$

Result: $p(\theta \mid y_{1:T})$ is recovered **exactly** as the marginal of the extended target distribution $\phi(\theta, u)$, despite the fact that we employ an SMC **approximation** of the likelihood using a finite number of particles N.

Particle Metropolis Hastings (PMH)

Based on the current sample $(\theta[m], u[m])$ a new sample (θ', u') is proposed according to

$$\theta' \sim q(\cdot \mid \theta[m], u[m]), \qquad u' \sim \psi(\cdot \mid \theta').$$

The probability of accepting this sample is given by

$$\alpha = \min\left(1, \frac{\widehat{p}_{\theta',u'}(y_{1:T})p(\theta')}{\widehat{p}_{\theta[m],u[m]}(y_{1:T})p(\theta[m])} \frac{q(\theta[m] \mid \theta', u')}{q(\theta' \mid \theta[m], u[m])}\right).$$

Note: Very importantly, α does not require evaluation of $\psi(u \mid \theta')$!

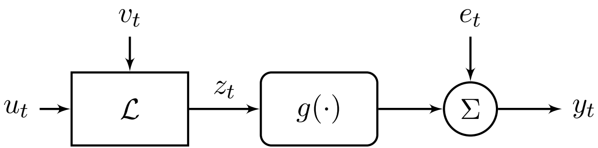
Originally appeared in (different derivation)

Christophe Andrieu, Arnaud Doucet and Roman Holenstein, **Particle Markov chain Monte Carlo methods**, *Journal of the Royal Statistical Society: Series B*, 72:269-342, 2010.

and further studied in,

Johan Dahlin, Fredrik Lindsten and Thomas B. Schön, **Particle Metropolis Hastings using gradient and Hessian information**, *Statistics and Computing*, 2014. (accepted for publication)

Example – semiparametric Wiener model



Parametric LGSS and a nonparametric static nonlinearity:

$$x_{t+1} = \underbrace{\begin{pmatrix} A & B \end{pmatrix}}_{\Gamma} \begin{pmatrix} x_t \\ u_t \end{pmatrix} + v_t, \qquad v_t \sim \mathcal{N}(0, Q),$$

$$z_t = C x_t.$$

$$y_t = g(z_t) + e_t, \qquad e_t \sim \mathcal{N}(0, R).$$

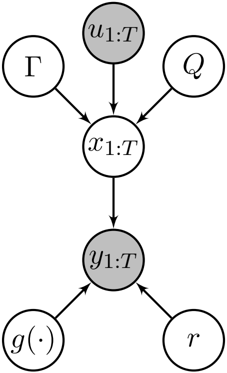
Example – semiparametric Wiener model

"Parameters": $\theta = \{A, B, Q, g(\,\cdot\,), r\}$.

Bayesian model specified by priors

- Conjugate priors for $\Gamma = [A \; B]$, Q and r,
  - $p(\Gamma, Q) =$ Matrix-normal inverse-Wishart
  - $p(r) =$ inverse-Wishart
- Gaussian process prior on $g(\,\cdot\,)$,

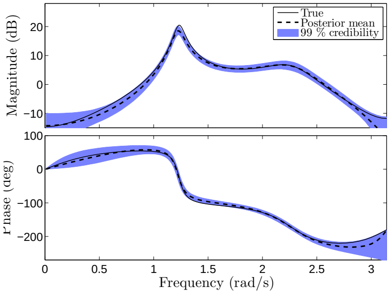
$$g(\,\cdot\,) \sim \mathcal{GP}(z, k(z, z')).$$



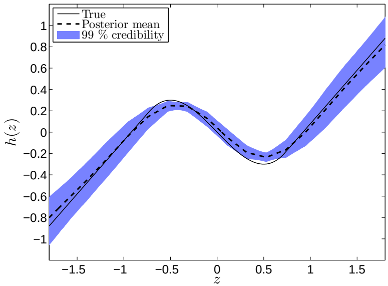
Inference using PGAS with $N = 15$ particles. $T = 1\,000$ measurements. We ran $15\,000$ MCMC iterations and discarded $5\,000$ as burn-in.

Example – semiparametric Wiener model

Show movie



Bode diagram of the 4th-order linear system. Estimated mean (dashed black), true (solid black) and 99% credibility intervals (blue).



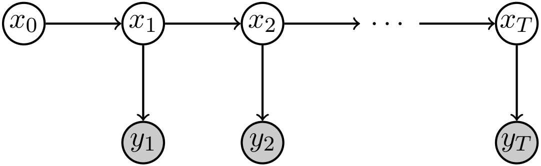
Static nonlinearity (non-monotonic), estimated mean (dashed black), true (black) and the 99% credibility intervals (blue).

Fredrik Lindsten, Thomas B. Schön and Michael I. Jordan. **Bayesian semiparametric Wiener system identification**. *Automatica*, 49(7): 2053-2063, July 2013.

The nonlinear SSM is just a special case...

A **graphical model** is a probabilistic model where a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ represents the conditional independency structure between random variables,

1. a set of **vertices** $\mathcal{V}$ (nodes) represents the random variables
2. a set of **edges** $\mathcal{E}$ containing elements $(i, j) \in \mathcal{E}$ connecting a pair of nodes $(i, j) \in \mathcal{V}$

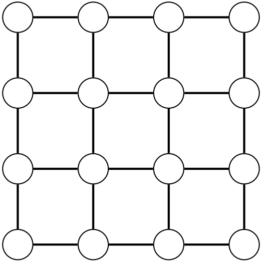


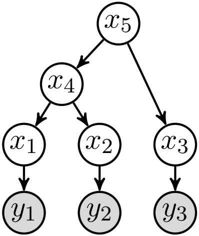
$$p(x_{0:T}, y_{1:T}) = p(x_0) \prod_{t=1}^{N} p(x_t \mid x_{t-1}) \prod_{t=1}^{N} p(y_t \mid x_t).$$

The nonlinear SSM is just a special case...

SMC samplers are used to approximate a sequence of probability distributions on a sequence of probability spaces.

Constructing an artificial sequence of intermediate target distributions for an SMC sampler is a powerful (and **quite possibly underutilized**) idea.





Christian A. Naesseth, Fredrik Lindsten and Thomas B. Schön, **Sequential Monte Carlo methods for graphical models**. *Advances in Neural Information Processing Systems (NIPS)* 27, Montreal, Canada, December, 2014.

Fredrik Lindsten, Adam M. Johansen, Christian A. Naesseth, Bonnie Kirkpatrick, Thomas B. Schön, John Aston and Alexandre Bouchard-Côté. **Divide-and-Conquer with Sequential Monte Carlo**. *arXiv:1406.4993*, June 2014.

Conclusion

1. Overview of identification strategies for nonlinear SSMs.
2. Focused on **marginalization** today, where we made use of the unbiased likelihood estimate $\widehat{p}_\theta(y_{1:T})$ from SMC within MH.
3. Powerful tools useful also outside the class of nonlinear SSMs.

A lot of interesting research that remains to be done!!

Information about a PhD course (*Computational learning in dynamical systems*) on the topic is available via

`user.it.uu.se/~thosc112/CIDS.html`

Manuscript is also available (ask me for a draft if you want)

Thomas B. Schön and Fredrik Lindsten. **Learning of dynamical systems – Particle filters and Markov chain methods**, 2014.

References to some of our work

Self-contained introduction to particle smoothing using BS and AS

Fredrik Lindsten and Thomas B. Schön, **Backward simulation methods for Monte Carlo statistical inference**, *Foundations and Trends in Machine Learning*, 6(1):1-143, 2013.

ML identification of nonlinear SSMs

F. Lindsten, **An efficient stochastic approximation EM algorithm using conditional particle filters**, *Proceedings of the 38th IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP)*, Vancouver, Canadan, May 2013.

Thomas B. Schön, Adrian Wills and Brett Ninness. **System Identification of Nonlinear State-Space Models**. *Automatica*, 47(1):39-49, January 2011.

PMCMC for Bayesian identification of nonlinear SSMs (and more)

Johan Dahlin, Fredrik Lindsten and Thomas B. Schön. **Particle Metropolis Hastings using gradient and Hessian information**. *Statistics and Computing*, 2014. (accepted for publication)

Fredrik Lindsten, Michael I. Jordan and Thomas B. Schön. **Particle Gibbs with ancestor sampling**. *Journal of Machine Learning Research (JMLR)*, 15:2145-2184, June 2014.

SMC methods for graphical models

Christian A. Naesseth, Fredrik Lindsten and Thomas B. Schön, **Sequential Monte Carlo methods for graphical models**. *Advances in Neural Information Processing Systems (NIPS)* 27, Montreal, Canada, December, 2014.

Seminar: `http://www.newton.ac.uk/seminar/20140425104011151`

Fredrik Lindsten, Adam M. Johansen, Christian A. Naesseth, Bonnie Kirkpatrick, Thomas B. Schön, John Aston and Alexandre Bouchard-Côté. **Divide-and-Conquer with Sequential Monte Carlo**. *arXiv:1406.4993*, June 2014.