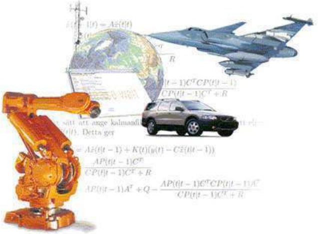
Learning models of nonlinear dynamical systems

– Strategies and concrete examples



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1. Dynamics modelled using a Markov process $\{x_t\}_{t \geq 1}$ (the state),

$$x_{t+1} \mid x_t \sim f_{\theta,t}(x_{t+1} \mid x_t, u_t), \qquad x_1 \sim \mu_\theta(x_1).$$

2. Observations modelled using a measurement process $\{y_t\}_{t \geq 1}$

$$y_t \mid x_t \sim h_{\theta,t}(y_t \mid x_t, u_t).$$

(3.) A Bayesian model also require $p(\theta), \theta \sim p(\theta)$.

Model = probability density function (pdf)

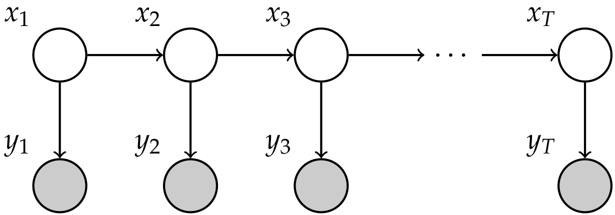

Figure: Graphical model for the SSM. Each stochastic variable is encoded using a node, where the nodes that are filled (gray) corresponds to variables that are observed and nodes that are not filled (white) are latent variables. The arrows pointing to a certain node encodes which variables the corresponding node are conditioned upon.

The SSM is an instance of a graphical model called **Bayesian network**, or **belief network**.

The time invariant linear Gaussian state space (LGSS) model is defined by

$$
\begin{aligned}
x_{t+1} &= Ax_t + Bu_t + v_t, \\
y_t &= Cx_t + Du_t + e_t,
\end{aligned}
$$

where $x_t \in \mathbb{R}^{n_x}$ denotes the state, $u_t \in \mathbb{R}^{n_u}$ denotes the known input signal and $y_t \in \mathbb{R}^{n_y}$ denotes the observed measurement. The initial state and the noise are distributed according to

$$
\begin{pmatrix} x_1 \\ v_t \\ e_t \end{pmatrix} \sim \mathcal{N}\left(\begin{pmatrix} \mu \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} P_1 & 0 & 0 \\ 0 & Q & S \\ 0 & S^T & R \end{pmatrix} \right).
$$

The filtering density $p(x_t \mid y_{1:t})$ is computed by the forward computations, summarized below in terms of the **measurement update**

$$p(x_t \mid y_{1:t}) = \frac{\overbrace{h(y_t \mid x_t)}^{\text{measurement}} \overbrace{p(x_t \mid y_{1:t-1})}^{\text{prediction pdf}}}{p(y_t \mid y_{1:t-1})},$$

and the **time update**

$$p(x_t \mid y_{1:t-1}) = \int \underbrace{f(x_t \mid x_{t-1})}_{\text{dynamics}} \underbrace{p(x_{t-1} \mid y_{1:t-1})}_{\text{filtering pdf}} \mathrm{d}x_{t-1},$$

Problem formulation:

- Maximum likelihood learning
- Bayesian learning
- Wiener model

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1. Solving the ML problem
   - Expectation maximization 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/smoother
   - Examples – learning a semiparametric Wiener model
3. Conclusions

Problem formulation

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 maximizes 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 $y_t \mid x_t \sim h_\theta(y_t \mid x_t)$ and $x_t \mid x_{t-1} \sim f_\theta(x_t \mid x_{t-1})$.
3. Assume that the stochastic variables $Y_1, \dots, Y_T$ are conditionally iid.

ML amounts to solving,

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

where the log-likelihood function is given by

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

Problem formulation – ML learning (II/II)

There are at least two challenges with the ML formulation:

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

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

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

Problem formulation – Bayesian learning

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

The **goal** in Bayesian modeling is to compute the posterior
$p(\underbrace{\theta, x_{1:T}}_{\triangleq \eta} \mid y_{1:T}) = p(\eta \mid y_{1:T})$ (or one of its marginals).

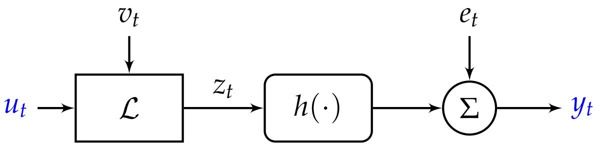
Bayesian modeling/learning amounts to:

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.

Example used – the Wiener model

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:

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

Measurements: Static nonlinearity:

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

Wiener model – common simplifying assumptions

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 restrictive assumptions.

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

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    - Expectation maximization combined with a particle smoother
    - Example – blind learning of a Wiener model.
2. Solving the Bayesian problem
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Expectation Maximization (EM) – strategy and idea

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 idea is to consider the joint log-likelihood function of 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

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

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

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

   (c) $i \leftarrow i + 1$

In computing the $\mathcal{Q}$-function

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

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 $\mathcal{Q}$-function

$$\mathcal{Q}(\theta, \theta^i) = I_1 + I_2 + I_3,$$

where

$$I_1 = \int \log p_\theta(x_1) p_{\theta^i}(x_1 \mid y_{1:N}) dx_1,$$

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

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

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

$$p_{\theta^i}(x_1 \mid y_{1:T}) \approx \widehat{p}^N_{\theta^i}(x_1 \mid y_{1:T}) = \sum_{i=1}^{N} w^i_{1|T} \delta_{x^i_1}(x_1),$$

$$p_{\theta^i}(x_{t:t+1} \mid y_{1:T}) \approx \widehat{p}^N_{\theta^i}(x_{t:t+1} \mid y_{1:T}) = \sum_{i=1}^{N} w^i_{t|T} \delta_{x^i_{t:t+1}}(x_{t:t+1}).$$

The particle smoother employed is the so called forward filtering backward simulation (FFBS) 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,

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

and similarly for I_2.

Algorithm 2 EM for learning nonlinear systems

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

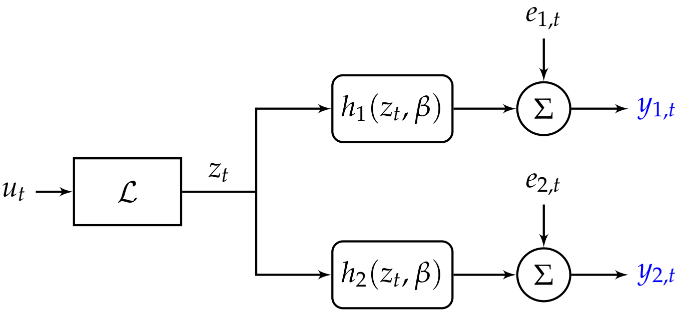
   $$\widehat{\mathcal{Q}}(\theta, \theta^i) = \widehat{I}_1(\theta, \theta^i) + \widehat{I}_2(\theta, \theta^i) + \widehat{I}_3(\theta, \theta^i)$$

   (b) **Maximization (M) step:** Compute $\theta^{i+1} = \underset{\theta \in \Theta}{\arg\max}\ \widehat{\mathcal{Q}}(\theta, \theta^i)$ using an off-the-shelf numerical optimization algorithm.

   (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.

Example – blind Wiener learning (I/III)



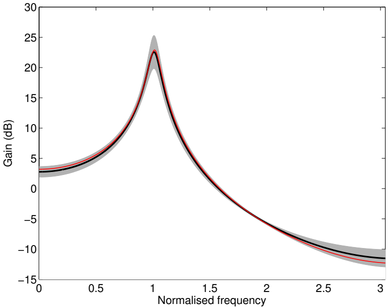
$$x_{t+1} = \begin{pmatrix} A & B \end{pmatrix} \begin{pmatrix} x_t \\ u_t \end{pmatrix}, \qquad u_t \sim \mathcal{N}(0, Q),$$

$$z_t = C x_t, \qquad y_t = h(z_t, \beta) + e_t, \qquad e_t \sim \mathcal{N}(0, R).$$

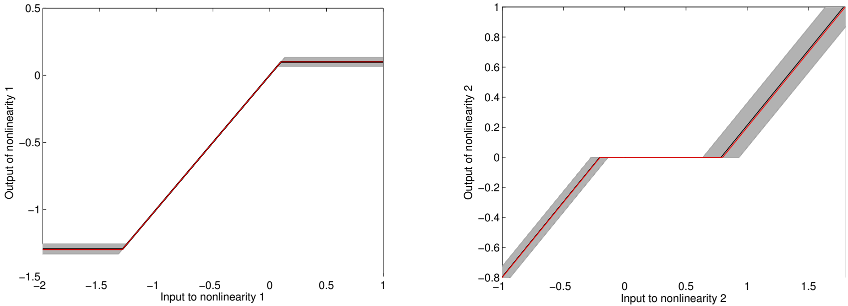
Learning problem: Find $\mathcal{L}$, β, r_1, and r_2 based on $\{y_{1,1:T}, y_{2,1:T}\}$.

Example – blind Wiener learning (II/III)

- 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).

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

Bayesian problem formulation again

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 (blocked) 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 parameterized LGSS model $(\theta \triangleq \{\Gamma, \Pi\})$.

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

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

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

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).

(Non-trivial) solution: Careful and clever analysis of how to combine MCMC and PF/PS results 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)**

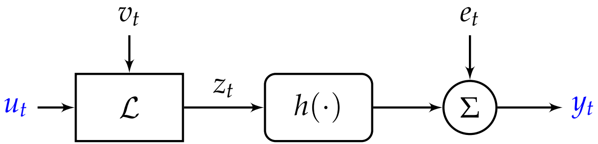
Christophe Andrieu, Arnaud Doucet and Roman Holenstein, **Particle Markov chain Monte Carlo methods**, *Journal of the Royal Statistical Society: Series B*, 72:269-342, 2010.

Particle Gibbs with backward simulation (PG-BS)

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

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

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



LGSS and a static nonlinearity:

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

$$z_t = Cx_t.$$

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

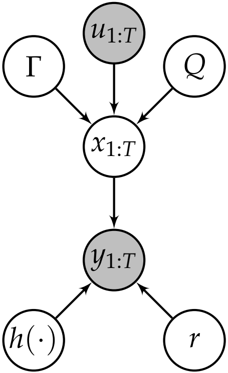
First step towards a fully data driven model (the order of the LGSS model is still assumed known).

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

Bayesian model specified by priors:

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

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

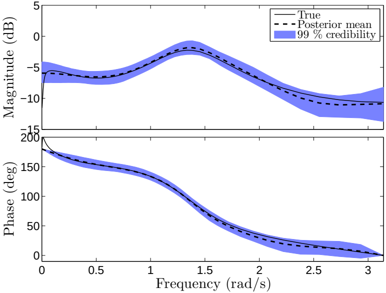


Gibbs sampler targeting $p(\theta, x_{1:T} \mid D_T)$.

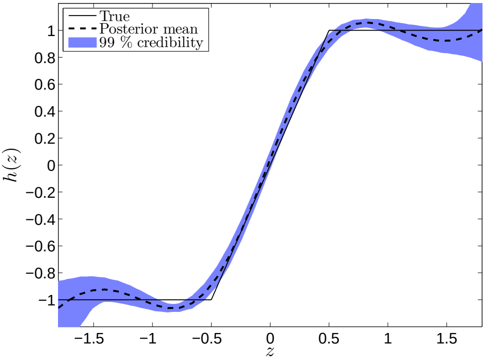
- Conditional particle filter and backwards simulation
  - Run a conditional PF, targeting $p(x_{1:T} \mid \theta, D_T)$;
  - Run a backward simulator to sample $x^\star_{1:T}$;
- Draw $\{\Gamma^\star, Q^\star, r^\star\} \sim p(\Gamma, Q, r \mid h, x^\star_{1:T}, D_T)$;
- Draw $h^\star \sim p(h \mid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

Example – known model order (I/II)

- Bayesian semiparametric model with conjugate prior (MNIW).
- 6^{th} 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.



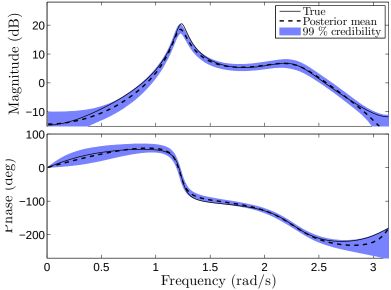
True Bode diagram of the linear system (solid black), estimated mean (dashed black) and 99% credibility interval (blue).



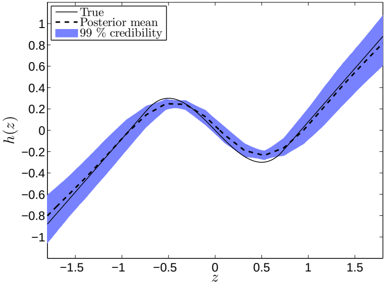
True static nonlinearity (solid black), estimated posterior mean (dashed black) and 99% credibility interval (blue).

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.

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*, 2012 (in revision).

Conclusions

- Maximum likelihood modeling learning:
  - EM (nonlinear optimization and PS)
- Bayesian modeling and learning:
  - PMCMC = combination of MCMC and PF/PS
  - PMCMC is systematic and provably correct
- Solved various Wiener learning problems for illustration.
- Much interesting research **remains to be done**!!

In this talk I introduced the strategies and showed a few concrete examples. Should you be interested in the details, I am offering a PhD course on this topic.

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

References to some of our work

- Maximum likelihood modeling learning:

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.

Some MATLAB code is available from `users.isy.liu.se/rt/schon/software.html`

- Bayesian modeling and learning:

Fredrik Lindsten, Thomas B. Schön and Michael I. Jordan. **Bayesian semiparametric 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.

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

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

MATLAB code is available from `users.isy.liu.se/rt/lindsten/code.html`