Newton-based maximum likelihood estimation in nonlinear SSMs SysId conference 2015, Beijing

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$$y_t = g_{\theta}(x_t, e_t),$$



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 $\begin{array}{l} x_t: \text{ latent state variables at time } t \\ y_t: \text{ measurements at time } t \\ f_{\theta}(\cdot), g_{\theta}(\cdot): \text{ (nonlinear) dynamic and measurement model} \end{array}$



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 $f_{\theta}(\cdot), g_{\theta}(\cdot)$: (nonlinear) dynamic and measurement model θ : parameters

 v_t, e_t : process and measurement noise



Maximum likelihood (ML) estimates of parameters in nonlinear SSMs

$$\widehat{\theta}_{\mathsf{ML}} = \operatorname*{arg\,max}_{\theta} \, \ell_{\theta}(y_{1:N})$$



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Maximum likelihood (ML) estimates of parameters in nonlinear SSMs

$$\widehat{ heta}_{\mathsf{ML}} = rg\max_{ heta} \, \ell_{ heta}(y_{1:N})$$

 $\widehat{ heta}_{ML}$: ML estimate of heta $\ell_{ heta}(y_{1:N})$: log-likelihood of the measurements $y_{1:N}$



Estimating $\boldsymbol{\theta}$ using Newton methods. Iteratively update:

$$\theta_{k+1} = \theta_k - \varepsilon_k \Big[\mathcal{H}(\theta_k) \Big]^{-1} \Big[\mathcal{G}(\theta_k) \Big],$$



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 $\begin{aligned} \mathcal{G}(\theta_k): \text{ gradient of } \ell_{\theta}(y_{1:N}) \\ \mathcal{H}(\theta_k): \text{ Hessian of } \ell_{\theta}(y_{1:N}) \\ \boldsymbol{\varepsilon}_k: \text{ Step size at iteration } k \end{aligned}$



Problem description

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- \Rightarrow Approximations are needed.



- Use Fisher's identity to estimate the gradient and Hessian / Extend the approach from Segal and Weinstein (1989)¹ to nonlinear SSMs.
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 - We explore two approximation methods: based on *linearization* and based on *sampling*.
- Show the workings of the methods on simulated data from two simple nonlinear SSMs.



$$\begin{aligned} \mathcal{G}(\theta_k) &= \frac{\partial}{\partial \theta} \ell_{\theta}(y_{1:N}) \big|_{\theta = \theta_k} \\ &= \int \frac{\partial}{\partial \theta} \log p_{\theta}(x_{1:N}, y_{1:N}) \big|_{\theta = \theta_k} p_{\theta}(x_{1:N} | y_{1:N}) \, \mathrm{d}x_{1:N} \end{aligned}$$



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$$p_{\theta}(x_{1:N}, y_{1:N}) = p_{\theta}(x_1) \prod_{t=1}^{N-1} f_{\theta}(x_{t+1}|x_t) \prod_{t=1}^{N} g_{\theta}(y_t|x_t),$$



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Estimate the two-step joint smoothing distribution!



$$\begin{aligned} \mathcal{G}(\theta_k) &= \frac{\partial}{\partial \theta} \ell_{\theta}(y_{1:N}) \big|_{\theta = \theta_k} \\ &= \sum_{t=1}^N \int \xi_{\theta_k}(x_{t+1:t}) p_{\theta_k}(x_{t+1:t} | y_{1:N}) \, \mathrm{d}x_{t+1:t} \triangleq \sum_{t=1}^N \mathcal{G}_t(\theta_k) \\ \widehat{\mathcal{H}}(\theta_k) &= \frac{1}{N} \Big[\mathcal{G}(\theta_k) \Big] \Big[\mathcal{G}(\theta_k) \Big]^\top - \sum_{t=1}^N \Big[\mathcal{G}_t(\theta_k) \Big] \Big[\mathcal{G}_t(\theta_k) \Big]^\top \end{aligned}$$

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1. Set k = 0

2. while exit condition is not satisfied do

- 1. Run an algorithm to estimate the log-likelihood $\hat{\ell}(\theta_k)$, its gradient $\hat{\mathcal{G}}(\theta_k)$ and its Hessian $\hat{\mathcal{H}}(\theta_k)$.
- 2. Determine ε_k .
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end while

3. Set $\widehat{\theta}_{ML} = \theta_k$.



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Linearization approximation

- Use extended Kalman filter to estimate $\widehat{\ell}(\theta_k)$.
- Compute the smoothed state estimates and covariances by solving the optimization problem

$$\widehat{x}_{t|N} = \underset{x_{1:N}}{\operatorname{arg\,max}} p_{\theta_k}(x_{1:N}, y_{1:N}).$$

using a standard Gauss-Newton solver.



Fixed lag smoother	Forward filter backward simu-
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Assumes that the SSM forgets about its past within a few time	Can be seen as the particle ap- proximation of the Rauch-Tung-
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More information: Dahlin, J. (2014). Sequential	More information: Lindsten, F. and Schön, T. B.
Monte Carlo for inference in nonlinear state space	(2013). Backward simulation methods for Monte
models. Licentiate's thesis no. 1652, Linköping Uni-	Carlo statistical inference. In Foundations and
versity, Linköping, Sweden.	Trends in Machine Learning, volume 6, 1–143.



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Estimate $\widehat{\ell}(\theta_k)$ using an EKF. Estimate $\widehat{\mathcal{G}}(\theta_k), \widehat{\mathcal{H}}(\theta_k)$ using Gauss- Newton optimization.	Estimate $\widehat{\mathcal{G}}(\theta_k), \widehat{\mathcal{H}}(\theta_k)$ using a particle smoother.		



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Newton optimization.	smoother.		
Determine ε_k using a line search.	Use a pre-defined schedule for ε_k .		

Simulation results: SSM1 1000 data points, 100 data sets

$$x_{t+1} = \arctan x_t + v_t,$$

$$y_t = \theta_1 x_t + \theta_2 + e_t,$$

$$v_t \sim \mathcal{N}(0, 1),$$

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 $1\,000$ data points, 100 data sets

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Parameters only in the linear part of the SSM.

 $\Rightarrow\,$ The linearization approach works very well.



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Alg.	Bias ($\cdot 10^{-4}$)		MSE ($\cdot 10^{-4}$)	
	θ_1	θ_2	θ_1	θ_2
Linearization	10	10	1	10
Sampling (FL)	38	-214	2	16
Sampling (FFBSi)	31	53	1	11



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Trace plot





Simulation results: SSM2 1000 data points, 100 data sets

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Parameters also in the nonlinear part of the SSM.

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- We determine the gradient and Hessian of the log-likelihood using Fisher's identity in combination with an algorithm to obtain smoothed state estimates.
- We approximate the log-likelihood and its gradient and Hessian using *linearizations* and using *sampling methods*.
- The *linearization approach* is computationally cheap. However, the quality of its estimates highly depends on the structure of the SSM.





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For more information: Manon Kok, Johan Dahlin, Thomas B. Schön and Adrian Wills, Newton-based maximum likelihood estimation in nonlinear state space models. Proceedings of the 17th IFAC Symposium on System Identification, Beijing, China, October 2015. Source code, data, slides and paper online on http://users.isy.liu.se/en/rt/manko/research.html



Thank you for your attention!

Questions?

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Vetenskapsrådet

