applied sciences

MDPI

Article

Use of Total Least Squares Adjustment in Geodetic Applications

Aleš Marjetič *, Tomaž Ambrožič and Simona Savšek

Faculty of Civil and Geodetic Engineering, University of Ljubljana, Jamova cesta 2, 1000 Ljubljana, Slovenia; tambrozi@fgg.uni-lj.si (T.A.); ssavsek@fgg.uni-lj.si (S.S.)
* Correspondence: amarjeti@fgg.uni-lj.si; Tel.: +386-41-392-604

Abstract: This article discusses the method of computing the values of the unknowns under the condition of the minimum sum of the squares of the residuals of the observations, also known as the least squares method, with the additional condition of taking into account the errors in the unknowns. The problem has already been treated by many authors, especially in the field of regression analysis and the computation of transformation parameters. We give an overview of the theoretical foundations of the least squares method and extensions of this method by considering the errors in the unknowns in the model matrix. So, the total least squares method is presented in this paper, fitting the regression line to a set of points and computing transformation parameters for the transition between the old and the new Slovenian national coordinate systems. Furthermore, for the first time, the method is also presented and tested in the S-transformation between different geodetic datum-dependent solutions. Also, for the first time, we systematically compare the results of the approach with conventional approaches in all three considered tasks. With the results based on relevant statistics, we confirm the suitability of the described method for dealing with the considered computational tasks.

Keywords: total least squares; errors; coordinate transformation; S-transformation

check for updates

Citation: Marjetič, A.; Ambrožič, T.; Savšek, S. Use of Total Least Squares Adjustment in Geodetic Applications. *Appl. Sci.* **2024**, *14*, 2516. https://doi.org/10.3390/app14062516

Received: 21 February 2024
Revised: 8 March 2024
Accepted: 14 March 2024
Published: 16 March 2024

Copyright: © 2024 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https://creativecommons.org/licenses/by/4.0/).

1. Introduction

In geodesy, the quantities we are interested in cannot usually be measured directly. However, we can compute these unknown quantities indirectly based on measurements. Due to the redundant measurements, the model that connects all measurements and unknown quantities consists of more equations than necessary and is therefore predetermined. The solution for the unknowns is usually obtained by adjusting the measurement residuals using the least squares (LS) method. In adjustment theory, this situation is described as the inverse problem, the goal of which is to determine the best-fitting parameters of the model that minimize the discrepancies between the observed values and those predicted by the model. The computational process involves iteratively adjusting the parameters to reduce the differences between observed and computed values until an optimal solution is achieved. Contrary to the inverse problem, the forward problem involves the prediction or computation of observed values based on known parameters and a mathematical model. We focus on the inverse problem.

Due to its non-linearity, the system of equations linking measured values and unknowns is converted into a system of linear equations for measurement residuals, called the Gauss–Markov model [1]. In the next step, it is transformed into a system of normal equations [1,2], which allows unambiguous determination of the values of the unknowns when the criterion of the least sum of the squares of measurement residuals is satisfied [2]. In this conventional LS adjustment approach, only measurement errors are taken into account. We assume the presence of normally distributed random errors, without gross errors. In geodesy, we have many methods to detect outliers and exclude them from the observations before the adjustment procedure. However, we can look for a solution by assuming that random errors are also present in the model on the side of unknowns or

variables. This approach has been considered by many researchers in the field [3–9]. It has been referred to as total least squares (TLS) adjustment and has proven to be very useful, especially in the field of regression fitting and transformation computations.

In this article, we tested the applicability of the TLS method for two applications which are also common to many other studies [6,7]. We start with best fitting the regression line to the set of points to practically demonstrate the TLS method explained theoretically with the equations and to clarify the geometrical meaning of the solutions. We used the same set of points as in [7] but our aim, unlike other studies, is to show the difference between different computational procedures. Moreover, the ordinary approaches (LS and LS using Singular Value Decomposition (SVD)) in computing the values of the unknowns under the condition of the minimum sum of the squares of the measurement residuals are also described and practically tested. The scope of the analysis and discussion of the different possibilities for the computation of the unknowns is also to evaluate the quality of each solution and comparison between them.

The same concept of testing the TLS approach and other computational methods as well as the analysis of differences between solutions is also applied in the field of coordinate transformation. We test the suitability of the TLS approach for computing the transformation parameters for transitioning between two coordinate systems. The topic is current, and unlike other authors, it is implemented in the specific task of finding the most appropriate solution for the transformation parameters between the old and the new official coordinate system in Slovenia, which has its own peculiarities.

Finally, by understanding the computational procedure involved in the task of transforming point coordinates, the TLS approach is also applied to the S-transformation of coordinate solutions from a free network into a datum-dependent solution. The problem of finding the correct geodetic datum is of utmost importance in the field of deformation analysis when comparing the coordinates of points in the geodetic network between different time epochs. The total least squares approach in the S-transformation has not yet been identified in the literature, and we believe not only is the topic appropriate, but our findings also indicate the possibility to identify the set of unstable points in the geodetic network, which are described in more details at the end of this article.

2. Solution of the Predetermined Model

2.1. Motivation

Measurements and unknowns are associated with mathematical expressions in the model of observations equations, Equation (1), where we connect them in linearized form [2]:

$$\mathbf{A}\mathbf{x} = \mathbf{b}, \begin{bmatrix} a_{11} & \cdots & a_{1u} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nu} \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ \vdots \\ x_u \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}, \quad (1)$$

where n is the number of measurements or the number of all equations of the considered model, u is the number of unknowns, $\mathbf{b}$ is the vector of observations or measurements, $\mathbf{A}$ is the design or the model matrix, which consists of coefficients belonging to each unknown and is treated as a forward operator, and $\mathbf{x}$ is the vector of unknowns. In model (1), the vector of observations $\mathbf{b}$ lies in multidimensional space, spanned by the columns of matrix $\mathbf{A}$ [2]. Rank of matrix $\mathbf{A}$ is $\text{rank}(\mathbf{A}) = r \leq \min(n, u)$.

In system (1), connecting unknowns and measurements, there are three possible situations for a system of n equations for u unknowns: a predetermined system when $n > u$, a uniquely determined system when $n = u$, and an underdetermined system when $n < u$ (the latter is not common when measurements are involved, since we always aim for a redundant number of measurements). System (1) can also be written in the form:

$$[\mathbf{A}|\mathbf{b}] \begin{bmatrix} \mathbf{x} \\ -1 \end{bmatrix} = \mathbf{0}. \quad (2)$$

Let us focus on a predetermined system and present it through finding the intersection of three lines in Figure 1:

- Three lines intersect at the same point T—the left in Figure 1: In this case, we deal with the system of n consistent equations. The property of system (1) is that $r = \text{rank}(\mathbf{A}) = \text{rank}([\mathbf{A}|\mathbf{b}]) = u$. In geometrical representation, vector $\mathbf{b}$ lies in a space spanned by the columns of matrix $\mathbf{A}$; or in other words, vector $\mathbf{b}$ can be represented as a linear combination of the columns of matrix $\mathbf{A}$.
- Three lines (blue) do not intersect at the same point—the right in Figure 1: In this case, we have $r = \text{rank}(\mathbf{A}) < \text{rank}([\mathbf{A}|\mathbf{b}]) = u + 1$ and the equality in Equation (1) does not apply. We can write $\mathbf{Ax} \cong \mathbf{b}$ instead. In geometrical representation, the observation vector $\mathbf{b}$ does not lie in the space spanned by the column vectors of matrix $\mathbf{A}$ or cannot be written as a linear combination of the column vectors of matrix $\mathbf{A}$. There is no unique solution as we have three non-consistent equations. The aim is to find the orthogonal projection of vector $\mathbf{b}$ in the above mentioned space; or in other words, our aim is to transform system (1) to the consistent form with the solution for $\mathbf{x} \rightarrow \hat{\mathbf{x}}$ and consequently $\mathbf{b} \rightarrow \hat{\mathbf{b}}$ (the right in Figure 1, red lines), where $\mathbf{A}\hat{\mathbf{x}} = \hat{\mathbf{b}}$, for which it would apply that $r = \text{rank}(\mathbf{A}) = \text{rank}([\mathbf{A}\hat{\mathbf{b}}]) = u$. Therefore, we want to reduce the system rank of $[\mathbf{A}|\mathbf{b}]$ by 1.

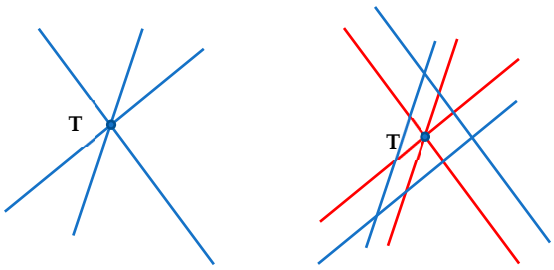

Figure 1. Left—system of consistent equations, **right**—system of non-consistent equations (blue lines) and the adjusted solution (red lines).

In addition, for the predetermined system of non-consistent equations, we search for a solution, which will fulfill the requirement of the minimal sum of the squares of measurement residuals $\|\mathbf{v}\|^2 = \mathbf{v}^{\mathrm{T}}\mathbf{Pv} = \text{min.}$, where $\mathbf{v} = \hat{\mathbf{b}} - \mathbf{b}$ are measurement residuals and $\mathbf{P}$ is the weight matrix of measurements. This solution is called the LS solution and can be obtained in different ways:

(a.) We search for the most probable LS solution for the vector of unknowns $\mathbf{x}$ through the system of normal equations [1,2]:

$$\mathbf{Ax} = \mathbf{b} + \mathbf{v},\ \mathbf{A}^{\mathrm{T}}\mathbf{PAx} = \mathbf{A}^{\mathrm{T}}\mathbf{Pb},\ \hat{\mathbf{x}} = (\mathbf{A}^{\mathrm{T}}\mathbf{PA})^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{Pb}. \quad (3)$$

In the case $\mathbf{P} = \mathbf{I}$, the solution is $\hat{\mathbf{x}} = (\mathbf{A}^{\mathrm{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}\mathbf{b}$.

(b.) We can also use a more general approach—general least squares (GLS). In this case, the solution to the unknowns is not sought directly from the measurements, but via a vector of equivalent observations, each of which is a linear combination of the original observations [2]. Model (1) would be written in the form $\mathbf{Bb} = \mathbf{Ax}$, and the solution would be computed using the expression:

$$\hat{\mathbf{x}} = (\mathbf{A}^{\mathrm{T}}(\mathbf{BQB}^{\mathrm{T}})^{-1}\mathbf{A})^{-1}\mathbf{A}^{\mathrm{T}}(\mathbf{BQB}^{\mathrm{T}})^{-1}\mathbf{b}, \quad (4)$$

where $\mathbf{B}$ represents the matrix of observations' coefficients, $\mathbf{A}$ is the design matrix or the matrix of coefficients of unknowns and $\mathbf{Q} = \mathbf{P}^{-1}$ is the cofactor matrix of observations.

This approach is useful, especially in procedures for approximating curves and surfaces to a certain set of points, where we treat as "one observation" the actual coordinate

pairs (x, y) or triplets (x, y, z), which, on the surface, are connected in a mathematical equation with unknowns in non-linear form. In this case, it would be very difficult to isolate each coordinate and express it in a linear form. The same situation applies to coordinate transformation, where each coordinate pair or triplet of all points are treated as observations. The GLS solution is much faster and simpler in this case.

(c.) We look for a solution with the help of SVD [10], which is a version of the computation according to the classical least squares method under a.). We can also take into account the weights of the observations (in matrix **P**) when using SVD. If we consider the fact that the matrix **P** for observations is a positive definite, then it holds that $\mathbf{P} = \mathbf{P}_c\mathbf{P}_c^*$ (Cholesky decomposition) and system (1) can be transformed to the form:

$$(\mathbf{P}_c\mathbf{b}) = (\mathbf{P}_c\mathbf{A})\mathbf{x}. \tag{5}$$

(d.) We use the adjustment method, which also takes into account the errors in unknowns and is described in detail in the following section and later practically tested on a few numerical examples.

2.2. Method of Taking into Account the Presence of Errors in Variables (EIV)

The method is called total least squares (TLS) [6,7,11]. In this case, we consider the predetermined system (1), which results in $\mathbf{Ax} \cong \mathbf{b}$ and $\{\text{rank}(\mathbf{A}) = u\} \neq \{\text{rank}([\mathbf{A}|\mathbf{b}]) = u + 1\}$ due to random errors in measurements. Classical treatment or searching for a solution for the vector of unknowns in the LS method only considers the presence of random errors in measured values (in vector **b**). If we assume, in addition to measurement errors, there is also the presence of errors in variables or unknowns [6,7], it can be written as:

$$\mathbf{b} + \mathbf{v} = (\mathbf{A} - \mathbf{E}_\mathrm{A})\mathbf{x}, \tag{6}$$

with the stochastic properties:

$$\begin{bmatrix} \mathbf{v} \\ \mathbf{e}_\mathrm{A} \end{bmatrix} := \begin{bmatrix} \mathbf{v} \\ \mathrm{vec}(\mathbf{E}_\mathrm{A}) \end{bmatrix} \sim \left(\begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix}, \sigma_0^2 \begin{bmatrix} \mathbf{Q}_\mathrm{b} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_\mathrm{A} \end{bmatrix} \right), \tag{7}$$

where $\mathbf{e}_\mathrm{A} = \mathrm{vec}(\mathbf{E}_\mathrm{A})$ is a vector, which consists of the columns of matrix $\mathbf{E}_\mathrm{A}$ of the dimensions $(n{\cdot}u \times 1)$. $\mathbf{Q}_\mathrm{b}$ represents the cofactor matrix of observations and $\mathbf{Q}_\mathrm{A}$ represents the cofactor matrix of unknowns.

The solution for **x** in Equation (6) can be derived with the help of Lagrange multiplication factors **k** of the dimensions $(n \times 1)$. The condition of the minimum sum of squares is written with a weighting function Φ [6]:

$$\Phi = \mathbf{v}^\mathrm{T}\mathbf{Q}_\mathrm{b}^{-1}\mathbf{v} + \mathbf{e}_\mathrm{A}^\mathrm{T}\mathbf{Q}_\mathrm{A}^{-1}\mathbf{e}_\mathrm{A} + 2\mathbf{k}^\mathrm{T}(\mathbf{b} + \mathbf{v} - \mathbf{Ax} + \mathbf{E}_\mathrm{A}\mathbf{x}) = \min. \tag{8}$$

If we unify $\mathbf{e}_\mathrm{A}$ and $\mathbf{E}_\mathrm{A}$ in Equation (8) with the use of the Kronecker product ($\bigotimes$), we obtain:

$$\Phi = \mathbf{v}^\mathrm{T}\mathbf{Q}_\mathrm{b}^{-1}\mathbf{v} + \mathbf{e}_\mathrm{A}^\mathrm{T}\mathbf{Q}_\mathrm{A}^{-1}\mathbf{e}_\mathrm{A} + 2\mathbf{k}^\mathrm{T}(\mathbf{b} + \mathbf{v} - \mathbf{Ax} + (\mathbf{x}^\mathrm{T} \bigotimes \mathbf{I}_n)\mathbf{e}_\mathrm{A}) = \min. \tag{9}$$

For the determination of the minimum of the weight function Φ, we must equate the partial derivatives with respect to the variables **v**, **x**, $\mathbf{e}_\mathrm{A}$ and **k** to **0** [7]:

$$\frac{1}{2}\frac{\partial\Phi}{\partial\mathbf{v}^\mathrm{T}} = \mathbf{Q}_\mathrm{b}^{-1}\mathbf{v} + \mathbf{k} = \mathbf{0}, \tag{10}$$

$$\frac{1}{2}\frac{\partial\Phi}{\partial\mathbf{e}_\mathrm{A}^\mathrm{T}} = \mathbf{Q}_\mathrm{A}^{-1}\mathbf{e}_\mathrm{A} + (\mathbf{x} \bigotimes \mathbf{I}_n)\mathbf{k} = \mathbf{0}, \tag{11}$$

$$\frac{1}{2}\frac{\partial \Phi}{\partial \mathbf{k}^{\mathrm{T}}} = \mathbf{b} + \mathbf{v} - \mathbf{A}\mathbf{x} + (\mathbf{x}^{\mathrm{T}} \bigotimes \mathbf{I}_n)\mathbf{e}_{\mathrm{A}} = \mathbf{0}, \tag{12}$$

$$\frac{1}{2}\frac{\partial \Phi}{\partial \mathbf{x}^{\mathrm{T}}} = -\mathbf{A}^{\mathrm{T}}\mathbf{k} + \mathbf{E}_{\mathrm{A}}^{\mathrm{T}}\mathbf{k} = \mathbf{0}. \tag{13}$$

From Equations (10) and (11) follows:

$$\mathbf{v} = -\mathbf{Q}_{\mathrm{b}}\mathbf{k}, \tag{14}$$

$$\mathbf{e}_{\mathrm{A}} = \mathrm{vec}(\mathbf{E}_{\mathrm{A}}) = -\mathbf{Q}_{\mathrm{A}}(\mathbf{x} \bigotimes \mathbf{I}_n)\mathbf{k}. \tag{15}$$

If we insert (14) and (15) to (12), we obtain:

$$\mathbf{k} = (\mathbf{Q}_{\mathrm{b}} + (\mathbf{x}^{\mathrm{T}} \bigotimes \mathbf{I}_n)\mathbf{Q}_{\mathrm{A}}(\mathbf{x} \bigotimes \mathbf{I}_n))^{-1}(\mathbf{b} - \mathbf{A}\mathbf{x}) = \mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}(\mathbf{b} - \mathbf{A}\mathbf{x}), \tag{16}$$

where

$$\mathbf{Q}_{\tilde{\mathrm{b}}} = \mathbf{Q}_{\mathrm{b}} + (\mathbf{x}^{\mathrm{T}} \bigotimes \mathbf{I}_n)\mathbf{Q}_{\mathrm{A}}(\mathbf{x} \bigotimes \mathbf{I}_n). \tag{17}$$

Taking into account Equation (16) from Equation (13), the solution for the vector of unknowns **x** under the assumption of EIV is:

$$\hat{\mathbf{x}} = ((\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\mathbf{A})^{-1}(\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\mathbf{b}, \tag{18}$$

where $((\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\mathbf{A})$ can represent the matrix of the normal equations of the extended model $\mathbf{b} + \mathbf{v} = (\mathbf{A} - \mathbf{E}_{\mathrm{A}})\mathbf{x}$, which also includes the errors in the model. But this matrix is neither symmetrical nor a positive definite unlike the matrix of normal equations $\mathbf{N} = \mathbf{A}^{\mathrm{T}}\mathbf{P}\mathbf{A}$ of the model $\mathbf{b} + \mathbf{v} = \mathbf{A}\mathbf{x}$. The solution can be found in the transformation of (18) taking into account $\widetilde{\mathbf{A}} = \mathbf{A} - \mathbf{E}_{\mathrm{A}}$ or $\mathbf{A} = \widetilde{\mathbf{A}} + \mathbf{E}_{\mathrm{A}}$:

$$(\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\mathbf{A}\hat{\mathbf{x}} = (\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\mathbf{b}. \tag{19}$$

Both sides can be subtracted by $(\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\mathbf{E}_{\mathrm{A}}\hat{\mathbf{x}}$:

$$(\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\mathbf{A}\hat{\mathbf{x}} - (\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\mathbf{E}_{\mathrm{A}}\hat{\mathbf{x}} = (\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\mathbf{b} - (\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\mathbf{E}_{\mathrm{A}}\hat{\mathbf{x}}, \tag{20}$$

$$(\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}(\mathbf{A} - \mathbf{E}_{\mathrm{A}})\hat{\mathbf{x}} = (\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}(\mathbf{b} - \mathbf{E}_{\mathrm{A}}\hat{\mathbf{x}}) \tag{21}$$

From Equations (20) and (21), the solution for the unknowns is:

$$\hat{\mathbf{x}} = \left((\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}(\mathbf{A} - \mathbf{E}_{\mathrm{A}})\right)^{-1}(\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}(\mathbf{b} - \mathbf{E}_{\mathrm{A}}\hat{\mathbf{x}}), \tag{22}$$

$$\hat{\mathbf{x}} = \left((\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}(\mathbf{A} - \mathbf{E}_{\mathrm{A}})\right)^{-1}(\mathbf{A} - \mathbf{E}_{\mathrm{A}})^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\widetilde{\mathbf{b}}, \tag{23}$$

where $\widetilde{\mathbf{b}} = \mathbf{b} - \mathbf{E}_{\mathrm{A}}\hat{\mathbf{x}}$.

The solution for the vector of observations and the vector of residuals of the model considering Equations (6) and (10) can be written as:

$$\hat{\mathbf{b}} = (\mathbf{A} - \mathbf{E}_{\mathrm{A}})\hat{\mathbf{x}}, \tag{24}$$

$$\hat{\mathbf{v}} = -\mathbf{b} + \mathbf{A}\hat{\mathbf{x}} = -\mathbf{Q}_{\tilde{\mathrm{b}}}\mathbf{k}\hat{\mathbf{b}} = (\mathbf{A} - \mathbf{E}_{\mathrm{A}})\hat{\mathbf{x}}. \tag{25}$$

If we consider Equation (15), that $\mathbf{E}_{\mathrm{A}}\hat{\mathbf{x}} = (\mathbf{x}^{\mathrm{T}} \otimes \mathbf{I}_n)\mathrm{vec}(\mathbf{E}_{\mathrm{A}}) = (\mathbf{x}^{\mathrm{T}} \otimes \mathbf{I}_n)\mathbf{e}_{\mathrm{A}}$, the matrices of cofactors for adjusted measurements can be written as

$$\mathbf{Q}_{\tilde{\mathrm{b}}} = \mathbf{Q}_{\mathrm{b}} + (\hat{\mathbf{x}}^{\mathrm{T}} \bigotimes \mathbf{I}_n)\mathbf{Q}_{\mathrm{A}}(\hat{\mathbf{x}} \bigotimes \mathbf{I}_n), \tag{26}$$

$$\mathbf{Q}_{\hat{\mathrm{x}}} = (\overset{\sim}{\mathbf{A}}^{\mathrm{T}} \mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{-1} \overset{\sim}{\mathbf{A}})^{-1}, \tag{27}$$

with the corresponding a posteriori reference variance as:

$$\hat{\sigma}_0^2 = \frac{\hat{\mathbf{v}}^{\mathrm{T}} \mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{-1} \hat{\mathbf{v}}}{n-u} = \frac{\mathbf{k}^{\mathrm{T}} \mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{-1} \mathbf{k}}{n-u}. \tag{28}$$

2.2.1. Computational Algorithm

This algorithm is an iterative procedure according to [7]:
Step 1: Set the initial value for the unknowns.

The initial values for the unknowns are taken from the common weighted LS solution (WLS) with the measurement precision $\mathbf{P} = \mathbf{\Sigma}_{\mathrm{b}}^{-1}$ (this refers to observations that are treated as observations in ordinary LS and this is all explained through the regression line in the following Section 3):

$$\hat{\mathbf{x}}^0 = (\mathbf{A}^{\mathrm{T}} \mathbf{P} \mathbf{A})^{-1} \mathbf{A}^{\mathrm{T}} \mathbf{P} \mathbf{b}. \tag{29}$$

Step 2: Set $i = 0$ (i—iteration).

$$\mathbf{v}^i = \mathbf{A}\hat{\mathbf{x}}^i - \mathbf{b}, \tag{30}$$

$$\mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{\ i} = \mathbf{Q}_{\mathrm{b}} + ((\hat{\mathbf{x}}^i)^{\mathrm{T}} \bigotimes \mathbf{I}_n) \mathbf{Q}_{\mathrm{A}} (\hat{\mathbf{x}}^i \bigotimes \mathbf{I}_n), \tag{31}$$

where matrix $\mathbf{Q}_{\mathrm{A}}$ depends on the precision of measurements which are included in the adjustment and can be computed as [6,7]:

$$\mathbf{Q}_{\mathrm{A}} = \sum_{i=1}^{u} \sum_{j=1}^{u} \mathbf{c}_i \mathbf{c}_j^{\mathrm{T}} \bigotimes \mathbf{Q}_{ij}, \tag{32}$$

with $\mathbf{c}_i$ and $\mathbf{c}_j$ as unit vectors with 1 in the position that belongs to the variable and 0 otherwise. Matrix $\mathbf{Q}_{ij}$ represents a cofactor matrix of measurements that appear alongside unknowns with the dimensions of $n \times n$. We compute vector $\mathbf{e}_{\mathrm{A}}^i$, which belongs to matrix $\mathbf{E}_{\mathrm{A}}^i$ in the i-th iteration:

$$\mathbf{e}_{\mathrm{A}}^i = -\mathbf{Q}_{\mathrm{A}} (\hat{\mathbf{x}}^i \bigotimes \mathbf{I}_n) (\mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{\ i})^{-1} \mathbf{v}^i, \tag{33}$$

$$\overset{\sim}{\mathbf{A}}^i = \mathbf{A} - \mathbf{E}_{\mathrm{A}}^i \hat{\mathbf{x}}^i, \tag{34}$$

$$\mathbf{b}^i = \mathbf{b} - \mathbf{E}_{\mathrm{A}}^i, \tag{35}$$

$$\mathbf{Q}_{\hat{\mathrm{x}}}^{i+1} = (\overset{\sim}{\mathbf{A}}^{i\mathrm{T}} (\mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{\ i})^{-1} \overset{\sim}{\mathbf{A}}^i)^{-1}, \tag{36}$$

$$\hat{\mathbf{x}}^{i+1} = \mathbf{Q}_{\hat{\mathrm{x}}}^{i+1} \overset{\sim}{\mathbf{A}}^{i\mathrm{T}} (\mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{\ i})^{-1} \mathbf{b}^i = (\overset{\sim}{\mathbf{A}}^{i\mathrm{T}} (\mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{\ i})^{-1} \overset{\sim}{\mathbf{A}}^i)^{-1} \overset{\sim}{\mathbf{A}}^{i\mathrm{T}} (\mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{\ i})^{-1} \mathbf{b}^i = \overset{\sim}{\mathbf{N}}^{-1} \overset{\sim}{\mathbf{A}}^{i\mathrm{T}} (\mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{\ i})^{-1} \mathbf{b}^i, \tag{37}$$

$$i = i + 1.$$

Step 3: Make a convergence test.

$$|\hat{\mathbf{x}}^{i+1} - \hat{\mathbf{x}}^i| < \delta, \tag{38}$$

where δ is a predetermined value to stop iterations.

2.2.2. Precision Estimation

System $\mathbf{b} + \mathbf{v} = \mathbf{A}\mathbf{x}$ was translated to system $\overset{\sim}{\mathbf{b}} + \overset{\sim}{\mathbf{v}} = \overset{\sim}{\mathbf{A}}\hat{\mathbf{x}}$. Taking into account Equations (24) and (25) in Equation (37), we have:

$$\hat{\mathbf{b}} = \overset{\sim}{\mathbf{b}} + \hat{\mathbf{v}} = \overset{\sim}{\mathbf{A}}\hat{\mathbf{x}} = (\mathbf{A} - \mathbf{E}_{\mathbf{A}})\hat{\mathbf{x}} = \overset{\sim}{\mathbf{A}} (\overset{\sim}{\mathbf{A}}^{\mathrm{T}} \mathbf{Q}_{\underset{\sim}{\mathrm{b}}}^{-1} \overset{\sim}{\mathbf{A}})^{-1} \overset{\sim}{\mathbf{A}}^{\mathrm{T}} (\mathbf{Q}_{\underset{\sim}{\mathrm{b}}})^{-1} \overset{\sim}{\mathbf{b}} = \mathbf{P}_{\breve{\mathrm{A}}} \overset{\sim}{\mathbf{b}}, \tag{39}$$

$$\hat{\mathbf{v}} = \overset{\sim}{\mathbf{b}} - \hat{\mathbf{b}} = -\mathbf{Q}_{\underset{\sim}{\mathrm{b}}} \mathbf{k} = \left(\mathbf{I} - \mathbf{P}_{\breve{\mathrm{A}}}\right) \overset{\sim}{\mathbf{b}}. \tag{40}$$

From Equations (39) and (40), the cofactor matrices are:

$$\mathbf{Q}_{\hat{\mathrm{b}}} = \mathbf{P}_{\check{\mathrm{A}}}\mathbf{Q}_{\tilde{\mathrm{b}}} = \widetilde{\mathbf{A}}\mathbf{Q}_{\hat{\mathrm{x}}}\widetilde{\mathbf{A}}^{\mathrm{T}}, \tag{41}$$

$$\mathbf{Q}_{\hat{\mathrm{v}}} = \left(\mathbf{I} - \mathbf{P}_{\check{\mathrm{A}}}\right)\mathbf{Q}_{\tilde{\mathrm{b}}} = \mathbf{Q}_{\tilde{\mathrm{b}}} - \mathbf{Q}_{\hat{\mathrm{b}}}. \tag{42}$$

The a posteriori reference variance is:

$$\hat{\sigma}_0^2 = \frac{\hat{\mathbf{v}}^{\mathrm{T}}\mathbf{Q}_{\tilde{\mathrm{b}}}^{-1}\hat{\mathbf{v}}}{n-u}. \tag{43}$$

2.3. Total Least Squares Using SVD

As we mentioned before, if we are looking for a solution for $\mathbf{x}$ in system (1), then we want to achieve $\mathrm{rank}(\widetilde{\mathbf{A}}) = \mathrm{rank}([\widetilde{\mathbf{A}}|\widetilde{\mathbf{b}}]) = u$. System (1), in its extended form, can be rewritten as:

$$[\widetilde{\mathbf{A}}|\widetilde{\mathbf{b}}]\begin{bmatrix}\widetilde{\mathbf{x}}\\ -1\end{bmatrix} = \mathbf{0}. \tag{44}$$

If we decompose the $[\widetilde{\mathbf{A}}|\widetilde{\mathbf{b}}]$ matrix using SVD [12], we obtain [11]:

$$[\widetilde{\mathbf{A}}|\widetilde{\mathbf{b}}] = \widetilde{\mathbf{U}}\widetilde{\mathbf{\Lambda}}\widetilde{\mathbf{V}} = \begin{bmatrix} | & | & | \\ \widetilde{\mathbf{u}}_1 & \widetilde{\mathbf{u}}_2 \cdots & \widetilde{\mathbf{u}}_n \\ | & | & | \end{bmatrix}\begin{bmatrix} \widetilde{\lambda}_1 & & & & 0 \\ & \ddots & & & \\ & & \widetilde{\lambda}_r & & \\ & & & \ddots & \\ 0 & & & & \widetilde{\lambda}_{u+1} \end{bmatrix}\begin{bmatrix} -\widetilde{\mathbf{v}}_1- \\ -\widetilde{\mathbf{v}}_2- \\ \vdots \\ -\widetilde{\mathbf{v}}_{u+1}- \end{bmatrix} = \sum_{i=1}^{u+1}\widetilde{\lambda}_i\widetilde{\mathbf{u}}_i\widetilde{\mathbf{v}}_i. \tag{45}$$

where $\mathbf{U}$ and $\mathbf{V}$ are quadratic and orthogonal matrices and the $\mathbf{\Lambda}$ diagonal matrix of singular values.

We want to achieve the rank of Equation (45) to decrease from $u+1$ to u with the smallest possible change in $[\widetilde{\mathbf{A}}|\widetilde{\mathbf{b}}]$. Therefore, the smallest value in Equation (45) $\widetilde{\lambda}_{u+1}$ must be changed to 0. Equation (45) is then:

$$\begin{bmatrix} | & | & | \\ \widetilde{\mathbf{u}}_1 & \widetilde{\mathbf{u}}_2 \cdots & \widetilde{\mathbf{u}}_n \\ | & | & | \end{bmatrix}\begin{bmatrix} \widetilde{\lambda}_1 & & & 0 \\ & \widetilde{\lambda}_2 & & \\ & & \ddots & \\ & & \widetilde{\lambda}_u & \\ 0 & & & 0 \end{bmatrix}\begin{bmatrix} -\widetilde{\mathbf{v}}_1- \\ -\widetilde{\mathbf{v}}_2- \\ \vdots \\ -\widetilde{\mathbf{v}}_{u+1}- \end{bmatrix} = \sum_{i=1}^{u}\widetilde{\lambda}_i\widetilde{\mathbf{u}}_i\widetilde{\mathbf{v}}_i. \tag{46}$$

We can write:

$$[\widetilde{\mathbf{A}}|\widetilde{\mathbf{b}}]\cdot\widetilde{\mathbf{v}}_{u+1}^{\mathrm{T}} = \left(\sum_{i=1}^{u}\widetilde{\lambda}_i\widetilde{\mathbf{u}}_i\widetilde{\mathbf{v}}_i\right)\cdot\widetilde{\mathbf{v}}_{u+1}^{\mathrm{T}} = \mathbf{0}, \tag{47}$$

where $\widetilde{\mathbf{v}}_i\cdot\widetilde{\mathbf{v}}_{u+1}^{\mathrm{T}} = 0$, because the rows in $\mathbf{V}$ are orthogonal to each other and $\widetilde{\mathbf{v}}_{u+1}^{\mathrm{T}} = \begin{bmatrix}v_{u+1,1} & v_{u+1,2} & \cdots v_{u+1,u} & v_{u+1,u+1}\end{bmatrix}^{\mathrm{T}}$ is the last column in $\mathbf{V}$.

If we connect Equations (44) and (47), we obtain:

$$[\widetilde{\mathbf{A}}|\widetilde{\mathbf{b}}]\cdot\begin{bmatrix}\widetilde{\mathbf{x}}\\ -1\end{bmatrix} = [\widetilde{\mathbf{A}}|\widetilde{\mathbf{b}}]\cdot\begin{bmatrix}v_{u+1,1} & v_{u+1,2} & \cdots & v_{u+1,u} & v_{u+1,u+1}\end{bmatrix}^{\mathrm{T}} = 0. \tag{48}$$

From Equation (48), the solution for the unknown vector can be derived when we are also taking into account the errors in variables:

$$\widetilde{\mathbf{x}}_{\mathrm{TLS}} = -\frac{1}{v_{u+1,u+1}}\begin{bmatrix} v_{u+1,1} & v_{u+1,2} & \dots & v_{u+1,u} \end{bmatrix}^{\mathrm{T}} \tag{49}$$

In this case, we find a solution without stochastic treatment. If we want to take into account the weights of the observations in the computation, both on the side of the vector **b** and on the side of the matrix **A**, a problem arises. In the extension (2) or (44), we cannot take into account both the weights of the observations and the weights of the unknowns, as indicated in Section 2.1 by the Cholesky decomposition of the matrix **P**. Here, we consider two different weight matrices.

3. Practical Examples

3.1. The Regression Line

We fit the regression line to ten points, which do not lie on a straight line. The mathematical equation connecting measurements and unknowns is represented by the equation of a straight line: $y = kx + r$. The unknowns are the coefficients k and r. In the classical adjustment approach (LS with or without weights), the x-coordinates represent a "constant" value, and the y-coordinates are treated as a "measured" value (Table 1). A numerical example of coordinates and associated weights in Table 1 is taken from [13,14] and is also presented in [7].

Table 1. "Measured" points with weights and elements of extended matrix $[\mathbf{A}|\mathbf{b}]$.

	"Constant"	"Measured"	Weights		$[\mathbf{A}\,\vert\,\mathbf{b}]$		
Point	x	y	p_x	p_y	**A**		**b**
T1	0.0	5.9	1000	1	0.0	1	5.9
T2	0.9	5.4	1000	2	0.9	1	5.4
T3	1.8	4.4	500	4	1.8	1	4.4
T4	2.6	4.6	800	8	2.6	1	4.6
T5	3.3	3.5	200	20	3.3	1	3.5
T6	4.4	3.7	80	20	4.4	1	3.7
T7	5.2	2.8	60	70	5.2	1	2.8
T8	6.1	2.8	20	70	6.1	1	2.8
T9	6.5	2.4	1.8	100	6.5	1	2.4
T10	7.4	1.5	1	500	7.4	1	1.5

The rank of **A** is 2 and 3 of the extended matrix $[\mathbf{A}|\mathbf{b}]$. This is the result of points that do not lie on the same straight line. We are looking for a solution for k and r by different adjustment approaches (Table 2):

- Least squares adjustment without weights (LS),
- Using SVD without weights as an alternative approach to LS (LS_SVD),
- Total least squares without weights using SVD (TLS_SVD),
- Least squares adjustment with weights (WLS),
- Total least squares with weights (WTLS), and
- Generalized LS (GLS) when both x- and y-coordinates are measurements.

Table 2. Adjustment of the regression line according to different approaches.

Method	Weights	k	r	σ_k	σ_r	$\hat{\sigma}_0$
LS	no	−0.53958	5.76119	0.04213	0.18949	0.316
LS_SVD	no	−0.53958	5.76119	/	/	
TLS_SVD	no	−0.54886	5.81004	/	/	
WLS	yes	−0.61081	6.10011	0.06234	0.42406	2.072
WTLS	yes	−0.48053	5.47991	0.07062	0.35925	1.218
GLS	yes	−0.46397	5.39746	0.07134	0.35427	1.154

The criterion for stopping the iterations for WTLS is $\delta = 10^{-12}$. In this case, we obtain eight iterations.

In Figure 2, it can be seen that when adjustment is performed according to the WLS (purple line), the solution is completely fitted to the points with larger weights for the y-coordinate. The solution by the WTLS method (green line) considers all weights equally, for both y and x. The solution in this case is much more reasonable. The solution of the generalized least squares model is numerically close to the WTLS solution.

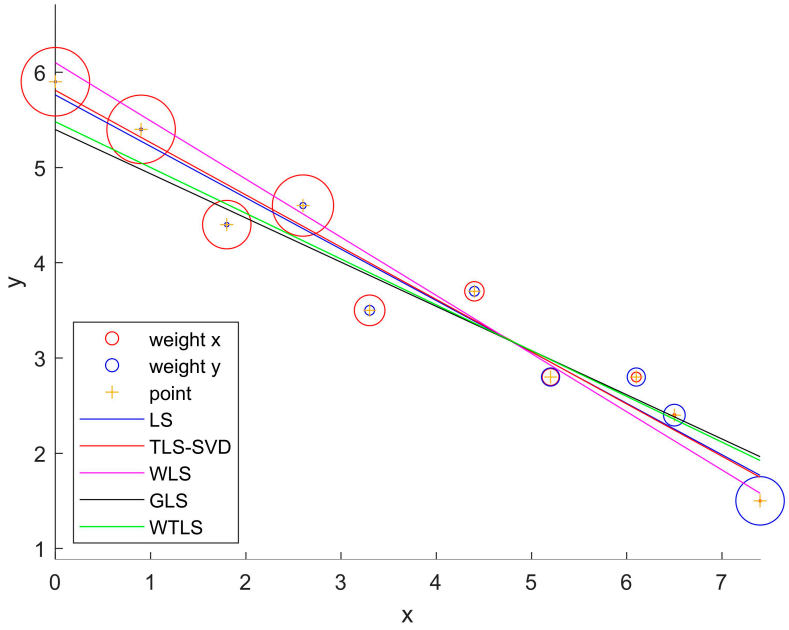

Figure 2. Solutions for the regression line.

The geometric meaning of adjustment by taking into account the errors in the unknowns (EIV) in the regression line can be explained as follows [11,15]: If we search for a solution by treating the coordinate y as a measured value and x as a constant, we obtain a solution under the condition of the minimum sum of the squares of the measured values. That is, the minimum sum of the squares of the corrections to the y-coordinates after adjustment (dashed line in Figure 3). If we also treat the x-coordinates as measured values, we are looking for the minimum of the sum of the squares of the corrections of the measured x- and y-coordinates simultaneously. Therefore, we minimize the sum of the squares of the perpendicular distances of the "measured" points from the regression line (dashed–dotted line in Figure 3).

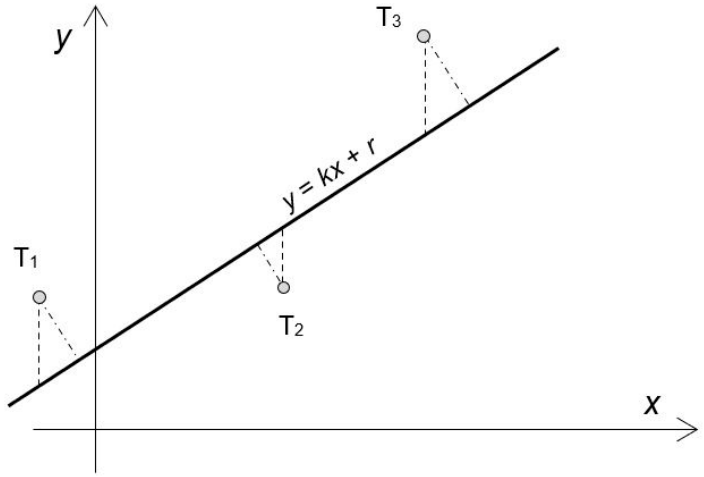

Figure 3. Geometrical representation for a solution of LS (dashed line) in comparison to TLS (dashed–dotted line).

The above comparison of "displacements" in the y-direction and perpendicular to it is, of course, only meaningful if we do not consider weights or if they are the same for all "measurements" ($\mathbf{P} = \mathbf{I}$). When considering weights, we are not dealing with perpendicular distances, but with some oblique ones. If we now consider the above example with a uniform weighting matrix, we see the difference in the results—the sum of the squares of the deviations of the points from the regression line:

- Perpendicular distance from line: $\sum_{LS} d_{\perp}^2 = \sum_{GLS} d_{\perp}^2 = 0.78748 > 0.78649 = \sum_{WTLS} d_{\perp}^2$;
- Distance from line in direction y: $\sum_{LS} d_y^2 = \sum_{GLS} d_y^2 = 0.89480 < 0.89593 = \sum_{WTLS} d_y^2$.

In the case of a uniform weighting matrix for the observation (=input point coordinates), the solution for the regression line for LS and GLS is the same. We can also see that the WTLS solution is such that it minimizes the perpendicular distances of the points from the computed line.

3.2. The Transformation of Coordinates

Considering the transition between the two versions of the coordinate systems is relevant because in everyday official geodetic practice data on points, both coordinate systems are interwoven—cadastral points, legacy points of different levels of geodetic networks, GNSS measurement points, etc. At the state level, or for the data of which the Surveying Authority of the Republic of Slovenia is the administrator, the country-wide triangular transformation model (sectional affine transformations [16]) was officially adopted. In this task, we set out to find the transformation parameters for the transformation in the local area of the part of Ljubljana city based on the points given in the old coordinate system (D48/GK, GK—Gauss–Krueger projection) and determined by the GNSS method in the new coordinate system (D96/TM, TM—transverse Mercator projection).

The precision for points in the old official coordinate system (D48/GK) is not listed in Table 3 as we do not have information about them. We estimate that the coordinates were determined with no better than the centimeter precision. This is due to the fact that at the time of determining the coordinates of these points in the old coordinate system (more than 40 years ago), the only measurement method used in geodetic networks for geodetic points of this class was triangulation. The precision of the coordinates of points in D96/TM comes from the results of our measurement and computations of the geodetic network, combining classical terrestrial (measurements of angles and distances) and GNSS surveying methods, and is generally several times more precise than in D48/GK (Table 3). Accordingly, we set the weights of individual points in both coordinate systems (Table 3), with the weights in the initial (D48/GK) coordinate system set to 1. The weights in the new (D96/TM) coordinate systems are presented by the ratio between the precision of points in

the old and new coordinate systems (e.g., for the e coordinate, $p_e = \sigma_e^{old\ cs} / \sigma_e^{new\ cs}$) rounded to the appropriate whole number to emphasize the difference in precision quality.

Table 3. List of points for transformation.

	D48/GK				D96/TM					
Point	y **[m]**	x **[m]**	p_y	p_x	e **[m]**	n **[m]**	σ_e **[mm]**	σ_n **[mm]**	p_e	p_n
T1	461,832.4600	99,989.5000	1	1	461,461.4803	100,475.9817	1.2	1.7	10	5
T2	461,849.9300	99,989.2200	1	1	461,478.8845	100,475.7180	1.4	2.0	8	5
T3	459,984.0200	99,868.1900	1	1	459,613.0262	100,354.6710	1.5	2.0	8	5
T4	459,937.1900	101,340.7500	1	1	459,566.2221	101,827.2837	0.4	0.8	25	10
T5	456,202.4000	99,557.5400	1	1	455,831.3858	100,044.0614	0.2	0.3	40	35
T6	454,777.1400	100,905.6500	1	1	454,406.2259	1013,92.2533	0.7	0.8	10	10

We consider four-parametric similarity transformation in the horizontal plane in the form:

$$\begin{bmatrix} e \\ n \end{bmatrix} = \begin{bmatrix} a & b \\ -b & a \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} + \begin{bmatrix} c \\ d \end{bmatrix}, \tag{50}$$

where e and n are the coordinates in new coordinate system, y and x are the coordinates in the old coordinate system, a and b are transformation parameters including scale and orientation change ($a = m{\cdot}\cos\alpha$, $b = m{\cdot}\sin\alpha$; m is scale, α is rotation) and c and d are translation parameters.

The transformation parameters are computed in four different ways (Table 4), which are discussed in this paper: according to the WLS, TLS using SVD (TLS_SVD), and with the weighted TLS approach (WTLS). In the computation, we consider reduced coordinates to the center of gravity of the grid in the initial coordinate system (D48/GK).

Table 4. Transformation parameters—results.

Method	**Weights**	a	b	c **[m]**	d **[m]**	α **["]**	m **[ppm]**	$\hat{\sigma}_0$ **[m]**
WLS	yes	0.9999986	0.0000132	−370.98998	486.51088	2.72229	−1.35	0.09911
TLS_SVD	no	0.9999942	0.0000143	−370.98587	486.51985	2.94140	−5.83	/
WTLS	yes	0.9999948	0.0000140	−370.98617	486.51914	2.89402	−5.18	0.04278
GLS	yes	0.9999948	0.0000140	−370.98617	486.51914	2.89398	−5.18	0.06051

From the results in Table 4, it can be seen that the WTLS method gives quite similar results in the considered case with or without considering the weights (TLS_SVD) in the adjustment and that they are also consistent with the results of the general adjustment model (GLS); only the a posteriori precision estimate and the rotation angle α are slightly different.

We are also interested in the evaluation of the transformation quality from the point of view of the comparison of the transformed coordinates based on the computed parameters (Tables 5 and 6). In this analysis, we restrict ourselves only to the computations that take into account the weights (WTLS and the WLS).

From the results of the transformation parameters (Tables 4–6), it can be seen that the results are slightly different if the adjustment is performed classically by the method of least squares, taking into account the weights (the WLS), or if the errors in the unknowns (WTLS) are also taken into account. The differences in the transformed coordinates in D96/TM between the WLS and WTLS are of the order of one centimeter. Using the SVD decomposition in the TLS method, we obtain very similar results to the WTLS method.

Table 5. Differences between transformed and given coordinates in the final coordinate system—using the WLS approach.

WLS	New Coordinate System (D96/TM)		Differences		Transformed to D96/TM	
Point	***e* [m]**	***n* [m]**	***de* [m]**	***dn* [m]**	***e* [m]**	***n* [m]**
T1	461,461.4803	100,475.9817	−0.0178	−0.0065	461,461.4625	100,475.9752
T2	461,478.8845	100,475.7180	0.0480	−0.0231	461,478.9325	100,475.6949
T3	459,613.0262	100,354.6710	−0.0028	0.0187	459,613.0235	100,354.6897
T4	459,566.2221	101,827.2837	−0.0092	−0.0354	459,566.2130	101,827.2484
T5	455,831.3858	100,044.0614	0.0187	0.0287	455,831.4045	100,044.0901
T6	454,406.2259	101,392.2533	−0.0617	−0.0363	454,406.1642	101,392.2170
		RMS [m]	0.0338	0.0268		

Table 6. Differences between transformed and given coordinates in the final coordinate system—using the WTLS approach.

WTLS	New Coordinate System (D96/TM)		Differences		Transformed to D96/TM	
Point	***e* [m]**	***n* [m]**	***de* [m]**	***dn* [m]**	***e* [m]**	***n* [m]**
T1	461,461.4803	100,475.9817	−0.0247	0.0005	461,461.4557	100,475.9822
T2	461,478.8845	100,475.7180	0.0411	−0.0160	461,478.9256	100,475.7020
T3	459,613.0262	100,354.6710	−0.0027	0.0278	459,613.0235	100,354.6988
T4	459,566.2221	101,827.2837	−0.0077	−0.0319	459,566.2144	101,827.2518
T5	455,831.3858	100,044.0614	0.0330	0.0421	455,831.4188	100,044.1035
T6	454,406.2259	101,392.2533	−0.0408	−0.0268	454,406.1851	101,392.2265
		RMS [m]	0.0292	0.0275		

Comparing the WLS and WTLS results: Which one is better? Some of the parameters computed here indicate a better quality of adjustment by the WTLS method. If the quality criterion is represented by the a posteriori estimate of precision computed from the vector of measurements/observations residuals (corrections for point coordinates), then the value is better when WTLS is used (Table 4). When the a priori value of the standard deviation is set to 0.020 m for the initial coordinates in D48/GK and 0.005 m for the coordinates in D96/TM, the a posteriori value with the WLS is approximately 10 cm, and 4 cm when taking into account errors in variables (WTLS). Also, the mean value of the squares of the deviations of the transformed coordinates (based on the computed parameters) from those in the final/target coordinate system (Tables 5 and 6) is smaller with WTLS. It follows that the values of the computed transformation parameters are determined/computed by the WTLS method in such a way that the transformed coordinates on average fit better to the final "measured" coordinates of points.

3.3. The S-Transformation

3.3.1. General information about the S-Transformation

The S-transformation is a computational method that transforms an arbitrary datum-dependent solution for the vector of unknowns (coordinates of points) in the adjustment of the geodetic network to a selected geodetic datum. The method has been developed and described in detail by many researchers [17,18]. The basic S-transformation equation that converts the solution for coordinate unknowns from one (*gdi*) to another (*gdj*) geodetic datum is:

$$\mathbf{x}_{gdj} = \mathbf{S}_{gdj}\mathbf{x}_{gdi}, \tag{51}$$

with

$$\mathbf{S}_{gdj} = \mathbf{I} - \mathbf{H}(\mathbf{H}^{\mathrm{T}}\mathbf{E}\mathbf{H})^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{E}, \tag{52}$$

where $\mathbf{H} = \begin{bmatrix} & \vdots & & \\ 1 & 0 & x_i & y_i \\ 0 & 1 & -y_i & x_i \\ & \vdots & & \end{bmatrix}$ is the matrix of inner constraints with dimension of $2m \times (datum\ defect)$.

If the datum defect is 3 (the scale is known in the case of measured distances in network), then we, for instance, omit the fourth column. **E** is the matrix of dimensions $2m \times 2m$ (m—number of points in network) with off-diagonal elements that are equal to 0; and on the diagonal, there are values of 1 only in places that belong to the individual coordinate component that represents the given quantity to define the geodetic datum gdi. Matrix **E** can be considered as a weight matrix and Equation (51) as a weighted S-transformation [19].

The functional model of the S-transformation is the Gauss–Markov model, which connects "observations" $\mathbf{x}_{gdi}$, "residuals" $\mathbf{x}_{gdj}$ and unknowns of transformation vector $\mathbf{t}_{\mathrm{S}}$ is:

$$\mathbf{x}_{gdj} + \mathbf{H}\mathbf{t}_{\mathrm{S}} = \mathbf{x}_{gdi}, \tag{53}$$

where the LS solution for $\mathbf{t}_S$ can be:

$$\mathbf{t}_{\mathbf{S}} = (\mathbf{H}^{\mathrm{T}}\mathbf{E}\mathbf{H})^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{E}\mathbf{x}_{gdi}, \tag{54}$$

The matrix of the S-transformation (52) and matrix $\mathbf{H}\left(\mathbf{H}^{\mathrm{T}}\mathbf{E}\mathbf{H}\right)^{-1}\mathbf{H}^{\mathrm{T}}\mathbf{E}$ represent the orthogonal projectors, which project the observation vector $\mathbf{x}_{gdi}$ onto two orthogonal components: $\mathbf{t}_{\mathrm{S}}$ and $\mathbf{x}_{gdj}$. To solve model (53), we look for a solution for $\mathbf{t}_{\mathrm{S}}$ under the conditions of the least squares, this time for the minimum of the sum of the squares of the elements of the vector $\mathbf{x}_{gdj}$ with the previously determined "weight matrix" **E**. Thus, the S-transformation model provides the solution that minimizes the Euclidean norm of the vector of the coordinate components of the points which determine the geodetic datum: $\mathbf{x}^{\mathrm{T}}\mathbf{x} = \min$.

Matrix **H** is the datum matrix of internal constraints which includes all points of the geodetic network; or in other words, a matrix that ensures that all points of the geodetic network define a geodetic datum (example: free network). This means that matrix **E**, as a "weight matrix", is the one that determines which points should have a greater or lesser influence in defining the geodetic datum. So, we want to define such a weighting matrix **E**, which defines the optimal geodetic datum via the matrix **S** or finally provides the optimal solution for the vector $\mathbf{x}_{gdj}$.

3.3.2. The Total Least Squares Solution for the S-Transformation

In addition to the solution in Equation (54), we can find the solution for $\mathbf{t}_{\mathbf{S}}$ from Equation (53) using SVD decomposition. According to Equation (44), we can extend the **H** matrix by vector $\mathbf{x}_{gdi}$ and take into account the "weighting" matrix **E**:

$$\widetilde{\mathbf{H}} = [\mathbf{E}\mathbf{H}|\mathbf{E}\mathbf{x}_{gdi}], \tag{55}$$

In this case, the solution can be found according to Equations (46)–(49). We must take care that the system is at least uniquely determined. This means that we have at least uniquely determined the geodetic datum; or in numbers, rank(**H**) should not be smaller than rank($\widetilde{\mathbf{H}}$). The solution for vector $\mathbf{t}_{\mathrm{S}}$ follows the solutions in Equations (44) to (49).

To illustrate the computation of different solutions for $\mathbf{t}_S$, we simulated (the Box–Muller approach [20]) measurements of horizontal angles and distances in a predefined 2D geodetic network (Figure 4) for two measurement epochs, t_1 and t_2. Epoch t_2 is compared to t_1, a network with forced point movements (Table 7). For each epoch, the network was adjusted as a free network with the same initial values of point coordinates to provide the same geodetic datum for both epochs.

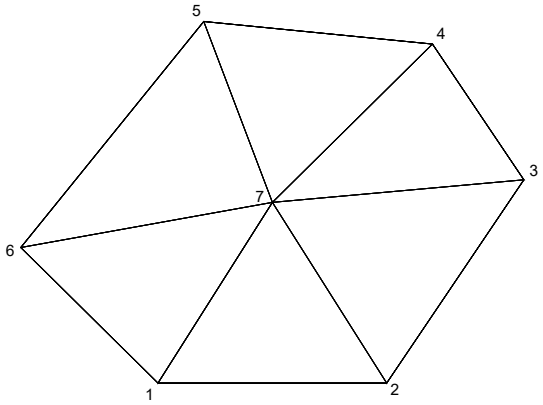

Figure 4. Geometry of the geodetic network.

Table 7. A simulated geodetic network with free network solutions for epochs t_1 and t_2.

	Initial Values		**Forced Movement**		**Epoch t_1**				**Epoch t_2**			
Point	x **[m]**	y **[m]**	dx **[mm]**	dy **[mm]**	x **[m]**	y **[m]**	σ_x **[mm]**	σ_y **[mm]**	x **[m]**	y **[m]**	σ_x **[mm]**	σ_y **[mm]**
1	1000	1000	/	/	999.9999	999.9984	0.5	0.6	999.9948	999.9906	0.5	0.6
2	2000	1000	/	/	1999.9998	1000.0010	0.5	0.6	1999.9948	999.9957	0.5	0.6
3	2600	1900	10	10	2600.0002	1899.9999	0.6	0.5	2600.0030	1900.0059	0.6	0.5
4	2200	2500	15	10	2199.9997	2499.9996	0.5	0.6	2200.0061	2500.0047	0.5	0.6
5	1200	2600	15	15	1200.0005	2600.0002	0.5	0.6	1200.0067	2600.0079	0.5	0.6
6	400	1600	/	/	400.0001	1600.0004	0.5	0.5	399.9936	1599.9913	0.5	0.5
7	1500	1800	8	10	1500.0000	1800.0005	0.4	0.4	1500.0011	1800.0039	0.4	0.4

Comparing solutions of free network adjustment for t_1 and t_2 in Table 7, it is obvious that we cannot obtain the right solution for displacements of points compared to forced values. Therefore, we usually use the S-transformation (51) with appropriately defined matrix **E**.

Model (53) can be solved in the same way as we performed computations for coordinate transformations using the described TLS approaches. We computed ordinary S-transformation, LS, and TLS using SVD and the WTLS solution of model (53). The results for differently defined geodetic datum (cases 1–3 with values 1 in matrix **E** in positions for selected datum points) are presented in Tables 8–10. For each solution, we also computed the sum of the squares of dx and dy coordinate differences $\mathbf{x}_{gdj}^{\mathrm{T}}\mathbf{x}_{gdj}$.

Table 8. Case 1—solutions for uniquely defined geodetic datum of points 1 and 2.

	Free Network		S-Transform.		LS		TLS_SVD		WTLS	
Point	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**
1	−0.00510	−0.00780	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
2	−0.00500	−0.00530	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000	0.00000
3	0.00280	0.00600	0.00999	0.00971	0.00999	0.00971	0.00999	0.00971	0.00999	0.00971
4	0.00640	0.00510	0.01513	0.00975	0.01513	0.00975	0.01513	0.00975	0.01513	0.00975
5	0.00620	0.00770	0.01528	0.01484	0.01528	0.01484	0.01528	0.01484	0.01528	0.01484
6	−0.00650	−0.00910	0.00016	0.00014	0.00016	0.00014	0.00016	0.00014	0.00016	0.00014
7	0.00110	0.00340	0.00815	0.00987	0.00815	0.00987	0.00815	0.00987	0.00815	0.00987
	$\mathbf{x}_{gdj}^{\mathrm{T}}\mathbf{x}_{gdj}$	0.00049		0.00114		0.00114		0.00114		0.00114

Table 9. Case 2—solutions for predetermined geodetic datum of points 1, 2 and 6.

	Free Network		S-Transform.		LS		TLS_SVD		WTLS	
Point	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**
1	−0.00510	−0.00780	−0.00004	−0.00007	−0.00004	−0.00007	−0.00004	−0.00007	−0.00004	−0.00007
2	−0.00500	−0.00530	0.00000	0.00004	0.00000	0.00004	0.00000	0.00004	0.00001	0.00003
3	0.00280	0.00600	0.00992	0.00985	0.00992	0.00985	0.00992	0.00985	0.00992	0.00986
4	0.00640	0.00510	0.01498	0.00987	0.01498	0.00987	0.01498	0.00987	0.01497	0.00987
5	0.00620	0.00770	0.01508	0.01486	0.01508	0.01486	0.01508	0.01486	0.01507	0.01486
6	−0.00650	−0.00910	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003	0.00003
7	0.00110	0.00340	0.00805	0.00989	0.00805	0.00989	0.00805	0.00989	0.00804	0.00989
	$\mathbf{x}_{gdj}^{\mathrm{T}}\mathbf{x}_{gdj}$	0.00049		0.00113		0.00113		0.00113		0.00113

Table 10. Case 3—solutions for predetermined geodetic datum of points 1, 2 and 7.

	Free Network		S-Transform.		LS		TLS_SVD		WTLS	
Point	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**	***dx* [m]**	***dy* [m]**
1	−0.00510	−0.00780	0.00137	−0.00412	0.00137	−0.00412	0.00138	−0.00412	0.00162	−0.00584
2	−0.00500	−0.00530	−0.00431	0.00057	−0.00431	0.00057	−0.00431	0.00057	−0.00436	0.00046
3	0.00280	0.00600	−0.00195	0.00798	−0.00195	0.00798	−0.00195	0.00798	−0.00362	0.00856
4	0.00640	0.00510	0.00265	0.00274	0.00265	0.00274	0.00265	0.00274	0.00014	0.00249
5	0.00620	0.00770	0.00801	0.00257	0.00801	0.00257	0.00801	0.00257	0.00564	0.00069
6	−0.00650	−0.00910	0.00213	−0.0102	0.00213	−0.0102	0.00213	−0.01020	0.00160	−0.01306
7	0.00110	0.00340	0.00293	0.00355	0.00293	0.00355	0.00293	0.00355	0.00175	0.00239
	$\mathbf{x}_{gdj}^{\mathrm{T}}\mathbf{x}_{gdj}$	0.00049		0.00032		0.00032		0.00032		0.00036

The comparison of the results in Table 8, Table 9 and Table 10 clearly shows that appropriate solutions for point displacements can only be obtained in the case of the appropriately defined geodetic datum. The results show that the solutions for the appropriate definition of geodetic datums are close to simulated/forced movements of points and are also the same (case 1 and 2—Tables 8 and 9) for all computational approaches. What is apparent from the results is that in case 3 (Table 10) of an inappropriately selected geodetic datum defined by the combination of points that are not all suitable for datum definition

(point 7 has moved), the values of point displacements (coordinate changes) and directions (Figure 5) and also the sum of the squares of all coordinate changes $\mathbf{x}_{gdj}^{T}\mathbf{x}_{gdj}$ are wrong and not the same for each solution. It can be seen from Table 10 (case 3) that the WTLS solution significantly differs from other solutions, which is not the case when the geodetic datum is appropriately defined (cases 1 and 2). Taking into account this finding, it is possible to find suitable combinations of points that appropriately define the geodetic datum and result in correct values of point displacements. Consequently, the solution for the appropriate combination of geodetic datums can therefore be found iteratively, combining different sets of datum points in matrix **E**.

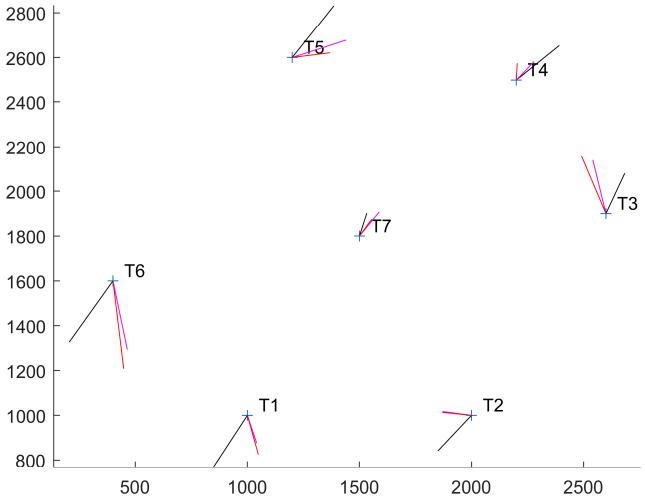

Figure 5. Case 3—vectors of point displacements in a geodetic network (black—free network, magenta—S-transf., LS and TLS_SVD solution, and red—WTLS solution).

4. Discussion and Conclusions

The problem of finding an optimal solution for the unknowns in a given system of equations combining observations and unknowns can be approached in several ways. In general, the closest approach to the surveyors is adjustment by the least squares method, in which observations, unknowns, and constants are connected in a linearized form via the Gauss–Markov model (1). In this case, the solution can be computed using a system of normal equations with or without taking into account precision or weights (no weights—similar to case when we give all measurements the same weights, e.g., 1) of the measurement. Such treatment is problematic in some cases. In finding a regression line for a set of points in a horizontal plane, only one coordinate component of the points can be treated as an observation, while the other is a constant. In certain cases, however, it makes sense for both coordinate components to be included in the regression model as observations/measurements. According to the mathematical relationship, the x-coordinate appears on the side of model matrix **A** and, in this way, also "forces" the treatment of errors on the side of the unknowns (EIV). A similar situation arises in the computation of the transformation parameters, where we want points in both the initial and target coordinate systems to have the status of observations in the adjustment. As an extension of the standard LS adjustment procedure, in addition to the well-known generalized adjustment model (GLS), an adjustment procedure based on the least squares method was investigated and developed by many researchers, and is referred to in the literature as "total least squares" or TLS. The method takes into account the errors on the side of the unknowns or in the matrix of adjustment model **A**, also with the possibility of taking into account weights (weighted total least squares —WTLS).

In this article, we presented the adjustment according to classical LS and the TLS approach using the computational example of finding the coefficients of the regression line and the computation of the transformation parameters and compared the results. The

regression line of the set of points in the plane computed by the TLS method adapts to the given precision of the x- and y-coordinates, which is reasonable and can be treated as a better solution than the LS solution.

When transforming the coordinates, based on the computed quality statistics, it can be stated that, in the case of adjustment using the WTLS method, the transformation is better adapted to the points in the final (target) coordinate system. Considering the precision of the given coordinates of the points, which are many times better in the final/newer coordinate system than in the original system (especially in the official state/national coordinate system developing over time), such a result is of course more appropriate due to the generally better quality of coordinates in the newer coordinate system.

The method was tested in transforming the positions of geodetic points from the old system to the new national coordinate system in Slovenia, which is quite problematic due to the characteristics of the old coordinate systems. The old system, dating back to the middle of the 20th century, was developed using totally different measuring and computational methods compared to the new system, which utilizes modern, up-to-date GNSS techniques. The transformation between them is very important due to the need to convert a vast amount of spatial data from various databases (cadastre, GIS, and others) to the new coordinate system.

For this purpose, the old geodetic points (e.g., churches), which have positions in the old coordinate system and can also be measured in the new system, are crucial for computing transformation parameters in a local area. In our opinion, the total least squares approach for determining the transformation parameters can represent a significant advancement in the phase of determining transformation parameters and consequently in the process of transforming all official spatial data to the new coordinate system on a national level.

Another application of the TLS approach that we wanted to emphasize in this article is in the field of deformation analysis, when computing the displacements of points in a geodetic network measured at different time epochs. The appropriately defined geodetic datum is very important when aiming to compute the correct values of point displacements. Many methods have been developed in the past in the field of deformation analysis, with the common task of determining the set of points that maintain their positions (are stable). Based on these points, the adjustment solution for displacements in a free geodetic network is then transformed to the correctly defined geodetic datum of stable points using the S-transformation.

In our research, we utilized the computational process of the TLS approach developed for coordinate transformations and implemented it into the process of the S-transformation. We compared this solution with the solutions for point displacements using the "ordinary" S-transformation, LS and SVD approaches.

We found that the different approaches yield the same results in the new geodetic datum when the selected reference or datum points have not moved between two compared epochs. In other cases, when there is a combination of stationary ('good') and moved ('bad') points, differences occur, which can also indicate an inadequately defined geodetic datum. Additionally, an iterative procedure can be utilized to find an appropriate set of 'good' geodetic datum points that can serve as the reference points for computing the displacement in a geodetic network. We consider this finding as a solid basis for further investigations in the field of computing the correct values of point displacements and consequently determining the true deformation state of the considered object.

In this article, we have focused only on the presence of normally distributed random errors in the model. The implications of outliers, which can cause distortions in estimates of unknown parameters, in the adjustment of observations could be also among the appropriate themes for further research. Investigating the response of the computational method to the presence of outliers could enhance the reliability and accuracy of adjustment results, thus contributing to the advancement of TLS data processing in geodetic applications.

Author Contributions: Conceptualization, A.M. and T.A.; methodology, A.M.; software, A.M.; validation, A.M., T.A. and S.S.; formal analysis, A.M., T.A. and S.S.; investigation, A.M., T.A. and S.S.; data curation, A.M.; writing—original draft preparation, A.M., T.A. and S.S.; writing—review and editing, A.M., T.A. and S.S.; visualization, A.M.; supervision, T.A. and S.S. All authors have read and agreed to the published version of the manuscript.

Funding: The authors acknowledge the financial support from the Slovenian Research and Innovation Agency-ARIS (research core funding No. P2-0227 Geoinformation infrastructure and sustainable spatial development of Slovenia).

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The original contributions presented in the study are included in the article, further inquiries can be directed to the corresponding author.

Conflicts of Interest: The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript; or in the decision to publish the results.

References

1. Kuang, S. *Geodetic Network Analysis and Optimal Design: Concepts and Applications*; Ann Arbor Press: Chelsea, MI, USA, 1996; ISBN 1575040441.
2. Teunissen, P. *Adjustment Theory: An Introduction*; Delft University Press: Delft, The Netherlands, 2000; ISBN 9040719748.
3. Fang, X.; Kutterer, H. On the Weighted Total Least Squares Solutions. In *The 1st International Workshop on the Quality of Geodetic Observation and Monitoring Systems (QuGOMS'11)*; Kutterer, H., Seitz, F., Alkhatib, H., Schmidt, M., Eds.; Springer International Publishing: Cham, Switzerland, 2015; pp. 45–50.
4. Amiri-Simkooei, A.R. Weighted Total Least Squares with Constraints: Alternative Derivation without Using Lagrange Multipliers. *J. Surv. Eng.* **2018**, *144*, 06017005. [CrossRef]
5. Akyilmaz, O. Total Least Squares Solution of Coordinate Transformation. *Surv. Rev.* **2007**, *39*, 68–80. [CrossRef]
6. Neitzel, F. Generalization of Total Least-Squares on Example of Unweighted and Weighted 2D Similarity Transformation. *J. Geod.* **2010**, *84*, 751–762. [CrossRef]
7. Amiri-Simkooei, A.; Jazaeri, S. Weighted Total Least Squares Formulated by Standard Least Squares Theory. *J. Geod. Sci.* **2012**, *2*, 113–124. [CrossRef]
8. Schaffrin, B.; Wieser, A. Empirical Affine Reference Frame Transformations by Weighted Multivariate TLS Adjustment. In *Geodetic Reference Frames: IAG Symposium, Munich, Germany, 9–14 October 2006*; Drewes, H., Ed.; Springer: Berlin/Heidelberg, Germany, 2009; pp. 213–218, ISBN 978-3-642-00860-3.
9. Fang, X. Weighted Total Least Squares Solutions for Applications in Geodesy. Ph.D. Thesis, Leibniz Universität Hannover, Hannover, Germany, 2011.
10. Van Loan, C.F. Generalizing the Singular Value Decomposition. *SIAM J. Numer. Anal.* **1976**, *13*, 76–83. [CrossRef]
11. Markovsky, I.; Van Huffel, S. Overview of Total Least-Squares Methods. *Signal Process.* **2007**, *87*, 2283–2302. [CrossRef]
12. Strang, G.; Borre, K. *Linear Algebra, Geodesy, and GPS*; Wellesley-Cambridge Press: Wellesley, MA, USA, 1997.
13. Lybanon, M. A Better Least-Squares Method When Both Variables Have Uncertainties. *Am. J. Phys.* **1984**, *52*, 22–26. [CrossRef]
14. Neri, F.; Saitta, G.; Chiofalo, S. An Accurate and Straightforward Approach to Line Regression Analysis of Error-Affected Experimental Data. *J. Phys. E* **1989**, *22*, 215. [CrossRef]
15. Golub, G.H.; Van Loan, C.F. An Analysis of the Total Least Squares Problem. *SIAM J. Numer. Anal.* **1980**, *17*, 883–893. [CrossRef]
16. Berk, S.; Komadina, Ž. *Trikotniško Zasnovana Transformacija Med Starim in Novim Državnim Koordinatnim Sistemom Slovenije [Triangle-Based Transformation between the Old and New National Coordinate Systems of Slovenia]*; REPUBLIKA SLOVENIJA PORTAL PROSTOR: Online, 2010; pp. 291–299, ISBN 978-961-254-210-8.
17. Baarda, W. *S-Transformations and Criterion Matrices*; Rijkscommissie voor Geodesie: Delft, The Netherlands, 1981; Volume 5.
18. Grafarend, E.; Schaffrin, B. Unbiased Free Net Adjustment. *Surv. Rev.* **1974**, *22*, 200–218. [CrossRef]
19. Chen, Y.Q.; Chrzanowski, A.; Secord, J.M. A Strategy for the Analysis of the Stability of Reference Points in Deformation Surveys. *CISM J.* **1990**, *44*, 141–149. [CrossRef]
20. Box, G.E.P.; Muller, M.E. A Note on the Generation of Random Normal Deviates. *Ann. Math. Stat.* **1958**, *29*, 610–611. [CrossRef]

Disclaimer/Publisher's Note: The statements, opinions and data contained in all publications are solely those of the individual author(s) and contributor(s) and not of MDPI and/or the editor(s). MDPI and/or the editor(s) disclaim responsibility for any injury to people or property resulting from any ideas, methods, instructions or products referred to in the content.