Joint sampling of states and parameters in state space models

William J. McCausland [*1] and Samuel Gingras [†1]

[1]Département de sciences économiques, Université de Montréal

June 5, 2017

Abstract

We consider the problem of sampling the posterior distribution in univariate non-linear, non-Gaussian state space models. We propose a new method that updates the parameter vector θ and the state vector x together as a single block. The proposal (θ^*, x^*) is drawn in two steps. The marginal proposal distribution for θ^* is constructed using approximations of the gradient and Hessian of the log posterior density of θ. The conditional proposal distribution for x^* given θ^* is that described in McCausland (2012). Computation of the approximate gradient and Hessian requires no simulation. Rather, it combines computational by-products of the x^* draw with a modest amount of additional computation. We compare the numerical efficiency of our posterior simulation with that of the Ancillarity-Sufficiency Interweaving Strategy (ASIS) described in Kastner and Frühwirth-Schnatter (2014), using the stochastic volatility model and the panel of 23 daily exchange rates from that paper. For computing the posterior mean of the volatility persistence parameter, our numerical efficiency is 4-19 times higher; for the volatility of volatility parameter, 15-36 times higher.

1 Introduction

We consider stationary univariate state space models with Gaussian states x_t,

$$x_1 \sim N(\mu, \sigma^2(1-\phi^2)^{-1}), \quad x_t \sim N(\mu(1-\phi) + \phi x_{t-1}, \sigma^2), \quad t = 2, \ldots, n,$$

and observations y_t with the following conditional independence structure:

$$p(y_1, \ldots, y_n | x_1, \ldots, x_n) = \prod_{t=1}^{n} p(y_t | x_t).$$

The y_t may be scalars or vectors, and the dimension of y_t may vary with t, to accommodate mixed-frequency observations or missing data. Any element of y_t may be a discrete, continuous or mixed random variable. There may be functions of y_t that are non-random.

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[*]william.j.mccausland@umontreal.ca, File: `theta_draw.tex`, Very preliminary.
[†]samuel.gingras@umontreal.ca

The most common examples are variations on the stochastic volatility (SV) model introduced by Taylor (1982). Some of these variations add flexibility to self-contained SV models, typically by allowing excess kurtosis in the measurement equation, jumps, or (negative) correlation between returns and the innovation of the state equation. In some variations, SV models are embedded in more complicated models.

Other examples of state space models include models with time-varying counts or durations. Durbin and Koopman (1997) study counts of deaths of van drivers in Britain; Frühwirth-Schnatter and Wagner (2006), casualties of pedestrians in Linz; and Jung, Kukuk, and Liesenfeld (2006), admissions for asthma to a hospital in Sydney. Bauwens and Veredas (2004), Strickland, Forbes, and Martin (2006) and Strickland, Forbes, and Martin (2008) study durations between transactions in financial markets.

Several methods for Bayesian posterior simulation in such state state models have been proposed. Direct methods sample latent states from their conditional posterior distribution. Sampling may be done one-at-a-time as in Jacquier, Polson, and Rossi (1994); in blocks, as in Shephard and Pitt (1997), Watanabe and Omori (2004), Strickland, Forbes, and Martin (2006) or Omori and Watanabe (2008); or all at once, as in McCausland (2012) or Djegnene and McCausland (2015). Auxiliary mixture methods involve transforming the model into a linear Gaussian model, approximating any non-Gaussian distributions in the transformed model by finite Gaussian mixtures. Kim, Shephard, and Chib (1998), Chib, Nardari, and Shephard (2002) and Omori, Chib, Shephard, and Nakajima (2007) use auxiliary mixture sampling for various SV models. Stroud, Müller, and Polson (2003) use it for Gaussian, but non-linear, state space models with state dependent variances; Frühwirth-Schnatter and Wagner (2006) for state space models with Poisson counts; and Frühwirth-Schnatter and Frühwirth (2007) for logit and multinomial logit models. (WJM: update this review.)

Numerical efficiency varies greatly across posterior simulation methods. Since there is often a great deal of posterior autocorrelation in x, and much posterior dependence between θ and x, it helps to update sequences of state values together in the same Gibbs block and to update parameters and states together. At the same time, the larger the block, the more difficult it is to approximate non-standard distributions. So, for example, a multivariate normal distribution is adequate for direct sampling of blocks of 20-50 state values, but not for the complete observed sequence x. McCausland (2012) and Djegnene and McCausland (2015) provide an approximation of $p(x|\theta, y)$ for generic state space models that is not multivariate normal and that proved highly efficient for drawing x in a single block. Auxiliary mixture models yield Gaussian x when one conditions on discrete mixture component indicators, and x can be drawn as a single block here too.

There have been previous attempts to draw θ and x together in a single block. For the Taylor SV model, Kim, Shephard, and Chib (1998) draw θ and x together, conditional on mixture component indicators, in what they call an "integration sampler" because x is marginalized out to draw parameters. Chib, Nardari, and Shephard (2002) analyse several SV models using a sampler in which x is marginalized out to draw μ, ϕ, σ and other parameters. McCausland (2012) draws parameters and x together, directly, as as single block in many state space models. One application replicates the analysis in Chib, Nardari, and Shephard (2002) of a 6-parameter Student's t SV model, the model from that paper with the highest Bayes factor for a sample of size $n = 8851$ of S&P 500 stock index returns. For the posterior sample mean of ϕ, Chib, Nardari, and Shephard (2002) achieve a numerical

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efficiency of 0.19 and McCausland (2012), 0.61. For the posterior sample mean of σ, the efficiencies are 0.10 and 0.87, respectively.

In all these cases, the SV model is a self-contained model for a single return series, not embedded in a larger model. This makes it easy to precompute the shape of the posterior distribution of parameters when x is marginalized out.

When the SV model is embedded in a larger model, the shape of this posterior distribution is a moving target. In part because of this issue, it is often desirable to update parameters and x—and mixture component indicators, if any—in separate Gibbs blocks. Kastner and Frühwirth-Schnatter (2014) do this as efficiently as possible by interleaving draws of two different parameterizations of θ to ensure that the update of θ is close to a pure Gibbs draw.

Our contribution is a method to draw parameters and states together, but in a way that does not rely on any pre-computation. Instead, it is based on computations of the local shape of the posterior distribution of parameters, with x marginalized out. The result is a sampler that is much more numerically efficient than that of Kastner and Frühwirth-Schnatter (2014) and not much less efficient than that of McCausland (2012), which does rely on pre-computing the shape of the posterior distribution of parameters.

We describe our new method in Section 2. We demonstrate it in Section 3, comparing its numerical efficiency with those of competing methods. We conclude in Section 4. The long and tedious work required to derive good approximations of the gradient and Hessian of the log posterior density of θ is relegated to the appendices. Once this is out of the way, the rest is quite simple.

2   Joint sampling of states and parameters

Our new simulation method takes advantage of close approximations of the gradient and Hessian of the log posterior density $\log p(\theta|y)$, where x has been marginalized out. The gradient and Hessian give a good idea of the shape of $p(\theta|y)$ at any point θ, allowing us to draw well targeted proposals of θ.

We describe our new methods in four parts. First, we describe a parameterization θ of the latent state process x that makes $p(\theta|y)$ well enough approximated by a Gaussian distribution. We then describe how we use the approximate gradient and Hessian of $\log p(\theta|y)$ to propose a candidate value θ^*. We then describe how we use the HESSIAN method to propose a candidate value x^*. Finally, we describe the Metropolis Hastings accept/reject decision that is applied to the joint proposal (θ^*, x^*).

2.1   Parameterizations

We will use two different parameterizations of the latent state process. One, ψ, is useful for computing analytic expressions. The other, θ, is useful for posterior simulation.

Let $\psi \equiv (\omega, \phi, \mu)$, where $\omega = \sigma^{-2}$, the precision of the state innovation. Since ω appears linearly in the quadratic (in x) term of $\log p(x|\theta)$, it is more convenient to work with than σ^2. However, the log posterior density $\ln p(\psi|x)$ is not well approximated by a quadratic in ψ. For one, its support is not $\mathbb{R}^3$; ψ lies in the space $\Psi \equiv [0, \infty] \times (-1, 1) \times \mathbb{R}$, and the ϕ parameter often has considerable posterior mass near the boundary of its support.

We prefer a parameterization whose log posterior density more closely resembles a positive definite quadratic function. This is for numerical efficiency, as it lets us better target the posterior density with a Gaussian approximation. With this in mind, let $\theta \equiv (\ln \omega, \tanh^{-1} \phi, \mu)$. The transformation $\theta(\psi)$ maps the parameter space Ψ to $\mathbb{R}^3$. We will use θ for posterior simulation, but we will need to transform θ back to ψ in order to evaluate $p(x|\omega, \phi, \mu)$. The reverse transformation is $(\omega, \phi, \mu) = \psi(\theta) = (e^{\theta_1}, \tanh \theta_2, \theta_3)$.

2.2   Drawing the proposal θ^*

The marginal proposal distribution for θ^* is based on a second order Taylor expansion of the log target density $\log p(\theta|y)$. The approach here is similar to that described in Robert and Casella (2010).

Let $g_{\theta|y}(\theta)$ and $H_{\theta|y}(\theta)$ be the gradient and Hessian of the log target density. We can write

$$g_{\theta|y}(\theta) = g_\theta(\theta) + g_{y|\theta}(\theta) \quad \text{and} \quad H_{\theta|y}(\theta) = H_\theta(\theta) + H_{y|\theta}(\theta),$$

where $g_\theta(\theta)$ and $H_\theta(\theta)$ are the gradient and Hessian of the log prior density $p(\theta)$; and $g_{y|\theta}(\theta)$ and $H_{y|\theta}(\theta)$ are the gradient and Hessian of $\log p(y|\theta)$ with respect to θ.

Unfortunately, $g_{y|\theta}(\theta)$ and $H_{y|\theta}(\theta)$ are not available. Instead, we use approximations $\tilde{g}_{y|\theta}(\theta)$ and $\tilde{H}_{y|\theta}(\theta)$, described in Appendix A. This gives the following approximations of the gradient and Hessian of the log target distribution:

$$\tilde{g}_{\theta|y}(\theta) = g_\theta(\theta) + \tilde{g}_{y|\theta}(\theta) \quad \text{and} \quad \tilde{H}_{\theta|y}(\theta) = H_\theta(\theta) + \tilde{H}_{y|\theta}(\theta).$$

Now let (θ_c, x_c) denote the current value of the parameter and state vectors in the MCMC chain. The values $\tilde{g}_{y|\theta}(\theta_c)$ and $\tilde{H}_{y|\theta}(\theta_c)$ will already be available from previous computations, as we will see.

Given the current value θ_c, we draw the proposal θ^* according to

$$\theta^*|\theta_c \sim N(\theta_c - \frac{1}{2}\gamma \tilde{H}_{\theta|y}(\theta_c)\tilde{g}_{\theta|y}(\theta_c), -\gamma \tilde{H}_{\theta|y}(\theta_c)^{-1}),$$

and evaluate the prior density $p(\theta^*)$ and the log proposal density $q(\theta^*|\theta_c)$. Since $\tilde{H}_{\theta|y}(\theta)$ depends on θ, we have to be careful not to ignore the normalization factor of $q(\theta^*|\theta_c)$.

The factor γ is present for robustness. Without it, numerical efficiency would be much lower: when θ_c is very far from its posterior mode, the gradient $\tilde{g}_{\theta|y}(\theta_c)$ is large, the mean of the proposal is far from θ_c, and the Hessian $\tilde{H}_{y|\theta}(\theta^*)$ may be quite different from $\tilde{H}_{y|\theta}(\theta_c)$ A consequence is that the acceptance probability may be extremely low. This situation is most likely to occur during a burn-in period where values of various variables may in regions of low posterior density.

Multiplying the Hessian matrix by γ reins in excessively large proposals. We use the following multiplier

$$\gamma = \coth\left(\frac{3 + 2\sqrt{6}}{-\tilde{g}_{\theta|y}(\theta)\tilde{H}_{\theta|y}^{-1}(\theta)\tilde{g}_{\theta|y}(\theta)}\right),$$

where coth is the hyperbolic cotangent. The function $\coth(1/x)$ is a "soft" $\min(x, 1)$, without a kink. The maximum value of $\gamma(-\tilde{g}_{\theta|y}(\theta)\tilde{H}_{\theta|y}^{-1}(\theta)\tilde{g}_{\theta|y}(\theta))$ is $3 + 2\sqrt{6}$, two standard

deviations above the mean of a $\chi^2(3)$ random variable. (WJM: explain why this makes sense, why it is scale invariant, how it might generalize to θ with more elements than three.)

2.3 Drawing the proposal $x^*|\theta^*$

We use the HESSIAN method to draw x^* from a close approximation $q(x^*|\theta^*, y)$ to the conditional posterior distribution $p(x^*|\theta^*, y)$ and to compute the proposal density $q(x^*|\theta^*, y)$ We also compute $p(x^*|\theta^*)$ and $p(y|x^*)$,

Using a modest amount of additional computation, described in the appendices, we can also compute $\tilde{g}_{y|\theta}(\theta^*)$ and $\tilde{H}_{y|\theta}(\theta^*)$ at the same time. We need these to evaluate the reverse proposal density $q(\theta_c|\theta^*)$. In the event that the proposal (θ^*, x^*) is accepted, the values of $\tilde{g}_{y|\theta}(\theta^*)$ and $\tilde{H}_{y|\theta}(\theta^*)$ can be kept for the next iteration.

2.4 Joint accept-reject

We then compute the reverse proposal density $q(\theta_c|\theta^*)$ using $\tilde{g}_{y|\theta}(\theta^*)$ and $\tilde{H}_{y|\theta}(\theta^*)$, and accept (θ^*, x^*) with probability

$$\min\left[1, \frac{p(\theta^*)p(x^*|\theta^*)p(y|x^*)q(\theta_c|\theta^*)q(x_c|\theta_c, y)}{p(\theta_c)p(x_c|\theta_c)p(y|x_c)q(\theta^*|\theta_c)q(x^*|\theta^*, y)}\right].$$

3 Results

3.1 Stochastic volatility

We apply our methods to daily exchange rate data for 23 currencies, from January 3rd, 2000 to April 4, 2012. The data, from the European Central Bank, are those used by Kastner and Frühwirth-Schnatter (2014) in their empirical application. We compute 3139 log returns using exchange rates against the Euro observed on 3140 consecutive trading days.

We use the following prior for θ:

$$\theta \sim N\left(\begin{bmatrix} 3.6 \\ 2.5 \\ -10.5 \end{bmatrix}, \begin{bmatrix} 1.25 & 0.5 & 0 \\ 0.5 & 0.25 & 0 \\ 0 & 0 & 0.25 \end{bmatrix}\right).$$

The prior is based on independent priors for $\tanh^{-1}\phi$ and $\log\omega(1-\phi^2)$. We do this because in practice, the unconditional precision $\omega(1-\phi^2)$ of x_t covaries less with ϕ than does the conditional precision ω, across financial return series. (WJM: Confirm and document this, using a more extensive collection of results.) Results (including efficiency) are fairly robust to setting the covariance $\text{Cov}[\theta_1, \theta_2]$ to zero.

Table 1 illustrates the results. For each currency, and the three parameters σ, ϕ and μ, we report the posterior sample mean and standard deviation, as well as the relative numerical efficiency for the posterior sample mean. The relative numerical efficiency is the ratio of the numerical variance of the mean of an iid sample to the numerical variance of the posterior sample mean. It is the reciprocal of the inefficiency factor used by Kastner and Frühwirth-Schnatter (2014) and others. We estimate the numerical variance of our

Currency	$E[\sigma|y]$	sd$[\sigma|y]$	rne	$\times$	$E[\phi|y]$	sd$[\phi|y]$	rne	$\times$	$E[\mu|y]$	sd$[\mu|y]$	rne
Australian dollar	0.155	0.021	0.33	31.9	0.981	0.006	0.18	12.5	-10.26	0.17	0.18
Canadian dollar	0.077	0.015	0.25	29.5	0.993	0.004	0.09	8.4	-10.12	0.25	0.15
Swiss franc	0.202	0.019	0.23	16.8	0.986	0.004	0.18	5.9	-12.01	0.27	0.26
Czech koruna	0.260	0.032	0.21	20.6	0.960	0.010	0.18	12.8	-11.50	0.12	0.23
Danish krone	0.409	0.040	0.23	16.5	0.912	0.017	0.19	11.0	-18.07	0.09	0.21
UK pound sterling	0.098	0.012	0.37	32.3	0.993	0.002	0.20	7.9	-10.84	0.28	0.20
Hong Kong dollar	0.064	0.010	0.35	26.2	0.996	0.002	0.13	4.7	-10.16	0.32	0.18
Indonesian rupiah	0.208	0.032	0.24	34.7	0.974	0.009	0.18	20.9	-9.86	0.16	0.15
Japanese yen	0.114	0.015	0.30	27.1	0.991	0.003	0.16	7.7	-9.95	0.26	0.22
Korean won	0.135	0.016	0.26	20.8	0.989	0.004	0.19	7.7	-10.03	0.24	0.25
Mexican peso	0.153	0.020	0.34	29.3	0.982	0.006	0.18	11.0	-9.76	0.16	0.20
Malaysian ringgit	0.074	0.012	0.33	29.3	0.994	0.003	0.11	6.3	-10.28	0.27	0.17
Norwegian krone	0.165	0.021	0.25	19.2	0.976	0.007	0.16	8.4	-11.14	0.14	0.22
New Zealand dollar	0.155	0.027	0.30	40.0	0.974	0.010	0.15	17.5	-10.01	0.13	0.13
Philippine peso	0.133	0.021	0.27	43.4	0.983	0.007	0.12	15.1	-10.11	0.16	0.10
Polish zloty	0.181	0.020	0.37	25.3	0.979	0.006	0.22	9.5	-10.42	0.17	0.22
Romanian leu	0.299	0.025	0.30	18.0	0.972	0.006	0.29	9.3	-11.08	0.20	0.22
Russian rouble	0.143	0.016	0.24	20.0	0.990	0.003	0.17	6.4	-10.62	0.27	0.23
Swedish krona	0.108	0.012	0.27	16.4	0.992	0.002	0.16	3.6	-11.33	0.28	0.22
Singapore dollar	0.067	0.010	0.32	31.9	0.996	0.002	0.17	8.2	-10.58	0.35	0.22
Thai baht	0.115	0.018	0.29	26.4	0.987	0.005	0.12	7.8	-10.17	0.18	0.15
Turkish lira	0.302	0.025	0.25	17.2	0.962	0.008	0.21	8.9	-9.78	0.15	0.25
US dollar	0.064	0.010	0.39	29.2	0.996	0.002	0.16	6.0	-10.14	0.32	0.19

Table 1: Posterior mean, standard deviation and numerical efficiency for the SV model and ECB exchange rate data.

posterior sample means using the overlapping batch means method—see Flegal and Jones (2010).

For σ and ϕ parameters, we also report the number of times more efficient the posterior sample means are, compared to those reported by Kastner and Frühwirth-Schnatter (2014). For computing the posterior mean of σ, our numerical efficiency is 15-36 times higher; for ϕ, 4-19 times higher.

For the μ parameter, numerical efficiency is high, although slightly lower than that reported by Kastner and Frühwirth-Schnatter (2014). Given that the conditional posterior distribution of μ, (i.e. $\mu|\phi, \sigma, x, y$) is Gaussian, the numerical efficiency for μ and higher moments could easily be greatly improved through antithetic sampling or Rao-Blackwellization.

3.2 High frequency counts with diurnal patterns.

WJM: to complete.

3.3 Stochastic volatility factors.

WJM: to complete.

4 Conclusions

With modest additional computation, we can compute approximations of the gradient and Hessian of $\log p(\theta|y)$ in univariate non-linear non-Gaussian state space models. This allows us to construct a one-block posterior sampler for (θ, x).

In an empirical application, we show that the approximation is good enough to achieve high numerical efficiency for the 23 return series we investigate.

A Computing approximate gradient and Hessian of $\log p(y|\theta)$

Our objective is to compute approximations to the following gradient and Hessian:

$$g_{y|\theta}(\theta) \equiv \frac{\partial \log p(y|\theta)}{\partial \theta}, \quad H_{y|\theta}(\theta) \equiv \frac{\partial^2 \log p(y|\theta)}{\partial\theta\partial\theta^\top}.$$

We will use the exact result, proved in Appendix B, that

$$g_{y|\theta}(\theta) = E_{x|\theta,y}[g_{x|\theta}(\theta)] \quad \text{and} \quad H_{y|\theta}(\theta) = E_{x|\theta,y}[H_{x|\theta}(\theta)] + \text{Var}_{x|\theta,y}[g_{x|\theta}(\theta)],$$

where

$$g_{x|\theta}(\theta) \equiv \frac{\partial \log p(x|\theta)}{\partial \theta}, \quad H_{x|\theta}(\theta) \equiv \frac{\partial^2 \log p(x|\theta)}{\partial\theta\partial\theta^\top}.$$

We first compute exact expressions for $g_{x|\theta}(\theta)$ and $H_{x|\theta}(\theta)$. Then we compute exact expressions for their means. Then we use approximate distributions for $x|\theta, y$ to approximate these means. Finally, we compute an approximation of the variance of $g_{x|\theta}$.

A.1 Computing $g_{x|\theta}(\theta)$ and $H_{x|\theta}(\theta)$

First decompose $\log p(x|\psi) = k + L(\psi)$, where

$$k \equiv \frac{n}{2}(\ln \omega - \ln 2\pi) + \frac{1}{2}\ln(1 - \phi^2)$$

and

$$L(\psi) = -\frac{\omega}{2}\left[(1 - \phi^2)(x_n - \mu)^2 + \sum_{t=1}^{n-1}[(x_t - \mu) - \phi(x_{t+1} - \mu)]^2\right].$$

We will compute all first and second order partial derivatives of $L(\psi)$ with respect to ω, ϕ and μ.

First order partial derivatives:

$$\frac{\partial L(\psi)}{\partial \omega} = -\frac{1}{2}\left[(1 - \phi^2)(x_n - \mu)^2 + \sum_{t=1}^{n-1}[(x_t - \mu) - \phi(x_{t+1} - \mu)]^2\right].$$

$$\frac{\partial L(\psi)}{\partial \phi} = \omega \left[\sum_{t=1}^{n-1} (x_t - \mu)(x_{t+1} - \mu) - \phi \sum_{t=2}^{n-1} (x_t - \mu)^2 \right]$$

$$\frac{\partial L(\psi)}{\partial \mu} = \omega(1 - \phi) \left[(x_1 + x_n - 2\mu) + (1 - \phi) \sum_{t=2}^{n-1} (x_t - \mu) \right]$$

Second order partial derivatives:

$$\frac{\partial^2 L(\psi)}{\partial \omega^2} = 0, \qquad \frac{\partial^2 L(\psi)}{\partial \phi^2} = -\omega \sum_{t=2}^{n-1} (x_t - \mu)^2, \qquad \frac{\partial^2 L(\psi)}{\partial \mu^2} = -\omega \left[2(1 - \phi) + (n - 2)(1 - \phi)^2 \right],$$

$$\frac{\partial^2 L(\psi)}{\partial \omega \partial \phi} = \frac{1}{\omega} \frac{\partial L}{\partial \phi}, \qquad \frac{\partial^2 L(\psi)}{\partial \omega \partial \mu} = \frac{1}{\omega} \frac{\partial L}{\partial \mu},$$

$$\frac{\partial^2 L(\psi)}{\partial \phi \partial \mu} = -\omega \left[(x_1 + x_n - 2\mu) + 2(1 - \phi) \sum_{t=2}^{n-1} (x_t - \mu) \right]$$

Now we compute gradient and Hessian of $L(\psi(\theta))$ with respect to θ, the vector of transformed parameter values. We can write

$$\frac{\partial L(\psi(\theta))}{\partial \theta} = \frac{\partial L(\psi)}{\partial \psi} \frac{\partial \psi}{\partial \theta}$$

$$\frac{\partial^2 L(\psi(\theta))}{\partial \theta_i^2} = \frac{\partial^2 L(\psi)}{\partial \psi_i^2} \left(\psi_i'(\theta_i) \right)^2 + \frac{\partial L(\psi)}{\partial \psi_i} \psi_i''(\theta_i)$$

For $i \neq j$,

$$\frac{\partial^2 L(\psi(\theta))}{\partial \theta_i \partial \theta_j} = \frac{\partial^2 L(\psi(\theta))}{\partial \psi_i \partial \psi_j} \psi_i'(\theta_i) \psi_j'(\theta_j)$$

The first two derivatives of $\omega = \exp(\theta_1)$ with respect to θ_1 are

$$\psi_1'(\theta_1) = \frac{\partial \omega}{\partial \theta_1} = \exp(\theta_1) = \omega, \qquad \psi_1''(\theta_1) = \frac{\partial^2 \omega}{\partial \theta_1^2} = \exp(\theta_1) = \omega,$$

and the first two derivatives of $\phi = \tanh \theta_2$ with respect to θ_2 are

$$\psi_2'(\theta_2) = \frac{\partial \phi}{\partial \theta_2} = 1 - \tanh^2 \theta_2 = 1 - \phi^2, \qquad \psi_2''(\theta_2) = \frac{\partial^2 \phi}{\partial \theta_2^2} = -2 \tanh \theta_2 (1 - \tanh^2 \theta_2) = -2\phi(1 - \phi^2).$$

The gradient with respect to θ is

$$\frac{\partial L(\psi(\theta))}{\partial \theta} = \begin{bmatrix} -\frac{\omega}{2} \left[(1 - \phi^2)(x_n - \mu)^2 + \sum_{t=1}^{n-1} [(x_t - \mu) - \phi(x_{t+1} - \mu)]^2 \right] \\ \omega(1 - \phi^2) \left[\sum_{t=1}^{n-1} (x_t - \mu)(x_{t+1} - \mu) - \phi \sum_{t=2}^{n-1} (x_t - \mu)^2 \right] \\ \omega(1 - \phi) \left[(x_1 + x_n - 2\mu) + (1 - \phi) \sum_{t=2}^{n-1} (x_t - \mu) \right] \end{bmatrix}$$

The elements of the Hessian are

$$\frac{\partial^2 L(\psi(\theta))}{\partial \theta_1^2} = \frac{\partial L(\psi(\theta))}{\partial \theta_1},$$

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$$\frac{\partial^2 L(\psi(\theta))}{\partial \theta_2^2} = (1-\phi^2)^2 \frac{\partial^2 L(\psi)}{\partial \phi^2} - 2\phi(1-\phi^2)\frac{\partial L(\psi)}{\partial \phi} = (1-\phi^2)\left[(1-\phi^2)\frac{\partial^2 L(\psi)}{\partial \phi^2} - 2\phi\frac{\partial L}{\partial \phi}\right]$$

$$\frac{\partial^2 L(\psi(\theta))}{\partial \theta_3^2} = \frac{\partial^2 L(\psi)}{\partial \mu^2}.$$

$$\frac{\partial^2 L(\psi(\theta))}{\partial \theta_1 \partial \theta_2} = (1-\phi^2)\frac{\partial L(\psi)}{\partial \phi} = \frac{\partial L(\psi(\theta))}{\partial \theta_2}.$$

$$\frac{\partial^2 L(\psi(\theta))}{\partial \theta_1 \partial \theta_3} = \frac{\partial L(\psi)}{\partial \mu} = \frac{\partial L(\psi(\theta))}{\partial \theta_3}.$$

$$\frac{\partial^2 L(\psi(\theta))}{\partial \theta_2 \partial \theta_3} = (1-\phi^2)\frac{\partial^2 L(\psi)}{\partial \phi \partial \mu}.$$

The log normalizing factor $k = \frac{n}{2}(\ln \omega - \ln 2\pi) + \frac{1}{2}\ln(1-\phi^2)$ also depends on θ. Noting that $\theta_1 = \ln \omega$, we have

$$\frac{\partial k}{\partial \theta_1} = \frac{n}{2}, \qquad \frac{\partial^2 k}{\partial \theta_1^2} = 0.$$

Then

$$\frac{\partial k}{\partial \theta_2} = (1-\phi^2)\frac{\partial k}{\partial \phi} = (1-\phi^2)\frac{1}{2}\frac{-2\phi}{(1-\phi^2)} = -\phi,$$

$$\frac{\partial^2 k}{\partial \theta_2^2} = (1-\phi^2)\frac{\partial}{\partial \phi}\frac{\partial k}{\partial \theta_2} = -(1-\phi^2).$$

A.2 Computing the mean of $g_{x|\theta}(\theta)$ and $H_{x|\theta}(\theta)$

We express the mean of L and its derivatives in terms of the decomposition $x_t \equiv c_t + e_t$, where $c_t \equiv E[x_t|\theta, y]$ and $e_t \equiv x_t - c_t$.

Here we just take the mean of $g_{x|\theta}(\theta)$ and $H_{x|\theta}(\theta)$ with respect to the distribution $x|\theta, y$, component by component. For the rest of this section, we will suppress conditioning on θ and y so that, for example, $E[x]$ denotes $E[x|\theta, y]$.

This gives

$$E\left[\frac{\partial L(\psi(\theta))}{\partial \theta_1}\right] = -\frac{\omega}{2}\left[(1-\phi^2)[(c_n - \mu)^2 + E[e_n^2]] + \sum_{t=1}^{n-1}(c_t - \phi c_{t+1} - \mu(1-\phi))^2 + E[(e_t - \phi e_{t+1})^2]\right]$$

$$E\left[\frac{\partial^2 L(\psi(\theta))}{\partial \theta_1^2}\right] = E\left[\frac{\partial L(\psi(\theta))}{\partial \theta_1}\right]$$

$$E\left[\frac{\partial L(\psi(\theta))}{\partial \theta_2}\right] = \omega(1-\phi^2)\left[\sum_{t=1}^{n-1}(c_t - \mu)(c_{t+1} - \mu) + E[e_t e_{t+1}] - \phi\sum_{t=2}^{n-2}(c_t - \mu)^2 + E[e_t^2]\right]$$

$$E\left[\frac{\partial^2 L(\psi(\theta))}{\partial \theta_2^2}\right] = -\omega(1-\phi^2)^2\left[\sum_{t=2}^{n-1}(c_t - \mu)^2 + E[e_t^2]\right] - 2\phi E\left[\frac{\partial L(\psi(\theta))}{\partial \theta_2}\right]$$

$$E\left[\frac{\partial^2 L(\psi(\theta))}{\partial \theta_1 \partial \theta_2}\right] = E\left[\frac{\partial L(\psi(\theta))}{\partial \theta_2}\right].$$

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$$E\left[\frac{\partial L(\psi(\theta))}{\partial \theta_3}\right] = \omega(1-\phi)\left[(c_1 + c_n - 2\mu) + (1-\phi)\sum_{t=2}^{n-1}(c_t - \mu)\right]$$

$$E\left[\frac{\partial^2 L(\psi(\theta))}{\partial \theta_3^2}\right] = -\omega[2(1-\phi) + (n-2)(1-\phi)^2]$$

$$E\left[\frac{\partial^2 L(\psi(\theta))}{\partial \theta_1 \partial \theta_3}\right] = E\left[\frac{\partial L(\psi(\theta))}{\partial \theta_3}\right]$$

$$E\left[\frac{\partial^2 L(\psi(\theta))}{\partial \theta_2 \partial \theta_3}\right] = -\omega(1-\phi^2)\left[(c_1 + c_n - 2\mu) + 2(1-\phi)\sum_{t=1}^{n-1}(c_t - \mu)\right]$$

To compute exact values of these expressions, we would need to compute all the $c_t = E[x_t]$ and the $E[e_t^2]$ and the $E[(e_t - \phi e_{t+1})^2]$. In the next section, we develop approximations.

A.3 Computing approximate moments of $g_{x|\theta}(\theta)$ and $H_{x|\theta}(\theta)$

First, let $x^\circ = (x_1^\circ, \ldots, x_n^\circ)$ be the mode of $x|\theta, y$ and $\epsilon = (\epsilon_1, \ldots, \epsilon_n) \equiv x - x^\circ$. Recall that we previously defined $c \equiv E[x]$ and $e \equiv x - c$. This implies that $e = \epsilon - E[\epsilon]$.

A.3.1 Introduce $\mu_{t|t+1}(\epsilon_{t+1})$ and $b_{t|t+1}(\epsilon_{t+1})$

Recall that $\epsilon_t = x_t - x_t^\circ$. All distributions in this appendix are conditional on y and θ, and the notation for this conditioning will be suppressed. Let $\mu_{t|t+1}(\epsilon_{t+1}) \equiv E[\epsilon_t | \epsilon_{t+1}]$. Let $b_{t|t+1}(\epsilon_{t+1})$ be the conditional mode of ϵ_t given ϵ_{t+1}. Let $v_t(\epsilon_{t+1}) = \epsilon_t - b_{t|t+1}(\epsilon_{t+1})$.

We have the following approximate Taylor expansions of $\mu_{t|t+1}(\epsilon_{t+1})$ and $b_{t|t+1}(\epsilon_{t+1})$. Definitions of coefficients are in McCausland (2012), and are already computed as by-products.

$$\mu_{t|t+1}(\epsilon_{t+1}) \approx \mu_t + \dot{\mu}_t \epsilon_{t+1} + \frac{1}{2}\ddot{\mu}_t \epsilon_{t+1}^2 + \frac{1}{6}\dddot{\mu}_t \epsilon_{t+1}^3$$

$$b_{t|t+1}(\epsilon_{t+1}) \approx b_t + \dot{b}_t \epsilon_{t+1} + \frac{1}{2}\ddot{b}_t \epsilon_{t+1}^2 + \frac{1}{6}\dddot{b}_t \epsilon_{t+1}^3$$

Centering to put these functions as polynomials in e_{t+1} gives, for example,

$$\mu_{t|t+1}(\epsilon_{t+1}) = \left(\mu_t + \dot{\mu}_t E[\epsilon_{t+1}] + \frac{1}{2}\ddot{\mu}_t E[\epsilon_{t+1}]^2 + \frac{1}{6}\dddot{\mu}_t E[\epsilon_{t+1}]^3\right) \tag{1}$$

$$+ \left(\dot{\mu}_t + \ddot{\mu}_t E[\epsilon_{t+1}] + \frac{1}{2}E[\epsilon_{t+1}]^2\right) e_{t+1}$$

$$+ \frac{1}{2}\left(\ddot{\mu}_t + \dddot{\mu}_t E[\epsilon_{t+1}]\right) e_{t+1}^2 + \frac{1}{6}\dddot{\mu}_t e_{t+1}^3.$$

A.3.2 Computing $E[\epsilon_t]$, $E[e_t e_{t+1}]$ and $\text{Var}[e_t]$

To compute $E[\epsilon_t]$, $E[e_t e_{t+1}]$ and $\text{Var}[e_t]$, we first use the laws of total expectation and total variance to obtain:

$$E[\epsilon_t] = E[E[\epsilon_t | x_{t+1}]], \tag{2}$$

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$$E[e_t e_{t+1}] = E[e_{t+1} E[e_t | x_{t+1}]], \tag{3}$$

$$\text{Var}[e_t] = E[\text{Var}[e_t | x_{t+1}]] + \text{Var}[E[e_t | x_{t+1}]]. \tag{4}$$

By definition, $E[\epsilon_t | x_{t+1}] = \mu_{t|t+1}$, so we have, taking expectations of both sides of (1),

$$E[\epsilon_t] = \left(\mu_t + \dot{\mu}_t E[\epsilon_{t+1}] + \frac{1}{2} \ddot{\mu}_t E[\epsilon_{t+1}]^2 + \frac{1}{6} \dddot{\mu}_t E[\epsilon_{t+1}]^3 \right) \tag{5}$$
$$+ \frac{1}{2} \left(\ddot{\mu}_t + \dddot{\mu}_t E[\epsilon_{t+1}] \right) \text{Var}\, e_{t+1} + \frac{1}{6} \dddot{\mu}_t E[e_{t+1}^3].$$

Now express the conditional expectation $E[e_t | x_{t+1}]$ as a third order polynomial in e_{t+1}:

$$E[e_t | x_{t+1}] = E[\epsilon_t | x_{t+1}] - E[\epsilon_t] \tag{6}$$
$$= (\dot{\mu}_t + \ddot{\mu}_t E[\epsilon_{t+1}]) e_{t+1} + \frac{1}{2} \ddot{\mu}_t (e_{t+1}^2 - E[e_{t+1}^2]) + \frac{1}{6} \dddot{\mu}_t (e_{t+1}^3 - E[e_{t+1}^3])$$

Then using (3),

$$E[e_t e_{t+1}] = (\dot{\mu}_t + \ddot{\mu}_t E[\epsilon_{t+1}]) \text{Var}[e_{t+1}] + \frac{1}{2} \ddot{\mu}_t E[e_{t+1}^3] + \frac{1}{6} \dddot{\mu}_t E[e_{t+1}^4]. \tag{7}$$

Similarly,

$$\text{Var}[E[e_t | x_{t+1}]] = \left(\dot{\mu}_t + \ddot{\mu}_t E[\epsilon_{t+1}] + \frac{1}{2} \dddot{\mu}_t E[\epsilon_{t+1}]^2 \right)^2 \text{Var}[e_{t+1}] \tag{8}$$
$$+ \left(\dot{\mu}_t + \ddot{\mu}_t E[\epsilon_{t+1}] + \frac{1}{2} \dddot{\mu}_t E[\epsilon_{t+1}]^2 \right) (\ddot{\mu}_t + \dddot{\mu}_t E[\epsilon_{t+1}]) E[e_{t+1}^3]$$
$$+ \frac{1}{4} (\ddot{\mu}_t + \dddot{\mu}_t E[\epsilon_{t+1}])^2 \text{Var}[e_{t+1}^2].$$

A.3.3 Derivatives of $h_t \equiv \log p(x_t | x_{t+1})$ with respect to e_t

Result from McCausland (2012):

$$h_1''(x_1) = -\omega(1 - \phi^2) + \psi_1''(x_1).$$

$$h_t''(x_t) = \omega \phi \mu_{t-1|t}'(x_t) - \omega + \psi_t''(x_t).$$

$$h_n''(x_n) = \omega \phi \mu_{n-1|n}'(x_t) - \omega(1 - \phi^2) + \psi_t''(x_n),$$

where

$$\psi_t''(x_t) = \frac{\partial \log p(y_t | x_t, \theta)}{\partial x_t}$$

is a computational byproduct of the HESSIAN method. We can write

$$h_t''(x_t^\circ + b_{t|t+1}) = -\Sigma_t^{-1} + \omega \phi (\mu_{t-1|t}(b_{t|t+1}) - \dot{a}_{t-1}) + \psi_t''(x_t^\circ + b_{t|t+1}),$$

where $\Sigma_t \equiv -(\omega \phi \dot{a}_{t-1} - \omega + \psi_t''(x_t^\circ))^{-1}$ is a by-product of Hessian method computations.

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Using the approximations

$$\mu_{t-1|t}(b_{t|t+1}) = \dot{\mu}_{t-1} + \ddot{\mu}_{t-1}b_{t|t+1}, \qquad \psi_t''(x_t^\circ + b_{t|t+1}) = \psi_t''(x_t^\circ) + \psi_t'''(x_t^\circ)b_{t|t+1},$$

we have

$$h_t''(x_t^\circ + b_{t|t+1}) \approx -\Sigma_t^{-1} + \omega\phi(\dot{\mu}_{t-1} - \dot{a}_{t-1}) + (\omega\phi\ddot{\mu}_{t-1} + \psi_t'''(x_t^\circ))b_{t|t+1}.$$

Then approximate

$$-h_t''(x_t^\circ + b_{t|t+1})^{-1} \approx \frac{\Sigma_t}{1 - \dot{a}_t(\dot{\mu}_{t-1} - \dot{a}_{t-1}) - (\dot{a}_t\ddot{\mu}_{t-1} + \psi_t'''(x_t^\circ)\Sigma_t)b_{t|t+1}}$$

$$\approx \Sigma_t[1 + \dot{a}_t(\dot{\mu}_{t-1} - \dot{a}_{t-1}) + (\dot{a}_t\ddot{\mu}_{t-1} + \psi_t'''(x_t^\circ)\Sigma_t)b_{t|t+1}]. \qquad (9)$$

We get the following special cases using a similar development, for $t = 1$ and $t = n$:

$$-h_1''(x_1^\circ + b_{1|2})^{-1} \approx \Sigma_1[1 + \psi_1'''(x_1^\circ)\Sigma_1 b_{1|2}],$$

$$-h_n''(x_n^\circ + b_n)^{-1} \approx \Sigma_n[1 + \dot{a}_n(\dot{\mu}_{n-1} - \dot{a}_{n-1}) + (\dot{a}_n\ddot{\mu}_{n-1} + \psi_n'''(x_n^\circ)\Sigma_n)b_n].$$

A.3.4 Computing $E[\epsilon_t]$, $E[\text{Var}[e_t|x_{t+1}]]$ and $E[e_t^3]$

First, we compute the conditional expectations $E[\epsilon_t|x_{t+1}]$, $\text{Var}[e_t|x_{t+1}]$ and $E[e_t^3|x_{t+1}]$, then we will take expectations again to get the unconditional expectations.

Now let $v_t \equiv \epsilon_t - b_{t|t+1}$ and $\delta_{t|t+1} = \mu_{t|t+1} - b_{t|t+1}$.

We can write $\epsilon_t = v_t - (\mu_{t|t+1} - b_{t|t+1}) = v_t - \delta_{t|t+1}$, and $e_t = v_t - (E[\epsilon_t] - b_{t|t+1})$.

We will base calculations on

$$E[v_t^2|x_{t+1}] = -h_t''(x_t^\circ + b_{t|t+1})^{-1}, \qquad E[v_t^3|x_{t+1}] = 0.$$

This implies (note that $E[v_t|x_{t+1}] = \delta_{t|t+1}$)

$$\text{Var}[e_t|x_{t+1}] = E[(\epsilon_t - \mu_{t|t+1})^2|x_{t+1}] = E[(v_t - \delta_{t|t+1})^2|x_{t+1}] = -h_t''(x_t^\circ + b_{t|t+1})^{-1} - \delta_{t|t+1}^2. \tag{10}$$

$$E[e_t^3|x_{t+1}] = E[(v_t - (E[\epsilon_t] - b_{t|t+1})^3)|x_{t+1}] \tag{11}$$
$$= E[-3v_t^2(E[\epsilon_t] - b_{t|t+1}) + 3v_t(E[\epsilon_t] - b_{t|t+1})^2 - (E[\epsilon_t] - b_{t|t+1})^3|x_{t+1}]$$
$$= 3h_t''(x_t^\circ + b_{t|t+1})^{-1}(E[\epsilon_t] - b_{t|t+1}) + 3\delta_{t|t+1}(E[\epsilon_t] - b_{t|t+1})^2 - (E[\epsilon_t] - b_{t|t+1})^3.$$

A.3.5 Computing the gradient

Start-up, $t = n$:

1. Set $E[\epsilon_n] = \mu_n$.

2. Compute $E[e_n^2] = -h_n''(b_n)^{-1}$.

3. Compute $E[e_n^3] = (\mu_n - b_n)^3$.

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Iterative step $t = n - 1, \ldots, 1$, where we have $E[\epsilon_t]$, $E[e_t^2]$ and $E[e_t^3]$ from the previous step:

1. Compute $E[\epsilon_t]$ using (5), $E[e_t e_{t+1}]$ using (7), and $\text{Var}[E[e_t|x_{t+1}]]$ using (8).

2. Compute coefficients giving $E[e_t^3|x_{t+1}]$ in (11) as a polynomial in e_{t+1}, take expectations to get $E[e_t^3]$.

3. Compute coefficient giving $\text{Var}[e_t|x_{t+1}]$ in (10) as a polynomial in e_{t+1}, take expectations to get $E[\text{Var}[e_t|x_{t+1}]]$. Combine this quantity with $\text{Var}[E[e_t|x_{t+1}]]$ using (**??**) to obtain $E[e_t^2]$.

B Derivation of gradient and Hessian of $\log p(y|\theta)$

We can write, for any function $q(x)$ with the same support as $p(x|\theta)p(y|x)$,

$$p(y|\theta) = \int \frac{p(x|\theta)p(y|x)}{q(x)} q(x)\, dx.$$

For convenience, let

$$w_\theta(x) = \frac{p(x|\theta)p(y|x)}{q(x)},$$

so that $p(y|\theta) = \int w_\theta(x)q(x)\, dx$. The notation is meant to evoke an importance weight, where $p(x|\theta)p(y|x)$ is the target and $q(x)$ is the importance distribution. Note that for $q(x) = p(x|\theta, y)$, $w_\theta(x) = p(\theta|y)$ for all values of x.

We can write the gradient of $\log p(y|\psi)$ as

$$\frac{\partial \log p(y|\theta)}{\partial \theta} = \frac{1}{p(y|\theta)} \frac{\partial p(y|\theta)}{\partial \theta} = \frac{1}{p(y|\theta)} \int \frac{\partial p(x|\theta)}{\partial \theta} \frac{p(y|x)}{q(x)} q(x)\, dx = \frac{\int \frac{\partial \log p(x|\theta)}{\partial \theta} w_\theta(x)q(x)\, dx}{\int w_\theta(x)q(x)\, dx}.$$

Taking the derivative of the second expression, with respect to ψ, yields the Hessian matrix,

$$\frac{\partial^2 \log p(y|\theta)}{\partial \theta \partial \theta^\top} = \frac{1}{p(y|\theta)} \frac{\partial^2 p(y|\theta)}{\partial \theta \partial \theta^\top} - \frac{1}{p(y|\theta)^2} \frac{\partial p(y|\theta)}{\partial \theta} \frac{\partial p(y|\theta)}{\partial \theta^\top}.$$

We can write the first term as

$$\begin{aligned}
\frac{1}{p(y|\theta)} \frac{\partial^2 p(y|\theta)}{\partial \theta \partial \theta^\top} &= \frac{1}{p(y|\theta)} \int \frac{\partial^2 p(x|\theta)}{\partial \theta \partial \theta^\top} \frac{p(y|x)}{q(x)} q(x)\, dx \\
&= \frac{1}{p(y|\theta)} \int \left[\frac{\partial^2 \log p(x|\theta)}{\partial \theta \partial \theta^\top} p(x|\theta) + \frac{1}{p(x|\theta)} \frac{\partial p(x|\theta)}{\partial \theta} \frac{\partial p(x|\theta)}{\partial \theta^\top} \right] \frac{p(y|x)}{q(x)} q(x)\, dx \\
&= \frac{1}{p(y|\theta)} \int \left[\frac{\partial^2 \log p(x|\theta)}{\partial \theta \partial \theta^\top} + \frac{\partial \log p(x|\theta)}{\partial \theta} \frac{\partial \log p(x|\theta)}{\partial \theta^\top} \right] w_\theta(x) q(x)\, dx
\end{aligned}$$

We can write the second term as

$$-\frac{1}{p(y|\theta)^2} \frac{\partial p(y|\theta)}{\partial \theta} \frac{\partial p(y|\theta)}{\partial \theta^\top} = -\frac{\partial \log p(y|\theta)}{\partial \theta} \frac{\partial \log p(y|\theta)}{\partial \theta^\top}.$$

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Putting it together, we have

$$\frac{\partial^2 \log p(y|\theta)}{\partial\theta\partial\theta^\top} = \frac{\int \left[\frac{\partial^2 \log p(x|\theta)}{\partial\theta\partial\theta^\top} + \frac{\partial \log p(x|\theta)}{\partial\theta}\frac{\partial \log p(x|\theta)}{\partial\theta^\top}\right] w_\theta(x)q(x)\,dx}{\int w_\theta(x)q(x)\,dx} - \frac{\partial \log p(y|\theta)}{\partial\theta}\frac{\partial \log p(y|\theta)}{\partial\theta^\top}.$$

Note that if we could use $q(x) = p(x|\theta, y)$, the weights $w_\theta(x)$ would not depend on x, and we would have

$$\frac{\partial \log p(y|\theta)}{\partial\theta} = E_{x|\theta,y}\left[\frac{\partial \log p(x|\theta)}{\partial\theta}\right],$$

$$\frac{\partial^2 \log p(y|\theta)}{\partial\theta\partial\theta^\top} = E_{x|\theta,y}\left[\frac{\partial^2 \log p(x|\theta)}{\partial\theta\partial\theta^\top}\right] + \mathrm{Var}_{x|\theta,y}\left[\frac{\partial \log p(x|\theta)}{\partial\theta}\right].$$

Or, in terms of the notation in Section A,

$$g_{y|\theta} = E_{x|\theta,y}[g_{x|\theta}], \qquad H_{y|\theta} = E_{x|\theta,y}[H_{x|\theta}] + V_{x|\theta,y}[g_{x|\theta}].$$

C Variance of $\partial L(\psi(\theta))/\partial\theta_1$

Let

$$m \equiv \begin{bmatrix} (c_1 - \mu) - \phi(c_2 - \mu) \\ (c_2 - \mu) - \phi(c_3 - \mu) \\ \vdots \\ (c_{n-1} - \mu) - \phi(c_n - \mu) \\ \sqrt{1 - \phi^2}(c_n - \mu) \end{bmatrix} \quad \text{and} \quad v \equiv \begin{bmatrix} e_1 - \phi e_2 \\ e_2 - \phi e_3 \\ \vdots \\ e_{n-1} - \phi e_n \\ \sqrt{1 - \phi^2}e_n \end{bmatrix}.$$

We want to find the variance of $(v+m)^\top \Lambda (v+m)$, where $\Lambda = I$. We can use the formula (assuming "Gaussianity")

$$\begin{aligned}
\mathrm{Var}[(v + m)^\top \Lambda (v + m)] &= 2\,\mathrm{tr}[\Lambda\Sigma\Lambda\Sigma] + 4m^\top\Lambda\Sigma\Lambda m \\
&= 2\,\mathrm{tr}[\Sigma^2] + 4m^\top\Sigma m \\
&\equiv 2k_1 + 4k_2,
\end{aligned}$$

where $\Sigma = \mathrm{Var}[v]$.

Note that $k_1 = \mathrm{tr}[\Sigma^2]$ is the sum of the squared elements of Σ. Now let's compute the elements of Σ.

The diagonal elements we already have from (**??**) and (**??**). The upper triangular elements are as follows. For $1 \le s < t < n$,

$$\begin{aligned}
\Sigma_{st} &= E[(e_s - \phi e_{s+1})(e_t - \phi e_{t+1})] \\
&= E[((\dot\mu_s - \phi)e_{s+1} + u_s)(e_t - \phi e_{t+1})] \\
&= (\dot\mu_s - \phi)\dot\mu_{s+1}\dot\mu_{s+2}\cdots\dot\mu_{t-1}(E[e_t^2] - \phi\dot\mu_t E[e_{t+1}^2]).
\end{aligned}$$

and

$$\begin{aligned}
\Sigma_{sn} &= E[((\dot\mu_s - \phi)e_{s+1} + u_s)\sqrt{1 - \phi^2}e_n] \\
&= (\dot\mu_s - \phi)\dot\mu_{s+1}\dot\mu_{s+2}\cdots\dot\mu_{n-1}\sqrt{1 - \phi^2}E[e_n^2].
\end{aligned}$$

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The sum of squared upper triangular elements—and by symmetry the sum of squared lower triangular elements—is

$$\sum_{s=1}^{n-1}\sum_{t=s+1}^{n}\Sigma_{st}^2 = \iota_{n-1}^\top DAz, \tag{12}$$

where $\iota_{n-1} = (1, 1, \ldots, 1)$, $D = \mathrm{diag}((\dot{\mu}_1 - \phi)^2, \ldots, (\dot{\mu}_{n-1} - \phi)^2)$,

$$A = \begin{bmatrix} 1 & \dot{\mu}_2^2 & \dot{\mu}_2^2\dot{\mu}_3^2 & \dot{\mu}_2^2\dot{\mu}_3^2\dot{\mu}_4^2 & \cdots \\ & 1 & \dot{\mu}_3^2 & \dot{\mu}_3^2\dot{\mu}_4^2 & \cdots \\ & & \ddots & & \\ & & & 1 & \dot{\mu}_{n-1}^2 \\ & & & & 1 \end{bmatrix} = \begin{bmatrix} 1 & -\dot{\mu}_2^2 & & & \\ & 1 & -\dot{\mu}_3^2 & & \\ & & 1 & \ddots & \\ & & & \ddots & -\dot{\mu}_{n-1}^2 \\ & & & & 1 \end{bmatrix}^{-1},$$

$$z = \begin{bmatrix} (E[e_2^2] - \phi\dot{\mu}_2 E[e_3^2])^2 \\ (E[e_3^2] - \phi\dot{\mu}_3 E[e_4^2])^2 \\ \vdots \\ (E[e_{n-1}^2] - \phi\dot{\mu}_2 E[e_n^2])^2 \\ (1 - \phi^2)(E[e_n^2])^2 \end{bmatrix}.$$

Now $v_2 = m^\top\Sigma m = m\Phi M^{-1}\,\mathrm{diag}(\sigma_1^2, \ldots, \sigma_n^2)M^{-1}\Phi^\top m$, where

$$\Phi = \begin{bmatrix} 1 & -\phi & & & \\ & 1 & -\phi & & \\ & & 1 & \ddots & \\ & & & \ddots & -\phi \\ & & & & 1 \end{bmatrix}, \quad \text{and} \quad M = \begin{bmatrix} 1 & -\dot{\mu}_2 & & & \\ & 1 & -\dot{\mu}_3 & & \\ & & 1 & \ddots & \\ & & & \ddots & -\dot{\mu}_{n-1} \\ & & & & 1 \end{bmatrix}.$$

WJM: write up variances and covariances of other terms.

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