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Asymmetric filters for analyzing time series of atmospheric constituent data

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ABSTRACT

We consider the design of asymmetric digital filters for extracting estimates of long-term trends and seasonal cycles from monthly mean values of atmospheric constituent data. It is possible to reduce the amount of data lost from the end of the records at the expense of a relatively small increase in the mean-square error in the estimated signals.

1. Introduction

Digital filtering provides a convenient framework for describing many types of analysis performed on time series records of atmospheric composition such as estimating long-term trends or changes in seasonal cycles (Cleveland et al., 1983; Enting, 1987a, b). It includes, as special cases, several other techniques that have previously been used in the analysis of atmospheric constituent data, e.g., spline smoothing (Enting, 1987c) and complex demodulation as used by Thompson et al. (1986) (see Enting, 1987a).

The design of digital filters involves a number of trade-offs such as resolution versus variance, resolution versus length of filter and bias versus variance. There are a variety of standard techniques for designing digital filters in order to optimize various criteria (Hamming, 1977). A particularly important criterion, which forms the basis of the Wiener (1949) approach, is to minimize the mean-square error in the signal that is extracted by the filter. When the signal and noise bands overlap, this optimization procedure gives biased estimates of the signal. Much of this bias can be removed (at the expense of increased variance) by following Bloomfield (1976) and rescaling all the filter coefficients. Small changes of this type will give only second-order changes in the mean-square error, because the mean-square error is a quadratic function of the filter coefficients.

In previous applications of digital filtering to atmospheric constituent records, symmetric filters have generally been used. This implies an inability to obtain estimates near the ends of records. There are several reasons for wishing to remove this limitation. In particular, analysing the results of ongoing observational programs in as near as possible to real time can provide a measure of quality control on the observations and allow the timely implementation of supplementary measurement programs if possible new phenomena are identified. Furthermore, while our discussion concentrates on filters that reduce data loss from the most recent part of the record, our filters can be used in a time-reversed manner to obtain estimates from near the beginnings of records.

2. Wiener and Kalman filtering

There are two standard approaches to constructing asymmetric filters: Wiener filtering and Kalman filtering. Kalman filtering (Anderson and Moore, 1979) is based on a state-space representation of the time series (Akaike, 1974). This approach is of some appeal in atmospheric constituent studies where we are often seeking to express a time series as a sum of a seasonal part, a long term variation and some "noise" term. It has the additional advantage of being applicable to more general non-stationary processes which are beyond the scope of this note. However, the Kalman filtering approach requires that these states be further subdivided until the evolution can be regarded as a first-order vector auto-regressive process. A lack of appropriate state-space models and a lack of information about the sensitivity of the Kalman filter formalism to departures from an assumed model preclude the general application of Kalman filtering to atmospheric constituent records without extensive further analysis. Kalman filtering has been applied to the analysis of CO_2 data by Surendran and Mulholland (1987).

Wiener filtering (Wiener, 1949) uses a frequency domain representation of a continuous stationary time series extending infinitely far into the past. Priestley (1981) gives the discrete time form. Zadeh and Ragazzini (1950) generalized the Wiener formalism to allow non-stationarity via polynomial variations and also allowed limits on the range of times required. Our approach can be regarded as a combination of these two generalizations. However we by-pass the analytic factorization used in these formalisms and treat the filter-design calculation as a finite-dimensional optimization problem defined in the terms of the filter coefficients.

3. Filter design

As emphasized in our previous studies (Enting, 1986, 1987a, b, c), any statistical analysis implies some statistical model of the time series. Following Zadeh and Ragazzini (1950) we shall assume that the observed time series, $z(t)$, can be expressed as

$$z(t) = p(t) + y(t) + \varepsilon(t), \tag{1}$$

where $p(t)$ is a polynomial, $y(t)$ is a statistically stationary signal and $\varepsilon(t)$ is a statistically stationary noise contribution that is independent of $y(t)$. In order to design a filter to analyse such records, we must make assumptions about the spectral density functions $f_y(\theta)$ and $f_\varepsilon(\theta)$ for $y(t)$ and $\varepsilon(t)$ and also the degree, J, of the polynomial $p(t)$. There are two distinct cases of interest in atmospheric constituent studies: low-pass filtering and band-pass filtering. In the former case we are seeking an estimate of the sum $p(t) + y(t)$; we require that the filter pass any polynomial variation exactly and act on the residual $y(t) + \varepsilon(t)$ so as to minimize the mean-square error in the estimate of $y(t)$. In the band-pass filtering case we are seeking an estimate of $y(t)$. We require a filter that completely removes any polynomial component $p(t)$ and acts on the residual $y(t) + \varepsilon(t)$ so as to minimize the mean-square error in the estimate of $y(t)$. The requirement that polynomials of degree J be passed or removed exactly involves $J + 1$ constraints on the filter. These can be expressed in terms of derivatives of the transfer function (Brillinger, 1965) or directly in terms of the coefficients (eqs. (5), (6) below).

A filter with coefficients c_k is characterized by its transfer function $H(\theta)$ where

$$H(\theta) = \sum_k c_k \exp(ik\theta). \tag{2}$$

Summations over k as in (2) are taken over the range $M \leqslant k \leqslant N$. In this note we consider only $N > 0$ and $M < 0$. The use of $M > 0$ would correspond to a "prediction" problem, i.e., estimating future levels of the signal given past observations. Our numerical examples will consider monthly data containing an annual cycle. We shall use $N = 24$ so as to span several cycles and consider the effect of varying M over the range -24 to -1. $|M|$ is the number of months "lost" from the recent end of a record in that the filter will not give a signal estimate for these last $|M|$ months.

We apply low-pass filters to time series data, z_k, to obtain estimates of the form:

$$p(t_j) + \hat{y}(t_j) = \sum_k c_k z(t_{j-k}), \tag{3a}$$

and band-pass filters to obtain estimates of the form

$$\hat{y}(t_j) = \sum_k c_k z(t_{j-k}). \tag{3b}$$

For the stationary component $y(t) + \varepsilon(t)$, the mean-square error in $\hat{y}(t)$, the estimate of y, is

$$\Phi = E[(\hat{y} - y)^2] = \Phi_{\text{bias}} + \Phi_{\text{var}}, \tag{4a}$$

where

$$\Phi_{\text{bias}} = \int_{-\pi}^{\pi} |1 - H(\theta)|^2 f_y(\theta)\,d\theta, \tag{4b}$$

$$\Phi_{\text{var}} = \int_{-\pi}^{\pi} |H(\theta)|^2 f_\varepsilon(\theta)\,d\theta. \tag{4c}$$

Here, Φ_{bias} represents the bias in $\hat{y}$ due to the filter failing to pass the signal exactly and Φ_{var} represents the variance in the estimate due to the filter failing to completely remove the "noise" contribution. The expression for the mean square error is often expressed in the time domain, using the autocorrelation functions instead of spectral densities (see for example Levinson, 1947). The frequency domain form given above is obtained from expression (10.3.10) of Priestly (1981) by changing the time origin and regrouping terms. The expression above can also be obtained by integrating expression (7.12) of Yaglom (1962).

The filter coefficients c_k for the two cases described above are obtained by minimizing Φ with respect to the c_k, subject to the constraints

$$\sum_k c_k k^m = 0, \quad m = 1 \text{ to } J, \tag{5}$$

$$\sum_k c_k = 1 \quad \text{for the "low-pass" case,} \tag{6a}$$

or

$$\sum_k c_k = 0 \quad \text{for the "band-pass" case,} \tag{6b}$$

which ensure that Jth-order polynomials are passed or stopped as required.

The constrained minimization is performed by introducing $J + 1$ Lagrange multipliers λ_m. This is a discrete-time version of the approach used by Zadeh and Ragazzini (1950). The resulting equations are linear in both the c_k and λ_m. In the examples considered below, rounding errors of about 2×10^{-7} lead to ill-conditioning of the equations when J was increased to 5. No such problems were apparent for smaller J values.

4. Filters for use in atmospheric constituent studies

We have used the formalism described above as a basis for designing filters for use in studies of monthly mean atmospheric constituent data. The analysis shows that if the signal and noise bands overlap then the optimal filter will be biased. The optimal amount of bias at a particular frequency depends on the signal-to-noise ratio at that frequency. Our basic model spectrum had a low frequency peak and a peak of the same amplitude at a frequency of 1 cycle per year. In some cases, it may be appropriate to use filters that extract harmonics as well as the fundamental (see for example Enting, 1987a, b). To these peaks was added a "white-noise" component with a power density of 10% of the peak heights. When designing the low-pass filters, this white-noise component was modified to go to zero at zero frequency. This was required to make the optimal filter consistent with our constraints of passing polynomials exactly, i.e., to remove the ambiguity as to whether the zero frequency component should be part of the signal or the noise. (The ill-conditioning that occurs for higher-order polynomials is a reflection of the same ambiguity effectively occurring for a range of frequencies.) Having $f_\varepsilon(\theta)$ go to zero at zero frequency leads to a filter that is unbiased at zero frequency. Similar modifications to the noise spectrum were tried when designing the band-pass filters but, because no exact constraint was applied away from zero frequency, not all the bias was removed. As noted above, the simplest way to produce a filter that is unbiased at some specified frequency seems to be to design an optimal (biased) filter and then rescale it. Thus the filter designs analysed here are based on the idealized spectra shown in Figs. 1a and 1b.

We have implemented the minimization procedure described above to obtain specific sets of filter coefficients given piecewise linear representations of $f_\varepsilon(\theta)$ and $f_y(\theta)$. This representation enables us to obtain analytic expressions for the integrals, eqs. (4b, 4c), and their partial derivatives with respect to the c_k. The filter coefficients c_k were restricted to the range $M \leqslant k \leqslant N$. Figs. 2a and 2b consider the case of $J = 2$ (i.e. 2nd order polynomials treated exactly), $N = 24$. M is allowed to range from -24 to -1 to show the effect of allowing asymmetry in the filter. The symmetry of the equations ensures that the $M = -N$ case will in fact be symmetric with $c_k = c_{-k}$. The figures show the mean-square error, Φ and the "bias" and "variance" contributions, Φ_{bias} and Φ_{var}. It will be seen that restricting M

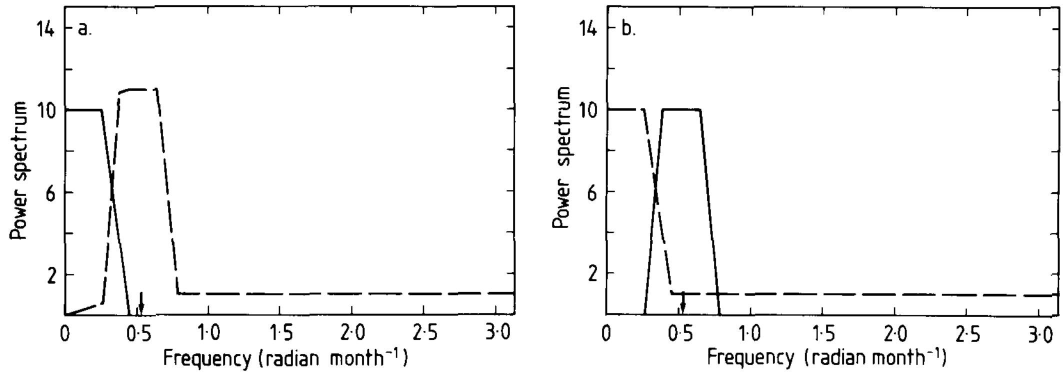

Fig. 1. Idealized power spectra used to define filters with the ordinates in arbitrary units. Solid curve is signal spectrum $f_y(\theta)$ and dashed curve is noise spectrum $f_\varepsilon(\theta)$. Frequency units are radian month^{-1}. The arrow at $\pi/6$ indicates the 12-month period. (a) Low frequency signal case used to specify low-pass filter. The annual peak is part of the "noise" term to be removed. (b) "Seasonal peak" case used to define band-pass filter. The slowly varying component is part of the "noise" to be removed.

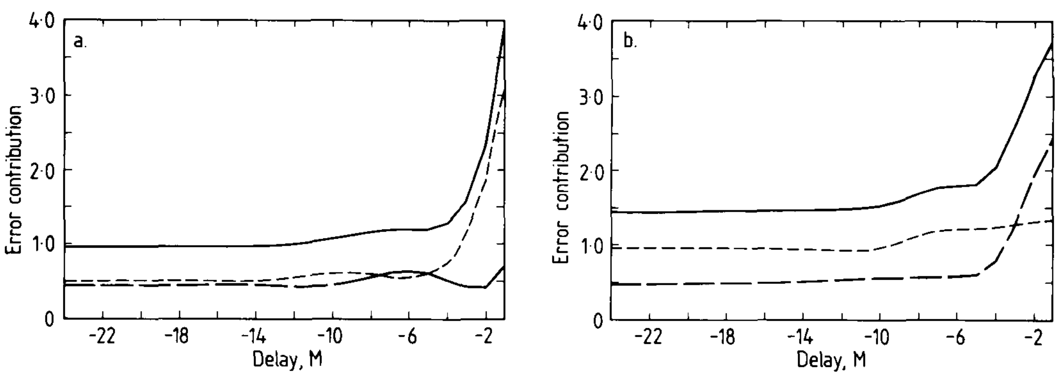

Fig. 2. Behaviour of filters optimized for spectra 1a, 1b respectively subject to the constraint of treating second order polynomials exactly and only using coefficients c_k with $M \leqslant k \leqslant 24$. The quantities shown are the mean square error Φ, (solid curve) the bias Φ_{bias} due to distortion of the signal (long dashes) and the variance Φ_{var} due to failure to suppress the noise (short dashes), each plotted as a function of M, the lower cutoff of the filters. Each is expressed in the same arbitrary units as are used for the power spectra. (a) For the low-pass filter derived using the spectra in Fig. 1a. (b) For the band-pass filter derived using the spectra in Fig. 1b.

gives very little degradation in the filtering properties until M is restricted to be greater than about -6. Our results for $M > -6$ suggest that when a Kalman filter approach is used, lagged estimates could be desirable. The conventional use of Kalman filtering corresponds to $M = 0$.

The coefficients for the two cases with $J = 2$, $N = 24$ and $M = -6$ are listed in Tables 1, 2. The respective transfer functions are plotted in Figs. 3a and 3b. The solid line shows the real part of the transfer function and the dashed line shows the imaginary part. Since the filter coefficients are real, $\text{Re}[H(\theta)]$ will be an even function of θ and $\text{Im}[H(\theta)]$ will be an odd function of θ. The dotted line shows the transfer function of the optimal filter for the unconstrained case with $M \to -\infty$, $N \to \infty$. This optimal filter has the transfer function (Yaglom, 1962, Eq. 5.29)

$$H(\theta)_{\text{opt}} = f_y(\theta)/(f_y(\theta) + f_\varepsilon(\theta)). \tag{7}$$

The presence of non-zero imaginary parts in the transfer functions of asymmetric filters means

Table 1. *Coefficients of low-pass filter whose transfer function is shown in Fig. 3a*

c_{-6} to c_1	c_2 to c_9	c_{10} to c_{17}	c_{18} to c_{24}
0.0195437	0.0991627	0.0019535	−0.0015664
0.0547763	0.0916603	−0.0034339	0.0010518
0.0724535	0.0790778	−0.0067296	0.0041404
0.0808757	0.0634538	−0.0081130	0.0064984
0.0864676	0.0471996	−0.0079577	0.0055657
0.0922081	0.0322411	−0.0068314	−0.0022196
0.0977541	0.0196141	−0.0052867	−0.0203996
0.1008513	0.0095689	−0.0035804	

Table 2. *Coefficients of the "optimal" band-pass filter whose transfer function is shown in Fig. 3b. If the filter is required to be unbiased for periods of one year, then these coefficients should be multiplied by 1.1611*

c_{-6} to c_1	c_2 to c_9	c_{10} to c_{17}	c_{18} to c_{24}
−0.0380936	0.0553766	0.0252247	0.0156365
−0.0904725	−0.0184901	0.0188898	0.0066558
−0.0766125	−0.0768208	0.0038185	−0.0066538
−0.0142243	−0.1023772	−0.0089688	−0.0164509
0.0649096	−0.0924411	−0.0121536	−0.0154090
0.1265904	−0.0579016	−0.0051437	0.0003969
0.1465702	−0.0168808	0.0066482	0.0305011
0.1186437	0.0137744	0.0154579	

that there will be phase errors in the estimated signals. The effect of such errors on an estimated signal is one of the contributions to the bias term which can be written as

$$\Phi_{\text{bias}} = \int_{-\pi}^{\pi} \{[1 - \text{Re}(H(\theta))]^2 f_y(\theta) + [\text{Im}(H(\theta))]^2 f_y(\theta)\}\,d\theta. \tag{8}$$

The small variation in Φ_{bias} for $M \leqslant -6$ shows that such phase errors are of relatively little importance in this range.

The transfer functions show some of the trade-offs involved in using asymmetric filters, particularly in the band-pass case. The filter is biased in that the response function is less than 1 over all of the pass-band. As noted above, modifying the "white-noise" component so that the optimal filter was unbiased gave little improvement in the amount of bias involved in the finite-length filters considered here. In contrast, our low-pass filter is unbiased at zero frequency by virtue of constraint (6a).

For many purposes, such as comparison with models, biased estimates are inconvenient even if they do have the minimum mean square error. If approximately unbiased band-pass filters are required, then a simple rescaling can be used. Multiplying all coefficients on Table 2 by 1.1611 gives a filter whose transfer function is close to 1 for frequencies around 1 cycle per year.

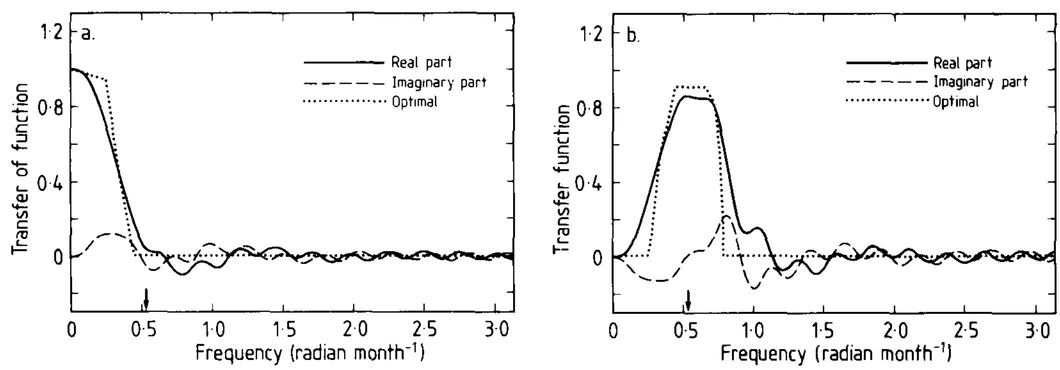

Fig. 3. Transfer functions of the filters constrained to treat second order polynomials exactly with coefficients c_k from the range $-6 \leqslant k \leqslant 24$. Solid curve is the real part of $H(\theta)$ and dashed curve is the imaginary part. The dotted curve is the transfer function for the optimal filter in the case of no constraints on either length or effect on polynomials. The arrow at $\pi/6$ indicates the 12-month period. (a) Low-pass filter obtained assuming the spectra of Fig. 1a. (b) Band-pass filter obtained assuming the spectra of Fig. 1b.

5. Summary

The analysis presented in this note shows the general possibility of obtaining asymmetric filters suitable for analysing time series of atmospheric constituent data, thus making it possible to estimate signals near the ends of available records. We have obtained specific sets of filter coefficients, suitable for analysing time series of monthly mean data containing a seasonal cycle, an approximately white noise contribution and a long-term trend consisting of a stationary part and a possible polynomial contribution. The two filters are suitable for (a) extracting the long-term trend in the presence of the noise and the seasonal cycle and (b) extracting the seasonal cycle in the presence of the noise and the long-term trend. For many applications, the rescaled form of the band-pass filter would be appropriate. While these filters have optimized for specific idealized spectra, they will be near-optimal for qualitatively similar spectra. Thus the coefficients presented in Tables 1, 2 can be used for analysing a wide range of atmospheric constituent data. In most cases little improvement will be obtained by recalculating the filter coefficients using the power spectrum estimated from the particular time series being studied. However the actual spectrum should be used firstly in confirming whether the assumed division into long-term trend and seasonal cycle is appropriate (Thompson et al., 1986; Enting, 1986, 1987a, b) and secondly in using expression (4) to obtain the mean square error in the estimated signal. This approach is currently being applied in the analysis of data from the observational programs conducted by the CSIRO Division of Atmospheric Research.

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