1 Basic Linear State Space

1.1 Definition

$$x_t = Fx_{t-1} + \epsilon_t^x \tag{1}$$
$$y_t = Hx_t + \epsilon_t^y \tag{2}$$

$x_t \in \mathbb{R}^{d_x}$ and $y_t \in \mathbb{R}^{d_y}$.

$$\epsilon_t^x \sim \mathcal{N}(0, Q) \tag{3}$$
$$\epsilon_t^y \sim \mathcal{N}(0, R) \tag{4}$$

Q and R are positive definite covariance matrices.

Equivalently in terms of transition and observation densities:

$$p(x_t|x_{t-1}, F, Q) = \mathcal{N}(x_t|Fx_{t-1}, Q) \tag{5}$$
$$p(y_t|x_t, H, R) = \mathcal{N}(y_t|Hx_t, R) \tag{6}$$

The initial state x_1 may be known or may be assigned a Gaussian prior.

1.2 Identifiability

1.3 Bayesian Learning with Gibbs Sampling

Target the joint distribution $p(F, Q, x_{1:T}|y_{1:T})$. Gibbs sampling can be used, targeting the state and parameter posterior conditionals alternately. State conditional sampled by Kalman filtering and backward simulation.

1.3.1 Parameter Conditional

The conjugate prior is:

$$p(F, Q) = p(F|Q)p(Q) \tag{7}$$

$$Q \sim \mathcal{IW}(\nu_0, \Psi_0) \tag{8}$$
$$F|Q \sim \mathcal{MN}(M_0, Q, \Omega_0) \tag{9}$$

So the prior densities are:

$$p(Q) = \frac{|\Psi_0|^{\frac{\nu_0}{2}}}{2^{\frac{\nu_0}{2}} \Gamma\left(\frac{\nu_0}{2}\right)} |Q|^{-\frac{\nu_0+d_x+1}{2}} \exp\left(-\frac{1}{2} \operatorname{Tr}\left[Q^{-1}\Psi_0\right]\right) \tag{10}$$

$$p(F|Q) = |2\pi Q|^{-\frac{1}{2}} |2\pi\Omega_0|^{-\frac{1}{2}} \exp\left(-\frac{1}{2} \operatorname{Tr}\left[Q^{-1}(F-M_0)\Omega_0^{-1}(F-M_0)^T\right]\right) \tag{11}$$

$\nu_0 \in \mathbb{R}, \nu_0 > d_x$. Ψ_0 and Ω_0 are $d_x \times d_x$ positive definite matrices. $M_0 \in \mathbb{R}^{d_x \times d_x}$.

The likelihood function is:

$$p(x_{1:T}|F, Q) = p(x_0) \prod_{t=2}^{T} p(x_t|x_{t-1}, F, Q)$$

$$\propto |Q|^{-\frac{1}{2}(T-1)} \exp\left(-\frac{1}{2} \sum_{t=2}^{T} (x_t - Fx_{t-1})^T Q^{-1}(x_t - Fx_{t-1})\right)$$

$$= |Q|^{-\frac{1}{2}(T-1)} \exp\left(-\frac{1}{2} \operatorname{Tr}\left[Q^{-1} \sum_{t=2}^{T} (x_t - Fx_{t-1})(x_t - Fx_{t-1})^T\right]\right)$$

$$= |Q|^{-\frac{1}{2}S_0} \exp\left(-\frac{1}{2} \operatorname{Tr}\left[Q^{-1}\left(FS_1 F^T - FS_2^T - S_2 F^T + S_3\right)\right]\right) \tag{12}$$

where the sufficient statistics are:

$$S_0 = T - 1 \tag{13}$$

$$S_1 = \sum_{t=2}^{T} x_{t-1} x_{t-1}^T \tag{14}$$

$$S_2 = \sum_{t=2}^{T} x_t x_{t-1}^T \tag{15}$$

$$S_3 = \sum_{t=2}^{T} x_t x_t^T \tag{16}$$

$$\tag{17}$$

The parameter posterior conditional is:

$$p(F, Q | x_{1:T}, y_{1:T}) = p(F|Q, x_{1:T}) p(Q|x_{1:T}) \tag{18}$$

$$Q|x_{1:T} \sim \mathcal{IW}\left(\nu, \Psi\right) \tag{19}$$
$$F|Q, x_{1:T} \sim \mathcal{MN}\left(M, Q, \Omega\right) \tag{20}$$

Hyperparameter updates:

$$\Omega^{-1} = \Omega_0^{-1} + S_1 \tag{21}$$
$$M\Omega^{-1} = M_0\Omega_0^{-1} + S_2 \tag{22}$$
$$\nu = \nu_0 + S_0 \tag{23}$$
$$\Psi = \Psi_0 + S_3 + M_0\Omega_0^{-1}M_0^T - M\Omega^{-1}M^T \tag{24}$$

Proof:

$$
\begin{aligned}
p(F, Q | x_{1:T}, y_{1:T}) &\propto p(x_{1:T}|F, Q) p(F|Q) p(Q) \\
&= |Q|^{-\frac{1}{2}S_0} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[Q^{-1}\left(FS_1F^T - FS_2^T - S_2F^T + S_3\right)\right]\right) \\
&\quad \times |Q|^{-\frac{\nu_0 + d_x + 1}{2}} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[Q^{-1}\Psi_0\right]\right) \\
&\quad \times |Q|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[Q^{-1}(F - M_0)\Omega_0^{-1}(F - M_0)^T\right]\right) \\
&= |Q|^{-\frac{(\nu_0 + S_0) + d_x + 1}{2}} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[Q^{-1}(\Psi_0 + S_3)\right]\right) \\
&\quad \times |Q|^{-\frac{1}{2}} \exp\Bigg(-\frac{1}{2}\operatorname{Tr}\Bigg[Q^{-1}\bigg(F(\Omega_0^{-1} + S_1)F^T - F(\Omega_0^{-1}M_0^T + S_2^T) \\
&\quad\quad\quad - (M_0\Omega_0^{-1} + S_2)F^T + M_0\Omega_0^{-1}M_0^T\bigg)\Bigg]\Bigg)
\end{aligned}
\tag{25}
$$

Finish by completing the square and comparing terms.

2 Degenerate Linear State Space Model

2.1 Definition and Complications

$$x_t = Fx_{t-1} + G\epsilon_t^x \tag{26}$$

$$\epsilon_t^x \sim \mathcal{N}\left(0, I\right) \tag{27}$$

This is equivalent to the basic case, except that $Q = GG^T$ is only positive semi-definite. This is not in itself a problem. The probability distribution associated with each transition is still well-defined, although it does not have a density on $\mathbb{R}^{d_x}$. The state perturbations $(x_t - Fx_{t-1})$ must all lie in a linear subspace.

There are two problems with extending the Gibbs sampling methodology to such a model. First, the state sequence and the transition covariance matrix are too strongly related. The sampled state sequence defines the subspace, so we cannot freely change Q. Second, the conjugate prior is tricky. The matrix-normal-inverse-wishart can be generalised to the case where Q is not full rank (using singular inverse Wishart and singular matrix normal distributions). However, this is not helpful, because it constrains the transition matrix to lie in a linear subspace.

We will need the eigen-decomposition of Q frequently.

$$Q = V\Lambda V^T \tag{28}$$

This is the "non-singular" part of the factorisation, where Λ is a diagonal $r \times r$ matrix with $r = \text{Rank}(Q)$, and V from the appropriate Stiefel manifold. The full decomposition will also be useful at times.

$$Q = \begin{bmatrix} V & V_\perp \end{bmatrix} \begin{bmatrix} \Lambda & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} V^T \\ V_\perp^T \end{bmatrix} \tag{29}$$

2.2 Conjugate Prior

2.2.1 Inverse Wishart Part

There are two ways to extend the inverse Wishart distribution to positive semi-definite matrices. Either let $\nu_0 \in \{z \in \mathbb{N}^+ | z < d_x\}$, in which case $\text{Rank}(Q) = \nu_0$, or let Ψ_0 be positive semi-definite. The latter makes it tricky to work out what we should set Ψ_0 to, so we'll go with the former. If we set ν_0 equal to a known value of the rank r, then the singular Wishart density is,

$$p(Q|r) = \frac{|\Psi_0|^{\frac{r}{2}}}{2^{\frac{1}{2}rd_x}\pi^{\frac{1}{2}r(d_x-r)}\Gamma_r\left(\frac{r}{2}\right)} |\Lambda|^{-\frac{1}{2}(3d_x-r+1)} \exp\left(-\frac{1}{2}Q^+\Psi_0\right). \tag{30}$$

- [7] covers the basic multivariate statistics for the full-rank case.

- [10] covers singular Wishart distributions, including the eigenvalue distribution, and base measure for positive semi-definite matrices.

- [3] covers singular and pseudo Wishart distributions in a thorough and unifying manner.

- [2] covers singular and pseudo inverse Wishart distributions.

- [1] contains a few useful properties.

Note that Ψ_0 is defined as the inverse of what it usually is, for consistency with the basic model case.

2.2.2 Matrix Normal Part

It's fine for the row-variance matrix in a matrix normal distribution to be less than full rank. That just means that the matrix is constrained to lie in a particular subspace. There's even a density associated with this. See [3]. But this is no good as a prior. We want to be able to change the transition matrix freely.

Instead we can use,

$$F|Q \sim \mathcal{MN}\left(M_0, Q + V_\perp\Lambda_\perp V_\perp^T, \Omega_0\right) \tag{31}$$

$\Lambda_\perp$ is a diagonal matrix of positive eigenvalues which relax the constraint to lie in the subspace. They control the rate at which the density decays as we move away from that subspace. Setting these extra eigenvalues might be tricky. I haven't really worked out how to do this well yet. But they can depend on the other ones, so we could take the minimum, maximum or average of the others. Making them really big is uninformative.

2.3 MCMC for Bayesian Learning

A sampled state trajectory $x_{1:T}$ defines the subspace in which the state perturbations must lie, which means that neither F nor Q can be freely changed, and Gibbs sampling alone does not work. However, we can still sample within the space specified by this constraint. Additional MCMC moves will then be needed which allow the subspace to be changed.

2.3.1 Factorising the Covariance

Using Givens rotations, we can efficiently factorise the covariance eigenvector matrix as follows.

$$\begin{bmatrix} V & V_\perp \end{bmatrix} = \begin{bmatrix} U & U_\perp \end{bmatrix} \begin{bmatrix} E & 0 \\ 0 & E_\perp \end{bmatrix} \begin{bmatrix} U_R & 0 \\ 0 & I \end{bmatrix} \begin{bmatrix} I & 0 \\ 0 & U_N \end{bmatrix} \tag{32}$$

So

$$V = UEU_R \tag{33}$$

$$V_\perp = U_\perp E_\perp U_N \tag{34}$$

Then defined the following, which is positive definite

$$D = EU_R \Lambda U_R^T E^T \tag{35}$$

So

$$Q = UDU^T \tag{36}$$

2.3.2 State Trajectory Likelihood

There is no proper transition density over $\mathbb{R}^{d_x}$ for the degenerate model. However, there is a density associated with the underlying state disturbances which allows us to write a likelihood function.

$$x_t = Fx_{t-1} + UD^{\frac{1}{2}}\epsilon_t^x \tag{37}$$

$$\tag{38}$$

$$\Rightarrow U^T(x_t - Fx_{t-1}) \sim \mathcal{N}(0, D) \tag{39}$$

$$p(x_t|x_{t-1}, F, Q) \propto |D|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}(x_t - Fx_{t-1})^T UD^{-1}U^T(x_t - Fx_{t-1})\right) \tag{40}$$

The likelihood function associated with the state trajectory is:

$$p(x_{1:T}|F, Q) = p(x_0) \prod_{t=2}^{T} p(x_t|x_{t-1}, F, Q)$$

$$\propto |D|^{-\frac{1}{2}(T-1)} \exp\left(-\frac{1}{2}\sum_{t=2}^{T}(x_t - Fx_{t-1})^T UD^{-1}U^T(x_t - Fx_{t-1})\right)$$

$$= |D|^{-\frac{1}{2}(T-1)} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[D^{-1}U^T \sum_{t=2}^{T}(x_t - Fx_{t-1})(x_t - Fx_{t-1})^T U\right]\right)$$

$$= |D|^{-\frac{1}{2}S_0} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[D^{-1}\left(U^T FS_1 F^T U - U^T FS_2^T U - U^T S_2 F^T U + U^T S_3 U\right)\right]\right) \tag{41}$$

$$= |D|^{-\frac{1}{2}S_0} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[D^{-1}\left(F_U S_1 F_U^T - F_U S_2^T U - U^T S_2 F_U^T + U^T S_3 U\right)\right]\right) \tag{42}$$

where

$$F_U = U^T F \tag{43}$$

This is all subject to the constraint that each state must be reachable from the previous one, which we can write concisely as,

$$X_{2:T} = FX_{1:T-1} + UZ \tag{44}$$

where $Z \in \mathbb{R}^{r \times d_x}$ and

$$X_{2:T} = \begin{bmatrix} x_2 & x_3 & \dots & x_T \end{bmatrix} \tag{45}$$

2.3.3 Transforming the Prior

If we transform from (F, Q) to (F_U, D), then the prior on these variables is as follows.

Using the transformation property of the matrix normal distribution:

$$F_U|Q = F_U|U, D \sim \mathcal{MN}\left(U^T M_0, D, \Omega_0\right) \tag{46}$$

Using the transformation property of the Wishart distribution:

$$D|U \sim \mathcal{IW}\left(r, (U^T \Psi_0^{-1} U)^{-1}\right) \tag{47}$$

Proof:

$$X \sim \mathcal{W}\left(\nu, \Sigma\right)$$
$$\Rightarrow Z \sim \mathcal{MN}\left(0, I, I\right)$$
$$\text{with } X = \Sigma^{\frac{1}{2}} ZZ^T \Sigma^{\frac{1}{2}}{}^T$$
$$\text{and } Z \in \mathbb{R}^{d \times \nu}$$
$$Y = X^+ = \Sigma^{\frac{1}{2}}{}^{-1}(ZZ^T)^+ \Sigma^{\frac{1}{2}}{}^{-T}$$
$$Y \sim \mathcal{IW}\left(\nu, \Sigma\right)$$
$$AYA^T = A\Sigma^{\frac{1}{2}}{}^{-1}(ZZ^T)^+ \Sigma^{\frac{1}{2}}{}^{-T} A^T$$
$$= (A\Sigma^{\frac{1}{2}}{}^{-1})(ZZ^T)^+(A\Sigma^{\frac{1}{2}}{}^{-1})^T$$
$$\Rightarrow AYA^T \sim \mathcal{IW}\left(\nu, \left((A\Sigma^{\frac{1}{2}}{}^{-1})(A\Sigma^{\frac{1}{2}}{}^{-1})^T\right)^{-1}\right)$$
$$AYA^T \sim \mathcal{IW}\left(\nu, \left((A\Sigma^{-1}A^T)^{-1}\right)\right)$$

$$\tag{48}$$

2.3.4 Within-Subspace Parameter Conditional

We can now get to the conditional distribution for $p(F_U, D|U, x_{1:T})$ which is well-behaved and can be sampled.

The parameter posterior conditional is:

$$p(F_U, D|U, x_{1:T}, y_{1:T}) = p(F_U|D, U, x_{1:T})p(D|U, x_{1:T}) \tag{49}$$

$$D|U, x_{1:T} \sim \mathcal{IW}\left(\nu, \Psi\right) \tag{50}$$
$$F_U|D, U, x_{1:T} \sim \mathcal{MN}\left(M, Q, \Omega\right) \tag{51}$$

Hyperparameter updates:

$$\Omega^{-1} = \Omega_0^{-1} + S_1 \tag{52}$$
$$M\Omega^{-1} = U^T\left(M_0\Omega_0^{-1} + S_2\right) \tag{53}$$
$$\nu = r + S_0 \tag{54}$$
$$\Psi = (U^T\Psi_0^{-1}U)^{-1} + U^T\left(S_3 + M_0\Omega_0^{-1}M_0^T\right)U - M\Omega^{-1}M^T \tag{55}$$

Proof:

$$
\begin{aligned}
p(F_U, D|U, x_{1:T}) &\propto p(x_{1:T}|F_U, D, U)p(F_U|D, U)p(D|U) \\
&\propto |D|^{-\frac{1}{2}S_0} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[D^{-1}\left(F_U S_1 F_U^T - F_U S_2^T U - U^T S_2 F_U^T + U^T S_3 U\right)\right]\right) \\
&\quad \times |D|^{-\frac{1}{2}(r+r+1)} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[D^{-1}(U^T \Psi_0^{-1}U)^{-1}\right]\right) \\
&\quad \times |D|^{-\frac{1}{2}} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[D^{-1}(F_U - U^T M_0)\Omega_0^{-1}(F_U - U^T M_0)^T\right]\right) \\
&= |D|^{-\frac{1}{2}((r+S_0)+r+1)} \exp\left(-\frac{1}{2}\operatorname{Tr}\left[D^{-1}\left((U^T \Psi_0^{-1}U)^{-1} + U^T S_3 U\right)\right]\right) \\
&\quad \times |D|^{-\frac{1}{2}} \exp\Bigg(-\frac{1}{2}\operatorname{Tr}\Bigg[D^{-1}\Bigg(F_U(\Omega_0^{-1} + S_1)F_U^T - F_U(\Omega_0^{-1}M_0^T + S_2^T)U \\
&\qquad\qquad\qquad\qquad - U^T(M_0\Omega_0^{-1} + S_2)F_U^T + U^T M_0 \Omega_0^{-1} M_0^T U\Bigg)\Bigg]\Bigg)
\end{aligned}
\tag{56}
$$

Finish by completing the square and comparing terms.

Of course, we want F, not F_U. We can recover the matrix uniquely using the constraint from the likelihood. The previous value of F from before we sampled must have satisfied this constraint. Let's call that matrix F^*.

$$
\begin{aligned}
X_{2:T} &= F^* X_{1:T-1} + U Z^* \\
X_{2:T} &= F X_{1:T-1} + U Z \\
\Rightarrow 0 &= (F - F^*)X_{1:T-1} + U(Z - Z^*) \tag{57} \\
\Rightarrow 0 &= (F_U - F_U^*)X_{1:T-1} + (Z - Z^*) \tag{58} \\
\Rightarrow 0 &= (F - F^*)X_{1:T-1} - U(F_U - F_U^*)X_{1:T-1} \tag{59} \\
0 &= \left[(F - F^*) - U(F_U - F_U^*)\right]X_{1:T-1} \tag{60} \\
\Rightarrow 0 &= (F - F^*) - U(F_U - F_U^*) \tag{61}
\end{aligned}
$$

$$
\begin{aligned}
F &= F^* + U(F_U - F_U^*) \\
&= F^* + U(F_U - U^T F^*) \\
&= (I - UU^T)F^* + U F_U \tag{62}
\end{aligned}
$$

2.3.5 Metropolis-Hastings for the Covariance Subspace

In order to change U, we can target $p(Q|F, y_{1:T})$ with Metropolis-Hastings, which is justified as a collapsed Gibbs move.

We sample a rotation matrix Ξ from some proposal distribution with density ς (w.r.t. Haar measure on orthogonal matrices) and then apply the following transformation,

$$
\begin{bmatrix} Q' \\ \Xi' \end{bmatrix} = \begin{bmatrix} \Xi Q \Xi^T \\ \Xi^T \end{bmatrix},
$$

which is clearly its own inverse. Since $|\Xi| = 1$, it is straightforward to show that the Jacobian of this transformation is 1, and hence using the reversible jump interpretation of Metropolis-Hastings [4,5], the acceptance probability is,

$$
\begin{aligned}
\alpha(Q \to Q') &= \min\left\{1, \frac{p(Q'|F, y_{1:T})\varsigma(\Xi')}{p(Q|F, y_{1:T})\varsigma(\Xi)}\right\} \tag{63} \\
&= \min\left\{1, \frac{p(y_{1:T}|F, Q')}{p(y_{1:T}|F, Q)} \times \frac{p(Q', F)}{p(Q, F)} \times \frac{\varsigma(\Xi')}{\varsigma(\Xi)}\right\}.
\end{aligned}
$$

The first term is simply a ratio of Kalman filter likelihoods.

There are numerous ways to sample the rotation matrix Ξ from a suitable proposal distribution ς. For example, we could use the Cayley transform [6], a bijective mapping from the skew-symmetric matrices to the rotation matrices, defined by,

$$
P(S) = (I - S)^{-1}(I + S). \tag{64}
$$

The matrix exponential would also work. Note that the Jacobian of the Cayley transformation is derived in [8], but this is not needed as it cancels out.

To sample from ς, we draw $\frac{1}{2}d_x(d_x - 1)$ independent scalar random variables $\{s_{i,j}\}_{0<i<j<d_x}$ from any zero-mean distribution; a nice choice is,

$$s_{k,l} \sim \mathcal{N}\left(0, \sigma_s^2\right). \tag{65}$$

Use these to construct a skew-symmetric matrix S,

$$S_{k,l} = \begin{cases} s_{k,l} & k < l \\ -s_{l,k} & k > l \\ 0 & k = l, \end{cases} \tag{66}$$

and then set $\Xi = P(S)$. The Cayley transform has the property that $P(-S) = P(S^T) = P(S)^{-1} = P(S)^T$, which implies that $\varsigma(\Xi) = \varsigma(\Xi^T) = \varsigma(\Xi')$, leading to a cancellation in the acceptance probability.

There is an alternative using Givens rotations. First sample $i \in [1, d_x]$, $j \in [1, d_x] \setminus i$, and $\gamma \in [-\pi/2, \pi/2]$ from some zero-mean distribution. Form the Givens matrix $\Gamma_{i,j}(\gamma)$ such that,

$$[\Gamma_{i,j}(\gamma) - I]_{k,l} = \begin{cases} \cos(\gamma) - 1 & k = l = i \text{ or } k = l = j \\ \sin(\gamma) & k = i, l = j \\ -\sin(\gamma) & k = j, l = i \\ 0 & \text{otherwise}, \end{cases} \tag{67}$$

and use $\Xi = \Gamma_{i,j}(\gamma)$. This also has the property that $\Gamma_{i,j}(-\gamma) = \Gamma_{i,j}(\gamma)^T$, meaning that we achieve the same cancellation of the proposals as before.

2.3.6 Metropolis-Hastings for the Transition Matrix

Define π as the posterior density, conditioning on $y_{1:T}$.

If we modify the covariance matrix slightly so that it is no longer singular, then we can use the existing sampling procedure from the basic linear model and treat the resulting value of F as a proposal in a Metropolis-Hastings kernel targeting $\pi(F, x_{1:T}|Q)$.

Suppose we start with sampled values of F,Q and $x_{1:T}$. A suitably modified non-singular covariance matrix is,

$$\widetilde{Q} = Q + \delta I, \tag{68}$$

where δ is a small positive constant. We propose a new value of F by sampling,

$$F' \sim \pi(F|\widetilde{Q}, x_{1:T}). \tag{69}$$

This distribution is simply a Gaussian and we can evaluate the density using (??). Finally, we also sample a new state trajectory using forward filtering backward sampling,

$$x'_{1:T} \sim \pi(x_{1:T}|F', Q). \tag{70}$$

The acceptance probability is simply,

$$\begin{aligned} \alpha\left(F, x_{1:T} \to F', x'_{1:T}\right) \\ = \min&\left\{1, \frac{\pi(F', x'_{1:T}|Q)\pi(x_{1:T}|F, Q)\pi(F|\widetilde{Q}, x'_{1:T})}{\pi(F, x_{1:T}|Q)\pi(x'_{1:T}|F', Q)\pi(F'|\widetilde{Q}, x_{1:T})}\right\} \\ = \min&\left\{1, \frac{\pi(F'|Q)\pi(F|\widetilde{Q}, x'_{1:T})}{\pi(F|Q)\pi(F'|\widetilde{Q}, x_{1:T})}\right\} \\ = \min&\left\{1, \frac{p(y_{1:T}|F', Q)}{p(y_{1:T}|F, Q)} \times \frac{p(F'|Q)}{p(F|Q)} \times \frac{\pi(F|\widetilde{Q}, x'_{1:T})}{\pi(F'|\widetilde{Q}, x_{1:T})}\right\}, \end{aligned} \tag{71}$$

in which the first term is a ratio of Kalman filter likelihoods.

2.3.7 Metropolis-Hastings for the Covariance Matrix Rank

It is unlikely that the rank of Q will be known a priori. We can learn this within the MCMC scheme by allowing the sampler to add and remove eigenvalue-eigenvector pairs using reversible jump moves [4, 5]. This can be achieved with a matching pair of moves. The eigenvalues are assumed to be sorted in descending order of magnitude, so that λ_1 is the largest.

Algorithm 1 Reversible Jump Move: Increase rank

Require: r, Q
   Set $r' = r + 1$.
   Sample a new eigenvector $v_{r'}$.
   Sample a new eigenvalue $\lambda_{r'} \in [0, \lambda_r]$.
   $Q' = Q + \lambda_{r'} v_{r'} v_{r'}^T$.
   return r', Q'

Algorithm 2 Reversible Jump Move: Decrease rank

Require: r', Q'
   $Q = Q' - \lambda_{r'} v_{r'} v_{r'}^T$.
   Set $r = r' - 1$.
   return r, Q

The acceptance probabilities are then,

$$\alpha(r, Q \to r', Q') = \min\{1, \beta\} \tag{72}$$

$$\alpha(r', Q' \to r, Q) = \min\{1, \beta^{-1}\}, \tag{73}$$

with,

$$\beta = \frac{\pi(r', Q'|F, x_{1:T}) J(Q, \lambda_{r'}, v_{r'} \to Q')}{\pi(r, Q|F, x_{1:T}) q_\lambda(\lambda_{r'}|Q) q_v(v_{r'}|Q)} \tag{74}$$

$$= \frac{p(x_{1:T}|F, Q') p(Q'|r', F) p(r') J(Q, \lambda_{r'}, v_{r'} \to Q')}{p(x_{1:T}|F, Q) p(Q|r, F) p(r) q_\lambda(\lambda_{r'}|Q) q_v(v_{r'}|Q)} \tag{75}$$

$$= \frac{p(x_{1:T}|F, Q') p(F, Q'|r') p(r')}{p(x_{1:T}|F, Q) p(F, Q|r) p(r)} \times \frac{J(Q, \lambda_{r'}, v_{r'} \to Q')}{q_\lambda(\lambda_{r'}|Q) q_v(v_{r'}|Q)}, \tag{76}$$

where $J(Q, \lambda_{r'}, v_{r'} \to Q')$ is the Jacobian of the transformation from Q to Q', and q_λ and q_v are the probability densities for the eigenvalue and eigenvector proposal distributions respectively, with respect to appropriate measures. The second term is a tricky beast, particularly the Jacobian.

The volume element (ignoring sign) on the set of positive semi-definite matrices can be written in terms of the eigen-decomposition as follows [2, 3, 10],

$$(dQ) = 2^{-r} \times \prod_{i=1}^{r} \lambda_i^{d_x - r} \times \prod_{j=1}^{r} \prod_{i=1}^{j-1} (\lambda_i - \lambda_j) \times (V^T dV) \wedge \bigwedge_{i=1}^{r} d\lambda_i, \tag{77}$$

where $(V^T dV)$ is the Haar measure on the appropriate Stiefel manifold [7],

$$(V^T dV) = \bigwedge_{i=1}^{r} \bigwedge_{j=i+1}^{d_x} v_j^T dv_i. \tag{78}$$

Similarly,

$$(dQ') = 2^{-r-1} \times \prod_{i=1}^{r+1} \lambda_i^{d_x - r - 1} \times \prod_{j=1}^{r+1} \prod_{i=1}^{j-1} (\lambda_i - \lambda_j) \times \left(V'^T dV'\right) \wedge \bigwedge_{i=1}^{r+1} d\lambda_i$$

$$= \left[2^{-1} \lambda_{r+1}^{d_x - r - 1} \prod_{i=1}^{r} \lambda_i^{-1} \prod_{i=1}^{r} (\lambda_i - \lambda_{r+1}) \right]$$

$$\times 2^{-r} \times \prod_{i=1}^{r} \lambda_i^{d_x - r} \times \prod_{j=1}^{r} \prod_{i=1}^{j-1} (\lambda_i - \lambda_j) \times \left(V'^T dV'\right) \wedge \bigwedge_{i=1}^{r+1} d\lambda_i,$$

where

$$\left(V'^T dV'\right) = \bigwedge_{i=1}^{r+1} \bigwedge_{j=i+1}^{d_x} v_j^T dv_i$$

$$= \bigwedge_{i=1}^{r} \bigwedge_{j=i+1}^{d_x} v_j^T dv_i \wedge \bigwedge_{j=r+2}^{d_x} v_j^T dv_i. \tag{79}$$

A suitable base measure for the new eigenvector can be formulated by considering the following generative procedure. This new eigenvector $v_{r'}$ must have unit magnitude and be orthogonal to the existing eigenvectors of Q. This can be achieved by sampling $u \in \{u \in \mathbb{R}^{d_x - r} : |u| = 1\}$ according to the Haar probability measure on this set and setting $v_{r'} = V_\perp u$. Since this is another Stiefel manifold, the volume element for this set is [7],

$$\left(u^T du\right) = \bigwedge_{j=2}^{d_x - r} u_j^T du \tag{80}$$

where $u_2, \ldots, u_{d_x - r}$ is any set of unit vectors orthogonal to u. Using the transformation,

$$\left(v_{r'}^T dv_{r'}\right) = \left(u^T V_\perp^T V_\perp du\right)$$

$$= \left(u^T du\right)$$

$$= \bigwedge_{j=2}^{d_x - r} u_j^T du$$

$$= \bigwedge_{j=2}^{d_x - r} u_j^T V_\perp^T dv_{r'}$$

$$= \bigwedge_{j=r+2}^{d_x} v_j'^T dv_{r'}, \tag{81}$$

where $v_j' = V_\perp u_{r+j}$ are the columns of the new $V_\perp'$.

The base measure for the new eigenvalue is Lesbegue.

Thus, the Jacobian is,

$$J(Q, \lambda_{r'}, v_{r'} \to Q') = \frac{(dQ')}{(dQ)\left(v_{r'}^T dv_{r'}\right)(d\lambda_{r'})}$$

$$= 2^{-1} \lambda_{r+1}^{d_x - r - 1} \prod_{i=1}^{r} \lambda_i^{-1} \prod_{i=1}^{r} (\lambda_i - \lambda_{r+1}) \tag{82}$$

The density of the proposal distribution for the new eigenvector is simply the reciprocal of the volume of the set, which is a half of a hypersphere (since we have to resolve the eigenvector sign ambiguity). Thus,

$$q_v(v_{r'}|Q) = \frac{\Gamma\left(\frac{d_x - r}{2}\right)}{\pi^{\frac{1}{2}(d_x - r)}}. \tag{83}$$

For the eigenvalue, we can use any distribution over $[0, \lambda_r]$, e.g. uniform.

So,

$$\beta = \frac{p(x_{1:T}|F, Q')p(F, Q'|r')p(r')}{p(x_{1:T}|F, Q)p(F, Q|r)p(r)} \times \frac{J(Q, \lambda_{r'}, v_{r'} \to Q')}{q_\lambda(\lambda_{r'}|Q)q_v(v_{r'}|Q)}$$

$$= \frac{p(x_{1:T}|F, Q')p(F, Q'|r')p(r')}{p(x_{1:T}|F, Q)p(F, Q|r)p(r)} \times \frac{\pi^{\frac{1}{2}(d_x - r)} \prod_{i=1}^{r} \lambda_i^{-1}}{2\,\Gamma\left(\frac{d_x - r}{2}\right)} \times \frac{\lambda_{r+1}^{d_x - r - 1} \prod_{i=1}^{r}(\lambda_i - \lambda_{r+1})}{q_\lambda(\lambda_{r+1}|Q)}.$$

3 Additional Notes

I originally focussed on methods where the prior dependence between F and Q was broken, and the two were sampled alternately. To do this efficiently (with matrix normal distribution for the transition matrix) requires using eigen-decompositions in a manner inspired by this paper: [9].

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