State Space Loglikelihood Gradient Calculation

Using the preferred (Harvey 1989) timing for the state space model,

$$
\begin{aligned}
y_t &= Z_t \alpha_t + d_t + \epsilon_t & \epsilon_t &\sim N(0, H_t) \\
\alpha_t &= T_t \alpha_{t-1} + c_t + R_t \eta_t & \eta_t &\sim N(0, Q_t)
\end{aligned}
$$

the likelihood of of data $\mathbf{Y}_t$ is given by $L_n \equiv \sum_{t=1}^n \ell_t$ where

$$
\ell_t = -\frac{p}{2}\log(2\pi) - \frac{1}{2}\log|F_t| + v_t' F_t^{-1} v_t
$$

$$
\begin{aligned}
a_t &= T_t a_{t-1} + c_t + K_t v_t & P_t &= T_t P_{t-1} L_{t-1} + R_t Q_t R_t' \\
v_t &= y_t - d_t - Z_t a_t & F_t &= Z_t P_t Z_t' + H_t \\
M_t &= P_t Z_t' F_t^{-1} & K_t &= T_{t+1} M_t \\
L_t &= T_{t+1} - K_t Z_t & w_t &= F_t^{-1} v_t
\end{aligned}
$$

From Nagakura (working paper), we can get the gradient:

$$
\begin{aligned}
G_\theta(\ell_t) = {} & G_\theta(a_t) Z_t' w_t \\
& + \frac{1}{2} G_\theta(P_t) \mathrm{vec}(Z_t' w_t w_t' Z_t - Z_t' F_t^{-1} Z_t) \\
& + G_\theta(d_t) w_t \\
& + G_\theta(Z_t) \mathrm{vec}(w_t a_t' + w_t v_t' M_t' - M_t') \\
& + \frac{1}{2} G_\theta(H_t) \mathrm{vec}(w_t w_t' - F_t^{-1})
\end{aligned}
$$

where

$$
\begin{aligned}
G_\theta(a_{t+1}) = {} & G_\theta(a_t) L_t' \\
& + G_\theta(P_t)(Z_t' w_t \otimes L_t') \\
& + G_\theta(c_{t+1}) \\
& - G_\theta(d_t) K_t' \\
& + G_\theta(Z_t)[P_t L_t' \otimes w_t - (a_t + M_t v_t) \otimes K_t'] \\
& - G_\theta(H_t)(w_t \otimes K_t') \\
& + G_\theta(T_{t+1})[(a_t + M_t v_t) \otimes I_m]
\end{aligned}
$$

$$
\begin{aligned}
G_\theta(P_{t+1}) = {} & G_\theta(P_t)(L_t' \otimes L_t') \\
& + G_\theta(H_t)(K_t' \otimes K_t') \\
& + G_\theta(Q_{t+1})(R_{t+1}' \otimes R_{t+1}') \\
& + [G_\theta(T_{t+1})(P_t L_t' \otimes I_m) \\
& \qquad - G_\theta(Z_t)(P_t L_t' \otimes K_t') \\
& \qquad + G_\theta(R_{t+1})(Q_{t+1} R_{t+1}' \otimes I_m)] N_m
\end{aligned}
$$

The initial conditions for the recursion are given by a simplification of the expressions above (which can also be easily derived from the explicit expressions for a_1 and P_1):

$$\begin{aligned} G_\theta(a_1) = G_\theta(a_0)T_1' \\ + G_\theta(c_1) \\ + G_\theta(T_1)[a_0 \otimes I_m] \end{aligned}$$

$$\begin{aligned} G_\theta(P_1) = G_\theta(P_0)(T_t' \otimes T_t') \\ + G_\theta(Q_1)(R_1' \otimes R_1') \\ + [G_\theta(T_1)(P_0T_1' \otimes I_m) \\ + G_\theta(R_1)(Q_1R_1' \otimes I_m)]N_m \end{aligned}$$

To determine $G_\theta(a_0)$ and $G_\theta(P_0)$ when a_0 and P_0 are set as the unconditional mean and variance of the state (i.e., when they are not explicitly provided and the system is stationary) use the definitions of the unconditional state:

$$\begin{aligned} a_0 &= (I_m - T)^{-1}c \\ G_\theta(a_0) &= G_\theta([I_m - T]^{-1}c) \\ &= G_\theta([I_m - T]^{-1})(c \otimes I_m) + G_\theta(c)(I_1 \otimes [(I_m - T)^{-1})]' \\ &= -G_\theta(I_m - T)[(I_m - T)^{-1} \otimes (I_m - T)^{-1}](c \otimes I_m) + G_\theta(c)(I_m - T)'^{-1} \\ &= G_\theta(T)[(I_m - T)^{-1} \otimes (I_m - T)^{-1}](c \otimes I_m) + G_\theta(c)(I_m - T)'^{-1} \end{aligned}$$

$$\begin{aligned} \text{vec}(P_0) &= (I_{m^2} - T \otimes T)^{-1}\text{vec}(RQR') \\ G_\theta(P_0) &= G_\theta(\text{vec}(P_0)) \\ &= G_\theta(S \ \text{vec}(RQR')) \\ &= G_\theta(S)[\text{vec}(RQR') \otimes I_{m^2}] + G_\theta(\text{vec}(RQR'))(I_1 \otimes S') \\ &= -G_\theta(I_{m^2} - T \otimes T)(S \otimes S')[\text{vec}(RQR') \otimes I_{m^2}] \\ &\quad + [G_\theta(R)(QR' \otimes I_m)N_m + G_\theta(Q)(R' \otimes R')]S' \\ &= G_\theta(T \otimes T)(S \otimes S')[\text{vec}(RQR') \otimes I_{m^2}] \\ &\quad + [G_\theta(R)(QR' \otimes I_m)N_m + G_\theta(Q)(R' \otimes R')]S' \end{aligned}$$

where $S = (I_{m^2} - T \otimes T)^{-1}$. Note that $G_\theta(T \otimes T)$ must be computed separately.