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ORIGINAL PAPER

PERFORMANCE COMPARISON OF LEAST SQUARES, ITERATIVE AND GLOBAL L_1 NORM MINIMIZATION AND EXHAUSTIVE SEARCH METHODS FOR OUTLIER DETECTION IN LEVELING NETWORKS

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ABSTRACT

Different approaches have been proposed to determine the possible outliers existing in a dataset. The most widely used consists in the application of the data snooping test over the least squares adjustment results. This strategy is very likely to succeed for the case of zero or one outliers but, contrary to what is often assumed, the same is not valid for the multiple outlier case, even in its iterative application scheme. Robust estimation, computed by iteratively reweighted least squares or a global optimization method, is other alternative approach which often produces good results in the presence of outliers, as is the case of exhaustive search methods that explore elimination of every possible set of observations. General statements, having universal validity, about the best way to compute a geodetic network with multiple outliers are impossible to be given due to the many different factors involved (type of network, number and size of possible errors, available computational force, etc.). However, we see in this paper that some conclusions can be drawn for the case of a leveling network, which has a certain geometrical simplicity compared with planimetric or three-dimensional networks though a usually high number of unknowns and relatively low redundancy. Among other results, we experience the occasional failure in the iterative application of the data snooping test, the relatively successful results obtained by both methods computing the robust estimator, which perform equivalently in this case, and the successful application of the exhaustive search method, for different cases that become increasingly intractable as the number of outliers approaches half the number of degrees of freedom of the network.

1. INTRODUCTION

The theory of statistical testing for outlier detection in a set of measurements has received considerable attention in the last half century (Rofatto et al., 2020). After the pioneering works by Baarda (1968) and Pope (1976), which established its foundations for the case of a single outlier, the theory of statistical testing after least squares adjustment has tried to be extended to the case of multiple outliers by many authors (e.g., Cross and Price, 1985; Ding and Coleman, 1996; Knight et al., 2010).

In the case of multiple outliers, sometimes called multiple gross errors (though the term gross error refers to an incorrect observation which may or not cause and outlier, and outliers are not always caused by gross errors), there is an inherent difficulty, however: since there are different sets of observations – contaminated by different numbers and sizes of outliers – leading to exactly the same least squares solution, the attempts to build a general, always successful approach solely based on the examination of the least squares solution with no additional or alternative assumptions are doomed to failure (Baselga, 2011b).

Robust estimation is built on one of such alternative assumptions: observations are no longer assumed to follow Normal distributions but other, to a certain extent similar, type of distribution so that the corresponding adjustment of observations is obtained by minimizing a particular function of residuals (e.g. the sum of absolute values, also known as L_1 norm) other than the sum of their squared values (Huber, 1981). This results in a solution maximally resistant to the occurrence of not only gross but also systematic errors. The particular shape of the function that

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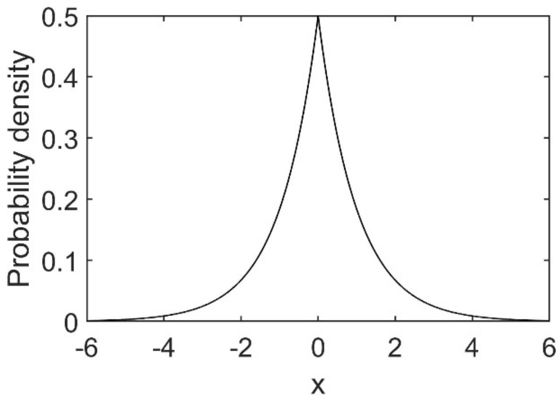

Fig. 1 Double exponential function.

observations are assumed to follow – more due to its practical performance in ruling out undesired errors than to fundamental reasons – is, however, one of the things that cannot be established with universal validity in view of the results obtained for different scenarios, although the double exponential function, Figure 1, leading to the minimization of the L_1 norm of residuals is one of the most commonly used functions in robust estimation (Fuchs, 1982; Harvey, 1993; and Yetkin, 2011, to name a few).

To achieve the minimum of the L_1 norm of residuals, a process based on iteratively reweighted least squares adjustments (with weights computed from the residuals in the previous iteration) is normally followed (Koch, 1996). This easy procedure may result, however, in a local rather than the global minimum of the function or, in other words, in a suboptimal solution due to the unsatisfactory computation process. In Baselga (2007b) it was proposed to abandon altogether the least squares adjustment, not only as the estimator entailed by the assumption that observations are normally distributed, but also as the working tool for achieving minimization of L_1 norm, in favor of the use of a global optimization method instead. This has the advantage of guaranteeing the solution to be not only a local but the global minimum.

In this paper we want to study the differences in the adjustment results obtained after the computation of the minimum L_1 norm by iteratively reweighted least squares and the computation of the minimum L_1 norm by global optimization methods. It is common practice to use the approach of iteratively reweighted least squares, basically due to its ease of implementation for those accustomed to using least squares theory, rather than approaches based on optimization methods, such as genetic algorithms, simulated annealing, the simplex method, etc., that should give the optimal solution. This solution will sometimes coincide with the one obtained by iteratively reweighted least squares and sometimes not, being the latter a suboptimal solution. Among all the existing optimization methods we have selected the simulated annealing method, understanding that it yields the global optimum (in fact this is only guaranteed in probabilistic terms, as explained later on) as it would be equally reached by the simplex method, genetic algorithms or other optimization methods. Comparisons among different optimization methods in terms of computational time are beyond the scope of the current paper, since they deviate from our current topic of research and can be found in other publications (see for instance Ingrassia et al., 2013).

Other robust estimators, such as Huber's estimator, may be more appropriate than the minimum L_1 norm as it has been shown in the extensive testing of robust methods based on M-estimates by Trasak and Stroner (2014); however, this idea will not be pursued in this paper as it is only concerned with the comparison of the minimum L_1 norm in two different computational approaches (iteratively reweighted least squares and global optimization methods), with the minimum L_2 norm (least squares) and the exhaustive search procedure.

Other strategies may also be followed for outlier detection. One very simple is the elimination of one (or several) observation(s) followed by the computation of the corresponding least squares adjustment and comparison with the least squares adjustment of the entire set of observations. This strategy has several drawbacks being one of them the need for a rigorous theoretical statistical foundation that permits to compare both solutions and decide when one solution is significantly better than the other (from a statistically rigorous point of view). Another inconvenience is the computational burden to exhaust all possibilities up to a reasonable number of observations to be eliminated, so that the analysis can be done in a thorough manner, independently of the user's intuition on where an outlier can be located. This strategy was named exhaustive search procedure in Baselga (2011a).

General rules or advice on which of these approaches should be followed in presence of a geodetic network contaminated by outliers cannot be made by and large. Factors as the type of geodetic network, number and size of possible errors, and available computational force prevent one to give any possible universal recipe. We would like to explore, however, if some conclusions could be drawn for the case of a leveling network.

Leveling networks have a particularly simple geometry compared with planimetric or three-dimensional networks, which makes it easier to discover the occurrence of possible outliers. Some cases may still be challenging, though, especially those where the number of outliers approaches half of the degrees of freedom number.

In the present work we compare the performances for the case of a leveling network of the least squares adjustment approach with possible application of Baarda's data snooping test (for one outlier or several of them after iterative elimination of the worst outlier indicated and subsequent readjustment), robust estimation by minimization of L_1 norm (be it by iteratively reweighted least squares as well as by using a global optimization method) and the exhaustive search procedure after exploration of all possible sets of observations containing outliers.

2. METHODS

The above-mentioned approaches are now reviewed before analyzing their application to a leveling network.

2.1. LEAST SQUARES WITH APPLICATION OF DATA SNOOPING TEST

The standard procedure to adjust an over-determined system of observation equations is the well-known least squares adjustment (e.g. Kaczmarek and Kontny, 2018; Li et al., 2019), which can be supplemented with the application of Baarda's data snooping test for outlier detection (one can resort to many general references here for obtaining the complete formulation, e.g. Leick et al., 2015). In short, for the system of m observation equations and n unknowns ($m > n$)

$$Ax - k = r \qquad (1)$$

with vector of unknowns x, matrix of coefficients A, vector of independent terms k and vector of residuals r, the least squares solution satisfying

$$min \sum_i r_i^2 \qquad (2)$$

in the case of observations of unit weight, or

$$min \sum_i r_i^2 p_i \qquad (3)$$

if every observation has a weight p_i, is

$$x = (A^T PA)^{-1} A^T Pk \qquad (4)$$

where P is the weight matrix for the system of equations (1) or the identity matrix if the observations are all of unit weight.

The variance of the unit weight observation is computed as

$$\hat{\sigma}_0{}^2 = \frac{r^T Pr}{m-n} \qquad (5)$$

Introducing the x vector obtained in (4) into (1) permits to obtain the least squares observation residuals, whose covariance matrix can be computed by

$$Q_r = P^{-1} - A(A^T PA)^{-1} A^T \qquad (6)$$

Every observation i can be checked for the occurrence of a possible error by means of the data snooping test, which evaluates the variable

$$\omega_i = \frac{r_i}{\sigma_{r_i}} \qquad (7)$$

comparing the residual of the observation, r_i, with its standard deviation computed from the cofactor matrix (the square root of its element i,i)

$$\sigma_{r_i} = \sqrt{Q_{r_{ii}}} \qquad (8)$$

If the absolute value of the data snooping variable ω_i exceeds a prefixed cutoff value (usually 3.29, for a level of significance of 0.001) then the observation is flagged as containing an outlier.

It is known that the data snooping test assumes the existence of only one outlier (or none) in the dataset (e.g. Caspary and Rüeger, 2000), although false negatives can also occur even with only one outlier (Rofatto et al., 2020) especially if observations are correlated (Baselga, 2007a). Therefore the application of the data snooping test to the case of multiple outliers — routinely done in the fashion of sequential data snooping eliminating the worst observation and readjusting — may result in incorrect identification, so that false positives (i.e. correct observations rejected by the test) and false negatives (i.e. wrong observations that go unnoticed by the test) may occur (Baselga, 2011b). Surprising as it may be, this fact is often overlooked in many works and computing software. As we will see in the application section this may lead to clearly wrong conclusions.

2.2. LEAST L_1 NORM

For using the formulation in this subsection, we assume that all observations have been previously reduced to unit weight so that their corresponding standard deviations are all unity. This prior unit-weight reduction is done by multiplying each equation of the system of equations (1) by the square root of its corresponding weight, so that every value of the coefficient matrix A and vector k are multiplied by $\sqrt{p_i}$, being p_i the weight of the corresponding row, so that an equivalent system of equations of unit weight is obtained (see e.g. Ingram (2010), p. 278). ¨

Now, for the resulting system of equations, finding the minimum of the function

$$min \sum_i |r_i| \qquad (9)$$

produces a more robust result than least-squares, that is, the result obtained is much more resistant to the appearance of outliers in the observations.

This robust estimator is often computed in the fashion of *iteratively reweighted least-squares* adjustments using an equivalent weight function. Hence, by weighing each observation as

$$p_i = \frac{1}{|r_i|} \qquad (10)$$

using the residual r_i of the previous iteration, one obtains a least-squares function $\sum_i r_i^2 p_i$ that tends to $\sum_i |r_i|$.

However, as shown in Baselga (2007b), this approach may yield suboptimal results if the solution of the initial iteration (i.e. the least-squares solution) is far away from the correct solution, possibly resulting in a local optimum only.

This is the reason why a *global optimization method* may be preferred instead. In this case an x

vector is found so that the resulting residuals in (1) entail a global minimum of the desired function (9). Among the different successful global optimization methods, we can choose, for example, the Simulated Annealing method. This method uses the Monte Carlo sampling, which is widely used in computing and engineering (e.g. Gruszczyński et al., 2019a, 2019b; Xiang et al., 2019; Rofatto et al., 2020), for attaining the global minimum of a function of many variables by following a scheme that emulates the way crystalline networks are self-constructed in nature (see e.g. Berné and Baselga, 2004).

Put in short, an initial configuration (starting vector x) is modified at random to obtain a new x vector and the resulting value for the objective function – that is (9) after having plugged the residuals obtained in (1) – is computed and compared with the previous value. If the new value for the objective function is smaller than the previous one then the new solution is accepted as base for the next iteration, otherwise the new solution is discarded (except in very few cases, for a prescribed low probability, e.g. 0.01, so that the occasional, rare adoption of worse solutions is permitted as observed in nature, which enables the algorithm not to remain trapped in a local optimum). The first modifications of the initial x vector (which need not be the least squares solution but can be taken as any vector at random inside the search domain) need to be considerably large in size, say one fifth of the search domain width, so that the algorithm can comfortably explore the entire domain. This search domain can be any arbitrarily large region (the larger the domain the more time consuming will result to be the algorithm) but it is customarily constructed for each unknown using its least squares solution x_{LS} and corresponding standard deviation σ_{LS} as $x_{LS} \pm k\sigma_{LS}$ with the conservative assumption of a relatively large k value (say 10). The subsequent modifications of the solution vector, Δx_i for iteration i, are increasingly smaller in size (for each coordinate random displacements taken from a normal distribution $N(0,\sigma)$ with σ evolving in accordance with a simple rule as $\sigma_i = \sigma_0\beta^i$, β taken e.g. as 0.99999, can be used), as emulating the increasingly smaller movements observed in nature as the solid reduces its temperature. The algorithm is finished where the current typical displacement size σ_i is negligible in size (say below 0.1 mm). For a sufficiently slow cooling scheme the desired solution can be eventually found since the convergence to the global optimum in a finite number of iterations is always guaranteed (van Laarhoven and Aarts, 1987; Granville et al., 1994). Subsequent executions of the algorithm (with different initial x vectors) should yield the same solution, which reinforces the security that the global optimum has indeed been reached, something than in practice can only be guaranteed in probabilistic terms. This is why, in what follows, we should understand that by global optimum we are only referring to our numerical determination of the global optimum. More details in the practical implementation of the Simulated Annealing method for solving the minimum L_1 norm problem can be found in Baselga (2007b).

In the present work, we will compute the minimum L_1 norm by both methods – iteratively reweighted least-squares and global optimization – and compare their performances for outlier detection in the case of leveling networks. As it will turn out, contrary to what is expected in general for more complex geodetic problems, where the global optimization method produces better results in the minimization of the L_1 norm, both methods produce here very similar results, which is due to the relatively geometrical simplicity of leveling networks.

2.3. EXHAUSTIVE SEARCH PROCEDURE

As demonstrated in Baselga (2011b), there are many initial observation sets, with different outlier number and sizes, leading to the same least squares solution, so that detection within the least squares framework is impossible without resort to additional or alternative hypotheses (such as, for example, minimization of L_1 norm). We can, however, use a strategy based not only on one least squares adjustment but on the comparison of multiple least squares adjustments (each of them with a number of observations eliminated) with respect to the least squares adjustment of the complete set of observations. This strategy, computed for all possible combinations of observations after having eliminated 1, 2… up to s observations is what was named exhaustive search in Baselga (2011a), where a programming code was also provided for the reader. We use an adaptation of that code for the present study.

To briefly summarize the procedure let us say that the variance of the unit weight observation, equation (5), is computed both for the complete adjustment affected by several outliers ($\hat{\sigma}_{0-global}{}^2$) and for a partial adjustment where several observations have been removed ($\hat{\sigma}_{0-partial}{}^2$). The statistic

$$r = \frac{\hat{\sigma}_{0-partial}{}^2}{\hat{\sigma}_{0-global}{}^2} \tag{11}$$

does not follow an F distribution (neither singly nor doubly noncentral) since numerator and denominator should be independent variables and they are clearly not. The characterization of this statistic in Baselga (2011b) permits to decide on the ascription of a particular result to any of the two existing possibilities with controlled statistical significance:

- The error-error case: when there are one or more outliers in both the numerator and the denominator
- The error-free case: when one of the variances is affected by outliers (the one in the denominator) and the other (the one for the partial adjustment) is free of them

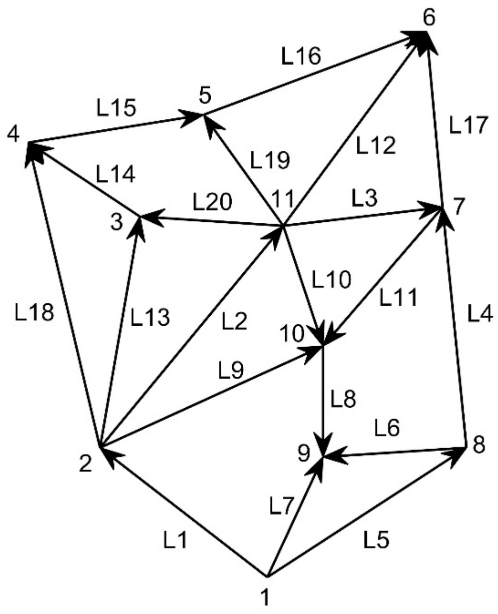

Fig. 2 Leveling network plot.

Also the approximate sizes of the corresponding outliers can be estimated in the process (as they are also given in standard deviation units by the working code accompanying Baselga, 2011b).

One should look for the minimum number of observations permitting to obtain an error-free solution; especially since, as said, one might not expect a unique multiple outlier vector, but, in general, a set of several feasible multiple outlier vectors.

3. EXAMPLES

In the present work we will work with the leveling network presented in Suraci et al. (2019), Figure 2, and personal programming code developed under Matlab R2019b (Matlab, 2019) to examine the performance of the different approaches outlined above for outlier detection. As we can see the situation will become increasingly intractable as the number of outliers approaches half the number of degrees of freedom of the network.

According to our preferences, we can imagine these measurements to be level differences appropriately corrected by means of the corresponding orthometric corrections, hence orthometric height differences using the geoid as reference; or imagine the measurements as normal height differences referred to the quasigeoid (Trojanowicz et al., 2020).

3.1. ONLY ACCIDENTAL ERRORS

The example network presented in Suraci et al. (2019) was simulated with zero error in its measurements; therefore, the least squares adjustment yields only null residual for all its observations. To resemble more a real network we must consider the accidental errors which are inherent to any measuring process, so that we add to each observation a random error extracted from the Normal distribution with zero mean and standard deviation σ_i, where $\sigma_i = 1.0(mm)\sqrt{K_i}$, with K_i the length of the leveling section in km.

Table 1 Example 1 (no outliers). Results of the least squares adjustment (values in mm).

Unknown	Adjusted height	Standard deviation
Z2	163856.5	4.5
Z3	216740.2	5.4
Z4	279641.0	5.5
Z5	283528.3	5.4
Z6	326232.7	5.3
Z7	227343.5	4.7
Z8	101128.7	3.3
Z9	398010.4	3.3
Z10	337572.6	4.6
Z11	170306.2	4.8

The *least squares adjustment* produces satisfactory results. The chi-square test with a level of significance of $\alpha = 0.001$ is passed for a posteriori unit weight variance of 0.880. Point heights for the unknown points (all points except Point 1 whose height is held fixed) are obtained with standard deviations in the range 3 to 5 mm (Table 1).

The residuals and reliability measures are displayed in Table 2. As expected being no outliers, none of the Baarda's data snooping test variables exceeds the critical value of ±3.29 which represents the minimum detectable values also displayed (for $\alpha = 0.001$ significance level and $\beta = 0.80$ power of test). The redundancy numbers range from 0.2930 for the less controlled observation (L6) to 0.7294 for the most controlled observation (L2).

There are minimum discrepancies, from -1.6 to +1.3 mm in residuals and from -2.0 to +2.0 mm in heights, from these values with respect to the ones obtained by minimizing *L_1 norm* (either by the iterative or the global method, since their results coincided completely).

The application of the *exhaustive search* procedure also concluded that there are no outliers, as it was expected.

3.2. ONE OUTLIER

One outlier is added over the previous example. The worst observation in terms of redundancy, observation L6, is selected, and a outlier of +35 mm, which is higher than the minimum detectable error for the observation, 27.5 mm, is added over the simulated measurement in the previous example, which already had been added a random error.

After the *least squares adjustment*, the chi-square test is still passed for an a posteriori unit weight variance of 2.957 but some observations are flagged by the data snooping test as potentially containing outliers (those indicated with an asterisk in Table 3).

Table 2 Example 1 (no outliers). Residuals and reliability measures: Baarda's data snooping test variable, redundancy numbers and minimum detectable errors (values in mm for residuals and minimum detectable errors and unitless for Baarda's test variables and redundancy numbers).

Line	From	To	Residual	wBaarda	Redund.No.	Min. Detectable Error
L1	1	2	1.4376	0.2820	0.5305	39.6930
L2	2	11	-0.0376	-0.0069	0.7294	30.9652
L3	11	7	-6.5034	-1.3287	0.6304	32.0649
L4	8	7	-3.7366	-1.0215	0.3936	38.3866
L5	1	8	-0.2668	-0.0847	0.4510	28.8456
L6	8	9	1.2710	0.6512	0.2930	27.5087
L7	1	9	-0.3958	-0.1208	0.4665	28.9990
L8	10	9	-3.8669	-0.7531	0.5493	38.6080
L9	2	10	-3.4664	-1.5003	0.3559	26.8126
L10	11	10	5.1711	1.4535	0.5273	27.8616
L11	7	10	-4.0255	-0.5999	0.7262	38.1620
L12	11	6	-0.3095	-0.0524	0.6974	34.9689
L13	2	3	3.4022	0.7571	0.5769	32.1681
L14	3	4	1.5994	0.3232	0.5696	35.8849
L15	4	5	4.0268	1.6345	0.3035	33.5269
L16	5	6	6.2245	1.8083	0.4232	33.5945
L17	7	6	-4.1061	-1.6999	0.3071	32.4852
L18	2	4	6.4016	1.3696	0.5602	34.4600
L19	11	5	0.566	0.1525	0.5103	30.0399
L20	11	3	-1.2602	-0.4355	0.3988	29.9707

Table 3 Example 2 (1 outlier simulated in L6 of +35 mm). Residuals and reliability measures: Baarda's data snooping test variable, redundancy numbers and minimum detectable errors (values in mm for residuals and minimum detectable errors and unitless for Baarda's test variables and redundancy numbers).

Line	From	To	Residual	wBaarda	Redund.No.	Min. Detectable Error
L1	1	2	1.5095	0.2961	0.5305	39.6930
L2	2	11	-1.0739	-0.1964	0.7294	30.9652
L3	11	7	-9.5509	-1.9514	0.6304	32.0649
L4	8	7	4.3652	1.1933	0.3936	38.3866
L5	1	8	-12.3805	-3.9305*	0.4510	28.8456
L6	8	9	-8.9848	-4.6035*	0.2930	27.5087
L7	1	9	12.2347	3.7351*	0.4665	28.9990
L8	10	9	7.6414	1.4882	0.5493	38.6080
L9	2	10	-2.4163	-1.0458	0.3559	26.8126
L10	11	10	7.2576	2.0400	0.5273	27.8616
L11	7	10	1.1086	0.1652	0.7262	38.1620
L12	11	6	-1.9267	-0.3263	0.6974	34.9689
L13	2	3	2.6955	0.5999	0.5769	32.1681
L14	3	4	1.4062	0.2841	0.5696	35.8849
L15	4	5	3.4754	1.4107	0.3035	33.5269
L16	5	6	5.0222	1.4590	0.4232	33.5945
L17	7	6	-2.6758	-1.1077	0.3071	32.4852
L18	2	4	5.5017	1.1771	0.5602	34.4600
L19	11	5	0.1510	0.0407	0.5103	30.0399
L20	11	3	-0.9306	-0.3216	0.3988	29.9707

It is worth recalling here that the data snooping test is based on the assumption of a possible single outlier only, although it is frequently used with the unjustified hope of a high efficiency for the multiple outlier case. As said before, its use is only rigorously justified for the case of a single outlier, however, and even then, false negatives can also occur.

Therefore, in this case we should eliminate only one observation, the one with the highest absolute value in the data snooping variable, that is L6, which was the one containing the outlier. After elimination of this observation, the least squares adjustment produces satisfactory results with no observations now flagged by the data snooping test. We see that, as expected, the data snooping test has succeeded in finding one outlier, even given the fact that the corresponding observation was the one with the lowest redundancy number.

Regarding the adjustments minimizing the L_1 *norm*, by the iteratively reweighted least squares as well as the global optimization method (Simulated Annealing), we obtained the residuals displayed in Table 4 in comparison with those of the initial least squares adjustment. The comparison between both

Table 4 Example 2 (1 outlier simulated in L6 of +35 mm). Residuals after the initial least squares adjustment (νLS), minimum L_1 norm by the iterative procedure (νL_{1i}) minimum L_1 norm by the global optimization method (νL_{1g}) and corresponding differences with respect the least squares values (values in mm). The sum of absolute values of the residuals Σ|ν| is given in the last row for each of the three different adjustments.

Line	νLS	νL_{1i}	νL_{1g}	νL_{1i}-νLS	νL_{1g}-νLS
L1	1.5	0.0	0.0	-1.5	-1.5
L2	-1.1	0.0	0.0	1.1	1.1
L3	-9.6	-10.2	-10.0	-0.6	-0.5
L4	4.4	0.0	0.0	-4.4	-4.4
L5	-12.4	-9.1	-8.9	3.3	3.5
L6	**-9.0**	**-20.7**	**-22.0**	**-11.8**	**-13.0**
L7	12.2	3.8	2.7	-8.5	-9.6
L8	7.6	0.0	0.0	-7.6	-7.6
L9	-2.4	-1.7	-2.9	0.7	-0.4
L10	7.3	6.9	5.7	-0.4	-1.5
L11	1.1	1.4	0.1	0.2	-1.0
L12	-1.9	0.0	0.0	1.9	1.9
L13	2.7	4.7	4.7	2.0	2.0
L14	1.4	0.0	0.0	-1.4	-1.4
L15	3.5	3.8	3.8	0.3	0.3
L16	5.0	7.1	7.1	2.1	2.1
L17	-2.7	-0.1	-0.3	2.6	2.4
L18	5.5	6.1	6.1	0.6	0.6
L19	0.2	0.0	0.0	-0.2	-0.1
L20	-0.9	0.0	0.0	0.9	0.9
Σ|ν|	92.4	75.6	74.3	-	-

approaches minimizing the L_1 norm is very slightly in favor of the global optimization method, since the value for the function to minimize, 74.3, is a bit smaller than for the other approach, 75.6, as it is expected for a method that must yield the global optimum, and the residual of the contaminated observation tends a little bit more towards the added error. These very slight discrepancies between both methods for computing the minimum L_1 norm may be considered perfectly negligible, however.

Since the values of the residuals should correct not only the outlier in observation L6 (-35 mm should be expected for this purpose) but also the inevitable accidental errors, one should expect values relatively close to zero for all observations except L6, that is values corresponding to their accidental errors, as well as a value relatively close to -35 for observation L6 (to account for the combination of the gross and the accidental error). In consequence, one can be moderately satisfied with the solution achieved here by both L_1 norm minimization methods since they improve the least squares solution (residual -9.0) but are still a bit far from the expected value, i.e. -35 plus or minus a small variation due to a reasonable accidental error, say an expected value from -25 to - 45, for example.

The exhaustive search method, by contrast, correctly identifies the outlier, indicating that there is only one possible error (one ratio value, in this case 0.31477, below the threshold) for observation L6 with approximate error size of 8.5042 times its initial standard deviation, i.e. some 30.6 mm.

3.3. TWO OUTLIERS

One additional outlier is added over the previous example, now to the second-worst observation in terms of redundancy, observation L15: an outlier of - 40 mm, which is higher than the minimum detectable error for the observation, 33.5 mm.

After the least squares adjustment, the chi-square test is rejected for an a posteriori unit weight variance of 6.775 and some observations are flagged by the data snooping test as potentially containing outliers (Table 5).

Again we should only eliminate one observation, the one with higher absolute value for the data snooping variable, in this case L15. Readjusting the remaining set of observations, we observe that there are still flagged observations, eliminating again the worst, L6, and readjusting we find that there are no more flagged observations. In this case, the iterative application of the data snooping test has succeeded in eliminating the two observations containing outliers (and only these two!) but, as said before, this success is not guaranteed and, as we will experience with more complicate examples, it will not always work.

Minimization of the *L_1 norm* by the iteratively reweighted least squares as well as the global optimization method (Simulated Annealing) produces the results displayed in Table 6, again being extremely similar between them.

In the results minimizing the L1 norm we still see the moderate success in correcting the +35 mm (plus the accidental error) in observation L6, along with

Table 5 Example 3 (2 outliers in L6 of +35 mm and in L15 of -40 mm). Residuals and reliability measures: Baarda's data snooping test variable, redundancy numbers and minimum detectable errors (values in mm for residuals and minimum detectable errors and unitless for Baarda's test variables and redundancy numbers).

Line	From	To	Residual	wBaarda	Redund.No.	Min. Detectable Error
L1	1	2	4.2471	0.8330	0.5305	39.6930
L2	2	11	-5.9861	-1.0947	0.7294	30.9652
L3	11	7	-10.5560	-2.1568	0.6304	32.0649
L4	8	7	2.0137	0.5505	0.3936	38.3866
L5	1	8	-13.2090	-4.1935*	0.4510	28.8456
L6	8	9	-8.5752	-4.3936*	0.2930	27.5087
L7	1	9	11.8158	3.6072*	0.4665	28.9990
L8	10	9	7.0032	1.3639	0.5493	38.6080
L9	2	10	-4.9344	-2.1357	0.3559	26.8126
L10	11	10	9.6517	2.7130	0.5273	27.8616
L11	7	10	4.5079	0.6718	0.7262	38.1620
L12	11	6	-5.7905	-0.9806	0.6974	34.9689
L13	2	3	3.3152	0.7378	0.5769	32.1681
L14	3	4	13.4947	2.7268	0.5696	35.8849
L15	4	5	15.6150	6.3380*	0.3035	33.5269
L16	5	6	11.3984	3.3114*	0.4232	33.5945
L17	7	6	-5.5343	-2.2911	0.3071	32.4852
L18	2	4	18.2099	3.8959*	0.5602	34.4600
L19	11	5	-10.0890	-2.7179	0.5103	30.0399
L20	11	3	4.6013	1.5900	0.3988	29.9707

Table 6 Example 3 (2 outliers in L6 of +35 mm and in L15 of –40 mm). Residuals after the initial least squares adjustment (νLS), minimum L_1 norm by the iterative procedure (νL_{1i}) minimum L_1 norm by the global optimization method (νL_{1g}) and corresponding differences with respect the least squares values (values in mm). The sum of absolute values of the residuals Σ|ν| is given in the last row for each of the three different adjustments.

Line	νLS	νL_{1i}	νL_{1g}	νL_{1i}-νLS	νL_{1g}-νLS
L1	4.2	0.0	0.0	-4.2	-4.2
L2	-6.0	0.0	0.0	6.0	6.0
L3	-10.6	-10.2	-10.2	0.3	0.4
L4	2.0	0.0	0.0	-2.0	-2.0
L5	-13.2	-9.1	-9.1	4.1	4.1
L6	**-8.6**	**-20.4**	**-21.8**	**-11.8**	**-13.2**
L7	11.8	4.1	2.7	-7.8	-9.1
L8	7.0	0.0	0.0	-7.0	-7.0
L9	-4.9	-1.4	-2.8	3.5	2.2
L10	9.7	7.2	5.8	-2.5	-3.8
L11	4.5	1.7	0.3	-2.8	-4.2
L12	-5.8	0.0	0.0	5.8	5.8
L13	3.3	4.7	4.7	1.4	1.4
L14	13.5	0.0	0.0	-13.5	-13.5
L15	**15.6**	**43.8**	**43.8**	**28.2**	**28.2**
L16	11.4	7.1	7.1	-4.3	-4.3
L17	-5.5	-0.1	-0.1	5.5	5.4
L18	18.2	6.1	6.1	-12.1	-12.1
L19	-10.1	0.0	0.0	10.1	10.1
L20	4.6	0.0	0.0	-4.6	-4.6
Σ|ν|	170.5	115.9	114.5	-	-

a highly satisfactory success in correcting the -40 mm (plus accidental error) in observation L15.

Regarding the *exhaustive search* procedure, again it correctly indicates that the possible set of outliers is precisely the one where outliers have been simulated, also giving reasonable estimates for their sizes (Table 7).

3.4. THREE OUTLIERS

One additional outlier is added over the previous example, now in the best observation in terms of redundancy, observation L2: an outlier of +35 mm, which is higher than the minimum detectable error for the observation, 31.0 mm.

Table 7 Example 3 (2 outliers in L6 of +35 mm and in L15 of –40 mm). Exhaustive search method: set of observations deduced to be affected by outliers and corresponding approximate error sizes.

Line	error size (times σ)	error size (mm)
L6	8.1165	29.26
L15	-11.5049	-51.45

Table 8 Example 4 (3 outliers in L2 +35 mm, L6 +35 mm, and L15 -40 mm). Residuals and reliability measures: Baarda's data snooping test variable, redundancy numbers and minimum detectable errors (values in mm for residuals and minimum detectable errors and unitless for Baarda's test variables and redundancy numbers).

Line	From	To	Residual	wBaarda	Redund.No.	Min. Detectable Error
L1	1	2	0.8812	0.1728	0.5305	39.6930
L2	2	11	-31.5134	-5.7628*	0.7294	30.9652
L3	11	7	-13.4287	-2.7437	0.6304	32.0649
L4	8	7	4.3150	1.1796	0.3936	38.3866
L5	1	8	-12.2759	-3.8973*	0.4510	28.8456
L6	8	9	-8.9038	-4.5620*	0.2930	27.5087
L7	1	9	12.4203	3.7917*	0.4665	28.9990
L8	10	9	6.9550	1.3545	0.5493	38.6080
L9	2	10	-0.9160	-0.3964	0.3559	26.8126
L10	11	10	4.1974	1.1799	0.5273	27.8616
L11	7	10	1.9261	0.2871	0.7262	38.1620
L12	11	6	-8.0220	-1.3584	0.6974	34.9689
L13	2	3	8.9829	1.9990	0.5769	32.1681
L14	3	4	12.6666	2.5595	0.5696	35.8849
L15	4	5	17.7117	7.1891*	0.3035	33.5269
L16	5	6	11.7034	3.4000*	0.4232	33.5945
L17	7	6	-4.8933	-2.0257	0.3071	32.4852
L18	2	4	23.0495	4.9313*	0.5602	34.4600
L19	11	5	-12.6254	-3.4012*	0.5103	30.0399
L20	11	3	0.7963	0.2752	0.3988	29.9707

After the *least squares adjustment*, the chi-square test is rejected for an a posteriori unit weight variance of 9.976 and some observations are flagged by the data snooping test as potentially containing outliers (Table 8).

There are many flagged observations but, again we try eliminating one and readjusting at a time. With this strategy we subsequently eliminate L15, L6 and L2 until the remaining set has no flagged observations after the adjustment. In this case, again, the iterative application of the data snooping test has succeeded in eliminating the three observations containing outliers (and only them), although as we know this success was not guaranteed.

Minimization of the *L_1 norm* by the iteratively reweighted least squares as well as the global optimization method (Simulated Annealing) produces the results displayed in Table 9. We can see that both solutions are exactly the same.

Again we see a moderate success in correcting the +35 mm (plus the accidental error) in observation L6, along with a great success in correcting the +35 mm (plus accidental error) in observation L2 and the -40 mm (plus accidental error) in observation L15. In the case of the observation with a high redundancy number, observation L2, we also see that the least squares residual already accounted satisfactorily for the simulated outlier.

The exhaustive search procedure, again, correctly indicates that there is only one possible set of outliers, which is precisely the one where outliers have been simulated (Table 10).

3.5. *FOUR OUTLIERS*

One additional outlier of -35 mm is added over the previous example, now in observation L3, which has the endpoint 11 in common with the observation L2, also affected by an outlier of +35 mm.

After the *least squares adjustment*, the chi- square test is rejected for an a posteriori unit weight variance of 9.535 and some observations are flagged by the data snooping test as potentially containing outliers (Table 11).

With the strategy of eliminating the worse and readjusting we subsequently eliminate L2, L15 and L5 until the remaining set has no flagged observations after the adjustment. Note that in this case the iterative application of the data snooping test fails since it eliminates one correct observation (L5) while retaining two incorrect observations (L3 and L6) in the final set.

Minimization of the *L_1 norm* by the two methods produces the results displayed in Table 12.

Minimization of L_1 norm by both methods produces better results than least squares, that is,

Table 9 Example 4 (3 outliers in L2 +35 mm, L6 +35 mm, and L15 -40 mm). Residuals after the initial least squares adjustment (νLS), minimum L_1 norm by the iterative procedure (νL_{1i}) minimum L_1 norm by the global optimization method (νL_{1g}) and corresponding differences with respect the least squares values (values in mm). The sum of absolute values of the residuals Σ|ν| is given in the last row for each of the three different adjustments.

Line	νLS	νL_{1i}	νL_{1g}	νL_{1i}-νLS	νL_{1g}-νLS
L1	0.9	0.0	0.0	-0.9	-0.9
L2	**-31.5**	**-31.8**	**-31.8**	**-0.3**	**-0.3**
L3	-13.4	-10.3	-10.3	3.1	3.1
L4	4.3	0.0	0.0	-4.3	-4.3
L5	-12.3	-6.0	-6.0	6.3	6.3
L6	**-8.9**	**-22.1**	**-22.1**	**-13.2**	**-13.2**
L7	12.4	5.5	5.5	-6.9	-6.9
L8	7.0	0.0	0.0	-7.0	-7.0
L9	-0.9	0.0	0.0	0.9	0.9
L10	4.2	5.4	5.4	1.2	1.2
L11	1.9	0.0	0.0	-1.9	-1.9
L12	-8.0	0.0	0.0	8.0	8.0
L13	9.0	7.9	7.9	-1.1	-1.1
L14	12.7	0.0	0.0	-12.7	-12.7
L15	**17.7**	**43.8**	**43.8**	**26.1**	**26.1**
L16	11.7	7.1	7.1	-4.6	-4.6
L17	-4.9	0.0	0.0	4.9	4.9
L18	23.0	9.3	9.3	-13.7	-13.7
L19	-12.6	0.0	0.0	12.6	12.6
L20	0.8	0.0	0.0	-0.8	-0.8
Σ|ν|	198.1	149.2	149.2	-	-

Table 10 Example 4 (3 outliers in L2 +35 mm, L6 +35 mm, and L15 -40 mm). Exhaustive search method: set of observations deduced to be affected by outliers and corresponding approximate error sizes.

Line	error size (times σ)	error size (mm)
L2	6.7479	43.21
L6	8.4276	30.39
L15	-13.0497	-58.36

Table 11 Example 5 (4 outliers: L2 +35 mm, L3 -35 mm, L6 +35 mm, and L15 -40 mm). Residuals and reliability measures: Baarda's data snooping test variable, redundancy numbers and minimum detectable errors (values in mm for residuals and minimum detectable errors and unitless for Baarda's test variables and redundancy numbers).

Line	From	To	Residual	wBaarda	Redund.No.	Min. Detectable Error
L1	1	2	4.5502	0.8925	0.5305	39.6930
L2	2	11	-28.4142	-5.1961*	0.7294	30.9652
L3	11	7	8.6357	1.7644	0.6304	32.0649
L4	8	7	-0.5007	-0.1369	0.3936	38.3866
L5	1	8	-13.6276	-4.3264*	0.4510	28.8456
L6	8	9	-7.8612	-4.0278*	0.2930	27.5087
L7	1	9	12.1112	3.6974*	0.4665	28.9990
L8	10	9	3.7505	0.7304	0.5493	38.6080
L9	2	10	-1.6895	-0.7312	0.3559	26.8126
L10	11	10	0.3247	0.0913	0.5273	27.8616
L11	7	10	10.9889	1.6377	0.7262	38.1620
L12	11	6	-15.3937	-2.6068	0.6974	34.9689
L13	2	3	10.5281	2.3429	0.5769	32.1681
L14	3	4	11.3829	2.3001	0.5696	35.8849
L15	4	5	17.2488	7.0012*	0.3035	33.5269
L16	5	6	7.6323	2.2173	0.4232	33.5945
L17	7	6	0.6705	0.2776	0.3071	32.4852
L18	2	4	23.3110	4.9873*	0.5602	34.4600
L19	11	5	-15.9261	-4.2903*	0.5103	30.0399
L20	11	3	-0.7578	-0.2619	0.3988	29.9707

Table 12 Example 5 (4 outliers: L2 +35 mm, L3 -35 mm, L6 +35 mm, and L15 -40 mm). Residuals after the initial least squares adjustment (νLS), minimum L_1 norm by the iterative procedure (νL_{1i}) minimum L_1 norm by the global optimization method (νL_{1g}) and corresponding differences with respect the least squares values (values in mm). The sum of absolute values of the residuals Σ|ν| is given in the last row for each of the three different adjustments.

Line	νLS	νL_{1i}	νL_{1g}	νL_{1i}-νLS	νL_{1g}-νLS
L1	4.6	0.0	0.0	-4.6	-4.6
L2	**-28.4**	**-26.4**	**-26.4**	**2.0**	**2.0**
L3	**8.6**	**14.9**	**17.5**	**6.3**	**8.9**
L4	-0.5	0.0	0.0	0.5	0.5
L5	-13.6	-10.4	-7.8	3.2	5.8
L6	**-7.9**	**-17.7**	**-20.3**	**-9.8**	**-12.4**
L7	12.1	5.5	5.5	-6.6	-6.6
L8	3.8	0.0	0.0	-3.8	-3.7
L9	-1.7	0.0	0.0	1.7	1.7
L10	0.3	0.0	0.0	-0.3	-0.3
L11	11.0	4.4	1.8	-6.6	-9.2
L12	-15.4	-9.8	-7.2	5.6	8.2
L13	10.5	13.3	13.3	2.8	2.8
L14	11.4	0.0	0.0	-11.4	-11.4
L15	**17.2**	**41.1**	**43.7**	**23.9**	**26.4**
L16	7.6	0.0	0.0	-7.6	-7.6
L17	0.7	0.0	0.0	-0.7	-0.7
L18	23.3	14.7	14.7	-8.6	-8.6
L19	-15.9	-2.7	-0.1	13.2	15.8
L20	-0.8	0.0	0.0	0.8	0.8
Σ|ν|	195.3	160.9	158.3	-	-

Table 13 Example 5 (4 outliers: L2 +35 mm, L3 -35 mm, L6 +35 mm, and L15 -40 mm). Exhaustive search method: set of observations deduced to be affected by outliers and corresponding approximate error sizes.

Line	error size (times σ)	error size (mm)
L2	6.0842	38.96
L3	-2.2222	-13.70
L6	7.4407	26.83
L15	-12.7086	-56.83

smaller values for the residuals of the observations free from outliers whereas larger residuals for those where outliers have been simulated, although these results seem to be insufficient to account for some of the outliers simulated (especially those in L3 and L6).

The *exhaustive search* procedure still works properly in this fairly complicated case: again, it correctly indicates that there is only one possible set of outliers, the correct one, and yields approximately correct estimates for most of their error sizes (Table 13).

One additional outlier of +35 mm is added over the previous example, now in observation L10, in order to make it a fairly intractable problem, now that the number of outliers equals half the number of degrees of freedom of the network.

After the *least squares adjustment*, the chi-square test is clearly rejected for an a posteriori unit weight variance of 12.132. Many observations are flagged by the data snooping test as potentially containing outliers (Table 14).

As with the previous example, the strategy of eliminating the worse and readjusting does not work either. In this way, we subsequently eliminate L2, L15, L5 and L10 until the remaining set has no flagged observations after the adjustment. Therefore, one correct observation, L5, has been eliminated, whereas two incorrect observations, L3 and L6, have been retained in the final set.

Minimization of the *L_1 norm* by the two methods produces the results displayed in Table 15.

The two methods for L_1 norm minimization still behave very similarly, but in this difficult case they are not always successful at correctly determining the affected observations: for in0stance, they find high residuals for the correct observation L5 while finding small residuals for the contaminated observation L6.

In this case the *exhaustive search* procedure also fails. It indicates that there is only one possible set of outliers formed with L6, L10 and L15, which are correctly identified, along with L17 and L20, which are indeed free from outliers. It is worth noting,

Table 14 Example 6 (5 outliers: L2 +35 mm, L3 -35 mm, L6 +35 mm, L10 +35 mm and L15 -40 mm). Residuals and reliability measures: Baarda's data snooping test variable, redundancy numbers and minimum detectable errors (values in mm for residuals and minimum detectable errors and unitless for Baarda's test variables and redundancy numbers).

Line	From	To	Residual	wBaarda	Redund.No.	Min. Detectable Error
L1	1	2	3.8075	0.7468	0.5305	39.6930
L2	2	11	-37.7318	-6.9000*	0.7294	30.9652
L3	11	7	14.7677	3.0172	0.6304	32.0649
L4	8	7	-4.0471	-1.1063	0.3936	38.3866
L5	1	8	-14.0097	-4.4477*	0.4510	28.8456
L6	8	9	-6.7310	-3.4487*	0.2930	27.5087
L7	1	9	12.8593	3.9258*	0.4665	28.9990
L8	10	9	-1.9837	-0.3863	0.5493	38.6080
L9	2	10	5.5356	2.3959	0.3559	26.8126
L10	11	10	-18.1326	-5.0969*	0.5273	27.8616
L11	7	10	21.3998	3.1893	0.7262	38.1620
L12	11	6	-11.3681	-1.9251	0.6974	34.9689
L13	2	3	5.0384	1.1212	0.5769	32.1681
L14	3	4	12.4766	2.5211	0.5696	35.8849
L15	4	5	15.5031	6.2926*	0.3035	33.5269
L16	5	6	8.4820	2.4641	0.4232	33.5945
L17	7	6	-1.4358	-0.5944	0.3071	32.4852
L18	2	4	18.9150	4.0468*	0.5602	34.4600
L19	11	5	-12.7501	-3.4348*	0.5103	30.0399
L20	11	3	3.0702	1.061	0.3988	29.9707

Table 15 Example 6 (5 outliers: L2 +35 mm, L3 -35 mm, L6 +35 mm, L10 +35 mm and L15 -40 mm). Residuals after the initial least squares adjustment (νLS), minimum L_1 norm by the iterative procedure (νL_{1i}) minimum L_1 norm by the global optimization method (νL_{1g}) and corresponding differences with respect the least squares values (values in mm). The sum of absolute values of the residuals Σ|ν| is given in the last row for each of the three different adjustments.

Line	νLS	νL_{1i}	νL_{1g}	νL_{1i}-νLS	νL_{1g}-νLS
L1	3.8	0.0	0.0	-3.8	-3.8
L2	**-37.7**	**-39.8**	**-39.7**	**-2.1**	**-2.0**
L3	**14.8**	**17.4**	**17.5**	**2.6**	**2.7**
L4	-4.0	0.0	0.0	4.0	4.0
L5	-14.0	-21.3	-21.2	-7.3	-7.2
L6	**-6.7**	**-6.8**	**-6.9**	**-0.1**	**-0.2**
L7	12.9	5.5	5.5	-7.4	-7.3
L8	-2.0	0.0	0.0	2.0	2.0
L9	5.5	0.0	0.0	-5.5	-5.5
L10	**-18.1**	**-21.6**	**-21.7**	**-3.5**	**-3.5**
L11	21.4	15.3	15.2	-6.1	-6.2
L12	-11.4	-7.3	-7.2	4.1	4.1
L13	5.0	0.0	0.0	-5.0	-5.1
L14	12.5	0.0	0.0	-12.5	-12.5
L15	**15.5**	**43.5**	**43.6**	**28.0**	**28.1**
L16	8.5	0.0	0.0	-8.5	-8.5
L17	-1.4	0.0	0.0	1.4	1.4
L18	18.9	1.4	1.4	-17.5	-17.5
L19	-12.8	-0.2	-0.1	12.6	12.6
L20	3.1	0.1	0.0	-3.0	-3.1
Σ|ν|	230.0	180.2	180.1	-	-

Table 16 Example 6 (5 outliers: L2 +35 mm, L3 -35 mm, L6 +35 mm, L10 +35 mm and L15 -40 mm). Exhaustive search method: set of observations deduced to be affected by outliers and corresponding approximate error sizes.

Line	error size (times σ)	error size (mm)
L6	6.3710	22.97
L10	7.0187	34.38
L15	-11.4224	-51.08
L17	1.0726	4.68
L20	-1.6801	-7.70

however, that it gives really small error sizes for these two observations, L17 and L20, incorrectly identified as affected by outliers (Table 16). This suggests the idea that the exhaustive procedure performance could be improved in the future by making use of information about error sizes.

All in all, in a case where such a high number of outliers is suspected the results are so highly unreliable that no other recommendation than repeating the measurements altogether could be given.

4. CONCLUSIONS

Least squares adjustment and the iterative application of the data snooping test correctly identifies the appearance of one outlier higher than the minimum detectable error but does not always succeed in the case of multiple outliers, occasionally committing false positives and false negatives. In consequence, one should prefer the least squares solution, after the possible elimination of up to one outlier by the data snooping test, when there can be reasonable evidence that no more than one outlier has been committed, and use other strategies otherwise, at least as a complement that might reinforce the results given by the least squares solution.

Among the alternative adjustment procedures, it has been shown that the adjustments by minimum L1- norm computed by iteratively reweighted least squares and by means of global optimization produce similar results in the case of leveling networks, where the number of unknowns is high and the geometrical consistency relatively low. This is a somehow unexpected conclusion inasmuch as global optimization normally improves the results from iteratively reweighted least squares. Overall, both approaches correctly identify the observations and sizes of the corresponding outliers here, improving the results given by the least squares estimator, except where the number of affected observations is very high. The linearity of the current model seems to be the reason for this equivalence, which could also be investigated in other linear models such as those for 3D adjustment of GNSS baselines.

The exhaustive search procedure produces the correct solution in all cases except for the one with the largest number of outliers, namely when they are half the number of the degrees of freedom of the network, a case that seems intractable for any procedure.

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