

Learning dynamical systems using SMC

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We automate the extraction of knowledge and understanding from data.

Both basic research and applied research (with companies).



Create **probabilistic models** of dynamical systems and their surroundings.

Develop methods to learn models from data.

The models can then be used by machines (or humans) to **understand** or **take decisions** about what will happen next. The state space model (SSM) is a **Markov** chain that makes use of a **latent** variable representation to describe dynamical phenomena.

It consists of two stochastic processes:

- 1. unobserved (state) process $\{x_t\}_{t\geq 0}$ modelling the dynamics,
- 2. observed process $\{y_t\}_{t\geq 1}$ modelling the measurements and their relationship to the unobserved state process.

 $\begin{aligned} x_t &= f(x_{t-1}, \theta) + v_t, \\ y_t &= g(x_t, \theta) + e_t, \end{aligned}$

where $\theta \in \mathbb{R}^{n_{\theta}}$ denotes static model parameters.

The SSM offers a practical representation not only for **modelling**, but also for **reasoning** and **inference**.

Ex) "what are x_t , θ and y_t "?

Aim (motion capture): Compute x_t (position and orientation of the different body segments) of a person (θ describes the body shape) moving around indoors using measurements y_t (accelerometers, gyroscopes and ultrawideband).



Show movie!

Manon Kok, Jeroen D. Hol and Thomas B. Schön. Using inertial sensors for position and orientation estimation, Foundations and Trends of Signal Processing, 11(1–2):1–153, 2017.

Three different representations of the SSM

Three alternative representations, using

- 1. graphical models,
- 2. probability distributions or
- 3. probabilistic programs.

1. Representing the SSM using a graphical model:



Representations using distributions or probabilistic programs

2. Representation using probability distributions

 $\begin{aligned} x_t \mid & (x_{t-1}, \theta) \sim p(x_t \mid x_{t-1}, \theta), \\ y_t \mid & (x_t, \theta) \sim p(y_t \mid x_t, \theta), \\ & x_0 \sim p(x_0 \mid \theta). \end{aligned}$

3. Representing the SSM using a probabilistic program

A **probabilistic program** encodes a **probabilistic model** (here an LG-SSM) according to the semantics of a particular probabilistic programming language (here Birch).

SSM – full probabilistic model

The full probabilistic model is given by

$$p(x_{0:T}, \theta, y_{1:T}) = \underbrace{p(y_{1:T} \mid x_{0:T}, \theta)}_{\text{data distribution}} \underbrace{p(x_{0:T}, \theta)}_{\text{prior}}$$

Distribution describing a parametric nonlinear SSM

$$p(x_{0:T}, \theta, y_{1:T}) = \prod_{\substack{t=1 \ \text{observation} \\ \text{data distribution}}}^{T} \underbrace{\prod_{\substack{t=1 \ \text{observation} \\ \text{dynamics}}}^{T} \underbrace{p(x_t \mid x_{t-1}, \theta)}_{\text{dynamics}} \underbrace{p(x_0 \mid \theta)}_{\text{state}} \underbrace{p(\theta)}_{\text{param.}}$$

Model = probability distribution!

Learning the states and the parameters

Based on our generative model, compute the posterior distribution

$$p(x_{0:T}, \theta \mid y_{1:T}) = \underbrace{p(x_{0:T} \mid \theta, y_{1:T})}_{\text{state inf.}} \underbrace{p(\theta \mid y_{1:T})}_{\text{param. inf.}}.$$

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

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

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

$$\widehat{\boldsymbol{\theta}} = \operatorname*{arg\,max}_{\boldsymbol{\theta}\in\Theta} p(y_{1:\mathcal{T}} \mid \boldsymbol{\theta}).$$

Central object - the likelihood

The likelihood is computed by marginalizing

$$p(\mathbf{x}_{0:T}, \mathbf{y}_{1:T} \mid \boldsymbol{\theta}) = p(\mathbf{x}_0 \mid \boldsymbol{\theta}) \prod_{t=1}^{T} p(\mathbf{y}_t \mid \mathbf{x}_t, \boldsymbol{\theta}) \prod_{t=1}^{T} p(\mathbf{x}_t \mid \mathbf{x}_{t-1}, \boldsymbol{\theta}),$$

w.r.t the state sequence $x_{0:T}$,

$$p(y_{1:T} \mid \boldsymbol{\theta}) = \int p(\boldsymbol{x}_{0:T}, y_{1:T} \mid \boldsymbol{\theta}) d\boldsymbol{x}_{0:T}.$$

(We are averaging $p(x_{0:T}, y_{1:T} | \theta)$ over all possible state sequences.)

Equivalently we have

$$p(y_{1:T} \mid \theta) = \prod_{t=1}^{T} p(y_t \mid y_{1:t-1}, \theta) = \prod_{t=1}^{T} \int p(y_t \mid x_t, \theta) \underbrace{p(x_t \mid y_{1:t-1}, \theta)}_{\text{key challenge}} dx_t.$$

Thomas B. Schön, Fredrik Lindsten, Johan Dahlin, Johan Wagberg, Christian A. Naesseth, Andreas Svensson and Liang Dai. Sequential Monte Carlo methods for system identification. In Proceedings of the 17th IFAC Symposium on System Identification (SYSID), Beijing, China, October 2015.

The nonlinear filtering problem involves the measurement update

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

and the time update

$$p(\mathbf{x}_t \mid y_{1:t-1}) = \int \underbrace{p(\mathbf{x}_t \mid \mathbf{x}_{t-1})}_{\text{dynamics}} \underbrace{p(\mathbf{x}_{t-1} \mid y_{1:t-1})}_{\text{filtering pdf}} d\mathbf{x}_{t-1}$$

Outline

Aim: 1. Give a (hopefully) intuitive explanation of sequential Monte Carlo (SMC) for probabilistic modelling of dynamical systems.
2. Derive a new stochastic optimization method that can for example be used to learn unknown parameters in nonlinear SSMs.

- 1. Probabilistic modelling of dynamical systems
- 2. Sequential Monte Carlo (SMC)
- 3. Stochastic optimization
- 4. Some ongoing research snapshots (if there is time)

Sequential Monte Carlo

The need for computational methods, such as SMC, is tightly coupled to the intractability of the integrals on the previous slides.

SMC provide approximate solutions to **integration** problems where there is a **sequential structure** present.

The particle filter approximates $p(x_t | y_{1:t})$ for

$$\begin{aligned} x_t &= f(x_{t-1}) + v_t, \\ y_t &= g(x_t) + e_t, \end{aligned}$$

by maintaining an empirical distribution made up of N samples (particles) $\{x_t^i\}_{i=1}^N$ and the corresponding weights $\{w_t^i\}_{i=1}^N$

$$\underbrace{\widehat{p}(\mathbf{x}_t \mid \mathbf{y}_{1:t})}_{\widehat{\pi}(\mathbf{x}_t)} = \sum_{i=1}^N \frac{w_t^i}{\sum_{j=1}^N w_t^j} \delta_{\mathbf{x}_t^i}(\mathbf{x}_t).$$

Consider a toy 1D localization problem.

Data



Model

Dynamic model:

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \mathbf{u}_t + \mathbf{v}_t,$$

where x_t denotes position, u_t denotes velocity (known), $v_t \sim \mathcal{N}(0, 5)$ denotes an unknown disturbance.

Measurements:

$$y_t = h(\mathbf{x}_t) + e_t$$

where $h(\cdot)$ denotes the world model (here the terrain height) and $e_t \sim \mathcal{N}(0, 1)$ denotes an unknown disturbance.

Task: Find the state x_t (position) based on the measurements $y_{1:t} \triangleq \{y_1, \ldots, y_t\}$ by computing the filter density $p(x_t | y_{1:t})$.

Highlights two key capabilities of the PF:

- Automatically handles an unknown and dynamically changing number of hypotheses.
- Work with nonlinear/non-Gaussian models.



SMC = sequential importance sampling + resampling

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

The ancestor indices $\{a_t^i\}_{i=1}^N$ are very useful auxiliary variables! They make the stochasticity of the resampling step explicit. **Aim:** Compute the position of a person moving around indoors using sensors (inertial, magnetometer, radio) located in an ID badge and a map.



The sensors (IMU and radio) and the DSP are mounted inside an ID badge.



pdf for an office environment, the bright areas are rooms and corridors (i.e., walkable space).

Application – indoor localization (II/III)



Show movie

Johan Kihlberg, Simon Tegelid, Manon Kok and Thomas B. Schön. Map aided indoor positioning using particle filters. Reglermöte (Swedish Control Conference), Linköping, Sweden, June 2014.

Application – indoor localization (III/III)

Aim: Compute the **position** 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.



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. In Proceedings of the European Navigation Conference 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 Transactions on Robotics*, 2018 (to appear).

A systematic way of combining SMC and MCMC.

Builds on an extended target construction.

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

A bit more precise: Construct a Markov chain with $p(\theta, x_{1:T} | y_{1:T})$ (or one of its marginals) as its stationary distribution. Also used for parameter learning.

Exact approximations

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.

Aim: 1. Give a (hopefully) intuitive explanation of **sequential Monte Carlo (SMC)** for probabilistic modelling of dynamical systems. 2. Derive a new **stochastic optimization** method that can for example be used to learn unknown parameters in nonlinear SSMs.

- 1. Probabilistic modelling of dynamical systems
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Quasi-Newton — A non-standard take

Our problem is of the form (note change of notation...)

 $\max_{\mathbf{x}} f(\mathbf{x})$

Idea underlying (quasi-)Newton methods: Learn a local quadratic model $q(x_k, \delta)$ of the cost function f(x) around the current iterate x_k

$$q(\mathbf{x}_{k},\delta) = f(\mathbf{x}_{k}) + g(\mathbf{x}_{k})^{\mathsf{T}}\delta + \frac{1}{2}\delta^{\mathsf{T}}H(\mathbf{x}_{k})\delta$$

A second-order Taylor expansion around x_k , where

$$g(\mathbf{x}_{k}) = \nabla f(\mathbf{x})\big|_{\mathbf{x}=\mathbf{x}_{k}},$$
$$H(\mathbf{x}_{k}) = \nabla^{2}f(\mathbf{x})\big|_{\mathbf{x}=\mathbf{x}_{k}},$$
$$\delta = \mathbf{x} - \mathbf{x}_{k}.$$

We have measurements of the

- cost function $f_k = f(x_k)$,
- and its gradient $g_k = g(\mathbf{x}_k)$.

Question: How do we update the Hessian model?

Line segment connecting two adjacent iterates x_k and x_{k+1} :

$$r_k(\tau) = \mathbf{x}_k + \tau(\mathbf{x}_{k+1} - \mathbf{x}_k), \qquad \tau \in [0, 1].$$

Useful basic facts

The fundamental theorem of calculus states that

$$\int_{0}^{1} \frac{\partial}{\partial \tau} \nabla f(r_{k}(\tau)) d\tau = \nabla f(r_{k}(1)) - \nabla f(r_{k}(0)) = \underbrace{\nabla f(x_{k+1})}_{g_{k+1}} - \underbrace{\nabla f(x_{k})}_{g_{k}}$$

and the chain rule tells us that

$$\frac{\partial}{\partial \tau} \nabla f(r_k(\tau)) = \nabla^2 f(r_k(\tau)) \frac{\partial r_k(\tau)}{\partial \tau} = \nabla^2 f(r_k(\tau)) (\mathbf{x}_{k+1} - \mathbf{x}_k).$$

$$\underbrace{g_{k+1}-g_k}_{=y_k}=\int_0^1\frac{\partial}{\partial\tau}\nabla f(r_k(\tau))\mathsf{d}\tau=\int_0^1\nabla^2 f(r_k(\tau))\mathsf{d}\tau(\underbrace{x_{k+1}-x_k}_{s_k}).$$

With the definitions $y_k \triangleq g_{k+1} - g_k$ and $s_k \triangleq x_{k+1} - x_k$ we have

$$y_k = \int_0^1 \nabla^2 f(r_k(\tau)) \mathrm{d}\tau s_k.$$

Interpretation: The difference between two consecutive gradients (y_k) constitute a *line integral observation of the Hessian*.

Problem: Since the Hessian is unknown there is no functional form available for it.

Solution 1 — recovering existing quasi-Newton algorithms

Existing quasi-Newton algorithms (e.g. BFGS, DFP, Broyden's method) assume the Hessian to be constant

$$abla^2 f(r_k(\tau)) \approx H_{k+1}, \qquad \tau \in [0,1],$$

implying the following approximation of the integral (secant condition)

$$y_k = H_{k+1}s_k.$$

Find H_{k+1} by regularizing H:

$$\begin{aligned} H_{k+1} &= \min_{H} \quad \|H - H_k\|_W^2, \\ \text{s.t.} \quad H &= H^{\mathsf{T}}, \quad Hs_k = y_k, \end{aligned}$$

Equivalently, the existing quasi-Newton methods can be interpreted as **particular instances of Bayesian linear regression**.

The approach used here is fundamentally different.

Recall that the problem is **stochastic** and **nonlinear**.

Hence, we need a model that can deal with such a problem.

Idea: Represent the Hessian using a Gaussian process learnt from data.

Two of the remaining challenges:

- 1. Can we use line integral observations when learning a GP?
- 2. How do we ensure that the resulting GP represents a Hessian?

GP prior for the Hessian

Stochastic quasi-Newton integral

$$y_k = \int_0^1 \underbrace{\mathcal{B}(r_k(\tau))}_{=\nabla^2 f(r_k(\tau))} s_k \mathrm{d}\tau + e_k,$$

corresponds to noisy (e_k) gradient observations.

Since $B(x)s_k$ is a column vector, the integrand is given by $\operatorname{vec}(B(x)s_k) = (s_k^{\mathsf{T}} \otimes I)\operatorname{vec}(B(x)) = (s_k^{\mathsf{T}} \otimes I)\operatorname{vec}(B(x))$, where $\operatorname{vec}(B(x)) = D \underbrace{\operatorname{vech}(B(x))}_{\widetilde{B}(x)}$.

Let us use a GP model for the unique elements of the Hessian $\widetilde{B}(x) \sim \mathcal{GP}(\mu(x), \kappa(x, x')).$

Resulting stochastic qN integral and Hessian model



The Hessian can now be estimated using tailored GP regression.

Linear transformations (such as an integral or a derivative) of a GP results in a new GP.

Resulting stochastic optimization algorithm

Standard non-convex numerical optimization loop with **non-standard components**.

Algorithm 1 Stochastic optimization

- 1. Initialization (k = 1)
- 2. while not terminated do
 - (a) Compute a search direction p_k using the current approximation of the gradient g_k and Hessian B_k.
 - (b) Stochastic line search to find a step length α_k and set

$$\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k.$$

(c) Set k := k + 1

- (d) Update the Hessian estimate (tailored GP regression)
- 3. end while

Identify the parameters $\theta = (a, c, q, r)^{\mathsf{T}}$ in

$$\begin{aligned} \mathbf{x}_{t+1} &= \mathbf{a}\mathbf{x}_t + \mathbf{w}_t, & \mathbf{w}_t \sim \mathcal{N}(0, \mathbf{q}), \\ \mathbf{y}_t &= \mathbf{c}\mathbf{x}_t + \mathbf{e}_t, & \mathbf{e}_t \sim \mathcal{N}(0, \mathbf{r}). \end{aligned}$$

Observations:

- The likelihood L(θ) = p(y_{1:τ} | θ) and its gradient ∇_θL(θ) are available in closed form via standard Kalman filter equations.
- Standard gradient-based search algorithms applies.
- Deterministic optimization problem $(L(\theta), \nabla_{\theta}L(\theta)$ noise-free).

ex) Simple linear toy problem



Classical BFGS alg. for noisy observations of $L(\theta)$ and $\nabla L(\theta)$.

100 independent datasets.

Clear blue – True system Red – Mean value of estimate Shaded blue – individual results



GP-based BFGS alg. with noisy observations of $L(\theta)$ and $\nabla L(\theta).30/41$

ex) laser interferometry



The classic Michelson-Morley experiment from 1887.

Idea: Merge two light sources to create an interference pattern by superposition.

Two cases:

- 1. Mirror B and C at the same distance from mirror A.
- 2. Mirror B and C at different distances from mirror A.

ex) laser interferometry

Dynamics: constant velocity model (with unknown force w)

$$\begin{pmatrix} \dot{p} \\ \dot{v} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} p \\ v \end{pmatrix} + \begin{pmatrix} 0 \\ w \end{pmatrix}.$$

Measurements: generated using two detectors

$$y_1 = \alpha_0 + \alpha_1 \cos(\kappa p) + e_1, \qquad e_1 \sim \mathcal{N}(0, \sigma^2),$$
$$y_2 = \beta_0 + \beta_1 \sin(\kappa p + \gamma) + e_2, \qquad e_2 \sim \mathcal{N}(0, \sigma^2).$$
Unknown parameters: $\theta = \begin{pmatrix} \alpha_0 & \alpha_0 & \beta_0 & \beta_1 & \gamma & \sigma \end{pmatrix}^{\mathsf{T}}.$

Resulting maximum likelihood system identification problem

$$\max_{\theta} p(y_{1:T} \mid \theta)$$

ex) laser interferometry

Research snapshots

What is the key limitation of our GP-based optimization algorithm?

It does not scale to large-scale problems!

Still highly useful and competitive for small to medium sized problems.

We have developed a **new** technique that scales to **very large** problems.

Key innovations:

- Replace the GP with a matrix updated using fast Cholesky routines.
- Exploit a receding history of iterates and gradients akin to L-BFGS.
- An auxiliary variable Markov chain construction.



Training a deep CNN for MNIST data.



Logistic loss function with an L2 regularizer, gisette, 6 000 observations and 5 000 unknown variables.



Logistic loss function with an L2 regularizer, URL, 2 396 130 observations and 3 231 961 unknown variables.

Adrian Wills and Thomas B. Schön. Stochastic quasi-Newton with adaptive step lengths for large-scale problems. arXiv:1802.04310, February, 2018.

Snapshot 2 – GP-based nonlinear state space model

"Inspired by the Gaussian process, enabled by the particle filter"

$$\begin{aligned} x_{t+1} &= f(x_t) + w_t, \qquad \text{ s.t. } f(x) \sim \mathcal{GP}(0, \kappa_{\eta, f}(x, x')), \\ y_t &= g(x_t) + e_t, \qquad \text{ s.t. } g(x) \sim \mathcal{GP}(0, \kappa_{\eta, g}(x, x')). \end{aligned}$$

Results in a **flexible** non-parametric model where the GP prior takes on the **role of a regularizer**.

We can now find the posterior distribution

 $p(f, g, Q, R, \eta | y_{1:T}),$

via some approximation (we use particle MCMC).

Frigola, Roger, Fredrik Lindsten, Thomas B. Schön, and Carl Rasmussen. Bayesian inference and learning in Gaussian process state-space models with particle MCMC. In Advances in Neural Information Processing Systems (NIPS), 2013.

Andreas Svensson and Thomas B. Schön. A flexible state space model for learning nonlinear dynamical systems, Automatica, 80:189-199, June, 2017.

Aim: Automate probabilistic modeling of dynamical systems (and their surroundings) via a formally defined **probabilistic modeling language**.



Keep the model and the learning algorithms separated.

Create a market place for SMC-based learning algorithms (think CVX).

Birch — Our prototype probabilistic programming language.

Lawrence M. Murray, Daniel Lundén, Jan Kudlicka, David Broman and Thomas B. Schön. Delayed sampling and automatic Rao-Blackwellization of probabilistic programs. In Proceedings of the 21st International Conference on Artificial Intelligence and Statistics (AISTATS), Lanzarote, Spain, April, 2018.

Birch - our prototype probabilistic programming language

- 1. The basic idea of **probabilistic programming** is to equate probabilistic models with the programs that implement them.
- 2. Just as we can think of doing inference over models, we can think of doing inference over programs.

The particular PPL used here is **Birch**, which is currently being developed at Uppsala University.

Probabilistic and object-oriented language.

An early pre-release of Birch is available

birch-lang.org

Constructing an artificial sequence of intermediate target distributions for an SMC sampler is a powerful (**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. Journal of Computational and Graphical Statistics (JCGS), 2017. 39/41

Snapshot 5 – Spatio-temporal modelling

Problem: predicting **spatio-temporal** processes with temporal patterns varying across spatial regions when data is obtained as a **stream**.

A **localized** spatio-temporal covariance model.



The predictor can be updated sequentially with each new data point.

Muhammad Osama, Dave Zachariah and Thomas B. Schön. Learning localized spatio-temporal models from streaming data. In Proceedings of the 35th International Conference on Machine Learning (ICML), Stockholm, Sweden, July, 2018.

Conclusion

Probabilistic modelling of nonlinear dynamical systems



SMC provide approximate solutions to **integration** problems where there is a **sequential structure** present.

Stochastic optimization:

- Non-standard interpretation of quasi-Newton.
- Represent the Hessian using a Gaussian process.
- We can scale up to larg(er) problems.