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Peter Thejll and Torben Schmith

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Limitations on regression analysis due to serially correlated residuals: Application to climate reconstruction from proxies.

Peter Thejll and Torben Schmith

Climate Division, Danish Meteorological Institute,

Copenhagen, Denmark*

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Abstract

The effects of serially correlated residuals on the accuracy of linear regression are considered, and remedies suggested. The *Cochrane-Orcutt* method specifically remedies the effects of serially correlated residuals and yields more accurate regression coefficients than does

*e-mail: thejll@dmi.dk and ts@dmi.dk

ordinary least squares. We illustrate the effects of serially correlated residuals, explain the application of the CO method, and evaluate the gains to be achieved in its use. We apply the method to an example from climate reconstruction, and show that the effects of serial correlation in residuals are present, and show the significantly improved result.

1 Introduction

Linear regression is central to most areas of quantitative science, and applied widely. In its simplest form two time series x_t and y_t, called the predictor and predictand respectively, are supposed to be related by the linear relationship $y_t = \alpha + \beta x_t + u_t$, where u_t is the error term. The parameters α and β are not known but must be estimated from the predictor and predictand series. This estimation procedure is often considered as being synonymous with the technique of 'ordinary least squares' (OLS), where the parameters in the regression model are estimated by minimizing the sum of the squared 'residuals' (observed error terms).

However, this is not a fruitful approach under all circumstances. There are conditions to be met, in order for the OLS estimate to the 'best' estimate of the model parameters. This is well known and described in statistical text books (e.g. [von Storch and Zwiers, 1999]), but in applications these conditions are not always met, or even considered.

Central to this is the Gauss-Markov theorem, which states that: *if the error term time series is stationary and has no serial correlation, then the OLS parameter estimate is the Best Linear Unbiased Estimate (BLUE)*, meaning that all other linear unbiased estimates will have a larger variance. The Gauss-Markov theorem thus points to the error term and not the time series themselves as being important to consider. Next, it states, that under these conditions, the OLS estimate has two nice properties, namely it is *unbiased* and has *the smallest possible variance* among the linear estimates.

The premise in the Gauss-Markov theorem essentially states that the error term must have no structure – for instance, the level of the residuals must not have a trend and the variance must be constant through time. There is no a priori reason to trust that residuals should be without structure – there are at least two ways in which it could happen. First, there is the effect of missing variables. Any factor that a model fails to incorporate, either by being unrecognized or by being unknown, will turn up in the residues. Therefore the nature of the residuals depends on the factors omitted. Some of these factors may be serially correlated and thus give rise to serially correlated residuals. Second, there is the effect of mixing variables with different levels of serial correlation. Because the residuals are a linear combination of the predictors and predictand it is possible that the residuals will be serially correlated if one of the dependent or independent variables also is.

When the error term in the regression does not fulfill the premise in the

Gauss-Markov theorem, OLS is still unbiased – however, it is not BLUE, i.e. OLS does not exploit the data at hand to give the most efficient estimate of the parameters in the model. In this situation, a strategy would be to transform the problem (i.e. the variables and their regression relationship) so that the error term in the transformed problem has no structure. This strategy will be adopted in the following section ending up in the procedure known as the *Cochrane-Orcutt algorithm*. Subsequently, we will illustrate this algorithm within the field of climate reconstruction by proxies. Here multi-regression techniques are widely applied in the 'standard OLS form', but the conditions for the Gauss-Markov theorem are usually not tested for. For example, in the past five volumes of Journal of Climate, four papers on climate reconstructions are published, but the serial correlation of residuals is considered in just one of them only.

2 The Cochrane-Orcutt algorithm

Consider a multiple regression model

$$y_t = \alpha + \sum_{k=1}^{K} \beta_k x_{t,k} + u_t, \tag{1}$$

where the error term u_t follows an AR(1) process with the autocorrelation at lag 1 being ρ (whose value is unknown at this stage):

$$u_t = \rho u_{t-1} + \epsilon_t, \tag{2}$$

where ϵ is a series of serially independent numbers with mean zero and constant variance.

If ρ is not zero then, as we have seen, OLS is not an efficient estimator of model parameters and other methods are called for. One such method is that suggested by Cochrane and Orcutt (1949), which modifies equation 1 by rewriting it for $t-1$ instead of t, multiplying all terms by ρ, subtracting the result from equation 1, using equation 2, and rearranging terms to obtain:

$$(y_t - \rho y_{t-1}) = \alpha(1-\rho) + \sum_{k=1}^{K} \beta_k (x_{t,k} - \rho x_{t-1,k}) + \epsilon_t, \tag{3}$$

for t=2,...,N.

Equation 3 is a regression equation with modified variables, coefficients, and an error term that satisfies the Gauss Markov theorem. We have, however, introduced one new parameter, namely ρ which prevents us from applying OLS directly.

We can solve the problem iteratively by first estimating (using OLS) α and the β's from equation 3 for an initial guess of ρ. Then, using the values of α, β just determined a new value for ρ is found (using equations 1 and 2), which is then held fixed and used to find new values for the α, β's, and so on, until

convergence occurs (see Ramanathan (2002) p. 393, for a detailed description of the algorithm). Discussions have appeared as to whether this technique guarantees convergence to a good solution (e.g. [Dufour, et al., 1980]) - the outcome of the discussion seems to be that a grid search through parameter space almost always reveals that the iterated solution is the best one.

The Cochrane-Orcutt method is well known in the econometrics literature, but has, it seems, not been widely appreciated outside this field. In the following sections we will show that there is reason to take notice of the method in geophysics, as it offers advantages in realistic situations where OLS is commonly applied without being wholly appropriate.

3 Illustrating the Cochrane-Orcutt algorithm by applying it to artificial series with known properties

3.1 Variables without serial or inter-correlation

We next show the results of applying the CO algorithm to artificial problems. We generate suitable regression problems from the following model

$$y_t = \alpha + \beta_1 x_t^{(1)} + \beta_2 x_t^{(2)} + u_t, \tag{4}$$

where $x_t^{(1,2)}$ are two predictor vectors generated from uniformly distributed random numbers, furthermore

$$u_t = \rho u_{t-1} + \epsilon_t, \tag{5}$$

is the noise, where ϵ is normally distributed white noise. Use of this generation technique (equation 5) for u requires care with 'spin-up' problems - a long sequence of numbers should be generated for the choices of ρ and starting value u_0 before a segment of the required length is selected.

After generating random vectors $x^{(1,2)}$ we generate T by picking values of α, β_1, β_2, and the auto-correlated series is generated by picking a value for ρ and generating the series u. We estimate α, β_1, β_2 using OLS and the CO method. Below, in Figure 1 we show the results of 1000 simulations of this procedure for $\rho = 0.87$.

First we note that the disturbance u causes a spread in the estimates of the coefficients, but that these are centered on the correct solutions - hence, there is no evidence of a bias on average, in accordance with theory. Next, we see (Figure 1) that in OLS the values found for β_1, β_2 have a larger spread than the CO values, while the OLS value for the constant term α appears less spread out than the CO value.

For a smaller value of the parameter determining the auto-correlation of the additive noise ($\rho = 0.57$) Figure 2 shows the results, which are that the constant term α is now almost equally well-determined with OLS and CO

while the larger spread in the regression coefficients β_1, β_2 for OLS compared to CO is still evident.

For a range of values of ρ Figure 3 summarizes the results. In general one sees that the spread in OLS determinations of regression constant and coefficients does not depend on the character of the added noise. However, the CO algorithm is highly sensitive to this and produces increasingly better regression coefficients for increasing ρ – the spread in the regression constant grows with ρ, however. It would appear that for these particular experiments there is much to gain by using CO, up to values of ρ just below 0.75, if one wants accurate regression constant as well as coefficients, because β_1, β_2 are much better determined in CO compared to OLS while the α's are about equally well determined.

For small ρ (in this example, for values less than 0.4, say) there is only a little to gain by using CO instead of OLS although CO is still the best method. For large ρ better regression coefficients are bought at the cost of less well determined regression constant. This means that in applications where accurate regression coefficients are sought, but the value of the regression constant, α, is not so important, CO will outperform OLS.

We end this experiment by reminding the reader that the variables used here - the predictors - are generated as normally distributed random numbers. They therefore have a 'white' spectrum and are probably, in the statistical sense, independent, given the length of series used here. In reality,

one is often left to perform regressions on variables that are neither 'white' nor independent of one another. The consequences of this situation will be discussed in the next section.

In summary, we have tested the performance of OLS versus the CO method in trials with independent and 'white' predictors with auto-correlated additive noise. We have shown that if residuals have structure - in the sense of having a serial correlation different from 0 - then the CO method will outperform OLS in determining regression coefficients more the larger ρ is. The regression constant's accuracy suffers in the CO method, however. But as regression coefficients (providing *rate information*) are generally of greater interest than the model offset, this is of little concern in some cases.

3.2 Variables that are independent but serially correlated

In the previous section we investigated how well CO does compared to OLS when the predictors in the problem are independent and white-noise like. What will happen if they are more realistic and, for instance, have their own serial correlation or when they are related to each other through correlation? We will separate these problems and first consider the case of auto-correlated variables that are not inter-correlated.

We will generate the variables $x^{(1,2)}$, in equation 4 iteratively, by

$$x_t = \alpha_1 x_{t-1} + \epsilon_t. \tag{6}$$

For simplicity we shall choose the same value for the autocorrelation at lag one, α_1, for both series. In order to avoid mix-up with the case treated in next section, we shall expressly test whether $x^{(1)}$ and $x^{(2)}$ are correlated and reject series that are. The likelihood that they are correlated by chance rises with α_1 because the number of independent points in the series decreases.

We choose α_1 in equation 6 to be 0.6 and repeat the exercises above. We accept series that are no more correlated to each other than $R = 0.1$, where R is the Pearson linear correlation coefficient. We perform a series of experiments similar to the previous section and show in Figure 4 a summary of results for autocorrelated but mutually un-correlated predictors. The results indicate that CO is always better for the regression coefficients than OLS, for values of ρ greater than about 0.4. For the regression constant there is the trade-off already seen above. One difference with the result using white noise series is that OLS gradually deteriorates as ρ increases - before it held constant. Therefore, not only does CO do better as ρ rises, but OLS does worse and worse. This seems a strong indication that CO is the preferable choice when series are auto-correlated and mutually un-correlated. Again, we note that results are centered on the correct values, so in the mean there is no coefficient bias in either OLS or CO.

3.3 Correlated and auto-correlated variables

We now consider what happens when the variables are not only auto-correlated but also correlate with one another. We proceed as above but this time accept only those sets of series that are more strongly correlated than $R = 0.3$. Figure 5 summarizes results from several runs. The results are very similar to Figure 4.

The final experiment in this section increases the mutual correlation substantially, to $R \geq 0.7$, and the results are summarized in Figure 6. We see in general that the predictor's correlations affect the result, but that for very large residual correlation CO wins out over OLS while following the patterns seen above.

We summarize this set of experiments by noting that correlation between the predictors, in the presence of auto-correlated noise in the model, has an increasing importance as the additive noise becomes more and more auto-correlated, and that for the largest values of serial noise correlation all regression coefficients are best determined with the CO method. Careful analysis of predictor's inter-correlations, and the level of residual auto-correlation thus plays a central role in the application of regression methods (OLS or CO).

A final note is due on the subject of the *quality of the model fit* vs. the *quality of the parameter estimations*. OLS will always give the best model fit to the data at hand whether residuals are autocorrelated or not, but CO will offer the most accurate estimates of regression coefficient values.

4 Application of the CO method to climate reconstruction using proxies

Instrumental climate series are not as long as are the 'proxy' series that can be developed from natural records, such as tree ring data, ice cores, lake varves, coral rings, and so on. These natural observables may reflect environmental conditions to some extent, and by calibrating these against instrumental series we can obtain climate information back in time, before instrumental records began. The calibration of the proxy can in its simplest form be performed by a regression, and the present discussion about how well regression methods perform is relevant.

One early attempt to calibrate temperature proxies against instrumental data was that of Landsberg and Groveman [Landsberg *et al*, 1978; Groveman and Landsberg, 1979], who utilized a technique whereby supposed proxies for global mean temperatures were related to an instrumental temperature curve, using multivariate linear regression. Although the data available to Landsberg and Groveman were limited compared to the much larger data-collections now used in climate-reconstructions, and the method, in the form chosen by those authors, is not now commonly used, we chose the example in order to show the need for CO instead of OLS for the calibration. The illustrative powers of the example are undiminished by the choice of data and the details of the method of that work.

Very briefly, the Landsberg and Groveman method consists of scaling or calibrating climate proxies against a constructed global- or hemispheric-mean instrumental record with multivariate regression. Not all proxies have the same length, so in the application of Landsberg and Groveman proxies were chosen that all ended near the end of the instrumental record but which started at different times from 1579 AD and forward in time. Sets of proxy time series were chosen on the basis of the years in which they overlapped. In this way a final reconstruction was patched together from many segments, each of which are the results of a calibration during the instrumental period, but being used only for a specific time interval before this era.

We first reconstructed the method of Landsberg and Groveman from the data published [Groveman, 1979]. The residuals were tested for auto-correlation using the Bartlett cumulated periodogram test [Bartlett, 1966] - the residuals are significantly auto-correlated for some choices of proxy data. This conclusion was also obtained using another test for serial correlation in time series - the Durbin Watson test [Draper and Smith, 1981]. The Durbin Watson test is a test of a statistic d against some null hypothesis. The statistic d is formed from the residuals $e_1, e_2, ..., e_n$:

$$d = \frac{\sum_{t=1}^{n}(e_t - e_{t-1})^2}{\sum_{t=1}^{n} e_t^2}. \tag{7}$$

The value of d obtained from the residuals is compared to critical values (e.g. the tables in Draper and Smith (1981)). If d is less than a lower limit then the null hypothesis of no serial correlation in the residuals can

be rejected, whereas if d is above an upper limit the hypothesis cannot be rejected. Values in between are indeterminate. A look at equation 7 shows that strongly autocorrelated series will give a small d statistic, while the opposite happens if the series are not serially correlated, going in the limit of long series to $d = 2$.

The DW test gave similar results to the Bartlett test - namely, that the residuals, in the instrumental calibration range, are serially correlated for those cases when a few proxy time series are used - notably the first period from 1579-1658 AD (at the 99% significance level). Values of the d statistic close to the lower limit, but inside the 'indeterminate range' were obtained for other early intervals, notably 1706-1764 and 1817-1820. There is therefore support for recalculating the temperature reconstruction with CO substituted for OLS, with the expectation that significantly different results could be obtained for the early years of the reconstruction.

We therefore replaced the OLS regressions used in the method, by the CO algorithm and derived a new reconstructed temperature curve. The original and the new curve are shown in Figure 7. The difference between the two results is shown in Figure 8. We see that there are considerable differences between the reconstructions in the early years (e.g. 0.4 degrees C near 1600 AD), and a tendency for a systematic upward slope in the difference towards nearly zero difference for years near to the instrumental record.

5 Summary and Discussion

We have by example shown how important the effects of serially correlated residuals can be for the results of regressions, and offered a remedy for situations when regression must be performed in the presence of such autocorrelated residuals, namely the Cochrane-Orcutt method.

In a climatological application we have shown the extent of the effects of using CO instead of OLS in a proxy reconstruction. Although the chosen proxy-based temperature reconstruction may no longer be current, the use of proxy-based reconstruction methods to build a description of past climate is growing. Most of these applications of proxy-scaling are potentially sensitive to the problems we have discussed in this paper, and most of them tend to use fewer proxies at the start of the time interval of reconstruction - furthest from the instrumental data scaled against. These are conditions under which OLS and CO will tend to give different results, and we therefore suggest that reconsideration of some climate reconstructions using regressions could profitably be undertaken.

We have highlighted the impact of CO on just one example chosen from a specific field. A whole family of analysis methods rely at heart on minimization of residuals, but are often performed without testing for compliance with the appropriate equivalent of the Gauss-Markov theorem. Such methods as Empirical Orthogonal Analysis, Canonical Correlation Analysis, the Empirical Mode Decomposition Method [Huang, N.E., 1998], Redundancy

Analysis (e.g. [Tyler, 1982]), and others, seem to be based on conditions that may as easily be violated as is the case for simple regression, and a revision of such methods in view of the potential impacts we have illustrated here, may prove profitable.

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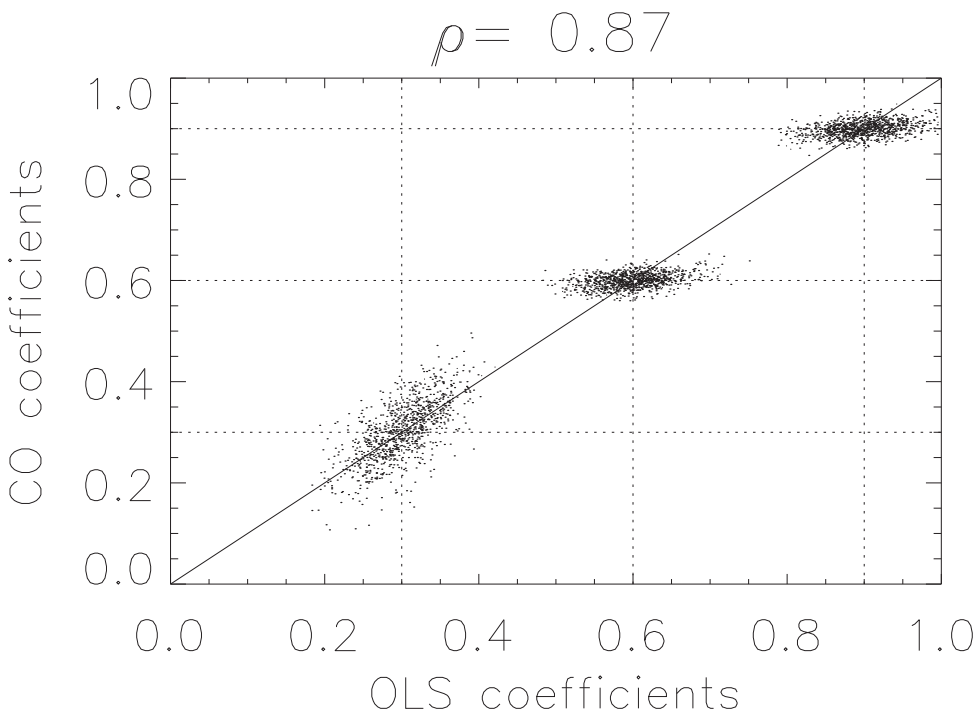

Figure 1: Results of simulations of OLS and CO regression on 1000 simulated data sets. From lower left to upper right, the cloud of points are the results for the constant term α and the regression coefficients β_1 and β_2 - these were assigned the values 0.3, 0.6 and 0.9 in the model, respectively (the dotted lines). Time series of length 100 points were used. The noise added to the model is auto-correlated, with ρ=0.87. There is clearly a larger spread in the OLS regression coefficients, while the OLS constant term is less spread out than the CO value. Bias in the estimate seems low - the clouds of points are centered on the model values.

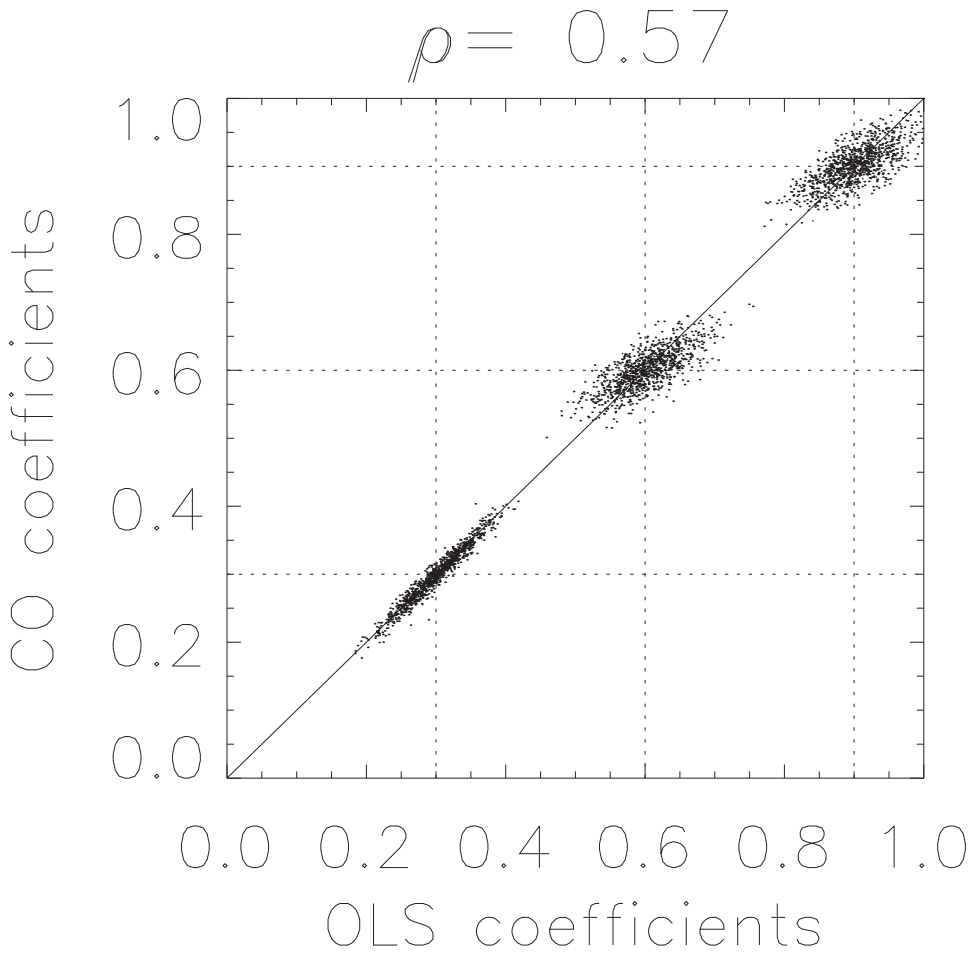

Figure 2: As in Figure 1, but for a lower value of the parameter describing the auto-correlation of the added noise. ρ=0.57.

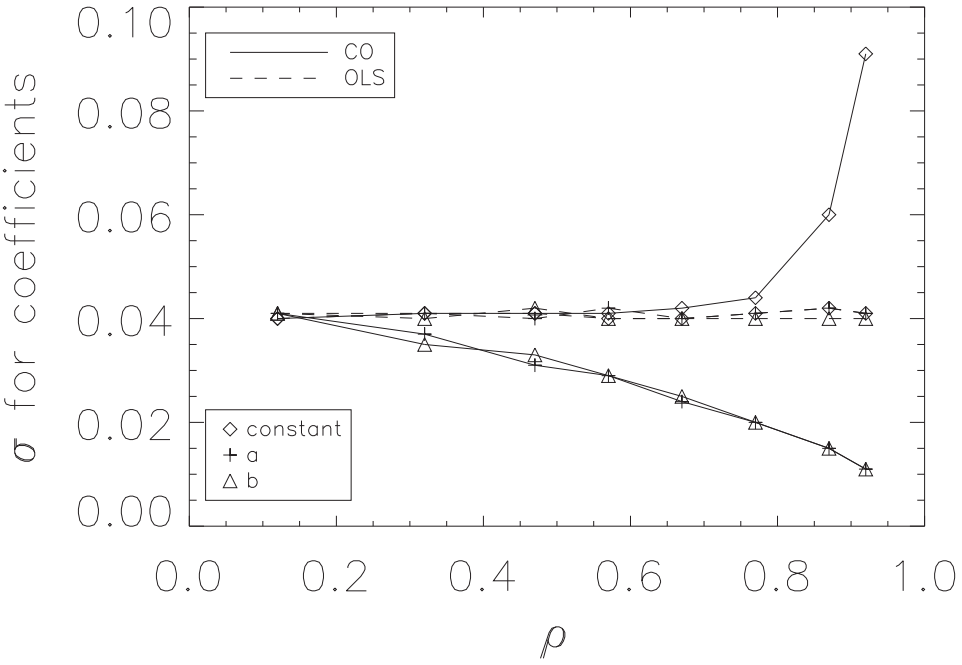

Figure 3: Results of several experimental trials comparing OLS and CO results, for selected values of the parameter controlling the serial correlation of the residuals, ρ, with variables that themselves are neither auto-correlated nor mutually correlated. The experiments are as in Figure 1. The ordinate gives the standard deviation in the OLS or CO determination of the regression constant and coefficients over 1000 trials. Solid lines connect CO results, dashed OLS.

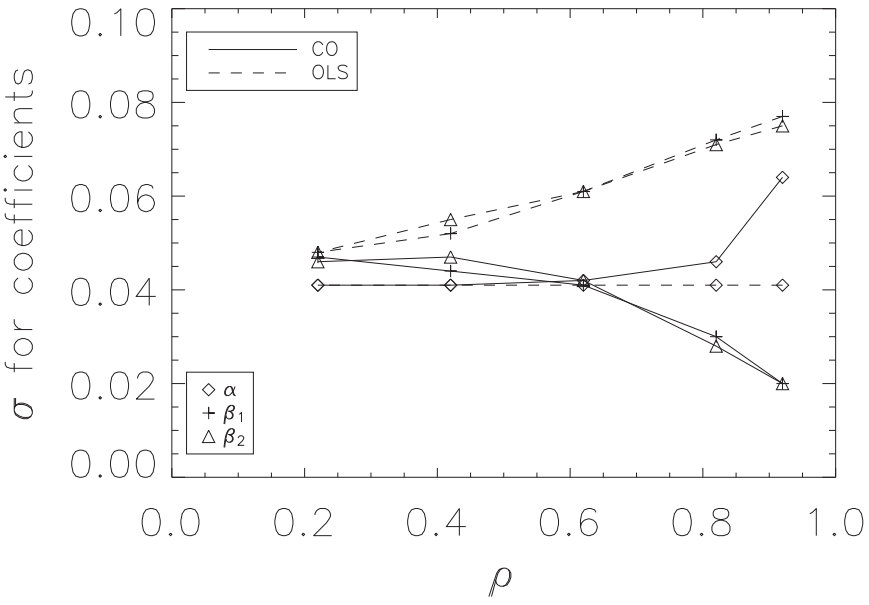

Figure 4: As Figure 3, a summary of results for the regression constant and coefficients, in 1000 trials of series 100 points long, using now series that each are auto-correlated (α_1=0.6) but mutually un-correlated - i.e. each set of series are selected for being not correlated above the level of $R = 0.1$.

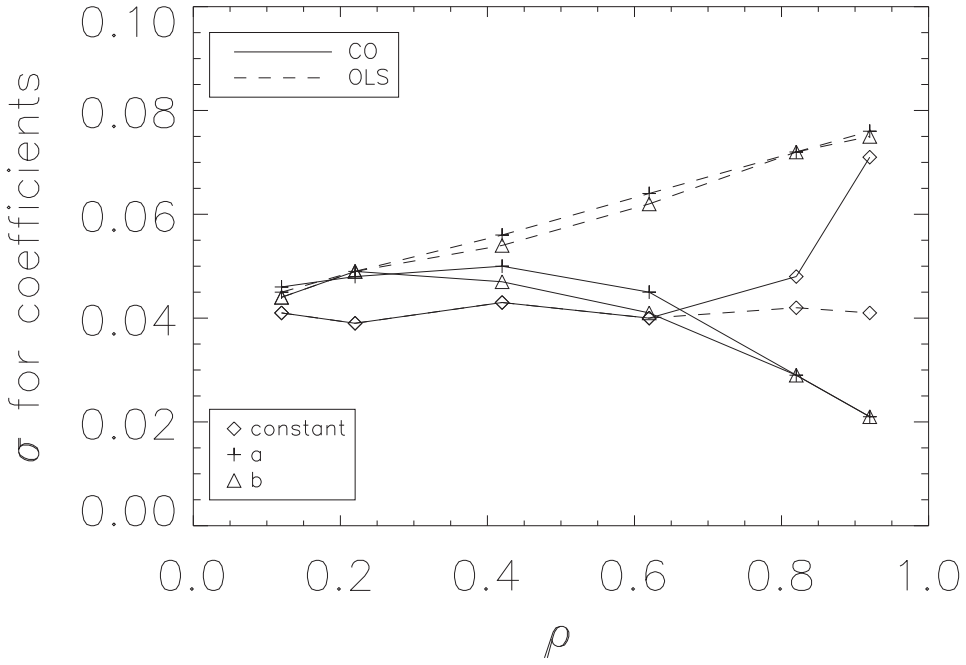

Figure 5: As Figure 3, a summary of results for the regression constant and coefficients, in 1000 trials of series 100 points long, using now series that each are auto-correlated (α_1=0.6) but also mutually correlated at least by $R = 0.3$.

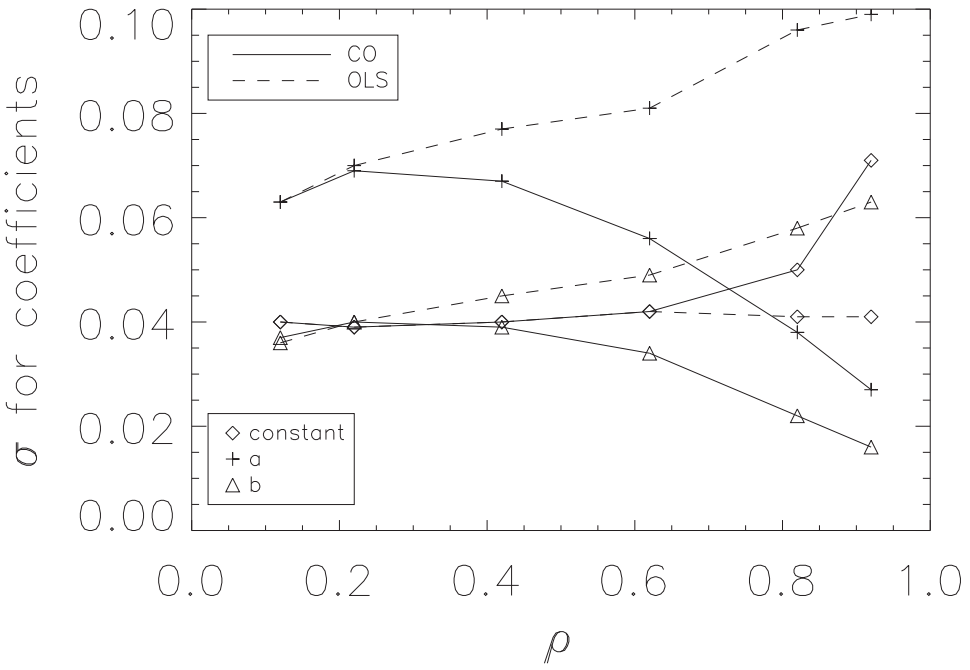

Figure 6: As Figure 5, a summary of results for the regression constant and coefficients, in 1000 trials of series 100 points long, using now series that each are auto-correlated (α_1=0.6) but also mutually correlated at least by $R = 0.7$.

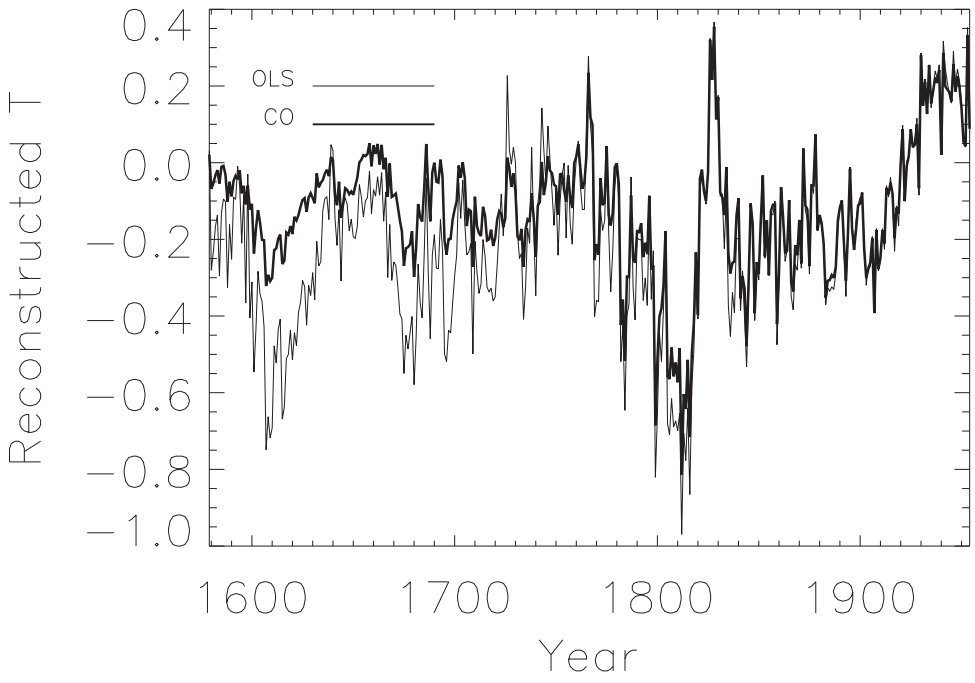

Figure 7: Proxy scaling example.

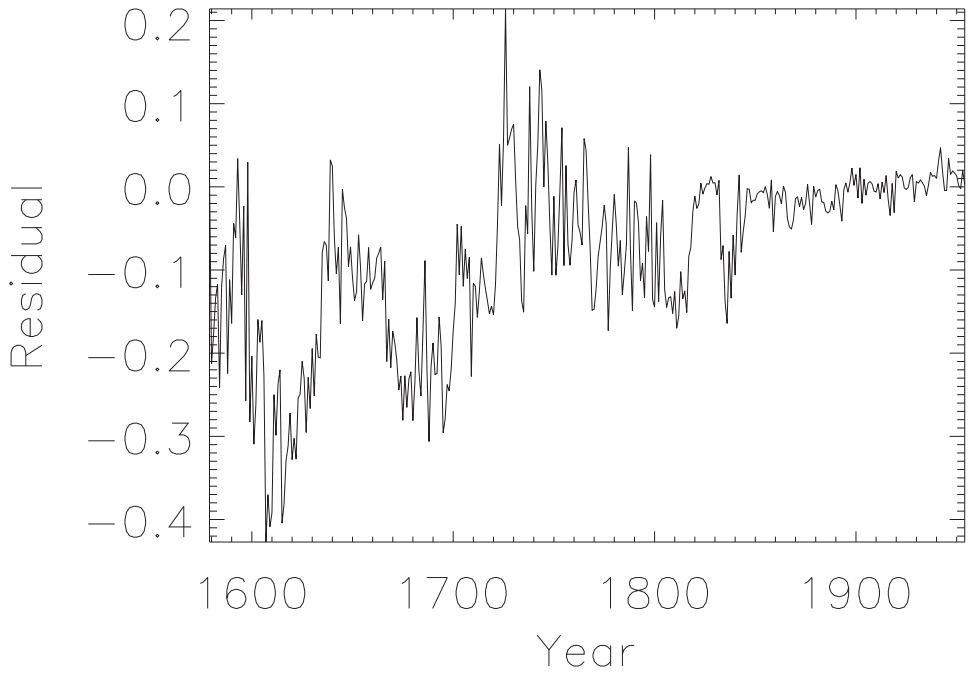

Figure 8: Proxy scaling example - Residuals (T_{OLS}-T_{CO}). The figure shows the difference (in degrees C) between the reconstruction in Landsberg and Groveman's method using OLS and CO.

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