



Seasonality with trend and cycle interactions in unobserved components models

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Summary. Unobserved components time series models decompose a time series into a trend, a season, a cycle, an irregular disturbance and possibly other components. These models have been successfully applied to many economic time series. The standard assumption of a linear model, which is often appropriate after a logarithmic transformation of the data, facilitates estimation, testing, forecasting and interpretation. However, in some settings the linear-additive framework may be too restrictive. We formulate a non-linear unobserved components time series model which allows interactions between the trend-cycle component and the seasonal component. The resulting model is cast into a non-linear state space form and estimated by the extended Kalman filter, adapted for models with diffuse initial conditions. We apply our model to UK travel data and US unemployment and production series, and show that it can capture increasing seasonal variation and cycle-dependent seasonal fluctuations.

Keywords: Diffuse initialization; Extended Kalman filter; Non-linear state space models; Seasonal interaction; Unobserved components

1. Introduction

A common practice in economic time series analyses and seasonal adjustment procedures is first to take logarithms of the data. Linear Gaussian models can often be fitted to the transformed data, whereas they are inappropriate for the series in the original metric. The log-additive framework appears to work successfully for time series modelling based on the decomposition into trend, seasonal, irregular and other components. The logarithmic transformation converts an exponentially growing trend into a linear trend. Further, it often eliminates or reduces growing seasonal variation and heteroscedasticity in seasonal time series. However, the log-transformation has various drawbacks. In decomposition models or in seasonal adjustment procedures such as the popular US census X-11 and X-12 programs, the logarithmic transformation presents a single rigid alternative to the untransformed linear additive specification; see Findley *et al.* (1998). In particular, it predicates that time series components combine multiplicatively in the implied model for the untransformed series. A full multiplicative model is not always intended or desired. Moreover, when some heteroscedasticity or changing seasonal variation remains after the transformation, applying the log-transformation again is usually not an attractive solution. Finally, if the data have already been supplied in units measuring proportional changes, applying the log-transformation can complicate model interpretation.

In empirical work we may encounter cases where the log-transformation does not remove all heteroscedasticity or growth in the seasonal component. For example, consider the data set of

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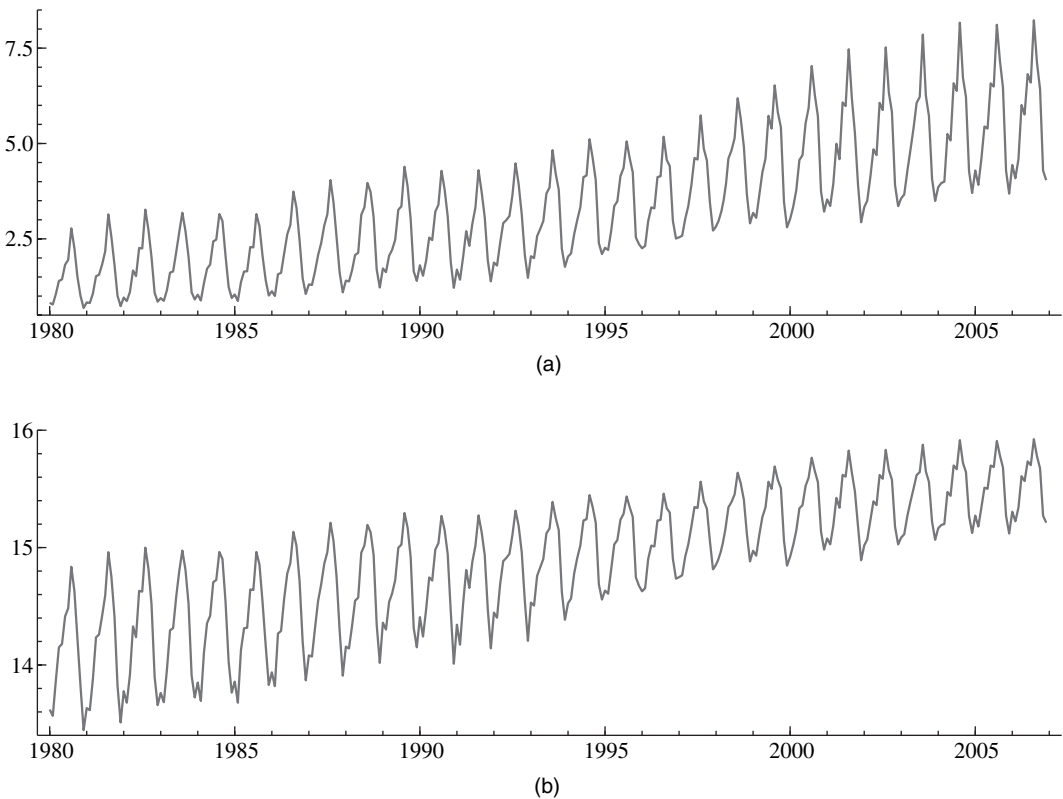


Fig. 1. Visits of UK residents abroad in (a) levels (millions) and (b) logarithms

monthly visits abroad by UK residents from January 1980 to December 2006. Fig. 1 presents time series plots of the data in levels and in logarithms. The time series of visits abroad shows a clear upward trend, a pronounced seasonal pattern and a steady increase in the seasonal variation over time. However, after applying the log-transformation, the increase of seasonal variation has been converted into a decrease. This may indicate that the log-transformation is not particularly appropriate for this series. An obvious course of action is to consider alternative data transformations.

In this paper however, we explore a different option by modelling the time series by using the class of unobserved components (UC) models; see Harvey (1989) for a detailed discussion. Searching for an appropriate data transformation is essentially a quest for a suitable functional form of the model. Our approach is to alter the functional form directly by relating the seasonal component to other components such as the trend. We introduce a simple multiplicative-additive extension to linear UC models, in which a transformation of the trend acts as a scaling factor to the seasonal component. Estimation is effectively performed by using the extended Kalman filter (EKF), which is a relatively simple estimation procedure compared with more elaborate simulation-based methods. As our model specification contains non-stationary components, we have adapted an exact diffuse initialization method to the EKF, which is a novelty in the literature. Unlike previous studies with multiplicative seasonality in UC models, we explicitly parameterize and estimate the degree of trend-season interaction. The basic linear form is a simple parameter restriction in our model.

When the data contain a cyclical component, the magnitude of the seasonal influence may vary

along the phase of the cycle. Although seasonal fluctuations and business cycles are traditionally assumed to be uncorrelated, for some macroeconomic series there is increasing evidence that this assumption is not valid. For example Cecchetti *et al.* (1997), Franses and de Bruin (1999), van Dijk *et al.* (2003) and Osborn and Matas-Mir (2004) have found varying amounts of interactions between cycles and seasonal adjustment in unemployment and industrial production series by using linear or non-linear smooth transition auto-regression models. With a straightforward extension of our trend–season interaction model, we also examine interactions between the seasonal component and the business cycle. Interactions between the season and the trend or the cycle are typically studied separately in the literature. The non-linear UC model allows us to model changes in seasonal variation along both trend and cycle fluctuations, as well as changes resulting from exogenous shocks, by using a single coherent framework.

In the next section, we describe the basic unobserved components model. We further review models with multiplicative seasonality that have been proposed in the literature. In Section 3 we introduce our non-linear specification and describe the EKF estimation procedure. Empirical applications of the new model are provided in Section 4. We conclude with Section 5.

2. The unobserved components time series model

The UC time series model has proven to be a valuable tool for seasonal adjustment; see for example Gersch and Kitagawa (1983) and Harvey and Scott (1994). Compared with model-free procedures, they offer the benefit of providing statistical tests and prediction algorithms. Additionally, it is simple to incorporate changing seasonal patterns and to introduce additional features such as explanatory variables, interventions and cyclical components. Estimation of parameters and measurement of the components are based on Kalman filtering and smoothing methods which can deal with multivariate series and data irregularities such as missing observations or unevenly recorded data. In this section we briefly introduce the basic form of the model and provide some details which are needed for the following sections.

The seasonal adjustment framework that is employed in this paper is based on the basic structural model (BSM) as described by Harvey (1989). We assume that the time series $\{Y_t\}$ is observed, which we routinely transform into logarithms, i.e.

$$y_t = \log(Y_t), \quad t = 1, \dots, n. \quad (1)$$

The BSM decomposes y_t into additive stochastic components and is given by

$$y_t = \mu_t + \gamma_t + \varepsilon_t, \quad \varepsilon_t \sim \text{NID}(0, \sigma_\varepsilon^2), \quad t = 1, \dots, n, \quad (2)$$

where μ_t represents the trend, γ_t the seasonal component and ε_t the irregular disturbance term. The linear model (2) can be regarded as a generalization of the classical time series decomposition in which deterministic components for trend and season are replaced by stochastic processes. The BSM is a simple example of a UC model. It can be extended by including deterministic and/or stochastic components. For example, explanatory variables, intervention effects and stochastic cycles can be a part of the UC model.

The trend component μ_t in model (2) is specified in our applications by the local linear trend model as given by

$$\begin{aligned} \mu_{t+1} &= \mu_t + \beta_t + \eta_t, & \eta_t &\sim \text{NID}(0, \sigma_\eta^2), \\ \beta_{t+1} &= \beta_t + \zeta_t, & \zeta_t &\sim \text{NID}(0, \sigma_\zeta^2), \end{aligned} \quad (3)$$

where β_t represents the drift or slope of the trend μ_t and the disturbances ε_t, η_t and ζ_t

are mutually uncorrelated at all lags and leads, for $t = 1, \dots, n$. Some notable limiting cases of this specification include the following: if $\sigma_\zeta \rightarrow 0$ while σ_η is non-zero the trend is a random walk with drift β_1 ; if $\sigma_\eta \rightarrow 0$ while σ_ζ is non-zero the trend follows a smooth integrated random walk; when both tend to 0, μ_t reverts to a deterministic linear trend. **In our empirical section we use a smooth trend specification by restricting σ_η^2 to 0.** The initial values of μ_1 and β_1 are generally unknown and will be represented by non-informative or *diffuse* initial distributions. We shall elaborate on this issue in Section 3.5, as the estimation procedure needs to take it into account.

The seasonal component γ_t can be specified as a sum of time varying trigonometric cycles. Specifically, in a model for a time series with seasonal length s , we have

$$\gamma_t = \sum_{j=1}^{\lfloor s/2 \rfloor} \gamma_{j,t} \quad (4)$$

where $\lfloor \cdot \rfloor$ denotes the floor function and the recursion of the components is given by

$$\begin{pmatrix} \gamma_{j,t+1} \\ \gamma_{j,t+1}^* \end{pmatrix} = \begin{pmatrix} \cos(\lambda_j) & \sin(\lambda_j) \\ -\sin(\lambda_j) & \cos(\lambda_j) \end{pmatrix} \begin{pmatrix} \gamma_{j,t} \\ \gamma_{j,t}^* \end{pmatrix} + \begin{pmatrix} \omega_{j,t} \\ \omega_{j,t}^* \end{pmatrix}, \quad \begin{pmatrix} \omega_{j,t} \\ \omega_{j,t}^* \end{pmatrix} \sim \text{NID}(0, \sigma_\omega^2 I_2), \quad (5)$$

with $\lambda_j = 2\pi j/s$ for $j = 1, \dots, \lfloor s/2 \rfloor$ and $t = 1, \dots, n$. The seasonal disturbances $\omega_{j,t}$ and $\omega_{j,t}^*$ are uncorrelated with the previously specified disturbances at all lags and leads. Note that the components $\gamma_{j,t+1}^*$ are not included in γ_t directly but are used as auxiliary variables to write the seasonal term in recursive form. In the absence of the disturbances $\omega_{j,t}$ and $\omega_{j,t}^*$, equation (5) reduces to a recursive expression of deterministic sine and cosine waves and $(\gamma_{j,t}, \gamma_{j,t}^*)$ follow a circle when they are projected on the orthogonal axes in two-dimensional Euclidean geometry. Further details of the seasonal components were discussed by Harvey and Scott (1994) and Proietti (2000) who also described alternative seasonal component models such as stochastic seasonal dummy variables. Although these alternative specifications can be considered in our non-linear UC model, we restrict ourselves to the trigonometric seasonal component (5) in our study. The seasonal components represent non-stationary processes and their initial conditions rely on diffuse distributions, similar to the trend components.

Many macroeconomic time series contain periodic fluctuations of a lower frequency than the seasonal frequencies. For example, fluctuations in economic time series that are associated with medium frequencies related to periods between 1.5 and 8 years are typically interpreted as the business cycle; see Baxter and King (1999). The dynamic effects that are related to these medium frequencies appear often moderately pronounced in the observed economic time series and tend to be of a stationary nature. To incorporate the cyclical dynamics in the time series model, the BSM can be extended by a stochastic cyclical component ψ_t . We then have the decomposition model

$$y_t = \mu_t + \gamma_t + \psi_t + \varepsilon_t, \quad t = 1, \dots, n, \quad (6)$$

with

$$\begin{pmatrix} \psi_{t+1} \\ \psi_{t+1}^* \end{pmatrix} = \rho \begin{pmatrix} \cos(\lambda^c) & \sin(\lambda^c) \\ -\sin(\lambda^c) & \cos(\lambda^c) \end{pmatrix} \begin{pmatrix} \psi_t \\ \psi_t^* \end{pmatrix} + \begin{pmatrix} \kappa_t \\ \kappa_t^* \end{pmatrix}, \quad \begin{pmatrix} \kappa_t \\ \kappa_t^* \end{pmatrix} \sim \text{NID}(0, \sigma_\kappa^2 I_2), \quad (7)$$

where the three unknown coefficients λ^c , ρ and σ_κ^2 in the cycle equation (7) represent the cyclical frequency, the damping factor and the cycle disturbance variance respectively. **The period of the**

cycle is given by $2\pi/\lambda^c$. For $|\rho| < 1$ and $0 < \lambda < \pi$, the cycle ψ_t and the auxiliary process ψ_t^* are stationary auto-regressive moving average (ARMA(2,1)) processes, with variance $\sigma_\kappa^2/(1-\rho^2)$. The cycle collapses into an AR(1) process when λ^c approaches 0. For stationary cycle processes represented by equation (7) the unconditional distributions provide the properly defined initial conditions for ψ_t and ψ_t^* . The disturbances κ_t and κ_t^* are specified to be uncorrelated with the disturbances of the other components at all lags and leads, and uncorrelated with the initial distributions. A more elaborate discussion of the BSM and other UC models has been provided by Harvey (1989).

The BSM, possibly extended with a cycle component, can be formulated as a linear state space model specified by the equations

$$\begin{aligned} y_t &= Z\alpha_t + \varepsilon_t, & \varepsilon_t &\sim \text{NID}(0, \sigma_\varepsilon^2), \\ \alpha_{t+1} &= T\alpha_t + \eta_t, & \eta_t &\sim \text{NID}(0, H), \quad t = 1, \dots, n, \end{aligned} \quad (8)$$

where the first equation relates the observation y_t to an unobserved state vector α_t , which contains the trend, season and other components that are required for describing the model. The state vector is modelled by the vector auto-regressive process that is specified in the second equation, together with an initial distribution for α_1 . The system variables Z , T , σ_ε^2 and H are chosen to represent a particular model and will usually depend on unknown parameters, which can be estimated by maximizing the Gaussian likelihood function of the model. After replacing the parameters by their estimated values, the unobserved components can be estimated by using the Kalman filtering and smoothing equations. The seasonal adjustment procedure based on the BSM simply consists of subtracting the estimated seasonal component γ_t from the time series y_t , i.e. $y_t^{\text{SA}} = y_t - \hat{\gamma}_t$ where y_t^{SA} is the seasonally adjusted time series and $\hat{\gamma}_t$ is the estimate of γ_t that is obtained from the Kalman smoothing equations. The filtering, smoothing and likelihood equations for linear Gaussian state space models are provided in Appendix A. For a more complete discussion of state space methods and their applications, we refer to Harvey (1989) and Durbin and Koopman (2001). An introductory text for UC models is Commandeur and Koopman (2007).

3. Seasonal interacting components

3.1. A review of non-linear trend–seasonal models

A mixed additive multiplicative seasonal adjustment procedure based on the classical trend–seasonal–irregular decomposition was considered by Durbin and Murphy (1975) for the modelling of a set of unemployment series. The Durbin–Murphy specification is given by

$$y_t = m_t + g_t + g_t^* m_t + \varepsilon_t, \quad \varepsilon_t \sim \text{NID}(0, \sigma_\varepsilon^2), \quad t = 1, \dots, n,$$

where m_t is a deterministic trend function, g_t is an additive seasonal fixed effect and g_t^* is a multiplicative seasonal fixed factor. A standard moving average filter can be derived to extract the various components from the data. Although this model was not based on a stochastic UC model, it can be regarded as an early precursor to our multiplicative seasonal component model that is presented in Section 3.2 below.

Bowerman *et al.* (1990) explored various approaches to deal with the problem of increasing seasonal variation in time series. Although all their suggestions are built on ARMA model-based methods, one of their models takes a similar direction to what we propose. In their seasonal interaction model, changes in the seasonal component are directly related to a deterministic trend by

$$y_t = \beta_0 + \beta_0^+ t + \sum_{j=1}^{s-1} \beta_j D_{j,t} + \sum_{j=1}^{s-1} \beta_j^+ D_{j,t} t + u_t,$$

where $\beta_0 + \beta_0^+ t$ is the fixed trend component with unknown coefficients β_0 and β_0^+ , $D_{j,t}$ is the seasonal dummy regression variable with unknown coefficients β_j and β_j^+ for $j = 1, \dots, s-1$ and u_t is modelled as an auto-regressive integrated moving average process. The coefficients β_j are associated with the seasonal effects that are independent of the trend whereas the coefficients β_j^+ are interacting with the trend.

In most current applications of UC models, the specifications are of the logarithmic additive type, which can be easily formulated as a linear state space model. An important practical advantage of linearity is that optimal estimates of the latent components, parameters and model predictions are easily obtained by using standard Kalman-filter-based methods. Estimation is a routine procedure for which easy-to-use graphical packages are available. Combining multiplicative and additive components may result in a better model fit. However, optimal estimation in such models can be quite complex and is often carried out by using elaborate and computationally expensive simulation methods. For example, Shephard (1994) formulated the multiplicative UC seasonal adjustment model

$$y_t = (1 + \gamma_t + \varepsilon_t^+) \mu_t + \varepsilon_t, \quad \varepsilon_t \sim \text{NID}(0, \sigma_\varepsilon^2), \quad \varepsilon_t^+ \sim \text{NID}(0, \sigma_{\varepsilon^+}^2),$$

for $t = 1, \dots, n$, where μ_t and γ_t are the trend and seasonal components and can possibly be modelled as in expressions (3) and (5) respectively. The two irregular terms ε_t and ε_t^+ are uncorrelated with each other and with all other disturbances at all leads and lags. The seasonal term γ_t interacts with the trend component through scaling whereas the irregular term ε_t^+ allows for additional heteroscedasticity. The multiplicative UC model was used to adjust seasonally the UK M4 money supply series based on parameter estimates obtained from Markov chain Monte Carlo methods. Durbin and Koopman (2001) used a similar additive–multiplicative specification as an exposition example for importance sampling techniques.

An alternative specification, which is called the pseudoadditive decomposition, was described in Findley *et al.* (1998). It was developed by the UK Office for National Statistics for seasonally adjusting series with very small, possibly zero, values in certain seasons. The decomposition is based on the representation

$$Y_t = T_t(S_t + I_t - 1)$$

where Y_t is the time series in levels and T_t , S_t and I_t are the trend, seasonal and irregular components respectively. The main feature of this decomposition is that the seasonal adjustment is carried out by subtracting the term $T_t(S_t - 1)$ rather than division by a seasonal factor which is unstable when the seasonal factor is very small. Moving-average-based filters to extract the components are implemented in the X-12-ARIMA program of the US Bureau of the Census.

Proietti and Riani (2007) considered the use of the Box–Cox transformation in seasonal UC models as a generalization of the log-transformation. This approach implies an inverse Box–Cox transformation on the sum of the components and it allows for a far wider range of options than the usual exponential transformation. However, interpretation in the original metric can be awkward for many values of the Box–Cox transformation parameter. The model was estimated with a combination of numerical integration and simulation techniques.

Finally, the methodology of Ozaki and Thomson (1994) is close to our non-linear UC model of Section 3.2 below although the specifics and motivations of the models are different. Ozaki and Thomson considered a UC model in levels, given by

$$Y_t = M_t(1 + G_t) \exp(\varepsilon_t - \sigma^2/2), \quad \varepsilon_t \sim \text{NID}(0, \sigma_\varepsilon^2), \quad t = 1, \dots, n,$$

where M_t is a linear Gaussian stochastic process for the trend whereas G_t is a stochastic seasonal component. When the log-transformation is applied to Y_t , the model for $y_t = \log(Y_t)$ becomes linear and is given by

$$y_t = \mu_t + \gamma_t + \varepsilon_t, \quad \mu_t = \log(M_t) - \sigma^2/2, \quad \gamma_t = \log(1 + G_t),$$

for $t = 1, \dots, n$. Parameter estimation is carried out on the basis of the non-linear model for Y_t , using the EKF rather than fitting the linear model to the log-transformed series y_t . The main motivation of this approach is to provide a model-based framework for the X-11 seasonal adjustment procedure.

3.2. Trend and cycle interactions in the basic structural model

The standard linear BSM of Section 2 is usually fitted to log-transformed data, implying a model with multiplicative components in the untransformed series. In the previous section we have discussed various alternative specifications that have been suggested in the literature. These non-linear model specifications can be considered when heteroscedasticity or changing seasonal variation is not adequately removed by the model-based seasonal adjustment procedure. We propose to generalize the BSM by scaling the amplitude of the seasonal component via an exponential transformation of the trend component. The time series, either in levels or in logarithms, is decomposed by the non-linear model

$$y_t = \mu_t + \exp(b\mu_t)\gamma_t + \varepsilon_t, \quad \varepsilon_t \sim \text{NID}(0, \sigma_\varepsilon^2), \quad t = 1, \dots, n, \quad (9)$$

where b is an unknown fixed coefficient and the dynamic specification of the trend component μ_t is given by expression (3) and the seasonal component γ_t is given by expression (5). The sign of the coefficient b determines whether the seasonal variation increases or decreases when a positive change in the trend occurs. The model reduces to the basic linear specification when b is 0. The overall amplitude of the seasonal component is determined by both $\exp(b\mu_t)$ and the disturbance variance σ_ε^2 in the stochastic seasonal equation (5). The two sources of seasonal amplitude can be made more explicit by restricting $\sigma_\varepsilon^2 = 1$ in expression (5) and replacing $\exp(b\mu_t)$ by $\exp(a + b\mu_t)$ as the scaling process in model (9) where a is a fixed unknown coefficient. However, we adopt specification (9) to remain close to the original linear BSM.

When the cycle component (7) is added to the BSM we obtain model (6). Similar to the introduction of the trend interaction, we can extend model (6) by a trend and cycle interaction to obtain the non-linear model

$$y_t = \mu_t + \psi_t + \exp(b\mu_t + c\psi_t)\gamma_t + \varepsilon_t, \quad (10)$$

where c is an unknown fixed coefficient. The seasonal term in model (10) is scaled by an exponential transformation of a linear combination of the trend and cycle components. In economic time series, the ψ_t -component can often be referred to as the business cycle. In this case, the sign of c determines whether seasonal effects are amplified or dampened during expansions and recessions. The restriction $b = c$ implies that the seasonal component is scaled by the combined trend-cycle component $\mu_t + \psi_t$. Model (10) reduces to model (6) when $b = c = 0$.

In specification (10) changes to the seasonal pattern can be due to either the random shocks of $\omega_{j,t}$ and $\omega_{j,t}^*$ in expression (5) or to changes in the trend and cycle components. It is possible to generalize the trend-cycle interaction model further. For instance, we can introduce a scaling process to the cyclical component based on the trend and seasonal components. We can also

include interactions based on exogenous intervention and regression variables. In this study, however, we limit ourselves to the specifications that are described in this section.

3.3. Seasonal interaction model in state space form

The non-linear seasonal interaction model cannot be formulated in the linear state space form (8). Therefore we consider a non-linear state space model where the observation equation $y_t = Z\alpha_t + \varepsilon_t$ in expression (8) is replaced by

$$y_t = Z(\alpha_t) + \varepsilon_t, \quad \varepsilon_t \sim \text{NID}(0, \sigma_\varepsilon^2), \quad t = 1, \dots, n. \quad (11)$$

Here $Z(\cdot)$ is a deterministic non-linear function whereas the state equation for α_{t+1} in expression (8) remains unaltered. The function $Z(\cdot)$ typically depends on unknown parameters.

The trend and cycle interaction model (10) has a state space representation with a state vector given by

$$\alpha_t = (\mu_t \quad \beta_t \quad \psi_t \quad \psi_t^* \quad \gamma_{1,t} \quad \gamma_{1,t}^* \quad \gamma_{2,t} \quad \gamma_{2,t}^* \quad \dots \quad \gamma_{\lfloor (s-1)/2 \rfloor, t} \quad \gamma_{\lfloor (s-1)/2 \rfloor, t}^* \quad \gamma_{\lfloor s/2 \rfloor, t})', \quad (12)$$

for s even and with the non-linear equation $Z(\alpha_t)$ in model (11) given by

$$Z(\alpha_t) = \mu_t + \psi_t + \exp(b\mu_t + c\psi_t)\gamma_t, \quad (13)$$

for $t = 1, \dots, n$. The dynamic specifications of the components are formulated in the state equation of expression (8) with system variables given by

$$T = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & T^\psi & 0 \\ 0 & 0 & 0 & T^\gamma \end{pmatrix}, \quad H = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \sigma_\zeta^2 & 0 & 0 \\ 0 & 0 & \sigma_\kappa^2 I_2 & 0 \\ 0 & 0 & 0 & \sigma_\omega^2 I_{s-1} \end{pmatrix}, \quad (14)$$

where

$$T^\psi = \rho C(\lambda^c), \quad T^\gamma = \text{diag}\{C(\lambda_1) \dots C(\lambda_{\lfloor (s-1)/2 \rfloor}) - 1\}, \quad (15)$$

for s even and with $\lambda_j = 2\pi j/s$ for $j = 1, \dots, \lfloor s/2 \rfloor$ and

$$C(\lambda) = \begin{pmatrix} \cos(\lambda) & \sin(\lambda) \\ -\sin(\lambda) & \cos(\lambda) \end{pmatrix}. \quad (16)$$

The elements of the initial state vector are diffuse except for ψ_t and ψ_t^* , which represent stationary variables. We therefore have $\alpha_1 \sim N(a_1, P_1)$ with

$$a_1 = 0, \quad P_1 = \begin{pmatrix} k & 0 & 0 & 0 \\ 0 & k & 0 & 0 \\ 0 & 0 & \{1/(1-\rho^2)\}\sigma_\kappa^2 I_2 & 0 \\ 0 & 0 & 0 & kI_{s-1} \end{pmatrix}, \quad (17)$$

and let $k \rightarrow \infty$. The state space formulation of the seasonal component with an odd seasonal length was discussed in Durbin and Koopman (2001).

3.4. Parameter estimation by the extended Kalman filter

Estimation of the parameters and unobserved components in the BSM usually proceeds by the procedure that was outlined at the end of Section 2. However, for the non-linear seasonal interaction model (10) the Kalman filter cannot be applied directly. Many methods to estimate non-linear state space models have been proposed in various disciplines. Early algorithms were based on linearization of the non-linear functions. Most of the recent work concentrates on simulation-based methods such as importance sampling and Markov chain Monte Carlo methods; see Frühwirth-Schnatter (1995), Carter and Kohn (1994), Shephard and Pitt (1997) and Durbin and Koopman (2000). In the engineering disciplines, the simulation-based particle filter is often employed for analysing non-linear state space models; see Gordon *et al.* (1993), Pitt and Shephard (1999) and de Freitas *et al.* (2001). In this paper we use the EKF for state estimation and likelihood evaluation. The EKF has the virtue of being relatively simple in concept and implementation while modest in terms of computational requirements. A review of the EKF method was provided in Anderson and Moore (1979).

The Kalman filter evaluates the conditional expectation of the state vector α_t given past observations y_1, \dots, y_{t-1} or given past and concurrent observations y_1, \dots, y_t . The evaluation of these state estimates is an intractable problem for general non-linear state space models. However, in many specific cases a practical approximation can be found. The EKF is based on a linearization of the non-linear effects in the model. For the seasonal interaction model, the smooth non-linear function $Z(\cdot)$ is expanded around an estimate of the state vector which we obtain from the Kalman filter. Since the Taylor series approximation is linear in the state vector α_t , it can be estimated by using the standard linear Kalman filter. The Kalman filter applied to the linearized model is termed the EKF for the non-linear state space model. Appendices A and B provide details of the EKF and its incorporation into the Kalman filter.

3.5. Discussion

In general non-linear state space models, the EKF provides suboptimal estimates in the mean-square error sense. In the engineering disciplines, from where the EKF originates, filtering is regularly used to track physical objects. The researcher is typically more certain about the model since it is derived from physical principles. The use of more sophisticated non-linear filtering techniques is therefore helpful to obtain more precise estimates. In economics applications, however, time series models are rarely interpreted as genuine descriptions of the real world dynamics that generated the data. The non-linear model is adopted to develop methods for improving the model fit compared with the linear specification. This inaccuracy due to the linearization step in the EKF does not need to be interpreted as an error. Although the non-linear model is easier to formulate and to explicate than the EKF linearization, it is not necessarily a better approximation to the processes underlying the data; nor need it be superior from a forecasting point of view. Nevertheless, when more accurate state estimates for the non-linear specification are desired, we can employ more computationally demanding simulation methods.

An important issue in estimating stochastic trends and seasonal components is the treatment of the initial state vector α_1 with mean a_1 and variance P_1 which are given by expression (17) for the seasonal interaction model. The trend and seasonal components are non-stationary processes and we therefore treat the associating elements in the state vector as diffuse variables,

i.e. $k \rightarrow \infty$ in expression (17). In practice, a simple approach is to replace k by a very large numerical value in expression (17), say $k = 10^7$. In our calculations, this approach has been detrimental to the numerical stability of the estimation procedure. We therefore have adopted the exact diffuse initialization algorithms of Koopman and Durbin (2003) and we have modified the EKF accordingly. Details of the diffuse recursions for the EKF together with an expression for the diffuse likelihood and the smoothing equations for the seasonal interaction model are given in Appendix B.

The maximum likelihood estimates in this paper are obtained by using the numerical optimization routines of the Ox matrix programming language by Doornik (2007). The diffuse EKF routines were programmed in Ox, with support from the functions in the suite of *SsfPack* routines by Koopman *et al.* (1999).

4. Applications

4.1. UK visits abroad

We first consider the data set of monthly visits abroad by UK residents from January 1980 to December 2006 that was introduced in Section 1. The data were compiled by the Office for National Statistics, based on the International Passenger Survey. Time series plots of the series in levels and in logarithms are presented in Fig. 1. A linear UC model with smooth trend, trigonometric seasonal and cycle components together with a normal white noise disturbance term as given by equations (3), (5), (6) and (7) is considered first for the number of visitors in levels. The maximum likelihood estimates of the parameters are

$$\begin{aligned} \hat{\sigma}_\varepsilon &= 0.106, & \hat{\sigma}_\zeta &= 0.00062, & \hat{\sigma}_\omega &= 0.0119, \\ \hat{\sigma}_\kappa &= 0.00050, & \hat{\rho} &= 0.958, & 2\pi/\hat{\lambda}^c &= 123, & \log(L) &= 48.2, \end{aligned} \quad (18)$$

where $\log(L)$ is the log-likelihood value of the model evaluated at the maximum likelihood estimates of the parameters. The estimated standard deviation of the trend disturbance is relatively small, which implies that the trend is quite steady. The cycle has period $2\pi/\lambda^c$ which is estimated by 123 months. Furthermore, the estimates of the cycle parameters include a relatively small disturbance and amplitude. Most of the variation in the series can be attributed to the seasonal component and to the disturbance term.

Alongside estimates of the unobserved state variables, the (extended) Kalman filter as described in Appendices A and B provides one-step-ahead prediction errors v_t and their variances f_t in each step of the recursion. Diagnostic tests can be based on the standardized prediction errors $v_t/\sqrt{f_t}$. Here, and in the following examples, we calculate the test statistics

$$N(\chi_2^2) = 6.21, \quad H_{104}(F_{104,104}) = 2.46, \quad Q_{12}(\chi_{11}^2) = 30.9, \quad Q_{24}(\chi_{23}^2) = 43.8, \quad (19)$$

where N , H and Q_l denote statistics for normality, heteroscedasticity and serial correlation up to lag l respectively. The null distributions of the tests are given in parentheses. The normality statistic that we use is based on the sample skewness and kurtosis, and was described in detail in Doornik and Hansen (1994). The statistic is a modification of the well-known asymptotic test by Bowman and Shenton (1975), with alternative distributional assumptions which are more suitable for small samples. The heteroscedasticity statistic is the classical Goldfeld–Quandt test, which is calculated as the ratio between the sum of squared prediction errors in two exclusive subsets of the sample. As suggested by Goldfeld and Quandt (1965), to increase the power of the test we do not use the entire sample. In all our examples, we only test for different variances between the first and last third of the series. Finally the serial correlation statistic is the standard

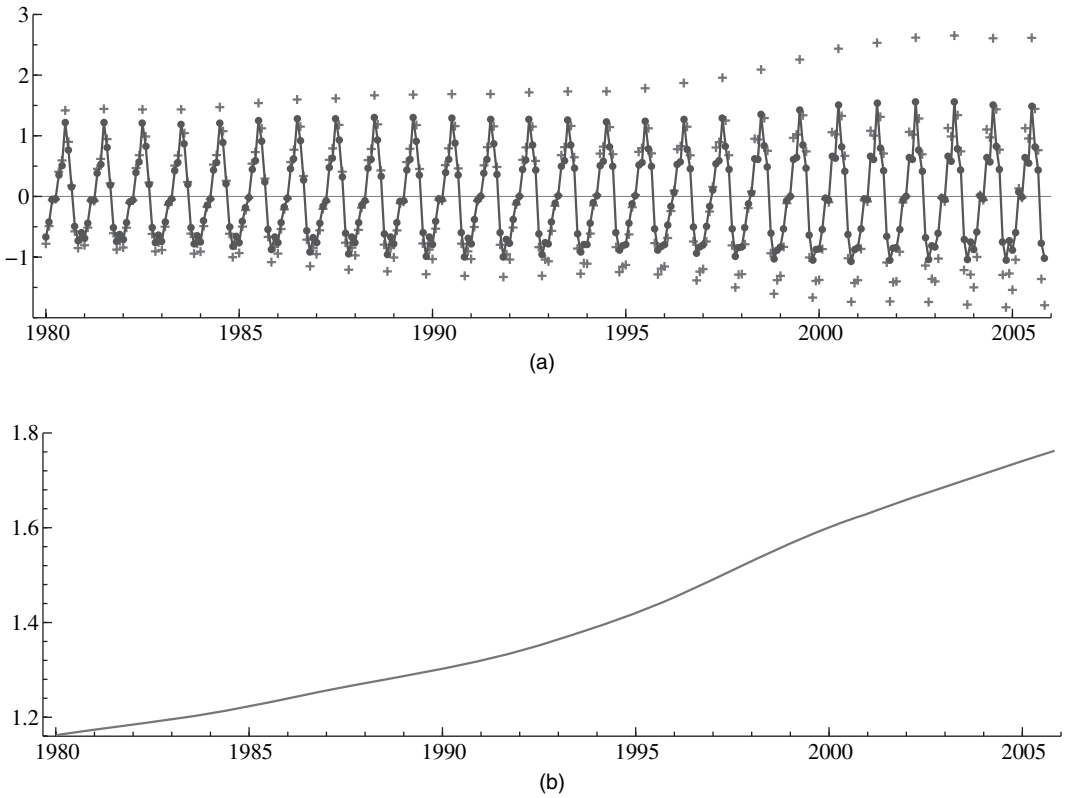


Fig. 2. Visits of UK residents abroad: (a) smooth estimates of the scaled (+) and unscaled (•) seasonal components obtained by the EKF and its associated smoothing equations; (b) scaling process $\exp(b\mu_t)$ with μ_t replaced by its smoothed estimate

portmanteau test based on the sum of squared sample auto-correlations that was derived by Ljung and Box (1978).

The diagnostics indicate that there is significant residual heteroscedasticity and serial correlation in the estimated linear model for the passenger survey series, as each is significant at the 5% level.

Next the non-linear specification

$$y_t = \mu_t + \psi_t + \exp(b\mu_t)\gamma_t + \varepsilon_t \quad (20)$$

is considered, for which parameter estimates are obtained by applying the EKF from Section 3.2. The parameter and likelihood estimates are given by

$$\begin{aligned} \hat{\sigma}_\varepsilon &= 0.116, & \hat{\sigma}_\zeta &= 0.00090, & \hat{\sigma}_\omega &= 0.00611, & \hat{b} &= 0.0984, \\ \hat{\sigma}_\kappa &= 0.00088, & \hat{\rho} &= 0.921, & 2\pi/\hat{\lambda}^c &= 589, & \log(L) &= 55.1. \end{aligned} \quad (21)$$

The most striking difference between the estimates of the linear model and model (20) is the large drop in the value of the standard deviation of the seasonal disturbances, from 0.0119 to 0.00611. The seasonal component γ_t in the non-linear model is scaled by the process $\exp(b\mu_t)$, which must account for most of the drop in σ_ω . The variation in μ_t is now factored in the seasonality through the scaling in $\exp(b\mu_t)\gamma_t$. The process for γ_t itself fluctuates less as a result.

Fig. 2(a) illustrates this by showing the scaled ($\exp(b\mu_t)\gamma_t$) and unscaled (γ_t) seasonal components as estimated by the extended Kalman smoother. The scaled component is changing largely because of the trend component, whereas the unscaled component shows much smaller movements and consequently does not require a large standard deviation in the disturbance. We confirm that the scaled component is roughly the same as the estimated γ_t from the linear model. In the non-linear model, the cycle frequency λ^c approaches 0, which implies that the period approaches ∞ and the cycle process ψ_t reduces to a first-order auto-regressive process. Relative to the sample size of the series, the estimated period of the cycle component was already quite large for the linear model. It highlights the difficulty in empirically identifying the cycle component from this data set accurately. We do not consider this a major problem, since relative to the other components the effect of the cycle is very modest in this series.

The diagnostic tests for the residuals of the non-linear model are given by

$$N(\chi_2^2) = 3.18, \quad H_{104}(F_{104,104}) = 1.85, \quad Q_{12}(\chi_{11}^2) = 21.9, \quad Q_{24}(\chi_{23}^2) = 31.0. \quad (22)$$

Compared with the previous linear model, all the diagnostic tests have improved. The Q_{12} - and the H -statistics are still significant at the 5% level, but the statistics indicate that auto-correlation and heteroscedasticity are less severe than they were in the initial specification. Taken together with the significant increase in the log-likelihood, we conclude that the non-linear model is a clear improvement over the linear specification.

4.2. US unemployment

In this section we apply the seasonal interaction model to the logarithm of the number of unemployed people in the USA. The monthly data set was obtained from the US Bureau of Labor Statistics and spans the period from January 1948 to December 2006.

A graph of the log-unemployment with the estimated trend from a linear decomposition model with trend, season, cycle and irregular components is shown in Fig. 3. Salient features in the series are an overall increasing trend that levels off towards the end, a distinct seasonal pattern and a large amount of medium frequency cyclical fluctuation. The estimated parameters from the linear decomposition model that is considered are given by

$$\begin{aligned} \hat{\sigma}_\varepsilon &= 0.00034, & \hat{\sigma}_\zeta &= 0.00150, & \hat{\sigma}_\omega &= 0.00120, \\ \hat{\sigma}_\kappa &= 0.00072, & \hat{\rho} &= 0.970, & 2\pi/\hat{\lambda}^c &= 57, & \log(L) &= 1082.3, \end{aligned} \quad (23)$$

with diagnostics

$$N(\chi_2^2) = 70.6, \quad H_{228}(F_{228,228}) = 4.43, \quad Q_{12}(\chi_{11}^2) = 18.5, \quad Q_{24}(\chi_{23}^2) = 33.9. \quad (24)$$

The business cycle is quite persistent, with a damping factor of 0.97 for a monthly frequency, which corresponds to 0.7 for a yearly frequency. The period of the cycle is close to 5 years, which is a typical business cycle frequency. In Fig. 3 the estimated trend is displayed, and it may be concluded that the series possibly contains a second cycle with a longer period that is currently captured by the trend component. The prediction-error-based diagnostic tests indicate that normality and homoscedasticity are strongly rejected, and the serial correlation statistics are not significant at the 5% level.

The non-linear model with interactions between the trend plus cycle and the seasonal component is given by equation (10) and is considered next. First we concentrate on the cycle-season interaction and estimate the parameters of this model under the constraint $b = 0$. Maximum

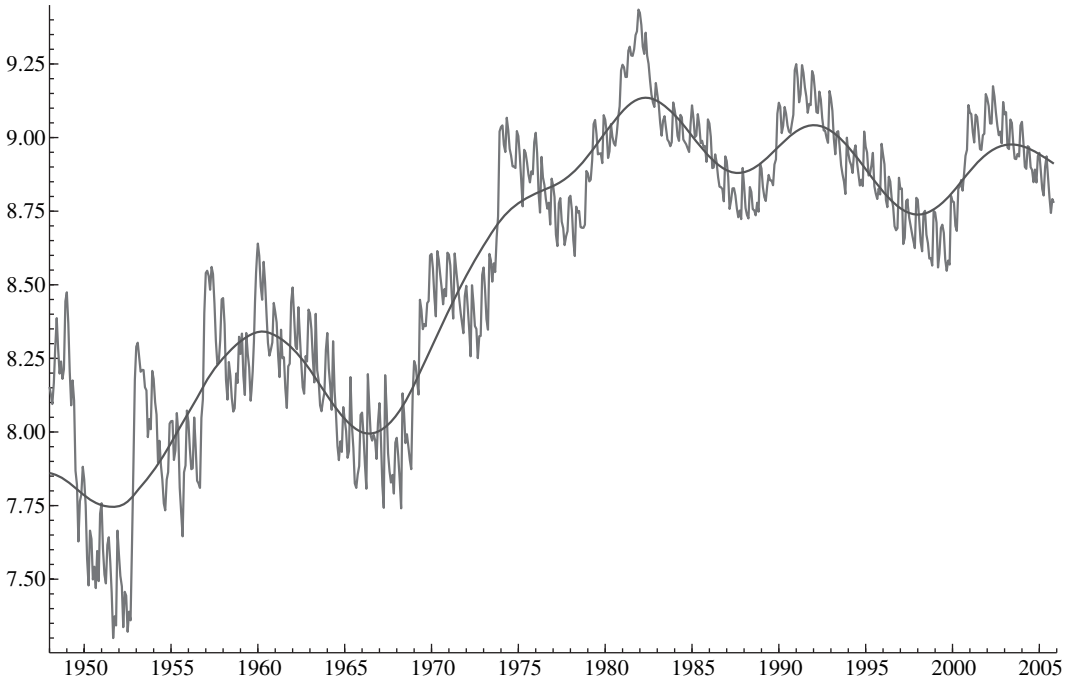


Fig. 3. US unemployed people with smooth trend obtained by the Kalman smoother, applied to a linear trend–cycle–season irregular UC decomposition model

likelihood estimates are given by

$$\begin{aligned} \hat{\sigma}_\varepsilon &= 0.00034, & \hat{\sigma}_\zeta &= 0.00217, & \hat{c} &= -0.58, & \hat{\sigma}_\omega &= 0.00117, \\ \hat{\sigma}_\kappa &= 0.00065, & \hat{\rho} &= 0.968, & 2\pi/\hat{\lambda}^c &= 53, & \log(L) &= 1098.0, \end{aligned} \quad (25)$$

with diagnostics

$$N(\chi^2_2) = 47.3, \quad H_{228}(F_{228,228}) = 4.22, \quad Q_{12}(\chi^2_{11}) = 15.0, \quad Q_{24}(\chi^2_{23}) = 32.5. \quad (26)$$

Compared with the estimates from the linear model, the cycle length becomes slightly shorter. The model fit has greatly improved in terms of the increase in the log-likelihood value, which gains almost 16 points at the cost of only one parameter. The diagnostic tests show small improvements, but the normality and heteroscedasticity tests remain highly significant. The negative value of the estimated coefficient \hat{c} indicates that the seasonal component is dampened during periods of high cyclical unemployment and attenuated in the negative phases of the cycle, which is consistent with the findings of Franses (1995). The smoothed scaling process is depicted in Fig. 4, together with the scaled and unscaled seasonal component. The plot shows that the scaling process adds about 20% cyclical variation to γ_t in the early parts of the series but levels off towards the end as the amplitude of the estimated cycle component wanes in the last decades.

We estimate a non-linear model with both trend–season and cycle–season interactions next by relaxing the restriction $b=0$. The parameters estimates are given by

$$\begin{aligned} \hat{\sigma}_\varepsilon &= 0.00033, & \hat{\sigma}_\zeta &= 0.00050, & \hat{b} &= -0.024, & \hat{c} &= -0.53, & \hat{\sigma}_\omega &= 0.00126, \\ \hat{\sigma}_\kappa &= 0.00074, & \hat{\rho} &= 0.980, & 2\pi/\hat{\lambda}^c &= 76, & \log(L) &= 1106.9, \end{aligned} \quad (27)$$

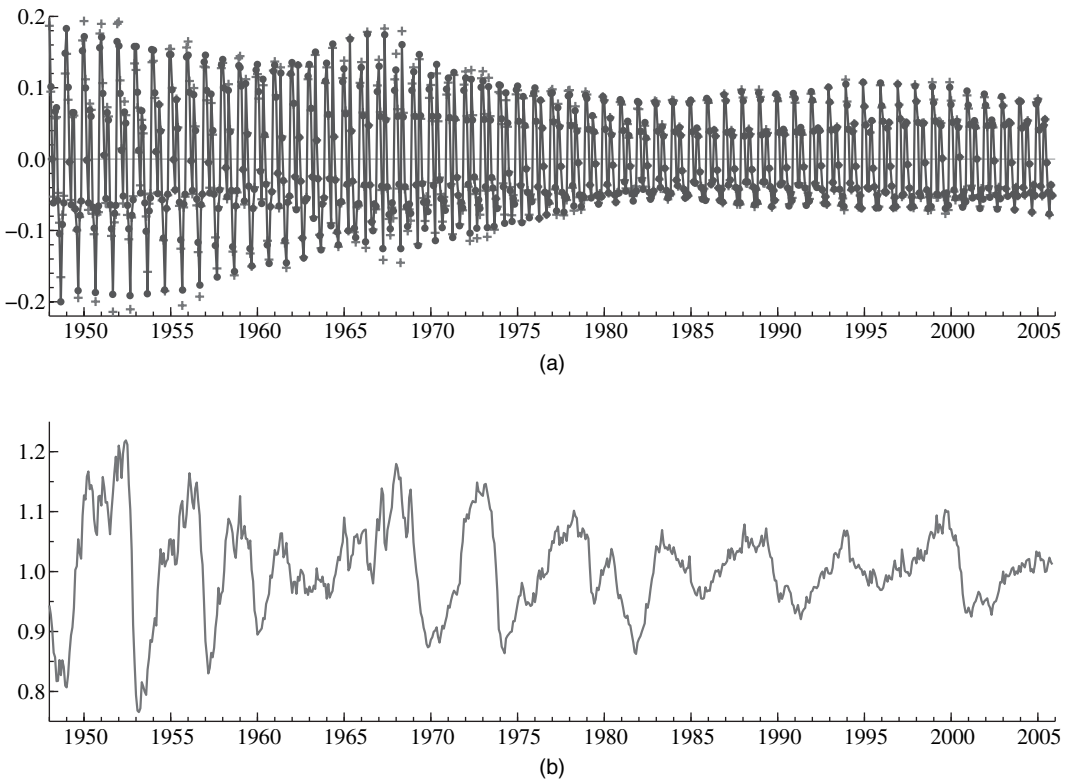


Fig. 4. US unemployed people: (a) scaled (+) and unscaled (•) seasonal component; (b) scaling process

with diagnostics

$$N(\chi^2_2) = 49.2, \quad H_{228}(F_{228,228}) = 4.47, \quad Q_{12}(\chi^2_{11}) = 23.3, \quad Q_{24}(\chi^2_{23}) = 45.9. \quad (28)$$

Although there is a considerable increase in the likelihood, not all the diagnostic statistics have improved. The most notable difference is that the serial correlation in the residuals is more severe than it was in the original linear specification, and both Q -tests are now significant at the 5% level. This may be attributed to the fact that, compared with previous estimates, there is a considerable change in the decomposition, as the trend is smoother, whereas the cycle period has lengthened over 6 years. Thus, a direct comparison with the linear specification is difficult, in contrast with the previous non-linear specification without a trend–season interaction. If we fix the cycle length at the value of the previous model and re-estimate, we obtain the results

$$\begin{aligned} \hat{\sigma}_\varepsilon &= 0.00034, & \hat{\sigma}_\zeta &= 0.00143, & \hat{b} &= -0.021, & \hat{c} &= -0.60, & \hat{\sigma}_\omega &= 0.00132, \\ \hat{\sigma}_\kappa &= 0.00067, & \hat{\rho} &= 0.973, & 2\pi/\lambda^c &= 53, & \log(L) &= 1104.6, \end{aligned} \quad (29)$$

and diagnostics

$$N(\chi^2_2) = 49.4, \quad H_{228}(F_{228,228}) = 4.04, \quad Q_{12}(\chi^2_{11}) = 17.6, \quad Q_{24}(\chi^2_{23}) = 34.2. \quad (30)$$

These diagnostic test statistics are very close to those obtained from the model with only cycle–season interaction. The Q -statistics have fallen below the 5% level of significance again, and

the model retains most of the improvement in the likelihood of the previous model. Thus, we prefer this decomposition to the previous one with an unrestricted cycle frequency parameter. Nevertheless, the diagnostics are still not quite satisfactory for this series, as non-normality and heteroscedasticity remain severe. As noted by Franses (1995), the US unemployment series exhibits several types of non-linearities that we have not incorporated in our model, such as asymmetry in the cycle and different shock persistence in different regimes. A complete treatment will probably require a more elaborate model, which we consider to be beyond the scope of this paper.

4.3. US industrial and dwellings production

In our final empirical application we consider the seasonal interaction model for the US industry and dwellings production series, which was obtained from Organisation for Economic Co-operation and Development main economic indicators 2007, release 07. Both monthly series start in January 1960 and end in December 2006. The production of total industry is an index series standardized at 100 in the year 2000, whereas the production of dwellings is measured in billion US dollars. We model both series in logarithms.

Table 1 presents the estimation results of linear and non-linear models for both series. For the industrial production series, we allow both trend–season and cycle–season interactions in the non-linear model. The estimates show that there is almost no improvement resulting from using the more general non-linear specification, as the log-likelihood value of the non-linear model increases by only 0.6. Since the linear model is a simple dimensional reduction in the parameter space of the non-linear model, we can use a likelihood ratio test to assess the significance of the linearity restriction. Under the null hypothesis that the parameter restrictions are valid, the likelihood ratio statistic is asymptotically χ_k^2 distributed. In this example, the statistic evaluates to 1.2, which would not be significant with two-parameter restrictions under any conventional significance level. We therefore conclude that no trend- or cycle-induced variations in the seasonal component of the US industrial production series are detected by our model.

Table 1. US monthly industrial and dwellings production, linear and non-linear model estimates and test statistics

Parameter	Results for industrial production		Results for dwellings production			
	Linear model	Trend–cycle model	Linear model	Trend model	Cycle model	Trend–cycle model
$\hat{\sigma}_\varepsilon (\times 10^{-3})$	0.0007	0.0007	0.001	0.001	0.001	0.001
$\hat{\sigma}_\zeta (\times 10^{-3})$	0.433	0.450	0.388	0.408	0.561	0.466
$\hat{\sigma}_\omega (\times 10^{-3})$	0.223	0.223	0.574	0.680	0.555	0.640
$\hat{\sigma}_\kappa (\times 10^{-3})$	0.029	0.029	0.236	0.232	0.232	0.230
$2\pi/\lambda^c$	60	60	73	72	72	72
$\hat{\rho}$	0.97	0.97	0.99	0.99	0.99	0.99
\hat{b}	—	0.0009	—	−0.063	—	−0.052
\hat{c}	—	−0.063	—	—	−0.289	−0.245
$\log(L)$	1742.0	1742.6	1182.7	1186.0	1187.5	1189.8
N	15.5	16.5	14.9	12.2	16.8	12.6
H	2.18	2.16	2.49	2.48	2.40	2.41
Q_{24}	34.7	35.2	130.7	128.1	120.6	120.5
Q_{48}	76.7	77.7	146.3	142.6	142.3	140.7

For the dwelling production series, we estimate the parameters for non-linear models with only a trend–season interaction ($c = 0$), only a cycle–season interaction ($b = 0$) and with both trend–season and cycle–season interactions. We learn from Table 1 that the models with only the trend–season interaction and only the cycle–season interaction improve the fit compared with the linear model. The model with both interactions provides a better fit than the two models with single interactions. Using the likelihood ratio test and starting from the unrestricted non-linear model, we can reject the restrictions $b = 0$ and $c = 0$ individually at the 5% level of significance. The joint restriction $b = c = 0$ can also be rejected at the 5% level. The fit of each interaction model provides a clear improvement when compared with the fit of the linear model. The residual diagnostic tests are all significant whereas those of the non-linear models show only small improvements. Therefore, we may conclude that the series may benefit from an even more elaborate modelling effort than we attempt here.

The estimated coefficient of the trend–season interaction is negative, which implies that the seasonal variation decreases with an increase in the trend. It can be argued that technological changes which may have reduced seasonal dependence in dwellings productions in the past decades have coincided with the trending behaviour in the series, which is probably caused by many unrelated factors such as demographic trends or changing preferences. Our model

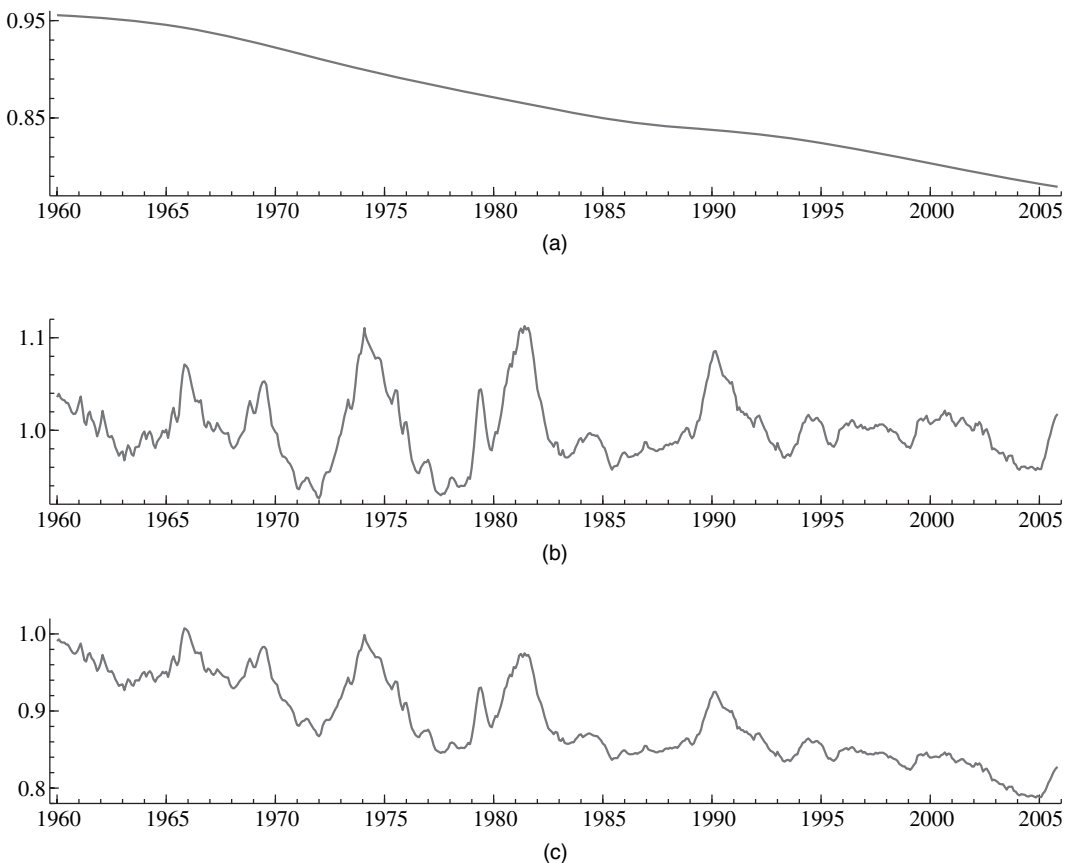


Fig. 5. US dwellings production, seasonal scaling process from the non-linear model with (a) trend interaction, (b) cycle interaction and (c) trend–cycle interaction

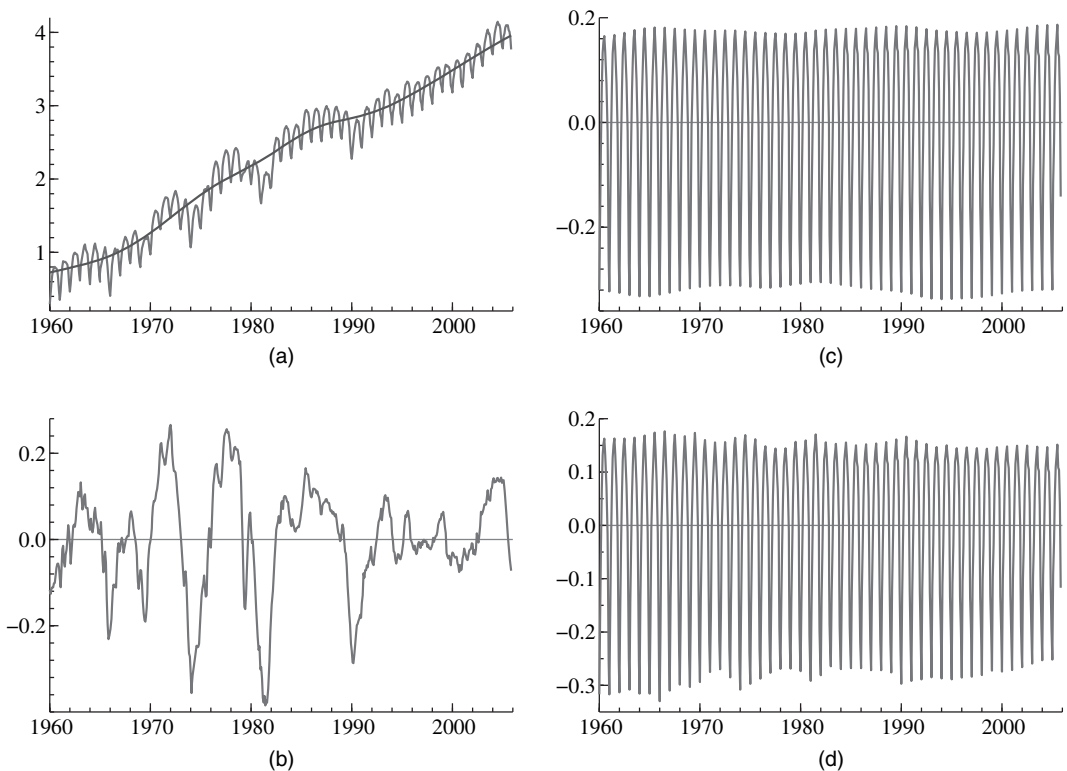


Fig. 6. Smooth estimates of non-linear UC decomposition of US dwellings production with interaction between the seasonal and the trend and cycle components: (a) data and trend component; (b) cycle components; (c) unscaled season component; (d) scaled season component

does not distinguish between underlying causes but merely reflects the effect of permitting the interaction.

The negative coefficient of the cycle–season interaction indicates that the seasonality in the dwellings productions is contracyclical, i.e. the seasonal amplitude decreases with upswings in the production. A similar effect has been documented in some other US industries by Cecchetti *et al.* (1997), who interpreted it as a capacity constraint in the sector when the inventory series of the sector does not show a decrease. However, in this paper we do not model inventory series.

Fig. 5 shows the estimated scaling process $\exp(b\mu_t + c\psi_t)$ from all three non-linear models. We observe that the trend-induced reduction in the seasonality is fairly uniform and is roughly 20% over the sample period. The cyclical swings contribute about 10% at their top in the mid-1970s and early 1980s. The cycle-induced variations in seasonality seem to have reduced since the early 1990s, as a direct result of the declining amplitude of the cyclical component. Finally, we present the unobserved components decomposition of the non-linear model with both trend–season and cycle–season interactions in Fig. 6, which includes the data and estimated trend, cycle-scaled and unscaled seasonal component.

5. Conclusion

In this paper we have presented a simple non-linear extension to the basic unobserved components model to allow the seasonal term to interact with the trend and cycle components.

The model that we propose addresses some functional misspecifications that may arise from imposing a (transformed) additive components structure. Starting from a basic linear unobserved components model with trend, season, cycle and irregular components, we include a transformed linear combination of trend and cycle components as a scaling factor for the seasonal component. In the resulting model, the seasonal amplitude is amplified or dampened along movements of the trend and cycle, depending on the estimated parameters.

In our empirical applications, we have considered models for UK travel, US unemployment and US production data. The travel data contain increasing seasonal variation, which is not adequately removed by a logarithmic transformation. Our non-linear model shows a significant improvement in the model fit and provides better residual diagnostics. In the unemployment series, we found significant interactions between the cycle and the seasonal term. Although the model improves on the linear specification, it does not capture all the non-linear dynamics in the series. The estimated coefficient sign indicates that seasonal effects are dampened during recessions. Finally our parameter estimates for the US production series do not show evidence of interactions between the total productions series. However, in the production of dwellings, we observe a significant contracyclical effect, as well as a dampening of seasonal fluctuations along the increasing trend.

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Appendix A: Kalman filter methods

A general formulation of a univariate linear Gaussian state space model is given by

$$\begin{aligned} y_t &= c_t + Z_t \alpha_t + \varepsilon_t, & \varepsilon_t &\sim \text{NID}(0, \sigma_\varepsilon^2), \\ \alpha_{t+1} &= d_t + T_t \alpha_t + \eta_t, & \eta_t &\sim \text{NID}(0, H_t), \quad t = 1, \dots, n, \end{aligned} \quad (31)$$

where the first equation relates the scalar observation y_t to the state vector α_t which is modelled as the vector auto-regressive (VAR(1)) process as given in the second of these equations. The state vector contains the unobserved components and additional variables to enable the specification of the dynamic processes of the components. The disturbance scalar ε_t and the disturbance vector η_t are assumed to be uncorrelated at all times. The scalars c_t and σ_ε^2 , the vectors Z_t and d_t and the matrices T_t and H_t are fixed system variables which are designed to represent a particular model. Some of the system variables may depend on unknown parameters which we collect in the vector θ . The initial state vector is distributed as $\alpha_1 \sim N(a_1, P_1)$.

The well-known Kalman filter equations for the state space model (31) are given by

$$\left. \begin{aligned} v_t &= y_t - Z_t a_t - c_t, & f_t &= Z_t P_t Z_t' + \sigma_\varepsilon^2, & K_t &= P_t Z_t' f_t^{-1}, \\ a_{t|t} &= a_t + K_t v_t, & P_{t|t} &= P_t - f_t K_t K_t', \\ a_{t+1} &= d_t + T_t a_{t|t}, & P_{t+1} &= T_t P_{t|t} T_t' + H_t, \end{aligned} \right\} \quad (32)$$

for $t = 1, \dots, n$, where v_t is the one-step-ahead prediction error with mean-square error (MSE) f_t , K_t is the Kalman gain vector and $a_{t|t}$ and a_{t+1} are conditional expectations of the state vector α_t with MSE matrices $P_{t|t}$ and P_{t+1} respectively. The Kalman filter recursions provide an efficient method for computing the filtered state $a_{t|t}$ and the predicted state a_{t+1} , which are the conditional expectation of respectively α_t and α_{t+1} given observations y_1, \dots, y_t , together with their MSEs. When the disturbances are Gaussian white noise, as we have assumed, the conditional expectations are the minimum MSE predictors of the state. Without the Gaussianity assumption, the state estimates are minimum MSEs among the set of linear predictors.

The Kalman gain K_t determines the appropriate weighting of the observations for the computation of the conditional expectations and variances. The smoothed state, i.e. the expectation of the state vector conditional on the entire sample y_1, \dots, y_n , can be computed with an additional set of recursions.

If the variables in α_t are stationary, the initial mean and covariance matrix are implied by their unconditional distributions. The distributions of non-stationary variables in α_t are degenerate and we let the associated diagonal elements in P_1 approach ∞ . We often refer to non-stationary variables in the state vector as diffuse variables, and the Kalman filter requires a diffuse initialization. Here, we describe the initialization method by Koopman and Durbin (2003). When the state vector contains diffuse variables, the MSE matrix P_t can be decomposed into a part that is associated with diffuse state elements $P_{\infty,t}$ and a part where the state has a proper distribution $P_{*,t}$, i.e.

$$P_t = kP_{\infty,t} + P_{*,t}, \quad k \rightarrow \infty. \quad (33)$$

For the diffuse initial state elements, the corresponding entries on the diagonal matrix $P_{\infty,1}$ are set to positive values, whereas the remainder of the matrix contains 0s. Koopman and Durbin (2003) showed that for models with diffuse state elements the standard Kalman filter can be split into two parts by expanding the inverse of $f_t = k f_{\infty,t} + f_{*,t}$ in k^{-1} . In the first d iterations of the filter, the state contains diffuse elements, which is indicated by a non-zero $P_{\infty,t}$. Separate update equations are maintained for the parts that are associated with $P_{\infty,t}$ and with $P_{*,t}$. Generally $P_{\infty,t}$ becomes 0 after some iterations, after which the standard Kalman filter can be used. The diffuse filter equations for the initial iterations are given by

$$\left. \begin{aligned} v_t &= y_t - Z_t a_t - c_t, \\ f_{\infty,t} &= Z_t P_{\infty,t} Z_t', & f_{*,t} &= Z_t P_{*,t} Z_t' + \sigma_\varepsilon^2, \\ K_{\infty,t} &= P_{\infty,t} Z_t' f_{\infty,t}^{-1}, & K_{*,t} &= (P_{*,t} Z_t' - K_{\infty,t} f_{*,t}) f_{\infty,t}^{-1}, \\ P_{\infty,t|t} &= P_{\infty,t} - f_{\infty,t} K_{\infty,t} K_{\infty,t}', & P_{*,t|t} &= P_{*,t} - K_{\infty,t} Z_t P_{*,t}' - K_{*,t} Z_t P_{\infty,t}', \\ P_{\infty,t} &= T_t P_{\infty,t|t} T_t', & P_{*,t} &= T_t P_{*,t|t} T_t' + H_t, \\ a_{t|t} &= a_t + K_{\infty,t} v_t, & a_{t+1} &= d_t + T_t a_{t|t}, \end{aligned} \right\} \quad (34)$$

when $f_{\infty,t} > 0$. In case $f_{\infty,t}$ is 0 $K_{\infty,t}$ does not exist, and the equations for $K_{*,t}$, $P_{\infty,t}$, $P_{*,t}$ and $a_{t|t}$ are given by

$$\begin{aligned} K_{*,t} &= P_{*,t} Z_t' f_{*,t}^{-1}, & a_{t|t} &= a_t + K_{*,t} v_t, \\ P_{\infty,t|t} &= P_{\infty,t}, & P_{*,t|t} &= P_{*,t} - K_{*,t} Z_t P_{*,t}'. \end{aligned} \quad (35)$$

Appendix B: Extended Kalman filter with diffuse initialization

A non-linear state space model for a univariate time series y_1, \dots, y_n can be defined by the equations

$$\begin{aligned} y_t &= Z_t(\alpha_t) + \varepsilon_t, & \varepsilon_t &\sim \text{NID}(0, \sigma_\varepsilon^2), \\ \alpha_{t+1} &= T_t(\alpha_t) + \eta_t, & \eta_t &\sim \text{NID}(0, H_t), \quad t = 1, \dots, n. \end{aligned} \quad (36)$$

The observations y_t are modelled as a transformation $Z_t(\cdot)$ of the latent stochastic state vector α_t plus observation noise ε_t . The state vector evolves according to the transformation $T_t(\cdot)$ and accumulates additional transition noise η_t at each time t . We also assume that all the noise terms and the initial state are mutually independent.

The EKF equations provide approximate estimates of the state by applying the standard Kalman filter to the Taylor series approximations of expression (36) expanded around the estimated state from the filter. The first-order approximations to the observation and transition equations are given by

$$\begin{aligned} y_t &\approx Z_t(a_t) + \tilde{Z}_t \cdot (\alpha_t - a_t) + \varepsilon_t, \\ \alpha_{t+1} &\approx T_t(a_{t|t}) + \tilde{T}_t \cdot (\alpha_t - a_{t|t}) + \eta_t, \end{aligned} \quad (37)$$

where

$$\begin{aligned} \tilde{Z}_t &= \left. \frac{\partial Z(x)}{\partial x} \right|_{x=a_t}, \\ \tilde{T}_t &= \left. \frac{\partial T(x)}{\partial x} \right|_{x=a_{t|t}}, \end{aligned} \quad (38)$$

as the predicted and filtered states a_t and $a_{t|t}$ respectively are the most recent state estimates available when the linearizations are required in the filter equations.

As the first-order approximation to the model is linear in α_t , we can apply the Kalman filter of expression (32) to expression (37), where the non-random terms $Z_t(a_t) - \tilde{Z}_t a_t$ and $T_t(a_{t|t}) - \tilde{T}_t a_{t|t}$ in the linearized model are incorporated into c_t and d_t respectively. This yields the equations

$$\left. \begin{aligned} v_t &= y_t - Z_t(a_t), & f_t &= \tilde{Z}_t P_t \tilde{Z}_t' + \sigma_\varepsilon^2, & K_t &= P_t \tilde{Z}_t' f_t^{-1}, \\ a_{t|t} &= a_t + K_t v_t, & P_{t|t} &= P_t - f_t K_t K_t', \\ a_{t+1} &= T_t(a_{t|t}), & P_{t+1} &= \tilde{T}_t P_{t|t} \tilde{T}_t' + H_t, \end{aligned} \right\} \quad (39)$$

which comprise the EKF for the non-linear state space model (36). A more detailed exposition of the EKF can be found in Jazwinski (1970) or Anderson and Moore (1979).

The filter equations provide estimates of the predicted and filtered state a_{t+1} and $a_{t|t}$ with approximate MSE matrices P_{t+1} and $P_{t|t}$. The smoothed states $\hat{\alpha}_t$, which are conditioned on the entire sample of observations, can be calculated with an additional set of recursions running from $t=n$ backwards to $t=1$; see Durbin and Koopman (2001). For the first-order approximation to the non-linear model, these take the form

$$\left. \begin{aligned} L_t &= \tilde{T}_t - \tilde{T}_t K_t \tilde{Z}_t', \\ r_{t-1} &= \tilde{Z}_t' f_t^{-1} v_t + L_t' r_t, \\ \hat{\alpha}_t &= a_t + P_t r_{t-1}, \end{aligned} \right\} \quad (40)$$

which is initialized by $r_n = 0$.

When we apply the diffuse filter to the linear approximation (37), we obtain the diffuse EKF for $t = 1, \dots, d$, which is given by

$$\left. \begin{aligned} v_t &= y_t - Z_t(a_t), \\ f_{\infty,t} &= \tilde{Z}_t P_{\infty,t} \tilde{Z}_t', & f_{*,t} &= \tilde{Z}_t P_{*,t} \tilde{Z}_t' + \sigma_\varepsilon^2, \\ K_{\infty,t} &= P_{\infty,t} \tilde{Z}_t' f_{\infty,t}^{-1}, & K_{*,t} &= (P_{*,t} \tilde{Z}_t' - K_{\infty,t} f_{*,t}) f_{\infty,t}^{-1}, \\ P_{\infty,t|t} &= P_{\infty,t} - f_{\infty,t} K_{\infty,t} K_{\infty,t}', & P_{*,t|t} &= P_{*,t} - K_{\infty,t} \tilde{Z}_t P_{*,t}' - K_{*,t} \tilde{Z}_t P_{\infty,t}', \\ P_{\infty,t} &= \tilde{T}_t P_{\infty,t|t} \tilde{T}_t', & P_{*,t} &= \tilde{T}_t P_{*,t|t} \tilde{T}_t' + H_t, \\ a_{t|t} &= a_t + K_{\infty,t} v_t, & a_{t+1} &= T_t(a_{t|t}), \end{aligned} \right\} \quad (41)$$

for $f_{\infty,t} > 0$, and

$$\left. \begin{aligned} K_{*,t} &= P_{*,t} \tilde{Z}_t' f_{*,t}^{-1}, \\ a_{t|t} &= a_t + K_{*,t} v_t, \\ P_{\infty,t|t} &= P_{\infty,t}, \\ P_{*,t|t} &= P_{*,t} - K_{*,t} \tilde{Z}_t P_{*,t}', \end{aligned} \right\} \quad (42)$$

for $f_{\infty,t} = 0$. When $P_{\infty,t}$ becomes 0 after d iterations, the standard EKF of expression (39) applies with $P_d = P_{*,d}$.

The state smoothing equations (40) can be split in a similar manner. The diffuse extended smoothing equations when $f_{\infty,t} > 0$ are

$$\left. \begin{aligned} L_{\infty,t} &= \tilde{T}_t - \tilde{T}_t K_{\infty,t} \tilde{Z}_t', \\ r_{t-1}^{(0)} &= L_{\infty,t}' r_t^{(0)}, \\ r_{t-1}^{(1)} &= \tilde{Z}_t' (f_{\infty,t}^{-1} v_t - K_{*,t}' r_t^{(0)}) + L_{\infty,t}' r_t^{(1)}, \end{aligned} \right\} \quad (43)$$

whereas for $f_{\infty,t} = 0$ we have

$$\left. \begin{aligned} L_{*,t} &= \tilde{T}_t - \tilde{T}_t K_{*,t} \tilde{Z}_t', \\ r_{t-1}^{(0)} &= \tilde{Z}_t' f_{*,t}^{-1} v_t + L_{*,t}' r_t^{(0)}, \\ r_{t-1}^{(1)} &= \tilde{T}_t' r_t^{(1)}, \end{aligned} \right\} \quad (44)$$

running from $t = d, \dots, 1$ with $r_d^{(0)} = r_d$ and $r_d^{(1)} = 0$. The smoothed state is calculated as

$$\hat{\alpha}_t = a_t + P_{*,t} r_{t-1}^{(0)} + P_{\infty,t} r_{t-1}^{(1)}. \quad (45)$$

We usually display the smoothed estimates of the state vector once the unknown parameters have been estimated. In models without diffuse variables, the parameter vector θ can be estimated by maximizing the Gaussian log-likelihood function as given by

$$\log\{L(\theta)\} = -\frac{1}{2} \sum_{t=1}^n \log(2\pi f_t) - \frac{1}{2} \sum_{t=1}^n \frac{v_t^2}{f_t}, \quad (46)$$

where the one-step prediction error v_t and its variance f_t are obtained from the linear Kalman filter or EKF. The diffuse likelihood function is given by

$$\log\{L(\theta)\} = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \sum_{t=1}^d w_t - \frac{1}{2} \sum_{t=d+1}^n \{\log(f_t) + f_t^{-1} v_t^2\}, \quad (47)$$

where $w_t = \log(f_{\infty,t})$ for $f_{\infty,t} > 0$ or $w_t = \log(f_{\infty,t}) + f_{*,t}^{-1} v_t^2$ when $f_{\infty,t} = 0$.

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