The effects of large data gaps on estimating linear trend in autocorrelated data

Troy A. Wynn and Dr. Vicent B. Wickwar
Utah State University, Department of Physics

Abstract

It is well known that atmospheric data is autocorrelated. Techniques for fitting a model to autocorrelated data without data gaps are well known. However in cases where large data gaps exist the analysis is more challenging. By large data gaps we mean 16-24% of the possible data present. This paper explores the challenges of estimating the correlation coefficient in an autocorrelated data set containing large data gaps and suggests ways to accurately estimate the autocorrelation and linear trend in a signal when such cases arise.

1. Introduction

The industrialization of the last 150 years has increased the amount of CO2 and other greenhouse gases in the earth's atmosphere. This large increase is expected to have a dramatic effect on the climate of the earth in the form of global warming. Model simulations predict that with increasing levels of greenhouse gases there should be a warming of the troposphere and a cooling of the stratosphere and mesosphere, and that the levels of cooling in the middle atmosphere should be greater than the warming in the lower atmosphere [Gruzdev and Brasseur, 2005]. The predicted cooling of the middle atmosphere has generated interest in detecting cooling trends in this region.

Many data sets span ten years or more. And data gaps are common. In cases where only a few points are missing interpolation is acceptable. However, upper atmospheric observations frequently depend on weather conditions and other factors that are not easily controlled, such as repair and funding availability. The USU Rayleigh lidar has been in regular operation since 1993 taking density measurements from 45 to 90 km; a data set has been collected spanning more than ten years with 593 nightly temperature profiles. The data set covers a span of 3623 days. This amounts to about 16.4% of possible observations. While this seems low it is not unusual. Over a similar time span (October 1978 through December 1989) the French lidar at Haute-Provence collected a total of 872 nights of observations out of 4110 possible, amounting to 21.3% of possible observations [Hauchecorne et al., 1991].

2. Assumptions

The length of a data set and large data gaps affect the confidence intervals for an estimated linear trend. When ordinary least squares (OLS) regression is used it is assumed that the errors are independent and identically distributed random variables (sometimes called the i.i.d. assumption) with zero mean and variance σ^2. In practice these assumptions rarely hold. For atmospheric temperature measurements the data are autocorrelated, there are sometimes large data gaps, and the variance is nonconstant (gravity wave activity during winter greatly increases the noise in the signal). For a simple linear model such as $y_i = \beta_0 + \beta_1 t_i + \varepsilon_i$, the estimated value for the β's are consistent if the y_i's are bounded, the t_i's are fixed, and the errors have zero mean; that is, the probability that the estimated value b will be close to the true value of β approaches one as the sample size approaches infinity [Hamilton, 1992].

Normal errors are an unnecessary assumption for OLS but are a convenient one for hypothesis testing. (The Student's t-distribution and the F distribution are justifiable under that assumption.) This is where the problem lies with fitting a linear trend to autocorrelated data. The estimation of the trend is consistent but the estimation of the standard error will be much larger than need be.

3. Autocorrelation

The atmosphere has memory, meaning the previous temperature influences the current temperature and so forth. The motivation behind times series analysis is to model this effect. In the atmosphere there are several sources of variability: seasonal variation, gravity waves, tidal effects, solar variation, secular trends, anthropogenic influence, and volcanic eruptions to name a few. All of these are known to influence atmospheric temperatures. Of these the greatest source of variability is seasonal: The annual oscillation (AO) in the mesosphere has an amplitude of 3 to 16 K and the semiannual oscillation (SAO) can have an amplitude of up to 5 K. The time scales of interest are on the order of days and therefore only autocorrelation in the noise need be considered. And though more complicated models are possible it best to first consider a simple AR(1) model.

The proposed model is

$$y_k = \beta t_k + N_k \qquad (k = 1, \ldots, n) \qquad (1)$$

where β is the linear trend, t_k is the time, and N_k is the residual term. The average of y and the average of t has been subtracted from y and t so that both vary around zero. The seasonal components have also been removed. The centering of the data on the origin permits the intercept to be left out of the regression equation and tends to give better results when fitting for

autocorrelation. The residuals are modeled as a first order autocorrelation process

$$N_k = \varphi N_{k-1} + \varepsilon_k, \quad \text{or as this} \tag{2}$$

$$N_k = \varepsilon_k + \varphi \varepsilon_{k-1} + \varphi^2 \varepsilon_{k-2} + \varphi^3 \varepsilon_{k-3} + \ldots + \varphi^{n-1} \varepsilon_{k-n-1} + \varphi^n \varepsilon_{k-n} \tag{3}$$

where the ε's are assumed to be random errors with constant variance and zero mean. Though it is possible to solve for the ε_k's in (3) using OLS, it was found to work only for autocorrelated data generated from random data. In practice solving for ε_k's using OLS is problematic. The linear term is assumed to constant whereas the errors are non-constant. This is also why the data was centered at the origin; the intercept would be very large as well as the ε_k's. Moreover, if more parameters are included in a model the R^2 value increases. Such a model would be a near perfect fit with outrageously large parameter values.

4. A Simple Case

First a simple case of purely autocorrelated data will be considered. The signal consists of first order autocorrelated Gaussian noise with no data gaps. This is represented by the following sequence.

$$\begin{aligned} N_0 &= \varepsilon_0 \\ N_1 &= \varphi N_0 + \varepsilon_1 \\ N_2 &= \varphi N_1 + \varepsilon_2 \\ N_3 &= \varphi N_2 + \varepsilon_3 \\ &\vdots \end{aligned} \tag{5}$$

where the ε 's are drawn from normal distribution with mean zero and unit variance, and φ is a selected correlation coefficient. Solving for the ε's will, in effect, "unzip" the series.

$$\begin{aligned} \varepsilon_0 &= N_0 \\ \varepsilon_1 &= N_1 - \varphi N_0 \\ \varepsilon_2 &= N_2 - \varphi N_1 \\ \varepsilon_3 &= N_3 - \varphi N_2 \\ &\vdots \end{aligned} \tag{6}$$

The ε's can be extracted by iterating the sequence shown in (6). However, if the correlation coefficient is unknown then solving for the errors is not a straightforward task. One could apply the Durbin-Watson statistic and use the relationship $d \approx 2(1-r)$, where d is the Durbin-Watson statistic and r is the correlation coefficient, but this would not work if there are large data gaps. The correlation coefficient can also be calculated using a formula similar to the one employed in solving for β in (1). But a different approach was better suited to this application.

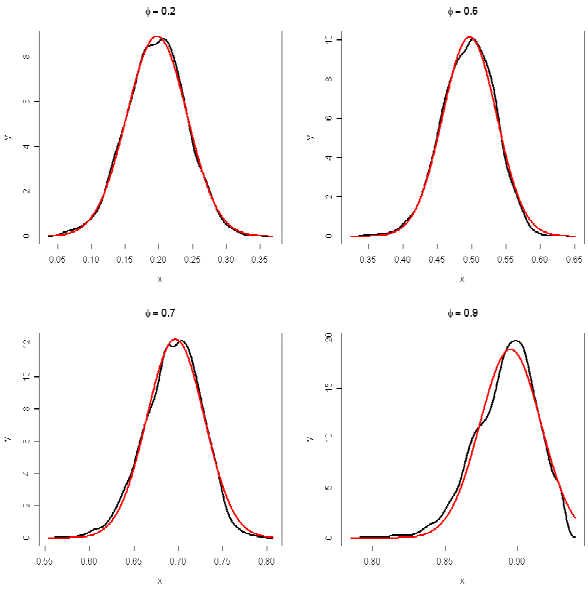

Figure 1. The distribution of the correlation coefficients (black) with fitted normal distribution (red).

The selected approach focuses on minimizing the errors. First a value for the autocorrelation coefficient is guessed; the sequence in (6) applied; and the variance σ^2 of the ε's is calculated. This process is repeated over a range of φ's; the one that minimized $\sigma^2(\varepsilon)$ is selected. Though a minimum variance of the ε's can always be found in this way, it was found that when σ^2 is minimized the correlation coefficient is often near its true value. A distribution of φ's was recovered (Figure 1). It can be seen from this figure that the distribution of the correlation coefficients are well approximated by a normal distribution.

To further validate this technique OLS was applied to (3), with the correlation terms 1, φ, φ^2, φ^3, … being the explanatory variables. It was found that if the data was centered at the origin then the coefficients ε_k, ε_{k-1}, ε_{k-2}, ε_{k-3},… were identical to the ε's recovered from unzipping (6); the sum of the absolute value of the differences being on the order of 10^{-14}.

5. Missing Data Points

The following equation can represent an AR(1) signal.

$$Z_n = \varepsilon_n + \sum_{i=1}^{n-1} \varphi^{n-i} \varepsilon_i \tag{7}$$

where Z_n is the measured signal, ε_n is the random component, and φ the correlation coefficient. This can be rewritten as

$$\varepsilon_n = Z_n - \sum_{i=1}^{n-1} \varphi^{n-i} \varepsilon_i \,. \tag{8}$$

To represent a data set containing missing data points multiply the terms in the summation by an indicator function.

$$\varepsilon_n = Z_n - \sum_{i=1}^{n-1} \varphi^{n-i} \varepsilon_i I_i \,. \tag{9}$$

The indicator function I_i has a value of 1 if the i'th data point is present and 0 if not. I^* is the converse: 0 if present and 1 if not. Note that $I_i + I_i^* = 1$ for all i. Z_n is a measured data point which contains no missing information. So replacing Z_n in (9) by (7) gives

$$\varepsilon_n = a_n' + \sum_{i=1}^{n-1} \xi^{n-i} a_i' - \sum_{i=1}^{n-1} \varphi^{n-i} \varepsilon_i I_i \tag{10}$$

where ζ is the true correlation value and a_i' is the true noise. Multiplying the terms in the first summation by $I + I^*$ gives

$$\begin{aligned} \varepsilon_n = a_n' &+ \sum_{i=1}^{n-1} \xi^{n-i} a_i' I_i^* \\ &+ \sum_{i=1}^{n-1} \xi^{n-i} a_i' I_i - \sum_{i=1}^{n-1} \varphi^{n-i} \varepsilon_i I_i \,. \end{aligned} \tag{11}$$

Then collecting terms

$$\begin{aligned} \varepsilon_n = a_n' &+ \sum_{i=1}^{n-1} \xi^{n-i} a_i' I_i^* \\ &+ \sum_{i=1}^{n-1} \left(\xi^{n-i} a_i' - \varphi^{n-i} \varepsilon_i \right) I_i \,. \end{aligned} \tag{12}$$

And finally taking the variance of (12)

$$\begin{aligned} Var[\varepsilon_n] = Var[a_n'] &+ \xi^{2(n-i)} Var\left[\sum_{i=1}^{n-1} a_i' I_i^* \right] \\ &+ Var\left[\sum_{i=1}^{n-1} \left(\xi^{n-i} a_i' - \varphi^{n-i} \varepsilon_i \right) I_i \right]. \end{aligned} \tag{13}$$

If the correlation coefficient is guessed correctly $\varphi \approx \zeta$. Expanding the variance gives

$$\begin{aligned} Var[\varepsilon_n] = Var[a_n'] &+ \xi^{2(n-i)} Var\left[\sum_{i=1}^{n-1} a_i' I_i^* \right] \\ &+ \xi^{2(n-i)} E\left[\sum_{i=1}^{n-1} \left(a_i' - \varepsilon_i \right)^2 I_i \right] - \xi^{2(n-i)} E\left[\sum_{i=1}^{n-1} \left(a_i' - \varepsilon_i \right) I_i \right]^2 . \end{aligned} \tag{14}$$

remembering that the last two expectation values are a variance, the sum being positive. If the errors ε_i can be recovered such that they are approximately equal to the true noise a_i then the variance of ε_n will have been minimized. Though this is not a proof it does serve to illustrate that an accurate guess of the correlation coefficient can minimize the variance.

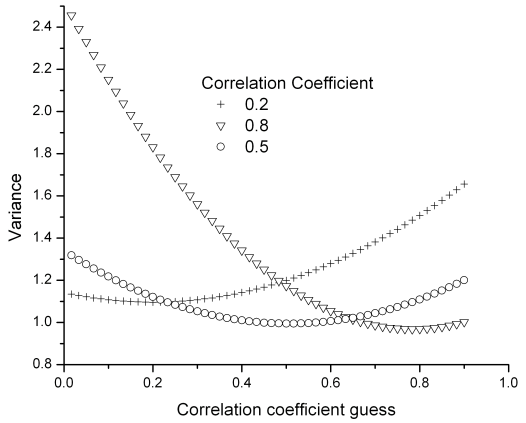

Figure 2. How the variance of the ε's change with (guessed) correlation coefficient. A minima can be seen near the true value of the correlation coefficient.

A procedure similar to the one described in the preceding section was applied to an AR(1) signal with USU data gaps. A total of 3623 data points were randomly drawn from a normal distribution and filtered to make an AR(1) signal. From this 593 data points were drawn matching the USU data gaps. It was found that even with these gaps the distributions of the correlation coefficient were reasonable. Furthermore the standard deviations for these distributions are nearly the same those for the no gaps case. And the standard deviation between the no data gaps cases were nearly the same.

6. Other Cases

In the USU data set of 593 data points 287 (48%) are consecutive, 89 have 2 day spacing, 46 have 3 day spacing, and 29 have 4 day spacing. If the procedures described above are applied to an uncorrelated signal the correlation coefficient distribution has a large spike near the origin (Figure 4) indicating that no autocorrelation is present in the data. For cases with evenly spaced data gaps of two, three, and four days a similar spike is found near the origin for the smaller values of correlation coefficients ($\varphi \sim 0.1$ to 0.3). (See Figure 5, Figure 6, and Figure 7.) With data gaps present the variance on the estimated autocorrelation coefficient is larger for smaller values of φ; and as φ gets larger the estimate of the variance becomes nearly equal to the no gaps case. (See Table 1.) This effect is due to the greater influence of previous information on the current measurement when autocorrelation is strong.

Further, as the size of the gaps increase so does the "zero spike" effect. Figure 5 shows that the zero spike is prominent up to φ = 0.3 for two-day gaps; Figure 6 shows a prominent spike up to φ = 0.4 for three-day gaps; and Figure 7 has a prominent spike up to φ = 0.5 for four-day gaps.

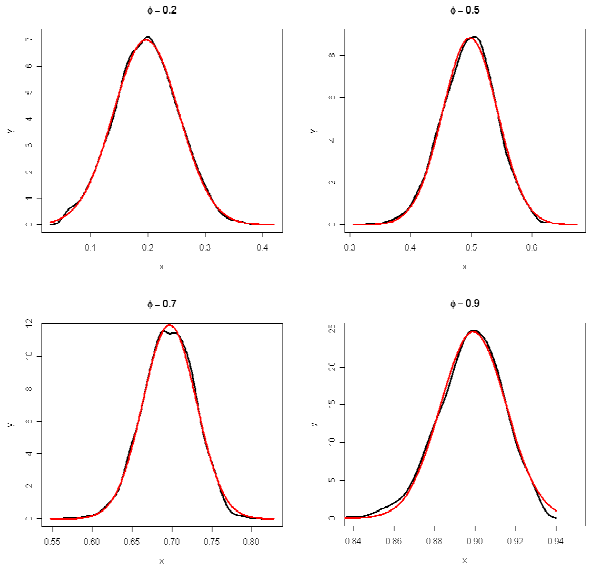

Figure 3. The distribution of the correlation coefficients with USU data gaps (black). Fitted normal distribution (red).

Table 1. The standard deviation of a Gaussian distribution fitted to the probability densities corresponding to no gaps, USU data gaps, two-day gaps, three-day gaps, and four-day gaps.

phi	No gaps	USU gaps	2 day gaps	3 day gaps	4 day gaps
0.1	0.0467	0.0600	0.1297	0.1917	0.2645
0.2	0.0447	0.0576	0.1578	0.2373	0.2846
0.3	0.0429	0.0526	0.0920	0.2389	0.3133
0.4	0.0422	0.0499	0.0727	0.1093	0.3142
0.5	0.0393	0.0454	0.0562	0.0738	0.1067
0.6	0.0371	0.0395	0.0466	0.0540	0.0648
0.7	0.0324	0.0334	0.0369	0.0377	0.0431
0.8	0.0270	0.0261	0.0286	0.0260	0.0260
0.9	0.0211	0.0161	0.0211	0.0178	0.0160

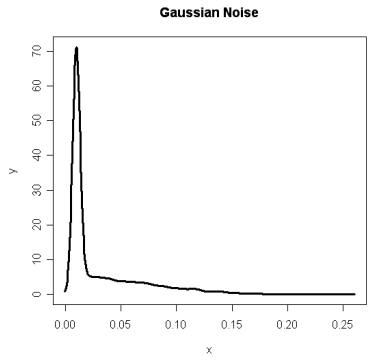

Figure 4. The distribution of correlation coefficients obtained from noise.

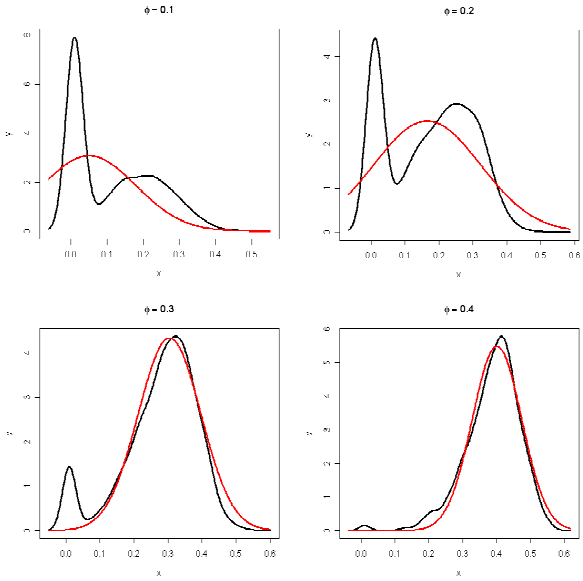

Figure 5. The probability densities for φ from two-day data gaps data. The probability densities are shown in black; the red is a Gaussian distribution fitted to the data.

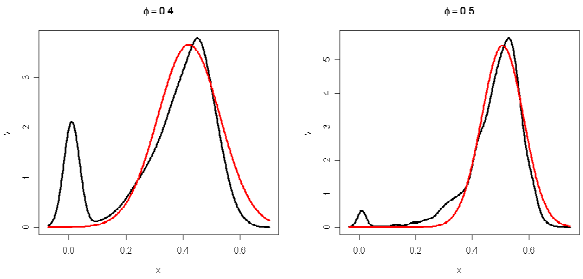

Figure 6. The probability densities for three-day data gaps. The densities for φ = 0.1, 0.2, and 0.3 are not shown as they are nearly identical to those in Figure 5.

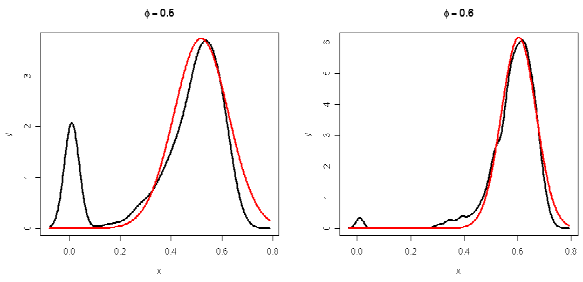

Figure 7. The probability densities for φ = 0.5-0.6 from four-day gaps data. The probability densities for less than φ = 0.5 are not shown as they are nearly identical to those in Figure 6 and Figure 5.

7. Effects on Detecting Linear Trends

The uncertainty on the autocorrelation coefficient has important consequences for estimating the significance of a linear trend. Frederic [1984] gives a formula for calculating the variance of an estimated trend for the following model

$$y_i = b_o + b_1 t_i + \varepsilon_i \,. \qquad (15)$$

The variance of b_1 is given by

$$\sigma^2(\hat{b}_1) = \frac{(1-\varphi^2)}{(1-\varphi)^2} \frac{\sigma^2(Y)}{\sum_i [(t-\bar{t})^2]} \qquad (16)$$

where the autocorrelation between consecutive measurements is given by $\varphi = e^{-\lambda \Delta t}$, where Δt is the time between measurements. This autocorrelation function shows that the autocorrelation decreases with increasing time between measurements. Thus closer spaced data points do not always result in a more accurate estimation of the standard error of the linear trend. If (16) is being used to estimate the variance of a linear trend then a good estimate of the autocorrelation function φ is needed. What this paper shows is that determining the autocorrelation coefficient from the data can be problematic. Especially when there are data gaps present in the data set.

The probability density functions shown above were estimated using kernel density estimation. In the cases with evenly spaced data gaps a spike near the origin is evident. The area under each probability density gives the probability of finding a range of values for the correlation coefficient. Estimating the area under the zero spike gives the probability that autocorrelation is not detectable in a signal. (See Figure 8 for example and Table 2 for probabilities.) From Table 2 it can be seen that the probability of being unable to detect autocorrelation in a signal with a correlation coefficient of 0.4 is 15% for three-day gaps and 31% for four-day gaps, suggesting that modeling autocorrelation becomes less useful with greater time intervals between measurements. However, the table is for evenly spaced data. In the case of USU data gaps where 48% of the data points are consecutive the probability density functions shown in Figure 3 have no zero spike. Hence, an autocorrelated model can be beneficial.

Table 2. The probabilities of not detecting autocorrelation with even gaps data.

φ	two-day	three-day	four-day
0.1	0.49	0.53	0.53
0.2	0.29	0.48	0.52
0.3	0.07	0.34	0.47
0.4	0.005	0.15	0.31

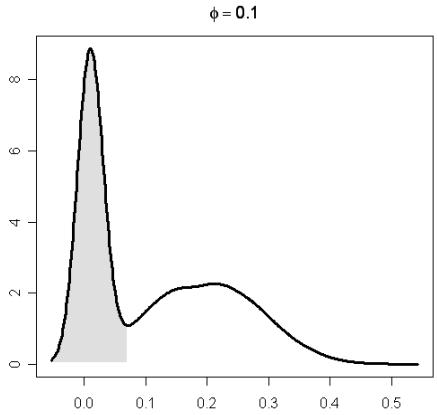

Figure 8. The area under the "zero spike". The plot above is for φ = 0.1 with two-day data gaps. The probability of no detectable autocorrelation is 49%.

Krzyścin [1997] proposed an iterative procedure for fitting a linear trend to autocorrelated data. The procedure is as follows. The model

$$y_k = \alpha^m + \beta^m t_k + \varphi^m (y_{k-1} - a^{m-1} - \beta^{m-1} t_{k-1}) + \varepsilon_k^m, \quad k = 1,2,3,\ldots n, \qquad (17)$$

where α^m, β^m, and φ^m are the fitted parameters at the mth step and $a^{m-1}$and β^{m-1} are the fitted parameters from the previous step is iterated. The term in the parenthesis approximates the N_{k-1} residual term. While this iterative technique converges quickly (two or three iterations) it is not clear how to handle missing data points. I have adapted Krzyścin's approach to handling missing data points by using a more involved method to approximate the N_{k-1} residual term. What I have sown in the previous sections of the this paper is that if a large percentage of the data points are consecutive, large data gaps notwithstanding, the approximation of the correlation coefficient is stable.

8. Problems approximating the N_{k-1} Residuals

First order autocorrelation can be modeled as

$$N_k = \varphi N_{k-1} + \varepsilon_k$$

where N_k is the kth residual, N_{k-1} is the previous residual, φ is the correlation coefficient, and ε_k is the random error component. The equation above can be rewritten as a series of equations

$$\begin{aligned} N_1 &= \varepsilon_1 \\ N_2 &= \varphi(\varepsilon_1) + \varepsilon_2 \\ N_3 &= \varphi(\varphi\varepsilon_1 + \varepsilon_2) + \varepsilon_3 \\ N_4 &= \varphi(\varphi^2\varepsilon_1 + \varphi\varepsilon_2 + \varepsilon_3) + \varepsilon_4 \\ &\vdots \end{aligned}$$

where the terms in the parenthesis approximates the Nth residual. If there are missing data points then summing the terms in the parenthesis while leaving out the missing data points can approximate the residuals. For example if the first 6 days in the data set are spaced 1, 2, 3, 5, 9, and 16 then we would have

$$\begin{aligned} N_1 &= \varepsilon_1 \\ N_2 &= \varphi(\varepsilon_1) + \varepsilon_2 \\ N_3 &= \varphi(\varphi\varepsilon 1 + \varepsilon_2) + \varepsilon_3 \\ N_5 &= \varphi(\varphi^3\varepsilon_1 + \varphi^2\varepsilon_2 + \varphi^1\varepsilon_3) + \varepsilon_5 \\ N_9 &= \varphi(\varphi^7\varepsilon_1 + \varphi^6\varepsilon_2 + \varphi^5\varepsilon_3 + \varphi^3\varepsilon_5) + \varepsilon_9 \\ N_{16} &= \varphi(\varphi^{14}\varepsilon_1 + \varphi^{13}\varepsilon_2 + \varphi^{12}\varepsilon_3 + \varphi^{10}\varepsilon_5 + \varphi^6\varepsilon_9) + \varepsilon_{16} \\ &\vdots \end{aligned} \qquad (18)$$

Again, the terms in the parenthesis approximating the N_{k-1} residual. (For convenience I shall refer to the N's as residuals and the ε's as errors.)

Three techniques for approximating the N terms in (18) were attempted. In the first the data gaps were ignored and the residuals were applied according to (17). But this was found to produced very inaccurate results. The two other methods were more productive and had results very similar to each other. The first method involved OLS regression on (1), then the correlation coefficient of the errors was found using the variance minimizing techniques described in this paper. The errors from the fit are then used to approximate the terms in the parenthesis in (18). This replaces the $y_{k-1} - a^{m-1} - \beta^{m-1}t_{k-1}$ term in (17). The process is iterated until no further improvement is detected. While it was found that a relatively accurate estimation of the correlation coefficient could be achieved the nature of the iteration introduces a small instability. Since the correlation coefficient from the previous step is used to calculate the residuals for the current step there is a tendency for the correlation coefficient to oscillate between two values. The oscillations however are small (0.01 or less). I shall refer to this first technique as residual simulation (RS).

The second technique is very similar to the first. In place of using the errors to estimate the N values, the residuals were estimated from $y_{k-1} - a^{m-1} - \beta^{m-1}t_{k-1}$ (17). These residuals were then put into equation (18) in place of the errors. OLS regression was performed and the procedure repeated. I shall refer to this second technique as hybrid residual simulation (HRS).

These techniques were applied to simulated data consisting of a linear trend of –0.5 K/year, an autocorrelation correlation of 0.7, and a standard deviation of 6.0 K in the noise (typical for the mesosphere). Gaussian noise was generated and then

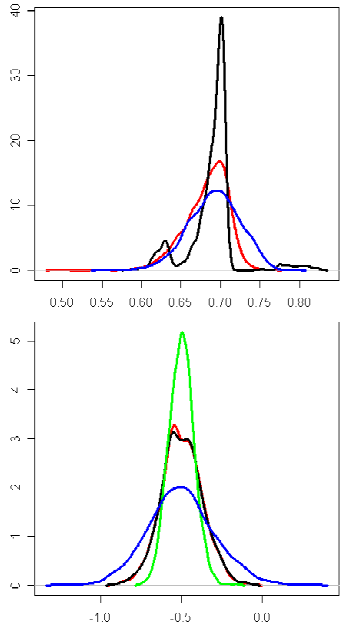

Figure 9. The probability densities for the correlation coefficient (above) and the linear trend (below). The green is the estimate for the no autocorrelation case. The red corresponds to RS; blue corresponds to the autocorrelated data with no data gaps; and the black is HRS.

autocorrelated and added to the linear component. Data was selected from this so as to duplicate the USU data gaps. A second autocorrelated data set was created with the same values but no data gaps. And a third was also created with no autocorrelation. This procedure was repeated 1300 times to create a distribution of the linear term as well as the correlation coefficient. The cooling rate of 0.5 K/year was selected because it is near the average value of cooling rates measured in the mesosphere [Beig et al., 2003].

As can be seen from Figure 9 the distribution of the correlation coefficient for the HRS is much tighter than the no gaps case and RS. The case with no data gaps is also broader than the case with USU data gaps. As far as the linear trend is concerned HRS and RS did equally

well and both produced a tighter distribution than the no gaps case. Using (16) to calculate the standard deviation of the linear term we get a value of 0.202 K/year which is very close to the measured value from the simulations of 0.205 K/year. As Frederick pointed out the number of measurement required to detect a significant linear trend decreases as the spacing between the measurements increases. Since the blue distribution is from consecutive measurements we would expect the standard deviation to be greater than a similar data set with data gaps. As was demonstrated earlier in this paper, evenly spaced data gaps make estimating the correlation function difficult. However, in the case of data sets where there are large data gaps but many consecutive measurements the best of both can be had. If a large portion of the measurements is consecutive then one can reasonably estimate the correlation coefficient; further, large data gaps decrease the number of data points needed to detect a significant trend. Thus Figure 9 shows a tighter distribution on the linear trend estimates for RS and HRS than for the no data gaps case. There is however the question of the distribution for the correlation coefficient, the distribution for RS and HRS are tighter than the no gaps case; and a markedly tighter distribution for HRS is obvious. This result is not intuitive. If there were no data gaps present one would expect a better estimation of the correlation function. It could be that the residual simulation and hybrid residual simulation are more accurate ways of approximating the residuals. But whatever the case may be the question remains open to inquiry.

9. Conclusions

It is possible to accurately measure the autocorrelation and the linear trend from a data set with large data gaps if certain conditions apply: if large data gaps are present in a data set and a large portion of the measurements are consecutive. If this be the case then an accurate estimation of the linear trend is possible. If the data is evenly spaced then estimating the correlation coefficient becomes problematic and fitting an autoregressive model to the data is questionable. Of the two techniques that were viable, namely residual simulation (RS) and hybrid residual simulation (HRS), HRS proved to estimate the correlation better than RS and estimated the linear trend equally well with RS. Modeling the autocorrelation in this way gave better results on linear trend estimation than the case with no data gaps. The question as to why HRS gave a much tighter distribution than RS is open to further investigation. It should be kept in mind that the equation for estimating the variance of the linear trend (16) is accurate only as far as the accuracy of the correlation coefficient will permit.

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