How to Detect a Change both on Global and Local Scale in Oceanographic Time Series

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Abstract

Analyzing change in climatic time series requires a more complete understanding of the different way that time series can vary over time, and the different kinds of 'trends' and 'pseudo-trends' that can occur. Time series can vary in the mean in either a deterministic or stochastic manner, they can vary in the seasonal component in either a deterministic or stochastic manner, and the underlying 'innovations variance' can also vary with time. Each of these types of changes in a series can produce similar kinds of behavior over a short period of observation, but are driven by very differing processes. Multiple time series, particularly those that are spatially distributed, may exhibit these types of behavior in a seemingly unrelated manner, yet can be shown to be driven by common underlying components. These types of dynamics will be very different from those that would be estimated by EOF's or other techniques based on principal component analysis. We discuss recent advances in time series analysis and econometrics that allow us to more fully explore how time series may vary and to test for and to estimate the underlying components of change.

Résumé

Pour analyser les changements dans une série climatique, il ne suffit pas de « repérer » les différentes sortes de « tendances » ou « pseudo-tendances » qui peuvent apparaître. Sous peine de profondes erreurs de compréhension, il est nécessaire de pouvoir caractériser correctement les différents processus d'évolution dans le temps. Une série temporelle peut évoluer de façon déterministe ou stochastique dans sa composante moyenne et/ou dans sa composante saisonnière. Les processus résiduels peuvent également avoir une variance qui évolue dans le temps. Ces différents processus d'évolution ont des propriétés très différentes et la caractérisation que l'on peut faire des changements temporels en dépend grandement. Malheureusement, sur de courtes périodes de temps, ces différents processus apparaissent très semblables. Il est donc primordial de pouvoir distinguer correctement les différentes composantes d'une série temporelle pour en caractériser les propriétés. Lorsqu'on examine conjointement un groupe de séries temporelles, par exemple des séries de température distribuées sur différentes latitudes adjacentes, il est possible de mettre en évidence des processus d'évolution sous-jacents qui leur sont communs. Ce type de dynamique est très différent de celui qui pourrait être estimé par des modèles EOF ou autres méthodes basées sur l'analyse en composante principale. Des avancées récentes en analyse des séries temporelles et en économétrie permettant d'explorer le type d'évolution d'une série temporelle, de tester et d'estimer les composantes sous-jacentes de ces changements temporels sont présentées.

Introduction

The earth's climate has been changing over the centuries, and coupled with these changes have been change in the ocean environment and in marine resources. Over the last several decades, concern has risen that anthropogenic effects, particularly in the atmosphere, may be altering or accelerating the natural pattern of climate change. However, the observed anthropogenic changes in the atmosphere are not necessarily producing concomitant changes in the ocean, or may be producing changes that are more complex than those observed in the atmosphere. Even without human influence, this natural progression of climate could have profound effects on the ocean and its resources. Understanding how the ocean has been changing, how the resources in the ocean have been changing, and detecting anthropogenic effects in either, are difficult problems that require careful thinking about what we mean by change, about the ways change can occur in the data we analyze, and whether even a global process of change could produce varying effects in different regions of the world. The types of dynamics we are presently witnessing in the ocean and the atmosphere raise questions that typically can not be answered by the usual methods of analysis. The term 'climate change' has been used loosely in the oceanographic literature, referring to almost any variation in the ocean environment. What is meant by 'climate change' must be more precisely defined if we want to characterize it properly.

Changes in the ocean environment can be transitory or relatively permanent. Even such large shocks as major El Niños can be transitory in nature when analyzed properly over a longer time-scale. Roy and Mendelssohn (this vol.) have shown that the major El Niños of 1972 and 1982 in the Humbolt Current, though large, were short-lived in their effects while the 1956-57 El Niño had long-lasting effects on the California Current system. ENSO events may be part and parcel of the long-term trend in the ocean, or they may be relatively frequent shocks to the ocean that in fact obscure the long-term signal. The upwelling regions of the world are of particular interest because of their high productivity. The upwelling process, which is local in scale, may be influenced by changes more global in scope. Bakun (1990), for example, has hypothesized that global warming would increase upwelling, making the upwelling regions cooler during the upwelling months, and perhaps affecting the oxygen content and other properties of the local ocean waters important to fish stocks. These changes, however, would not be reflected in the ocean as a whole. A change observed in the ocean environment at a particular area can be unique to that area, or part of a process observed over an entire region, or part of a process occurring over the entire globe. Moreover, there could be regional or global processes that are causing the observed change in the local environment, but with a different manifestation depending on the site it is occurring. It is then necessary to analyze variability at different spatial scales. Separating out common trends or common seasonal components from local trends and season is important to handle this type of question. Changes in the upwelling process can occur not only in the intensity of the upwelling, but also in the timing of crucial events such as the seasonal cycle, the onset of the spring transition in the California Current system for example. Identifying the proper source of these changes needs to be able to separate what pertains to a trend and what pertains to some cycle around this trend.

To properly deal with these types of problems requires precise definitions of the types of changes that might be observed and careful thinking about how change can be manifested in the data we analyze. Similar problems arose in economics where highlighting common features among variables, isolating source and timing of changes among any of numerous and always moving explicative factors, separating out a proper trend from some cycle and distinguishing a shifting trend from other cyclical fluctuations are crucial questions. Great advances have been made in econometrics and time series analysis to handle such a challenge. These new statistical techniques, which at least begin to deal with some of these issues, must be used also to analyze changes in oceanographic data, or else the results could be misleading. The aim of this paper is to describe some of these concepts and techniques; examples of their use are also presented.

1. What is change?

From the previous section, it is clear that change, particularly in the context of climate change, can be very complex in nature. Yet, when the term 'change' is mentioned, it is firstly as opposed to some sort of relatively stable state and change is therefore associated with some sort of non-stationary state. Climate change is often used in contexts such as 'global warming', meaning that the weather worldwide is progressively becoming warmer. In other words, the worldwide mean temperature has a positive time trend in the long-term. In this sense, 'change' and 'trend' in a series are almost synonymous. This is a limited view of what constitutes a 'change', particularly in regards to the climatic changes in the ocean. Only some of the examples presented in the Introduction correspond to this notion of change. Models that focus on the long-term change in the mean will not lend insight to the other problems discussed.

Even restricting ourselves to 'trends' in the data, the problem of defining the trend is more complex than finding the change in the overall mean. If a large region is being examined, this assumes that the entire region is changing in a homogeneous, uniform manner. In the ocean, due to the complex interactions between circulation processes and atmospheric forcing, the observed changes in different areas could be in different directions even if the underlying process is global in scope. Aggregate methods, or even disaggregate methods that assume a uniform trend will be misleading in identifying the change. Shifting trends are also changes that are very difficult to put to the fore if the trends are not correctly measured. 'Trend' can occur in the mean, the usual way people think of trend, but 'trend' can also occur in the seasonal component, and in the variance of the series. Properly identifying a trend will help to better characterize a change. More formally, a time series random variable is said to be stationary if its distribution does not depend on time. A time series is said to be weakly stationary if the mean and variance of the series do not depend on time. A time series is non-stationary, or has a 'trend', if either the mean or the variance of the time series (or both) are functions of time. Changes in the mean and the variance of a series can come about in several ways, for example, changes can be either deterministic or stochastic. Changes at intermediate frequencies can occur due to changes in the seasonal component. For non-stationary series, a series that has a trend in the mean has different properties than a series that has a trend in the variance. While over the short run the dynamics can appear similar, this difference has important consequences both for model building and for our understanding of the behavior of the process.

1.1. Deterministic and stochastic trends

The common understanding of trend is a changing mean level that varies deterministically. Let y_t be an observed time series, then a deterministic trend in the series y_t would be given for example by:

$$y_t = \mu + \alpha t + \varepsilon_t \qquad \text{where } \varepsilon_t \to \mathrm{N}(0, \sigma^2) \qquad (1)$$

The mean or expected value of this series is $E(y_t) = \mu + \alpha t$. This mean evolves with time while the variance is constant, $Var(y_t) = \sigma^2$. Such a series is said to have a deterministic trend or to be "trend stationary" since a simple regression on time will detrend or stationarize the series, the resulting detrended series will have a constant mean μ. The mean level of a deterministic trended series increases by some fixed amount every period (Fig.1c).

However, a time series can behave in the short-run as if it has a deterministic trend in the mean, yet be generated by a different mechanism. The simplest case of such a series is the so-called "random walk" which is of the form:

$$y_t = y_{t-1} + \varepsilon_t \qquad (2)$$

where the ε_t are independent, identically distributed random variables with mean of zero and variance σ^2 (Fig.1b). The series y_t can be rewritten as:

$$y_t = y_0 + \sum_{t=0}^{\infty} \varepsilon_t \qquad (3)$$

Such a series has a constant mean, $E(y_t) = y_0$, and a variance which increases towards infinity over time: $Var(y_t) = \sigma^2 t$

If the ε_t are zero mean stationary but autocorrelated, the series y_t is no longer a pure random walk but the trend of the y_t series will still behave as a random walk. These types of trends are called stochastic trends. In the econometric literature, they are also referred to as 'unit root', since the random walk model is equivalent to an autoregressive model with a root of modulus one in the autoregressive polynomial (i.e. roots of $\varphi(B) = 0$ in a series such as: $\varphi(B)y_t = \phi(B)\varepsilon_t$), see Hatanaka (1996) for details. In the above example (Eq. 2), it can be noticed that the coefficient in lag term is equal to 1. Differencing the series will remove the stochastic trend, leaving the series stationary. Processes that become stationary when differenced are called 'integrated' or 'difference stationary'. Let the backshift operator B be defined as:

$$By_t = y_{t-1} \tag{4}$$

Then differencing a series can be expressed as $\Delta y_t = (1 - B)y_t$. Sometimes a series needs to be differenced d times to become stationary. It will be then necessary to calculate $\Delta^d y_t = (1 - B)^d y_t$. These series are said to be 'integrated of order d', denoted by I(d). A random walk process is a very simple case. Generally, observed series exhibit more complex behavior than that of a pure random walk. A random walk with drift process can be given by:

$$y_t = \mu + y_{t-1} + \varepsilon_t \tag{5}$$

where ε_t is given as in Equation 2. Rewriting y_t as:

$$y_t = y_0 + \mu t + \sum_{t=0}^{\infty} \varepsilon_t \tag{6}$$

we see that this series has both a deterministic trend (i.e. a trend in mean given by $E(y_t) = y_0 + \mu t$) and a stochastic trend (i.e. a trend in variance given by $Var(y_t) = \sigma^2 t$). Since differencing will cancel out both trends, $E(y_t - y_{t-1}) = \mu$ and $Var(y_t - y_{t-1}) = \sigma^2$, such a series with both a deterministic and a stochastic trend is also an integrated series (Fig.1d). A random walk with drift will change in each period by some fixed amount *on average*. The change in each period will be by a predictable amount μ, which is called the drift, plus an unpredictable random amount. For this reason it is referred to as a 'stochastic trend'.

The different behaviors produced by these types of time series can be understood by examining artificial time series generated from closely related equations (Fig. 1a,b,c,d). The SST series at 36-38°N was whitened and the resulting residuals were used as the innovations (errors) in each of the simulations. The first series (Fig.1a) is a stationary autoregressive series with one lag and an autoregressive parameter equal to 0.5. The series has a constant mean and a constant variance. When the autoregressive parameter is set to 1, a unit root is introduced in the series. The random walk nature of the series is evident (Fig.1b). Adding a deterministic trend to the stationary series (Fig.1c) and adding an intercept to the random walk series, which becomes a random walk with drift (Fig.1d), highlights the problem of differentiating between deterministic and stochastic trend. The behavior of the two last series is very similar yet generated by two very different processes. Most people would say that the random walk with drift has a deterministic trend and would wrongly detrend this series by a regression on time.

In the case of a Trend Stationary series, it is only the mean of the series which will bring information on the long-term evolution of the process. The variance of forecast errors is finite, the uncertainty attached to these forecast is then bounded. It is indeed not the case for a Difference Stationary series since the variance of a series with a unit root is infinite. The best forecast of the future value of an integrated series we can make is its present value since the prediction error is going to infinity with time. The important difference between these two classes of non-stationarity lies on the fact that a 'shock' at any given period on a trend stationary process will only have a transitory effect while it will have a lasting effect on a difference stationary process. Integrated series are 'long memory' processes since any short-lived event will influence definitively the future level of such series.

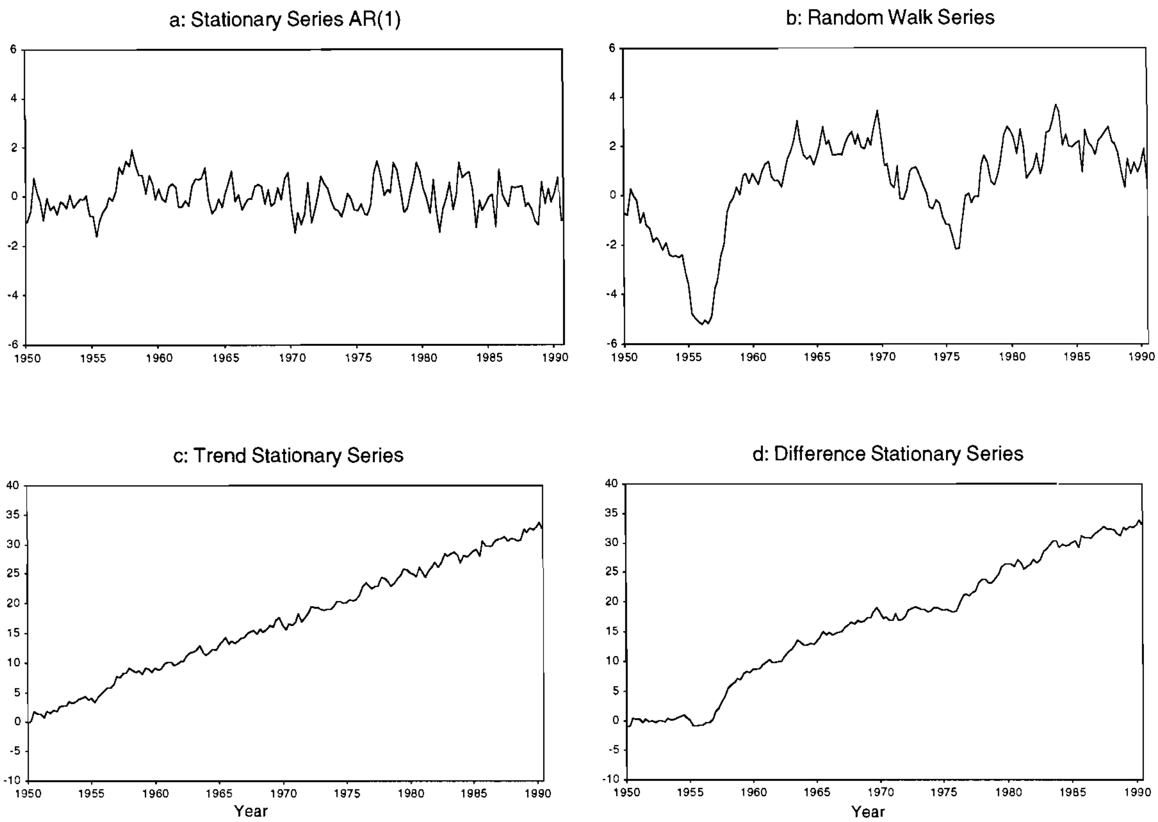

Fig. 1: Four artificial series generated from the same white noise ε_t (t is the time term trend).
a : Stationary : $X_t = 0.5X_{t-1} + \varepsilon_t$
b : Random walk : $X_t = X_{t-1} + \varepsilon_t$
c : Trend Stationary : $X_t = 0.1T + 0.5X_{t-1} + \varepsilon_t$
d : Difference Stationary : $X_t = 0.2 + X_{t-1} + \varepsilon_t$

1.2. Stationary and non-stationary seasonal component

Oceanographic data, particularly series such as SST, are characterized by their strong seasonality. In the oceanographic literature, seasonal components are usually estimated by taking monthly means or by fitting one or several harmonics to the data. Another method, more recently advocated, to deseasonalize monthly oceanographic time series is to transform the series to 12th-differences (Bakun, 1996, p. 165). Each of these two deseasonalizing methods suppose very different seasonal processes. The first one assumes that the seasonal component is deterministic and stationary, while the second one assumes a stochastic and non stationary seasonal component. To use a method in an inappropriate case will lead to spurious results. Prior to any deseasonalization or to any study of the seasonal pattern, it is then important to be able to decide which seasonal process is suitable for the observed time series. Some testing procedures have been recently developed for that purpose.

The concept of seasonality is, unless we have a precise and formal definition, as vague as that of a trend. Yet finding a precise definition for seasonality is not as simple as it appears. Despite a long history in analyzing seasonality, there is no generally agreed upon definition, nor is there a widely accepted view about how seasonality should be treated in empirical work. The main definitions offered by the literature (see for example Hylleberg *et al.*, 1990; Franses, 1996) are:

- A *deterministic seasonal process* : This seasonal process is stationary with a mean that varies by season. It is modeled by a regression on seasonal dummy variables such as the following quarterly series : $Y_t = m_0 + m_1S_{1t} + m_2S_{2t} + m_3S_{3t} + \varepsilon_t$ where ε_t is stationary. Seasonal dummy models imply a regular and non-changing seasonal pattern which can be perfectly forecast though some changes in phase and amplitude may appear in raw series due to the error process and to the existence of an autoregressive structure.
- A *stationary stochastic seasonal process* is a process generated by an equation such as : $\varphi\ (B)\ y_t = \varepsilon_t$ where ε_t are independent and identically distributed with all the roots of $\varphi\ (B)= 0$ lying outside the unit circle and with peaks in its spectrum at seasonal frequencies, as for example: $Y_t = \rho Y_{t-s} + \varepsilon_t$ with $|\rho|<1$. The mean of such series does not differ across seasons; however, if the initial values are seasonally different and the degree of serial correlation is high, such series may become very similar to the previous one. In such cases, a practical way to remove seasonality in stationary seasonal time series is to regress the series on seasonal dummy variables.
- A *non-stationary stochastic (or integrated) seasonal process* is generated by an autoregressive process like $\varphi(B)y_t = \varepsilon_t$ with one or several unit roots at some seasonal frequencies and ε_t stationary. As for example: $Y_t = -Y_{t-2} + \varepsilon_t$ for a quarterly time series seasonally integrated at one cycle per year. Such process describes changing seasonal patterns where sometimes 'spring' becomes 'summer'. The means in each season are not well-defined, they are an accumulation of all the past random shocks. These shocks which last forever may change permanently the seasonal pattern.
- A *periodic process* is generated by an autoregressive process such as:

  $$y_t = \mu_s + \sum_{i=1}^{p} \varphi_{is} y_{t-i} + \varepsilon_t$$

  where μ_s and φ_{is} are parameters that may vary across the seasons and ε_t are independent and identically distributed. These processes with periodically varying parameters describe a time series which has different properties in different seasons. A periodic process is non-stationary since the autocovariance function is not constant over time. Unit roots can also be present in a periodic process which nests the integrated seasonal model mentioned above.

This classification into deterministic and non-stationary stochastic seasonality parallels the trend classification already presented. The seasonal counterpart to treat with deterministic or integrated process will be to regress the series on seasonal dummy variables if the seasonality is assumed to be deterministic and/or stationary; and to difference the series with the appropriate $(1 - B^s)$ operator, where **s** is the number of seasons, if the seasonality is assumed to be integrated. The dynamics of the seasonal component, however, is more complex than that of a trend component. If we assume we have quarterly data (s=4), and examine the appropriate differencing operator, it can be factored into a product of backshift operators at smaller time lags as:

$$(1-B^4)y_t = (1-B)(1+B+B^2+B^3)y_t = (1-B)(1+B)(1-iB)(1+iB)y_t = (1-B)S(B)y_t \qquad (7)$$

The term $(1 - B)$ removes the longer-run trend while $S(B) = (1 + B + B^2 + B^3)$ removes the seasonal structure. This operator has four roots with modulus one, (1, -1, i, -i), which correspond respectively to zero frequency ("long-run" or non seasonal), 1/2 cycle per quarter or 2 cycles per year (Π) and 1/4 cycle or 3/4 cycle per quarter or one cycle per year (Π/2) for the pair of conjugate complex roots which cannot be distinguished. When monthly data are involved, the factored backshift operator $(1 - B^{12})$ contains many more roots than does Equation 7.

When modelling seasonality in empirical work, the key question is therefore to firstly establish if the data exhibit more evidence of seasonal dummies or seasonal unit roots. However, the choice of the proper model is not so direct and requires further care. The seasonal differencing operator removes unit roots at all frequencies although unit roots may exist only at some of the seasonal frequencies. In this case, the Δ_S differencing filter induces an over-differencing which further introduces unit roots in the moving average part of the series. In observed non-stationary time series deterministic and stochastic components are often both present. The seasonal pattern can be a combination of stationary deterministic part (seasonal dummies) and of non-stationary stochastic part (seasonal unit roots). All these configurations have to be taken in account when testing for seasonal roots, leading to many possible combinations of tests.

Deterministic, periodic and stochastic seasonal processes generate very different seasonal behaviors but, as with the trend component, over a relatively short time period, they can look very similar when examined visually (Fig. 2).

- The Fig. 2a series is a deterministic seasonal time series governed by four (in this case of quarterly data) alternating linear trends with identical slopes. The 'average' seasonal pattern remains constant. This series has been generated from a white noise and a very slight trend in the mean has been also added. The fluctuations that can be noted in this series are due to the perturbations of the error process.
- The Fig. 2b series is a periodic series where the trends vary with the season producing a changing seasonal pattern.
- The Fig. 2c series is an integrated seasonal series which yields four circularly merged random walks with identical drift, implying persistent and unpredictable changes in the seasonal pattern.
- The Fig. 2d series is the observed SST time series off the Canary Current at 30-32°N reduced to quarterly data. Comparing this last SST series to the three previous seasonal models highlights the difficulties that exists in attributing the observed changes to any type of seasonal process and to disentangle seasonal changes from trend changes when these changes are slow.

Although they can appear similar on small sample, deterministic, periodic and integrated seasonal processes have fundamentally different statistical properties which have to be taken in account when detecting and interpreting seasonal changes. A deterministic seasonal process is a stationary process. Some shifts or fluctuations due to exogenous shocks can appear but these changes will not persist in the seasonal pattern. When a seasonal time series is proven to be seasonally deterministic, each observed change in the seasonal component can be attributed to an exogenous cause that can therefore be investigated. The changing seasonal patterns in periodic processes are more difficult to interpret. The observed changes in the seasonal pattern of a periodic series are endogenous but may also be caused by some external sources. An integrated seasonal process allows a very changing seasonal pattern. The existence of a unit root in the seasonal component, as in the non-seasonal component, implies that a short-lived shock will perturbate definitively the pattern of season and the best prediction we can make of its future shape is always its present one.

For mathematical convenience, most analytical methods assume that the seasonal component is deterministic and unchanging, except for relatively small independent errors around the mean seasonal cycle. Our experience with the ocean is otherwise. Timing of events, such as the spring transition, in upwelling periods, shift over decades in a non-random manner. The intensity of upwelling may increase or decrease over quite a few years, without a corresponding change during the non-upwelling period. This 'trend' which is only during spring (or winter, or summer, etc.) is actually a change in the seasonal component. It seems then that the seasonal pattern in oceanographic variables is not constant over time and also that seasonal and non-seasonal variations are not independent.

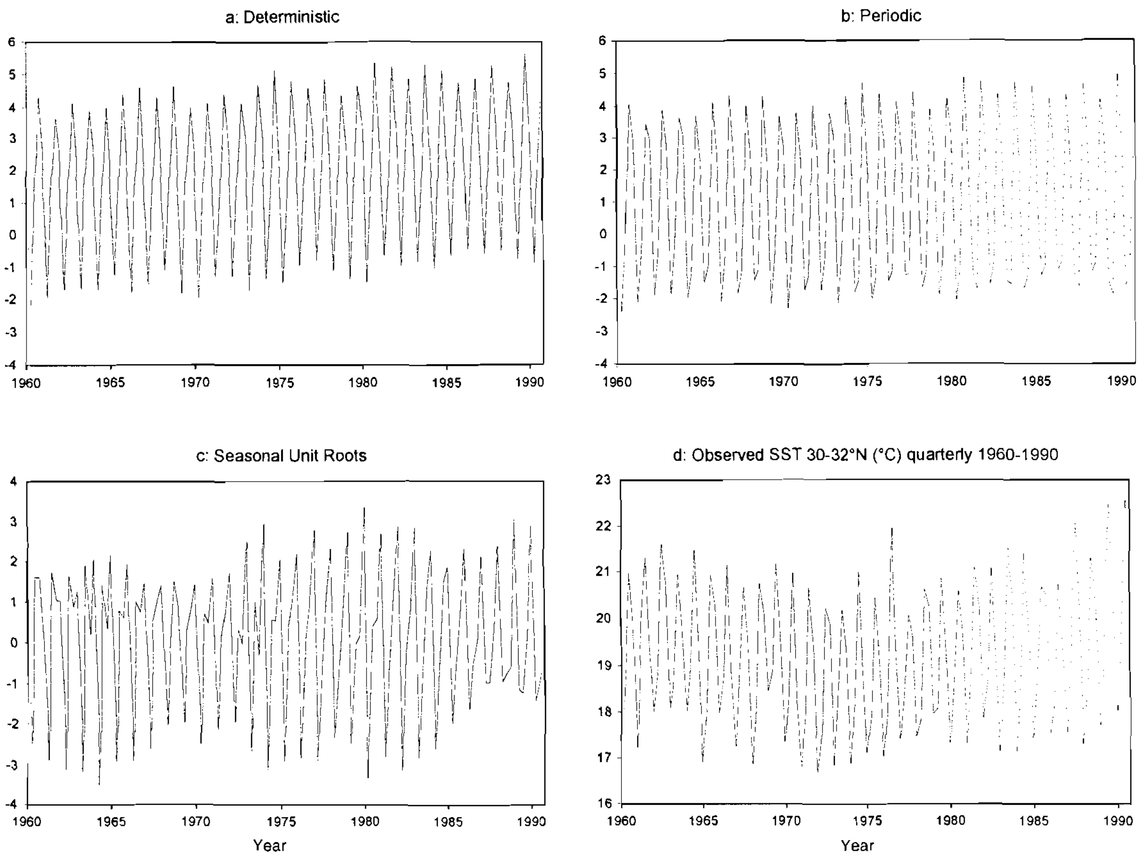

Fig. 2 : Deterministic, periodic and integrated seasonal time series generated from the same white noise ε_t and the observed SST series off the Canary Current at 30-32°N (T is the time term trend).

a : Deterministic : $X_t = 2D_1 - 3D_2 - D_3 + 3D_4 + 0.001T + \varepsilon_t$

b : Periodic : $X_t = 2D_1 - 3D_2 - D_3 + 3D_4 + \left((0.01 + 0.001T)D_1 + (0.05 + 0.005T)D_2 - (0.1 + 0.006T)D_3 + (0.04 + 0.007T)D_4\right)X_{t-1} + \varepsilon_t$

c : Integrated : $X_t = -X_{t-1} - X_{t-2} - X_{t-3} + \varepsilon_t$

1.3. Change in the variance of a series

A random walk (see Section 1.1) is a time series whose variance is a function of time, in that case a simple linear function of time. There are other cases where the underlying variance evolves with time in a non-linear fashion. For example, the variance can be a step function of time, it changes at a given time period and remains at its new level over a period of time. It is important when analyzing changes in a time series, and particularly when studying climatic changes, to be able to model the evolution process of the variability of the series. These type of non-linear time series processes with changing variance in the residuals are referred to as autoregressive conditional heteroscedastic process (ARCH) in the econometric literature (see Engle, 1982 and Bollerslev, 1986 for the first models), and as red noise in physics (see Steele, 1984 and Bakun, 1996, for reference in oceanography). ARCH or red noise process means that the conditional variance of a series is a function of time. It seems that these non-linear dynamics are frequent in the oceans where waters masses inertia produce endogeneous cycles. In fish catch time series it is often noted that the variability increases with the mean. This is also a conditional heteroscedasticity phenomenon which has to be represented with the appropriate models. More generally when a time series does not follow normal laws, the usual ARMA linear models are not suitable and it is necessary when forecasting or simulating such a series to refer to a class of non-linear time series models. A red noise process can be expressed as:

$$Y_t = \varepsilon_{t-1}^2 \varepsilon_t \qquad \text{Where } \varepsilon_t \to N(0,\sigma^2) \qquad (8)$$
$$E(Y_t) = 0 \qquad E(Y_t / \underline{Y_{t-1}}) = 0$$
$$V(Y_t) = 3\sigma^6 \qquad V(Y_t / \underline{Y_{t-1}}) = \sigma^2 \varepsilon_{t-1}^4$$

$\underline{Y_{t-1}}$ define the set of all the past values of Y_t. This process is stationary since the marginal mean and variance are constant and so do not depend upon time but the conditional variance is function of the history of the series.

Along with conditional heteroscedasticity, a time series can also contain deterministic trends or unit roots at some frequencies. All these features can be combined in more complex classes of ARCH models. Bollerslev and Ghysels (1996) have recently proposed a seasonal ARCH model with a periodic structure. A simple example of ARCH(1) process may be given by :

$$Y_t = (\alpha_0 + \alpha_1 Y_{t-1}^2)^{1/2} \varepsilon_t \qquad \text{Where } \varepsilon_t \to N(0,1) \qquad (9)$$
$$E(Y_t) = 0 \qquad E(Y_t / \underline{Y_{t-1}}) = 0$$
$$V(Y_t) = \alpha_0 / (1 - \alpha_1) \qquad V(Y_t / \underline{Y_{t-1}}) = \alpha_0 + \alpha_1 Y_{t-1}^2$$

Two examples of such ARCH(1) time series are shown in Figure 3. These are SST times series off the Canary Current at 28-30 and 30-32°N (Fig. 3a and Fig. 3d). They have been decomposed into trend, seasonal and residual components by the STL algorithm (Cleveland *et al.*, 1990). It can be noticed, both on the original series and on the residual series, that once the trend and the seasonality have been removed, the variability of the series is much greater before 1962 and after 1979 for the first 28-30°N SST series and greater before 1962 for the 30-32°N SST series.

These changes, which do not pertain to the trend nor to the seasonal component, have to be taken into account. Interpreting an observed change in a time series requires to be able to disentangle correctly the different components of the series if we want to attribute correctly which part comes from a change in the global mean (trend), in the seasonal cycle or from the behavior of the variance.

2. Detecting and modeling changes

Oceanographical data are generally considered as stationary or having a deterministic trend although it is a question whether freak events such as El Niños do not have lasting effect on the dynamics of the ocean. It is then important to be

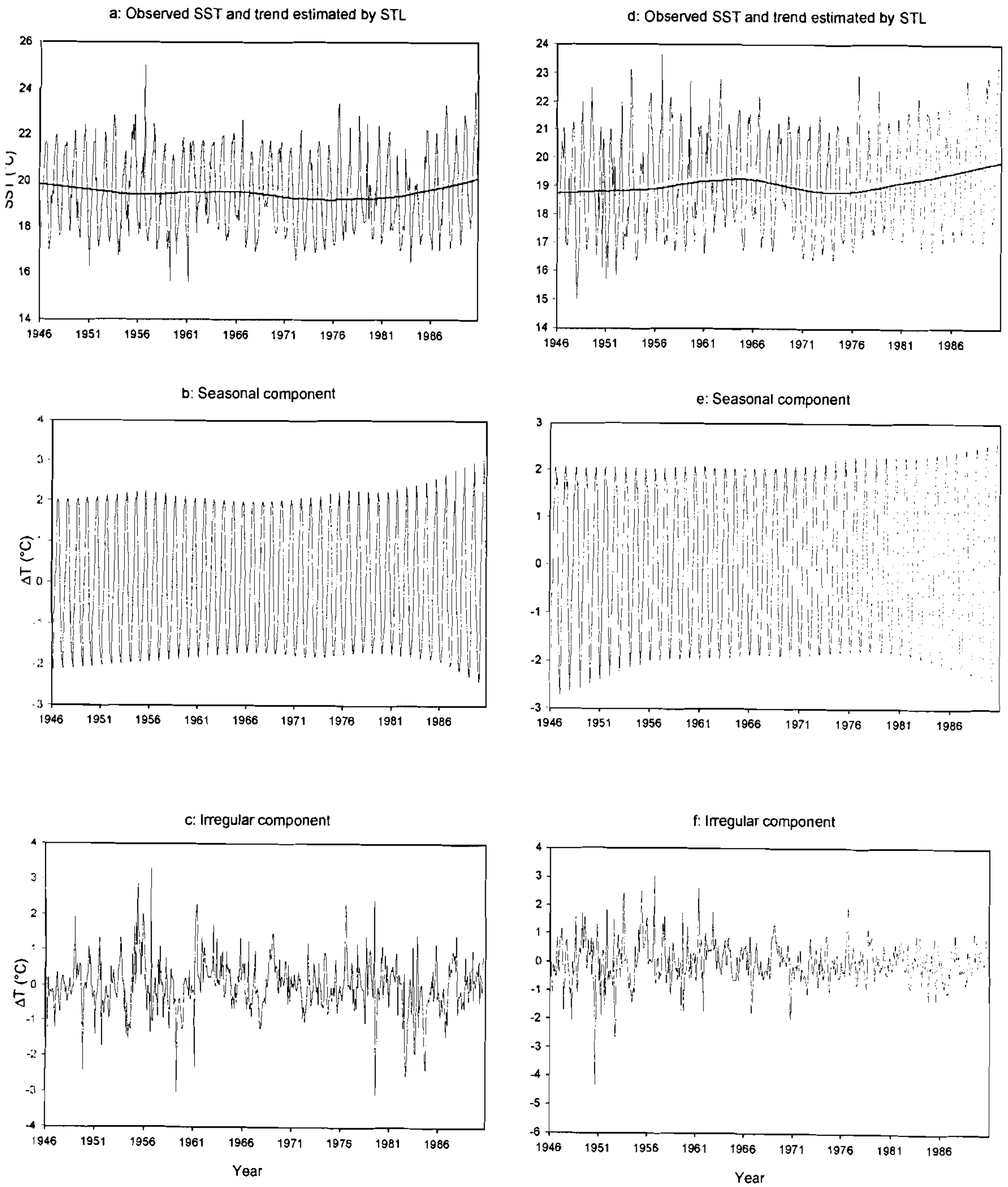

Fig. 3: Decomposition trough STL of two SST observed series off Canary Current at 28-30 (left panels) and 30-32°N (right panels).

able to identify what sort of non-stationarity, deterministic or stochastic, is operating in a series. There is no single method that will correctly model all of these possibilities for non-stationary behavior in a time series. However, several methods have been developed over the last decade that begin to deal with some of these issues, and thereby extend our ability to analyze the past behavior of oceanographic and biological time series. In the next sections, we discuss two possible approaches. Random walk, unit root, integrated series are all terms referring to stochastic trends. An integrated series is a series which has a unit root at some frequency in its autoregressive part. Analyzing the non-stationarity of a series will be then testing for unit root at any of its seasonal or non-seasonal frequencies. An other approach, allowing to avoid a delicate testing procedure, is to decompose a series in its unobservable components using a structural class of models developed by Harvey (1989). These models which treat seasonality as an unobserved component and separate non-seasonal from seasonal factors, are particularly adapted for series with a slowly changing seasonal pattern.

2.1. Testing for unit roots

Searching for unit roots at the zero frequency consists of testing the null hypothesis H_0: $\rho=1$ in a regression equation such as:

$$Y_t = \rho Y_{t-1} + \varepsilon_t \qquad (10)$$

where ε_t are independent and distributed as $N(0,\sigma^2)$. In order to whiten the residuals, autoregressive terms have to be added. The usual test regression is:

$$\Delta Y_t = \alpha + \beta t + \varphi Y_{t-1} + \sum_{i=1}^{q} a_i \Delta Y_{t-i} + \varepsilon_t \qquad (11)$$

The null hypothesis is now $\boldsymbol{H_0}$: $\varphi = 0$, since with the transformation to first difference, $\varphi = 1\text{-}\rho$. If the series has additional deterministic components, such as a deterministic trend for example, they have to be added to the regression test ($\alpha + \beta$t), along with the autoregressive structure $\sum_{i=1}^{q} a_i \Delta Y_{t-i}$

When φ=0, the problem examined is no more in a stationary framework. The ordinary least square (OLS) estimates of φ are not distributed as the usual regression test statistics. Instead, the appropriate t-statistics of φ are functions of Brownian motions. The asymptotic distributions of the test statistics will then depend on the different parameters included (constant, linear or quadratic trends). Because the statistical tests change depending on the model, testing for unit root must be done with care. Whatever may be the regression test, the null hypothesis is always the same. A procedure that sequentially tests reduced models is then highly recommended. These tests do not discriminate well between trend stationary and difference stationary series. This is still an open question and new tests are under discussion (see Cochrane, 1988, 1991; Hwang and Schmidt, 1996; Kwiatkowiski *et al.*, 1992; Leybourne and McCabe, 1994; Perron, 1989; Schmidt and Phillips, 1992). Critical values for the test statistics can be found in Fuller (1976) and Dickey and Fuller (1981) or in the above-cited literature for modified tests. Results of these tests may vary with the number of lags included in the model. To avoid this problem, Phillips and Perron (1988) has proposed a non-parametric test where the ε_t may be autocorrelated. Unit root tests have been revised by Kim and Schmidt (1993) in the case of conditional heteroscedastic errors.

Searching for unit roots at seasonal frequencies is a little more complicated and will depend on the periodicity of the series, either quarterly or monthly. As noted earlier a quarterly seasonal integrated process may have four unit roots (1, -1, i, -i) at the frequencies 0, 1/4, 1/2, 3/4. (see Section 1.2). A monthly seasonal integrated process may have 12 unit roots. The testing procedure for unit roots in the seasonal component at their different frequencies has been established for quarterly data by Hylleberg *et al.* (1990) and for monthly data by Beaulieu and Miron (1993). These authors have proven that the autoregressive polynomial of a quarterly seasonal series $\varphi(B)y_t = \varepsilon_t$ can be decomposed as:

$$\varphi(B) = -\pi_1 B(1+B+B^2+B^3) - \pi_2(-B)(1-B+B^2-B^3) - (\pi_4+\pi_3 B)(-B)(1-B^2) + \varphi^*(B)(1-B^4)$$

Then the deseasonalized y_t series can be decomposed as:

$$\varphi^*(B)y_{4t} = \pi_1 y_{1t-1} + \pi_2 y_{2t-1} + \pi_3 y_{3t-2} + \pi_4 y_{3t-1} + \varepsilon_t \qquad (12)$$

Where:

$y_{1t} = (1 + B + B^2 + B^3)y_t = S(B)\, y_t$ removes the seasonal unit roots at the frequency 1/4, 1/2, 3/4, while keeping the unit root at the zero frequency

$y_{2t} = (1 - B + B^2 + B^3)y_t$ removes the seasonal frequencies 0, 1/4, 3/4, while maintaining the unit root at the semi-annual frequency.

$y_{3t} = (1 - B^2)y_t$ removes the seasonal unit roots at the frequency 0, 1/2, while maintaining the annual frequency.

$y_{4t} = (1 - B^4)y_t$ is the deseasonalized series.

Under the null hypothesis of stochastic seasonality, all the π_i are zero. Testing that the autoregressive polynomial has a root of 1 is equivalent to testing $\pi_1 = 0$, testing that it has a unit root at the semi-annual frequency, root -1, is equivalent to testing $\pi_2 = 0$ and a joint test $\pi_3 = \pi_4 = 0$ will test for a unit root at the annual frequency. Intercept, trend and seasonal dummies have to be added to the regression equation (12), giving the model deterministic as well as stochastic components. This allows the possibility to discriminate between deterministic and stochastic trend model. Autoregressive terms must be added if the errors are not accepted as being a white noise process. As we are no more in a stationary framework, the test statistics do not follow anymore the usual laws. For different configurations of the test regression, critical values are provided by Hylleberg *et al.* (1990) for quarterly data and by Miron and Beaulieu (1993) for monthly data (see Frances and Hobijn (1994) for a detailed revue of critical values). Testing for seasonal unit root is more delicate than testing for the long-term unit root. Discussions of this test procedure and alternative are proposed by Canova and Hansen (1995), Franses (1996), Ghysels *et al.* (1994), Harvey and Scott (1994), Hylleberg (1995), Barthelemy and Lubrano (1996), Osborn *et al.* (1988). Franses (1994) has proposed a test for periodic integration which nests the usual seasonal unit root tests.

2.2. Decomposition of a time series

A simple starting point for modeling an observed time series Y_t such that the series can exhibit some of the more complex behavior of the previous section is to assume that the observed series is additively composed of independent components:

$$y_t = T_t + S_t + I_t + e_t \qquad t=1,T \qquad (13)$$

where T_t is the unobserved time-dependent mean-level (trend) at time t, S_t is the seasonal component at time t, I_t is the irregular term (stationary but autocorrelated) at time t, and e_t is the stationary, uncorrelated component at time t, which here can be viewed as 'observation' or 'measurement' error.

The model (Eq. 13) states mathematically the assumed form of the observed time series, but leaves open the question of the form of each component and how to estimate the component series from the observed data. The components could be modeled parametrically - the trend by a polynomial of a given order, the seasonal by harmonics, for example, but this approach is very limited in handling series with the types of dynamics discussed above. Ideally the components would be defined as flexibly as possible while allowing the model to be estimated. One way to achieve this is to put a constraint on the 'smoothness' (in this case through time) of the component. In the case of continuous functions of time, this implies constraining the derivatives of the function to be estimated. When time is discrete, the equivalent would be to put a smoothness constraint on the differences of the components, or other relevant linear combinations through time.

The use of such piecewise continuous 'smoothing splines' to estimate unobserved components dates back to Thiele (1880), see Lauritzen (1981), and in the more modern era to a paper by Whittaker (1923). Shiller (1973) modeled the distributed lag (impulse response) relationship between the input and output of a time series under difference equation 'smoothness' constraints on the distributed lags. He termed these constraints 'smoothness priors', but did not offer an objective method of choosing the smoothing parameter. Akaike (1979) developed a Bayesian interpretation of the model and used maximum likelihood to estimate the smoothness parameter. Brotherton and Gersch (1981) showed how the Kalman filter and maximum likelihood could be used to solve the smoothing problem. Kitagawa and Gersch (1984, 1985, 1988), in a series of papers, extended the Kalman filter-maximum likelihood approach to a variety of nonstationary problems, and Harvey (1989) developed similar models under the title « structural time series models ».

2.3. Smoothness priors and the trend component

How a smoothness constraint can allow for both a flexible and for a well-defined model can be most clearly understood in terms of estimating a 'smooth' but unknown function which has been observed with 'noise', that is data of the form:

$$y_t = f_t + e_t \tag{14}$$

where the y_t are the observed data, f_t is an unknown smooth function and e_t are independent gaussian errors. In this model there is no seasonal component and no autoregressive component. Whittaker (1923) suggested that the solution should balance fidelity to the data with fidelity to constraint on the smoothness of the unknown function f_t:

$$\left[\sum_{t=1}^{T} (y_t - f_t)^2 + \mu^2 \sum_{t=1}^{T} (\nabla^k f_t)^2 \right] \tag{15}$$

Equation 15 is equivalent to solving the least-squares problem subject to a constraint on the differences of the unknown function, using Lagrangean multipliers. The first term in Equation 15 is the usual sum-of-squares criterion, while the second term constrains the k-th order finite differences of the unknown function (the discrete equivalent of splines where the k-th order derivatives are constrained). The two parts are balanced by the 'smoothness parameter' μ. As μ goes to zero, the smoothness constraint disappears, and the estimate of the unknown function exactly interpolates the data. As μ approaches infinity, the sum-of-squares term becomes negligible, and the solution is the appropriate k-th order polynomial of time (e.g., linear for k=1, quadratic for k=2, etc.)

Equation 15 leaves unanswered the crucial question of how to estimate the smoothness parameter μ. Akaike (1979) gave the problem a Bayesian interpretation. He viewed the constraint as a stochastic, zero mean difference equation, that is:

$$\nabla^k f_t \rightarrow N(0,\sigma^2) \quad (16)$$

where the notation $N(0,\sigma^2)$ denotes a normal random variate with mean zero and variance σ^2, and where $\mu^2 = 1/\sigma^2$ (which can be interpreted as a signal-to-noise-ratio), is a hyperparameter that can be estimated using maximum likelihood methods. (See the reference above for a demonstration that for a fixed value of μ, the Bayesian model is equivalent to Equation 15). Akaike termed this a 'smoothness prior', because the smoothness constraint is given a prior distribution and is then estimated by likelihood methods.

The 'local trend' fit by the smoothness priors approach can be shown to be a linear smoother — for a given value of the smoothness parameter the estimate of the unknown function at any time period is linear in the data — that is it can be calculated as a weighted linear combination of the observed time series. This estimate differs from a running mean, for example, which is also a linear smoother, in that the window used to smooth the data can vary as can the weights (see Hastie and Tibshirani, 1990). Though the smoothing spline fit by this model is more complex than a running mean, the basic idea is the same: estimate the unobserved component by a linear smoother. We will return to this idea in order to model the seasonal component.

The 'smoothness prior' formulation clarifies the connection between the methods of this section and those of the next section. When k=1, Equation 16 reduces to:

$$y_t - y_{t-1} \rightarrow N(0,\sigma^2) \quad (17)$$

which is the same as Equation 2 if ε_t is assumed to be a normal random variable. The two methods are different approaches to dealing with the same problem.

2.4. Smoothness priors and the seasonal component

In Section 2.3, the trend was modeled by placing a prior distribution on low-order differences of the data, which constrains the smoothness of the trend component. This smoothness constraint yields a solution that is a linear smoother of the time series. If we have a time series that is known to have only a seasonal component plus noise, a similar idea can be used by constraining the seasonal differences of the time series (c.f. Eq. 7) as:

$$S_t - S_{t-s} \rightarrow N(0,\sigma^2{}_s) \qquad t=1,T \quad (18)$$

where s is the relevant number of periods in a year. If the series were monthly data, Equation 18 would be the same as individually fitting a trend to each monthly difference series, except now there is the added constraint that the amount of smoothing allowed must be the same for each month. Thus the calculated 'trend' for each monthly difference series is suboptimal if considered apart from the rest of the data. As with the trend term, the value of $\sigma^2{}_s$ determines if the differences have no trend, leading to a deterministic seasonal cycle, or a stochastic trend.

Constraining the seasonal differences is not the only way to define a sensible seasonal component. Assuming a series with no trend and a strictly deterministic seasonal component of periods (say, for example, a cosine curve with a period of 12 months), then the seasonal component has the property of having a zero mean if we average over the s-periods, and zero difference if we calculate the difference y_t-y_{t-s} (for example taking 12th differences for monthly data). The equivalent constraint would be to want the s-period running sum to have a mean of zero, but to allow it to vary, that is a constraint of the form:

$$\sum_{i=0}^{s-1} S(t-i) \rightarrow N(0,\sigma^2{}_s) \qquad t=1,T \qquad (19)$$

If $\sigma^2{}_s$ is zero, then the result is a deterministic seasonal cycle, in fact the mean for that season, while if $\sigma^2{}_s$ goes to infinity, then the seasonal component interpolates the data. In between, the estimate of the seasonal component is a smoothing spline, a linear smoother of the observed seasonal time series.

The smoothness constraint of Equation 18 explicitly smoothes the s-differenced time series and thereby implicitly smooths the s-period running sum. Similarly, the smoothness prior of Equation 18 explicitly smoothes the s period sums and thereby implicitly smoothes the time trends.

2.5. Combining trend and seasonal components

The previous examples have considered series that are composed of either a trend component plus noise or a seasonal component plus noise. Most oceanographic and biological time series are likely to have both components present, so the problem arises of simultaneously estimating the trend and the seasonal component. (The discussion that follows is not the algorithm actually used, which is given in Appendix A and which estimates all components simultaneously. However, the backfitting type algorithm described here could be used, and makes the ideas clearer). Start with initial estimates of the trend and seasonal components, say the mean of the series and the monthly means of the demeaned series. Then define the partial residuals as:

$$\begin{aligned} y_{1,t} &= y_t - \hat{S}_t \\ y_{2,t} &= y_t - \hat{T}_t \end{aligned} \qquad (20)$$

where S_t, T_t are respectively the present estimates of the seasonal component and of the trend. Each partial residual series is simply the observed series less the present estimate of the other component. Then iteratively, to get a new estimate for the trend, we calculate $y_{1,t}$ and use the approach of Section 2.3 to estimate the trend term for the partial residual series. The estimated trend in the partial residual series is then used as the new estimate of the trend component T. This new value of T is then used to calculate the partial residual $y_{2,t}$ and the methods of Section 2.4 are used to estimate the seasonal component for this partial residual series. The estimated seasonal component is then used as the new estimate of S and the process is iterated until convergence.

The algorithm can be viewed as iteratively fitting smoothing splines to the partial residuals of the series until convergence is achieved. In the examples (Section 4) we examine the original series and the partial residual series with the components to help understand output of the algorithm. This type of algorithm is not limited to using smoothing splines as the smoother. Cleveland *et al.* (1990) use a similar procedure and the LOWESS smoother in the STL algorithm for time series decomposition. If an autoregressive component (i.e., I_t) is also included in the model, then three partial residuals could be defined, and at each iteration a maximum likelihood estimate of the autoregression parameters would be estimated.

The actual algorithm used (Appendix A) sets up the entire model in state-space form and uses a combination of the Kalman filter and the EM algorithm (Dempster *et al.*, 1977) to calculate the maximum likelihood estimates of the parameters. Given the final estimates of the parameters, the Kalman smoother gives the minimum mean-square error estimates of the different components.

3. Multivariate analysis: cointegration

3.1. Cointegration

The existence of unit roots in a time series is not only important in understanding which type of trends is affecting the behavior of the series and its pattern of seasonality, but also has interesting consequences when several time series are modeled jointly (Granger, 1986, 1988a,, 1988b). For a general survey see Hatanaka (1996), Lütkepohl (1991) and Dolado *et al.* (1990).

All linear combinations of zero order integrated series will also be integrated of zero order. Likewise a linear combination of a group of I(d) series will generally be an I(d) series also. But sometimes it is possible to find a particular linear combination of non-stationary series which produces a new series which is integrated of lower order and which can be stationary. This particular linear combination of the series removes some or all the trends from some or all the series. These series are said to have 'common trends' or to be cointegrated. Ignoring cointegration in a group of series can lead to misspecified models. Since co-movements among time series indicate the existence of common components, this implies a more parsimonious and informative structure in a joint model (Engle and Yoo, 1987; Johansen, 1988).

The term 'integrated series' refers explicitly to unit roots or stochastic trends in a series and 'cointegration' to the existence of common trends in a group of integrated series. These ideas have been extended to a more general framework that tests for the presence of some 'feature' in a time series and whether this feature is common to a group of series. 'Features' are data properties such as serial correlation, trends, seasonality, heterocedasticity, autoregressive conditional heteroscedasticity and excess kurtosis. The idea is the same, if a linear combination of featured variables does not possess the feature any more, the featured variables will be said to have a 'common feature' (Engle and Kozicki, 1993; Vahid and Engle, 1993; Escribano and Pena, 1994).

For notational and presentational convenience, we will only present the case of order-1 integrated series. Let Y_t denote a n-vector of I(1) variables whose first difference is autoregressive.

$$\Phi(B)\Delta Y_t = \Theta(B)\varepsilon_t \qquad (21)$$

where Δ=(1-B) and ε_t is white noise. The stationary process ΔY_t has a moving average representation and can be rewritten as:

$$\Delta Y_t = \Phi^{-1}(B)\Theta(B)\varepsilon_t = H(B)\varepsilon_t \qquad (22)$$

H(B) is a polynomial matrix in B, and may be decomposed as *H(B) = H(1) + (1 - B) H* (B)* (see Engle and Granger, 1987). Integrating (taking the integrand of) both sides of equation 22 to solve for ΔY_t yields :

$$Y_t = H(1)\frac{\varepsilon_t}{(1-B)} + H^*(B)\varepsilon_t = H(1)\sum_{s=0}^{\infty}\varepsilon_{t-s} + H^*(B)\varepsilon_t \qquad (23)$$

which shows that an I(1) process is a sum of a random walk and a stationary process. Similarly, an I(d) process can be decomposed as a sum of d-1 random walks of order d, d-1, d-2, ...1, plus a stationary process.

If we can find a n-vector α_i such that $\alpha'_i H(1) = 0$, meaning that the matrix H(1) is not of full rank. Pre-multiplying Y_t by α'_i will cancel-out the random walk part of Yt and $\alpha'_i Y_t = \alpha'_i H^*(B)\varepsilon_t$ will be stationary. In that case, the multivariate process Y_t is said integrated order 1, cointegrated order 1, denoted C(1,1), and α_i is a cointegration vector stationarizing the process. There can exist r (r<n), linearly independent cointegration vectors, meaning that r different subsets of the variables in the

multivariate process Y_t are linked in stationary fashion. The collection of all linearly independent cointegration vectors form the (n,r) matrix α where $\alpha' Y_t$ is I(0). The existence of cointegration vectors implies that the rank of H(1) is n-r, so that testing for cointegration is equivalent to testing the rank of the matrix of H(1). This test is known as 'Johansen's test' (see for details Johansen and Juselius, 1990; Johansen, 1991; Phillips and Ouliaris, 1990 and Stock and Watson, 1988, for similar approach). Procedure and critical value are available in most of the econometric packages like E-Views, PC-Give or RATS.

Engle and Granger (1987) have presented several equivalent representations of cointegrated series. The most interesting one is the 'error-correction representation':

$$A(B)\Delta Y_t = -\gamma z_{t-1} + d(B)\varepsilon_t \qquad (24)$$

where $z_{t-1} = \alpha' Y_{t-1}$ and d(B) is a scalar polynomial in B. The series z_t is a random stationary process that measures the deviations or errors around the so called 'equilibrium relationship' defined by $\alpha' Y_{t-1}$ which is assumed to be null when realised. Stationarity in a linear combination of variables can be intuitively associated with the static notion of a long-term equilibrium relationship between these variables. This error-correction representation shows clearly a system directed by a 'long-term relationship' around with short-term variations adjust for the deviations at the equilibrium which have occurred at the previous period. Non-stationary series when cointegrated can never diverge far from each other over time. They are linked by a steady-state relationship that keeps them close in the long-term.

The presence of both deterministic and stochastic trends in a time series changes the distributional properties of the cointegration test as well as the form of the error-correction model. The appropriate modified procedures must be used in this instance.

The model considered here is linear and with time-invariant parameters. It can be generalized by allowing for time-varying parameters (see for example Granger,1986). The concept of cointegrated system has also been extended to the cases of seasonally integrated series by Hylleberg *et al.* (1990).

3.2. Seasonal cointegration

Seasonal cointegration occurs when a group of time series with changing seasonal pattern exhibit a 'parallel movement' in their seasonal component.

Assume that Y_t is an n-vector of zero mean quarterly variables which are all I(1) at the frequencies Θ=0, 1/4, 1/2, 3/4. The autoregressive-moving average representation of Y_t is:

$$(1-B^4)Y_t = C(B)\varepsilon_t \qquad (25)$$

where the ε_t are independant random n-vectors identically distributed as NID(0,Ω) and C(B) is an (n,n) matrix of lag polynomials. As in the previous univariate case (Section 1.4), the polynomial matrix C(B) can be expanded as:

$$C(B) = \Psi_1[1+B+B^2+B^3] + \Psi_2[1-B+B^2-B^3] + (\Psi_3+\Psi_4 B)[1-B^2] + C^*(B)(1-B^4) \qquad (26)$$

where $\Psi_1 = \frac{C(1)}{4}, \Psi_2 = \frac{C(-1)}{4}, \Psi_3 = \frac{\mathrm{Re}[C(i)]}{2}, \Psi_4 = \frac{\mathrm{Im}[C(i)]}{2}$.

To examine a group of series for seasonal cointegration requires analyzing the properties of the model:

$$(1-B^4)\alpha' Y_t = \alpha' C(B)\varepsilon_t \quad (27)$$

Seasonal cointegration exists when :

- The existence of an (n,r_1) matrix α_1, with $r_1<n$, such that $\alpha'_1 \Psi_1 = \alpha'_1 C(1) = 0$ implies cointegration at the zero frequency.
- The existence of an (n,r_2) matrix α_2, with $r_2<n$, such that $\alpha'_2 \Psi_2 = \alpha'_2 C(-1) = 0$ implies cointegration at the 1/2 frequency.
- The existence of an (n,r_3) matrix α, $r_3<n$, such that $\alpha'(\Psi_3 + \Psi_4 B) = \alpha' C(i) = 0$. Implies cointegration at the 1/4 and 3/4 frequencies without being distinguishable.

The columns in α_1 and α_2 form the cointegrating vectors at the zero and 1/2 frequencies. Columns in α will be called "polynomial cointegrating vectors" since they are of the form $\alpha(B)= \alpha_3 + \alpha_4 B$.

There is an error correction representation for seasonal cointegration which varies with the number and frequencies of unit roots which are canceled out by the cointegrating vectors α's (see example in Hylleberg *et al.*, 1990).

Testing for seasonal cointegration is still in an early age of development. The critical values for seasonal cointegration based on unit root test are already available for quarterly data (Engle *et al.*, 1993) but not for monthly data. Furthermore, the only procedure presently available for estimating the cointegration vectors and error correction representation is the two-step procedure similar to that of Engle and Granger (1987) and developed by Engle *et al.* (1993). Unfortunately this procedure works only in the bivariate case. A new method has been recently developed by Franses (1994) in order to test for seasonal unit roots. This method consists of a multivariate decomposition of a univariate time series into its different seasonal components allowing to use the Johansen's test procedure. This approach could be fruitfully extended in order to test for seasonal cointegration but will necessitate huge sample sizes.

Deseasonalizing time series by using a seasonal difference operator, which a priori assumes a changing seasonal pattern, has been increasingly preferred to diseasonalizing the series by a regression on seasonal dummy variables which assumes a deterministic seasonality. However, if the time series are seasonaly integrated and cointegrated at some frequencies, then both methods would lead to incorrect results. The appropriate method would be to use seasonally unadjusted data and jointly model the series.

4. APPLICATIONS

4.1. Interpretation of cointegration in oceanography

Cointegration models have a meaningful economic interpretation explaining why such an approach is burgeoning in economics. Economic theory postulates that economic variables will eventually reach an 'equilibrium relationship'. These 'target equilibrium' are generally not observed but there is strong belief that these variables should not diverge from equilibrium by too great an extent. Most of the time an economy is in disequilibrium, but market mechanisms and other economic forces bring about a dynamic adjustment of the variables towards their equilibrium.

Considered in a spatial context, theses new techniques in time series analysis could be usefully applied to oceanographic data. Identifying and estimating trends in oceanographic time series which are common to an entire region (global change) and separating these from stationary cyclical swings or non-stationary components which are unique to a local area (local dynamics) is an important problem in the studies of climatic change in oceanography. For example, if we can show that SST series at different adjacent latitudes are both integrated (i.e., non-stationary) either in their seasonal component or in the mean, as well as cointegrated either in their trend or seasonal component, then the estimated common trends can be viewed as 'global changes' since they affect all the SST series in the same manner over the region. The remaining variations of each individual SST series around these common trends can be viewed as 'local changes'. Identifying over a large region which group of SST series enter or do not enter in cointegration relationships, can also allow to better determine and characterize transition zones in the ocean's dynamic.

Since seasonality is driven by broad processes in the ocean, and if seasonal integration explain the varying and changing structure of seasonal pattern in oceanographical data, then seasonal cointegration should not be uncommon.

4.2. Decomposition of time series: examples

To illustrate the consequencies of misusing the different detrending and deseasonalizing methods previously exposed, they have been applied to the SST time series off the Canary Current at 22-24°N. Results obtained can be compared on Figure 4. This series have been tested for unit roots at long-term and seasonal frequencies. When deterministic term are included in the regression equation, the series appears to be deterministic although the results seem ambiguous for the zero frequency. To accept the hypothesis of a deterministic series (absence of unit roots at all frequencies) implies that the 12-difference operator must not be used to deseasonalize the series. A deterministic trend and season have been therefore estimated (Fig. 4d and 4e). Trend, although small, is significantly negative. Most of variations remain in the errors process. The error process is non-stationary which testify for a wrong decomposition of the series (Fig. 4f).

Decomposing the series through the STL algorithm, the behavior of the trend appears quite different, decreasing from 19.92°C in 1946 to 19.26°C in 1972 and increasing regularly again after this date (Fig. 4a). Without having seasonal unit roots, the seasonal pattern appear quite changing. This series has time varying parameters in the season (Fig. 4b). The irregular term is stationary yet proved to be conditionally heteroscedastic after being tested. This time series is non linear with time varying parameters and it could be modeled by a periodic conditionnally heteroscedastic model.

Changes in the series, both in the trend (inter-year changes) and in the season (intra-year changes) can be easily seen and interpreted with the results issued of the STL decomposition of the series. Although this series can be accepted as deterministic, it is in fact non linear and to estimate a deterministic trend and season will lead to spurious results and to the incapacity to really detect changes.

Two other examples will help to clarify some of these ideas. We calculate the decomposition for SST and the north-south component of the wind stress at 36-38°N, an area off the California coast between Monterey and San Francisco. SST in this region displays relatively little variation as compared to the mean level. If the overall series mean is removed from the SST series, then the residuals over the entire time period are less than three degrees in absolute value, compared to a mean level of roughly 14 degrees. So the trend likely to dominate any other component SST in this region is also highly seasonal and strongly autocorrelated. The seasonal component may vary to a degree, but winters are colder than summers etc. so that the basic pattern will be fairly deterministic. Wind stress, in contrast, is highly variable, with the variability around the overall mean

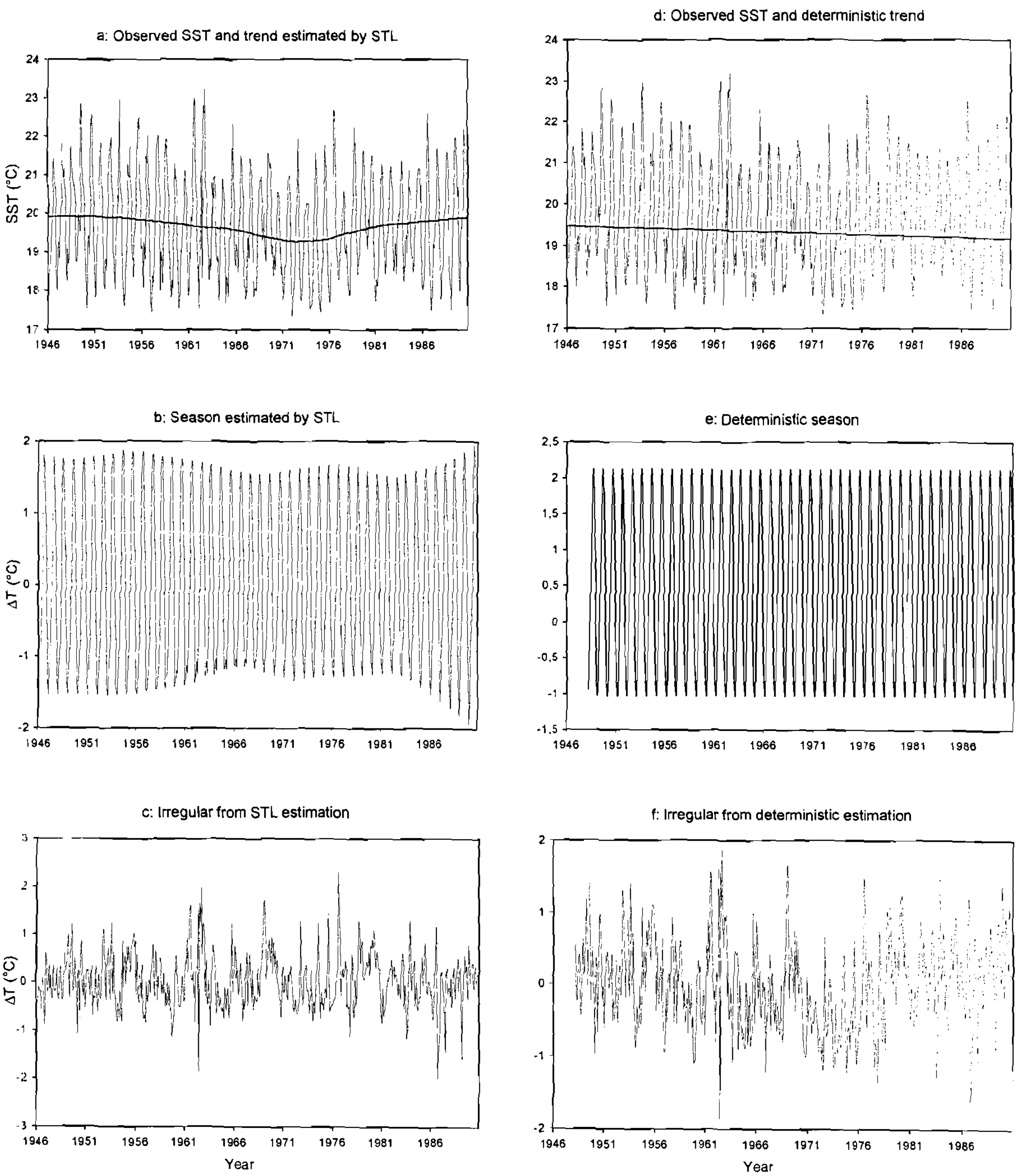

Fig. 4: SST time series off the Canary Current at 22-24°N. Decomposition in trend, season and irregular components through the STL algorithm (a,b,c), estimation of a deterministic trend (d), a deterministic seasonal (e), and irregular (f).

larger than the mean itself. Wind stress is not highly seasonal and with a low degree of autocorrelation, particularly when compared to SST. A reasonable procedure should at minimum reproduce these features of the ocean in this region.

The raw SST series and the estimated components (Fig. 5a-e) have the desired characteristics. The seasonal component is nearly deterministic and only varies by 3 degrees. The autoregressive term is nearly as large as the seasonal component, while the noise component is very small, less than 0.25 degree Celsius in absolute value.

When the estimated trend is plotted against the raw series (Fig. 6a), some of the features of the trend term are apparent in the raw time series, but others are more obscure. When the estimated seasonal component is removed (Fig. 6b), the estimated trend is clear in the partial residual series, and it is evident that the trend component is a smoother of the partial residual. When both the seasonal and the AR components are removed (Fig. 6c), the estimated trend differs from the partial residual series only by the relatively small noise series.

The estimated SST seasonal component (Fig. 7a) is a mean zero series (as desired, so that the trend component has at least one desired property), and when compared to the detrended series differs from it by roughly the AR component. The SST component can be seen to smooth the resulting partial residual series. The basic features of the series are deterministic, but the component series does vary, such as in the timing of the occurrence of the spring transition and other secondary maximum and minimum. Variations in the timing of such events can have significant implications for fish stocks, and would not be as easily identified if a purely deterministic model were used. Note that if the AR and trend components are removed, then the seasonal component differs from the partial residual series only by the amount of the noise series.

When both the estimated SST trend and seasonal components are removed, the resulting series is highly autocorrelated (Fig. 8a) and very close to the estimated AR component. The interplay of the three components and how each smoothes the appropriate partial residual series can be seen clearly in this example.

If we look at a similar sequence of graphs for north-south pseudo-stress in this region (Fig. 9, 10, 11), the seasonal component is closer to the trend in absolute value, while the AR component is very small and the uncorrelated noise series is as large in value as any of the other components. The trend is not as obvious from the data and the seasonal component is more variable.

These examples demonstrate the consistency of the procedure, how the different components interact in forming the estimates of the other components. Also, this example illustrates that the decomposition can estimate components that are consistent with what was known a priori, and which have very different dynamics.

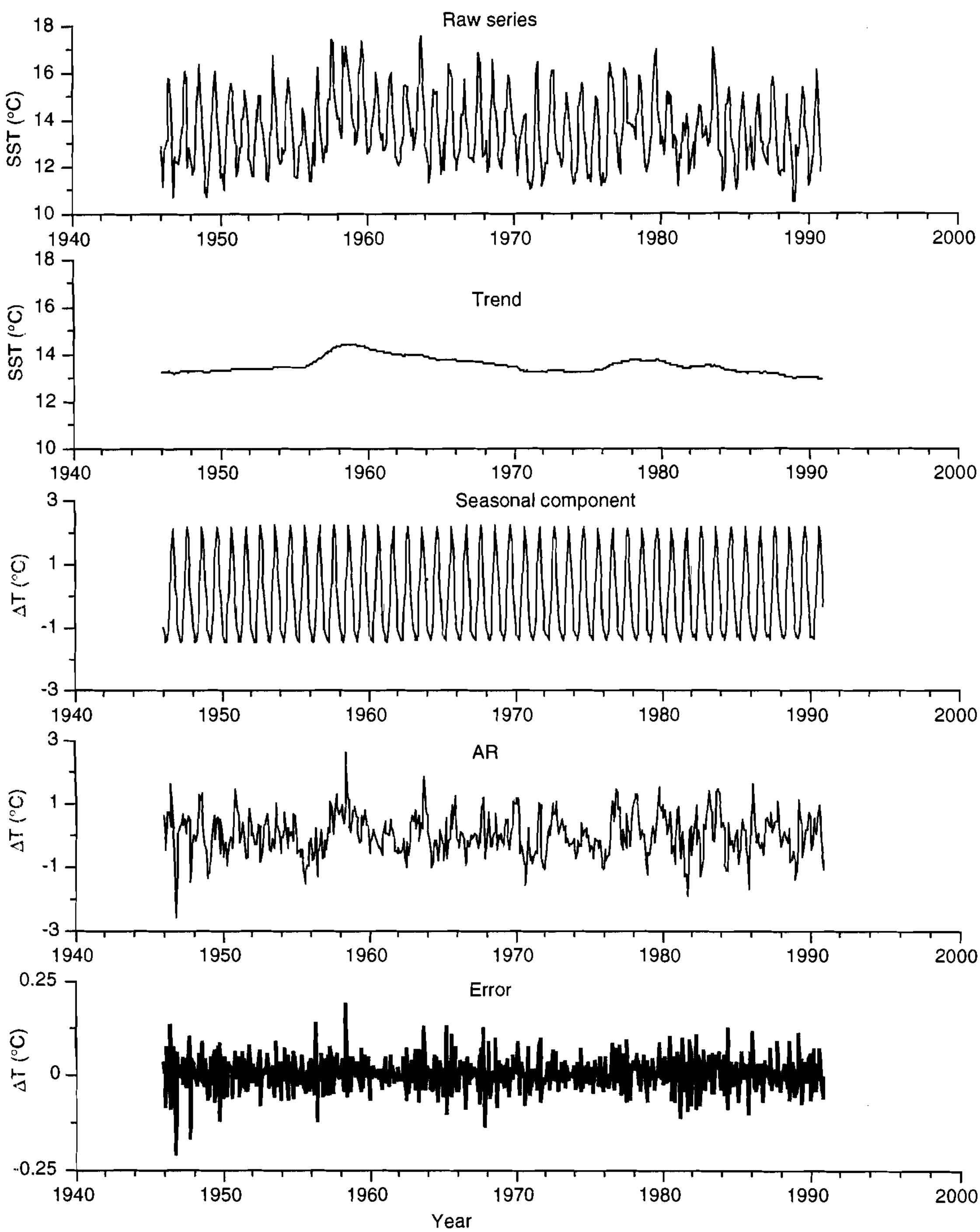

Fig. 5: Time series of SST (°C) off the California coast (36-38°N) and its decomposition into a non-parametric trend (°C); a non stationary seasonal component (ΔT; °C); and an autoregressive component (ΔT; °C); and an error term.

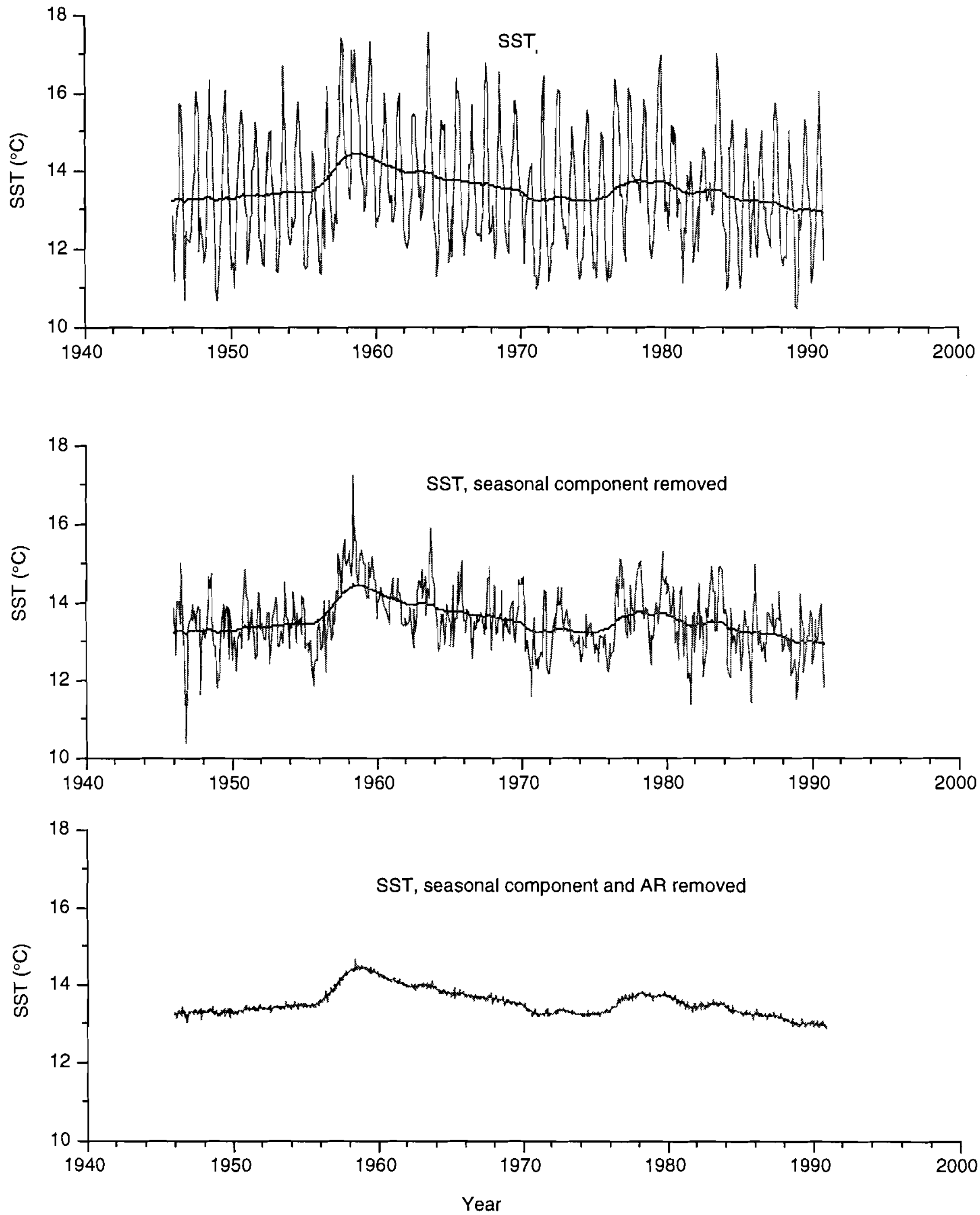

Fig. 6: California Current SST (°C) time series at 36-38°N : calculation of the trend from the partial residuals . The top panel shows the trend versus the original series; the middle panel the trend versus the original series minus the estimated seasonal component; the bottom panel the trend versus the original series minus both the estimated seasonal and the autoregressive components.

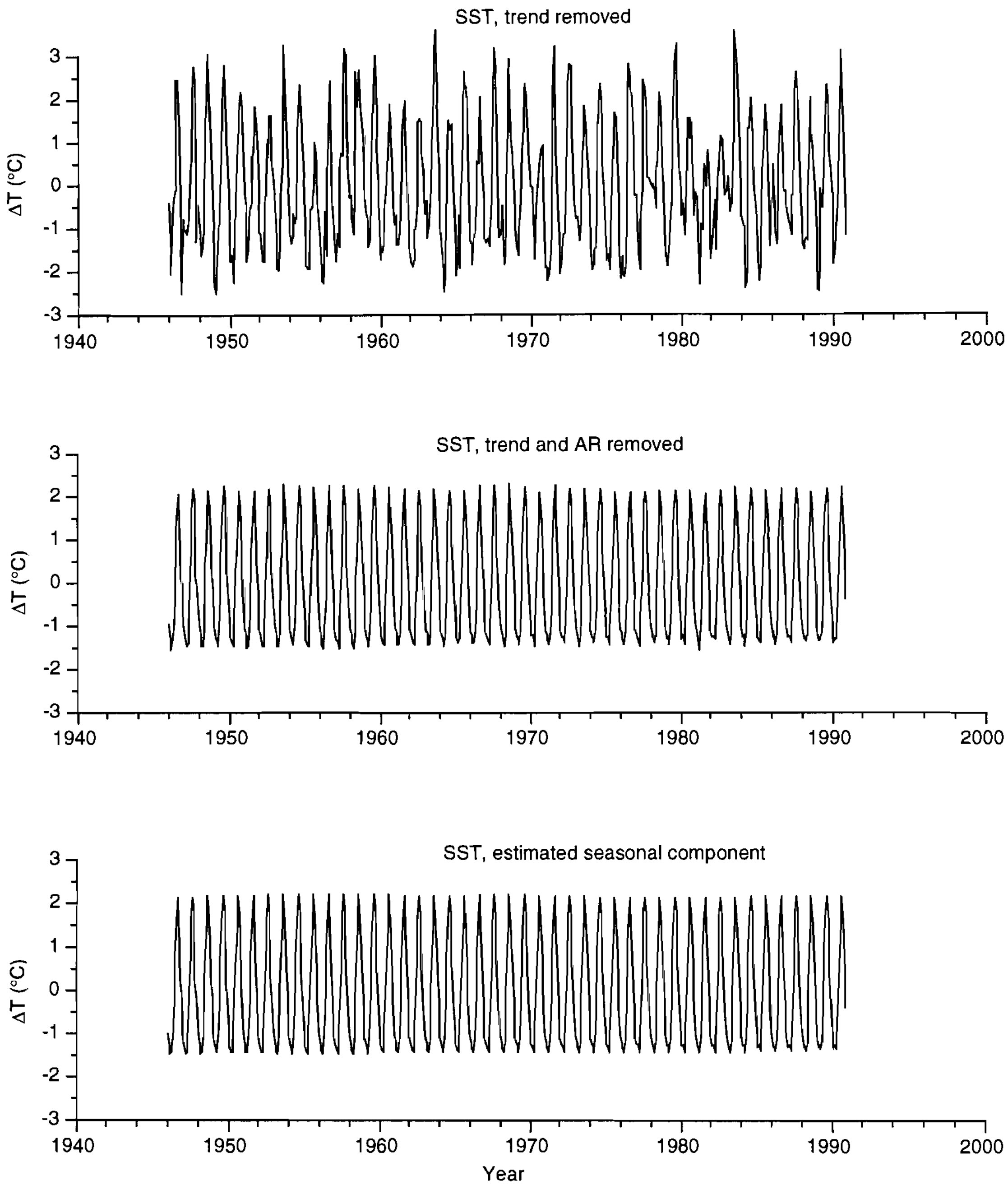

Fig. 7: California Current SST time series at 36-38°N: calculation of the seasonal component (ΔT; °C) from the partial residual series. The upper panel shows the detrended series; the middle panel shows the original series minus the trend and autoregressive components; the bottom panel shows the estimated seasonal component versus the original series, with the trend and AR components removed.

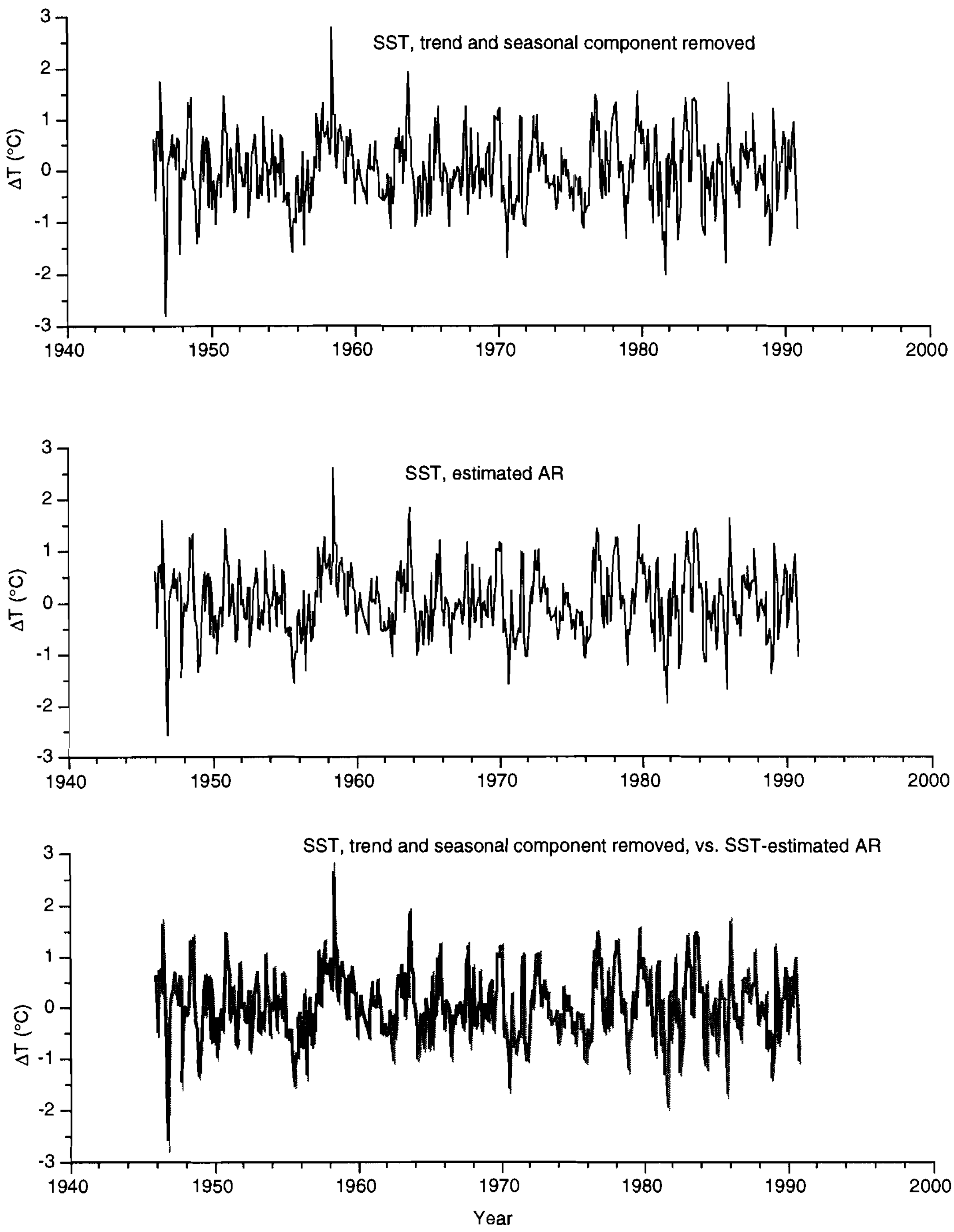

Fig. 8: California Current SST time series at 36-38°N: calculation of the AR component from the partial residual series (ΔT; °C). The upper panel shows the original series with the trend and seasonal component removed; the middle panel shows the estimated AR components; and the bottom panel shows the estimated AR component versus the original series with the trend and seasonal component removed.

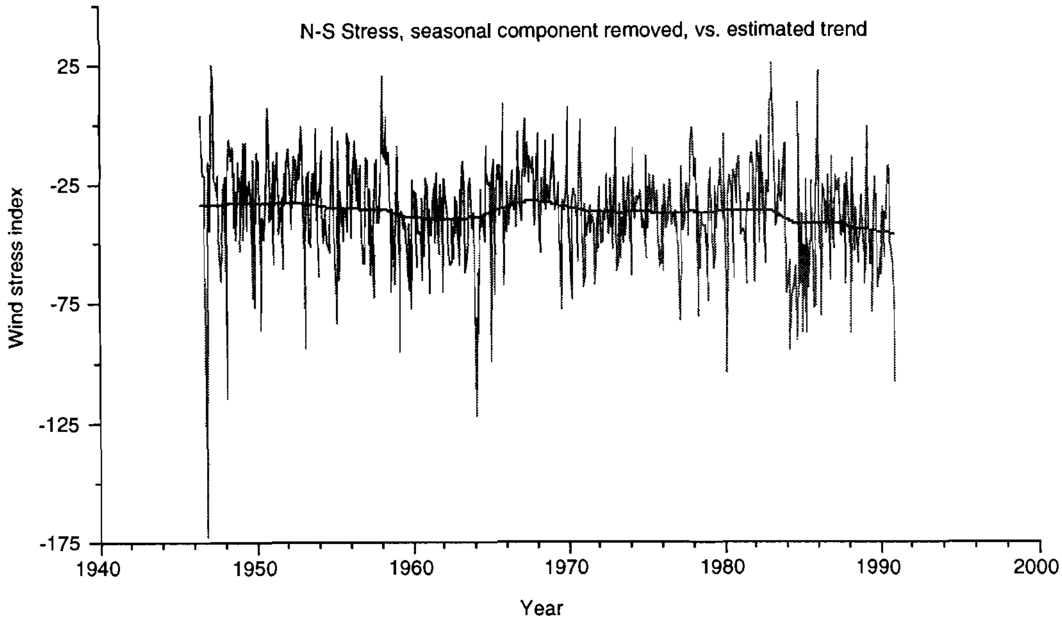

Fig. 9: California Current north-south wind stress time series at 36-38°N: calculation of the trend from the partial residuals. The panel shows the trend versus the original series minus the estimated seasonal component.

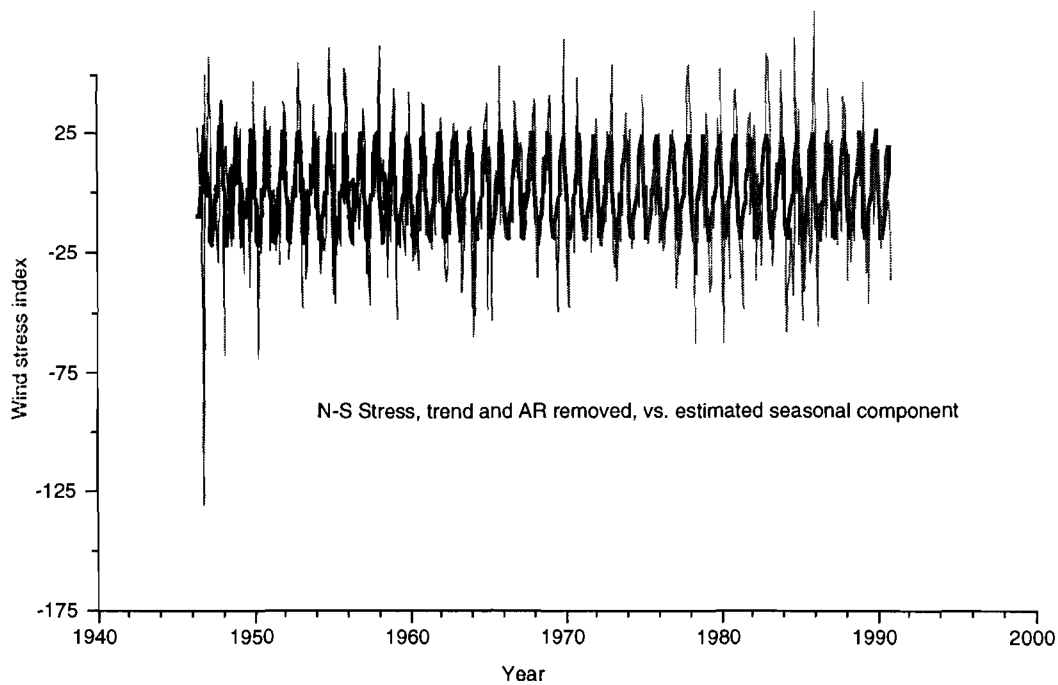

Fig. 10: California Current north-south wind stress time series at 36-38°N: calculation of the seasonal component from the partial residual series. The panel shows the estimated seasonal component versus the original series, with the trend and AR components removed.

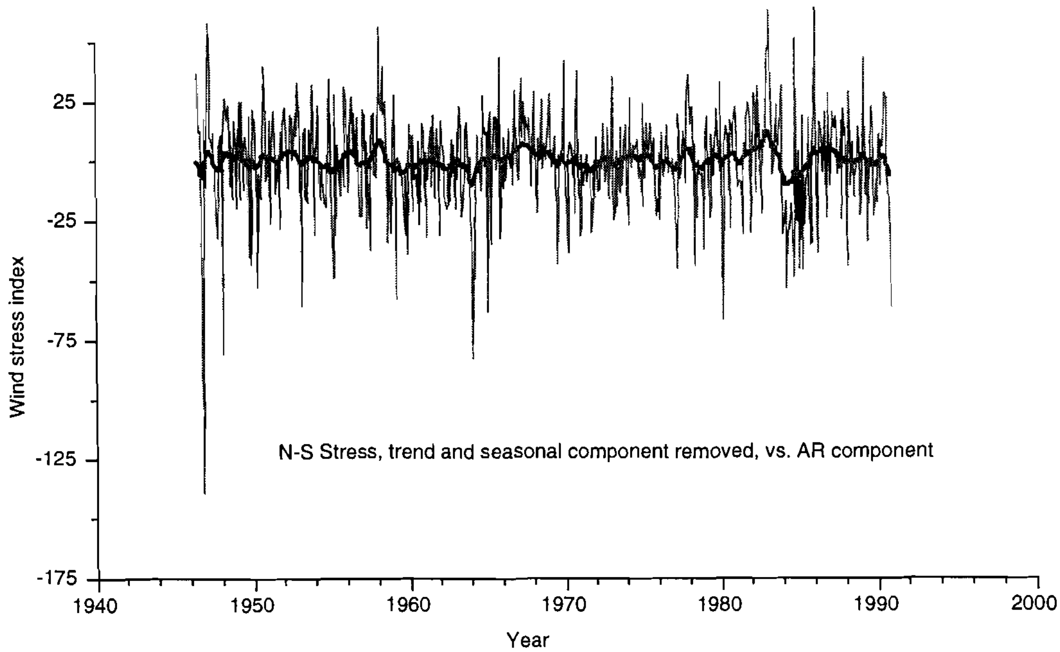

Fig. 11: California Current north-south wind stress time series at 36-38°N: calculation of the AR component from the partial residual series. The panel shows the estimated AR component versus the original series with the trend and seasonal components removed.

APPENDIX A: STATE-SPACE DECOMPOSITION OF TIME SERIES

The linear state-space model that is amenable to the Kalman filter takes the form:

$$y_t = A_t x_t + \upsilon_t \qquad (28a)$$

$$x_t = \Phi x_{t-1} + \omega_t \qquad (28b)$$

where the *observation equation* (Eq. 28a) has y_t a qx1-vector of the observed data (in this case $q=1$), A_t is a qxp matrix which relates the data to the unobserved components x_t, which is a vector of dimension px1, and ν_t is a qx1-vector of independent, identically distributed gaussian random variables with $E\nu_t = 0$ and noise covariance matrix:

$$R = E\left(\upsilon_t \upsilon_t^{'}\right) \qquad (29)$$

The evolution of the unobserved components or states x_t is governed by the initial value x_0 and the *state equation* (Eq. 28b). The matrix $\mathbf{\Phi}$ is a *pxp transition matrix* and the *p*x1-vector ω_t is another independent, identically distributed gaussian random variable with $E(\omega_t) = 0$ and:

$$Q = E(\omega_t \omega_t^{'}) \tag{30}$$

The specification of the model is completed by assuming that X_0 is also gaussian with $E(x_0) = \mu$ and:

$$\Sigma = E(x_0 - \mu)(x_0 - \mu)^{'} \tag{31}$$

See Shumway (1988, Section 3.4) for further details on the state-space model. Kitagawa and Gersch (1984) show how to put the smoothness priors assumptions of Equations 17-19 into state-space form. The model for k=1, and with a first order autoregression will be given. The model for other values follows analogously. The vector y_t is a scalar, the observed value of the time series at time t. The state vector x_t is of dimension 13 and is of the form:

$$x_t^{'} = (T_t, S_t, \ldots, S_{t-11}, I_t) \tag{32}$$

and the transition matrix $\mathbf{\Phi}$ is given by

$$\begin{pmatrix} 1 & 0 & 0 & \ldots & 0 & 0 \\ 0 & -1 & -1 & \ldots & -1 & 0 \\ 0 & 1 & 0 & \ldots & 0 & 0 \\ 0 & 0 & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 1 & 0 \\ 0 & 0 & 0 & \ldots & 0 & \phi \end{pmatrix} \tag{33}$$

where ϕ is the autoregressive parameter which is to be estimated. The observation matrix (from Eq. 13) is given by :

$$A = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{34}$$

The specification is complete by setting the observation error covariance matrix equal to $R = \sigma^2{}_e$ and by setting the state noise covariance matrix equal to:

$$\begin{pmatrix} \sigma^2{}_T & 0 & 0 & \ldots & 0 & 0 \\ 0 & \sigma^2{}_S & 0 & \ldots & 0 & 0 \\ 0 & 0 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 0 & \sigma^2{}_I \end{pmatrix} \tag{35}$$

For given values of the vector of parameters $\Theta = (\phi, \sigma^2_T, \sigma^2_S, \sigma^2_I, \sigma^2_e)$, the minimum mean-square-error estimates of each of the components of the state vector can be estimated using the Kalman filter and smoother. A particularly efficient form of the algorithm was developed independently by Ansley and Kohn (1985, 1990), Kohn and Ansley (1987) and De Jong (1989, 1990, 1991). Both algorithms include the case where $\Sigma \to \infty$, a diffuse or noninformative prior (see above references).

Let $X_{t|\tau}$ denote the expected value of the state vector given the data up to and including time τ, let $P_{t|\tau}$ denote the covariance matrix of the state vector conditional on the data up to and including time τ. Let r_t be a vector of dimension p, and R_t a pxp matrix. Then the filter and smoothing steps proceed as follows:

FILTERING:
Initialize:

$$\begin{aligned} x_0 &= \mu \\ P_0 &= \Sigma \end{aligned} \tag{36}$$

Iterate for t=1,T:

$$\begin{aligned} e_t &= y_t - Ax_{t/t-1} \\ D_t &= AP_{t/t-1}A + R \\ K_t &= \Phi P_{t/t-1}A' D_t^{-1} \\ x_{t+1/t} &= \Phi x_{t/t-1} + K_t e_t \\ L_t &= \Phi - K_t A \\ P_{t+1/t} &= \Phi P_{t/t-1} L_t' + Q \end{aligned} \tag{37}$$

SMOOTHING
Initialize:

$$\begin{aligned} r_T &= 0 \\ R_T &= 0 \end{aligned} \tag{38}$$

Iterate for t=T-1,0:

$$\begin{aligned} r_{t-1} &= A' D_t^{-1} e_t + L_t' r_t \\ R_{t-1} &= A' D_t^{-1} A + L_t' R_t L_t \\ x_{t/T} &= x_{t/t-1} + P_{t/t-1} r_{t-1} \\ P_{t/T} &= P_{t/t-1} + P_{t/t-1} R_{t-1} P_{t/t-1} \end{aligned} \tag{39}$$

The log-likelihood L(Y;Θ) given all the data Y and the parameter vector Θ is given by (see for example Shumway, 1988, page 178):

$$\ln L(Y;\Theta) = -\frac{1}{2}\sum_{t=1}^{T} \ln|D_t| - \frac{1}{2}\sum_{t=1}^{T} e_t' D_t^{-1} e_t \tag{40}$$

In order to use the EM algorithm (Dempster *et al.*, 1977) it is necessary to derive the complete data likelihood; here the components x_t are viewed as unobserved or "missing". After some manipulation, this can be shown to be (Shumway 1988, page 179):

$$\begin{aligned}
&-\frac{1}{2}\ln|\Sigma|-\frac{1}{2}tr\left\{\Sigma^{-1}\left[P_{0/T}+(x_{0/T}-\mu)(x_{0/T}-\mu)'\right]\right\}\\
&-\frac{T}{2}|\ln Q|\\
&-\frac{1}{2}tr\left\{Q^{-1}\left[S_t(0)-S_t(1)\Phi'-\Phi S_t(1)'+\Phi S_{t-1}\Phi'\right]\right\}\\
&-\frac{T}{2}\ln|R|\\
&-\frac{1}{2}tr\left\{R^{-1}\sum_{t=1}^{T}\left[(y_t-Ax_{t/T})(y_t-Ax_{t/T})'+AP_{t/T}A'\right]\right\}
\end{aligned} \quad (41)$$

where the terms $S_t(0)$, $S_t(1)$, and $S_{t-1}(0)$ are defined as:

$$\begin{aligned}
S_t(0)&=\sum_{t=1}^{T}\left(P_{t/T}+x_{t/T}x_{t/T}'\right)\\
S_{t-1}(0)&=\sum_{t=0}^{T-1}\left(P_{t-1/T}+x_{t/T}x_{t/T}'\right)\\
S_t(1)&=\sum_{t=1}^{T}\left(P_{t,t-1/T}+x_{t/T}x_{t-1/T}'\right)
\end{aligned} \quad (42)$$

and:

$$P_{t,t-1/T}=E\left[\left(x_t-x_{t/T}\right)\left(x_{t-1}-x_{t-1/T}\right)'/y_1,y_2,\ldots,y_T\right] \quad (43)$$

A recursion for $P_{t,t-1|T}$ is given in Shumway and Stoffer (1982) and De Jong (1990). The complete data likelihood is maximized by setting:

$$\begin{aligned}
\Phi&=S_t(1)\left[S_{t-1}(0)\right]^{-1}\\
Q&=T^{-1}\left[S_t(0)-S_t(1)\Phi'-\Phi S_t(1)'+\Phi S_{t-1}(0)\Phi'\right]\\
R&=T^{-1}\sum_{t=1}^{T}\left[\left(y_t-Ax_{t/T}\right)\left(y_t-Ax_{t/T}\right)'+AP_{t/T}A'\right]
\end{aligned} \quad (44)$$

In the model of this paper, since most of $\mathbf{\Phi}$ is fixed, the new estimate of $\mathbf{\Phi}$ is the (13,13) element of $\mathbf{\Phi}$, and since most of Q is fixed to zero, the new estimates of Q are the (1,1), (2,2) and (13,13) elements of the above matrix, with all other elements set to zero. Here R is a scalar. The complete algorithm then consists to

1. Choose initial values for x_0, $\mathbf{\Sigma}$ and $\mathbf{\Phi}$;
2. Calculate the Kalman filter and smoother for the given parameter values;
3. Update the parameters by Equations 42;
4. Iterate until convergence.

The Kalman smoothers, calculated at the final parameter estimates, produce the component time series.

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