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Singular Value Decomposition - A Tool for VLBI Simulations

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Abstract

Usually VLBI observations are adjusted by least-squares approaches like the Gauss-Markoff model with the use of normal equations. It is well known that parameter estimation methods based on this strategy show some numerical disadvantages. To overcome these problems a new approach makes use of a more stable least-squares algorithm, called singular value decomposition (SVD) and provides interesting insight into the composition of the estimated parameters and shows the impact of particular observations on the parameters.

For an example VLBI session the results of the new method will be presented and the suitability of the SVD approach for simulations and for the improvement of VLBI schedules will be shown.

1. Introduction

In many scientific analyses or engineering problems it is necessary to determine parameters of a linear (or linearized) model after performing (many) more measurements than necessary for a unique solution. This leads to an overdetermined system of linear equations which is commonly solved in a least-squares sense by e.g. using the Gauss-Markoff-Model (see e.g. Koch, [2]). Many VLBI data analysis software packages use this approach for the determination of e.g. earth orientation parameters, site positions, etc. One of the most common (and simple) methods for the estimation of the parameters in the model

$$A\mathbf{x} = \mathbf{b} \quad \text{with} \quad \Sigma_{bb} = \sigma_0^2 \cdot P^{-1} \tag{1}$$

is based on solving a system of normal equations, i.e. by using the well-known formula

$$\hat{\mathbf{x}} = (\mathbf{A}'\mathbf{P}\mathbf{A})^{-1}\mathbf{A}'\mathbf{P}\ \mathbf{b} \quad \text{and} \quad \Sigma_{\hat{\mathbf{x}}\hat{\mathbf{x}}} = \hat{\sigma}_0^2 \cdot (\mathbf{A}'\mathbf{P}\mathbf{A})^{-1}, \tag{2}$$

with

$\mathbf{A}$	the design matrix (or Jacobi matrix) containing the partial derivatives of the observations equation with respect to the parameters to be determined (= functional model). $\mathbf{A}'$ means the transpose of this matrix,
$\mathbf{P}$	the weight matrix as the inverse of the variance/covariance matrix (= stochastical model),
$\mathbf{b}$, Σ_{bb}	the vector of observations (also known as O-C-vector) and its variance-covariance matrix and
$\hat{\mathbf{x}}$, $\Sigma_{\hat{\mathbf{x}}\hat{\mathbf{x}}}$	the (estimated) vector of unknowns and its variance/covariance matrix.

Equation (2) yields a least-squares solution, i.e. it determines $\hat{\mathbf{x}}$ while minimizing the square sum of the residuals: $\| A\mathbf{x} - \mathbf{b} \|^2$.

In the language of linear algebra the least squares principle can be visualized geometrically by vector spaces and projections on the so-called column space of $\mathbf{A}$, i.e. the vector sub-space formed by the columns of the design matrix $\mathbf{A}$ (see e.g. ADAM, [1] or STRANG/BORRE, [6]).

In the following a quite unknown (at least in geodesy) approach for a least-squares solution of the system (1) is used which avoids normal equations and which reveals a lot more of geometrical information about the adjustment problem. This approach is based on the direct analysis of the design matrix by **Singular Value Decomposition (SVD)** which both preserves the numerical stability of the system to be solved and yields important information about the impact of certain observations on particular parameters.

The goal of these investigations is the application of an uncommon algebraic parameter estimation method in order to get deeper insight into the adjustment process and to give a 'geometrical' interpretation of the adjustment process. Furthermore, interesting auxiliary means for the assessment of the functional model can be derived from SVD and can be applied to the adjustment of VLBI sessions. This approach can be regarded as further development of existing simulation strategies. The information gained from these analyses will support the improvement of VLBI schedules.

2. Basics of Linear Algebra

2.1. Least-squares Solutions of Overdetermined Systems of Linear Equations

For the solution of an (usually) inconsistent system of linear equations like (1) Linear Algebra provides different approaches which are more or less numerically stable (see e.g. STRANG/BORRE, [6]). As mentioned above in geodetic applications the most common approach is the computation and solution of the associated system of normal equations. Other –so-called direct–methods as e.g. QR-decomposition are directly applied to the design matrix and preserve the lengths of the vectors associated with the system to be solved.

One of these length preserving, direct approaches is the singular value decomposition which decomposes an arbitrary matrix of dimension $m \times n$ into

$$\mathbf{A} = \mathbf{U} \cdot \mathbf{S} \cdot \mathbf{V}' = \mathbf{U} \begin{pmatrix} \mathbf{D} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \mathbf{V}' \qquad \text{with } \sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0. \tag{3}$$

$\mathbf{U}$ is an orthogonal matrix of dimension $m \times m$ whose columns form the so-called left singular vectors $\mathbf{u}_i$. $\mathbf{S}$ is an $m \times n$-matrix only containing the so-called singular values σ_i on its main diagonal and $\mathbf{V}$ is an orthogonal $n \times n$-matrix whose columns $\mathbf{v}_i$ form the so-called right singular vectors. By definition, the singular values σ_i are ordered in decreasing order.

Although $\mathbf{A}$ might be of arbitrary dimension for the following only the overdetermined case $(m > n)$ is considered.

Decomposition (3) can be understood as a generalization of an eigenvalue decomposition of a rectangular matrix. MEYER, [4] shows that the singular values are just the square roots of the eigenvalues of $\mathbf{A}' \cdot \mathbf{A}$ and the right singular vectors correspond to the eigenvectors of $\mathbf{A}' \cdot \mathbf{A}$. The left singular vectors correspond to the eigenvectors of $\mathbf{A} \cdot \mathbf{A}'$.

Especially in geophysical and geological applications the algebraic terms 'row and column space' are replaced by the more descriptive terms 'model space' and 'data space', respectively, since they depict the most important vector spaces associated with the adjustment process (see e.g. STRANG/BORRE, [6], MENKE, [3]).

After transforming the column space and the row space of **A** to the new bases formed by the left and the right singular vectors respectively the system is called to be transformed to its canonical form in which the least squares problem becomes simpler and thus more lucid (see e.g. STRANG/BORRE, [6]).

2.2. Geometrical Interpretations

Instead of using equation (2) the decomposition of the design matrix (formula (3)) can be used to solve (1) in a least-squares sense by:

$$\hat{\mathbf{x}} = \mathbf{V}_r \cdot \mathbf{S}_r^{-1} \cdot \mathbf{U}_r' \cdot \mathbf{b} = \sum_{n=1}^{r} \frac{\mathbf{u}_i \cdot \mathbf{b}}{\sigma_i} \cdot \mathbf{v}_i \tag{4}$$

where

r	denotes the rank of the system,
$\mathbf{V}_r$	is an $n \times r$ matrix formed by the first r columns of $\mathbf{V}$,
$\mathbf{U}_r$	is an $m \times r$ matrix formed by the first r columns of $\mathbf{U}$ and
$\mathbf{S}_r$	is an $r \times r$ matrix formed by the first r rows and columns of $\mathbf{S}$.

Equation (4) shows that the least-squares solution is formed by superimposing r 'slices' $\mathbf{v}_i$ i.e., the ith 'slice' of the solution vector consists of the respective $\mathbf{u}_i, \mathbf{v}_i, \sigma_i$ and the vector of observations $\mathbf{b}$.

According to STRANG/BORRE, [6] the first r left singular vectors $\mathbf{u}_i$ $(i = 1, \ldots, r)$ are called canonical vectors and "reveal observations which should have been performed with larger weight" since they have a large impact on the adjustment results. This can also be seen in the so-called "Data resolution matrix" described below. The first r right singular vectors $\mathbf{v}_i$ $(i = 1, \ldots, r)$ depict those parameters (or linear combinations of parameters) which are best determined. Right singular vectors $\mathbf{v}_i$ belonging to zero- (or very small) singular values show parameters which are totally undetermined.

2.3. Resolution Matrices

One of the analysis tools derived from SVD are so-called *resolution matrices* (see e.g. MENKE, [3]): For example,

$$DRM = U_r \cdot U_r' \tag{5}$$

is called **Data Resolution Matrix (DRM)** and serves as a projection operator onto the column space/data space of the design matrix. This matrix (also known as 'hat-matrix' in statistics) deserves a closer look since it provides a lot of information of the adjustment problem. The main diagonal of this matrix reveals the *importances* of the observations and thus the sensitivity of certain observations. Errors in observations with large importance values strongly impact the estimation results.

Furthermore

$$MRM = V_r \cdot V_r' \tag{6}$$

represents the so-called **Model resolution Matrix (MRM)** and serves as a projection operator onto the row space/model space of the design matrix. The MRM can be used for better investigation of separability of the parameters compared to the well-known correlation matrix (see e.g. KOCH, [2]).

3. Application Example

The methods described above have been applied to the analysis of the baseline Kokee - Wettzell within the Multi-Intensive session RD0404 (04JUN16XA). During 24 hours 415 observations have been performed on this baseline which have been used to estimate four parameters: (1) clock offset for Kokee, (2) tropospheric zenith path delay for Kokee (3) and for Wettzell, and (4) $dUT1$.

The design matrix for this (quite unusual but appropriate) parametrisation has been generated by using OCCAM 6.1 and the singular value decomposition has been performed with additional software written in Fortran 95.

Figure 1 shows a part of the components of the singular value decomposition of the design matrix of this session: the four right singular vectors $\mathbf{v}_1$ through $\mathbf{v}_4$ together with their respective singular values reveal the estimability and separability of the four estimated parameters (or some linear combinations of them). These components can be used for so-called model space investigations.

The first right singular vector $\mathbf{v}_1$ (together with the corresponding singular value σ_1 and the left singular vector $\mathbf{u}_1$, which is not shown here) mostly affects the second and the third parameter: the tropospheric zenith path delay for both Kokee and Wettzell. The second component ($\mathbf{v}_2$, σ_2 and $\mathbf{u}_2$) mostly affects the fourth parameter, which is the earth rotation $dUT1$[1]. In the same way $\mathbf{v}_3$, σ_3 and $\mathbf{u}_3$ as well as $\mathbf{v}_4$, σ_4 and $\mathbf{u}_4$ offer some insight into the generation of parts of the solution vector concerning the remaining parameters. $\mathbf{v}_4$ and σ_4 depict the least precisely determined parameter which is the clock offset at Kokee station.

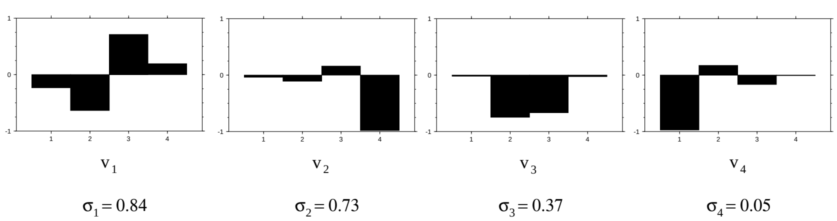

Figure 1. Right singular vectors v_1 through v_4 and singular values σ_1 through σ_4 (order of parameters: clock offset Kokee, zenith path delay Kokee and Wettzell, $dUT1$).

Figure 2 shows the main diagonal of the data resolution matrix (see equation (5)). Large values reveal observations which are (due to their geometry) of special importance for the parameter estimation process in general and thus need further considerations. Comparing Figure 2 with a list of all observations performed on this baseline, for this parametrisation (i.e. for this set of parameters to be estimated) especially observations to sources with low declinations are important. Assuming the rule of thumb that baselines with a long equatorial extension are mostly suitable for

[1]Analysis of the corresponding left singular vector $\mathbf{u}_2$ would reveal observations which are mostly important for earth rotation determination (since -in this case- the so-called 'importances' shown below almost give the same information $\mathbf{u}_2$ is not explicitly shown here).

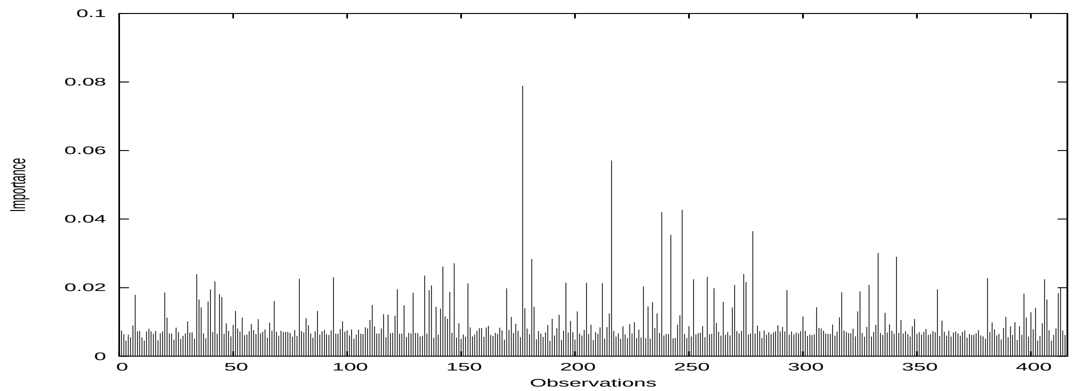

Figure 2. “Importances” of observations for R0404-baseline Kokee - Wettzell

the determination of earth rotation this result agrees with the theoretical results e.g. described by SCHUH, [5] and other authors.

4. Conclusions & Outlook

Investigations have shown that least-squares solutions of overdetermined systems of linear equations computed by singular value decomposition can be used as a tool for simulations in VLBI data analysis. SVD yields ‘geometrical’ insight into the adjustment problem and gives important information which can be used to improve VLBI observation schedules. Disadvantages of this approach might be larger memory requirements and longer computation times compared to the normal equation approach.

This method and the analysis tools derived from SVD will be applied to larger adjustment problems / larger observation networks in order to better understand the analysis of VLBI observations and to improve scheduling in general. A user-friendly software tool (for any type of adjustment problem) based on the graphical user interface-toolkit QT is being developed at GIUB and will be applied to the analysis of other VLBI sessions. The results will be presented in the future.

References

[1] Adam, J.: A detailed study of the duality relation for the least squares adjustment in euclidean spaces, Bull. Geod. 56, pp. 180-195, 1982.

[2] Koch, K. R.: Parameter Estimation and Hypothesis Testing in Linear Models, Second, Updated and Enlarged Edition, Springer, 1999.

[3] Menke, W.: Geophysical Data Analysis: Discrete Inverse Theory, Academic Press Inc., 1984.

[4] Meyer, C. D.: Matrix Analysis and Applied Linear Algebra, Society for Industrial and Applied Mathematics (siam), 2000.

[5] Schuh, H.: Die Radiointerferometrie auf langen Basen zur Bestimmung von Punktverschiebungen und Erdrotationsparametern, Ph.D. thesis, Rheinische Friedrich-Wilhelms-Universität zu Bonn, 1987.

[6] Strang, G., K. Borre: Linear Algebra, Geodesy and GPS, Wellesley-Cambridge Press, 1997.