Diagnosing Shocks in Time Series

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Efficient means of modeling aberrant behavior in times series are developed. Our methods are based on state-space forms and allow test statistics for various interventions to be computed from a single run of the Kalman filter smoother. The approach encompasses existing detection methodologies. Departures commonly observed in practice, such as outlying values, level shifts, and switches, are readily dealt with. New diagnostic statistics are proposed. Implications for structural models, autoregressive integrated moving average models, and models with explanatory variables are given.

KEY WORDS: Dynamic regression models; Interventions; Kalman filter; Outliers; Smoothing; State-space models.

1. INTRODUCTION

Many time series are subject to external influences. Our interest lies with sudden or unexpected events such as natural disasters, strikes, wars, the introduction of new legislation, or mistakes in recording data. Interventions are by nature hard to characterize in terms of quantities that can be measured. They are often modeled using dummy variables.

The problem is often viewed as one of diagnostic checking or outlier detection. Given a fitted model, are there movements in the series that are not adequately accounted for? Early methods were based on assumptions of independence. Fox (1972) pointed out that this is inadequate. He developed two models for outliers: additive and innovative. Iterative procedures for detecting additive, and innovative outliers and distinguishing between them were proposed by Chang, Tiao, and Chen (1988) and Tsay (1986). Tsay (1988) extended his method to include level shifts and changes in variance. All of the these methods are based on autoregressive integrated moving average (ARIMA) models. Many authors, including LeFrançois (1991) and Tsay (1986) have pointed out that outliers or structural changes can introduce serious bias in the sample autocorrelation function, leading to problems with model identification. Balke (1993) established that using Tsay's approach, level shifts may be labelled as innovative outliers.

Harvey and Durbin (1986) provided a practical example of intervention analysis using structural models. Details of the general approach have been given by Harvey (1989). The use of smoothed disturbances as a means of diagnostic checking was put forward by Harvey and Koopman (1992).

Intervention analysis in regression is typically carried out using deletion diagnostics (Atkinson 1985; Cook 1977; Cook and Weisberg 1982). An estimate of the regression parameter using the full dataset is compared with an estimate based on the data with observations removed. Statistics based on the difference, such as Cook's distance (Cook 1977), are used to identify outlying points. To detect stretches of overinfluential observation, Bruce and Martin (1989) put forward leave-k-out diagnostics. But in time series many types of intervention do not fit into the leave-k-out approach. The method also requires a great deal of computationally intensive parameter reestimation. These problems have been considered by Atkinson, Koopman, and Shephard (1997), who used score statistics to approximate the changes in hyperparameters when interventions are introduced into a series.

Recently, methods have been proposed (Carter and Kohn 1994; McCulloch and Tsay 1993; Shephard 1994) in which all hyperparameters, including those associated with the possible location and size of shocks, are estimated simultaneously within a single framework. Estimation is based on Markov chain Monte Carlo, an approach more computationally expensive than conventional parameter estimation. The resulting estimated model is typically of state-space form and can be checked using the diagnostics described in this article.

Diagnostic checking implicitly involves comparison of a fitted null model to an alternative. This article proposes a method in which the null can be any model that has a state-space representation. The alternative reflects the suspected inadequacy in the null. The addition of shocks can be used to model a large range of potential structural changes. We demonstrate that all statistics associated with these interventions can be generated from a single run of the Kalman filter smoother (KFS) applied to the null model.

The proposed statistics for detecting aberrant behavior are calculated directly from the fitted null model output. If unusual behavior is found, the model can be refitted taking into account the additional structure and the diagnostic procedure repeated, in the spirit of Box and Jenkins (1976). In general, statistics for detecting structural changes in time series are serially correlated. Plots of test statistics against time provide a useful alternative to formal testing. Here we focus on general multivariate time series; however, for simplicity, the results can be thought of in terms of univariate series. Conditional expectation is defined in the linear predictor sense, and conditional covariance is the covariance of the prediction errors. Both of these quantities are defined with respect to the null model.

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The layout of this article is as follows. Terminology is defined and estimation of interventions discussed in Section 2. An efficient representation of interventions via shocks in state-space models is put forward in Section 3. This leads to the key result that diagnostics can be generated from the output of a single null model KFS run. New statistics are suggested in Section 4, and the application of our results to structural time series and ARIMA models is explored in Section 5. Models with explanatory variables are discussed in Section 6, and the general composite intervention case is covered in Section 7. Proofs are given in the Appendix.

2. INTERVENTIONS

Assume that there is a model that is thought, at least initially, to be an appropriate representation of the process that generates the data $\mathbf{y} = (\mathbf{y}_1', \ldots, \mathbf{y}_n')'$. This is referred to as the null model. Assume that the null model states that $\mathbf{y}$ has mean $\mathbf{0}$ and covariance matrix $\sigma^2\mathbf{\Sigma}$, denoted by $\mathbf{y} \sim (\mathbf{0}, \sigma^2\mathbf{\Sigma})$. The matrix $\mathbf{\Sigma}$ gives the serial correlation of the series. Explanatory variables, such as mean effects or exogenous observed series, can readily be included and are dealt with in Section 6. We want to check for departures from the null model. These are modeled by the addition of an intervention variable, $\mathbf{D} = (\mathbf{D}_1', \ldots, \mathbf{D}_n')'$. The alternative is denoted by $\mathbf{y} \sim (\mathbf{D}\boldsymbol{\delta}, \sigma^2\mathbf{\Sigma})$ which reduces to the null if $\boldsymbol{\delta} = \mathbf{0}$.

For a univariate series with δ scalar, $\mathbf{D}$ is a column vector called the *intervention signature.* More generally, each column of $\mathbf{D}$ defines an intervention signature. Figure 1 illustrates the shape of three common signatures. The simplest is a measurement intervention that models a single outlying point caused by, for example, a mistake in recording the data. A level shift, characterized by a permanent shift in the mean of the series, is modeled by a signature that takes the value 0 up to point of the shift and 1 thereafter. Examples of series with level shifts are the Nile data of Cobb (1978) and the seatbelt data analyzed by Harvey and Durbin (1986). The third intervention displayed in Figure 1 is a switch intervention, consisting of consecutive extreme values on either side of the current level of the series. This could be caused by increased production after a strike or a collapse in stock values after a sudden rise. Thus interventions are characterized by origin (i.e., the first point of impact) and shape. Magnitude is determined by estimation.

Given $\mathbf{D}$ and $\mathbf{\Sigma}$, the intervention parameter $\boldsymbol{\delta}$ can be estimated using generalized least squares (GLS),

$$\hat{\boldsymbol{\delta}} = \mathbf{S}^{-1}\mathbf{s}, \qquad \operatorname{cov}(\hat{\boldsymbol{\delta}}) = \sigma^2\mathbf{S}^{-1}, \tag{1}$$

where

$$\mathbf{s} = \mathbf{D}'\mathbf{\Sigma}^{-1}\mathbf{y}, \qquad S = \mathbf{D}'\mathbf{\Sigma}^{-1}\mathbf{D}.$$

The quantity s is called the *intervention contrast.* The test of the hypothesis of no shock, $\boldsymbol{\delta} = \mathbf{0}$, is based on

$$\hat{\boldsymbol{\delta}}'\{\operatorname{cov}(\hat{\boldsymbol{\delta}})\}^{-1}\hat{\boldsymbol{\delta}} = \sigma^{-2}\mathbf{s}'\mathbf{S}^{-1}\mathbf{s}.$$

In practice, σ^2 is often replaced by the normal based maximum likelihood estimate (MLE), $\hat{\sigma}^2 = (\mathbf{y}'\mathbf{\Sigma}^{-1}\mathbf{y})/n$, yielding the test statistic

$$\tau^2 = \hat{\sigma}^{-2}\mathbf{s}'\mathbf{S}^{-1}\mathbf{s}. \tag{2}$$

The estimate of σ^2 can be adjusted to take into account the intervention, so $\hat{\sigma}^2 = n^{-1}(\mathbf{y}'\mathbf{\Sigma}^{-1}\mathbf{y} - \mathbf{s}'\mathbf{S}^{-1}\mathbf{s})$. The statistic τ^2 has an approximate χ_p^2 distribution, where p is the rank of $\mathbf{S}$ or, equivalently, the number of linearly independent columns in $\mathbf{D}$. Dividing each component of $\hat{\boldsymbol{\delta}}$ by its estimated standard error gives τ, the analog of the usual regression t statistic.

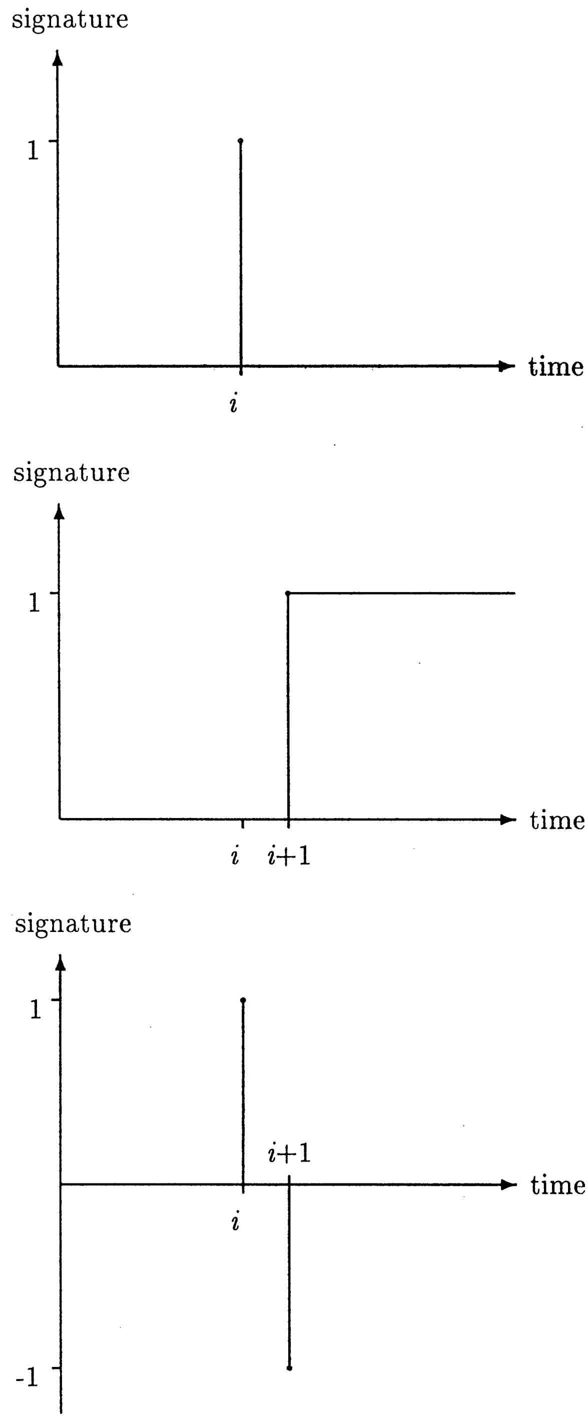

Figure 1. Some Common Intervention Signatures.

In practice, neither $\mathbf{D}$ nor $\boldsymbol{\Sigma}$ is known. Typically, $\boldsymbol{\Sigma}$ is a function of hyperparameters estimated under the null. The presence of shocks may distort these estimates and thus affect the test statistics. Our experience is that, at least for structural time series models, this distortion is not usually sufficient to obscure outliers and structural breaks.

To illustrate the detection process, consider the well-known Nile data (Cobb 1978). These data consist of readings of the annual flow volume of the Nile River at Aswan for 1871 to 1970; see Figure 2. A random walk plus noise model,

$$y_t = \alpha_t + \varepsilon_t, \qquad \varepsilon_t \sim \mathrm{N}(0, \sigma_\varepsilon^2)$$

and

$$\alpha_{t+1} = \alpha_t + \eta_t, \qquad \eta_t \sim \mathrm{N}(0, \sigma_\eta^2), \tag{3}$$

with $\hat{\sigma}_\varepsilon^2 = 15{,}099$ and $\hat{\sigma}_\eta^2 = 1{,}469.2$, appears to fit the data well. Suppose that outliers or level shifts in these data are suspected. The detection procedure consists of computing the τ^2 statistic (2) for these two interventions, at each point of the series; see Figure 3. The plots indicate outlying values in 1877 and 1913 and a level shift in 1899. Refitting the model including these interventions results in an estimate of 0 for the variance of the level component. The next section describes an efficient method for computing these statistics. In Section 4 we propose a chi-squared test statistic τ^{*2}. This statistic indicates, at the start of the diagnostic procedure, whether any further investigation is necessary. The large peak around 1900 in the τ^{*2} statistic for the Nile series suggests unusual behavior in the data; see Figure 4.

3. SHOCKS IN STATE-SPACE MODELS

The null state-space form of $\mathbf{y}_t$ is

$$\mathbf{y}_t = \mathbf{Z}_t \boldsymbol{\alpha}_t + \mathbf{G}_t \boldsymbol{\varepsilon}_t \tag{4}$$

and

$$\boldsymbol{\alpha}_{t+1} = \mathbf{T}_t \boldsymbol{\alpha}_t + \mathbf{H}_t \boldsymbol{\varepsilon}_t, \qquad t = 1, \ldots, n, \tag{5}$$

where $\boldsymbol{\varepsilon}_t \sim (\mathbf{0}, \sigma^2 \mathbf{I}), \boldsymbol{\alpha}_1 \sim (\mathbf{a}_1, \sigma^2 \mathbf{P}_1)$, and the $\boldsymbol{\varepsilon}_t$ and $\boldsymbol{\alpha}_1$ are mutually uncorrelated. The system matrices $\mathbf{Z}_t, \mathbf{T}_t, \mathbf{G}_t$, and $\mathbf{H}_t$ are deterministic quantities that, as the notation indicates, may vary over time. For a univariate model with an $m \times 1$ state vector $\boldsymbol{\alpha}_t$ and $p \times 1$ vector of errors $\boldsymbol{\varepsilon}_t$, the matrices $\mathbf{Z}_t, \mathbf{T}_t, \mathbf{G}_t$, and $\mathbf{H}_t$ are $1 \times m, m \times m, 1 \times p$, and $p \times p$. Equations (4) and (5) serve to define $\mathrm{cov}(\mathbf{y}) = \sigma^2 \boldsymbol{\Sigma}$.

An important tool for the state-space model is the well-known Kalman filter (Anderson and Moore 1979). For $t = 1, \ldots, n$,

$$\mathbf{v}_t = \mathbf{y}_t - \mathbf{Z}_t \mathbf{a}_t,$$

$$\mathbf{F}_t = \mathbf{Z}_t \mathbf{P}_t \mathbf{Z}_t' + \mathbf{G}_t \mathbf{G}_t',$$

$$\mathbf{K}_t = (\mathbf{T}_t \mathbf{P}_t \mathbf{Z}_t' + \mathbf{H}_t \mathbf{G}_t') \mathbf{F}_t^{-1},$$

$$\mathbf{a}_{t+1} = \mathbf{T}_t \mathbf{a}_t + \mathbf{K}_t \mathbf{v}_t,$$

and

$$\mathbf{P}_{t+1} = \mathbf{T}_t \mathbf{P}_t \mathbf{L}_t' + \mathbf{H}_t \mathbf{J}_t', \tag{6}$$

where $\mathbf{L}_t = \mathbf{T}_t - \mathbf{K}_t \mathbf{Z}_t$ and $\mathbf{J}_t = \mathbf{H}_t - \mathbf{K}_t \mathbf{G}_t$. Closely related to Kalman filtering is smoothing, which is efficiently implemented using the smoothing recursions put forward by de Jong (1988a, 1989) and Kohn and Ansley (1989). These recursions use output from the Kalman filter and are initialized with $\mathbf{r}_n = \mathbf{0}$ and $\mathbf{N}_n = \mathbf{0}$ and then, for $t = n, \ldots, 1$,

$$\mathbf{u}_t = \mathbf{F}_t^{-1} \mathbf{v}_t - \mathbf{K}_t' \mathbf{r}_t,$$

$$\mathbf{M}_t = \mathbf{F}_t^{-1} + \mathbf{K}_t' \mathbf{N}_t \mathbf{K}_t,$$

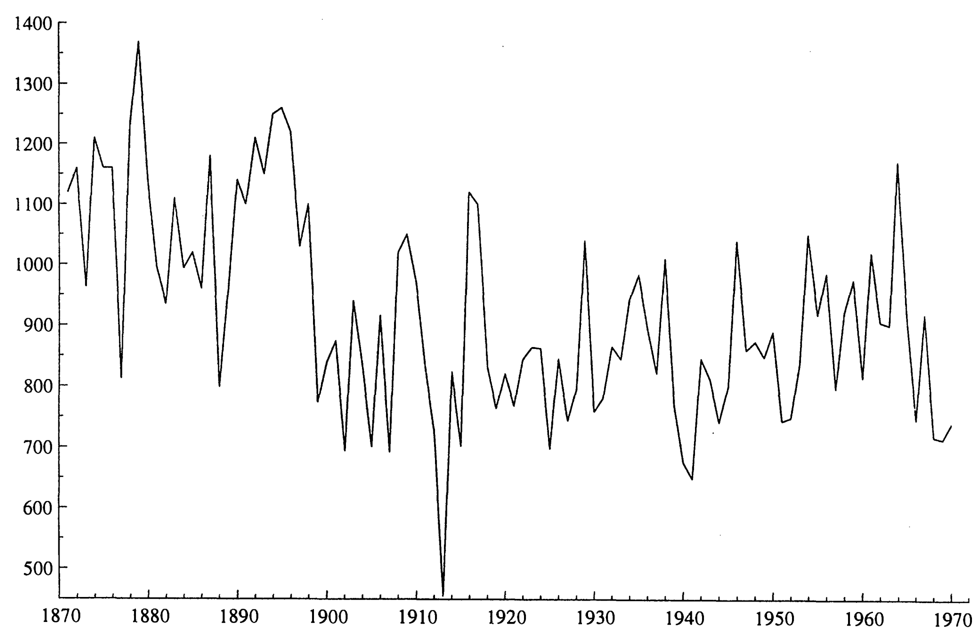

Figure 2. Nile Example: The Flow Volume of the Nile.

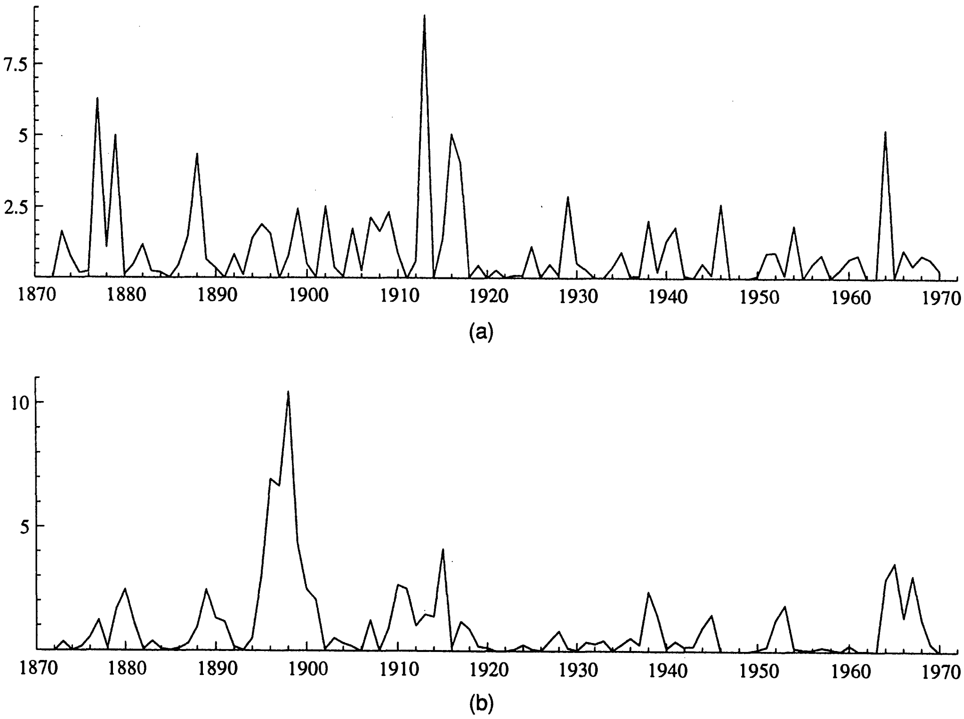

Figure 3. Nile Example: τ^2 Statistic for Measurement (a) and Level (b) Shocks.

$$\mathbf{r}_{t-1} = \mathbf{Z}_t'\mathbf{u}_t + \mathbf{T}_t'\mathbf{r}_t,$$

and

$$\mathbf{N}_{t-1} = \mathbf{Z}_t'\mathbf{F}_t^{-1}\mathbf{Z}_t + \mathbf{L}_t'\mathbf{N}_t\mathbf{L}_t. \tag{7}$$

The combined recursions (6) and (7) are called the Kalman filter smoother (KFS). The smoothing recursion output—in particular, the *smoothations,* $\mathbf{u}_t$—are fundamental for shock detection. Smoothations have the same dimensions as the observations and thus for a univariate series, each u_t is scalar. The $\mathbf{r}_t$ have the same dimension as the state vector. The properties of smoothations are described by the following theorem.

Theorem 1. The smoothations $\mathbf{u}_t$ are such that

$$\mathbf{u}_t = \mathbf{M}_t\{\mathbf{y}_t - E(\mathbf{y}_t|\mathbf{y}^t)\}$$

and

$$\mathbf{M}_t = \sigma^{-2}\mathrm{cov}(\mathbf{u}_t) = \{\sigma^{-2}\mathrm{cov}(\mathbf{y}_t|\mathbf{y}^t)\}^{-1}, \tag{8}$$

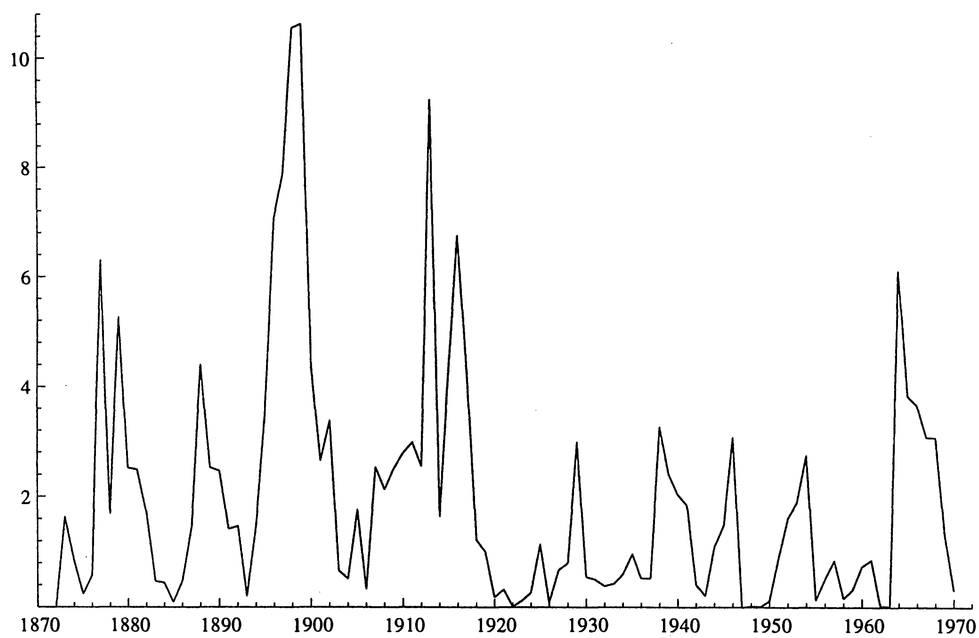

Figure 4. Nile Example: Maximal Statistic τ^{*2}.

where $\mathbf{y}^t$ is $\mathbf{y}$ excluding $\mathbf{y}_t$. Further, if $\mathbf{u} = (\mathbf{u}_1', \ldots, \mathbf{u}_n')'$, then $\mathbf{u} = \boldsymbol{\Sigma}^{-1}\mathbf{y}$ and $\text{cov}(\mathbf{u}) = \sigma^2\boldsymbol{\Sigma}^{-1}$.

The alternative model is defined by addition to the measurement and transition equations of a vector of shocks $\boldsymbol{\delta}$,

$$\mathbf{y}_t = \mathbf{X}_t\boldsymbol{\delta} + \mathbf{Z}_t\boldsymbol{\alpha}_t + \mathbf{G}_t\boldsymbol{\varepsilon}_t \tag{9}$$

and

$$\boldsymbol{\alpha}_{t+1} = \mathbf{W}_t\boldsymbol{\delta} + \mathbf{T}_t\boldsymbol{\alpha}_t + \mathbf{H}_t\boldsymbol{\varepsilon}_t, \tag{10}$$

where $\mathbf{X}_t$ and $\mathbf{W}_t$ are called the *shock design* matrices and $\boldsymbol{\delta}$ is the shock magnitude. Many departures observed in practice can be represented by a *simple intervention;* that is, by taking all $\mathbf{X}_t$ and $\mathbf{W}_t$ to be $\mathbf{0}$ except at a single point $t = i$. The signature of a simple intervention with origin i is

$$\mathbf{D}_t(i) = \begin{cases} \mathbf{0}, & t = 1, \ldots, i-1 \\ \mathbf{X}_i, & t = i \\ \mathbf{Z}_t\mathbf{T}_{t-1,i+1}\mathbf{W}_i, & t = i+1, \ldots, n, \end{cases} \tag{11}$$

where $\mathbf{T}_{j,t} \equiv \mathbf{T}_j \ldots \mathbf{T}_t$ for $j \geq t$ and $\mathbf{T}_{t-1,t} \equiv \mathbf{I}$. The matrix $\mathbf{D}(i) = (\mathbf{D}_1(i)', \ldots, \mathbf{D}_n(i)')'$ is the intervention signature corresponding to a shock $\boldsymbol{\delta}$ at $t = i$. The corresponding GLS estimate (1) is $\hat{\boldsymbol{\delta}}_i = \mathbf{S}_i^{-1}\mathbf{s}_i$, where the i subscripts indicate the origin i of the intervention. The following theorem shows how the shock contrast $\mathbf{s}_i$ is directly available from null model KFS output.

Theorem 2. Suppose that the null model KFS output is available. The shock contrast $\mathbf{s}_i$ and covariance matrix $\mathbf{S}_i$ corresponding to a simple shock at $t = i$ are

$$\mathbf{s}_i = \mathbf{D}(i)'\mathbf{u} = \mathbf{X}_i'\mathbf{u}_i + \mathbf{W}_i'\mathbf{r}_i$$

and

$$\mathbf{S}_i = \sigma^{-2}\text{cov}(\mathbf{s}_i) = \mathbf{X}_i'\mathbf{F}_i^{-1}\mathbf{X}_i + \mathbf{Q}_i'\mathbf{N}_i\mathbf{Q}_i, \tag{12}$$

where $\mathbf{Q}_i = \mathbf{W}_i - \mathbf{K}_i\mathbf{X}_i$.

The expression for $\mathbf{s}_i$ is established by noting, from (7), that

$$\mathbf{r}_t = \sum_{j=t+1}^{n} \mathbf{T}_{j-1,t+1}'\mathbf{Z}_j'\mathbf{u}_j. \tag{13}$$

Applying Theorem 1 yields $\mathbf{s}_i = \mathbf{D}(i)'\boldsymbol{\Sigma}^{-1}\mathbf{y} = \mathbf{D}(i)'\mathbf{u}$. Combining these results with expression (11) for the signature yields

$$\begin{aligned}\mathbf{s}_i = \mathbf{D}(i)'\mathbf{u} &= \mathbf{X}_i'\mathbf{u}_i + \mathbf{W}_i' \sum_{j=i+1}^{n} \mathbf{T}_{j-1,i+1}'\mathbf{Z}_j'\mathbf{u}_j \\ &= \mathbf{X}_i'\mathbf{u}_i + \mathbf{W}_i'\mathbf{r}_i,\end{aligned}$$

as required. The proof of the expression for $\mathbf{S}_i$ is given in the Appendix.

Varying i (i.e., running the simple intervention along the series) allows detection of sudden or unexpected movements. Theorem 2 yields the GLS estimate of $\boldsymbol{\delta}_i$ and the test statistic τ_i^2 for origins i from 1 to n. No assumptions about the nature of the intervention are made in the filtering and smoothing process. Thus intervention statistics for any number of interventions can be computed without doing any additional KFS runs.

Theorem 2 provides a concrete interpretation of the quantities involved in the smoothing recursions. For example, the case where $\mathbf{X}_i = \mathbf{I}$ and $\mathbf{W}_i = \mathbf{0}$ denotes a pure measurement shock at $t = i$. The shock contrast is $\mathbf{s}_i = \mathbf{u}_i$, and $\mathbf{M}_i^{-1}\mathbf{u}_i = \mathbf{y}_i - E(\mathbf{y}_i|\mathbf{y}^i)$ is the GLS estimate of shock. This result is intuitively appealing, because it states that the estimate $\hat{\boldsymbol{\delta}}_i$ is the difference between the observation $\mathbf{y}_i$ and the estimate of $\mathbf{y}_i$ based on all other data points. Peña (1990) stated this in a less general context, as a well-known result. The case $\mathbf{X}_i = \mathbf{0}$ and $\mathbf{W}_i = \mathbf{I}$, where each component of the state is shocked separately, is called a pure state shock. Here $\mathbf{s}_i = \mathbf{r}_i$, and the GLS estimate of the shock is $\mathbf{N}_i^{-1}\mathbf{r}_i$. Finally, consider an aberrant disturbance,

$$\mathbf{y}_i = \mathbf{Z}_i\boldsymbol{\alpha}_i + \mathbf{G}_i(\boldsymbol{\varepsilon}_i + \boldsymbol{\delta})$$

and

$$\boldsymbol{\alpha}_{i+1} = \mathbf{T}_i\boldsymbol{\alpha}_i + \mathbf{H}_i(\boldsymbol{\varepsilon}_i + \boldsymbol{\delta}).$$

Then $\mathbf{X}_i = \mathbf{G}_i$ and $\mathbf{W}_i = \mathbf{H}_i$, and so $\mathbf{s}_i = \mathbf{G}_i'\mathbf{u}_i + \mathbf{H}_i'\mathbf{r}_i$ and $\mathbf{S}_i = \mathbf{G}_i'\mathbf{F}_i^{-1}\mathbf{G}_i + \mathbf{J}_i'\mathbf{N}_i\mathbf{J}_i$.

Our approach can be contrasted with existing methods. From de Jong (1988), Kohn and Ansley (1989), and Koopman (1993), $E(\boldsymbol{\varepsilon}_i|\mathbf{y}) = \mathbf{G}_i'\mathbf{u}_i + \mathbf{H}_i'\mathbf{r}_i$. For structural time series models, Harvey and Koopman (1992) suggested the scaled $E(\boldsymbol{\varepsilon}_i|\mathbf{y})$ as diagnostics called auxiliary residuals. Their scaling amounts to multiplying by the inverse square root of $\text{cov}(\boldsymbol{\varepsilon}_i|\mathbf{y}) = \sigma^2\mathbf{I} - \text{cov}\{E(\boldsymbol{\varepsilon}_i|\mathbf{y})\}$. By the foregoing argument, scaling based on $\sigma^2(\mathbf{G}_i'\mathbf{F}_i^{-1}\mathbf{G}_i + \mathbf{J}_i'\mathbf{N}_i\mathbf{J}_i)$ is more appropriate. Note that $\sigma^2(\mathbf{G}_i'\mathbf{F}_i^{-1}\mathbf{G}_i + \mathbf{J}_i'\mathbf{N}_i\mathbf{J}_i) = \text{cov}\{E(\boldsymbol{\varepsilon}_i|\mathbf{y})\}$. From the preceeding paragraph, using the appropriate scaling yields the analog of the regression t statistics. General state-space methods have been proposed by Willsky and Jones (1976) and later by Atkinson et al. (1997), who use the fact that the Kalman filter is a linear transformation $\mathbf{L}\mathbf{y} = \mathbf{v}$, where $\mathbf{v} = (\mathbf{v}_1', \ldots, \mathbf{v}_n')'$ is the stack of the innovations. It follows that $\boldsymbol{\Sigma}^{-1} = \mathbf{L}'\mathbf{F}^{-1}\mathbf{L}$, where $\mathbf{F} = \text{diag}(\mathbf{F}_1, \ldots, \mathbf{F}_n) = \sigma^{-2}\text{cov}(\mathbf{v})$. Thus

$$\mathbf{s}_i = \mathbf{D}(i)'\boldsymbol{\Sigma}^{-1}\mathbf{y} = \{\mathbf{L}\mathbf{D}(i)\}'\mathbf{F}^{-1}\mathbf{v}$$

can be computed by filtering $\mathbf{D}(i)$ for each i and for every intervention structure of interest. This approach is clearly inefficient, because it requires the explicit construction and filtering of $\mathbf{D}(i)$ for every signature and origin i of interest. The relationship between filtering the signature and the smoother based methods that we develop is illustrated by Figure 5.

4. TEST STATISTICS

The shock design matrices $\mathbf{X}_i$ and $\mathbf{W}_i$ determine the type of simple intervention resulting from a shock, and the previous sections assume that $\mathbf{X}_i$ and $\mathbf{W}_i$ are given. Instead, the data can be used to suggest appropriate shock designs.

Theorem 3. For given i and the null state-space model, the maximum of $\rho_i^2 = \mathbf{s}_i'\mathbf{S}_i^{-1}\mathbf{s}_i$ with respect to $\mathbf{X}_i$ and $\mathbf{W}_i$

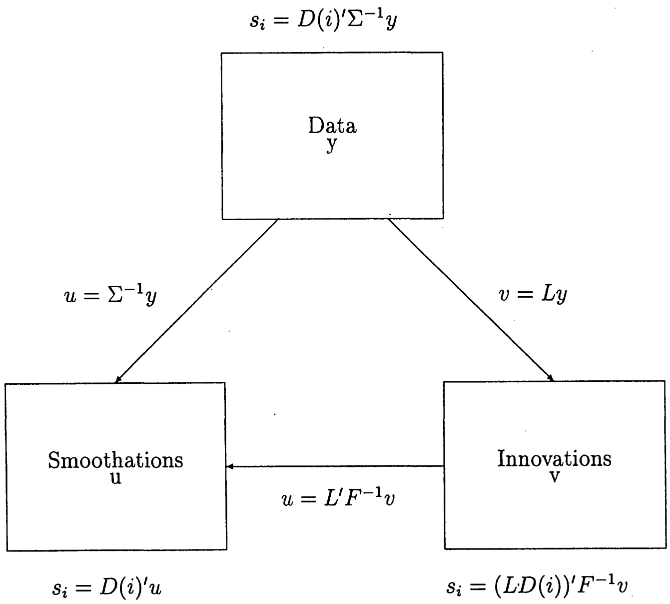

Figure 5. The Relationship Between Observations, Innovations, and Smoothations.

is

$$\rho_i^{*2} = \mathbf{v}_i'\mathbf{F}_i^{-1}\mathbf{v}_i + \mathbf{r}_i'\mathbf{N}_i^{-1}\mathbf{r}_i, \tag{14}$$

where $\mathbf{v}_i, \mathbf{F}_i, \mathbf{r}_i$, and $\mathbf{N}_i$ are computed with the KFS applied to the null model. The maximum is attained when $\mathbf{X}_i = \mathbf{v}_i$ and $\mathbf{W}_i = \mathbf{K}_i\mathbf{v}_i + \mathbf{N}_i^{-1}\mathbf{r}_i$, and hence when $\boldsymbol{\delta}$ is scalar.

The maximization is with respect to all matrices $\mathbf{X}_i$ and $\mathbf{W}_i$ of fixed row dimension. The maximum is attained when δ is scalar with $\mathbf{X}_i$ and $\mathbf{W}_i$ as indicated earlier, distributing the scalar shock over the measurement and state equations. The proof of Theorem 3 shows that the maximum is also attained when $(\mathbf{X}_i', \mathbf{W}_i') = \mathbf{I}$, corresponding to separate shocks to the measurement and each component of the state equation. It also follows from the proof that if $\mathbf{X}_i = \mathbf{0}$, then the maximum of ρ_i^2 is $\mathbf{r}_i'\mathbf{N}_i^{-1}\mathbf{r}_i$ attained at $\mathbf{W}_i = \mathbf{N}_i^{-1}\mathbf{r}_i$, whereas if $\mathbf{W}_i = \mathbf{0}$, then the maximum is $\mathbf{u}_i'\mathbf{M}_i^{-1}\mathbf{u}_i$ attained at $\mathbf{X}_i = \mathbf{M}_i^{-1}\mathbf{u}_i$.

These results provide a means of identifying the origin and shape of possible interventions. The test statistic (2) has maximum value $\tau_i^{*2} = \hat{\sigma}^{-2}\rho_i^{*2}$ regardless of whether $\hat{\sigma}^2$ is adjusted to take the intervention into account. A plot of τ_i^{*2} against i shows, for each i, the value of τ_i^2 under the shock design that has maximum impact at that point. The values of $\mathbf{X}_i$ and $\mathbf{W}_i$ that maximize ρ_i^2 can be used to suggest plausible intervention signatures.

The components of $\mathbf{v}_i'\mathbf{F}_i^{-1}\mathbf{v}_i$ and $\mathbf{r}_i'\mathbf{N}_i^{-1}\mathbf{r}_i$ are, given the model parameters, approximate independent chi-squared random variables with degrees of freedom equal to the number of components in the measurement equations and the state equations. Thus τ_i^{*2} is also approximately chi-squared. This provides a yardstick for judging the significance of plotted values of τ_i^{*2}. However, when many points i are considered, issues of serial correlation and simultaneous testing arise.

5. INTERVENTIONS IN PRACTICAL MODELS

This section deals with shocks in the context of two time series models frequently used in practice: structural components models (Harvey 1989) and ARIMA models. These models are time invariant, so $\mathbf{T}_t = \mathbf{T}$ and $\mathbf{H}_t = \mathbf{H}$ are independent of time t.

5.1 Structural Time Series Model

The local linear trend model has state-space form

$$y_t = (1 \quad 0)\boldsymbol{\alpha}_t + (1 \quad 0 \quad 0)\boldsymbol{\varepsilon}_t$$

and

$$\boldsymbol{\alpha}_{t+1} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}\boldsymbol{\alpha}_t + \begin{pmatrix} 0 & h_1 & 0 \\ 0 & 0 & h_2 \end{pmatrix}\boldsymbol{\varepsilon}_t. \tag{15}$$

The components of the state vector $\boldsymbol{\alpha}_t$ are the level and slope of the series. The signature from a pure measurement shock represents a single outlying value. A level intervention is modeled by taking $X_i = 0$ and $\mathbf{W}_i = (1,0)'$. In this case s_i and S_i correspond to the first element of $\mathbf{r}_i$ and the first diagonal entry of $\mathbf{N}_i$. Adding a shock to the level is equivalent to adding a step function in the measurement equation with a single step at $t = i$. Changes in the slope of the series are handled by taking $X_i = 0$ and $\mathbf{W}_i = (0,1)'$. From (11), the resulting shock signature has the form $D_t(i) = t - i - 1$ for $t > i$. The relevant shock contrast is now the second element of the vector $\mathbf{r}_i$, and S_i is the second diagonal entry in $\mathbf{N}_i$. Taking $X_i = 0$ and $\mathbf{W}_i = \mathbf{I}$ yields a pure state shock with shock estimate $\mathbf{N}_i^{-1}\mathbf{r}_i$. This is different from the estimates generated using separate level and slope shocks.

Our methods apply to seasonal series. To simplify the discussion, consider a model with a single component. The general case follows by combining components. A structural representation of a pure cycle has $Z = (1, 0)$,

$$\mathbf{T} = \phi\begin{pmatrix} \cos\omega & \sin\omega \\ -\sin\omega & \cos\omega \end{pmatrix},$$

$$\mathbf{T}^j = \phi^j\begin{pmatrix} \cos\omega j & \sin\omega j \\ -\sin\omega j & \cos\omega j \end{pmatrix},$$

and $\phi \le 1$. Apart from measurement noise, y_t is a cosine function with fixed frequency ω but slowly varying amplitude and phase. At time t, the amplitude and phase are the polar coordinates of $\boldsymbol{\alpha}_t$. The signature of a state shock at i is

$$D_t(i) = \phi^{t-i}\{\delta_1\cos\omega(t-i) + \delta_2\sin\omega(t-i)\}$$

for $t > i$. This is equivalent to adding a damped cycle with damping factor ϕ, amplitude $\sqrt{(\delta_1^2 + \delta_2^2)}$, and phase $\arctan(\delta_2/\delta_1)$. If $\phi = 1$, then the shock effect is persistent. The polar coordinates of δ measure the aberrant changes in amplitude and phase. If $\delta_2 = 0$, then there is a change in amplitude but no change in the positioning of the peaks or troughs of the cycle, a type of behavior that may be observed in practice. If $\delta_1 = 0$, then the change is a $\pm\pi$ radian shift in the phase, which is of limited practical relevance.

5.2 Autoregressive Integrated Moving Average Models

An ARIMA(p,d,q) model is written as $\phi(B)(1-B)^d y_t = \theta(B)\varepsilon_t$, where B is the backshift operator, $\phi(B) = 1 - \sum_{i=1}^{p}\phi_i B^i$ with all roots outside the unit circle, $\theta(B) = 1 + \sum_{i=1}^{q}\theta_i B^i$, and the ε_t are uncorrelated $(0,\sigma^2)$ random variables. Consider initially the stationary case $d = 0$. The usual state-space representation is $\mathbf{Z}_t = \mathbf{Z} = (1,0,\ldots,0), G_t = G = 0$,

$$\mathbf{T}_t = \mathbf{T} = \begin{pmatrix} \phi_1 & 1 & 0 & \cdots & 0 \\ \phi_2 & 0 & 1 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 0 \\ \vdots & 0 & \cdots & 0 & 1 \\ \phi_m & 0 & \cdots & \cdots & 0 \end{pmatrix},$$

and

$$\mathbf{H}_t = \mathbf{H} = \begin{pmatrix} 1 \\ \theta_1 \\ \vdots \\ \vdots \\ \theta_{m-1} \end{pmatrix},$$

where $m = \max(p, q+1)$. From (11), a shock to the state disturbance, $X_i = 0$ and $\mathbf{W}_i = \mathbf{H}$, yields

$$D_t(i) = \mathbf{Z}\mathbf{T}^{t-i}\mathbf{H} = \sum_{j=0}^{q}\pi_{t-i-j}\theta_j,$$

where π_k is the coefficient of B^k in the expansion of $1/\phi(B)$ for $k \geq 0$ and $\pi_k = 0$ for $k < 0$. Thus the signature $D_t(i)$ is made up of coefficients in the polynomial expansion of $\theta(B)/\phi(B)$; that is, the coefficients in the infinite MA representation. A measurement shock corresponds to $X_i = 1$ and $\mathbf{W}_i = \mathbf{0}$ with shock signature $D_t(i) = 0$ for $t \neq i$ and $D_i(i) = 1$. The corresponding estimates of δ for each i are generated using a single run of the KFS, as described in Section 3.

Our approach can be compared to ARIMA-based methods, including the method of Tsay (1988). He studied shocks by considering models of the form

$$y_t = D_t(i)\delta + \frac{\theta(B)}{\phi(B)}\varepsilon_t, \tag{16}$$

where $\phi(B)$ and $\theta(B)$ are the AR and MA polynomials of the null ARIMA model and $D_t(i) = \omega(B)\xi_t(i)$ is the shock signature with $\xi_t(i) = 0$ for $t \neq i$ and $\xi_i(i) = 1$. The cases $\omega(B) = 1$ and $\omega(B) = \theta(B)/\phi(B)$ are called additive and innovative outliers, and are equivalent to our measurement and state disturbance shocks. To estimate δ, the model is rewritten by multiplying both sides of (16) by $\phi(B)/\theta(B)$, yielding $\tilde{v}_t = \lambda_t(i)\delta + \varepsilon_t$, where $\tilde{v}_t = \{\phi(B)/\theta(B)\}y_t$ and $\lambda_t(i) = \{\phi(B)/\theta(B)\}D_t(i)$. The approximate innovations $\tilde{v}_t$ are regressed on the filtered innovation signature $\lambda_t(i)$ for each origin i. In the innovational outlier case, $\omega(B) = \theta(B)/\phi(B)$, implying that $\lambda_t(i) = \xi_t(i)$ and hence $\hat{\delta}_i = \tilde{v}_i$. With additive outliers, $\omega(B) = 1$, so $\lambda_t(i) = \{\phi(B)/\theta(B)\}\xi_t(i)$, the coefficients of the infinite AR representation.

The first difference between the ARIMA approach and our KFS-based method is that the latter is exact. Multiplying by $\phi(B)/\theta(B)$ is the polynomial approximation to the transformation $\mathbf{Ly} = \mathbf{v}$ discussed at the end of Section 3. Using $\tilde{v}_i$ gives poor results when the roots of $\theta(B), \phi(B), \omega(B)$, or $1/\omega(B)$ are close to the unit disc and the data series is short. Second, our approach does not involve explicit regression for each origin i but achieves this implicitly by appropriate interpretation of the null model KFS output. Third, the state-space methodology allows for a much wider class of shock designs. Finally, the KFS method applies to any model that can be cast in the state-space form, not just to ARIMA models.

A nonstationary ARIMA(p,d,q), where $d \geq 1$, can be treated as a structural model with stationary autoregressive moving average [ARMA(p,q)] disturbances. In the state-space form, the $\mathbf{T}$ matrix can be taken to have two blocks on the diagonal, the first block representing the nonstationary structural component and the second block modeling the ARMA disturbances. Introducing a level shock to this model is equivalent to a level intervention where $\omega(B) = (I-B)^{-1}$.

6. TIME SERIES MODELS WITH EXPLANATORY VARIABLES

Diagnostic tools for regression models with uncorrelated disturbances have been dealt with extensively in the literature (Atkinson 1985; Cook and Weisberg 1982). This section generalizes predicted residuals and influence to the time series regression setting. As in uncorrelated errors case, statistics are readily computed from the null model fit.

An example model is regression with ARMA(p,q) errors, $y_t = \mathbf{X}_{t,\beta}\boldsymbol{\beta} + \{\theta(B)/\phi(B)\}\varepsilon_t$, where the additional $\boldsymbol{\beta}$ subscript on $\mathbf{X}_t$ distinguishes this matrix from that used to denote a shock to the measurement equation. Harvey (1989) provided another model and a practical case of a time series influenced by observed exogenous variables—namely, monthly traffic fatalities, which are dependent on the price of fuel and the total number of kilometers travelled by all cars each month. The general state-space formulation including regression variables is

$$\mathbf{y}_t = \mathbf{X}_{t,\beta}\boldsymbol{\beta} + \mathbf{Z}_t\boldsymbol{\alpha}_t + \mathbf{G}_t\boldsymbol{\varepsilon}_t$$

and

$$\boldsymbol{\alpha}_{t+1} = \mathbf{W}_{t,\beta}\boldsymbol{\beta} + \mathbf{T}_t\boldsymbol{\alpha}_t + \mathbf{H}_t\boldsymbol{\varepsilon}_t,$$

where $\mathbf{X}_{t,\beta}$ and $\mathbf{W}_{t,\beta}$ contain the explanatory variables. The state-space equations imply that for some matrix $\mathbf{B}, \mathbf{y} \sim (\mathbf{B}\boldsymbol{\beta}, \sigma^2\boldsymbol{\Sigma})$. A simple mean effect is modeled by taking $\mathbf{X}_{t,\beta} = \mathbf{I}$ and $\mathbf{W}_{t,\beta} = \mathbf{0}$ for all t.

A null model run of the KFS now includes additional recursions relating to the explanatory variables,

$$\mathbf{V}_t = \mathbf{X}_{t,\beta} - \mathbf{Z}_t\mathbf{A}_t, \qquad \mathbf{A}_{t+1} = -\mathbf{W}_{t,\beta} + \mathbf{K}_t\mathbf{V}_t + \mathbf{T}_t\mathbf{A}_t, \qquad t = 1,\ldots,n, \tag{17}$$

where $\mathbf{A}_1 = \mathbf{0}$, and in the smoother

$$\mathbf{U}_t = \mathbf{F}_t^{-1}\mathbf{V}_t - \mathbf{K}_t'\mathbf{R}_t, \qquad \mathbf{R}_{t-1} = \mathbf{Z}_t'\mathbf{U}_t + \mathbf{T}_t'\mathbf{R}_t, \qquad t = n, \ldots, 1, \quad (18)$$

where $\mathbf{R}_n = \mathbf{0}$. The recursions (17) and (18) are the data-dependent part of the ordinary KFS applied to the explanatory variables. The smoothations of the columns of $\mathbf{B}$ are given by $\mathbf{U} = (\mathbf{U}_1', \ldots, \mathbf{U}_n')'$. The KFS together with (17) and (18) is called the diffuse or augmented KFS (de Jong 1991).

Shocks are included using the method described in Section 3. The vectors $\boldsymbol{\delta}$ and $\boldsymbol{\beta}$ are stacked as $\boldsymbol{\gamma} = (\boldsymbol{\delta}', \boldsymbol{\beta}')'$, and the regression matrix incorporating all external effects is denoted by $\mathbf{X}_\gamma = (\mathbf{D}(i), \mathbf{B})$. The GLS estimate of $\boldsymbol{\gamma}$ corresponding to an intervention with origin i is

$$\begin{aligned}\hat{\boldsymbol{\gamma}}_i &= (\mathbf{X}_\gamma'\boldsymbol{\Sigma}^{-1}\mathbf{X}_\gamma)^{-1}\mathbf{X}_\gamma'\boldsymbol{\Sigma}^{-1}\mathbf{y} \\ &= \begin{pmatrix} \sigma^{-2}\mathrm{cov}(\mathbf{D}(i)'\mathbf{u}) & \mathbf{D}(i)'\boldsymbol{\Sigma}^{-1}\mathbf{B} \\ \mathbf{B}'\boldsymbol{\Sigma}^{-1}\mathbf{D}(i) & \sigma^{-2}\mathrm{cov}(\mathbf{B}'\mathbf{u}) \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{D}(i)'\mathbf{u} \\ \mathbf{B}'\mathbf{u} \end{pmatrix} \\ &= \begin{pmatrix} \mathbf{S}_i & \mathbf{S}_{i,\beta} \\ \mathbf{S}_{i,\beta}' & \mathbf{S}_\beta \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{s}_i \\ \mathbf{s}_\beta \end{pmatrix}, \qquad (19)\end{aligned}$$

where (19) defines $\mathbf{s}_\beta, \mathbf{S}_\beta$, and $\mathbf{S}_{i,\beta}$. Thus $\hat{\boldsymbol{\gamma}}_i$ contains the estimate of both shock and regression parameters associated with the explanatory variables, adjusted for all other effects.

Quantities in (19) are evaluated in a single run of the augmented KFS. The contrast $\mathbf{s}_i$ and $\mathbf{S}_i$ is calculated as in (12). The quantities associated with the explanatory variables alone—that is, $\mathbf{s}_\beta = \mathbf{B}'\mathbf{u}$ and $\mathbf{S}_\beta = \sigma^{-2}\mathrm{cov}(\mathbf{s}_\beta)$—are not dependent on i, the origin of the intervention. In fact,

$$\mathbf{s}_\beta = \mathbf{B}'\boldsymbol{\Sigma}^{-1}\mathbf{y} = (\mathbf{L}\mathbf{B})'\mathbf{F}^{-1}\mathbf{L}\mathbf{y} = \sum_{t=1}^{n} \mathbf{V}_t'\mathbf{F}_t^{-1}\mathbf{v}_t$$

and

$$\mathbf{S}_\beta = \sum_{t=1}^{n} \mathbf{V}_t'\mathbf{F}_t^{-1}\mathbf{V}_t$$

are calculated in the augmented Kalman filter pass. Here $\mathbf{L}$ and $\mathbf{F}$ are as defined at the end of Section 3. The quantity $\mathbf{S}_{i,\beta} = \mathbf{D}(i)'\boldsymbol{\Sigma}^{-1}\mathbf{B}$ can be computed by noting that the components of $\boldsymbol{\Sigma}^{-1}\mathbf{B}$ are the smoothations $\mathbf{U}_t$ of the columns of $\mathbf{B}$. Using the expression for $\mathbf{D}(i)$ given in (11) yields

$$\mathbf{S}_{i,\beta} = \mathbf{X}_i'\mathbf{U}_i + \mathbf{W}_i' \sum_{t=i+1}^{n} \mathbf{T}_{j-1,i+1}'\mathbf{Z}_j'\mathbf{U}_j = \mathbf{X}_i'\mathbf{U}_i + \mathbf{W}_i'\mathbf{R}_i,$$

where $\mathbf{U}_i$ and $\mathbf{R}_i$ are given in (18).

The null model GLS estimate of $\boldsymbol{\beta}$ is $\hat{\boldsymbol{\beta}} = \mathbf{S}_\beta^{-1}\mathbf{s}_\beta$. When interventions are included, (19) yields the estimate of $\boldsymbol{\beta}$ that partials out shock effects. A partitioned matrix inversion of (19) shows that

$$\hat{\boldsymbol{\delta}}_i = (\mathbf{S}_i - \mathbf{S}_{i,\beta}\mathbf{S}_\beta^{-1}\mathbf{S}_{i,\beta}')^{-1}(\mathbf{s}_i - \mathbf{S}_{i,\beta}\hat{\boldsymbol{\beta}})$$

and

$$\hat{\boldsymbol{\beta}}_i = \hat{\boldsymbol{\beta}} - \mathbf{S}_\beta^{-1}\mathbf{S}_{i,\beta}'\hat{\boldsymbol{\delta}}_i. \qquad (20)$$

As before, GLS estimates of the parameters associated with all regression variables are generated with a single null model KFS run.

When $\boldsymbol{\Sigma} = \mathbf{I}$, observations are uncorrelated and $\mathbf{B} = \mathbf{X}_\beta \equiv (\mathbf{X}_{1,\beta}', \ldots, \mathbf{X}_{n,\beta}')'$. The only meaningful signature corresponds to a measurement shock, and then the estimates in (20) reduce to the well-known regression diagnostics (Atkinson 1985)

$$\hat{\boldsymbol{\delta}}_i = \{\mathbf{I} - \mathbf{X}_{i,\beta}(\mathbf{X}_\beta'\mathbf{X}_\beta)^{-1}\mathbf{X}_{i,\beta}'\}^{-1}(\mathbf{y}_i - \mathbf{X}_{i,\beta}\hat{\boldsymbol{\beta}})$$

and

$$\hat{\boldsymbol{\beta}}_i = \hat{\boldsymbol{\beta}} - (\mathbf{X}_\beta'\mathbf{X}_\beta)^{-1}\mathbf{X}_{i,\beta}'\hat{\boldsymbol{\delta}}_i,$$

and $\hat{\boldsymbol{\delta}}_i$ is the predicted or cross-validation residual at i. The quantity $(\mathbf{X}_\beta'\mathbf{X}_\beta)^{-1}\mathbf{X}_{i,\beta}'\hat{\boldsymbol{\delta}}_i$ is proportional to the sample influence curve. Thus the quantities in (20) generalize these notions to the case where the errors in the linear model are correlated.

Measures of influence of a shock on the parameter estimate $\hat{\boldsymbol{\beta}}$ can be defined from the expressions in (20). For example, a quantity analogous to Cook's distance (Cook 1977) is

$$(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_i)'\{\sigma^{-2}\mathrm{cov}(\hat{\boldsymbol{\beta}})\}^{-1}(\hat{\boldsymbol{\beta}} - \hat{\boldsymbol{\beta}}_i) = \hat{\boldsymbol{\delta}}_i'\mathbf{S}_{i,\beta}\mathbf{S}_\beta^{-1}\mathbf{S}_{i,\beta}'\hat{\boldsymbol{\delta}}_i.$$

This statistic is typically scaled by division by $p\hat{\sigma}^2$, where p is the number of explanatory variables and $\hat{\sigma}^2 = n^{-1}(\mathbf{v}'\mathbf{F}^{-1}\mathbf{v} - \mathbf{s}_\beta'\mathbf{S}_\beta^{-1}\mathbf{s}_\beta)$, the null model estimate of σ^2. The alternative model estimate of σ^2,

$$\hat{\sigma}^2 - n^{-1}(\mathbf{s}_i - \mathbf{S}_{i,\beta}\hat{\boldsymbol{\beta}})'(\mathbf{S}_i - \mathbf{S}_{i,\beta}\mathbf{S}_\beta^{-1}\mathbf{S}_{i,\beta}')^{-1}(\mathbf{s}_i - \mathbf{S}_{i,\beta}\hat{\boldsymbol{\beta}}),$$

which takes into account the effect of the shock, may also be used. Cook described several extensions of his method for measuring influence. Time series generalizations of these statistics are readily computed using the foregoing KFS framework.

7. COMPOSITE INTERVENTIONS

For a simple intervention, the signature is constrained by the form $\mathbf{Z}_t\mathbf{T}_{t-1,i+1}$ for $t > i$. More general shock signatures are generated by allowing the $\mathbf{X}_t$ and $\mathbf{W}_t$ in (9) and (10) to be nonzero for $t = i, \ldots, i+q$. Because the same intervention is considered for different origins i, it is convenient to adopt the notation

$$\mathbf{y}_t = \mathbf{X}_t(i)\boldsymbol{\delta} + \mathbf{Z}_t\boldsymbol{\alpha}_t + \mathbf{G}_t\boldsymbol{\varepsilon}_t$$

and

$$\boldsymbol{\alpha}_{t+1} = \mathbf{W}_t(i)\boldsymbol{\delta} + \mathbf{T}_t\boldsymbol{\alpha}_t + \mathbf{H}_t\boldsymbol{\varepsilon}_t,$$

where $\mathbf{X}_t(i) = 0$ and $\mathbf{W}_t(i) = 0$ for $t < i$ and $t > i + q$. The shock signature is then

$$\mathbf{D}_t(i) = \begin{cases} \mathbf{0}, \\ \quad t = 1, \ldots, i-1 \\ \mathbf{X}_t(i) + \mathbf{Z}_t \sum_{j=i}^{t-1} \mathbf{T}_{t-1,j+1}\mathbf{W}_j(i), \\ \quad t = i, \ldots, i+q \\ \mathbf{Z}_t \sum_{j=i}^{i+q} \mathbf{T}_{t-1,j+1}\mathbf{W}_j(i), \\ \quad t = i+q+1, \ldots, n. \end{cases}$$

The case $q = 0$ yields a simple intervention.

As an example, consider the local linear trend model (15). Temporary changes in the structure of this type of series can be represented using just two shocks, one to initiate the change and the other q periods later to turn it off. For example, a slope change that affects only q periods is generated by applying a shock to the second component of the state vector at $t = i$ and then an equivalent reverse shock at $t = i + q$. Taking $X_t(i) = 0$ and $\mathbf{W}_t(i) = \mathbf{0}$, except for $\mathbf{W}_i(i) = (0,1)'$ and $\mathbf{W}_{i+q}(i) = (0,-1)'$, yields the intervention signature,

$$D_t(i) = \begin{cases} 0, & t = 1,\ldots,i \\ t-i-1, & t = i+1,\ldots,i+q \\ q, & t = i+q+1,\ldots,n. \end{cases}$$

The signature indicates a linear increase in the level for periods $t = i$ through to $t = i + q$, after which the series reverts to its normal dynamics but starting from a level $q\delta$ higher than in the absence of an intervention. This signature is illustrated by Figure 6.

Estimation and testing of shock effects under the more general model is based on the intervention contrast

$$\mathbf{s}_i = \sum_{j=i}^{i+q} \{\mathbf{X}_j(i)'\mathbf{u}_j + \mathbf{W}_j(i)'\mathbf{r}_j\}, \tag{21}$$

where $\mathbf{u}_j$ and $\mathbf{r}_j$ are generated by the KFS applied to the null model. The covariance, $\mathbf{S}_i = \sigma^{-2}\mathrm{cov}(\mathbf{s}_i)$, can be generated recursively. Details and proofs are given in the Appendix.

To illustrate, consider a state shock at $t = i$ with an equivalent reverse shock at $t = i + q$; that is, $\mathbf{W}_i(i) = \mathbf{I}$ and $\mathbf{W}_{i+q}(i) = -\mathbf{I}$. Using (21) yields

$$\mathbf{s}_i = \mathbf{s}_{i,i} + \mathbf{s}_{i,i+q} = \mathbf{r}_i - \mathbf{r}_{i+q},$$

and thus

$$\begin{aligned}\mathbf{S}_i &= \sigma^{-2}\mathrm{cov}(\mathbf{r}_i - \mathbf{r}_{i+q}) \\ &= \mathbf{N}_i + \mathbf{N}_{i+q} - \mathbf{L}'_{i+q,i+1}\mathbf{N}_{i+q} - \mathbf{N}_{i+q}\mathbf{L}_{i+q,i+1},\end{aligned}$$

where $\mathbf{L}_{j,t} \equiv \mathbf{L}_j \ldots \mathbf{L}_t$ for $j \geq t$.

Another approach to composite interventions is to exploit the idea of model multiplicity. The null model can be written in an overelaborate form including components that under the null, play no role in the measurements. These additional state elements introduce structure into the transition matrix $\mathbf{T}$, allowing more general signatures to be propagated. For example, suppose that the null is a random walk plus noise (3). The null corresponds to (15) where the slope is constrained to be 0; that is, $\alpha_{1,2} = h_2 = 0$. Statistics to detect slope changes can be computed by using simple interventions in this overelaborate form of the null model.

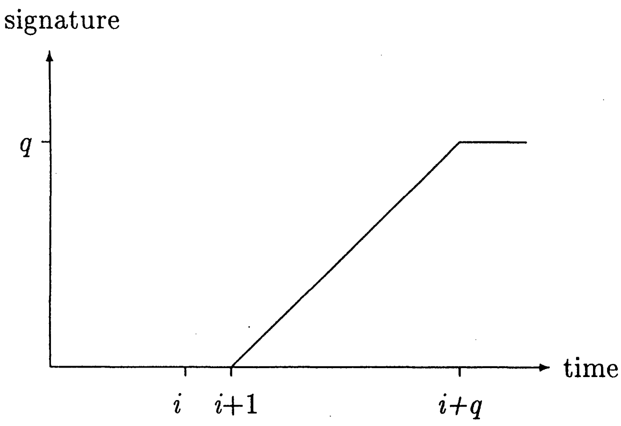

Figure 6. Intervention Signature for a Temporary Level Shift.

8. CONCLUSION

The introduction of shocks is a powerful tool for analyzing departures from a fitted null model. Many forms of aberrant behavior can be modeled efficiently by shocks to the transition equation of a state-space representation. We have established that alternative model statistics take simple forms when viewed as functions of the smoothations. Test statistics for any number of interventions can be generated using the output of a single null model KFS run.

Many authors (e.g., Ansley and Kohn 1985; de Jong 1988b, 1991; Harvey and Phillips 1979) have described the problem of filtering a series with diffuse initial conditions. They put forward a number of related algorithms that involve adjustments to the filtering equations. Diffuse initial conditions can be modeled by the introduction of a shock at $t = 0$. Running the KFS, using an arbitrary initialization, will provide an updated estimate of the starting conditions. This step can be incorporated into the optimization algorithm. Thus, on convergence of the maximization process, the estimate of the initial conditions will be computed along with the MLEs of the hyperparameters.

APPENDIX: PROOFS

Proof of Theorem 1

The proof of this theorem is based on the following lemma.

Lemma. Suppose that $\mathrm{cov}(\mathbf{y}) = \sigma^2\boldsymbol{\Sigma}$. Let $\mathbf{Jy}$ be any selection of the components of $\mathbf{y}$ with $\mathbf{Ky}$ denoting the remaining components. Then

$$\mathbf{J}\boldsymbol{\Sigma}^{-1}\{\mathbf{y} - E(\mathbf{y})\} = \mathbf{J}\boldsymbol{\Sigma}^{-1}\mathbf{J}'\{\mathbf{Jy} - E(\mathbf{Jy}|\mathbf{Ky})\} \tag{A.1}$$

and

$$\mathbf{J}\boldsymbol{\Sigma}^{-1}\mathbf{J}' = \{\sigma^{-2}\mathrm{cov}(\mathbf{Jy}|\mathbf{Ky})\}^{-1}. \tag{A.2}$$

Proof. Put $\mathbf{y}_1 = \mathbf{Ky}$ and $\mathbf{y}_2 = \mathbf{Jy}$ and, without loss of generality, assume that $\mathbf{y} = (\mathbf{y}_1', \mathbf{y}_2')'$. Partition $\boldsymbol{\Sigma}$ conformal to the partition of $\mathbf{y}$. By the inverse of a partitioned matrix,

$$\begin{aligned}\boldsymbol{\Sigma}^{-1} &= \begin{pmatrix} \boldsymbol{\Sigma}_1 & \boldsymbol{\Sigma}_{12} \\ \boldsymbol{\Sigma}_{21} & \boldsymbol{\Sigma}_2 \end{pmatrix}^{-1} \\ &= \begin{pmatrix} \boldsymbol{\Sigma}_1^{-1} + \boldsymbol{\Sigma}_1^{-1}\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{2|1}^{-1}\boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_1^{-1} & -\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\Sigma}_{12}\boldsymbol{\Sigma}_{2|1}^{-1} \\ -\boldsymbol{\Sigma}_{2|1}^{-1}\boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_1^{-1} & \boldsymbol{\Sigma}_{2|1}^{-1} \end{pmatrix},\end{aligned}$$

where

$$\boldsymbol{\Sigma}_{2|1} = \boldsymbol{\Sigma}_2 - \boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_1^{-1}\boldsymbol{\Sigma}_{12} = \sigma^{-2}\mathrm{cov}(\mathbf{y}_2|\mathbf{y}_1),$$

which establishes (A.2). By definition,

$$E(\mathbf{y}_2|\mathbf{y}_1) = E(\mathbf{y}_2) + \boldsymbol{\Sigma}_{21}\boldsymbol{\Sigma}_1^{-1}\{\mathbf{y}_1 - E(\mathbf{y}_1)\},$$

and hence the lower block of $\Sigma^{-1}\{\mathbf{y} - E(\mathbf{y})\}$ is given by

$$\Sigma_{2|1}^{-1}[\{\mathbf{y}_2 - E(\mathbf{y}_2)\} - \Sigma_{21}\Sigma_1^{-1}\{\mathbf{y}_1 - E(\mathbf{y}_1)\}] = \{\sigma^{-2}\text{cov}(\mathbf{y}_2|\mathbf{y}_1)\}^{-1}\{\mathbf{y}_2 - E(\mathbf{y}_2|\mathbf{y}_1)\},$$

which establishes (A.1).

Returning to Theorem 1, let $\mathbf{v}$ be the stack of innovations, $\mathbf{u}$ be the stack of smoothations, and $\text{cov}(\mathbf{y}) = \sigma^2\Sigma$. The innovations are given by $\mathbf{v} = \mathbf{L}\mathbf{y}$, where $\mathbf{L}$ is a lower triangular matrix with identity matrices on the diagonal. Thus

$$\text{cov}(\mathbf{v}) = \text{cov}(\mathbf{L}\mathbf{y}) = \sigma^2\mathbf{L}\Sigma\mathbf{L}' = \sigma^2\text{diag}(\mathbf{F}_1, \ldots, \mathbf{F}_n) \equiv \sigma^2\mathbf{F}.$$

The Kalman filter equations (6) for $\mathbf{v}_t$ and $\mathbf{a}_{t+1}$ can be written as

$$\begin{pmatrix} \mathbf{v}_t \\ \mathbf{a}_{t+1} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & -\mathbf{Z}_t \\ \mathbf{K}_t & \mathbf{L}_t \end{pmatrix} \begin{pmatrix} \mathbf{y}_t \\ \mathbf{a}_t \end{pmatrix}.$$

Similarly, combining the equations (8) for $\mathbf{u}_t$ and $\mathbf{r}_{t-1}$ yields

$$\begin{pmatrix} -\mathbf{u}_t \\ \mathbf{v}_{t-1} \end{pmatrix} = \begin{pmatrix} \mathbf{I} & -\mathbf{Z}_t \\ \mathbf{K}_t & \mathbf{L}_t \end{pmatrix}' \begin{pmatrix} -\mathbf{F}_t^{-1}\mathbf{v}_t \\ \mathbf{r}_t \end{pmatrix},$$

which works through the data, in reverse order, with $\mathbf{r}_n = 0$ and $-\mathbf{F}_t^{-1}\mathbf{v}_t$ as input. Thus if $\mathbf{v} = \mathbf{L}\mathbf{y}$, then

$$\mathbf{u} = \mathbf{L}'\mathbf{F}^{-1}\mathbf{v} = \Sigma^{-1}\mathbf{y}, \qquad \text{cov}(\mathbf{u}) = \sigma^2\mathbf{L}'\mathbf{F}^{-1}\mathbf{L} = \sigma^2\Sigma^{-1}. \tag{A.3}$$

Now $\text{cov}(\mathbf{u}_t) = \sigma^2\mathbf{M}_t$, so from (A.3), it follows that $\mathbf{M}_t$ is the tth diagonal block of Σ^{-1}. That $\mathbf{u}_t = \mathbf{M}_t\{\mathbf{y}_t - E(\mathbf{y}_t|\mathbf{y}^t)\}$ now follows from the lemma.

Proof of Theorem 2

That $\mathbf{s}_i = \mathbf{X}_i'\mathbf{u}_i + \mathbf{W}_i'\mathbf{r}_i$ has been established in Section 3. It follows that

$$\mathbf{s}_i = \mathbf{X}_i'(\mathbf{F}_i^{-1}\mathbf{v}_i - \mathbf{K}_i'\mathbf{r}_i) + \mathbf{W}_i'\mathbf{r}_i = \mathbf{X}_i'\mathbf{F}_i^{-1}\mathbf{v}_i + \mathbf{Q}_i'\mathbf{r}_i.$$

Now $\mathbf{r}_i$ is linear in the future innovations, and hence $\mathbf{v}_i$ and $\mathbf{r}_i$ are uncorrelated with covariance matrices $\mathbf{F}_i$ and $\mathbf{N}_i$. Hence $\text{cov}(\mathbf{s}_i) = \sigma^2\mathbf{S}_i$ is as asserted.

Proof of Theorem 3

Put $\mathbf{A} = (\mathbf{X}_i', \mathbf{W}_i')$ and $\mathbf{x} = (\mathbf{u}_i', \mathbf{r}_i')'$; then

$$\rho_i^2 = (\mathbf{A}\mathbf{x})'\{\sigma^{-2}\text{cov}(\mathbf{A}\mathbf{x})\}^{-1}(\mathbf{A}\mathbf{x}).$$

Define $\mathbf{A}^-$ as a generalized inverse of $\mathbf{A}$. If $\mathbf{A}$ has full column rank, then $\mathbf{A}^-\mathbf{A} = \mathbf{I}$ and

$$\begin{aligned} \rho_i^2 &= \mathbf{x}'\mathbf{A}'\{\mathbf{A}\sigma^{-2}\text{cov}(\mathbf{x})\mathbf{A}'\}^{-1}\mathbf{A}\mathbf{x} \\ &= \mathbf{x}'(\mathbf{A}^-\mathbf{A})'\{\sigma^{-2}\text{cov}(\mathbf{x})\}^{-1}(\mathbf{A}^-\mathbf{A})\mathbf{x} \\ &= \mathbf{x}'\{\sigma^{-2}\text{cov}(\mathbf{x})\}\mathbf{x} \\ &= (\mathbf{u}_i' \quad \mathbf{r}_i')[\sigma^{-2}\text{cov}\{(\mathbf{u}_i' \quad \mathbf{r}_i')'\}]^{-1}(\mathbf{u}_i' \quad \mathbf{r}_i')', \end{aligned}$$

where

$$\text{cov}\{(\mathbf{u}_i' \quad \mathbf{r}_i')'\} = \sigma^2 \begin{pmatrix} \mathbf{M}_i & -\mathbf{K}_i'\mathbf{N}_i \\ -\mathbf{N}_i\mathbf{K}_i & \mathbf{N}_i \end{pmatrix}.$$

Partitioned matrix inversion yields

$$\rho_i^2 = \mathbf{v}_i'\mathbf{F}_i^{-1}\mathbf{v}_i + \mathbf{r}_i'\mathbf{N}_i^{-1}\mathbf{r}_i.$$

Thus the maximum is as stated in (14) when $\mathbf{A}$ has full column rank. If $\mathbf{A}$ has rank 1, then

$$\rho_i^2 = (\mathbf{A}\mathbf{x})^2/\{\sigma^{-2}\mathbf{A}\ \text{cov}(\mathbf{x})\mathbf{A}'\}$$

attains the stated maximum (Rao 1973) at

$$\mathbf{A} = \mathbf{x}'\{\sigma^{-2}\text{cov}(\mathbf{x})\}^{-1} = (\mathbf{u}_i' \quad \mathbf{r}_i')[\sigma^{-2}\text{cov}\{(\mathbf{u}_i' \quad \mathbf{r}_i')'\}]^{-1} = (\mathbf{v}_i' \quad \mathbf{v}_i'\mathbf{K}_i' + \mathbf{r}_i'\mathbf{N}_i^{-1})'.$$

For $\mathbf{A}$ with rank between 1 and full column rank, the maximum must be equal to (14), because it must lie between the rank 1 and full column rank maxima.

Correlation of Shock Estimates

We can exploit the fact that the $\mathbf{v}_t$ are uncorrelated and $\mathbf{r}_t = \sum_{k=t+1}^n \mathbf{L}_{k-1,t+1}'\mathbf{Z}_k'\mathbf{F}_k^{-1}\mathbf{v}_k$ to derive a simple expression for $\text{cov}(\mathbf{s}_i, \mathbf{s}_j)$. For $i < j$,

$$\begin{aligned} \text{cov}(\mathbf{s}_i, \mathbf{s}_j) &= \text{cov}(\mathbf{X}_i'\mathbf{F}_i^{-1}\mathbf{v}_i + \mathbf{Q}_i'\mathbf{r}_i, \mathbf{X}_j'\mathbf{F}_j^{-1}\mathbf{v}_j + \mathbf{Q}_j'\mathbf{r}_j) \\ &= \mathbf{Q}_i'\text{cov}(\mathbf{r}_i, \mathbf{v}_j)\mathbf{F}_j^{-1}\mathbf{X}_j + \mathbf{Q}_i'\text{cov}(\mathbf{r}_i, \mathbf{r}_j)\mathbf{Q}_j \\ &= \mathbf{Q}_i'\mathbf{L}_{j-1,i+1}'\mathbf{Z}_j'\mathbf{F}_j^{-1}\text{cov}(\mathbf{v}_j, \mathbf{v}_j)\mathbf{F}_j^{-1}\mathbf{X}_j \\ &\quad + \mathbf{Q}_i'\mathbf{L}_{j-1,i+1}'\mathbf{L}_j'\text{cov}(\mathbf{r}_j, \mathbf{r}_j)\mathbf{Q}_j \\ &= \sigma^2\mathbf{Q}_i'\mathbf{L}_{j-1,i+1}'(\mathbf{Z}_j'\mathbf{F}_j^{-1}\mathbf{X}_j + \mathbf{L}_j'\mathbf{N}_j\mathbf{Q}_j). \end{aligned}$$

Noting that $\text{cov}(\hat{\delta}_i, \hat{\delta}_j) = \mathbf{S}_i^{-1}\text{cov}(\mathbf{s}_i, \mathbf{s}_j)\mathbf{S}_j^{-1}$ yields

$$\text{cov}(\hat{\delta}_i, \hat{\delta}_j) = \sigma^2\mathbf{S}_i^{-1}\mathbf{Q}_i'\mathbf{L}_{j-1,i+1}'(\mathbf{Z}_j'\mathbf{F}_j^{-1}\mathbf{X}_j + \mathbf{L}_j'\mathbf{N}_j\mathbf{Q}_j)\mathbf{S}_j^{-1}, \tag{A.4}$$

where $\mathbf{L}_{j,t} \equiv \mathbf{L}_j \ldots \mathbf{L}_t$ for $j \geq t, \mathbf{L}_{t-1,t} \equiv \mathbf{I}$ and $\mathbf{L}_{j,t} \equiv \mathbf{0}$ for $j < t-1$.

More on Composite Interventions

The expression for s_i is proved by noting that the intervention signature is given by $\mathbf{D}(i) = \sum_{j=i}^{i+q}\mathbf{D}(i,j)$, where $\mathbf{D}(i,j)$ is the shock signature arising from the shock entry at $t = j$, and $\mathbf{s}_i = \sum_{j=i}^{i+q}\mathbf{s}_{i,j}$, where

$$\mathbf{s}_{i,j} = \mathbf{D}(i,j)'\mathbf{u} = \mathbf{X}_j(i)'\mathbf{u}_j + \mathbf{W}_j(i)'\mathbf{r}_j = \mathbf{X}_j(i)'\mathbf{F}_j^{-1}\mathbf{v}_j + \mathbf{Q}_j(i)'\mathbf{r}_j.$$

Inspection of the covariances between the $\mathbf{s}_{i,j}$ leads to the recursion to compute $\mathbf{S}_i$. Set $\mathbf{S}_i \leftarrow \mathbf{0}$ and $\mathbf{C} \leftarrow \mathbf{0}$ and for $j = i+q, \ldots, i$, compute recursively

$$\mathbf{S}_i \leftarrow \mathbf{S}_i + \mathbf{X}_j(i)'\mathbf{F}_j^{-1}\mathbf{X}_j(i) + \mathbf{Q}_j(i)'\mathbf{N}_j\mathbf{Q}_j(i) + \mathbf{Q}_j(i)'\mathbf{C} + \mathbf{C}'\mathbf{Q}_j(i)$$

and

$$\mathbf{C} \leftarrow \mathbf{Z}_j'\mathbf{F}_j^{-1}\mathbf{X}_j(i) + \mathbf{L}_j'\{\mathbf{N}_j\mathbf{Q}_j(i) + \mathbf{C}\},$$

where $\mathbf{Q}_j(i) = \mathbf{W}_j(i) - \mathbf{K}_j\mathbf{X}_j(i)$.

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