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Learning dynamical systems using SMC

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Nonlinear state space model (SSM)

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.

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

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**.

Three different representations of the SSM

Three alternative representations, using

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

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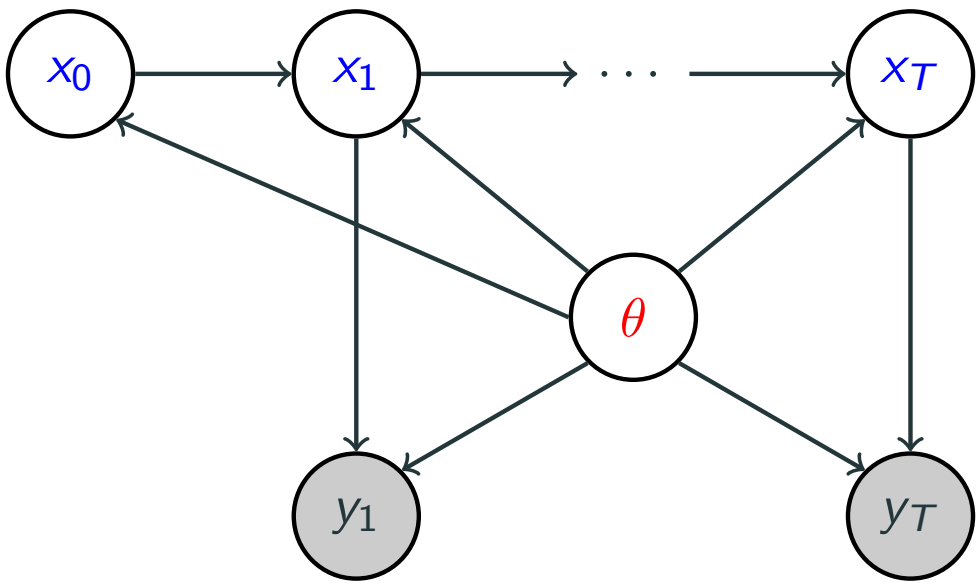
1. Representing the SSM using a graphical model:



Representations using distributions or probabilistic programs

2. Representation using probability distributions

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

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3. Representing the SSM using a probabilistic program

x[1] ∼ Gaussian(0.0, 1.0);	$p(x_1)$
y[1] ∼ Gaussian(x[1], 1.0);	$p(y_1 \mid x_1)$
for (t in 2..T) {	
x[t] ∼ Gaussian(a*x[t - 1], 1.0);	$p(x_t \mid x_{t-1})$
y[t] ∼ Gaussian(x[t], 1.0);	$p(y_t \mid x_t)$
}	

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

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

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

$$\widehat{\theta} = \arg\max_{\theta \in \Theta} p(y_{1:T} \mid \theta).$$

Central object – the likelihood

The likelihood is computed by marginalizing

$$p(x_{0:T}, y_{1:T} \mid \theta) = p(x_0 \mid \theta) \prod_{t=1}^{T} p(y_t \mid x_t, \theta) \prod_{t=1}^{T} p(x_t \mid x_{t-1}, \theta),$$

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

$$p(y_{1:T} \mid \theta) = \int p(x_{0:T}, y_{1:T} \mid \theta) \mathrm{d}x_{0:T}.$$

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

Equivalently we have

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

TS, 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.

State inference – nonlinear filtering problem

The nonlinear filtering problem involves the **measurement update**

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

and the **time update**

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

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 above.

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

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

$$x_t = f(x_{t-1}) + v_t,$$
$$y_t = g(x_t) + e_t,$$

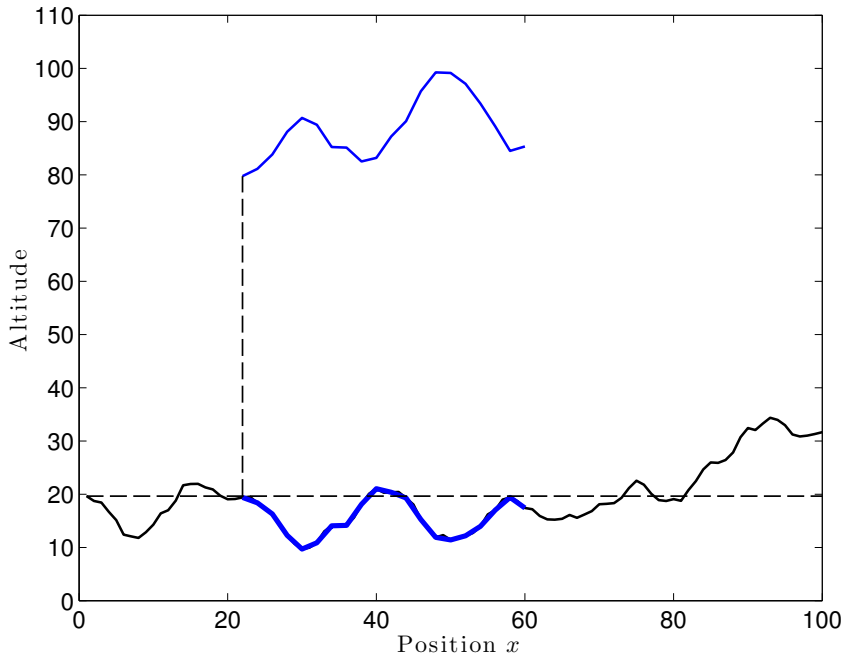
by maintaining an empirical distribution made up of N samples (particles) $\{x_t^i\}_{i=1}^N$ and the corresponding weights $\{w_t^i\}_{i=1}^N$

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

Particle filter – introductory example (I/II)

Consider a toy 1D localization problem.

Data



Model

Dynamic model:

$$x_{t+1} = x_t + u_t + v_t,$$

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

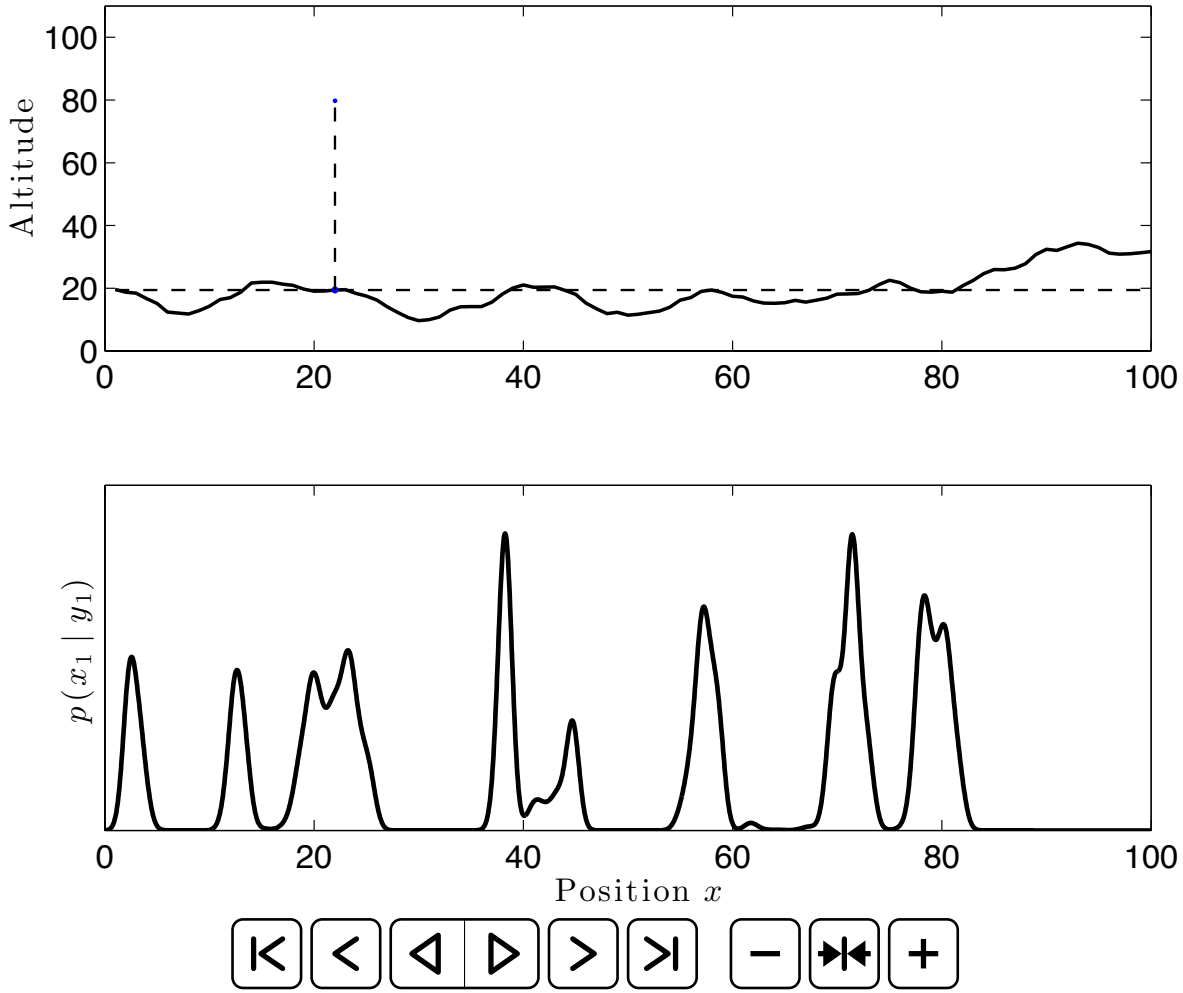
Measurements:

$$y_t = h(x_t) + e_t.$$

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 $p(x_t \mid y_{1:t})$.

Particle filter – introductory example (II/II)



Highlights two **key capabilities** of the PF:

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

Sequential Monte Carlo – particle filter

SMC = sequential importance sampling + resampling

1. **Propagation:** $x_t^i \sim p(x_t \mid x_{1:t-1}^{a_t^i})$ and $x_{1:t}^i = \{x_{1:t-1}^{a_t^i}, x_t^i\}$.
2. **Weighting:** $\bar{w}_t^i = W_t(x_t^i) = p(y_t \mid x_t^i)$.
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.

Application – indoor localization

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

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, TS and Simo Särkkä. **Modeling and interpolation of the ambient magnetic field by Gaussian processes.** *IEEE Transactions on Robotics*, 34(4):1112–1127 2018.

Particle MCMC = SMC + MCMC

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 $\mathcal{X}^T$.

A bit more precise: Construct a Markov chain with $p(\theta, x_{1:T} \mid y_{1:T})$ (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.

Sequential Monte Carlo (SMC) – abstract

The distribution of interest $\pi(x)$ is called **target distribution**.

(Abstract) problem formulation: **Sample from a sequence** of probability distributions $\{\pi_t(x_{0:t})\}_{t\geq 1}$ defined on a sequence of spaces of increasing dimension, where

$$\pi_t(x_{0:t}) = \frac{\widetilde{\pi}_t(x_{0:t})}{Z_t},$$

such that $\widetilde{\pi}_t(x_t) : \mathcal{X}^t \to \mathbb{R}^+$ is known point-wise and $Z_t = \int \pi(x_{0:t})\mathrm{d}x_{0:t}$ is often computationally challenging.

1. Approximate the normalizing constant Z_t.
2. Approximate $\pi_t(x_t)$ and compute integrals $\int \varphi(x_t)\pi_t(x_t)\mathrm{d}x_t$.

Important question: How general is this formulation?

Automation via a probabilistic programming language

1. Basic idea of **probabilistic programming**: equate probabilistic models with the computer programs that implement them.
2. Just as we can think of doing inference over models, we can now think of doing **inference over programs**.

Provides a means for **separating** the model and the learning algorithms.

We are developing a probabilistic programming language called **Birch**

`birch-lang.org`

Lawrence Murray and TS. **Automated learning with a probabilistic programming language: Birch.** *Annual Reviews in Control*, 2018. (Accepted for publication)

Outline

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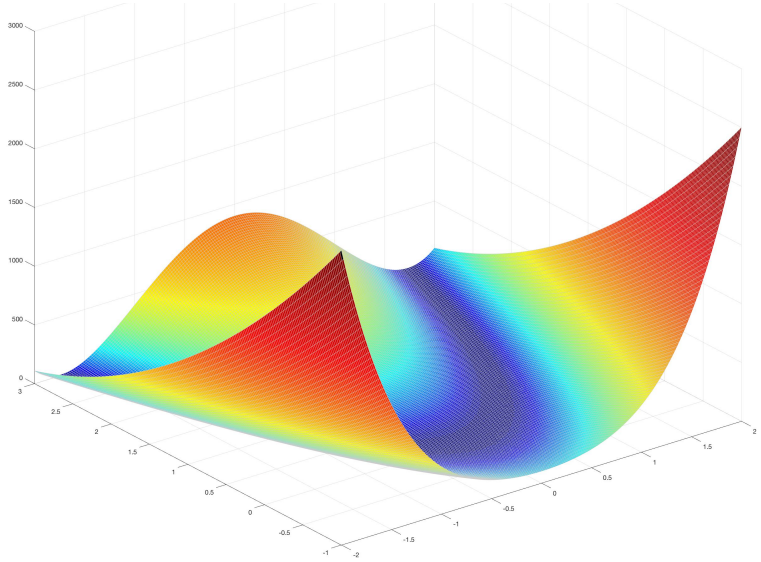
1. Probabilistic modelling of dynamical systems
2. Sequential Monte Carlo (SMC)
3. **Stochastic optimization**
4. Some ongoing research snapshots (if there is time)

Intuitive preview example – Rosenbrock's banana function

Let $f(\theta) = (1 - \theta_1)^2 + 100(\theta_2 - \theta_1^2)^2$.

Deterministic problem

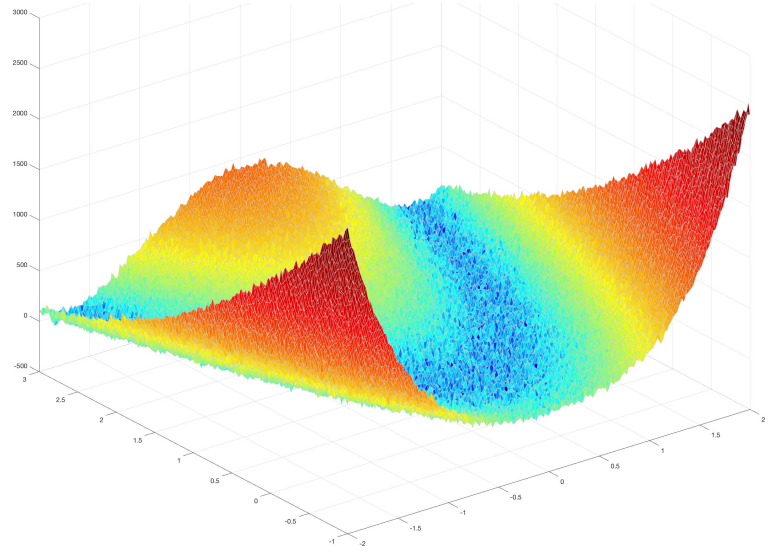
$$\min_{\theta} f(\theta)$$



Stochastic problem

$$\min_{\theta} f(\theta)$$

when we only have access to noisy versions of the cost function ($\widetilde{f}(\theta) = f(\theta) + e$, $e = \mathcal{N}(0, 30^2)$) and its noisy gradients.



Quasi-Newton – A non-standard take

Our problem is of the form

$$\min_{\theta} f(\theta)$$

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

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

$$g(\theta_k) = \nabla f(\theta)\big|_{\theta=\theta_k}, \qquad H(\theta_k) = \nabla^2 f(\theta)\big|_{\theta=\theta_k}, \qquad \delta = \theta - \theta_k.$$

We have measurements of

- the cost function $f_k = f(\theta_k)$,
- and its gradient $g_k = g(\theta_k)$.

Question: How do we update the Hessian model?

Useful basic facts

Line segment connecting two adjacent iterates θ_k and θ_{k+1}:

$$r_k(\tau) = \theta_k + \tau(\theta_{k+1} - \theta_k), \qquad \tau \in [0, 1].$$

---

1. The **fundamental theorem of calculus** states that

$$\int_0^1 \frac{\partial}{\partial \tau} \nabla f(r_k(\tau)) \mathrm{d}\tau = \nabla f(r_k(1)) - \nabla f(r_k(0)) = \underbrace{\nabla f(\theta_{k+1})}_{g_{k+1}} - \underbrace{\nabla f(\theta_k)}_{g_k}.$$

2. The **chain rule** tells us that

$$\frac{\partial}{\partial \tau} \nabla f(r_k(\tau)) = \nabla^2 f(r_k(\tau)) \frac{\partial r_k(\tau)}{\partial \tau} = \nabla^2 f(r_k(\tau))(\theta_{k+1} - \theta_k).$$

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

Result – the quasi-Newton integral

With the definitions $y_k \triangleq g_{k+1} - g_k$ and $s_k \triangleq \theta_{k+1} - \theta_k$ 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

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

implying the following approximation of the integral (**secant condition**)

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

Find H_{k+1} by **regularizing** H:

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

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

Solution 2 – use a flexible nonlinear model

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?

Resulting stochastic qN integral and Hessian model

Summary: resulting stochastic quasi-Newton integral:

$$y_k = D_k \int_0^1 \widetilde{B}(r_k(\tau))\mathrm{d}\tau + e_k,$$

with the following model for the Hessian

$$\widetilde{B}(\theta) \sim \mathcal{GP}(\mu(\theta), \kappa(\theta, \theta')).$$

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 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
   $$\theta_{k+1} = \theta_k + \alpha_k p_k.$$
   (c) **Update the Hessian model** (tailored GP regression).
   (d) Set $k := k + 1$.
3. **end while**

Curvature information is useful also for stochastic optimization.

ex) Simple linear toy problem

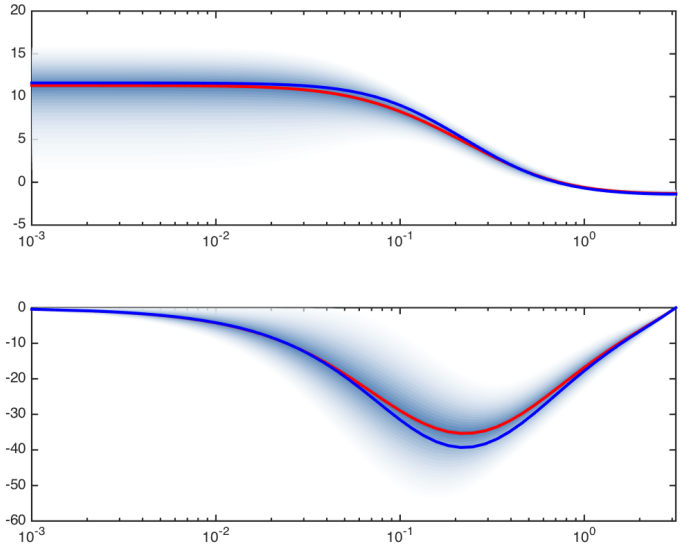
Identify the parameters $\theta = (a, c, q, r)^{\mathsf{T}}$ in

$$x_{t+1} = a x_t + w_t, \qquad w_t \sim \mathcal{N}(0, q^2),$$
$$y_t = c x_t + e_t, \qquad e_t \sim \mathcal{N}(0, r^2).$$

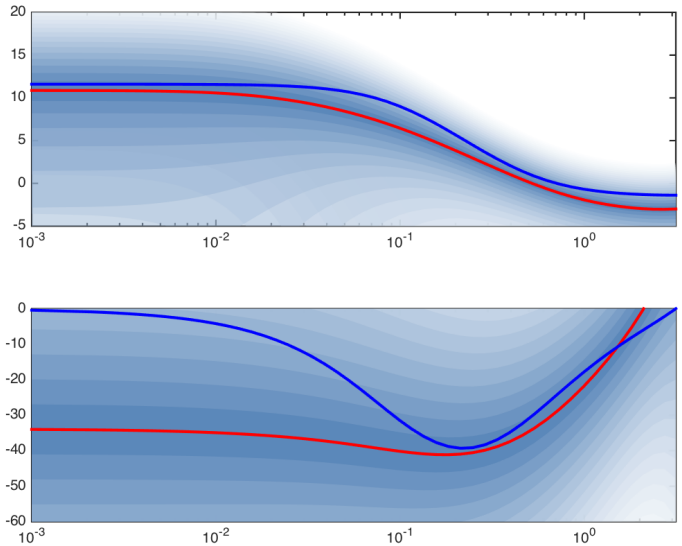
Observations:

- The likelihood $L(\theta) = p(y_{1:T} \mid \theta)$ and its gradient $\nabla_\theta L(\theta)$ 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



Both alg. in the noise-free case.



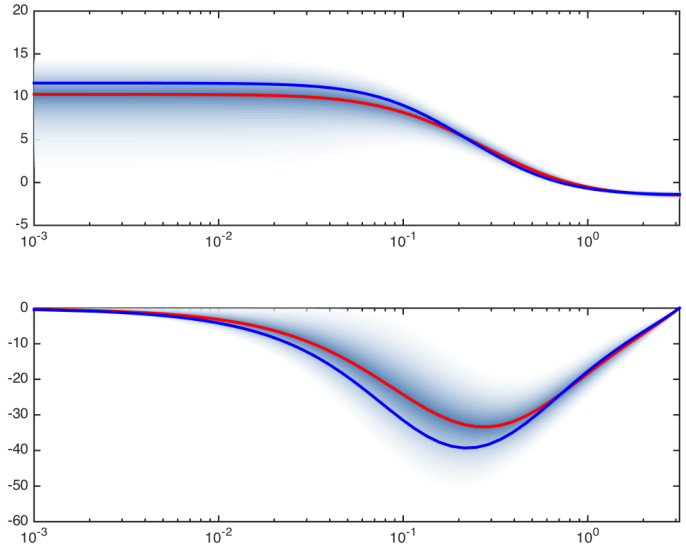
Classical BFGS alg. for noisy observations of $L(\theta)$ and $\nabla L(\theta)$.

100 independent datasets.

Clear blue – True system

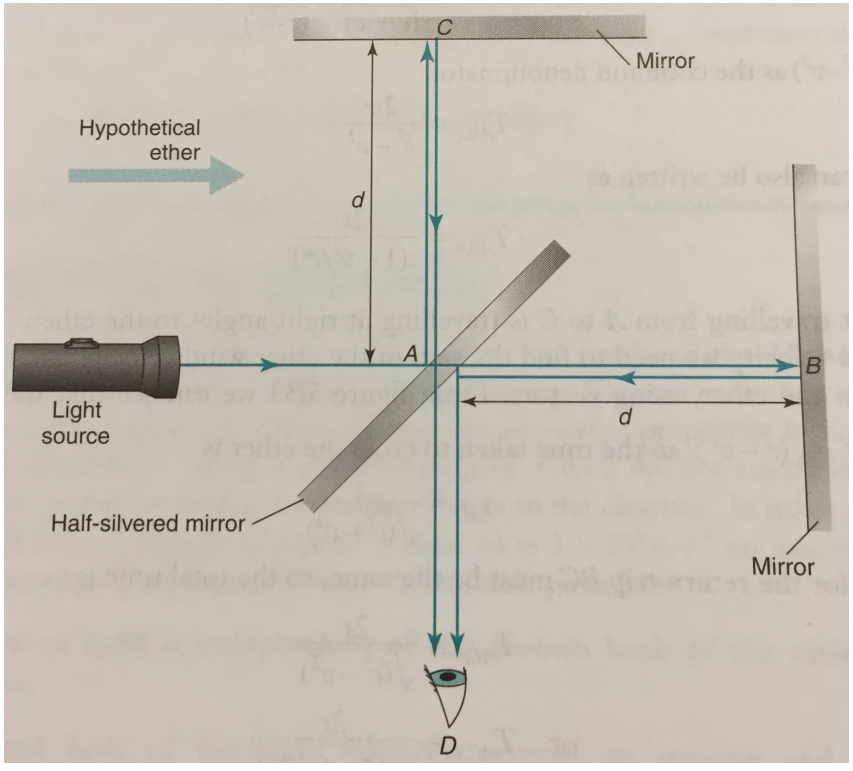
Red – Mean value of estimate

Shaded blue – individual results



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

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

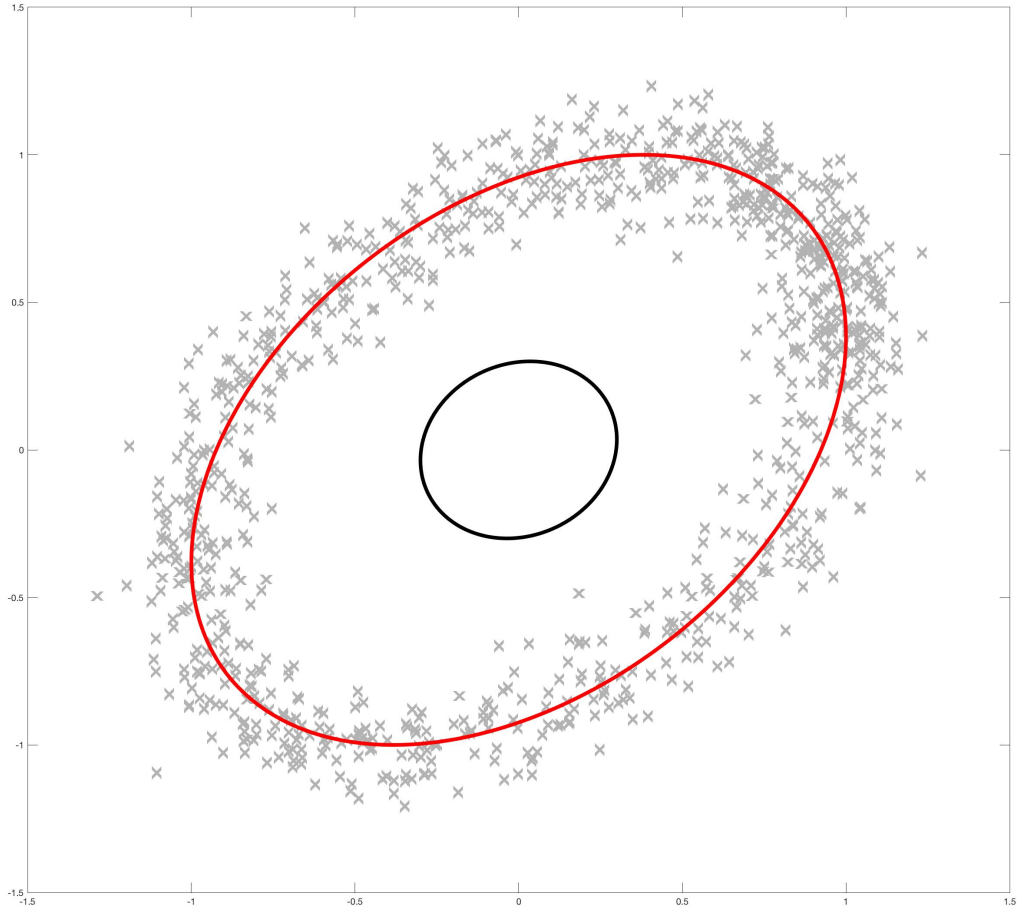
$$y_1 = \alpha_0 + \alpha_1 \cos(\kappa p) + e_1, \qquad e_1 \sim \mathcal{N}(0, \sigma^2),$$
$$y_2 = \beta_0 + \beta_1 \sin(\kappa p + \gamma) + e_2, \qquad e_2 \sim \mathcal{N}(0, \sigma^2).$$

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

Snapshot – Scaling up to large(r) problems

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

It **does not** scale to large-scale problems!

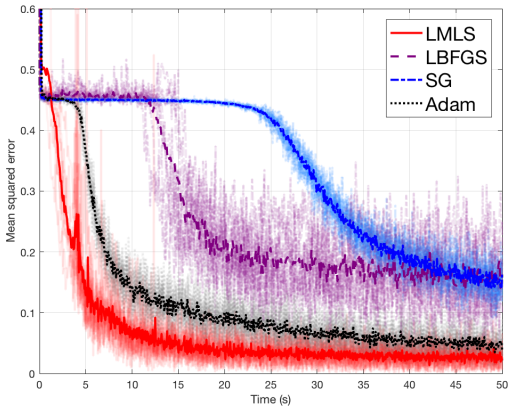
Still highly useful and competitive for **small to medium** sized problems.

We have developed a **new** technique that scales to **large(r)** problems.

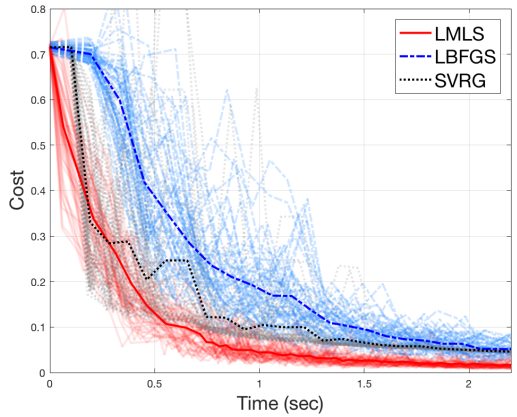
Snapshot – Scaling up to large(r) problems

Key innovations:

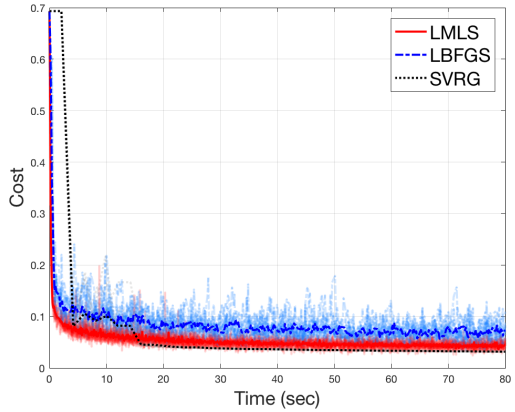
- Replace the GP with a matrix updated using fast Cholesky routines.
- Exploit a receding history of iterates and gradients akin to L-BFGS.
- Same stochastic line search applicable.



Training a deep CNN for MNIST data.



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

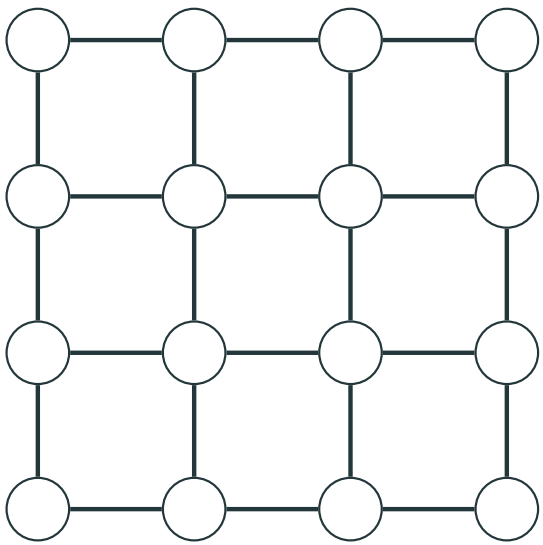


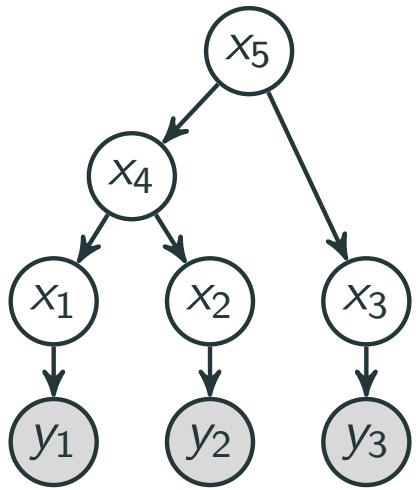
Logistic loss function with an L2 regularizer, `URL`, 2 396 130 observations and 3 231 961 unknown variables.

Adrian G. Wills, Carl Jidling and TS. **A fast quasi-Newton-type method for large-scale stochastic optimisation**. *arXiv:1810.01269*, September, 2018.

Snapshot – The nonlinear SSM is just a special case...

Constructing an artificial sequence of intermediate target distributions for an SMC sampler is a powerful (**quite possibly underutilized**) idea.





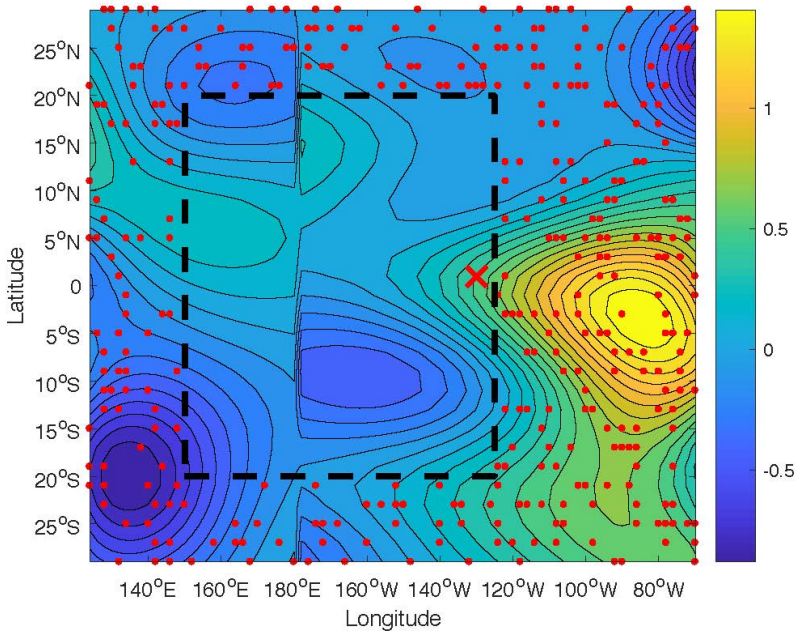
Christian A. Naesseth, Fredrik Lindsten and TS, **Sequential Monte Carlo methods for graphical models**. *Advances in Neural Information Processing Systems (NIPS)* 27, Montreal, Canada, December, 2014.

Fredrik Lindsten, Adam M. Johansen, Christian A. Naesseth, Bonnie Kirkpatrick, TS, John Aston and Alexandre Bouchard-Côté. **Divide-and-Conquer with Sequential Monte Carlo**. *Journal of Computational and Graphical Statistics (JCGS)*, 2017.

Snapshot – 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.

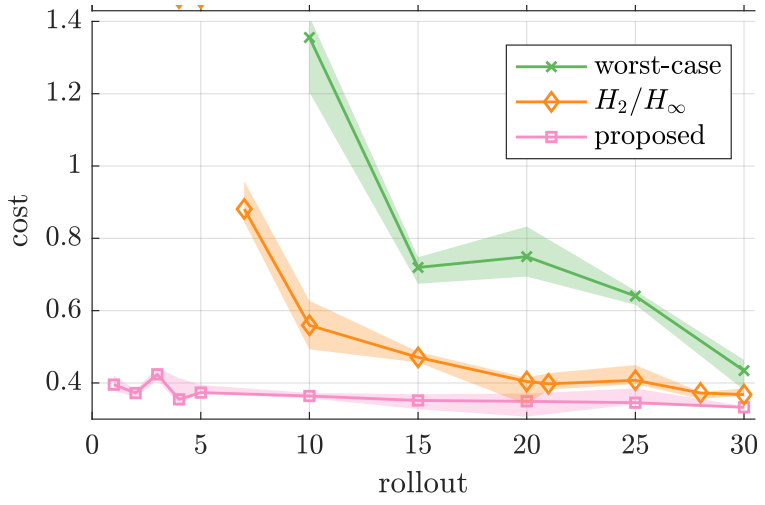
Muhammad Osama, Dave Zachariah and TS. **Learning localized spatio-temporal models from streaming data.** In *Proceedings of the 35th International Conference on Machine Learning (ICML)*, Stockholm, Sweden, July, 2018.

Snapshot – Using probabilistic models for control

Problem: Decision making for dynamical systems (control) in the presence of uncertainty.

Intersection of reinforcement learning (RL) and robust control (RC).

Problem: Given observations from an unknown dynamical system, we seek a policy to **optimize the expected cost** (as in RL), subject to certain **robust stability guarantees** (as in RC).



Jack Umenberger and TS. **Learning convex bounds for linear quadratic control policy synthesis.** *In Neural Information Processing Systems (NIPS)*, Montréal, Canada, December 2018.

Conclusion

Probabilistic modelling of nonlinear dynamical systems

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

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.

Looking for new PhD students

We are looking for 2 PhD students:

1. Probabilistic programming deployment of deep learning
2. Causality

Link to the opening is available on my website.