Bayesian model comparison with the Hyvärinen score

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Setting and examples

Goal: compare models in a Bayesian framework

- Given T observations $Y_{1:T} = (Y_1, ..., Y_T) \in (\mathbb{R}^{d_y})^T$.
- We want to compare candidate models from a finite set $\{M_1, ..., M_q\}$.
- Each model M_j is a collection of distributions $p_j(dy_{1:T}|\theta_j)$ parametrized by $\theta_j \in \mathbb{T}_j$ with a prior distribution $p_j(d\theta_j)$ on the parameter.
- We are interested in settings where the prior may be vague or improper.

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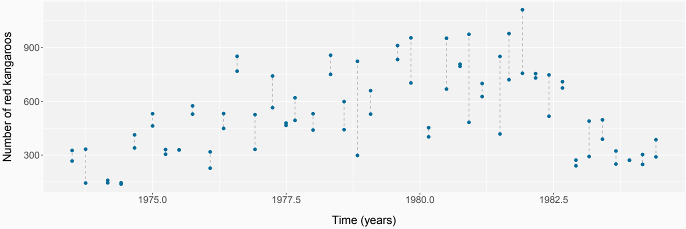
- **Example 1**. Normal i.i.d. models (*O'Hagan, 1995*)

Model 1	Model 2
$Y_1, \ldots, Y_T \mid \theta_1 \overset{\text{i.i.d.}}{\sim} \mathcal{N}(\theta_1, 1)$	$Y_1, \ldots, Y_T \mid \theta_2 \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, \theta_2)$
$\theta_1 \sim \mathcal{N}(0, \sigma_0^2)$	$\theta_2 \sim \text{Inv-}\chi^2(\nu_0, s_0^2)$

with known hyperparameters $\sigma_0 > 0$, $\nu_0 > 0$, and $s_0 > 0$.

What kind of models ? i.i.d. models, state-space models, ...

- **Example 2.** Population dynamics of red kangaroos (*Knape & de Valpine, 2012*)



Model 1	Model 2	Model 3
Given parameters (b,r,σ,τ):	Given parameters (r,σ,τ):	Given parameters (σ,τ):
$X_1 \sim \mathrm{LN}(0,5)$	$X_1 \sim \mathrm{LN}(0,5)$	$X_1 \sim \mathrm{LN}(0,5)$
$dX_t/X_t = (r - bX_t + \frac{\sigma^2}{2})\,dt + \sigma dW_t$	$dX_t/X_t = (r + \frac{\sigma^2}{2})\,dt + \sigma dW_t$	$dX_t/X_t = (\frac{\sigma^2}{2})\,dt + \sigma dW_t$
$Y_{1,t}\,,\,Y_{2,t} \mid X_t \overset{\text{i.i.d.}}{\sim} \mathrm{NB}(X_t, X_t + \tau X_t^2)$	$Y_{1,t}\,,\,Y_{2,t} \mid X_t \overset{\text{i.i.d.}}{\sim} \mathrm{NB}(X_t, X_t + \tau X_t^2)$	$Y_{1,t}\,,\,Y_{2,t} \mid X_t \overset{\text{i.i.d.}}{\sim} \mathrm{NB}(X_t, X_t + \tau X_t^2)$
with independent priors:	with independent priors:	with independent priors:
$b, \sigma, \tau \sim \mathrm{Unif}(0,10)$	$\sigma, \tau \sim \mathrm{Unif}(0,10)$	$\sigma, \tau \sim \mathrm{Unif}(0,10)$
$r \sim \mathrm{Unif}(-10,10)$	$r \sim \mathrm{Unif}(-10,10)$	

Why not use Bayes factors ?

Limitations of Bayes factors: sensitivity to vague priors

- Bayes factors favor the model M_j with the largest *evidence*

$$p_j(y_{1:T}) = \int p_j(y_{1:T}|\theta_j)\, p_j(\theta_j)\, d\theta_j$$

(a.k.a. the *marginal likelihood* of M_j)

Sensitivity to the choice of prior

- The evidence of any model can be made arbitrarily small by making the prior arbitrarily vague, regardless of the sample size.
- Bayes factors do not allow for improper priors.

Yet, vague or improper priors often stem from reasonable approaches
(genuine non-informativeness, Jeffreys prior, …)

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A new criterion: the Hyvärinen score

Bayes factors relate to a particular choice of scoring rule

- Bayes factors favor the model minimizing $-\log p(y_{1:T})$ or equivalently

$$\sum_{t=1}^{T} -\log p(y_t|y_{1:t-1})$$

- This is a particular case of a more general decision rule that favors the model with the smallest prequential score

$$\sum_{t=1}^{T} \mathcal{S}\left(y_t,\, p(dy_t|y_{1:t-1})\right)$$

with the choice of scoring rule $\mathcal{S}(y, p) = -\log p(y)$ called the log-score

Key idea: use the Hyvärinen score (H-score) instead (*Dawid & Musio, 2015*)

$$\sum_{t=1}^{T} \mathcal{H}\left(y_t,\, p(dy_t|y_{1:t-1})\right)$$

with $\mathcal{H}(y, p) = 2\,\Delta \log p(y) + \|\nabla \log p(y)\|^2$, where the Laplacian Δ and the gradient ∇ are taken with respect to the observation y

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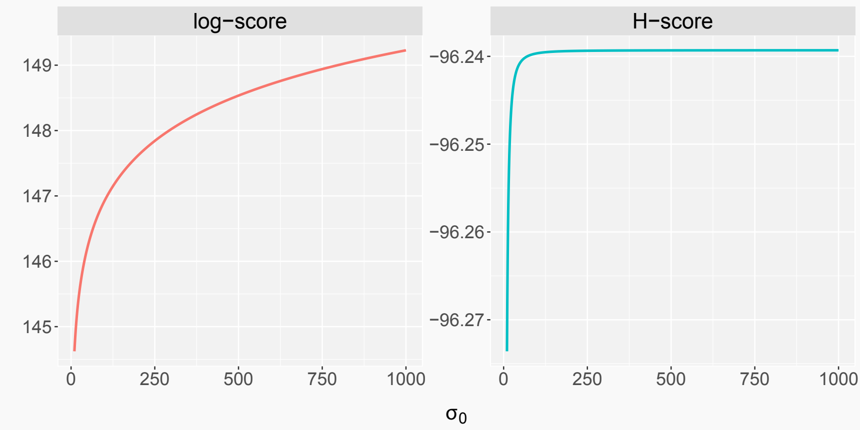
H-scores are robust to prior vagueness

- **Example**. Given i.i.d. realizations $y_1, \ldots, y_{100}$ from a $\mathcal{N}(0,1)$, consider the model describing $Y_1, \ldots, Y_{100} \mid \mu \overset{\text{i.i.d.}}{\sim} \mathcal{N}(\mu, 1)$ with prior $\mu \sim \mathcal{N}(0, \sigma_0^2)$.



Using H-scores is principled and justified non-asymptotically

- For univariate observations, the H-score can be written explicitly as

$$\sum_{t=1}^{T}\left(2\,\frac{\partial^2 \log p(y_t|y_{1:t-1})}{\partial {y_t}^2}+\left(\frac{\partial \log p(y_t|y_{1:t-1})}{\partial y_t}\right)^2\right)$$

- Similarly to the log-score, the H-score is
  - Proper: the expected loss $\mathbb{E}_\star\left[\mathcal{H}(Y, p)\right]$ under $Y \sim p_\star$ is minimized at $p = p_\star$
  - m-local: $\mathcal{H}(y, p)$ is a function of y and $p(y), p'(y), \ldots, p^{(m)}(y) \quad$ (with $m = 2$)
- The H-score has the additional advantage of being 0-homogeneous
  - $\mathcal{H}(y, p)$ is unchanged when multiplying $p(y), p'(y), \ldots, p^{(m)}(y)$ by any $\lambda > 0$
- The H-score is the simplest scoring rule satisfying propriety, m-locality, and 0-homogeneity (*Parry, Dawid & Lauritzen, 2012*)
- It can be extended to discrete observations via finite differences, while preserving all the above properties (*Dawid, Parry & Lauritzen, 2012*)
- **But it involves derivatives of typically intractable predictive densities $p(y_t|y_{1:t-1})$ at every $t \in \{1, \ldots, T\}$. This calls for sequential estimation.**

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How to estimate H-scores ?

H-scores via SMC if likelihoods can be evaluated

- By differentiating under the integral sign, the H-score turns out to be

$$\sum_{t=1}^{T}\left(2\,\mathbb{E}_t\left[\frac{\partial^2 \log p(y_t|y_{1:t-1},\Theta)}{\partial y_t^2}+\left(\frac{\partial \log p(y_t|y_{1:t-1},\Theta)}{\partial y_t}\right)^2\right]-\left(\mathbb{E}_t\left[\frac{\partial \log p(y_t|y_{1:t-1},\Theta)}{\partial y_t}\right]\right)^2\right)$$

where $\mathbb{E}_t$ denotes posterior expectations with respect to $\Theta \sim p(d\theta|y_{1:t})$

Estimation using SMC (*Chopin, 2002; Del Moral, Doucet & Jasra, 2006*)

H-scores can be consistently estimated using standard SMC samplers, as long as one can evaluate the incremental likelihoods $p(y_t|y_{1:t-1},\Theta)$

- However, incremental likelihoods $p(y_t|y_{1:t-1},\Theta)$ are typically intractable for general state-space models.

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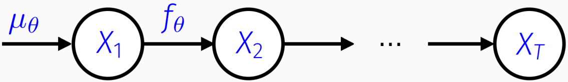
What is so challenging about state-space models ?



- Unobserved Markov chain of latent states $X_1, \ldots, X_T$ with

$$X_1 \sim \mu_\theta \quad \text{and} \quad X_t \,|\, X_{t-1} \sim f_\theta(\cdot|X_{t-1}) \quad \text{for } t \geq 2$$

- Observations $Y_1, \ldots, Y_T$ conditionally independent given $X_1, \ldots, X_T$ with

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The likelihood is generally intractable

$$p(y_{1:T}|\theta) = \int \mu_\theta(x_1) \prod_{t=2}^{T} f_\theta(x_t|x_{t-1}) \prod_{t=1}^{T} g_\theta(y_t|x_t)\, dx_{1:T}$$

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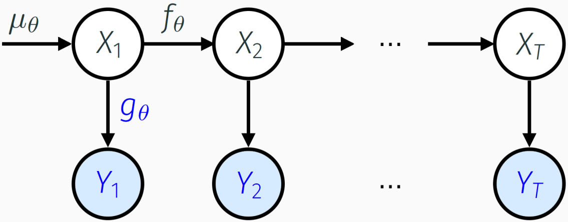

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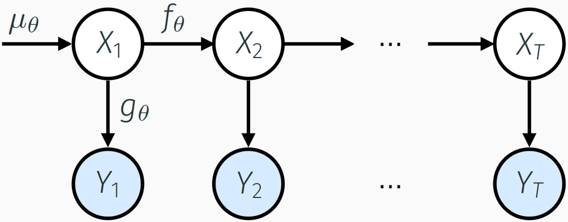

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H-scores via SMC^2 for general state-space models

- Under further integrability conditions, the H-score proves to equal

$$\sum_{t=1}^{T}\left(2\,\mathbb{E}_t\left[\frac{\partial^2 \log g_\Theta(y_t|X_t)}{\partial y_t^2}+\left(\frac{\partial \log g_\Theta(y_t|X_t)}{\partial y_t}\right)^2\right]-\left(\mathbb{E}_t\left[\frac{\partial \log g_\Theta(y_t|X_t)}{\partial y_t}\right]\right)^2\right)$$

where the expectations $\mathbb{E}_t$ are now with respect to the joint posterior distributions $(\Theta, X_t) \sim p(d\theta|y_{1:t})p(dx_t|y_{1:t},\theta)$

Estimation using SMC^2 (*Chopin, Jacob & Papaspiliopoulos, 2013*)

H-scores can be consistently estimated for state-space models, as long as one can simulate transitions from f_θ and evaluate g_θ

- SMC and SMC^2 can be used similarly in the case of discrete observations.

H-scores via SMC^2 for general state-space models

- Under further integrability conditions, the H-score proves to equal

$$\sum_{t=1}^{T}\left(2\,\mathbb{E}_t\left[\frac{\partial^2 \log g_\Theta(y_t|X_t)}{\partial y_t^2}+\left(\frac{\partial \log g_\Theta(y_t|X_t)}{\partial y_t}\right)^2\right]-\left(\mathbb{E}_t\left[\frac{\partial \log g_\Theta(y_t|X_t)}{\partial y_t}\right]\right)^2\right)$$

where the expectations $\mathbb{E}_t$ are now with respect to the joint posterior distributions $(\Theta, X_t) \sim p(d\theta|y_{1:t})p(dx_t|y_{1:t}, \theta)$

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Asymptotic guarantees

Consistency of the H-score for model selection

- Assume the true data generating process is $Y_1, \ldots, Y_T \overset{\text{i.i.d.}}{\sim} p_\star$
- Consider two non-nested i.i.d. models M_1 and M_2 with respective posterior distributions concentrating around $\theta_1^\star$ and $\theta_2^\star$. Let $p_{\theta_j^\star} = p_j(dy|\theta_j^\star)$
- Under regularity conditions, the H-scores $\mathcal{H}_T$ of M_1 and M_2 satisfy

$$\frac{1}{T}\Big(\mathcal{H}_T(M_2) - \mathcal{H}_T(M_1)\Big) \xrightarrow[T\to+\infty]{\mathbb{P}_\star - a.s.} \Delta(p_\star, M_2) - \Delta(p_\star, M_1)$$

where $\Delta(p_\star, M_j) = \mathbb{E}_\star[\mathcal{H}(Y, p_{\theta_j^\star})] - \mathbb{E}_\star[\mathcal{H}(Y, p_\star)]$
with $\Delta(p_\star, M_j) \geq 0$ and $\Delta(p_\star, M_j) = 0$ if and only if $p_{\theta_j^\star} = p_\star$

- By analogy, the log-Bayes factor of M_1 against M_2 satisfies

$$\frac{1}{T}\bigg(\Big(-\log p_2(Y_{1:T})\Big) - \Big(-\log p_1(Y_{1:T})\Big)\bigg) \xrightarrow[T\to+\infty]{\mathbb{P}_\star - a.s.} \mathrm{KL}(p_\star, M_2) - \mathrm{KL}(p_\star, M_1)$$

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- Similar results hold for dependent data and state-space models.

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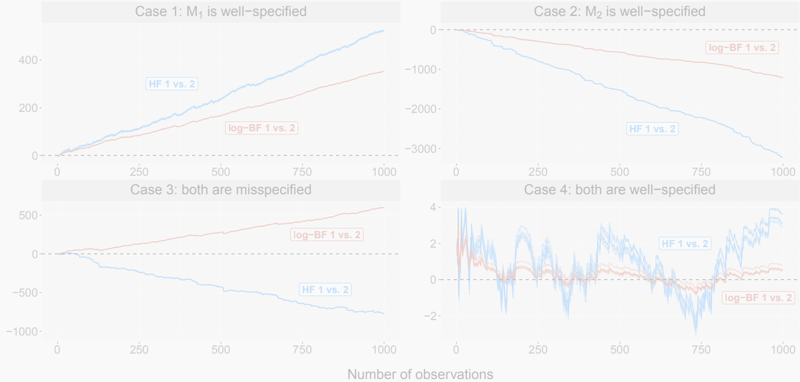
Illustration of consistency for i.i.d. models

- **Example 1**. Given simulated $y_1, \ldots, y_{1000} \sim \mathcal{N}(\mu_\star, \sigma_\star^2)$, we compare

$$M_1 : \quad Y_1, \ldots, Y_T \,|\, \theta_1 \overset{\text{i.i.d.}}{\sim} \mathcal{N}\left(\theta_1, 1\right), \quad \theta_1 \sim \mathcal{N}\left(0, 10\right)$$

$$M_2 : \quad Y_1, \ldots, Y_T \,|\, \theta_2 \overset{\text{i.i.d.}}{\sim} \mathcal{N}\left(0, \theta_2\right), \quad \theta_2 \sim \text{Inv-}\chi^2\left(0.1, 1\right)$$

in the following four cases $(\mu_\star, \sigma_\star^2) = (1,1), (0,5), (4,3), (0,1)$.



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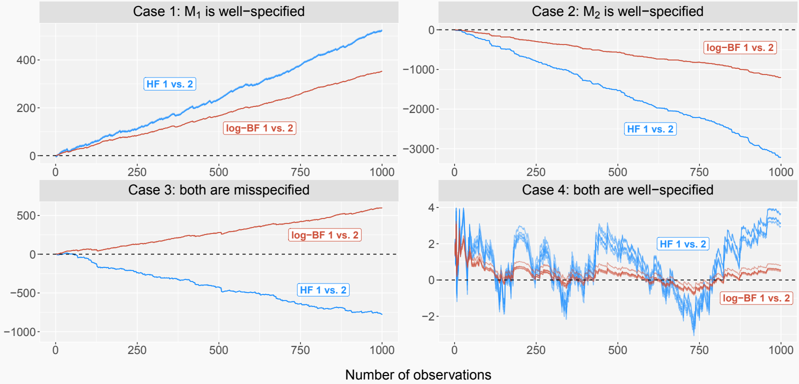
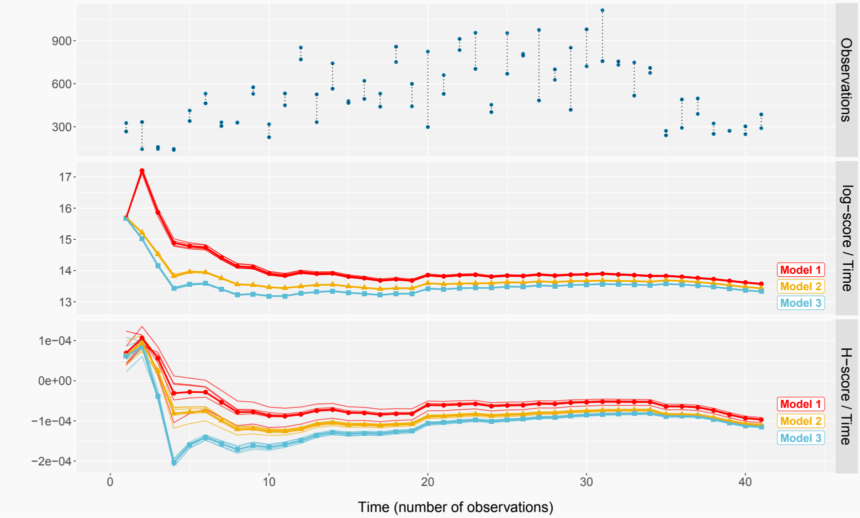


Applications and discussion

Jumping back to kangaroos

- **Example 2.** Population dynamics of red kangaroos (*Knape & de Valpine, 2012*)



Summary

Advantages of using the H-score

- Robust to prior vagueness and allows for improper priors
- Justified non-asymptotically and generally consistent asymptotically
- Can be estimated sequentially for a wide class of parametric models by using SMC methods

Limitations and avenues for future research

- Requires additional smoothness conditions on the densities
- Tends to require a larger number of particles than the log-evidence for accurate estimation via SMC methods
- Extension to nonparametric models ?

- More details in the manuscript: arxiv.org/pdf/1711.00136
- R package available at: github.com/pierrejacob/bayeshscore

Questions ?

References (1/2)

O. E. Barndorff-Nielsen and N. Shephard.
Non-Gaussian Ornstein–Uhlenbeck-based models and some of their uses in financial economics.
Journal of the Royal Statistical Society: Series B, 63(2):167––241, 2001.

N. Chopin.
A sequential particle filter method for static models.
89:539–552, 2002.

N. Chopin, P. E. Jacob, and O. Papaspiliopoulos.
SMC^2: an efficient algorithm for sequential analysis of state-space models.
Journal of the Royal Statistical Society, 75 (3):397–426, 2013.

A. P. Dawid, S. Lauritzen, and M. Parry.
Proper local scoring rules on discrete sample spaces.
The Annals of Statistics, 40 (1):593–608, 2012.

A. P. Dawid and M. Musio.
Bayesian model selection based on proper scoring rules.
Bayesian Analysis, 10 (2):479–499, 2015.

References (2/2)

P. Del Moral, A. Doucet, and A. Jasra.
Sequential Monte Carlo samplers.
Journal of the Royal Statistical Society: Series B (Statistical Methodology), 68(3):411–436, 2006.

J. Knape and P. D. Valpine.
Fitting complex population models by combining particle filters with markov chain monte carlo.
Ecology, 93 (2):256–263, 2012.

F. B. Lempers.
Posterior Probabilities of Alternative Linear Models.
Rotterdam University Press, 1971.

A. O'Hagan.
Fractional bayes factor for model comparison.
Journal of the Royal Statistical Society, 57 (1):99–138, 1995.

M. Parry, A. P. Dawid, and S. Lauritzen.
Proper local scoring rules.
The Annals of Statistics, 40 (1):561–592, 2012.

What kind of models ? i.i.d. models, state-space models, ...

- **Example 3.** Lévy-driven stochastic volatility models for log-returns of financial assets (*Barndorff-Nielsen & Shephard, 2001*)

Given parameters (λ, ξ, ω), generate random variables $(V_t, Z_t)_{t\geq 1}$ recursively as

$$\left.\begin{array}{c} k\sim\text{Poisson}(\lambda\xi^2/\omega^2)\,; \quad C_{1:k}\overset{\text{i.i.d.}}{\sim}\text{Unif}(t-1,t)\,; \quad E_{1:k}\overset{\text{i.i.d.}}{\sim}\text{Exp}(\xi/\omega^2)\,; \quad Z_0\sim\Gamma(\xi^2/\omega^2, \xi/\omega^2) \\ Z_t=e^{-\lambda}Z_{t-1}+\sum_{j=1}^{k} e^{-\lambda(t-C_j)}E_j\,; \quad V_t=\lambda^{-1}(Z_{t-1}-Z_t+\sum_{j=1}^{k} E_j) \end{array}\right\} \quad (⚙)$$

Model 1

Given parameters $(\lambda,\xi,\omega,\mu,\beta)$:

$$(V_t, Z_t) \sim (⚙)$$

$$X_t=(V_t, Z_t)$$

$$Y_t \mid X_t \sim \mathcal{N}(\mu+\beta V_t, V_t)$$

with independent priors:

$\lambda\sim\text{Exp}(1)$; $\xi, \omega^2\sim\text{Exp}(1/5)$; $\mu, \beta\sim\mathcal{N}(0,10)$

Model 2

Given parameters $(\lambda_1,\lambda_2,\text{w}_1,\text{w}_2,\xi,\omega,\mu,\beta)$:

$$(V_{1,t}, Z_{1,t}) \sim (⚙) \text{ with } (\lambda_1,\ \xi\text{w}_1,\ \omega\text{w}_1)$$

$$(V_{2,t}, Z_{2,t}) \sim (⚙) \text{ with } (\lambda_2,\ \xi\text{w}_2,\ \omega\text{w}_2)$$

$$X_t=(V_{1,t}, V_{2,t}, Z_{1,t}, Z_{2,t})$$

$$V_t=V_{1,t}+V_{2,t}$$

$$Y_t \mid X_t \sim \mathcal{N}(\mu+\beta V_t, V_t)$$

with independent priors:

$\lambda_1\sim\text{Exp}(1)$; $\lambda_2-\lambda_1\sim\text{Exp}(1/2)$; $\xi, \omega^2\sim\text{Exp}(1/5)$

$1-\text{w}_2=\text{w}_1\sim\text{Unif}(0,1)$; $\mu, \beta\sim\mathcal{N}(0,10)$

Illustration of consistency for state-space models

- **Example 3**. Lévy-driven stochastic volatility models, given $T = 1000$ observations simulated from a single-factor model with $\lambda = 0.01$, $\xi = 0.5$, $\omega^2 = 0.0625$, $\mu = 0$, and $\beta = 0$ (*Barndorff-Nielsen & Shephard, 2001*)

Model 1 (single-factor)

Given parameters $(\lambda, \xi, \omega, \mu, \beta)$:

$$(V_t, Z_t) \sim (\;)$$

$$X_t = (V_t, Z_t)$$

$$Y_t \mid X_t \sim \mathcal{N}(\mu + \beta V_t, V_t)$$

with independent priors:

$\lambda \sim \mathrm{Exp}(1)$; $\xi, \omega^2 \sim \mathrm{Exp}(1/5)$; $\mu, \beta \sim \mathcal{N}(0, 10)$

Model 2 (multi-factor)

Given parameters $(\lambda_1, \lambda_2, \mathrm{w}_1, \mathrm{w}_2, \xi, \omega, \mu, \beta)$:

$$(V_{1,t}, Z_{1,t}) \sim (\;) \text{ with } (\lambda_1,\ \xi \mathrm{w}_1,\ \omega \mathrm{w}_1)$$

$$(V_{2,t}, Z_{2,t}) \sim (\;) \text{ with } (\lambda_2,\ \xi \mathrm{w}_2,\ \omega \mathrm{w}_2)$$

$$X_t = (V_{1,t}, V_{2,t}, Z_{1,t}, Z_{2,t})$$

$$V_t = V_{1,t} + V_{2,t}$$

$$Y_t \mid X_t \sim \mathcal{N}(\mu + \beta V_t, V_t)$$

with independent priors:

$\lambda_1 \sim \mathrm{Exp}(1)$; $\lambda_2 - \lambda_1 \sim \mathrm{Exp}(1/2)$; $\xi, \omega^2 \sim \mathrm{Exp}(1/5)$

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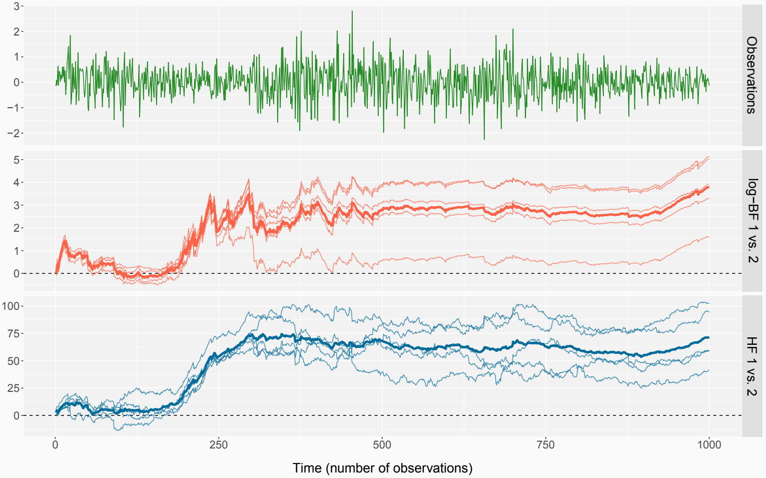

Prequential vs. Batch approach

- Notice that, unlike for the log scoring rule, here we have:

$$\mathcal{H}\left(y_{1:T}, p(dy_{1:T})\right) \quad \neq \quad \sum_{t=1}^{T} \mathcal{H}\left(y_t, p(dy_t|y_{1:t-1})\right)$$

- Batch version:
  - Easier to compute, as it only requires to estimate final evidence $p(y_{1:T})$
  - But typically inconsistent for model selection
- Prequential version:
  - Generally consistent for model selection
  - Requires to estimate all the intermediary predictive densities $p(dy_t|y_{1:t-1})$, but this can be achieved using algorithms such as SMC or SMC^2

Partial Bayes factors (Lempers, 1971)

- Split the data $y_{1:T}$ into a training set $y_{1:m}$ and another set $y_{m+1:T}$ for some choice of m
- Idea: condition on the training set to make the prior proper (or less vague) then compute the Bayes factor on the remaining data
- Essentially we replace the prior $p(\theta|M)$ by the posterior given the training set $p(\theta|y_{1:m}, M)$, and compute the usual Bayes factor on the remaining data set $y_{m+1:T}$
- The partial Bayes factor between Models M_1 and M_2 is defined as:

$$\frac{p(y_{m+1:T}|y_{1:m}, M_1)}{p(y_{m+1:T}|y_{1:m}, M_2)}$$

- Drawback: choice of m is a bit ad-hoc, undesirable to "waste" data for the training set especially in settings where the number of observations is small (e.g. Example 2 where $T = 41$)

Fractional Bayes factors (O'Hagan, 1995)

- In the setting of partial Bayes factors, if m and T are both large, the likelihood $p(y_{1:m}|\theta, M)$ of the training set will approximate (at least in the i.i.d. case) the full likelihood raised to a power $b \equiv m/T$
- For a given model M we define:

$$q_b(y_{1:T}|M) := \frac{\int p(\theta|M)p(y_{1:T}|\theta, M)d\theta}{\int p(\theta|M)p(y_{1:T}|\theta, M)^b d\theta}$$

  which approximates $p(y_{m+1:T}|y_{1:m}, M)$ for large m and T
- The fractional Bayes factor between Models M_1 and M_2 is defined as:

$$\frac{q_b(y_{1:T}|M_1)}{q_b(y_{1:T}|M_2)}$$

- Drawback: choice of b is a bit ad-hoc, not very principled for small sample size since the main justification relies on asymptotics