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## A Multivariate Dynamic Statistical Model of the Global Carbon Budget 1959—2020

### A note on the minimal representation of the linear state space model

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In the paper, we have specified a state vector of 17 entries, many of them redundant in a mathematical sense ( $G\_ATM^*$ ,  $S\_LND^*$ ,  $S\_OCN^*$  are all linear functions of  $C^*$ ). Many constant states were added to the state vector as an implementation device for model parameters. It is often interesting to consider the representation of a state space model with a minimum number of states, see, for example, Hannan and Deistler (2012). This is the representation that we present in this note.

## 1 The state equation

The three key budget variables are placed in the  $3 \times 1$  vector  $B_t^* = (C_t^*, E_t^*, X_t^E)'$ . The state space formulation requires Markovian (first-order autoregressive) updating equations for the  $3 \times 1$  vector  $B_t^*$  and for the  $4 \times 1$  vector  $X_t$  with its  $i$ th element given by  $X_{i,t}$ , for  $i = 1, \dots, 4$ . Given the established dynamic properties for the GCB variables, we can represent all variables as a first-order vector autoregressive model. In case of the concentration variable  $C_t^*$ , using the state equations defined in Section 2.4 in the paper, we can write  $(1 + \beta)C_{t+1}^* = k + C_t^* + E_t^* - \beta \text{ENSO}_{t+1} + \beta_5 \Delta \text{ECON}_{t+1} + X_t^E$ , for constants  $k = -c_1 - c_2$  and  $\beta = (\beta_1 + \beta_2)/C_{1750}$ . We recall that ENSO and ECON are treated as exogenous to the system. The autoregressive equation for CO<sub>2</sub> concentrations is then given by

$$C_{t+1}^* = \delta k + \delta C_t^* - \delta \beta \text{ENSO}_{t+1} + \delta E_t^* + \delta \beta_5 \Delta \text{ECON}_{t+1} + \delta X_t^E, \quad (1)$$

with  $\delta := (1 + \beta)^{-1} < 1$ . The vector autoregressive equation for  $B_t^*$  is then given by

$$B_{t+1}^* = b + \Xi B_t^* + \tilde{\Gamma} U_t + V \kappa_t,$$

where  $U_t = (\text{ENSO}_{t+1}, \Delta \text{ECON}_{t+1})'$  contains the exogenous variables, and

$$b = \begin{pmatrix} \delta k \\ d \\ 0 \end{pmatrix}, \quad \Xi = \begin{bmatrix} \delta & \delta & \delta \\ 0 & 1 & 1 \\ 0 & 0 & \phi_E \end{bmatrix}, \quad \tilde{\Gamma} = \begin{bmatrix} -\delta \beta & \delta \beta_5 \\ 0 & \beta_5 \\ 0 & 0 \end{bmatrix}, \quad V = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

The updating equation for  $X_t$  is given by

$$X_{t+1} = \Phi X_t + \eta_t,$$

where  $\Phi$  is a diagonal  $4 \times 4$  matrix with entries  $\phi_1, \dots, \phi_4$  and  $\eta_t$  is a  $4 \times 1$  vector with its  $i$ th element  $\eta_{i,t}$  for  $i = 1, \dots, 4$ .

The linear state space representation of the GCB model is obtained by defining the state vector  $\alpha_t = (B_t^*, X_t')'$  that contains all unobserved variables in the GCB model and the innovation vector  $\xi_t = (\kappa_t, \eta_t')'$ . The updating or state equation is then given by

$$\alpha_{t+1} = a + T\alpha_t + \Gamma U_t + R\xi_t, \quad a = \begin{pmatrix} b \\ 0 \end{pmatrix}, \quad T = \begin{bmatrix} \Xi & 0 \\ 0 & \Phi \end{bmatrix}, \quad \Gamma = \begin{bmatrix} \tilde{\Gamma} \\ 0_{4 \times 2} \end{bmatrix}, \quad R = \begin{bmatrix} V & 0 \\ 0 & I_4 \end{bmatrix}, \quad (2)$$

where  $I_4$  is the  $4 \times 4$  identity matrix,  $0_{4 \times 2}$  is a  $4 \times 2$  matrix of zeroes, and  $U_t$  is treated as exogenous regressors (Durbin and Koopman, 2012, section 3.2.5). The variance matrix of the zero mean innovation vector  $\xi_t$  is given by

$$\text{Var}(\xi_t) = Q = D \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & r_{12} & r_{13} & r_{14} \\ 0 & r_{12} & 1 & r_{23} & r_{24} \\ 0 & r_{13} & r_{23} & 1 & r_{34} \\ 0 & r_{14} & r_{24} & r_{34} & 1 \end{bmatrix} D,$$

where  $D$  is a diagonal  $5 \times 5$  matrix with elements  $\sigma_\kappa, \sigma_1, \dots, \sigma_4$ . Conditional on the variables  $E_t^*$  and  $U_t$ , the variable  $C_t^*$  follows a stationary process, while all remaining variables in the vectors  $B_t^*$  and  $X_t$  are also stationary. This implies that the initial conditions for all variables in the state vector  $\alpha_t$  are properly defined except the one for  $E_t^*$ , which can be treated using a *diffuse prior* (Durbin and Koopman, 2012, section 5.2).

## 2 The observation vector equation

The observation equation for  $y_t = (C_t, S\_LND_t, S\_OCN_t, E_t)'$  follows immediately from the definitions in Section 2.5 of the paper; it is given by

$$y_t = z + Z\alpha_t + PU_t, \quad z = \begin{pmatrix} 0 \\ c_1 \\ c_2 \\ 0 \end{pmatrix}, \quad Z = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 0 \\ \bar{\beta}_1 & 0 & 0 & 0 & 1 & 0 & 0 \\ \bar{\beta}_2 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad P = \begin{bmatrix} 0 & 0 \\ \beta_3 & 0 \\ \beta_4 & 0 \\ 0 & 0 \end{bmatrix},$$

where  $\bar{\beta}_j = \beta_j / C_{1750}$ , for  $j = 1, 2$ . We emphasize that this observation equation has no additive disturbance vector: the *signal* is constructed from the elements in  $B_t^*$  and the *noise* is represented by the elements in  $X_t$ . Both the signal and noise variables are contained in the state vector  $\alpha_t$ . Finally, we notice that for the identification (or estimation) of the signal, the observation variables  $C_t$  and  $E_t$  are sufficient. However, the land and ocean sink observation variables,  $S\_LND_t$  and  $S\_OCN_t$ , need to be included in the model, since they are instrumental for the budget equation to hold. The observation vector equation can easily be extended with exogenous effects such as explanatory and dummy variables (Durbin and Koopman, 2012, section 3.2.5).

The state space framework facilitates the signal extraction of the variables of interest such as those in vector  $B_t^*$ , but also  $S\_LND_t^*$ ,  $S\_OCN_t^*$  and other functions of  $B_t^*$ , the estimation of the parameters in the system matrices, and forecasting. Assuming that the innovation vector  $\xi_t$  in equation (2) is normally distributed, the log-likelihood function is evaluated by the Kalman filter via the prediction error decomposition. We adopt the method of maximum likelihood for parameter estimation, where the maximization of the log-likelihood function relies on a numerical optimization method. When the model is correctly specified, the standardized prediction errors should be normally, independently

and identically distributed with zero mean and unit variance. Various residual diagnostics can be used to verify these properties. Finally, the smoothed estimates of the state vector (based on all data) are obtained from the Kalman filter and a related smoothing method.

## References

**Durbin, J. and S. J. Koopman**, *Time series analysis by state space methods*, 2nd ed., Oxford University Press, 2012.

**Hannan, E.J. and M. Deistler**, *The statistical theory of linear systems*, SIAM, 2012.