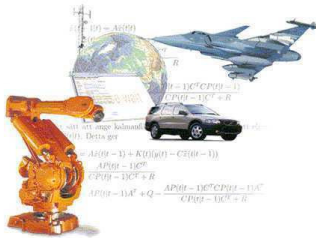


Learning nonlinear dynamical models using computational methods

– Strategies and a few concrete examples



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Joint work with (alphabetical order): **Michael I. Jordan** (UC Berkeley), **Fredrik Lindsten** (Linköping University), **Lennart Ljung** (Linköping University), **Brett Ninness** (University of Newcastle, Australia) and **Adrian Wills** (MRA, Newcastle, Australia).



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

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

Learning problem: Find θ based on $\{u_{1:T}, y_{1:T}\}$.

We will study two different learning problems for finding static parameters θ in SSMs:

1. **Maximum likelihood:** Find the value for θ that maximises the likelihood function $p_{\theta}(y_{1:T})$.
2. **Bayesian:** Compute the posterior distribution $p(\theta \mid y_{1:T})$.



The three steps of ML learning (applied to SSMS) are:

1. Model the obtained measurements y_1, \dots, y_T as a realisation from the stochastic variables Y_1, \dots, Y_T .
2. Assume $y_t \sim h_{\theta}(y_t | x_t, u_t)$ and $x_t \sim f_{\theta}(x_t | x_{t-1}, u_t)$.
3. Assume that the stochastic variables Y_1, \dots, Y_T are conditionally iid.

ML amounts to solving,

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

where the log-likelihood function is given by

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



There are at least two challenges with the ML formulation:

1. The one-step prediction pdf $p_{\theta}(y_t | y_{1:t-1})$ has to be computed.
2. In solving the optimisation problem

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

the derivatives $\frac{\partial}{\partial \theta} p_{\theta}(y_t | y_{1:t-1})$ are useful.



Bayesian model: θ is a random variable with a prior density $p(\theta)$.

The **goal** in Bayesian modeling is to compute the posterior

$$p(\underbrace{\theta, x_{1:T}}_{\triangleq \eta} \mid y_{1:T}) = p(\eta \mid y_{1:T}) \text{ (or one of its marginals).}$$

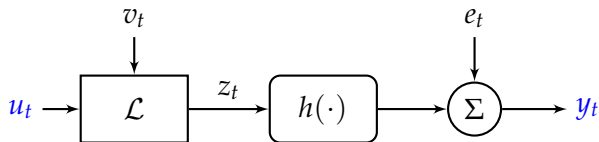
Bayesian modeling/learning amounts to:

1. Find an expression for the likelihood $p(y_{1:T} \mid \eta)$.
2. Assign priors $p(\eta)$ to all unknown stochastic variables η present in the model.
3. Determine the posterior distribution $p(\eta \mid y_{1:T})$.

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



As an example we will study how to learn a **Wiener model**.



A Wiener model is a linear dynamical model (\mathcal{L}) followed by a static nonlinearity ($h(\cdot)$).

Learning problem: Find \mathcal{L} and $h(\cdot)$ based on $\{u_{1:T}, y_{1:T}\}$.



Dynamics: Linear Gaussian state space (LGSS) model:

$$x_{t+1} = \begin{pmatrix} A & B \end{pmatrix} \begin{pmatrix} x_t \\ u_t \end{pmatrix} + v_t, \quad v_t \sim \mathcal{N}(0, Q),$$
$$z_t = Cx_t.$$

Measurements: Static nonlinearity:

- Parametric: $y_t = h(z_t, \beta) + e_t, \quad e_t \sim \mathcal{N}(0, R).$
- Non-parametric: $y_t = h(z_t) + e_t, \quad e_t \sim \mathcal{N}(0, R).$



Most of the existing work deals with special cases of the general problem. Typical restrictions imposed are:

- The nonlinearity $h(\cdot)$ is assumed to be invertible.
- The measurement noise e_t is absent.
- The LGSS model is deterministic (v_t is absent).
- The LGSS model is stochastic, but v_t is assumed white.

In the models and solutions provided here we do **not** have to make any of these assumptions.



Presents solutions to the two problems just formulated. These solutions are illustrated using the special case of the Wiener model.

1. Solving the ML problem

- Expectation maximisation combined with a particle smoother
- Example – blind learning of a Wiener model.

2. Solving the Bayesian problem

- Markov chain Monte Carlo (MCMC) combined with a particle filter/smoothing
- Examples – learning two semiparametric Wiener models

3. Conclusions



The strategy underlying the EM algorithm is to separate the original ML problem into **two closely linked subproblems**, each of which is hopefully more tractable than the original problem.

This separation is accomplished by exploiting the **structure** inherent in the probabilistic model.

The **key idea** is to consider the joint log-likelihood function of both the observed variables $y_{1:T}$ and the latent variables $Z \triangleq \{x_1, \dots, x_T\}$,

$$\ell_{\theta}(x_{1:T}, y_{1:T}) = \log p_{\theta}(x_{1:T}, y_{1:T}).$$



Algorithm 1 Expectation Maximization (EM)

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

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

$$\begin{aligned} Q(\theta, \theta^i) &= E_{\theta^i} [\log p_{\theta}(x_{1:T}, y_{1:T}) \mid y_{1:T}] \\ &= \int \log p_{\theta}(x_{1:T}, y_{1:T}) p_{\theta^i}(x_{1:T} \mid y_{1:T}) dx_{1:T} \end{aligned}$$

(b) **Maximization (M) step:** Compute

$$\theta^{i+1} = \arg \max_{\theta \in \Theta} Q(\theta, \theta^i)$$

(c) $i \leftarrow i + 1$



In computing the Q -function

$$\begin{aligned} Q(\theta, \theta^i) &= E_{\theta^i} [\log p_{\theta}(x_{1:T}, y_{1:T}) \mid y_{1:T}] \\ &= \int \log p_{\theta}(x_{1:T}, y_{1:T}) p_{\theta^i}(x_{1:T} \mid y_{1:T}) dx_{1:T}, \end{aligned}$$

we start by noting that

$$\begin{aligned} \log p_{\theta}(x_{1:T}, y_{1:T}) &= \log p_{\theta}(y_{1:T} \mid x_{1:T}) + \log p_{\theta}(x_{1:T}) \\ &= \log p_{\theta}(x_1) + \sum_{t=1}^{T-1} \log p_{\theta}(x_{t+1} \mid x_t) + \sum_{t=1}^T \log p_{\theta}(y_t \mid x_t) \end{aligned}$$



This results in the following expression for the Q -function

$$Q(\theta, \theta_k) = I_1 + I_2 + I_3,$$

where

$$I_1 = \int \log p_\theta(x_1) p_{\theta_k}(x_1 | y_{1:N}) dx_1,$$

$$I_2 = \sum_{t=1}^{T-1} \int \int \log p_\theta(x_{t+1} | x_t) p_{\theta_k}(x_{t+1}, x_t | y_{1:N}) dx_t dx_{t+1},$$

$$I_3 = \sum_{t=1}^T \int \log p_\theta(y_t | x_t) p_{\theta_k}(x_t | y_{1:N}) dx_t.$$

This leads us to a nonlinear state smoothing problem, which we can solve using sequential Monte Carlo (here, **particle smoothers**).



Using particle filters and particle smoothers we straightforwardly obtain the following approximations

$$p_{\theta_k}(x_1 | y_{1:T}) \approx \hat{p}_{\theta_k}^N(x_1 | y_{1:T}) = \sum_{i=1}^N w_{1|T}^i \delta_{x_1^i}(x_1),$$

$$p_{\theta_k}(x_{t:t+1} | y_{1:T}) \approx \hat{p}_{\theta_k}^N(x_{t:t+1} | y_{1:T}) = \sum_{i=1}^N w_{t|T}^i \delta_{x_{t:t+1}^i}(x_{t:t+1}).$$

The particle smoother employed is the so called forward filtering backward simulation (FFBSi) particle smoother derived by

R. Douc, A. Garivier, E. Moulines, and J. Olsson. **Sequential Monte Carlo smoothing for general state space hidden Markov models.** *Annals of Applied Probability*, 21(6):2109–2145, 2011.



Inserting the above approximations into the integrals yields the approximation we are looking for,

$$\begin{aligned}\hat{I}_1 &= \int \log p_\theta(x_1) \sum_{i=1}^N w_{1|T}^i \delta_{x_1^i}(x_1) dx_1 \\ &= \sum_{i=1}^N w_{1|T}^i \log p_\theta(x_1^i), \\ \hat{I}_3 &= \sum_{t=1}^T \int \log p_\theta(y_t | x_t) \sum_{i=1}^N w_{t|T}^i \delta_{x_t^i}(x_t) dx_t \\ &= \sum_{t=1}^T \sum_{i=1}^N w_{t|T}^i \log p_\theta(y_t | x_t^i),\end{aligned}$$

and similar for I_2 .



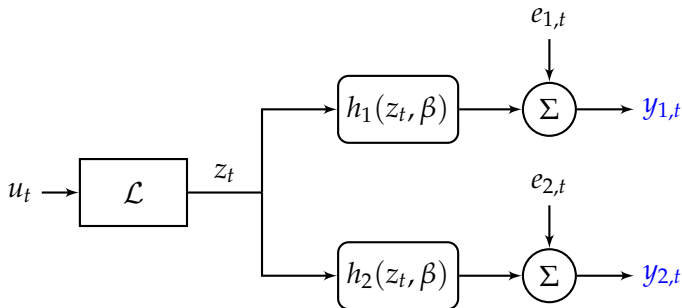
Algorithm 2 EM for nonlinear system identification

1. **Initialise:** Set $i = 1$ and choose an initial θ^1 .
2. **While** not converged **do:**
 - (a) **Expectation (E) step:** Run a FFBS PS and compute

$$\hat{Q}(\theta, \theta^i) = \hat{I}_1(\theta, \theta^i) + \hat{I}_2(\theta, \theta^i) + \hat{I}_3(\theta, \theta^i)$$

- (b) **Maximization (M) step:** Compute $\theta^{i+1} = \arg \max_{\theta \in \Theta} \hat{Q}(\theta, \theta^i)$
using an off-the-shelf numerical optimisation algorithm.
 - (c) $i \leftarrow i + 1$
-



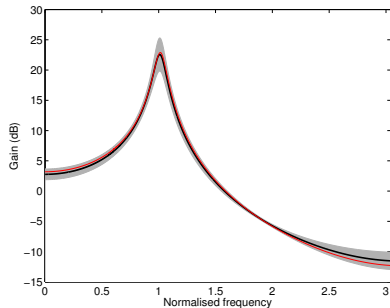


$$\begin{aligned}
 x_{t+1} &= \begin{pmatrix} A & B \end{pmatrix} \begin{pmatrix} x_t \\ u_t \end{pmatrix}, & u_t &\sim \mathcal{N}(0, Q), \\
 z_t &= Cx_t, & y_t &= h(z_t, \beta) + e_t, & e_t &\sim \mathcal{N}(0, R).
 \end{aligned}$$

Learning problem: Find \mathcal{L} and β, r_1, r_2 based on $\{y_{1,1:T}, y_{2,1:T}\}$.

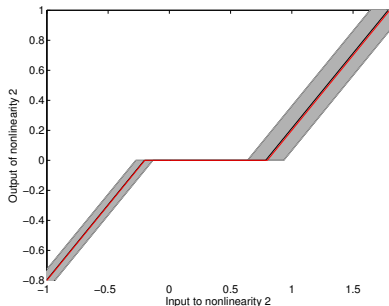
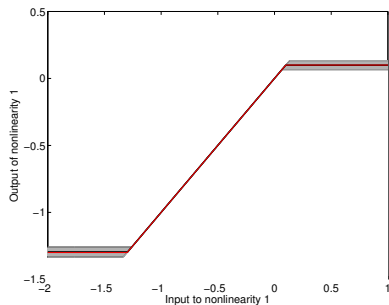


- Second order LGSS model with complex poles.
- Employ the EM-PS with $N = 100$ particles.
- EM-PS was terminated after 100 iterations.
- Results obtained using $T = 1000$ samples.
- The plots are based on 100 realisations of data.
- Nonlinearities (dead zone and saturation) shown on next slide.



Bode plot of estimated mean (black), true system (red) and the result for all 100 realisations (gray).





Estimated mean (black), true static nonlinearity (red) and the result for all 100 realisations (gray).



Consider a Bayesian SSM

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

We observe $D_T \triangleq \{u_{1:T}, y_{1:T}\}$.

Goal: Compute the posterior $p(\theta, x_{1:T} \mid D_T)$.



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

Gibbs sampling for SSMs amounts to iterating

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

The result is a Markov chain

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

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



Whenever you are working on an algorithm for nonlinear systems, **always** make sure that it solves the simple LGSS systems first!

Consider a fully parameterised LGSS model ($\theta \triangleq \{\Gamma, \Pi\}$).

$$\begin{pmatrix} x_{t+1} \\ y_t \end{pmatrix} | x_t \sim \mathcal{N} \left(\begin{pmatrix} x_{t+1} \\ y_t \end{pmatrix} | \underbrace{\begin{pmatrix} A & B \\ C & D \end{pmatrix}}_{\Gamma} \begin{pmatrix} x_t \\ u_t \end{pmatrix}, \underbrace{\begin{pmatrix} Q & S \\ S^T & R \end{pmatrix}}_{\Pi} \right).$$

The posterior distribution $p(\theta | D_T)$ is computed using Gibbs sampling,

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

Adrian Wills, Thomas B. Schön, Fredrik Lindsten and Brett Ninness, **Estimation of Linear Systems using a Gibbs Sampler**, *Proceedings of the 16th IFAC Symposium on System Identification (SYSID)*, Brussels, Belgium, July 2012.



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

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

Problem: $p(x_{1:T} \mid \theta, D_T)$ is not available!!

Idea: Approximate $p(x_{1:T} \mid \theta, D_T)$ using a particle smoother (PS).

Solution: Careful and clever analysis of how to combine MCMC and PF/PS resulted in the PMCMC family of algorithms.



Facts about Particle Markov Chain Monte Carlo (PMCMC) samplers:

- Provides a systematic and provably correct combination of PF/PS and MCMC.
- Standard MCMC samplers on non-standard spaces.
- Constitutes a family of Bayesian inference methods, including
 - Particle Independent Metropolis Hastings (PIMH)
 - Particle Marginal Metropolis Hastings (PMMH)
 - **Particle Gibbs (PG)**

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.

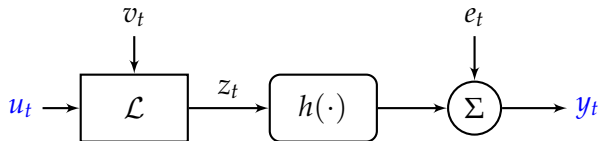


PG-BS sampler targeting $p(\theta, x_{1:T} \mid D_T)$.

- Conditional Particle filter and backwards simulation
 - Run a conditional PF, targeting $p(x_{1:T} \mid \theta, D_T)$;
 - Run a backward simulator to sample $x_{1:T}^*$;
- Draw $\theta^* \sim p(\theta \mid x_{1:T}^*, D_T)$.

Powerful and important properties of PG-BS: Provably convergent for any $N \geq 2$ particles and it works in practice!





LGSS and a static nonlinearity:

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

$$z_t = Cx_t.$$

$$y_t = h(z_t) + e_t,$$

$$e_t \sim \mathcal{N}(0, R).$$



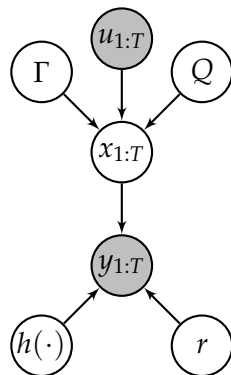
First step towards a fully data driven model (the order of the LGSS model is still assumed known).

Parameters: $\theta = \{\Gamma, Q, r, h(\cdot)\}$.

Bayesian model specified by priors:

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

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

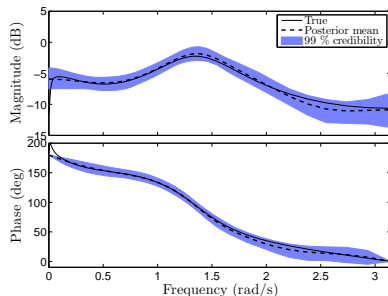


Gibbs sampler targeting $p(\theta, x_{1:T} \mid D_T)$.

- Conditional Particle filter and backwards simulation
 - Run a conditional PF, targeting $p(x_{1:T} \mid \theta, D_T)$;
 - Run a backward simulator to sample $x_{1:T}^*$;
- Draw $\{\Gamma^*, Q^*, r^*\} \sim p(\Gamma, Q, r \mid h, x_{1:T}^*, D_T)$;
- Draw $h^* \sim p(h \mid r^*, x_{1:T}^*, D_T)$.

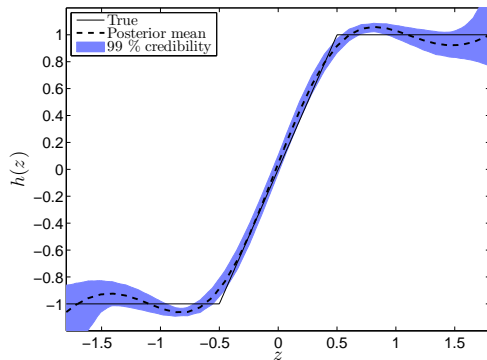


- Bayesian semiparametric model with conjugate prior (MNIW).
- 6th order LGSS model and a saturation.
- Using $T = 1000$ measurements.
- Employ the PG-BS sampler with $N = 15$ particles.
- Run 15000 MCMC iterations, discard 5000 as burn-in.



True Bode diagram of the linear system (black), estimated Bode diagram (dashed black) and 99% credibility interval (blue).





True static nonlinearity (black), estimated posterior mean (dashed black) and 99% credibility interval (blue).



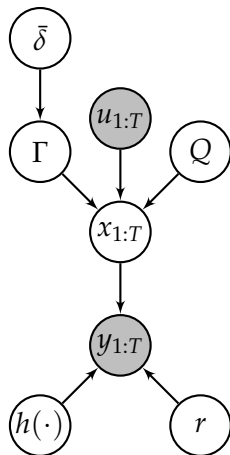
Everything is learned from the data, by introducing the possibility to switch specific model components on and off.

Parameters: $\theta = \{\Gamma, Q, \bar{\delta}, r, h(\cdot)\}$.

Bayesian model specified by priors

- Sparseness prior (ARD) on $\Gamma = [A \ B]$,
 - $p(\Gamma \mid \bar{\delta}) = \prod_{j=1}^{n_x+n_u} \mathcal{N}(\gamma_j \mid 0, \delta_j^{-1} I_{n_x+n_u})$
 - $\bar{\delta} = \{\delta_j\}_{j=1}^{n_x+n_u}$, $p(\delta_j) = \text{Gam}(\delta_j; a, b)$
- Inverse-Wishart prior on Q and r
- Gaussian process prior on $h(\cdot)$,

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

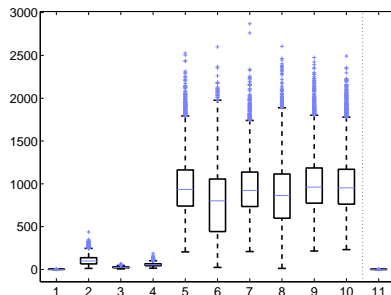


Gibbs sampler targeting $p(\theta, x_{1:T} \mid D_T)$.

- Conditional Particle filter and backwards simulation
 - Run a conditional PF, targeting $p(x_{1:T} \mid \theta, D_T)$;
 - Run a backward simulator to sample $x_{1:T}^*$;
- Draw $\{\Gamma^*, \bar{\delta}^*, Q^*, r^*\} \sim p(\Gamma, \bar{\delta}, Q, r \mid h, x_{1:T}^*, D_T)$;
- Draw $h^* \sim p(h \mid r^*, x_{1:T}^*, D_T)$.



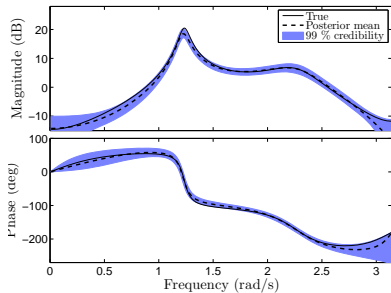
- Bayesian semiparametric model with ARD prior.
- 4th order LGSS model.
- Using $T = 1000$ measurements.
- Employ the PG-BS sampler with $N = 15$ particles.
- Run 15000 MCMC iterations, discard 5000 as burn-in.



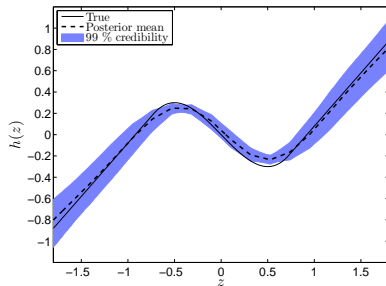
ARD precision parameters
 $\delta_j = 1, \dots, 11$. The rightmost box plot corresponds to the input signal.



Show movie



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



Estimated mean (thick black), 99% credibility intervals (blue) and the true static nonlinearity (non-monotonic) (black).



- Maximum likelihood learning:
 - EM combined with a particle smoother
 - Bayes modeling and learning:
 - PMCMC = combination of MCMC and PF/PS
 - PMCMC is systematic and provably correct
 - Solved various Wiener identification problems for illustration.
 - Much interesting research **remains to be done!!**
-

Should you be interested in the details, I am offering a PhD course on this topic at the University of Sydney next week. **Welcome!**

`users.isy.liu.se/rt/schon/course_CIDSusyd.html`



- Maximum Likelihood approach (EM-PS)

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*, 2012. (Accepted for publication)

MATLAB code is available from www.control.isy.liu.se/~schon/ressoftware.html

- Bayesian approach (PG-BS)

Fredrik Lindsten, Thomas B. Schön and Michael I. Jordan. **Data driven Wiener system identification**. *Automatica*, 2012 (in revision).

Fredrik Lindsten, Thomas B. Schön and Michael I. Jordan. **A semiparametric Bayesian approach to Wiener system identification**. *Proceedings of the 16th IFAC Symposium on System Identification (SYSID)*, Brussels, Belgium, July 2012.

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.

Fredrik Lindsten, Michael I. Jordan and Thomas B. Schön, **Ancestral Sampling for Particle Gibbs**, *Proceedings of Neural Information Processing Systems (NIPS)*, Lake Tahoe, NV, US, December, 2012. (Accepted for publication)

MATLAB code is available from www.control.isy.liu.se/~lindsten/code.html

