Nonlinear system identification enabled via sequential Monte Carlo

UPPSALA
UNIVERSITET

Thomas Schön (with significant input from Fredrik Lindsten)

Division of Systems and Control
Department of Information Technology
Uppsala University

Joint work with (alphabetical order): **Roger Frigola** (University of Cambridge, UK) **Michael I. Jordan** (UC Berkeley), **Fredrik Lindsten** (Linköping University), **Lennart Ljung** (Linköping University), **Brett Ninness** (University of Newcastle, Australia), **Carl E. Rasmussen** (University of Cambridge, UK), **Andreas Svensson** (Uppsala University), **Adrian Wills** (MRA, Newcastle, Australia) and **Johan Wågberg** (Uppsala University).

Dynamical systems are everywhere!

Some of the dynamical systems we have been working with,

We first have to learn the models. Then we can use them.

Learning nonlinear dynamical systems from data

A state space model (SSM) consists of a Markov process $\{x_t\}_{t\geq 1}$ and a measurement process $\{y_t\}_{t\geq 1}$, related according to

$$\begin{aligned} x_{t+1} \mid x_t &\sim f_t(x_{t+1} \mid x_t), \\ y_t \mid x_t &\sim g_t(y_t \mid x_t), \\ x_1 &\sim \mu(x_1). \end{aligned}$$

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

We observe

$$y_{1:T} \triangleq \{y_1, \ldots, y_T\},$$

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

Identification problem: Find f, g, μ (or θ) based on $y_{1:T}$.

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

Frequentists:

- Find $\widehat{\theta}_{\mathrm{ML}} = \arg\max_{\theta} p_\theta(y_{1:T})$.
- Use e.g. the expectation maximization (EM) algorithm.

Bayesians:

- Find $p(\theta \mid y_{1:T})$.
- Use e.g. Gibbs sampling.

Outline

1. Maximum Likelihood (ML) identification
   - Problem formulation
   - Solution using EM and a particle smoother
2. Bayesian identification
   - Problem formulation
   - Gibbs sampling
3. Sequential Monte Carlo (SMC), the particle filter
4. Particle Gibbs with ancestor sampling (PG-AS)
   - Example: Identifying Wiener systems
   - Bayesian nonparametric dynamical models

The sequential Monte Carlo samplers are fundamental to **both** the ML and the Bayesian approaches.

Problem formulation – ML

A state space model (SSM) consists of a Markov process $\{x_t\}_{t\geq 1}$ and a measurement process $\{y_t\}_{t\geq 1}$, related according to

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

Identification problem: Find θ based on $y_{1:T}$.

ML amounts to solving,

$$\widehat{\theta}^{\mathrm{ML}} = \arg\max_{\theta} \ \log p_\theta(y_{1:T})$$

where the log-likelihood function is given by

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

The **EM** algorithm computes ML estimates of unknown parameters in probabilistic models involving latent variables.

The latent variables in an SSM are given by the states,

$$\{x_1, \ldots, x_T\}.$$

Strategy: Use the *structure* inherent in the SSM to separate the original problem into *two closely linked subproblems*, each of which is hopefully in some sense more tractable than the original problem.

Algorithm 1 EM for identifying nonlinear dynamical systems

1. **Initialise:** Set $i = 1$ and choose an initial θ^1.
2. **While** not converged **do:**

   (a) **Expectation (E) step:** Compute

$$\begin{aligned} Q(\theta, \theta^i) &= \mathrm{E}_{\theta^i}\left[\log p_\theta(x_{1:T}, y_{1:T}) \mid y_{1:T}\right] \\ &= \int \log p_\theta(x_{1:T}, y_{1:T}) \underbrace{p_{\theta^i}(x_{1:T} \mid y_{1:T})}\, \mathrm{d}x_{1:T} \end{aligned}$$

   using **PS** (forward filter/**backward simulation**, FFBS).

   (b) **Maximization (M) step:** Compute $\theta^{i+1} = \arg\max_{\theta \in \Theta} Q(\theta, \theta^i)$

   (c) $i \leftarrow i + 1$

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

Problem formulation – Bayesian

Consider a Bayesian SSM (θ is now a random variable with a prior density $p(\theta)$)

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

Identification problem: Compute the posterior $p(\theta, x_{1:T} \mid y_{1:T})$, or one of its marginals.

The **key challenge** is that there is no closed form expression available for the posterior.

Gibbs sampler for SSMs

Markov chain Monte Carlo (MCMC) methods allow us to generate samples from a target distribution by simulating a Markov chain.

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!

Gibbs sampler for a general SSM

What would a Gibbs sampler for a general nonlinear/non-Gaussian SSM look like?

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

Problem: $p(x_{1:T} \mid \theta[m], y_{1:T})$ not available!

Idea: Approximate $p(x_{1:T} \mid \theta[m], y_{1:T})$ using a sequential Monte Carlo method!

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2. Bayesian identification
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   - Gibbs sampling
3. **Sequential Monte Carlo (SMC), the particle filter**
4. Particle Gibbs with ancestor sampling (PG-AS)

The sequential Monte Carlo samplers are fundamental to **both** the ML and the Bayesian approaches.

The particle filter

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

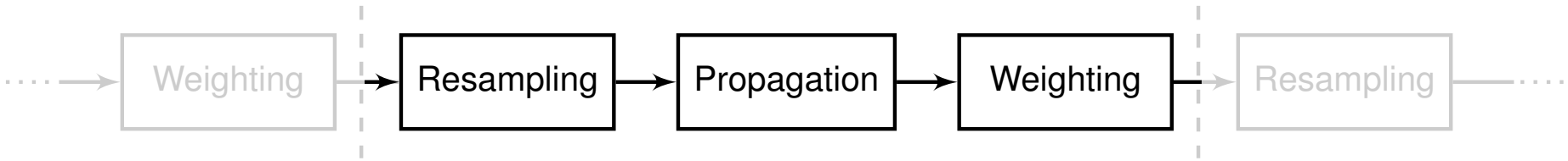
$$\begin{aligned} x_{t+1} \mid x_t &\sim f_t(x_{t+1} \mid x_t), \\ y_t \mid x_t &\sim g_t(y_t \mid x_t), \\ x_1 &\sim \mu(x_1). \end{aligned}$$

The particle filter maintains an empirical distribution made up N samples (particles) $\{x_t^i\}_{i=1}^N$ and corresponding weights $\{w_t^i\}_{i=1}^N$

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

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

The particle filter



1. **Resampling:** $\{x^i_{1:t-1}, w^i_{t-1}\}_{i=1}^N \rightarrow \{\tilde{x}^i_{1:t-1}, 1/N\}_{i=1}^N$.
2. **Propagation:** $x^i_t \sim R_t(x_t \mid \tilde{x}^i_{1:t-1})$ and $x^i_{1:t} = \{\tilde{x}^i_{1:t-1}, x^i_t\}$.
3. **Weighting:** $w^i_t = W_t(x^i_{1:t})$.

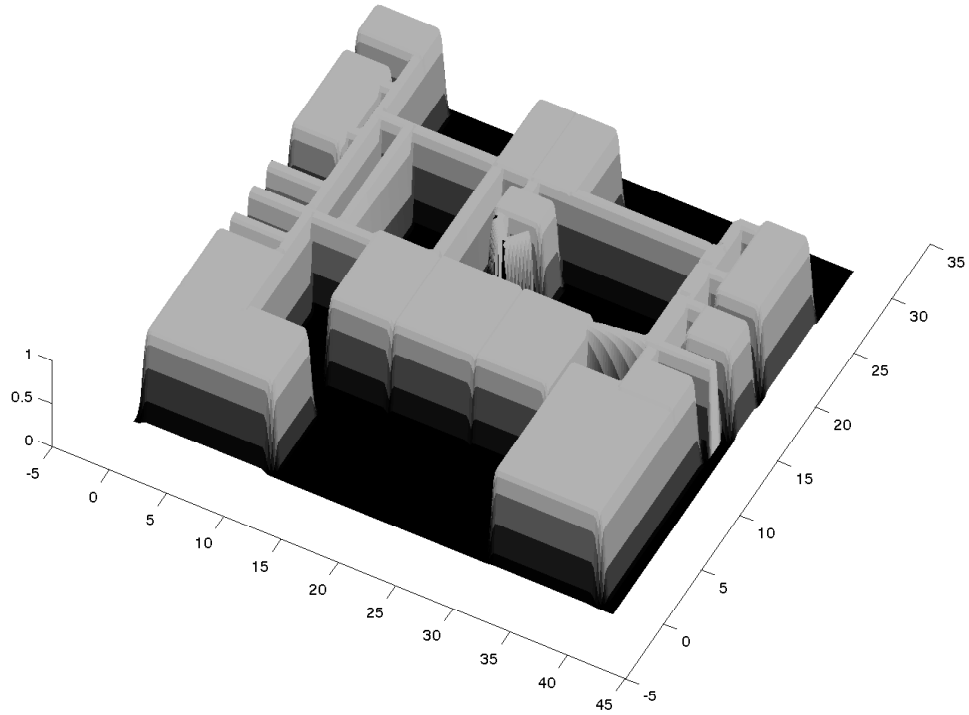
The result is a new weighted set of particles $\{x^i_{1:t}, w^i_t\}_{i=1}^N$.

A systematic way of obtaining approximations that converge

Xiao-Li Hu, Thomas B. Schön and Lennart Ljung. **A basic convergence result for particle filtering**. *IEEE Transactions on Signal Processing*, 56(4):1337-1348, April 2008.

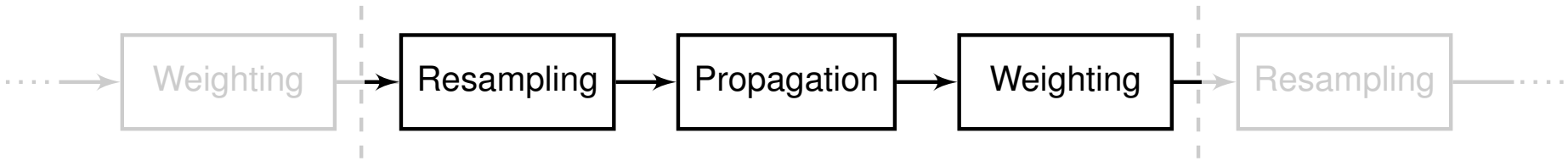
Example – Indoor localization

Aim: Compute the position of a person moving around indoors using sensors (inertial, magnetometer and radio) located in an ID badge and a map.



Show movie

The particle filter – alternative formulation



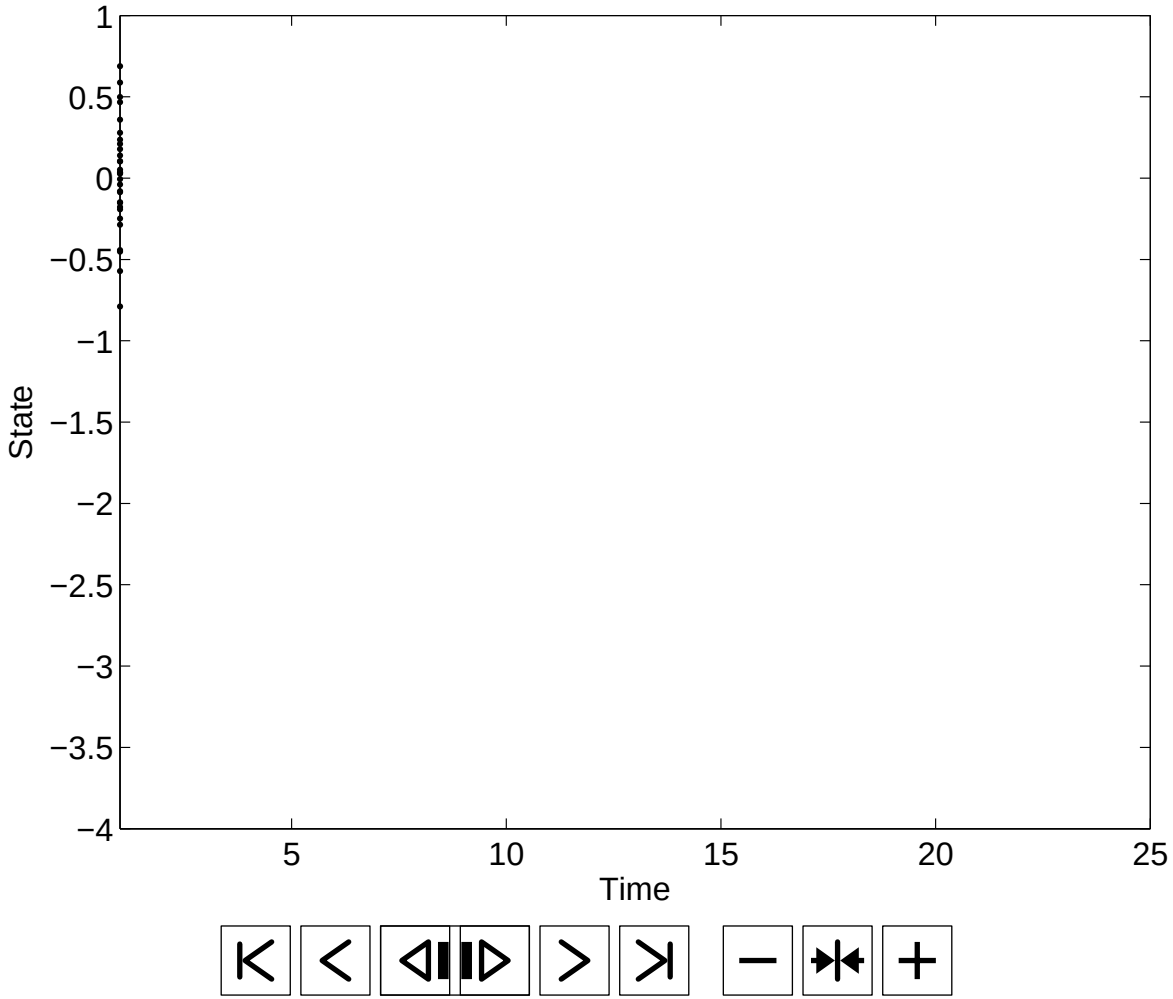
1. **Resampling + Propagation:**

$$(a_t^i, x_t^i) \sim M_t(a_t, x_t) = \frac{w_{t-1}^{a_t}}{\sum_l w_{t-1}^l} R_t(x_t \mid x_{1:t-1}^{a_t}).$$

2. **Weighting:** $w_t^i = W_t(x_{1:t}^i)$.

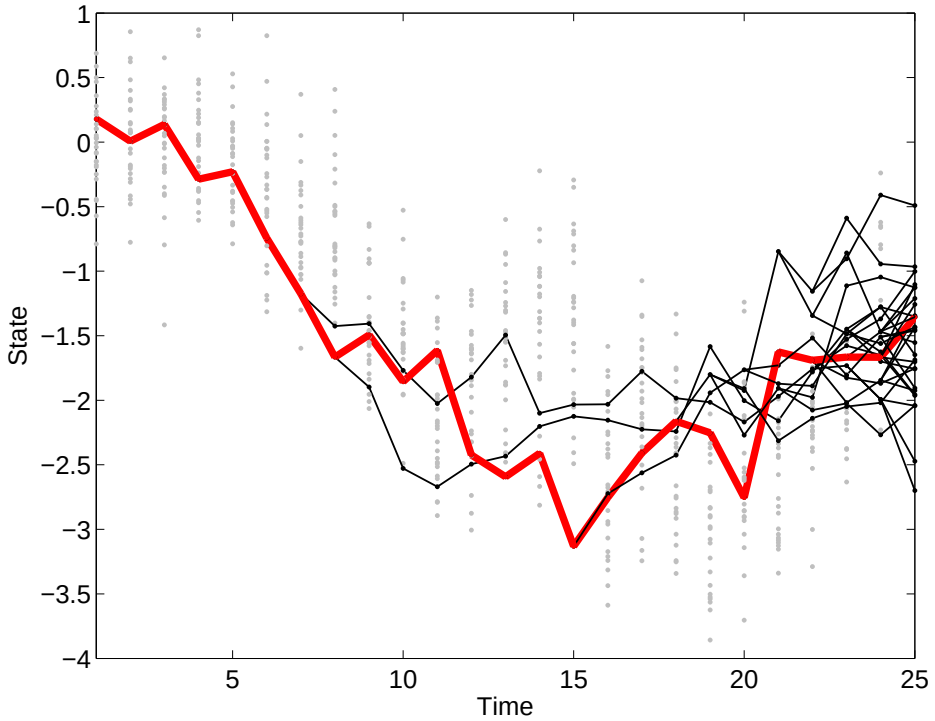
The result is a new weighted set of particles $\{x_{1:t}^i, w_t^i\}_{i=1}^N$.

The particle filter – illustrating particle degeneracy



Sampling based on the PF

With $P(x'_{1:T} = x^i_{1:T}) \propto w^i_T$ we get, $x'_{1:T} \overset{\text{approx.}}{\sim} p(x_{1:T} \mid \theta, y_{1:T})$.



Problems

Problems with this approach,

- Based on a PF $\Rightarrow$ approximate sample.
- Does not leave $p(\theta, x_{1:T} \mid y_{1:T})$ invariant!
- Relies on large N to be successful.
- A lot of wasted computations.

To get around these problems,

Use a conditional particle filter (CPF). One pre-specified path is retained throughout the sampler.

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.

Particle Markov Chain Monte Carlo (PMCMC)

The idea underlying **PMCMC** is to make use of a certain SMC sampler to construct a Markov kernel leaving the joint smoothing distribution $p(x_{1:T} \mid \theta, y_{1:T})$ invariant.

This Markov kernel is then used in a standard MCMC algorithm (e.g. Gibbs, results in the **Particle Gibbs (PG)**).

Three SMC samplers leaving $p(x_{1:T} \mid \theta, y_{1:T})$ invariant:

1. Conditional particle filter (CPF)
   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.
2. CPF with backward simulation (CPF-BS)
   Fredrik Lindsten and Thomas B. Sch Schön. **On the use of backward simulation in the particle Gibbs sampler**. *Proc. of the 37th Internat. Conf. on Acoustics, Speech, and Signal Processing (ICASSP)*, Kyoto, Japan, March 2012.
3. **CPF with ancestor sampling (CPF-AS)**
   Fredrik Lindsten, Michael I. Jordan and Thomas B. Schön, **Ancestor sampling for particle Gibbs**, *Advances in Neural Information Processing Systems (NIPS) 25*, Lake Tahoe, NV, US, December, 2012.

Conditional PF with ancestor sampling

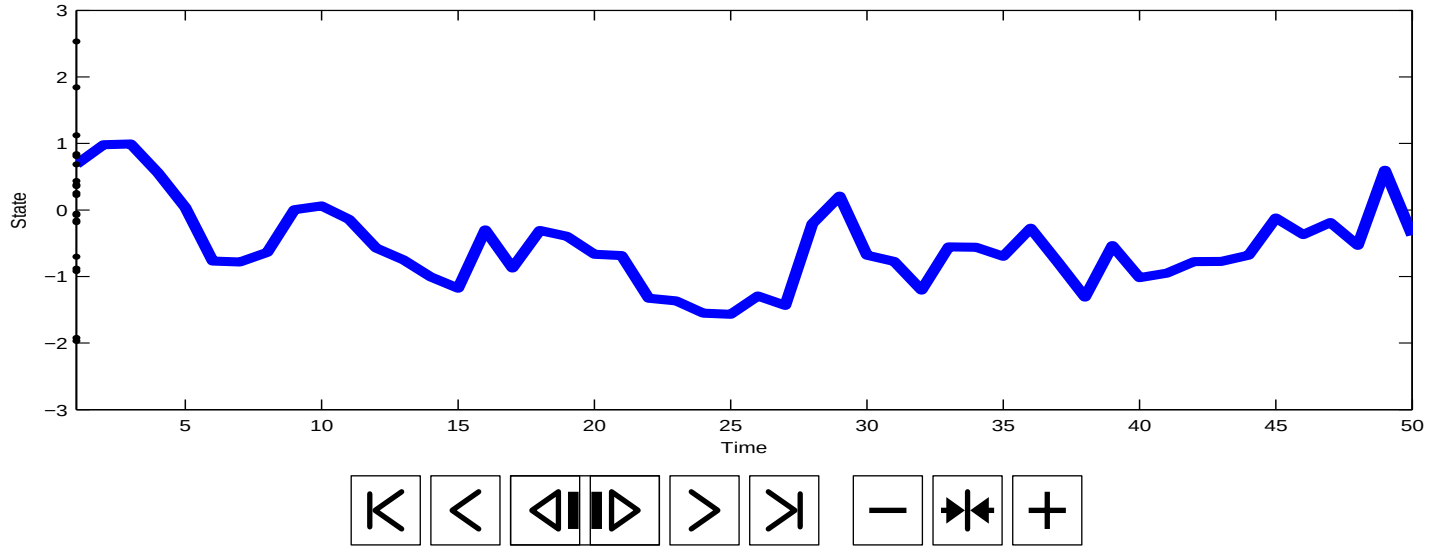
Algorithm CPF w. ancestor sampling (CPF-AS), conditioned on $x^\star_{1:T}$

1. **Initialize ($t = 1$):**
   (a) Draw $x^i_1 \sim R^\theta_1(x_1)$ for $i \neq N$ and set $x^N_1 = x^\star_1$.
   (b) Set $w^i_1 = W^\theta_1(x^i_1)$ for $i = 1, \ldots, N$.
2. **for** $t = 2, \ldots, T$**:**
   (a) Draw $(a^i_t, x^i_t) \sim M^\theta_t(a_t, x_t)$ for $i \neq N$ and set $x^N_t = x^\star_t$.
   (b) Draw a^N_t with $P(a^N_t = i) \propto w^i_{t-1} p(x^\star_t \mid \theta, x^i_{t-1})$.
   (c) Set $x^i_{1:t} = \{x^{a^i_t}_{1:t-1}, x^i_t\}$ and $w^i_t = W^\theta_t(x^i_{1:t})$ for $i = 1, \ldots, N$.

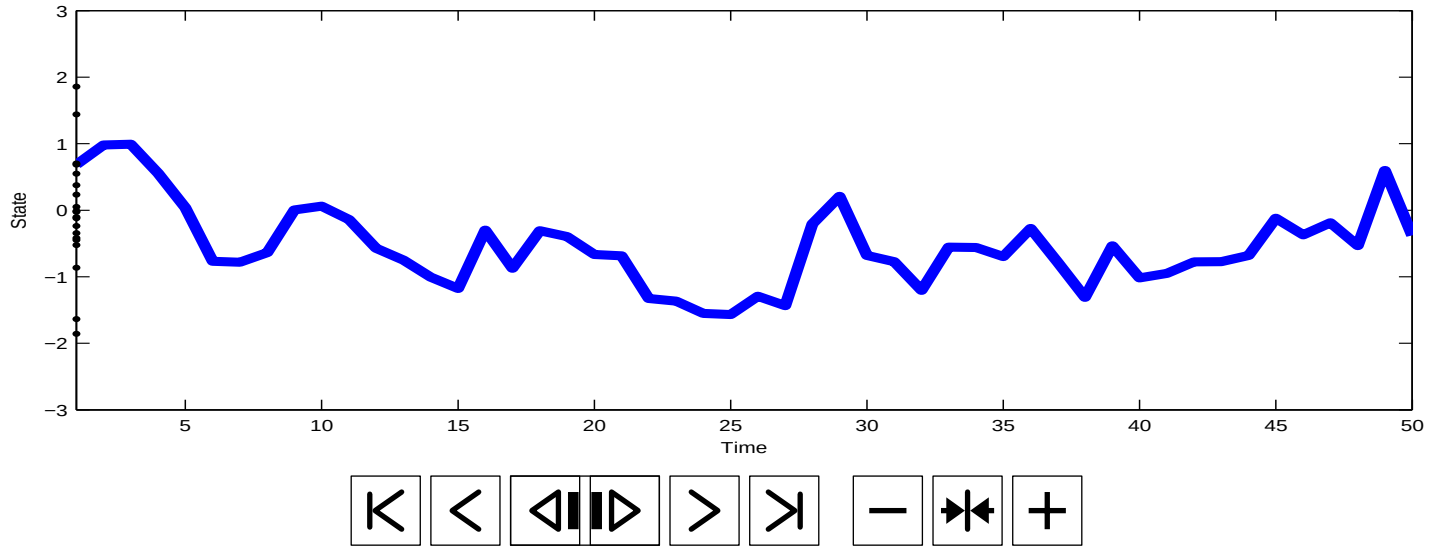
(The red text highlights the difference to the standard PF)

CPF vs. CPF-AS

CPF



CPF-AS



Conditional PF with ancestor sampling

Theorem

For any $N \geq 2$, the procedure;

(i) *Run CPF-AS$(x^{\star}_{1:T})$;*

(ii) *Sample $P(x'_{1:T} = x^{i}_{1:T}) \propto w^{i}_{T}$;*

defines a Markov kernel on X^T which leaves $p(x_{1:T} \mid \theta, y_{1:T})$ invariant.

Three additional reasons for using CPF-AS:

1. Significantly improves the mixing compared to CPF.
2. The computational complexity is linear in N.
3. Opens up for non-Markovian models.

Bayesian identification: Gibbs + CPF-AS = PG-AS

Algorithm PG-AS: Particle Gibbs with ancestor sampling

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1. **Initialize:** Set $\{\theta[0], x_{1:T}[0]\}$ arbitrarily.
2. **For** $m \geq 1$**, iterate:**
   (a) Draw $\theta[m] \sim p(\theta \mid x_{1:T}[m-1], y_{1:T})$.
   (b) Run CPF-AS$(x_{1:T}[m-1])$, targeting $p(x_{1:T} \mid \theta[m], y_{1:T})$.
   (c) Sample with $P(x_{1:T}[m] = {x_{1:T}}^i) \propto w_T^i$.

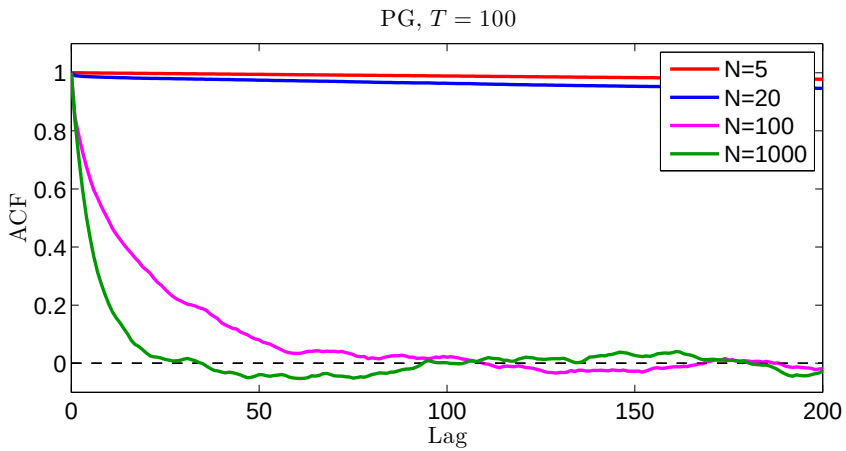
For any number of particles $N \geq 2$, the Markov chain $\{\theta[m], x_{1:T}[m]\}_{m \geq 1}$ has stationary distribution $p(\theta, x_{1:T} \mid y_{1:T})$.

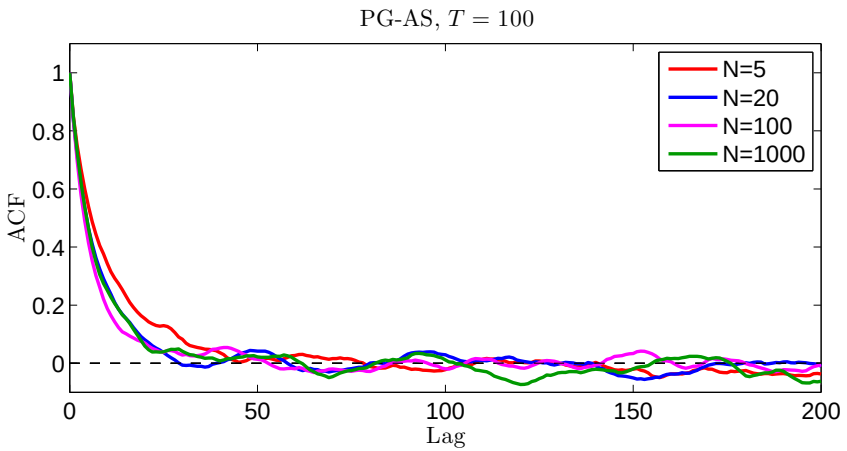
Toy example – stochastic volatility (I/II)

Consider the stochastic volatility model,

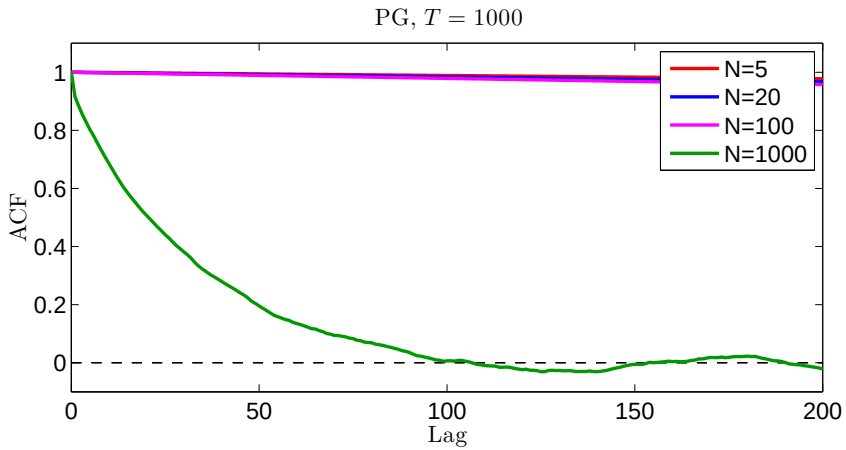
$$x_{t+1} = 0.9x_t + w_t, \qquad w_t \sim \mathcal{N}(0, \theta),$$
$$y_t = e_t \exp\left(\frac{1}{2}x_t\right), \qquad e_t \sim \mathcal{N}(0,1).$$

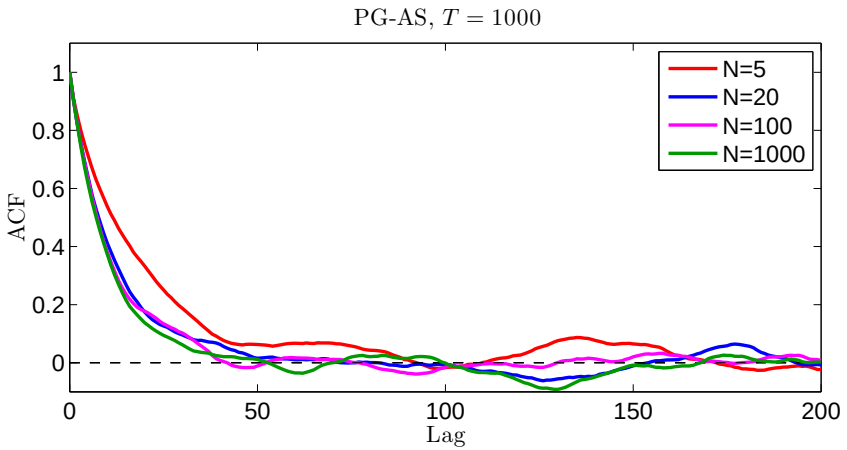
Let us study the ACF for the estimation error, $\widehat{\theta} - \mathrm{E}\left[\theta \mid y_{1:T}\right]$





Toy example – stochastic volatility (II/II)

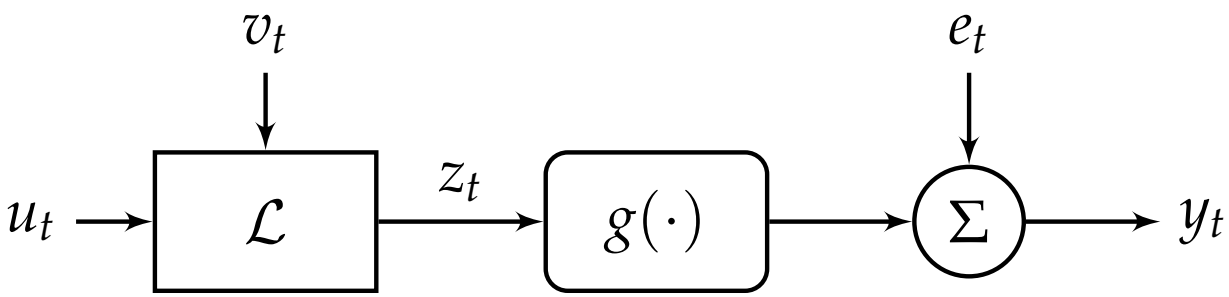




Some observations:

- We want the ACF to decay to zero as rapidly as possible (indicates good mixing in the PG sampler).
- Note the superior mixing of PG-AS compared to PG-CPF (already for just $N = 5$ particles!).

Example – semiparametric Wiener model (I/III)



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 (II/III)

Everything is learned from the data, by introducing the possibility to switch specific model components on and off.

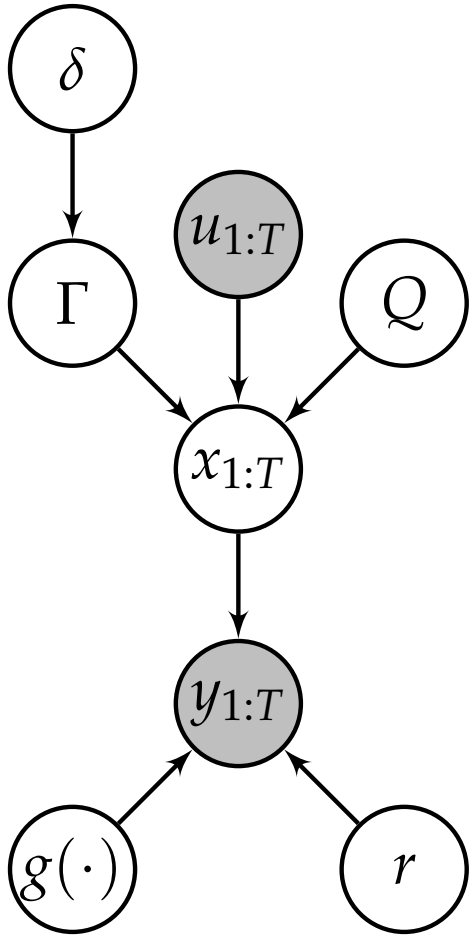
"Parameters": $\theta = \{A, B, Q, \delta, g(\cdot), r\}$.

Bayesian model specified by priors

- Sparseness prior (ARD) on $\Gamma = [A\ B]$,
- Inverse-Wishart prior on Q and r
- Gaussian process prior on $g(\cdot)$,

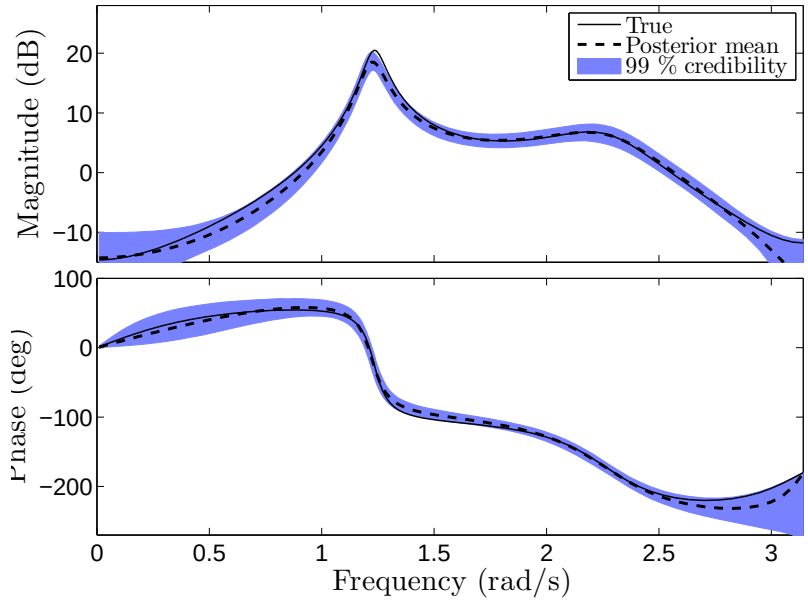
$$g(\cdot) \sim \mathcal{GP}(z, k(z, z')).$$

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

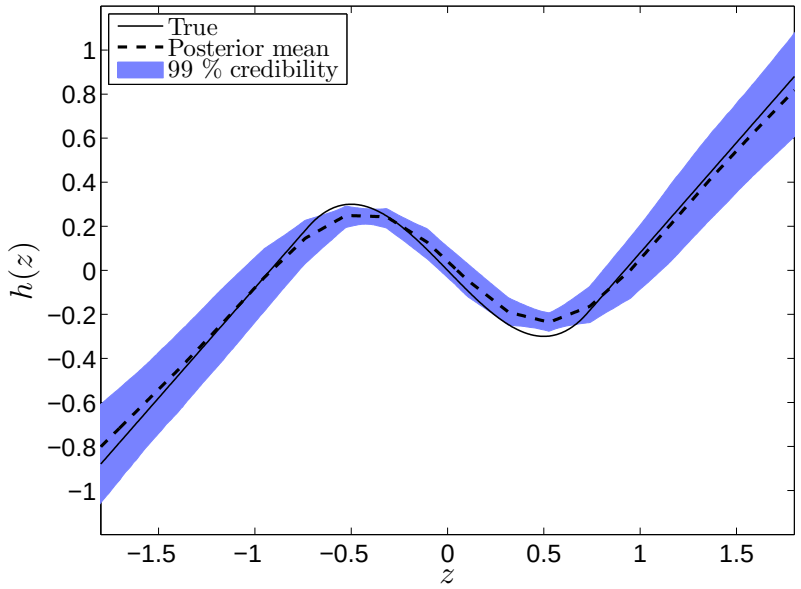


Example – semiparametric Wiener model (III/III)

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.

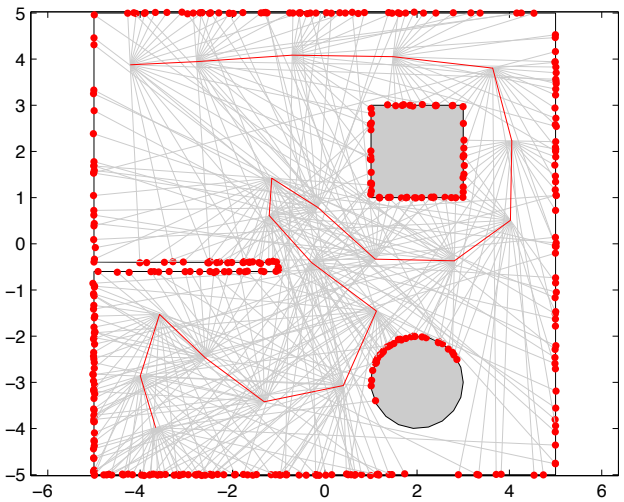
Bayesian nonparametric models

Bayesian nonparametric (BNP) models allow us to build **flexible** models where the **structure grows and adapts** to data.

BNP models: Gaussian, Dirichlet and Beta processes.

Opens up for systematic reasoning of uncertainty not only over parameters, but also orders, segmentations (clustering), etc.

DP model example from Johan Wågberg.



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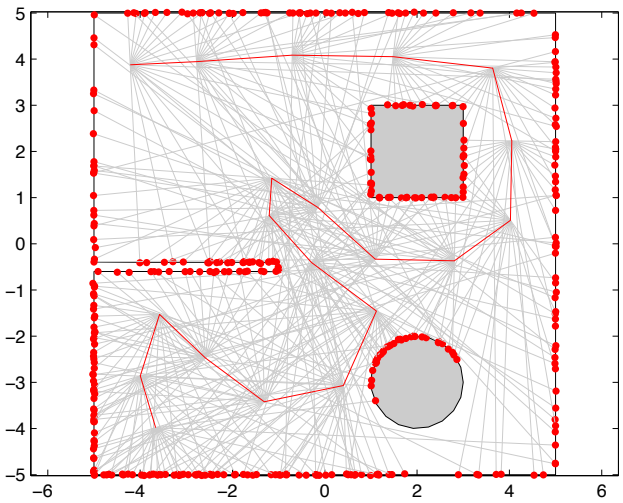

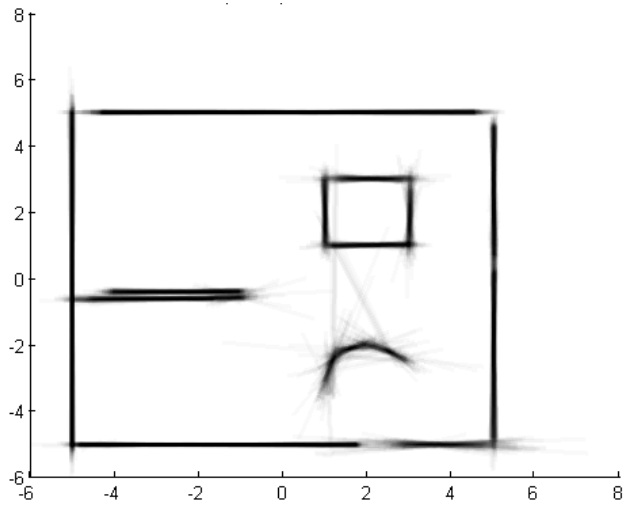

Bayesian nonparametric dynamical models

New result: We have been able to construct and learn a Gaussian process (GP) state space model

$$\begin{aligned} f(x_t) &\sim \mathcal{GP}(m_{\theta_x}(x_t), k_{\theta_x}(x_t, x_t')), \\ x_{t+1} \mid f_t &\sim \mathcal{N}(x_{t+1} \mid f_t, Q), \\ y_t \mid x_t &\sim p(y_t \mid x_t, \theta_y). \end{aligned}$$

Key idea: Marginalize out the function f.

Problem: Renders the model non-Markovian. **Solution:** PG-AS

Roger Frigola, Fredrik Lindsten, Thomas B. Schön and Carl E. Rasmussen, **Bayesian inference and learning in Gaussian process state-space models with particle MCMC**. In *Advances in Neural Information Processing Systems (NIPS) 26*, Lake Tahoe, NV, USA, December 2013. (accepted for publication)

Ongoing work: Construct and learn

- models based on the Dirichlet process to automatically capture segmented data,
- change-point models based on the GP-SSM.

Stochastic approximation EM

Assume for the time being that we can sample from $p_\theta(x_{1:T} \mid y_{1:T})$.

Stochastic approximation EM (SAEM): Replace the E-step with,

$$\widehat{Q}_m(\theta) = \widehat{Q}_{m-1}(\theta) + \gamma_m \left(\frac{1}{M} \sum_{j=1}^{M} \log p_\theta(\tilde{x}_{1:T}^j, y_{1:T}) - \widehat{Q}_{m-1}(\theta) \right),$$

where $\tilde{x}_{1:T}^j \overset{\text{i.i.d.}}{\sim} p_\theta(x_{1:T} \mid y_{1:T})$ for $j = 1, \ldots, M$.

SAEM converges to a maximum of $p_\theta(y_{1:T})$ for any $M \geq 1$ under standard stochastic approximation conditions.

B. Delyon, M. Lavielle and E. Moulines, **Convergence of a stochastic approximation version of the EM algorithm**, *The Annals of Statistics*, 27:94-128, 1999.

Stochastic approximation EM using CPF-AS

- **Bad news:** We cannot sample from $p_\theta(x_{1:T} \mid y_{1:T})$.
- **Good news:** It is enough to sample from a uniformly ergodic Markov kernel, leaving $p_\theta(x_{1:T} \mid y_{1:T})$ invariant.

We can use CPF-AS to sample the states!

Results in an interesting and useful **combination** of frequentist and Bayesian ideas. We will see more combinations like this in the future.

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

Conclusions

- EM-PS for ML learning in nonlinear SSMs.
- Conditional particle filters (CPF) are useful for identification!
- CPF-AS defines a kernel on X^T leaving $p_\theta(x_{1:T} \mid y_{1:T})$ invariant.
- CPF-AS consists of two parts:
  - **Conditioning:** Ensures correct stationary distribution for any N.
  - **Ancestor sampling:** Mitigates path degeneracy and enables movement around the conditioned path.
- Both Bayesian (PG-AS) and maximum likelihood inference (SAEM-AS) works with very few particles!

- We are working on a book project,

  Thomas B. Schön and Fredrik Lindsten, **Computational learning in dynamical systems**, 2013.

  Send me an e-mail if you are interested in a draft.
- Course: `users.isy.liu.se/rt/schon/course_CIDS.html`

Some references

Forthcoming book

Thomas B. Schön and Fredrik Lindsten, **Computational learning in dynamical systems**, 2013.

Novel introduction of PMCMC (very nice paper!)

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.

Self-contained introduction to BS and AS (not limited to SSMs)

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.

PG-AS (and the Wiener identification example)

Fredrik Lindsten, Michael I. Jordan and Thomas B. Schön, **Ancestor sampling for particle Gibbs**, *Advances in Neural Information Processing Systems (NIPS) 25*, Lake Tahoe, NV, US, December, 2012.

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

ML identification of nonlinear SSMs (and Wiener example)

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

Adrian Wills, Thomas B. Schön, Lennart Ljung and Brett Ninness. **Identification of Hammerstein-Wiener Models**. *Automatica*, 49(1): 70-81, January 2013.

Bayesian inference using Gaussian processes

Roger Frigola, Fredrik Lindsten, Thomas B. Schön and Carl E. Rasmussen, **Bayesian inference and learning in Gaussian process state-space models with particle MCMC**. In *Advances in Neural Information Processing Systems (NIPS) 26*, Lake Tahoe, NV, USA, December 2013. (accepted for publication)