7 Detrending

Trend in a time series is a slow, gradual change in some property of the series over the whole interval under investigation. Trend is sometimes loosely defined as a long term change in the mean (Figure 7.1), but can also refer to change in other statistical properties. For example, treering series of measured ring width frequently have a trend in variance as well as mean (Figure 7.2). Traditionally, seasonal or periodic components, and irregular fluctuations, and the various parts were studied separately. Modern analysis techniques frequently treat the series without such routine decomposition, but separate consideration of trend is still often required. Detrending is the statistical or mathematical operation of removing trend from the series. Detrending is often applied to remove a feature thought to distort or obscure the relationships of interest. In climatology, for example, a temperature trend due to urban warming might obscure a relationship between cloudiness and air temperature. Detrending is also sometimes used as a preprocessing step to prepare time series for analysis by methods that assume stationarity. Many alternative methods are available for detrending. Simple linear trend in mean can be removed by subtracting a least-squares-fit straight line. More complicated trends might require different procedures. For example, the cubic smoothing spline is commonly used in dendrochronology to fit and remove ring-width trend that might not be linear, or not even monotonically increasing or decreasing over time. In studying and removing trend, it is important to understand the effect of detrending on the spectral properties of the time series. This effect can be summarized by the frequency response of the detrending function.

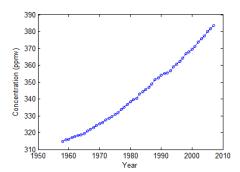


Figure 7.1. Trend in mean. A strong trend dominates the December atmospheric CO2 concentration at Mauna Loa, Hawaii, 1958-2007. Source: http://cdiac.ornl.gov/ftp/trends/co2/maunaloa.co2

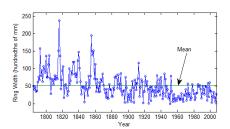


Figure 7.2. Trend in mean and variance. Ring widths from a Douglas-fir tree in Jemez Mountains, New Mexico, 1785-2007. Both mean ring width and variance of ring width decline with age of tree.

7.1 Identifying trend

Identification of trend in a time series is subjective because trend cannot be unequivocally distinguished from low frequency fluctuations. What looks like trend in a short segment of a time series segment often proves to be a low-frequency fluctuation – perhaps part of a cycle -- in the longer series. By extension, we can view the entire observed time series as a segment of an unknown infinitely long series, and cannot be sure that an observed change in mean over that segment is not part of some low-frequency fluctuation imparted by a stationary process.

Sometimes knowledge of the physical system helps in identifying trend. For example, a decrease of ring width of a tree with time is expected partly on geometrical grounds: the annual increment of wood is being laid down on an ever-increasing circumference. If the volume of wood produced annually levels off as the tree ages, ring width would still be expected to decline.

A hypothetical "age curve" in ring width can be computed assuming the cross-sectional area of wood added each year is constant (Figure 7.3). Such a conceptual model was used in dendrochronology as justification for "modified negative exponential" detrending (Fritts 1976).

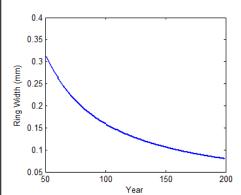


Figure 7.3. Mathematical form of expected ring width as function of time assuming constant increment of cross-sectional area.

If a physical basis is lacking, we need to rely on statistical methods to quantify trend. Statistical methods can help distinguish trend from other variations.

A simple statistical technique of identifying linear trend is to regress the observed time series against time and test the estimated slope coefficient of the regression equation for significance (Haan 2002). The null hypothesis is that the slope coefficient is zero (no linear trend) and the alternative hypothesis is that the slope differs from zero. A t-test applied to the estimated slope coefficient will indicate rejection or acceptance of the null hypothesis. This approach can be extended to multiple linear regression for trends in mean more complex

than simple linear trend (Haan 2002). Nonparametric tests are also available for identifying trend. The Mann-Kendall test is one such test commonly used in climatology and hydrology (Salas 1993).

The frequency domain is particularly useful here. Granger and Hatanaka (1964 p. 130) give some insight into spectral interpretation of trend. They conclude that we are unable to differentiate between a true trend and a very low frequency fluctuation, and give the following advice:

It has been found useful by the author to consider as "trend" in a sample of size n all frequencies less than 1/(2n) as these will all be monotonic increasing if the phase is zero, but it must be emphasized that this is an arbitrary rule. It may also be noted that it is impossible to test whether a series is stationary or not, given only a finite sample as any apparent trend in mean *could* arise from an extremely low frequency fluctuation.

If we apply the above reasoning to a 500-year tree-ring series, we would say that variations with period longer than twice the sample size, or 1000 years, should be regarded as trend. In another paper, Granger (1966) defines 'trend in mean' as comprising all frequency components whose wavelength exceeds the length of the observed time series. Cook et al. (1990) refer to Granger's (1966) "trend in mean" concept in giving suggestions for detrending tree-ring data:

Given the above definition of trend in mean, another objective criterion for selecting the optimal frequency response of a digital filter is as follows. Select a 50% frequency-response cutoff in years for the filter that equals some large percentage of the series length, n. This is the %n criterion described in Cook (1985). The results of Cook (1985) suggest that the percentage is 67%n to 75%n based on using the cubic smoothing spline as a digital filter. The %n criterion ensures that little low-frequency variance, which is resolvable in the standardized tree rings, will be lost in estimating and removing the growth trend. This criterion also has a bias of sorts because of the stiff character of the low-pass filter estimates of the growth trend. It will not necessarily guarantee and, in fact, will rarely possess any kind of optimal goodness-of-fit.

7.2 Fitting the trend

Four alternative approaches to detrending are: 1) first differencing, 2) curve-fitting, 3) digital filtering and 4) piecewise polynomials. This section is weighted heavily toward the piecewise polynomials approach, which is widely used in dendrochronology.

First differencing. A time series that is non-stationary in mean (e.g., trend in mean) can be made stationary by taking the first difference. The first-difference is the time series at time t minus the series at time t-1:

$$w_{t} = x_{t} - x_{t-1} \tag{1}$$

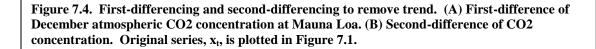
where x_i is the original time series and w_i is the first-differenced series. If the series is nonstationarity in not just the mean but in the rate of change of the mean (the slope), stationarity can be induced by taking the second difference, or the first difference of the first difference:

$$u_{\cdot} = w_{\cdot} - w_{\cdot, \cdot} \tag{2}$$

Higher orders of differencing can likewise be applied. First differencing has been applied in hydrology in the context of ARIMA (Autoregressive-Integrated-Moving-Average) modeling of streamflow series (Salas et al. 1980). As with any detrending method, first differencing can be expected to strongly attenuate the variance at the lowest frequencies in a time series. Salas et al. (1980) report that first differencing can be problematic in hydrology because it tends to introduce spurious high-frequency variation.

Anderson (1975) describes differencing as a way to remove nonstationarity from time series in general. According to Anderson (1975), each successive differencing will decrease the variance of the series, but at some point, higher-order differencing will lead to an increase in variance. When variance increases, the series has been *over-differenced*. First-differencing is most applicable with a linear trend in mean.

First-differencing can be illustrated with the trend-dominated Mauna Loa CO₂ time series plotted in Figure 7.1. In this case, first-difference fails to remove the trend. The first-differenced series is positive at all times, reflecting the accelerating rate of increase in the original CO2 curve (Figure 7.4a). Second-differencing appears to remove the trend (Figure 7.4b). The variance, however, increases with second-differencing, suggesting possible over-differencing: standard deviations of the original, first-differenced and second-differenced series are 20.89, 0.60 and 0.68. The huge drop in variance from the original series to the first-differenced series attests to the overwhelming importance of trend to variance of the Mauna Loa CO2 time series.



It is important to recognize that first-differencing implies that all the useful information in the time series is in the change from one observation from next, and that the level of the original series is unimportant. For example, if a time series of ring widths is first-differenced, a change from a very wide tree ring to a moderately wide ring can yield the same "detrended" value as a change from a moderately narrow ring to very narrow ring. First-differencing of ring widths ignores the fact that a year-to-year drop in tree-ring width toward the inner part of the radius or core is more likely attributable to "growth trend" than the same drop toward the outer part of the core.

Curve-fitting. If a time series changes in level gradually over time, it makes sense to summarize trend by some simple function of time itself. A simple and widely used function of time is the least-squares-fit straight line, which assumes linear trend. Simple linear regression is used to fit the model

$$x_{t} = a + bt + e_{t} \tag{3}$$

where x_i is the original time series at time t, a is the regression constant, b is the regression coefficient, and e_i are the regression residuals. The trend is then described by

$$\hat{g}_{t} = \hat{a} + \hat{b}t \tag{4}$$

where \hat{g}_i is the fitted trend, \hat{a} is the estimated regression constant, and \hat{b} is the estimated regression coefficient.

While the straight-line method has the virtue of simplicity, the straight line may unrealistic, in restricting the functional form of the trend. Other functions of t (e.g., quadratic) might be better depending on the type of data. Sometimes the mathematical form of the trend function has physical basis. For example, a modified negative exponential curve with conceptual basis in the change of tree-geometry with time has been used to remove the "age trend" from ring-width series (Fritts 1976). The modified exponential follows the equation

$$\hat{g}_{t} = \hat{a}e^{-\hat{b}t} + \hat{k} \tag{5}$$

where the coefficients, \hat{a} , \hat{b} , and \hat{k} are estimated such that the sum of square of differences of the smooth curve \hat{g} , and the original time series is minimized.

Ring-width trend alternatively described by a straight line and a modified negative exponential is illustrated in Figure 7.5. The curvature in the time plot of ring width is so slight that the choice of curve makes little difference for this example. At the recent end of the time series, however, the expected ring width according to trend is about 30 percent higher for the modified exponential than for the straight line.

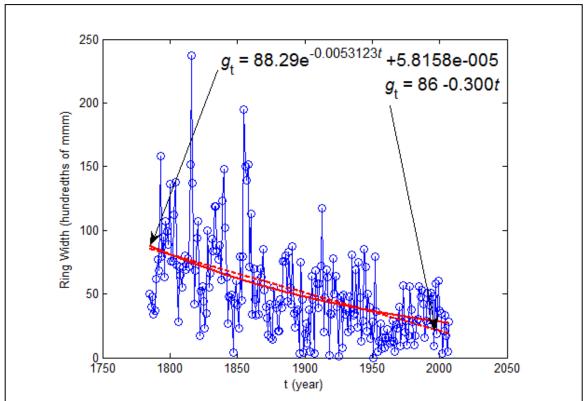


Figure 7.5. Trend in measured tree-ring width fit by straight line and modified negative exponential curve. Tree-ring series is same series described in caption to Figure 7.2. Time variable (year) was shifted to begin with 1 before estimating parameters annotated on figure.

Digital filtering. Another procedure for dealing with trend is to describe the trend as a linearly filtered version of the original series. The original series is converted to a smooth "trend line" by weighting the individual observations, x_i :

$$g_{t} = \sum_{r=-q}^{s} a_{r} x_{t+r} \tag{6}$$

where $\{a_r\}$ is a set of filter weights (summing to 1), and g_r is the smooth trend line. The weights are often symmetric, with s = q and $a_j = a_{-j}$. If the weights are all equal, the filter is a simple moving average, which generally is <u>not</u> recommended for measuring trend (Chatfield 1975). Preferable is a symmetric filter with weights decreasing from the central weight.

Piecewise polynomials. An alternative to fitting a curve to the entire time series (curve fitting) is to fit polynomials of time to different parts of the time series. Polynomials used this way are called piecewise polynomials. The *cubic smoothing spline* is a piecewise polynomial of time, *t*, with the following properties:

- The polynomial is cubic (t raised to third power)
- A separate polynomial is fit to every sequence of three points in the series
- The first and second derivatives are continuous at each point
- The "spline parameter" specifies the flexibility and depends on the relative importance given to "smoothness" of the fitted curve, and "closeness of fit", or how close the fitted curve passes to the individual data points

Given the approximate values $y_i = g(x_i) + \varepsilon_i$ of some supposedly smooth function g at data points x_1, \dots, x_N and an estimate δy_i of the standard deviation of y_i , the problem is to recover the smooth function from the data. Let $s(x_i)$ be the spline curve, or the approximation to the smooth function g. Following De Boor (1978, p. 235), the spline curve is derived by minimizing the quantity

$$p\sum_{i=1}^{N} \left[\frac{y_{i} - s(x_{i})}{\delta y_{i}} \right]^{2} + (1 - p) \int_{x_{i}}^{x_{n}} \left[D^{2} s \right]^{2}$$
 (7)

over all functions s for a given *spline parameter*, p, where D^2 s refers to the second derivative of s with respect to time. The first term in (7) is similar to a sum-of-squares of deviations. The second term integrates curvature contributions (second derivative). Minimizing establishes a compromise between staying close to the given data (first term) and obtaining the smoothest possible curve (second term). The choice of p, where p can range from 0 to 1, depends on which of those two goals is given the greater importance. For p = 0, s is the least squares straight-line fit to the data. At the other extreme, p = 1, s is the cubic spline interpolant, and passes through each data point. As p ranges from 0 to 1, the smoothing spline changes from one extreme to the other (Figure 7.6). The term s s allows for differential weighting of data points. Following recommendations of Cook and Peters (1981) we use equal weighting of 1 to all points (this is the default in Matlab).

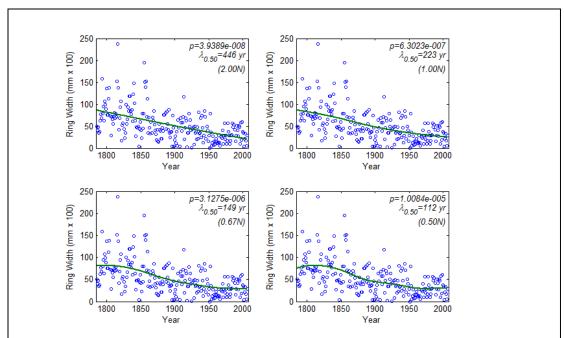


Figure 7.6. Cubic smoothing splines of differing stiffness fit to a time series of tree-ring ring width. Spline parameter is p. Spline has a frequency response of 0.50 at wavelength $\lambda_{0.50}$, which is expressed as a decimal fraction of the series length, N, in parentheses. Spline p for upper left plot is small enough that straight line is approximated.

7.3 Frequency response

The frequency response function describes how a linear system responds to sinusoidal inputs at different frequencies (Chatfield 2004, p. 198). The frequency response function has two components -- the *gain* and the *phase*. The gain at a given frequency describes how the amplitude of a sinusoid at that frequency is damped or amplified by the system. The phase describes how a wave at that frequency is shifted in absolute time.

For a cubic smoothing spline, the phase is zero, such that the "frequency response" merely describes the gain, or the amplitude, of the response function. The input to the "system" in this case is the original time series; the output is the smoothed curve intended to represent the trend. The frequency response measures how strongly the spline curve responds to or "tracks" a periodic component at a given frequency, should the time series have such a component. The amplitude of frequency response at a given frequency is the ratio of the amplitude of the sinusoidal component in the smoothed series (the spline curve) to the amplitude in the original time series.

Relation of frequency response to spline parameter

The cubic smoothing spline has become increasingly popular as a detrending method in dendrochronology because the spline is adaptable and easily applied to a wide range of types of "age trend" or "growth trend" found in tree-ring data. Application of the spline to dendrochronology was first proposed by Cook and Peters (1981), who derived a mathematical relationship between a spline parameter and the frequency response of the spline. Jean-Luc Dupouey (INRA, Forest Ecology and Ecophysiology Unit, Champenoux, France), has pointed out (personal communication) that the spline parameter p is defined somewhat differently in Matlab

Spline Toolbox¹ than in Cook and Peters (1981), and has provided equations that give the correct relationship for use with Matlab.

In terms of the parameter p in equation (7), the frequency response of the spline is given by

$$u(f) = \frac{1}{\left[1 + 12\left(\frac{1-p}{p}\right) \frac{\left(\cos 2\pi f - 1\right)^{2}}{\left(\cos 2\pi f + 2\right)}\right]}$$
(8)

where u(f) is the amplitude of frequency response at frequency f, and p is the spline parameter as defined earlier. A plot of u(f) against f shows the relative response of the spline to hypothetical input variations at different frequencies. For a smoothing spline, this response is higher toward the low-frequency end of the spectrum (Figure 7.7).

Equation (8) can be rearranged with p on the left-hand side to get the spline parameter corresponding to a spline with a desired amplitude of frequency response at a specified frequency:

$$p_{u_0(f_0)} = \frac{1}{\left\{ \left[\left(\frac{1 - u_0(f_0)}{u_0(f_0)} \right) \left(\frac{(\cos 2\pi f_0 + 2)}{12(\cos 2\pi f_0 - 1)^2} \right) \right] + 1 \right\}}$$
(9)

where f_0 is the target frequency, $u_0(f_0)$ is the desired amplitude of response at that frequency, and $p_{u_0(f_0)}$ is the corresponding spline parameter. Cook and Peters (1981) define an "*n*-year spline" as the spline whose frequency response is 50%, or 0.50, at a wavelength of *n* years.

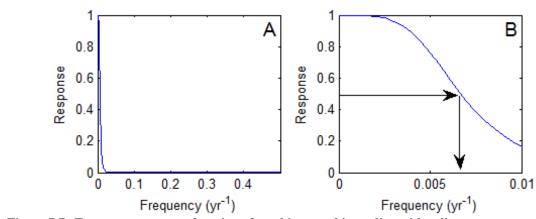


Figure 7.7. Frequency response function of a cubic smoothing spline with spline parameter p=3.1257E-6 as applicable to an annual time series. (A) Full frequency response. (B) Frequency response zoomed to frequency range 0 to 0.01 (periods ∞ to 100 years). Response rises above 0.2 at a wavelength slightly longer than 100 years, and reaches 0.5 at a wavelength of about 149 years (frequency of 0.0067). Plot of full response emphasizes that this spline tracks only low frequencies.

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¹ Spline Toolbox was discontinued with release 2010b of Matlab. Spline functions are now available from the Curve Fitting Toolbox.

Equation (9) can be used to compute the required spline parameter for the "n-year spline" by setting $u_0(f_0) = 0.50$, where $f_0 = 1/n$. For example, substitution into equation (9) for the "100-year" spline yields:

$$p = \frac{1}{\left\{ \left[\left(\frac{0.5}{0.5} \right) \left(\frac{\left(\cos 2\pi f_0 + 2 \right)}{12 \left(\cos 2\pi f_0 - 1 \right)^2} \right) \right] + 1 \right\}}$$

$$= \frac{1}{\left\{ \left[\left(\frac{\left(\cos \left(2\pi \left[1/100 \right] \right) + 2 \right)}{12 \left(\cos \left(2\pi \left[1/100 \right] \right) - 1 \right)^2} \right] \right] + 1 \right\}}$$

$$= \frac{1}{\left\{ \left[\left(\frac{\left(0.99802672842827 + 2 \right)}{12 \left(0.99802672842827 - 1 \right)^2} \right) \right] + 1 \right\}}$$

$$= 1.5585e-005$$

Function csaps in the Curve Fitting Toolbox of Matlab can be used generate the spline-smoothed curve for a given input time series and spline parameter (middle curve, Figure 7.8). It is important to keep in mind that the spline parameter in equation (9) will <u>not</u> give the desired spline smoothness if applied in tree-ring standardization program ARSTAN; for that application, the correct versions of the equations for the spline parameter and frequency response are those in Cook and Peters (1981).

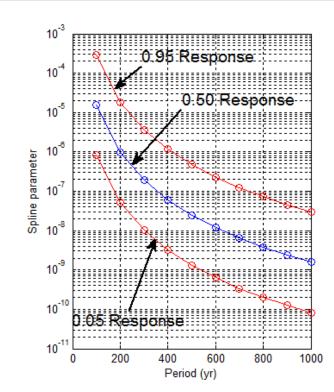


Figure 7.8. Spline parameter as a function of wavelength of frequency response. Curves shown correspond to amplitude of frequency response 0.05, 0.50 and 0.95. For example, a spline with parameter p=2E-07 has a frequency response of 0.50 at wavelength 300 years, a response of 0.95 at wavelength slightly longer than 600 years, and response of 0.05 at wavelength of about 150 vears. Such a spline strongly tracks variations with wavelength longer than 600 yr and hardly tracks at all variations with wavelength shorter than 150 vr. If the original time series were a sine wave with wavelength 300 years, the smooth curve would be a damped sine wave with 25 percent (0.50 squared) of the variance of the original series. The detrended series—the difference of the original series and smooth curve-- would have 75 percent of the variance of the original series.

7.4 Removal of trend

Once a trend line has been fit to the data, we can regard that line as representing the "trend." The question remains, how to remove the trend? If the trend-identification method has identified a trend line, two options are available. First is to subtract the value of the trend line from the original data, giving a time series of residuals from the trend. This "difference" method of removing trend is attractive for simplicity, and for giving a convenient breakdown of the variance: the residual series is in the same units as the original series, and the total sum of squares of the original data can be expressed as the trend sum-of-squares plus the residual sum-of-squares.

The other method of removing trend is to compute the ratio of the time series to the trend line at every point in time. This ratio will exceed 1.0 when the series is above the trend line and will below 1.0 when the series is below the trend line. The "ratio" option is attractive for some kinds of data because the ratio is dimensionless, and because the ratio operation tends to remove trend in variance that might accompany trend in mean. Treering width is one such data type: variance of ring width tends to be high when mean ring width is high, and low when mean ring width is low. Ratio-detrending should not be

used if the original time series contains negative values, and can become problematic when the fitted trend line crosses zero (e.g., division by zero yields infinity). These issues are addressed in the context of detrending tree-ring width by Cook and Peters (1997).

7.5 Effect of detrending on spectrum

Whether the "detrended" series is a difference of the original series and a fitted smooth curve or a ratio of the original series to the smooth curve, the effect is removal of the gradual, or low-frequency, fluctuations tracked by the smooth curve. The effect is therefore to remove low-frequency variance. Detrending in essence is equivalent to high-pass filtering. That is, the variance at low frequencies is diminished relative to variance at high frequencies. In detrending

by a cubic smoothing spline, the frequency response of the spline is high for those frequencies *tracked* closely by the spline. In the subsequent removal of the trend line, these frequencies are mostly *removed*. Frequencies at which the frequency response of the spline is high are therefore those at which variance is most suppressed or damped in the spectrum of the detrended series. In general, at the lowest frequencies, the spectrum of the detrended series will be diminished relative to the spectrum of the original data. The more *flexible* the spline, the higher the frequency-range affected by the detrending.

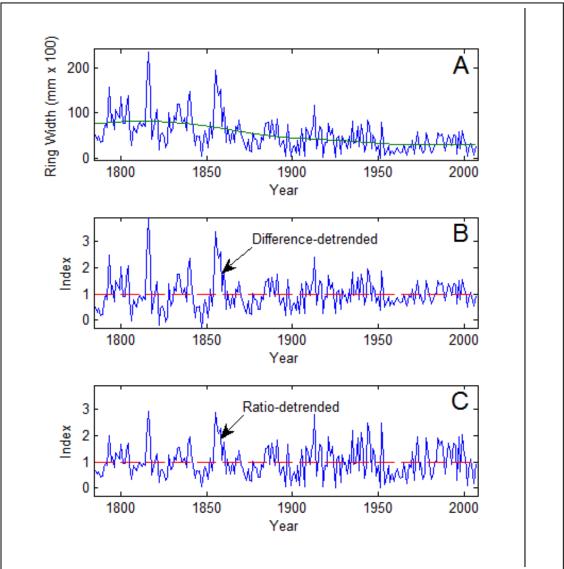


Figure 7.9. Contrast of time series detrended as difference and ratio. (A) Ring-width time series and fitted spline with 0.50 frequency response at 70 percent of series length. (B) Index computed as difference of original time series and fitted trend line. (C) Index computed as ratio of original time series to fitted trend line. Ratio-detrended series converted to same overall mean and variance as difference-detrended series before plotting. Time trend of variance evident in original ring width and difference-detrended series is not evident in ratio-detrended series. Data: ring-width from New Mexico, USA, described in caption to Figure 7.2.

Normalized spectrum. The objective in comparing two spectra is sometimes restricted to discerning differences in the *relative* distribution of variance as a function of frequency. The

visual comparison can be muddied by differences in *total* variance of the two series. To eliminate spectrum differences due to differences in total series variance, the spectra in this case are best plotted as *normalized spectra*. The total areas under two normalized spectra are by definition equal, as the spectra are standardized to have a unit area of 1.0². The normalized spectrum is computed by dividing each ordinate of the original spectrum by the area under the spectrum (Figure 7.10). A normalized spectrum can also be arrived at by first converting a time series to "Z-scores" (zero mean, unit standard deviation) before spectral estimation. (Recall that the area under the spectrum equals or is proportional to the variance.)

7.6 Quantifying the importance of trend

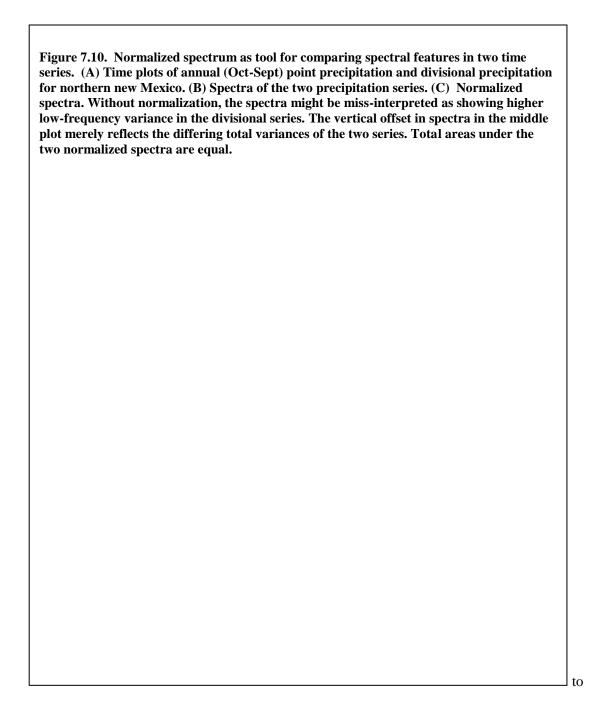
A simple measure of the practical importance of trend in a time series is the fraction of original variance of the series accounted for by the fitted trend line, which can be computed by

$$R^{2} = 1 - \frac{\operatorname{var}(e_{t})}{\operatorname{var}(x_{t})}$$
 (10)

where $var(x_t)$ is the variance of the original time series, and $var(e_t)$ is the variance of the residuals from the trend line.

Equation (10) measures the importance of the tend component in a time series time series, and can range from 0 for no importance to 1 if the series is pure trend (Figure 7.11). Note that for ratio detrending, the total variance of the original series cannot be decomposed into variance due to trend and residual variance because the detrended series is NOT a residual.

² Depending on plotting convention, the area under a plotted normalized spectrum may appear to differ from 1.0. For example, areas under the normalized spectra in Figure 7.10 are 1.0 only if the frequency axis is scaled such that the range $\{0\ 0.5\}$ is scaled to $\{0\ 1\}$. The important point is that the total area under the normalized spectrum is the same regardless of total variance of the time series.



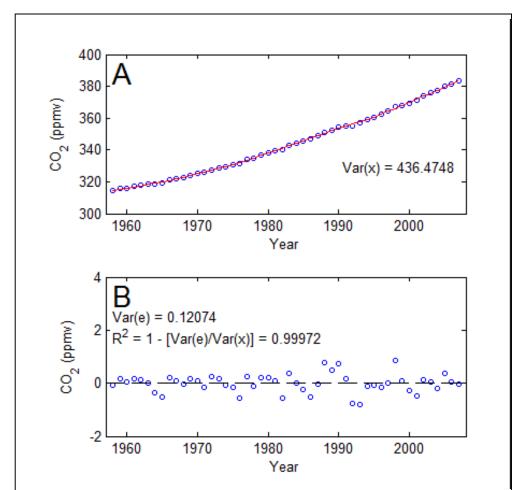


Figure 7.11. Variance due to trend in a trend-dominated series. (A) December free-air CO2 concentration at Mauna Loa, fit with cubic smoothing line to describe monotonic trend. (B) Residuals from the fitted trend line. While original time series varies over a range of more than 60 parts per million by volume (ppmv), the residuals have a range of less than 2 ppmv. The percentage of variance due to estimated trend according to equation (10) exceeds 99.9 percent.

7.7 References

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