



UPPSALA
UNIVERSITET

Welcome to Sequential Monte Carlo methods!!

Lecture 1 – Introduction and probabilistic modelling

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Who are you?

85 participants registered for the course, representing 11 different countries and 23 different universities/companies.

Use this week not only to learn about SMC methods, but also to get to know new friends. Hopefully new research ideas will be initiated.

Aim of this course

Aim: To provide an introduction to the theory and application of sequential Monte Carlo (SMC) methods.

After the course you should be able to derive your own SMC-based algorithms allowing you to do inference in nonlinear models.

Day 1-3: Focus on state space models (SSMs). How to learning them from data and how to estimate their hidden states.

Day 4: Using SMC for inference in general probabilistic models.

Ex) Indoor positioning (engineering)

Aim: Compute the **position** of a person moving around indoors using variations in the ambient magnetic field and the motion of the person (acceleration and angular velocities). All of this observed using sensors in a standard smartphone.



Ex) Indoor positioning (engineering)

Key ingredients of the solution:

1. The **particle filter** for computing the position
2. The **Gaussian process** for building and representing the map of the ambient magnetic field
3. **Inertial sensor** signal processing

Movie – map making: www.youtube.com/watch?v=enlMiUqPVJo

Movie – indoor positioning result



Arno Solin, Simo Särkkä, Juho Kannala and Esa Rahtu. **Terrain navigation in the magnetic landscape: Particle filtering for indoor positioning.** *Proc. of the European Navigation Conf. (ENC)*, Helsinki, Finland, June, 2016.



Arno Solin, Manon Kok, Niklas Wahlström, Thomas B. Schön and Simo Särkkä. **Modeling and interpolation of the ambient magnetic field by Gaussian processes.** *IEEE Trans. on Robotics*, 34(4):1112–1127, 2018.



Carl Jidling, Niklas Wahlström, Adrian Wills and Thomas B. Schön. **Linearly constrained Gaussian processes.** *Advances in Neural Information Processing Systems (NIPS)*, Long Beach, CA, USA, December, 2017.

Ex) Epidemiological modelling (statistics)

Aim: To learn a model explaining the seasonal influenza epidemics and then make use of this model to compute predictions.

Susceptible/infected/recovered (SIR) model:

$$S_{t+dt} = S_t + \mu \mathcal{P} dt - \mu S_t dt - (1 + F v_t) \beta_t S_t \mathcal{P}^{-1} I_t dt,$$

$$I_{t+dt} = I_t - (\gamma + \mu) I_t dt + (1 + F v_t) \beta_t S_t \mathcal{P}^{-1} I_t dt,$$

$$R_{t+dt} = R_t + \gamma I_t dt - \mu R_t dt,$$

$$\beta_t = R_0 (\gamma + \mu) (1 + \alpha \sin(2\pi t/12)),$$

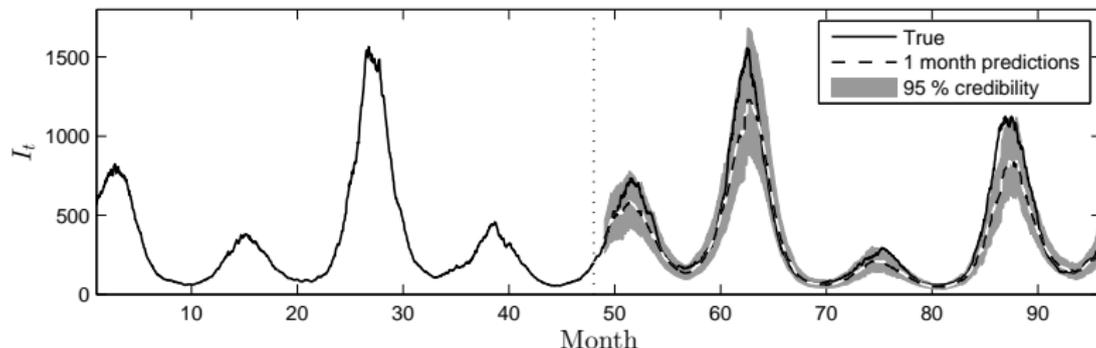
Measurements:

$$y_k = \rho \text{logit}(\bar{I}_k / \mathcal{P}) + e_k, \quad e_k \sim \mathcal{N}(0, \sigma^2).$$

Information about the unknown parameters $\theta = (\gamma, R_0, \alpha, F, \rho, \sigma)$ and states $x_t = (S_t, I_t, R_t)$ has to be learned from measurements.

Ex) Epidemiological modelling (statistics)

Compute $p(\theta, x_{1:T} | y_{1:T})$, where $y_{1:T} = (y_1, y_2, \dots, y_T)$ and use it to compute the predictive distribution.



Disease activity (number of infected individuals I_t) over an eight year period.



Ex) Probabilistic programming (machine learning)

A **probabilistic program** encodes a **probabilistic model** according to the semantics of a particular probabilistic programming language, giving rise to a **programmable model**.

The memory state of a running probabilistic program evolves dynamically and stochastically in time and so is a **stochastic process**.

SMC is a common inference method for programmable model.

Creates a clear separation between the model and the inference methods. Opens up for the automation of inference!

```
x ~ Bernoulli(p);   assume(x)
if (x) {           value(x)
  y ~ N(0,1);      assume(y)
} else {
  y <- 0;
```

More during lecture 17 and 18.

Course structure – overview

- 18 lectures (45 min. each)
- Credits offered: 6ECTS (Swedish system)
- Practicals (solve exercises and hand-in assignments, **discuss and ask questions**)
- Hand-in assignments. You can collaborate, but the reports with the solutions are individual.
- Complete course information (including lecture slides) is available from the course website:
www.it.uu.se/research/systems_and_control/education/2019/smc
- **Feel free to ask questions at any time!**

The only way to really learn something is by
implementing it on your own.

Outline – 4 days

Day 1 – Probabilistic modelling and particle filtering basics

- a) Probabilistic modelling of dynamical systems and filtering
- b) Introduce Monte Carlo and derive the bootstrap particle filter

Day 2 – Particle filtering and parameter learning

- a) Auxiliary particle filter, full adaptation and practicalities
- b) Maximum likelihood parameter learning, convergence

Day 3 – Bayesian parameter learning

- a) Particle Metropolis Hastings
- b) Particle Gibbs

Day 4 – Beyond state space models (outlooks)

- a) General target sequences and SMC samplers
- b) Probabilistic programming and applications to phylogenetics

Aim: Introduce the course and provide background on probabilistic modelling.

Outline:

1. Course introduction and practicalities
2. Probabilistic modelling
3. Key probabilistic objects
4. Ex. probabilistic autoregressive modelling (if there is time)

Probabilistic modelling

Mathematical model: A compact representation—set of assumptions—of the data that in precise mathematical form captures the key properties of the underlying situation.

Most of the course (day 1-3) is concerned with dynamical phenomena. The methods are more general than that and during the last day we will broaden the scope significantly.

Dynamical phenomena produce temporal measurements (data) arriving as a **sequence**

$$y_{1:t} = (y_1, y_2, \dots, y_t).$$

Nice introduction to probabilistic modelling in Machine Learning

Ghahramani, Z. **Probabilistic machine learning and artificial intelligence**. *Nature* 521:452-459, 2015.

Representing and modifying uncertainty

It is important to maintain a solid representation of uncertainty in all mathematical objects and throughout all calculations.



The two basic rules from probability theory

Let X and Y be continuous random variables¹. Let $p(\cdot)$ denote a general probability density function.

1. Marginalization (integrate out a variable): $p(x) = \int p(x, y)dy$.
2. Conditional probability: $p(x, y) = p(x | y)p(y)$.

Combine them into Bayes' rule:

$$p(x | y) = \frac{p(y | x)p(x)}{p(y)} = \frac{p(y | x)p(x)}{\int p(y | x)p(x)dx}$$

¹Notation: Upper-case letters for random variables (r.v.) X when we talk about models. Lower-case letters for realizations of the r.v., $X = x$ and in algorithms. We will not use bold face for vectors.

Basic variables classes

Measurements $y_{1:T} = (y_1, y_2, \dots, y_T)$: The measured data somehow obtained from the phenomenon we are interested in.

Unknown (static) model parameters θ : Describes the model, but unknown (or not known well enough) to the user.

Unknown model variables x_t (changing over time): Describes the state of the phenomenon at time t (in the indoor positioning example above x_t includes the unknown position).

Explanatory variables u : Known variables that we do not bother to model as stochastic.

A key task is often to learn θ and/or x_t based on the available measurements $y_{1:T}$.

Computational problems

The problem of learning a model based on data leads to computational challenges, both

- **Integration:** e.g. the high-dimensional integrals arising during marg. (averaging over all possible parameter values θ):

$$p(y_{1:T}) = \int p(y_{1:T} | \theta) p(\theta) d\theta.$$

- **Optimization:** e.g. when extracting point estimates, for example by maximizing the posterior or the likelihood

$$\hat{\theta} = \arg \max_{\theta} p(y_{1:T} | \theta)$$

Typically impossible to compute exactly, use approximate methods

- Monte Carlo (MC), Markov chain MC (MCMC), and sequential MC (SMC).
- Variational inference (VI).

Probabilistic autoregressive model

Probabilistic autoregressive model

An autoregressive model of order n is given by

$$Y_t = A_1 Y_{t-1} + A_2 Y_{t-2} + \dots + A_n Y_{t-n} + E_t, \quad E_t \sim \mathcal{N}(\mu, \tau^{-1})$$

where μ and τ are known explanatory variables ($\mu = 0, \tau \neq 0$).

The unknown model variables are collected as

$$\theta = (A_1, A_2, \dots, A_n)^T$$

with the prior

$$\theta \sim \mathcal{N}(0, \rho^{-1} I_n), \quad \text{where } \rho \text{ assumed to be known.}$$

Task: Compute the posterior $p(\theta | y_{1:T})$.

Probabilistic autoregressive model

Full probabilistic model $p(\boldsymbol{\theta}, y_{1:T}) = p(y_{1:T} | \boldsymbol{\theta})p(\boldsymbol{\theta})$, where the data distribution is given by

$$p(y_{1:T} | \boldsymbol{\theta}) = p(y_T | y_{1:T-1}, \boldsymbol{\theta})p(y_{1:T-1} | \boldsymbol{\theta}) = \cdots = \prod_{t=1}^T p(y_t | y_{1:t-1}, \boldsymbol{\theta}).$$

From the model we have that

$$p(y_t | y_{1:t-1}, \boldsymbol{\theta}) = \mathcal{N}(y_t | \boldsymbol{\theta}^T \mathbf{z}_t, \tau^{-1}),$$

where $\mathbf{z}_t = (Y_{t-1}, Y_{t-2}, \dots, Y_{t-n})^T$. Hence,

$$p(y_{1:T} | \boldsymbol{\theta}) = \prod_{t=1}^T \mathcal{N}(y_t | \boldsymbol{\theta}^T \mathbf{z}_t, \tau^{-1}) = \mathcal{N}(\mathbf{y} | \mathbf{z}\boldsymbol{\theta}, \tau^{-1}I_T),$$

where we have made use of $\mathbf{Y} = (Y_1, Y_2, \dots, Y_T)^T$ and $\mathbf{Z} = (Z_1, Z_2, \dots, Z_T)^T$.

Probabilistic autoregressive model

$$\begin{aligned} p(\boldsymbol{\theta}, \mathbf{y}) &= \underbrace{\mathcal{N}(\mathbf{y} \mid \mathbf{z}\boldsymbol{\theta}, \tau^{-1}I_T)}_{p(\mathbf{y} \mid \boldsymbol{\theta})} \underbrace{\mathcal{N}(\boldsymbol{\theta} \mid 0, \rho^{-1}I_n)}_{p(\boldsymbol{\theta})} \\ &= \mathcal{N}\left(\begin{pmatrix} \boldsymbol{\theta} \\ \mathbf{y} \end{pmatrix} \middle| \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \rho^{-1}I_2 & \rho^{-1}\mathbf{z}^T \\ \rho^{-1}\mathbf{z} & \tau^{-1}I_T + \rho^{-1}\mathbf{z}\mathbf{z}^T \end{pmatrix}\right). \end{aligned}$$

The posterior is given by

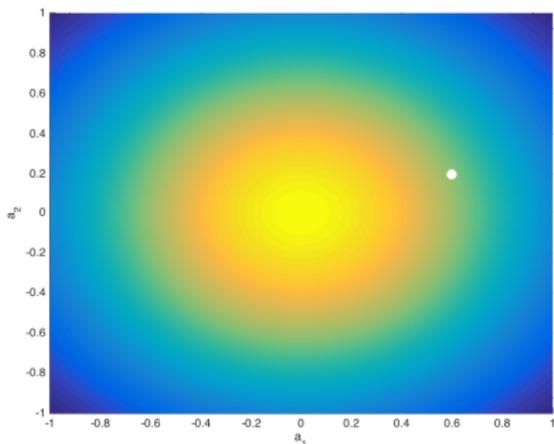
$$p(\boldsymbol{\theta} \mid \mathbf{y}) = \mathcal{N}(\boldsymbol{\theta} \mid m_T, S_T),$$

where

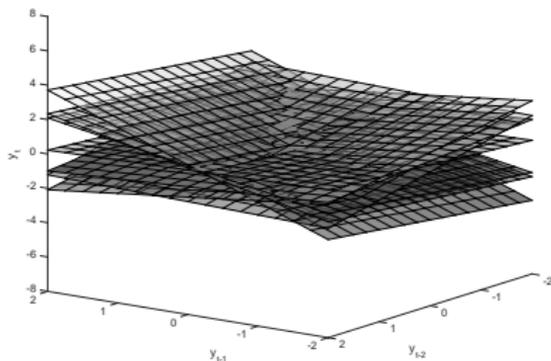
$$\begin{aligned} m_T &= \tau S_T \mathbf{z}^T \mathbf{y}, \\ S_T &= (\rho^{-1}I_2 + \sigma \mathbf{z}^T \mathbf{z})^{-1}. \end{aligned}$$

Ex) Situation before any data is used

$$Y_t = A_1 Y_{t-1} + A_2 Y_{t-2} + E_t, \quad E_t \sim \mathcal{N}(0, 0.2).$$



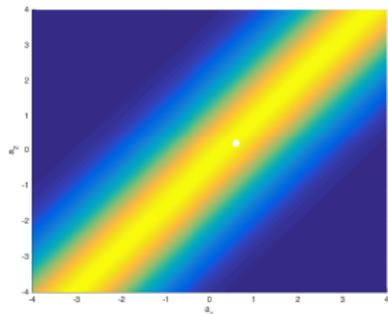
Prior



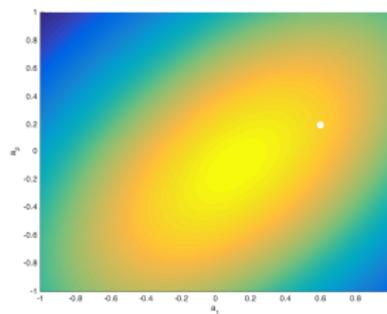
7 samples from the prior

White dot – true value for $\theta = (0.6, 0.2)$.

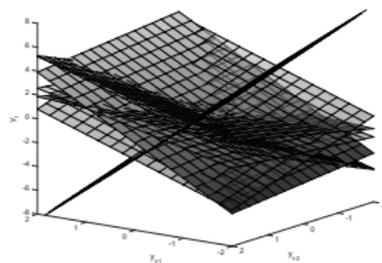
Ex) Situation after y_1 is obtained



Likelihood

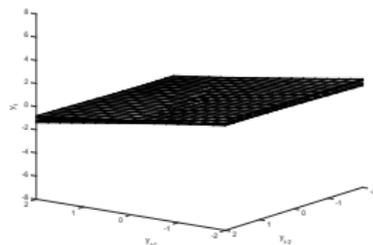
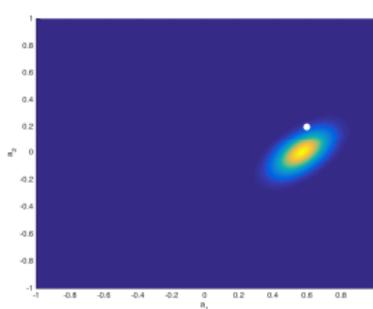
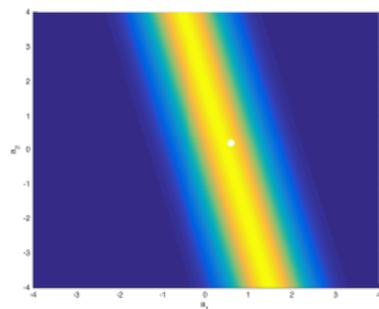
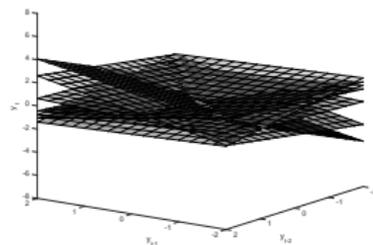
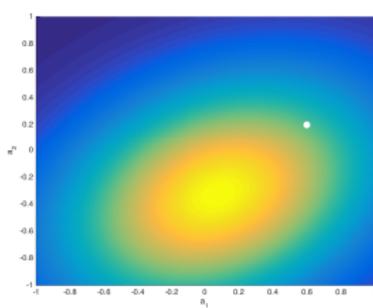
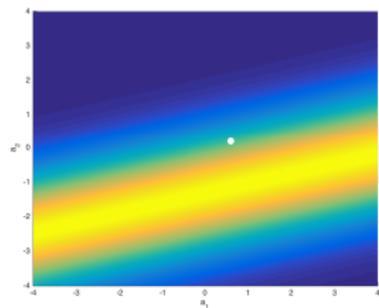


Posterior



7 samples from the
posterior

Ex) Situation after $y_{1:2}$ and $y_{1:20}$



Likelihood

Posterior

7 samples from the posterior

A few concepts to summarize lecture 1

Mathematical model: A compact representation—set of assumptions—of some phenomenon of interest.

Probabilistic modelling: Provides the capability to represent and manipulate **uncertainty** in data, models, decisions and predictions.

Full probabilistic model: The joint distribution of all observed (here $y_{1:T}$) and unobserved (here θ) variables.

Data distribution/likelihood: Distribution describing the observed data conditioned on unobserved variables.

Prior distribution: Encodes initial assumptions on the unobserved variables.

Posterior distribution: Conditional distribution of the unobserved variables given the observed variables.