From Eötvös to mGal

Study Team 2 – Workpackage 4

Scientific Data Production Quality Assessment using local space-wise preprocessing

FINAL REPORT

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A. Albertella, F. Migliaccio, F. Sansó

DIIAR, Politecnico di Milano

C.C. Tscherning

University of Copenhagen, Dept. of Geophysics

Summary

In WP4 the problem of quality assessment for GOCE data has been studied. Basically, procedures for outliers detection and removal have been identified, from two different points of view. In Sec. 4.1 the problem was studied in a track-wise approach, by the group of POLIMI. In Sec. 4.2 the problem was studied in an area-wise approach by C.C.Tscherning (UCPH). While the track-wise approach can be applied to the data on-the-fly, in the area-wise approach data of different types can be used as a whole. However, the second approach requires that characteristic values constant over an area be a-priori computed and subsequently updated as GOCE data become available.

4.1 Rejecting outliers in a series of time-wise regularly distributed data

4.1.1 The problem and the proposal

We have a regular time series of observed data

$$
\begin{aligned}
F_0(t_i) &= f(t_i) + \nu_i \\
f(t_i) &= \text{signal} \\
\nu_i &= \text{white noise} \\
t_i &= i \qquad (i = 1, 2, \cdots N) \ ,
\end{aligned}
\tag{4.1}
$$

and we want to test this series for the presence of a possible outlying value at k.

To this purpose we make the following hypotheses of extreme simplification:

Hp. 1 : the signal to noise ratio is very high so that we can neglect ν in (4.1),

Hp. 2 : the signal $f(t_i)$ is a stationary time series with zero mean and with a finite correlation function of an a-priori specified form,

Hp. 3 : the signal belongs to a normal family.

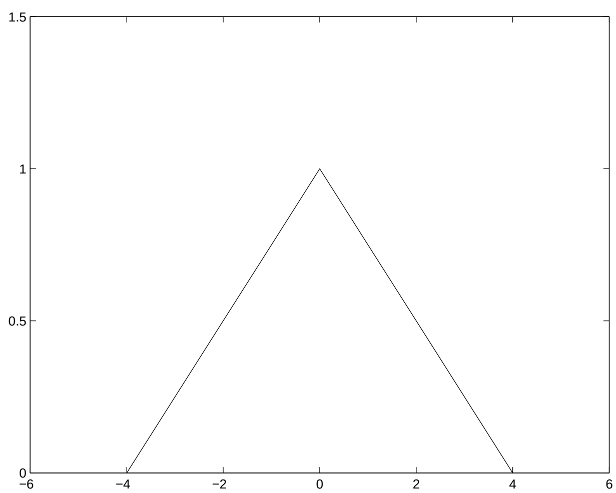

Figure 4.1: The correlation function (4.2) for $\Delta = 4$

In particular in this paper we shall discuss the case that

$$R(\tau) = \frac{E\{f(t+\tau)f(t)\}}{E\{f^2(t)\}} = \begin{cases} 1 - \dfrac{|\tau|}{\Delta} & |\tau| < \Delta \\ 0 & |\tau| \geq \Delta \ . \end{cases} \tag{4.2}$$

Obviously the family $R(\tau;\Delta)$ needs to be adjusted to the data only through the integer parameter Δ, which means the distance at which the true correlation function drops to zero.

Remark 1. To test $F_0(t_k)$ we will consider only data inside the window $[k-\Delta, k+\Delta]$; therefore it is irrelevant that (4.2) could be very different from the true correlation outside the window.

Our proposal is to use (4.2) to perform the prediction $\widehat{F}(t_k)$ from neighbouring data and to compare the prediction error $e_k = F(t_k) - \widehat{F}(t_k)$ with its estimated variance $\mathcal{E}_k^2$; since this in turn depends solely from the estimate $\widehat{C}$ of

$$C = E\{f^2(t)\} \ , \tag{4.3}$$

which is providing together with (4.2) the full covariance information

$$C(\tau) = E\{f(t+\tau)f(t)\} = CR(\tau) \ , \tag{4.4}$$

and since $\widehat{C}$ turns out to be independent of e_k, a sample variable of known distribution can be constructed, suitable to test a deviation from the $E\{F_0(t_k)\} = 0$ hypothesis, i.e. the presence of an outlier.

4.1.2 The prediction, the prediction error and the sample test statistic

We call

$$F_k = F(t_k) = f(t_k), \qquad \underline{F}_0 = \begin{vmatrix} F(t_{k-\Delta}) \\ \vdots \\ F(t_{k+\Delta}) \ , \end{vmatrix} \tag{4.5}$$

$$\underline{C}_{k0} = E\{F_k \underline{F_0}\} = C\underline{r}_0 = C \begin{vmatrix} 0 \\ R(\Delta-1) \\ \vdots \\ R(1) \\ R(1) \\ \vdots \\ R(\Delta-1) \\ 0 \end{vmatrix} \tag{4.6}$$

$$C_{00} = E\{\underline{F}_0 \underline{F}_0^T\} = CR = C \begin{vmatrix} 1 & r_1 & \cdots & r_{\Delta-1} & 0 & 0 & \cdots & 0 \\ r_1 & 1 & r_1 & \cdots & r_{\Delta-1} & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & r_{\Delta-1} & \cdots & r_1 & 1 \end{vmatrix} . \tag{4.7}$$

Then the best prediction of F_k in terms of $\underline{F}_0$ is given by

$$\widehat{F}_k = \underline{C}_{k0}^T C_{00}^{-1} \underline{F}_0 = \underline{r}_0^T R^{-1} \underline{F}_0 \ ; \tag{4.8}$$

as we can see, due to Hp. 1, $\widehat{F}_k$ does not depend on the signal variance C.

On the other hand the estimation error e_k is given by:

$$e_k = F_k - \widehat{F}_k = F_k - \underline{r}_0^T R^{-1} \underline{F}_0 \ . \tag{4.9}$$

As for the variances and covariances the following formulas are easily derived from (4.5), (4.6), (4.7). (4.8);

$$\begin{aligned} \mathcal{E}_k^2 &= E\{e_k^2\} = C - 2\underline{r}_0^T R^{-1} C_{F_0 F_k} + \underline{r}_0^T R^{-1} C_{F_0 F_0} R^{-1} \underline{r}_0 = \\ &= C - 2C\underline{r}_0^T R^{-1} \underline{r}_0 + C\underline{r}_0^T R^{-1} \underline{r}_0 = \\ &= C\{1 - \underline{r}_0^T R^{-1} \underline{r}_0\} \ , \end{aligned} \tag{4.10}$$

$$E\{e_k \underline{F}_0^T\} = E\{F_k \underline{F}_0^T\} - \underline{r}_0^T R^{-1} C_{F_0 F_0} = C\underline{r}_0^T - C\underline{r}_0^T R^{-1} R = 0 \ . \tag{4.11}$$

Since by Hp.3 $\begin{vmatrix} F_k \\ \underline{F}_0 \end{vmatrix}$ is a normal variate and its linear transform (cf. (4.9))

$$\begin{vmatrix} e_k \\ \underline{F}_0 \end{vmatrix} = \begin{vmatrix} 1 & -r_0^T R^{-1} \\ 0 & I \end{vmatrix} \begin{vmatrix} F_k \\ \underline{F}_0 \end{vmatrix} ,$$

is normal too, we may conclude that

$$e_k = \mathcal{N}[0, C(1 - \underline{r}_0^T R^{-1} \underline{r}_0)] \tag{4.12}$$

$$\underline{F}_0 = \mathcal{N}[0, CR] \ , \tag{4.13}$$

and furthermore e_k and $\underline{F}_0$ are stochastically independent.

Moreover from (4.13) we see that

$$\frac{1}{C} \underline{F}_0^T R^{-1} \underline{F}_0 = \chi^2_{2\Delta} \ , \tag{4.14}$$

where Δ is the width of the data window around $t_k = k$.

From (4.14) we read that an estimator $\widehat{C}$ of C is given by

$$\widehat{C} = \frac{1}{2\Delta}\underline{F}_0^T R^{-1}\underline{F}_0 = \frac{C}{2\Delta}\chi^2_{2\Delta} \ . \tag{4.15}$$

We stress again that e_k is independent of $\widehat{C}$, because $\widehat{C}$ is function of $\underline{F}_0$ only. Then a standard result of testing theory is that

$$T = \frac{e_k}{\sqrt{C(1-\underline{r}_0^T R^{-1}\underline{r}_0)}} \cdot \frac{1}{\sqrt{\dfrac{\widehat{C}}{C}}} = t_{2\Delta} \ , \tag{4.16}$$

with $t_{2\Delta}$ a student t with 2Δ degrees of freedom.

The relation (4.16) writes

$$\frac{e_k}{\sqrt{\widehat{C}(1-\underline{r}_0^T R^{-1}\underline{r}_0)}} = t_{2\Delta} \ ; \tag{4.17}$$

clearly (4.17) holds if (4.12) is true and in particular if

$$H_0: \quad E\{e_k\} = 0 \ . \tag{4.18}$$

Therefore (4.17) is a relation among sample variables, suitable to test (4.18); since the presence of an outlier in F_k (and not in the nearby observations) will tend to increase the empirical value of T, we can test (4.18), at a given significance level α, by accepting it if

$$\frac{|e_k|}{\sqrt{\widehat{C}(1-\underline{r}_0^T R^{-1}\underline{r}_0)}} \leq t_{2\Delta,1-\alpha/2} \tag{4.19}$$

and refusing it if (4.19) doesn't hold true.

Remark 2. In many cases the hypothesis that $E\{F(t_k)\} = 0 \quad \forall t_k$, can be significantly untrue and in particular it can be clearly false for the data in the window $[k-\Delta, k+\Delta]$, so that before applying (4.19) it is advisable to subtract the mean on the interval.

As it is known this has only the effect of modifying (4.15) and (4.19) in the degrees of freedom of the t variate, namely we have

$$\widehat{C} = \frac{1}{2\Delta - 1}\underline{F}_0^T R^{-1}\underline{F}_0 \tag{4.20}$$

$$\frac{|e_k|}{\sqrt{\widehat{C}(1-\underline{r}_0^T R^{-1}\underline{r}_0)}} \leq t_{2\Delta-1,1-\alpha/2} \ ; \tag{4.21}$$

as the correct acceptance test at the level α.

Remark 3. We note that the test proposed here is not intended to be used on raw data where very large outliers could occur and we shall assume that large deviations are eliminated by a simple threshold procedure.

In this case empirical estimates of the first correlation coefficients r_1, r_2 on sufficiently long rows is not too much disturbed by the presence of residual outliers, therefore a simple interpolation procedure can be applied to estimated Δ.

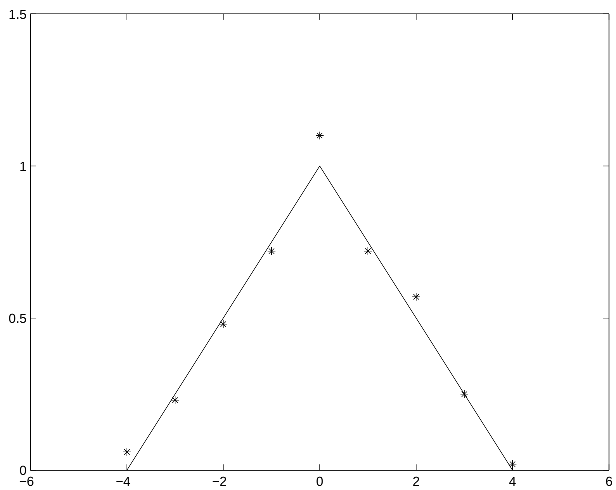

Figure 4.2 : Estimation of the interval Δ

We note also that Δ, rounded to an integer value, gives the width of the window in which we consider the data entering into the test procedure.

4.1.3 Numerical experiments

In order to test the procedure for outlier rejection described in the previous Sections we decided to synthesize time series of GOCE data. Our simulations were performed in a simplified way, yet they were useful to check our equations.

For each simulation we fixed the value of longitude λ, and generated values of T_{zz} at time intervals $\Delta t = 1\ s$, using the EGM96 gravity model from $\ell_{\text{min}} = 10$ to $\ell_{\text{max}} = 90$. The empirical covariance function was computed for several sets of data, to analyze the behaviour in the different cases and try to find out any characteristic pattern. What we found out was either that the function was equal to zero after about 50 seconds or that, after this time span, a point of inflection appeared. A typical result is represented in Fig. 4.3, for two time series of values, respectively belonging to the northern hemisphere and to the southern hemisphere.

In the first case the first zero appears after 98 seconds, and at about 50 seconds a point of inflection is present. In the second case the first zero appears after 74 seconds.

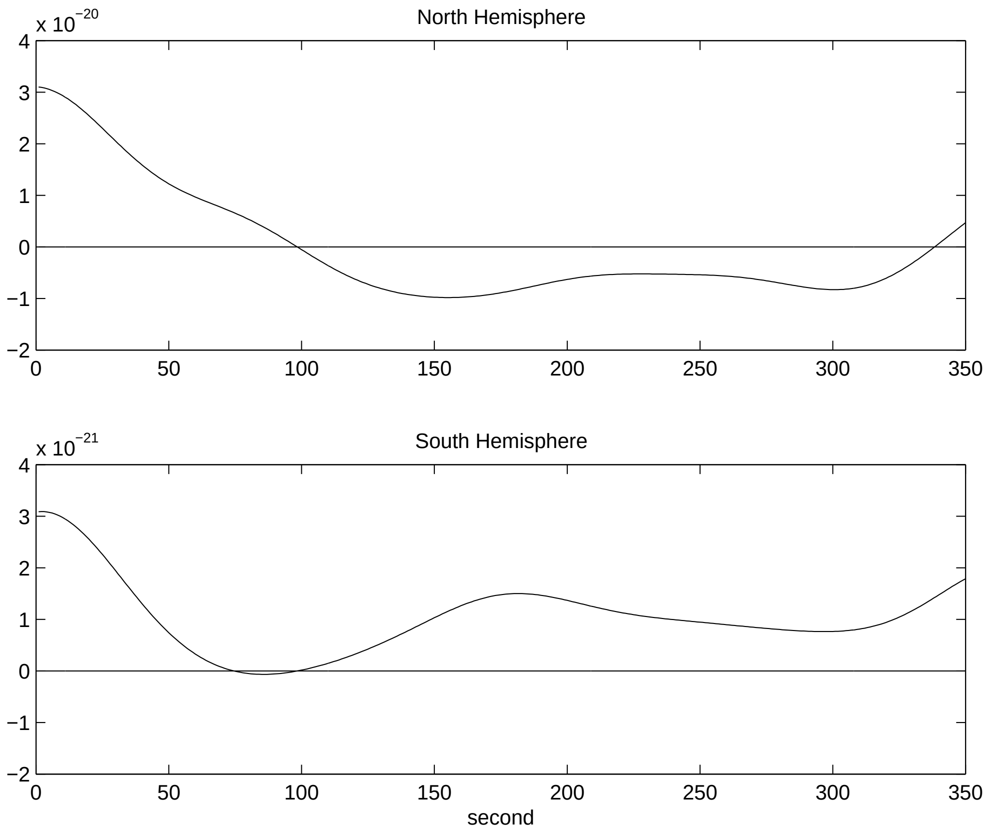

Figure 4.3 : Empirical covariance functions for time series in the Northern hemisphere ($\vartheta = 45° \div 90°$, $\lambda = 35°$) and in the Southern hemisphere ($\vartheta = 100° \div 140°$, $\lambda = 200°$)

However when we try to interpolate the empirical covariance function with a triangular function (as the one used in the approach described before) the first zero is always reached at a position very near 50 seconds. Consequently, it seemed useful to fix a unique value of the parameter Δ (namely $\Delta = 50\ s$) for all the arcs we simulated. This could be useful in the analysis of real series of GOCE data, in order to have procedures as automated as possible.

We performed the test (4.21) for the two series of data corresponding to the empirical covariance functions of Fig. 4.3. As a first test, we added to the simulated data white noise of the order of 10^{-3}. No outliers were included in the series. The student t variate obtained for the data belonging to the two series are represented in Fig. 4.4 as a function of colatitude. As one can see, the “empirical” values are always below the value $t = 2$, which corresponds to a significance level $\alpha = 5\%$ for the t test, with 99 degrees of freedom.

Afterwards, outliers were added to both data series, with a standard deviation of 10^{-2}. Namely, three outliers were included in each set of data at the positions corresponding to 110, 200 and 310 seconds.

Looking at the uppermost graphs of Fig. 4.5 and Fig. 4.6 (for the Northern hemisphere

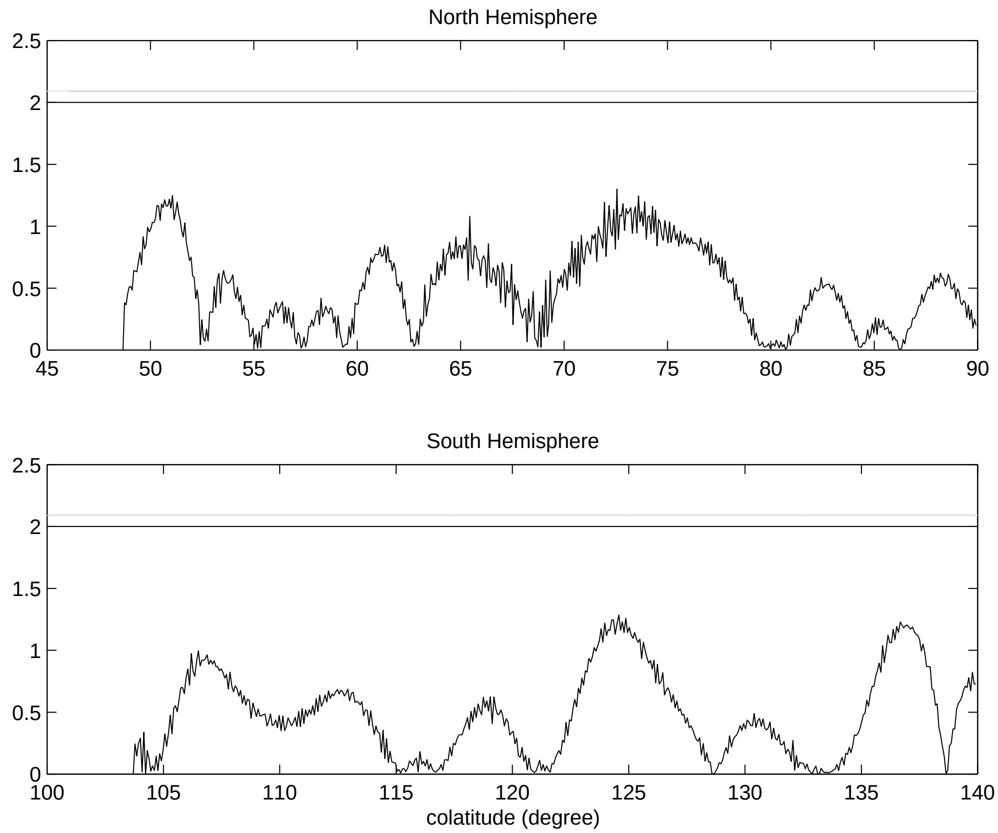

Figure 4.4 : Comparison of empirical t values with the critical value $t = 2$ corresponding to the covariance functions of Fig. 4.3, without outliers and with noise std $= 10^{-3}$

set of data and for the Southern hemisphere set of data, respectively) one sees the results of the t test after including these outliers. One would expect to have the rejection of the hypothesis only at the positions corresponding to the simulated outliers ($\vartheta = 52°.60,\ 58°.82,\ 66°.43$ for Fig. 4.5 and $\vartheta = 107°.60,\ 113°.82,\ 121°.42$ for Fig. 4.6). On the contrary, in both cases there are several points for which the value of t (cf. Eq. (4.21)) exceeds the threshold value $t = 2$ and are therefore reported as further outliers.

Looking at the graphs, it is evident that these points correspond to the positions at a distance of $\pm\Delta$ from the simulated outliers. This is a typical resonance behaviour, due to the fact that for the theoretical covariance function a very simplified model has been chosen; in particular, the function is not smoothed in the neighbourhood of its zero points.

The problem now is to discriminate between "real" and "fictitious" outliers. A simple procedure was devised to this purpose. Namely, the suspected outliers are rejected starting from the one corresponding to the highest value of t. This not only eliminates the "real" outlier, but also the resonance peaks it generates. The result is seen in the second graph of Fig. 4.5 and Fig. 4.6 respectively. The procedure is iterative, and at each step the observation with the highest value of t is eliminated. After the third step

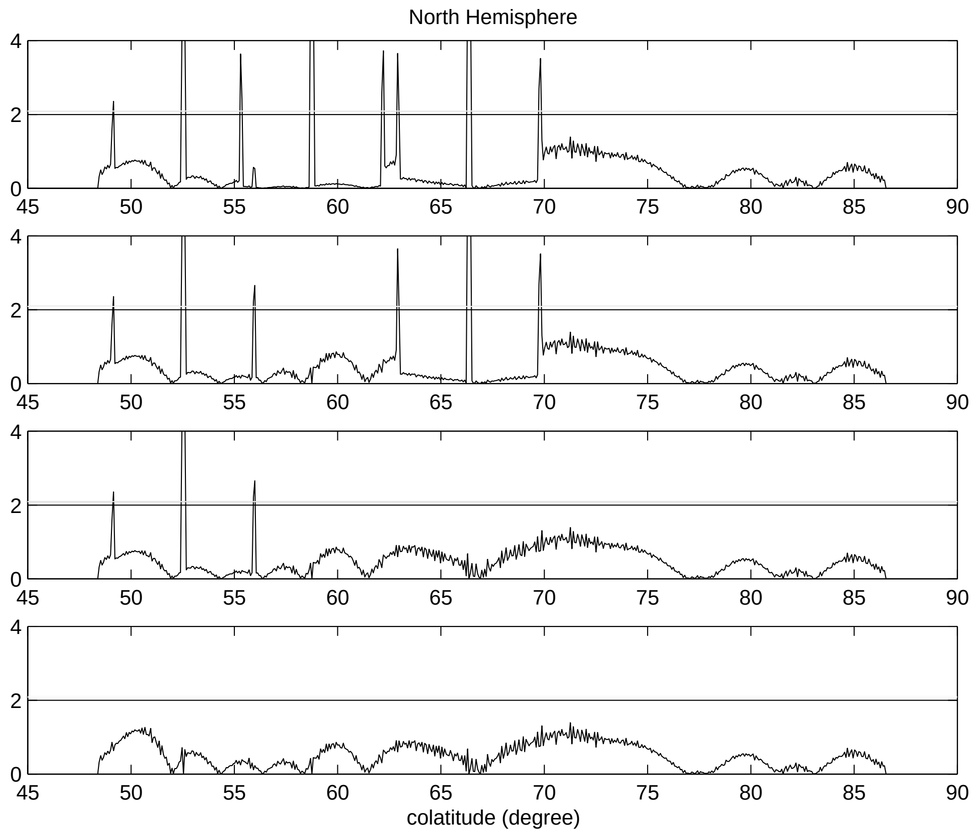

Figure 4.5 : Results of the t test performed on the data in the Northern hemisphere, including three outliers with noise std $= 10^{-2}$. The sequence shows the iterative procedure applied.

(as we had three outliers in the data), no points are left exceeding the threshold value, even if the "critical" points were far more than three.

4.1.4 Conclusions on outliers rejection in the track-wise approach

A procedure for outlier rejection has been devised, based on a hypothesis test which uses a statistics (cf. Eq. (4.21)) with student t distribution.

Though the procedure has been purposely designed in a simple way, it is effective in the identification and removal of outliers. Besides, its plain concept makes it suitable for automatic implementation.

Finally, we like to point out that the computing time needed to complete the procedure seems to be quite short even for long series of data.

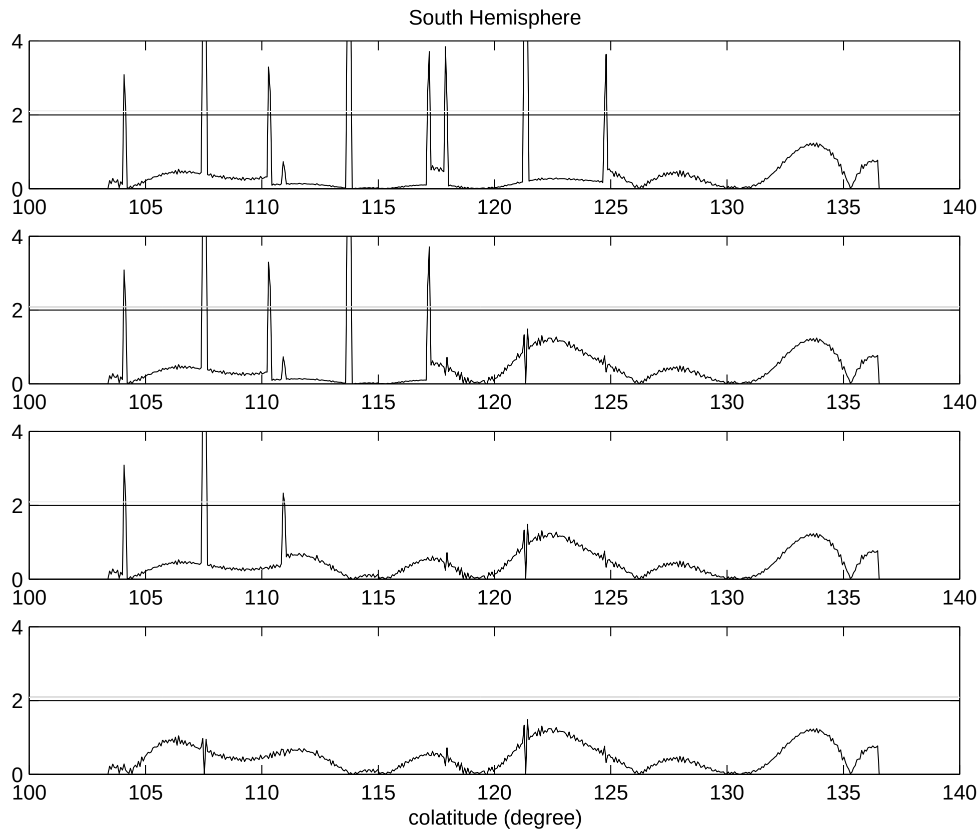

Figure 4.6 : Results of the t test performed on the data in the Southern hemisphere, including three outliers with noise std $= 10^{-2}$. The sequence shows the iterative procedure applied.

4.2 Local Preprocessing

4.2.1 General remarks

The quality assessment of the GOCE data has two aspects: (1) detection of gross-errors and (2) verification (or rejection) of the a-priori error model of the data. We will here primarily deal with the first aspect.

When searching for gross-errors it is advisable to work with data which have a signal to noise ratio as small as possible. This implies that we are making here a hypothesis which is different from Hp.1 (see Sec. 4.1.1). The knowledge of the value of the actual signal variance becomes important and we will now suppose that a general harmonic covariance model is available such as the one described in [14].

A small signal to noise ratio may be achieved by

- removing the contribution from a global gravity field model (EGM96 and iteratively the first GOCE-models);
- removing the contribution from ground gravity data by upward continuation;
- removing the contribution from the potential of the residual topography (residual, because the long-wave-length parts are already contained in the global models).

Software to carry out these tasks is included in the GRAVSOFT package [13].

4.2.2 Identification of point or area related errors

Already by calculating the differences with respect to such up-ward continued data, we may be able to detect the larger gross-errors, simply by inspecting the change of the residuals in the along-track direction.

The software in the GRAVSOFT package also includes programs for error-detection, which for example are used by the Bureau Gravimetrique Internationale in Toulouse, France. See for example [10] and [11].

The method (Least-Square Collocation, LSC), see Eq. (4.8) predicts a quantity associated with a point or an area from its neighbouring values, contingently just from the data on the same tracks as discussed in Section 4.1. We will as mentioned above not accept Hp.1, so the solution will depend on the signal variance, and the (contingently correlated) noise matrix must be added to the C_{00} matrix.

LSC also has the capability of calculating the error-estimate, cf. Eq.(4.10) and may take into account local biases or trends (like Kriging). If the difference between observed and predicted (interpolated) value (cf. Eq.(4.9)) is larger than the noise-level multiplied by a factor (typically 3), the point is flagged. The prediction may be carried out

(a) from the neighbouring (same track or same area) values only, or

(b) by including the point itself in the prediction.

If the points are close, the physical correlation with the neighbours will assure that the predicted value is heavily dependent on these values, and a residual will occur. Both procedures have been implemented.

Method (a) has been implemented in a version of the program GEOGRID, called GEOGRIDE. It has the disadvantage, that only one quantity can be used, i.e. one can not mix gravity gradient components. The program predicts a value from the N (typically 10) closest points. This means that N equations with N unknowns have to be calculated for each point or area element. However, systems of such a small size are very fast to invert.

Method (b) is implemented in the program GEOCOL. This program is not set up to handle small batches of data, but GEOGRIDE could be modified to do this. The program has the advantage that data of different types can be mixed. This means than not only neighbouring values may be used in the error-detection, but also values of a different kind, i.e. one gradient component may aid in detecting an error in the other. (This is in some way related to the fact that one may use the condition that the 3 diagonal elements in the gravity gradient matrix must sum to zero after removal of rotation).

Both procedures are feasible, but have some problems. The prediction will - depending on the magnitude of the gross-error - not only identify the erroneous value, but frequently also the neighbouring values as candidates for being considered gross errors. An iterative technique must there be used, which has not yet been automated.

The most simple method is to sequentially remove the largest suspected outliers. This is a drastic method, and it is preferably to perform a down-weighting, which is a function of the magnitude of the residual, as done in geodetic network adjustment, [7], [6]. The proper function to be used with SGG and SST data has not yet been found.

Furthermore, both procedures depend on the knowledge of the physical correlation between the data values. This correlation may be estimated and used. This is however quite demanding computationally, and statistical characteristics constant for an area (e.g. 5 deg. x 5 deg.) are frequently used. These characteristics may be initially pre-computed from ground data and stored in a data-base (see [8]). The characteristics (signal variance and correlation distance) may then be updated when satellite data become available. Alternatively a global statistical model may be constructed as discussed in [12].

4.2.2.1 Case study

Experiments have been carried out with 242 vertical gravity gradient data (T_{zz}) at 300 km altitude, generated from EGM96. The data were located on 2 meridians and had a spacing of 0.25 degrees. The data (removing the contribution of the low harmonics) had a mean of -0.01 EU and a standard deviation of 0.1 EU, i.e. quite a typical "residual value" data set.

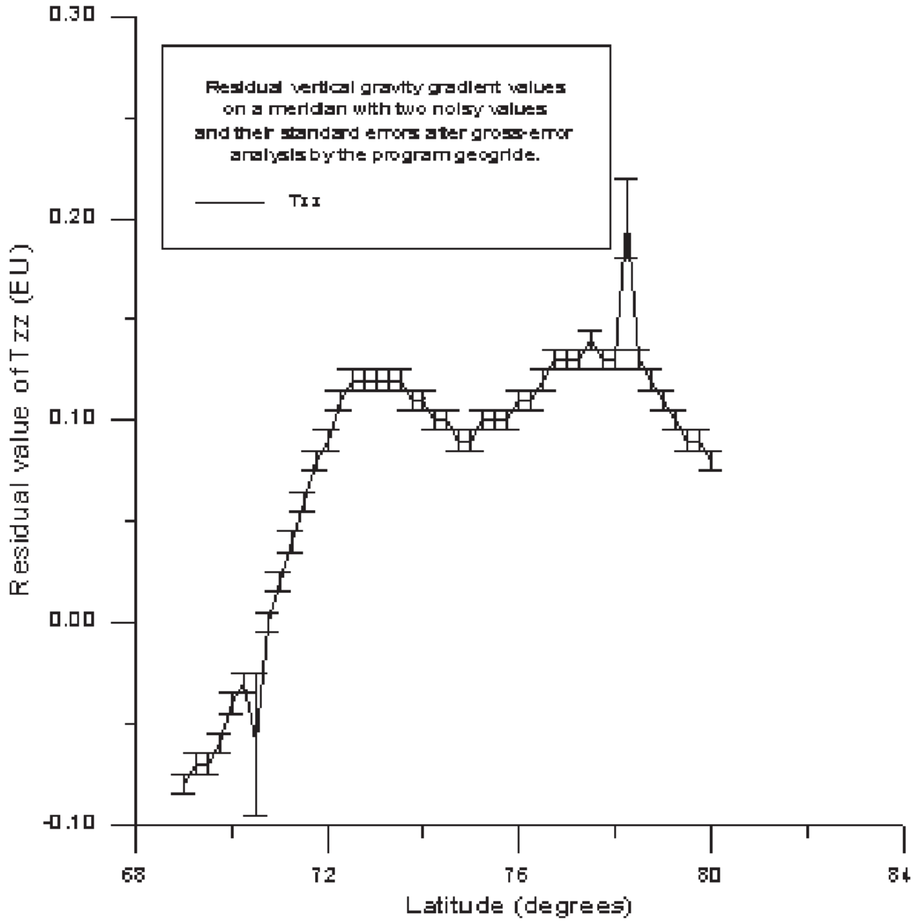

Figure 4.7 : Showing data with a-posteriori error bars.

A number of tests were performed, using correlation lengths between 2.0 degree and 3.5 degree.

The data were initially supposed to have an error of 0.005 EU in one case and 0.01 in the following test. For two values an outlier was added (0.03 and subsequently 0.07 EU). The two points were identified as errors in both cases. But for the case with an error of 0.07, also a neighbouring value was identified as having a possible gross-error.

When the standard-deviation was raised to three times the error of interpolation for the largest residuals the neighbour was not anymore identified as a “suspect”. The use of a short correlation distance did result in the identification of a neighbouring point as an outlier, while the use of the longer distance did not result in this. This is quite natural, considering that the larger correlation results in an increased influence of “good” data on the result.

4.2.3 Identification of systematic errors (biases, tilts)

The identification of systematic errors is a very difficult procedure. It requires that independent data are available. Such data are available in some land areas with modern gravity measurements tied to the IGSN71 global reference system.

In such areas gravity data may be used to calculate upward continued SGG and SST data, and then used together with the satellite data for the detection of e.g. biases and tilts [5]. The program GEOCOL may be used for this purpose, but also procedures which do not demand the same computational effort might be used. Upward continuation using a global gravity model or by FFT should be feasible, but these methods do not give error-estimates. However, a simple comparison of upward continued data with the SST and SGG data might give the first hints about contingent systematic errors.

4.2.4 Data filtering

The data will probably have different assigned errors, e.g. depending on the solar activity, the air density variations and the varying altitude. This must be taken into account when deriving various products from the data. Furthermore we know that the errors will be correlated.

The LSC method includes the capability for handling these problems, and it has been demonstrated (see [5]) using airborne gravity gradiometer data that the proper treatment of correlated errors gives improved results.

In theory - and as verified in practice - LSC is the optimal method for the filtering of the data. It will probably at the time of the launch of GOCE be difficult to construct global solutions using this methods, but regional solutions are easily constructed. Furthermore the local prediction of block-averages (to be used in a weighted integration procedure) is easily performed using GEOCOL.

4.2.5 Conclusions on local preprocessing

We have proposed and analyzed a simple and fast method of error detection which uses minimal a-priori information. This method may be very useful when analysing the first GOCE data. Further software developments and tests are necessary to assure the functionality of the technique.

General least-squares collocation with a-priori modeled covariance functions and known error characteristics require a somewhat larger numerical effort. However GRAVSOFT programs exist which are capable of local preprocessing of GOCE data. Both data filtering and regional predictions of all relevant quantities may be executed.

Supporting statistical information should be made available at the time of the launch, i.e. local statistical parameters, and updated as a part of the data-processing chain.

The use of several SST or SGG components in local preprocessing in an automatic manner requires certain software developments, which should be finished before the launch of GOCE.

4.3 Final conclusions and perspectives

Concerning the specific WP4 we believe that the capability of testing and assessing the quality of gradiometer data by the space-wise approach has been demonstrated.

This, when developed into a final form, together with the proposed cross overs analysis, can constitute a sound basis for data preprocessing and data quality assessment in the framework of space-wise data analysis.

In general the whole space-wise approach has done some significant steps forward, although we still have some points to clarify and analyze more in dept. In particular

- the integration procedures will be re-analized, in the light of some new ideas, also criticizing the standard block averaging processes;
- the whole theoretical basis of the space-wise approach has to be revisited, by providing a thorough numerical proof that the knowledge of low degree models, can completely resolve the restrictions imposed by the use of observations with measurement bandwidth.

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