Total singular value decomposition.
Robust SVD, regression and location-scale

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Abstract
Singular Value Decomposition (SVD) is the basic body of many statistical algorithms and few users question whether SVD is properly handling its job.

SVD aims at evaluating the decomposition that best approximates a data matrix, given some rank restriction. However often we are interested in the best components of the decomposition rather than in the best approximation. This conflict of objectives leads us to introduce Total SVD, where the word “Total” is taken as in “Total” least squares.

SVD is a least squares method and, therefore, is very sensitive to gross errors in the data matrix. We make SVD robust by imposing a weight to each of the matrix entries. Breakdown properties are excellent.
Algorithmic aspects are handled; they rely on high dimension fixed point computations.

1 Introduction
The presented approach goes upside-down. Indeed, starting with our ultimate goal, SVD, we precisely define the ingredients we need and, then, we keep them in mind in the course of actions. The two main principles will be

- Be robust. This will be understood as limiting the effect of each observation on the estimations in a way such that it cannot unduly pull on the result.

- Keep it simple. We would appreciate to plunge the Singular Value Decomposition (SVD) problem in a M-estimation setup. However, this does not seem possible without imposing heavy restrictions on the data matrices. We will remain pragmatic and be oriented toward the numerical aspects.

We observe that our natural use of weights is fully consistent with the theories developed in the field of robustness. Without any effort, we come with the concepts of Breakdown point and M-estimation.

1.1 SVD
There are many ways to look at data matrices and, thinking at principal components, most of the ways favor either the rows or the columns of the data matrix; they are either observation- or variable-oriented. Some analysis methods try to be more balanced, for instance the (non-robust) biplot as defended by Bradu and Gabriel (1978), Gabriel (1998), Gower (2004) or Le Roux and Gardner (2005). Considering a $[m \times n]$-data matrix $X$, a low-rank approximation is estimated (typically of rank 2) and graphically presented. Strangely, the approximation is worked out without taking into account the scatter of the matrix entries. Let us explain.

The singular value decomposition

$$X \approx U \Lambda V', \quad p \leq \min\{m, n\}$$

where

$$U' U = V' V = I_p \quad \text{and} \quad \Lambda = \text{diag}\{\lambda_1, ..., \lambda_p\}, \quad \lambda_1 \geq ... \geq \lambda_p \geq 0$$

is conveniently worked out with the help of an intermediate step

$$X \approx A B' = U \Lambda V'$$

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and an alternating computational scheme. This paper is centered on the approximation

\[ X \approx AB' \]  

and essentially ignores the last step,

\[ AB' = U \Lambda V' \]

seeing that it does not involve any approximation and can be performed by any (least squares) method. Works on alternating computational schemes are referred to in Ke and Kanade (2005) and Croux et al. (2003), for instance, and have flourished since the criss-crossing of Bradu and Gabriel (1978).

The goal is to estimate \( AB' \) as it appears in Eq. \((1)\) by a minimisation procedure

\[ \hat{A}\hat{B}' = \arg\min_{A B'} \{ \| X - AB' \| \} \]  

where \( \| \cdot \| \) is a norm. This problem is solved by alternating between

\[ A \text{ being known, } \hat{B}' = \arg\min_{B'} \{ \| X - A B' \| \} \]  

and

\[ B \text{ being known, } \hat{A} = \arg\min_{A} \{ \| X - A B' \| \} . \]

Unfortunately, the norm in Eq. \((2)\) is ill-defined and, except in the least squares set-up, it has little to do with those of Eq. \((3)\) and Eq. \((4)\). Moreover, the two latter are inconsistent seeing that, at the end of the convergence, the two errors with respect to the approximated entry \( X_{ij} \), namely

\[ [X_{ij} - (A \hat{B}')_{ij}] \text{ given } A \quad \text{ and } \quad [X_{ij} - (\hat{A} B')_{ij}] \text{ given } B \]

often differ. In fact, when robust estimation is of concern, very generally, they differ.

1.2 Regression

Besides the inconsistency of norms, an other little observed hindrance appears in the solving of Eq. \((3)\) and Eq. \((4)\). For the former, we wrote \( A \text{ being known} \) and, of course, it is estimated rather than known. Considering the \( n \) columns of \( X \) in Eq. \((3)\), the \( n \) columns of \( B' \) are solution of

\[ A \text{ being estimated, } (\hat{B}')_j = \arg\min_{B'} \{ \| x_j - A (B')_j \| \} \]

where \( X = (x_1, ..., x_n) \). In the more familiar regression notation, this is

\[ D \text{ being estimated, } \hat{\beta} = \arg\min_{\beta} \{ \| y - D \beta \| \} \]

under an error-in-variables model.

As seen by Huber (1973), the robust treatment of linear regression is a simple extension of his approach in (1972, 1996) in the location-scale set-up.

1.3 The location-scale set-up

This is at the root of all investigations in robustness and, in Section 2, we report a very simple-minded view that is exceptionally rich in spite of being little traditional. In some sense, we address the reader as if he was not already familiar with all developments made in the robustness field.

The location-scale set-up is further extended to handle regressions and this let unexpected features appear in Section 3. Section 4 concludes the exposition of the approach with the SVD treatment.
2 The location-scale set-up

2.1 The weighted approach.

We consider a set of \( m \) observations \( \{x_1, \ldots, x_m\} \) that are, as we all assume, distributed according to a so-called Gaussian distribution. We are interested in their location and their scatter, entities that can be assessed by their mean \( n \) and their standard deviation (again, ‘as we all know’), namely by

\[
n = \frac{1}{m} \sum_{i=1}^{m} x_i \quad \text{and} \quad s_x = \left( \frac{1}{m} \sum_{i=1}^{m} (x_i - n)^2 \right)^{1/2}.
\] (5)

Some might prefer to divide by \((m - 1)\) rather than by \(m\) in the second expression but, for the time being, we consider this idea as a sheer refinement. Rather, we are concerned by the possibility of gross errors of estimation due to possible errors in our data set \( \{x_1, \ldots, x_m\} \).

This is what robustness is about. To avoid that a few observations pull too much the mean toward them, it suffices to limit their influences on, for instance, the sum \( \sum_{i=1}^{m} x_i \) in Eq. (5).

Inserting weights \( w_i \), the sum becomes \( \sum_{i=1}^{m} w_i x_i \).

Clearly, the weighting must have little effect on the ‘central’ observations and must bound the extreme observations. Assuming that we bound to some constant \( q \), namely by

\[
w(x) = \begin{cases} \frac{c}{n-x}, & \text{if } x \ll m, \\ 1, & \text{if } |x-m| \ll s, \\ \frac{c}{x-n}, & \text{if } x \gg m. \end{cases}
\] (6)

Remark, already at this level, that the weights are allocated with help of the mean and standard deviation estimates. Further on, we apply the weight definitions

\[
w(x) = (1 + |u|^q)^{-1/q} \quad \text{where} \quad u = \frac{x - n}{k_1 s_x}, \quad 0 < q < \infty
\] (7)

and, at the limit \( q = \infty \),

\[
w(x) = \begin{cases} 1, & \text{if } |u| \leq 1, \\ 1/|u|, & \text{if } |u| \geq 1. \end{cases} \quad \text{where} \quad u = \frac{x - n}{k_1 s_x},
\]

that imply for the above constant

\[
c = \lim_{|x-n| \to \infty} w(x) |x| = k_1 s_x.
\]

The so-called ‘tuning constant’ \( k_1 \) controls the level of robustness that is desired. The parameter \( q \) will be numerically tried at five different values, \(1, 2, 4, 8\) and \(\infty\), in order to select the most appropriate one. The weights of \( q = 1 \) were already implemented in the numerical package of Klema (1978) and they are presented by Coleman et al. (1980) under the name ‘Fair’. At \( q = \infty \), the weighting is identical to what Huber (1964) found as optimal in the near-vicinity of the Gaussian distribution.

Clearly having inserted weights, Eq. (5) must be adapted and, at first sight, the next writings could appear appropriate

\[
n = \frac{1}{\sum_{i=1}^{m} w_i} \sum_{i=1}^{m} w_i x_i \quad \text{and} \quad s_x^2 = \frac{1}{\sum_{i=1}^{m} w_i} \sum_{i=1}^{m} [w_i (x_i - n)]^2.
\]

The above estimator of the population variance is severely biased on two grounds: On the one hand, it is greatly underestimating \( s_x^2 \) due to systematically down-weighting the large terms \((x - n)^2\) and, on the other hand, we have omitted to take the correct number of degrees freedom into account. We now deal with these two issues.

The severe underestimation is taken into account by inserting a correction factor

\[
k_2^2 = \frac{\int_{-\infty}^{\infty} w(x)^2 m(x) dx}{\int_{-\infty}^{\infty} w(x)^2 x^2 m(x) dx} \quad \text{where} \quad m(x) = \exp^{-x^2/2}/\sqrt{2 \pi}.
\] (8)
Rather than dividing by \( m \), at least in the linear context, we know that we must take into account a reduced number of degrees of freedom. In this approach with weights, it is less clear how the situation must be handled. We have opted for a correction term \( \frac{N}{N-1} \) where \( N \) stands for the ‘effective’ number of observations, the number of observations that play a role in the variance estimate. Very generally, whatever an item \( (u_i) \) can be, a weighted average takes the form \( \sum_{i=1}^{m} w_i (u_i)/\sum_{i=1}^{m} w_i \), therefrom come the expressions of the average weight \( \bar{w} \) and the ‘effective’ sample size \( \bar{w} = \frac{1}{\sum_{i=1}^{m} w_i} \). 

Further on, we compare estimators with respect to how many observations influence their taken values. Very simply, this can be measured by:

\[
\text{Efficacy} = \frac{N}{m}.
\]

It is now time to gather the various items we met with. The mean \( n \) and the scatter \( s_x \) are the solution of a fixed-point problem where, given previous estimates \( (n, s_x) \), the weights and the new \( (n, s_x) \) are estimated according to

\[
\begin{cases}
\text{Given } n \text{ and } s_x, \\
\quad w_i = (1 + |u_i|^q)^{-1/q}, \quad \text{where } u_i = (x_i - n)/(k_1 s_x), \\
\quad n = \frac{1}{\sum_{i=1}^{m} w_i} \sum_{i=1}^{m} w_i x_i, \\
\quad s_x^2 = k_2^2 \frac{1}{\sum_{i=1}^{m} w_i^2} \sum_{i=1}^{m} w_i^2 (x_i - n)^2.
\end{cases}
\] (10)

The unbiased estimator of the variance is

\[
\hat{\sigma}_x^2 = \frac{N}{N-1} s_x^2 \quad \text{where } \quad N = \left( \sum_{i=1}^{m} w_i \right)^2 / \sum_{i=1}^{m} w_i^2.
\]

For \( k_1 \to \infty \), the above expressions collapse in the familiar least squares formulae

\[
\begin{cases}
\text{Whatever a priori values } n \text{ and } s_x, \quad w_i = 1 \\
\quad n = \frac{1}{m} \sum_{i=1}^{m} x_i \\
\quad s_x^2 = \frac{1}{m} \sum_{i=1}^{m} (x_i - n)^2, \quad \text{where } \quad k_2 = 1.
\end{cases}
\]

We observe that the set of equations (10) in terms of the two variables \( n \) and \( s_x \) describes a contracting mapping when the weights satisfy Eq. (6). Hence, the numerical convergence can easily be accelerated in the vicinity of the fixed-point solution.

2.2 Theory and numerical experiments

Some aspects of the theory will be briefly sketched and further details can be found in very many places as, for instance, in Rey (1978, 1983). They will often be supported by numerical experiments.

2.2.1 Contamination model.

Rather than assuming that the variates \( x_i \) are distributed according to a nominal probability density function \( f_{\text{main}} \), Tukey (1960) considers that a few observations could possibly be drawn from another distribution \( f_{\text{rubbish}} \):

\[
x_i \sim f, \quad f = (1 - \epsilon) f_{\text{main}} + \epsilon f_{\text{rubbish}} \quad \text{where } \quad \epsilon \ll \frac{1}{2}.
\]
The contaminated distribution is a mixture distribution. The objective of robust estimation consists in being as little sensitive as possible to rubbish. As is usual, we assume a Gaussian distribution and outliers

\[ f_{\text{main}} = \mathcal{N}(\mu, \sigma^2) \quad \text{and} \quad f_{\text{rubbish}} \ll \mathcal{N}(\mu, \sigma^2). \]

### 2.2.2 M-estimation.

The above weights were introduced as an intuitive manner of limiting the influence of any extreme observation on the estimates of the mean and the variance. They also appear very naturally in the context of M-estimation.

Many estimators can be seen as solutions of minimization problems and, in the context of location estimation, it takes the form

\[ \hat{\theta} = \arg\min_{\theta} \left\{ \sum_{i=1}^{m} \rho(x_i - \theta) \right\}. \] (11)

Then, under differentiability conditions,

\[ \sum_{i=1}^{m} \Psi(x_i - \theta) = 0 \quad \text{where} \quad \Psi(u) = \frac{d}{du} \rho(u). \]

In order to let the weights appear, we transform the left hand member,

\[ \sum_{i=1}^{m} \Psi(x_i - \theta) = \sum_{i=1}^{m} \frac{\Psi(x_i - \theta)}{x_i - \theta} (x_i - \theta) = \sum_{i=1}^{m} w(x_i) (x_i - \theta) = 0 \]

and see that the weights

\[ w(x_i) = \frac{\Psi(x_i - \theta)}{x_i - \theta} \] (12)

naturally appears in a minimization framework.

In order to have a minimum, Eq. (11) must be convex and this is certainly realized when each of its terms in \( \rho(.) \) is convex. Then, seeing Eq. (12), the restriction (6) on the weights turns out.

All least squares approaches are based on \( \rho(u) = u^2 \) and that corresponds with no weighting (or equal non-zero weights).

### 2.2.3 Breakdown point.

This is a concept developed by Hampel (1968) that has a natural motivation. Robust estimators remain stable in spite of (very) extreme observations in the sample. The breakdown is a measure of how many very extreme observations can be tolerated.

To illustrate, consider the weighted mean estimator

\[ n = \frac{1}{\sum_{i=1}^{m} w_i} \sum_{i=1}^{m} w_i \ x_i \]

and suppose that you add \( k \) very extreme points on the right side of \( n \). Seeing Eq. (6), the estimator becomes

\[ n(m, k) = n \approx \frac{1}{\sum_{i=1}^{m} w_i} \left[ \sum_{i=1}^{m} w_i \ x_i + k \ c \right], \]

the approximation being valid as long as the point addition little influences the values of the weights \( w_i \). The breakdown point, \( \text{BP}_a \), is the fraction such that \( \text{Offset}_n \) be very large or, precisely

\[ \text{BP}_a = \lim_{m \to \infty} \frac{k_{\text{BP}}}{m + k_{\text{BP}}} \quad \text{such that} \ \{\text{Offset}_n = a\} . \] (13)

The exact value of \( a \) is immaterial as indicated in Note[2]
2.2.4 Numerical convergence

How fast the iterative process (10) converges is of great practical importance. Noting by \( l \) the iteration number, we observe that the mapping

\[
... \rightarrow (n^{l-1}, s_x^{l-1}) \rightarrow (n^l, s_x^l) \rightarrow (n^{l+1}, s_x^{l+1}) \rightarrow ... \rightarrow (n^\infty, s_x^\infty)
\]

is contracting. The rates \( b_n \) and \( b_s \) indicate the convergence speed,

\[
n^{l+1} - n^\infty \approx b_n (n^l - n^\infty) \quad \text{and} \quad s_x^{l+1} - s_x^\infty \approx b_s (s_x^l - s_x^\infty),
\]

(14) when process (10) is not accelerated. In the near-vicinity of \((n^\infty, s_x^\infty)\) and for symmetrical distributions, expressions (14) are exact.

2.2.5 Numerical experiments

All the reported experiments are with respect to the standard Gaussian distribution and this is further documented in Note 1. The tabulated results are asymptotic, \( m \rightarrow \infty \), as described in Note 3.

It is time to focus on better specifying the weight function given by the family (7). Clearly, any given weight definition has consequences on the number of outliers that can be tolerated without dramatically spoiling the estimations. Hence, the breakdown point appears to be a natural gauge. Of course, comparing the performances of various powers must be done under similar conditions. Table 1 proposes a summary of the observations and the power-value \( q = 4 \) turns out to be an interesting selection, although results with \( q = 2 \) or \( q = 8 \) are little different.

Table 1: Selecting the power \( q \) in the weight definition (7).

| Efficacy | \( q \) | BP1 |
|----------|-------|-----|
| Eq. (9)  | Eq. (7) | Eq. (13) |
| 0.80     | 1     | 0.276 |
|          | 2     | 0.352 |
|          | 4     | 0.375 |
|          | 8     | 0.382 |
|          | \( \infty \) | 0.383 |
| 0.90     | 1     | 0.195 |
|          | 2     | 0.294 |
|          | 4     | 0.329 |
|          | 8     | 0.339 |
|          | \( \infty \) | 0.342 |
| 0.95     | 1     | 0.124 |
|          | 2     | 0.235 |
|          | 4     | 0.282 |
|          | 8     | 0.293 |
|          | \( \infty \) | 0.297 |

Table 2 reports further details with the selected weight definition,

\[
w(x) = (1 + u^4)^{-1/4} \quad \text{where} \quad u = \frac{x - n}{k_1 s_x}.
\]

(15)

The parameters \( k_1 \) and \( k_2 \) control the degree of robustness of estimation by Eq. (10). As indicated by the last two columns of Table 2, the convergence of process (10) is somewhat slow and acceleration is welcome. We observe at the last rows that a small loss of Efficacy already yields a serious protection against possible outliers.

3 Regression

As indicated in the introduction, we consider the regression model

\[
y \in \mathbb{R}^n \quad D \in \mathbb{R}^{n \times p} \quad \beta \in \mathbb{R}^p \quad \text{error} \in \mathbb{R}^n
\]

\[
y = D \beta + \text{error}
\]
Table 2: Data with the weights of Eq. (15)

| Efficacy | $k_1$ | $k_2$ | $k_3$ | $k_1 \times k_2$ | BP | $b_n$ | $b_s$ |
|----------|-------|-------|-------|------------------|----|-------|-------|
| Eq. (9)  | 0.0987 | 3.7227 | 0.3673 | 0.4110           |    | 0.7220 | 0.4777 |
| Eq. (7)  | 0.1497 | 3.0541 | 0.4571 | 0.4062           |    | 0.6810 | 0.4723 |
| Eq. (8)  | 0.2244 | 2.5258 | 0.5669 | 0.3960           |    | 0.6275 | 0.4648 |
| Eq. (13) | 0.2760 | 2.2954 | 0.6336 | 0.3881           |    | 0.5933 | 0.4592 |
| Eq. (14) | 0.3428 | 2.0798 | 0.7130 | 0.3754           |    | 0.5515 | 0.4513 |
| Eq. (14) | 0.4336 | 1.8730 | 0.8122 | 0.3575           |    | 0.4984 | 0.4391 |
| Eq. (14) | 0.5686 | 1.6673 | 0.9480 | 0.3294           |    | 0.4265 | 0.4178 |
| Eq. (14) | 0.6456 | 1.5825 | 1.0217 | 0.3138           |    | 0.3893 | 0.4043 |
| Eq. (14) | 0.7472 | 1.4937 | 1.1161 | 0.2936           |    | 0.3442 | 0.3853 |
| Eq. (14) | 0.8942 | 1.3973 | 1.2494 | 0.2662           |    | 0.2869 | 0.3563 |
| Eq. (14) | 1.1537 | 1.2843 | 1.4817 | 0.2246           |    | 0.2063 | 0.3036 |
| Eq. (14) | 1.4227 | 1.2116 | 1.7238 | 0.1885           |    | 0.1458 | 0.2510 |
| Eq. (14) | 0.6418 | 0.1773 | 2.8198 | 0.4028           |    | 0.6605 | 0.4695 |
| Eq. (14) | 0.8202 | 0.3758 | 1.9955 | 0.3690           |    | 0.5317 | 0.4471 |
| Eq. (14) | 0.9145 | 0.6227 | 1.6059 | 0.3184           |    | 0.4001 | 0.4084 |
| Eq. (14) | 0.9601 | 0.8948 | 1.3970 | 0.2660           |    | 0.2867 | 0.3562 |
| Eq. (14) | 0.9811 | 1.1537 | 1.2843 | 0.2246           |    | 0.2063 | 0.3036 |
| Eq. (14) | 0.9907 | 1.4227 | 1.2116 | 0.1885           |    | 0.1458 | 0.2510 |
| Eq. (14) | 0.9953 | 1.7234 | 1.1605 | 0.1559           |    | 0.0991 | 0.1985 |

where the solution $\hat{\beta}$ satisfies

$$D \text{ being estimated}, \quad \hat{\beta} = \arg\min_{\beta} \{ \| y - D \beta \| \}$$

under an error-in-variables model. It is a topic that includes quite a few refinements that we here ignore inasmuch as feasible (by implicitly assuming independency properties).

### 3.1 Generalised least squares.

The ordinary least squares approach is based on the norm

$$\| y - D \beta \|^2 = (y - D \beta)' (y - D \beta) = \sum_{i=1}^{n} (y_i - d_i' \beta)^2 \quad \text{with} \quad D = \begin{pmatrix} d_1' \\ \vdots \\ d_n' \end{pmatrix},$$

a norm where the row-vectors $d_i'$ are seen as fully known. The terms $(y_i - d_i' \beta)^2$ measure the fit-errors and, when we desire to take into account the total error, we must add the errors due to the variability of the row-vectors $d_i'$. Namely, we must complete the terms into

$$(y_i - d_i' \beta)^2 + \beta' S_i \beta \quad \text{where} \quad S_i = \text{Cov}(d_i').$$

Thinking at robustness, in the weighted case the form

$$\sum_{i=1}^{n} (y_i - d_i' \beta)^2 \quad \text{becomes} \quad \sum_{i=1}^{n} w_i^2 (y_i - d_i' \beta)^2 + \beta' \left( \sum_{i=1}^{n} w_i^2 S_i \right) \beta$$

and the above norm $\| y - D \beta \|^2$ definition eventually is modified into

$$(y - D \beta)' W (y - D \beta) + \beta' S_D \beta, \quad \text{where} \quad S_D = \sum_{i=1}^{n} w_i^2 S_i.$$

Note that matrix $W$ is with respect to the squared weights,

$$W = \text{diag}\{w_1^2, ..., w_n^2\}.$$
Thus, the generalised least squares approach takes the form

\[
\hat{\beta} = \arg\min_\beta \{ (y - D\beta)' W (y - D\beta) + \beta' S_D \beta \}
\]

that yields to the estimator

\[
\hat{\beta} = J^{-1} D' W y
\]

with the next sandwich estimator of covariance

\[
\text{Cov}(\hat{\beta}) = \frac{N}{N - 1} J^{-1} \left\{ \sum_{i=1}^{n} w_i^4 \left[ e_i d_i - S_i \hat{\beta} \right] \left[ e_i d_i - S_i \hat{\beta} \right]' \right\} J^{-1}
\]

where

\[
J = D' W D + S_D = \sum_{i=1}^{n} w_i^2 \left[ d_i d_i' + S_i \right] \quad \text{and} \quad e_i = y_i - d_i' \hat{\beta}.
\]

The connections with ridge regression and with total least squares are evident.

The derivation of above \( \text{Cov}(\hat{\beta}) \) has been made by the infinitesimal jackknife of Jaeckel (1972) according to Rey (1983, Eq. 4.36) and sandwich estimators are surveyed by Freedman (2006). Their lack of efficiency is notorious as investigated by Kauermann and Carrol (2001) and it can be associated to the high stochastic variability of the central factor between the curled braces. In order to stabilize this factor, we imply in dependence conditions similar to those assumed in ordinary linear regression. We approximate the central factor and eventually obtain the covariance estimator (see further details at Note 4)

\[
\text{Cov}(\hat{\beta}) = \frac{N}{N - p} J^{-1} \left\{ \sum_{i=1}^{n} w_i^4 \left[ s^2 d_i d_i' + (S_i \hat{\beta})(S_i \hat{\beta})' \right] \right\} J^{-1}
\]

with

\[
N = \frac{\left( \sum_{i=1}^{n} w_i^2 \right)^2}{\sum_{i=1}^{n} w_i^4} \quad \text{and} \quad s^2 = \frac{\sum_{i=1}^{n} w_i^2 (y_i - d_i' \hat{\beta})^2}{\sum_{i=1}^{n} w_i^2}.
\]

### 3.2 Robust generalised least squares.

The extension to the robust context is natural and follows closely the above presentation for the one-dimension location estimator by the set of equations (10).

Given previous estimates of \((\beta, s)\), the weights and the new \((\beta, s)\) are estimated according to

\[
\begin{aligned}
\text{Given } \beta \text{ and } s, \\
J &= \sum_{i=1}^{n} w_i^2 \left[ d_i d_i' + S_i \right], \\
\beta &= J^{-1} D' W y, \\
s^2 &= \left[ \sum_{i=1}^{n} w_i^2 (y_i - d_i' \hat{\beta})^2 \right] / \left[ \sum_{i=1}^{n} w_i^2 \right].
\end{aligned}
\]

The associated covariance estimator

\[
\text{Cov}(\hat{\beta}) = k_2^2 \frac{N}{N - p} J^{-1} \left\{ \sum_{i=1}^{n} w_i^4 \left[ s^2 d_i d_i' + (S_i \hat{\beta})(S_i \hat{\beta})' \right] \right\} J^{-1} \quad \text{where} \quad N = \frac{\left( \sum_{i=1}^{n} w_i^2 \right)^2}{\sum_{i=1}^{n} w_i^4}
\]

is corrected for underestimation. It turns out that the constants \(k_3\) of and \(k_2\) are the same as for the one-dimension location estimator. Hence, the values of Table 2 are relevant in regression as well.
4 Singular Value Decomposition, SVD

We deal with the minimisation (2),

\[
\widehat{A} B' = \arg\min_{A,B'} \{ \| X - A B' \| \},
\]

where the approximation has rank \(p\)

\[
X \approx AB'.
\]

As we know, matrices \(A\) and \(B\) can be scaled and rotated in any convenient way; to limit this indeterminacy, we impose the weak condition that \(A\) be an orthonormal basis.

4.1 Total SVD, in view of statistical applications

First, in order to illustrate the inconsistencies that we mentioned in the introduction, we consider a simple numerical example. Let the data matrix to be analysed by singular value decomposition be next \(X\). Except for a minor perturbation at level of the second decimal place and an outlier, it is of Rank 1; the last entry should have been \(x_{5,3} = 15\).

\[
X = \begin{pmatrix}
1 & 2 & 3 \\
2 & 4 & 6 \\
3 & 6 & 9 \\
4 & 8 & 12 \\
5 & 10 & 0
\end{pmatrix} + 0.001 \begin{pmatrix}
92 & 3 & -17 \\
48 & 6 & -8 \\
26 & -4 & -64 \\
8 & -2 & 92 \\
17 & -3 & 0
\end{pmatrix} = \begin{pmatrix}
0.908 & 2.003 & 2.983 \\
2.048 & 4.006 & 5.992 \\
3.026 & 5.996 & 8.936 \\
4.008 & 7.998 & 12.09 \\
5.017 & 9.997 & 0
\end{pmatrix}.
\]

Applying the ordinary (least squares) SVD, the approximation is \(A B'\)

\[
\begin{array}{c|c|c}
\text{Ordinary SVD} & X & AB' = \\
\text{Rank 1, nonrobust} & & \\
\end{array}
\]

\[
\begin{pmatrix}
1.167 & 2.326 & 2.574 \\
2.364 & 4.710 & 5.212 \\
3.527 & 7.027 & 7.777 \\
4.741 & 9.445 & 10.45 \\
2.536 & 5.053 & 5.592
\end{pmatrix}.
\]

The outlier has completely spoiled the evaluation.

Initialising with this least squares approximation, we bring the attention on the two norms used in the evaluations of \(A\) and \(B'\). Running Eqs. (17) with \(k_3 = 1.5\), they induce robust weights on the data entries,

\[
\widehat{B'} = \arg\min_{B'} \{ \| X - A B' \| \} \rightarrow \text{weights} = \begin{pmatrix}
0.931 & 0.984 & 0.999 \\
0.997 & 1.000 & 0.997 \\
0.999 & 0.988 & 0.977 \\
1.000 & 0.982 & 0.980 \\
0.039 & 0.009 & 0.010
\end{pmatrix}
\]

and

\[
\widehat{A} = \arg\min_{A} \{ \| X - A B' \| \} \rightarrow \text{weights} = \begin{pmatrix}
0.987 & 0.975 & 0.869 \\
0.998 & 0.949 & 0.870 \\
0.997 & 0.953 & 0.868 \\
0.997 & 0.956 & 0.867 \\
0.997 & 0.955 & 0.867
\end{pmatrix}.
\]

Clearly these two norms do not match. Moreover, this does not help for better defining the norm of Eq. (13). As will soon be seen and in order to avoid the above incompatibility between the norms, we allocate the same set of weights for the evaluations of

\[
\widehat{B'} = \arg\min_{B'} \{ \| X - A B' \| \} \quad \text{and} \quad \widehat{A} = \arg\min_{A} \{ \| X - A B' \| \}.
\]
The second issue we raised in the introduction is with respect to the decomposition into an $A B'$ product. Each of the two components is estimated "as if" the other one was properly "known" rather than "estimated".

We now further detail and, momentarily for the simplicity, we place ourselves in the ordinary least squares context. The squared Frobenius norm of Eq. (2) can be written as the double summation

$$\{\hat{A}, \hat{B}\} = \text{argmin}_{\{A,B\}} \left\{ \sum_{i=1}^{m} \sum_{j=1}^{n} (x_{ij} - a_i' b_j)^2 \right\}$$

(19)

where the residuals of all approximated $X$-entries are minimized. Clearly, Eq. (19) guarantees a good approximation, namely a good estimation of the $A B'$ product. However in very many cases and, specifically for statistics in most low-rank reduction applications of SVD, we are interested in good estimations of $A$ and $B$. The qualities of the two components have the utmost importances rather than the quality of their product. Then, it leads to minimize

$$\{\hat{A}, \hat{B}\} = \text{argmin}_{\{A,B\}} \left\{ \sum_{i=1}^{m} \sum_{j=1}^{n} [(x_{ij} - a_i' b_j)^2 + a_i' \text{Cov}(b_j) a_i + b_j' \text{Cov}(a_i) b_j] \right\}$$

(20)

that has a total least squares flavour; the minimisations takes place on the $p$ columns of $A$ and the $p$ rows of $B'$. Accordingly, we call "Total SVD", the singular value decomposition based on the norm Eq. (20) (or Eq. (21), further on).

Seeing that the alternating process of Eq. (3) and Eq. (4) can yield informations on $\text{Cov}(b_j)$ and $\text{Cov}(a_i)$, the present set-up is less general although many of the arguments of Golub and van Loan (1980), most of them also reviewed in the classroom note of Nievergelt (1994), still hold. In some sense, Eq. (20) describes a trade-off between best approximating and best estimating the components of the approximation. The increased complexity of Eq. (20) compared to Eq. (19) induces practical difficulties that are already reported in Gabriel and Zamir (1979). In fact, the information we obtain on $\text{Cov}(b_j)$ and $\text{Cov}(a_i)$ is less rich than the full estimations of these matrices. For instance, the estimation of $B$ by Eq. (3) provides $n$ covariance matrices of dimensions $[p \times p]$, whereas $\text{Cov}(b_j)$ in Eq. (20) has dimensions $[m \times m]$. This mismatch of dimensions clearly displays a difficulty; we estimate $A$ and $B$ column-wise, but we use them row-wise in Eq. (20). However we can make use of the variances of the $A$- and $B$-entries, their covariances are not suitably available. This leads to substitute

$$\text{DiaCov}(a_i) = \text{diag}\{\sigma^2(a_{1,i}), ..., \sigma^2(a_{m,i})\}$$

in place of $\text{Cov}(a_i)$,

and similarly for $\text{Cov}(b_j)$. Hence, Eq. (20) takes the form

$$\{\hat{A}, \hat{B}\} = \text{argmin}_{\{A,B\}} \left\{ \sum_{i=1}^{m} \sum_{j=1}^{n} [(x_{ij} - a_i' b_j)^2 + a_i' \text{DiaCov}(b_j) a_i + b_j' \text{DiaCov}(a_i) b_j] \right\}$$

(21)

Cancelling $\text{DiaCov}(b_j)$ and $\text{DiaCov}(a_i)$, Eq. (21) collapses into the ordinary problem statement given by Eq. (2).

4.2 Estimation of Total SVD

In view of the past expositions, first we introduce the general algorithm in a few lines as being the solving of a fixed point problem.

Given previous estimates of $\{A, \text{DiaCov}(a_i)_{i=1...m}, B, \text{DiaCov}(b_j)_{j=1...n}\}$, the weights and
We review the four steps and this gradually leads us to the compact algorithm stated by Eqs. (20).

- **Given** \( \{ A, \text{DiaCov}(a_i)_{i=1...m}, B, \text{DiaCov}(b_j)_{j=1...n} \} \).

In fact, the algorithm does not do any use of any assumed \( \text{DiaCov}(b_j)_{j=1...n} \). The past estimation of \( A \) is entered in the next algorithmic step and, for the re-estimation of \( A \), we enter a \( \text{DiaCov}(b_j)_{j=1...n} \) as found while \( B \) was estimated.

Hence, a better formulation would have been “**Given** \( \{ A, \text{DiaCov}(a_i)_{i=1...m}, B \} \)”. Taking into account the definition \( \text{DiaCov} = \text{diag} \{ \sigma^2(a_{1,i}), ... , \sigma^2(a_{m,i}) \} \), we observe that we only need to enter the variances of the \( A \)-entries. Eventually, the proper formulation is “**Given** \( \{ A, \sigma^2(a_{i,k})_{i=1...m,k=1...p}, B, s \} \)”. The last parameter, \( s \), is incidental; it is entered to speed up the evaluation of the weights.

- **Evaluate the weights** \( w_{ij} \).

As indicated, we allocate the same set of weights for the evaluations of the two norms

\[
\widehat{B'} = \arg\min_{B'} \left\{ \| X - A B' \| \right\} \quad \text{and} \quad \widehat{A} = \arg\min_{A} \left\{ \| X - A B' \| \right\}.
\]

They are derived from the \( m \times n \) approximation residuals \( (X - A B')_{ij} \) and depends on their scatter \( s \) in a way that is familiar to the reader. Formally, this gives the following algorithmic piece.

\[
\begin{aligned}
\text{Given} & \quad \{ A, B, s \} . \\
\text{Evaluate the residuals} & \quad f_k = (X - A B')_{ij}, \quad k = 1, ..., m n. \\
\text{Iterate on the expressions:} & \\
\begin{align*}
w_k &= (1 + [f_k / (k_3 s)]^4)^{-1/4}, \\
N &= \frac{\sum_{k=1}^{m n} w_k^2}{\sum_{k=1}^{m n} w_k^2}, \\
\nu &= \left( m + n - \frac{\nu + 1}{2} \right) p, \\
\sigma^2 &= \frac{N}{N - \nu} \frac{\sum_{k=1}^{m n} w_k^2 f_k^2}{\sum_{k=1}^{m n} w_k^2}. \\
\text{Allocate the} & \quad w_k : \quad w_{ij} = w_k. 
\end{align*}
\end{aligned}
\]

The iterations converge linearly and should be accelerated.

- **Given** \( A \) and \( \text{DiaCov}(a_i)_{i=1...m} \), estimate \( B \) and \( \text{DiaCov}(b_j)_{j=1...n} \).

The generalised least squares context of Section [5.7] here is relevant and, without further delay, we present the corresponding algorithmic piece that solves

\[
\widehat{B'} = \arg\min_{B'} \left\{ \| X - A B' \| \right\}.
\]
Given \( \{ A, \sigma^2(a_{ik})_{i=1...m, k=1...p} \} \),

Successively, for each of the columns \( x_j \) of \( X \),

\[
S_i = \text{diag} \left\{ \sigma^2(a_{i1}), ..., \sigma^2(a_{ip}) \right\}, \quad \text{Dim.: } [p \times p].
\]

\[
J = \sum_{i=1}^m w_{ij}^2 \left[ a_i a'_i + S_i \right], \quad \text{Dim.: } [p \times p].
\]

\[
W_j = \text{diag} \left( w_{1j}, ..., w_{nj} \right), \quad \text{Dim.: } [m \times m].
\]

\[
(B')_j = J^{-1} A' W_j x_j, \quad \text{Dim.: } [p \times 1],
\]

\[
s^2_j = \left[ \sum_{i=1}^m w^2_{ij} (x_{ij} - a_j (B')_j) \right]^2 / \left[ \sum_{i=1}^m w^2_{ij} \right].
\]

\[
N_j = \left( \sum_{i=1}^m w^2_{ij} \right)^2 / \sum_{i=1}^m w^2_{ij}.
\]

\[
\text{Cov} \left[ (B')_j \right] = k_2 \frac{N_j}{N_{j-p}} \left( \sum_{i=1}^m w^4_{ij} \left( s^2_i a_i a'_i + [S_i (B')_j] \right) \right) J^{-1}. \quad (24)
\]

\[
\sigma^2(b_{jk}) = \text{Cov} \left[ (B')_j \right]_{kk}. \quad \text{(24)}
\]

The notation distinguishing rows from columns requiring some attention, as well as for convenience, we noted the matrix dimensions between square brackets.

- Given \( B \) and \( \text{DiaCov}(b_{j})_{j=1...n} \), estimate \( A \) and \( \text{DiaCov}(a_{i})_{i=1...m} \).

Except for matrix transpositions, we mimic very closely Eq. (24) and present the corresponding algorithmic piece. It solves

\[
\hat{A}' = \arg\min_{A'} \left\{ \| X' - B A' \| \right\}.
\]

Furthermore, we complete by imposing the condition that \( A \) be an orthonormal basis.

Given \( \{ B, \sigma^2(b_{jk})_{j=1...n, k=1...p} \} \),

Successively, for each of the columns \( x_i \) of \( X' \),

\[
S_j = \text{diag} \left\{ \sigma^2(b_{j1}), ..., \sigma^2(b_{jp}) \right\}, \quad \text{Dim.: } [p \times p].
\]

\[
J = \sum_{j=1}^n w^2_{ij} \left[ b_j b'_j + S_j \right], \quad \text{Dim.: } [p \times p].
\]

\[
W_i = \text{diag} \left( w_{i1}, ..., w_{in} \right), \quad \text{Dim.: } [n \times n].
\]

\[
(A')_i = J^{-1} B' W_i x_i, \quad \text{Dim.: } [p \times 1],
\]

\[
s^2_i = \left[ \sum_{j=1}^n w^2_{ij} (x_{ij} - b_j (A')_i) \right]^2 / \left[ \sum_{j=1}^n w^2_{ij} \right].
\]

\[
N_i = \left( \sum_{j=1}^n w^2_{ij} \right)^2 / \sum_{j=1}^n w^2_{ij}.
\]

\[
\text{Cov} \left[ (A')_i \right] = k_2 \frac{N_i}{N_{i-p}} \left( \sum_{j=1}^n w^4_{ij} \left( s^2_i b_j b'_j + [S_j (A')_i] \right) \right) J^{-1}. \quad (25)
\]

\[
\sigma^2(a_{ik}) = \text{Cov} \left[ (A')_i \right]_{kk}.
\]

Transform \( A \) into an orthonormal basis.
At the end of the convergence of Eqs. (22), the orthonormalisation of $A$ becomes an identity operation.

Summing up, the above algorithmic parts obtain the Total SVD solution as a fixed point of $\{A, \sigma^2(a_{i,k})_{i=1...m,k=1...p}, B, s\}$ according to

\[
\begin{align*}
\text{Evaluate the weights } w_{ij} \text{ by Eqs. (23).} \\
\text{Estimate } B \text{ and by Eqs. (24).} \\
\text{Estimate } A \text{ by Eqs. (25).}
\end{align*}
\]

(26)

Before leaving this presentation, it must be noted that some difficulties of convergence can occur (see Note 5).

We apply the variants of the above algorithm on the $[5 \times 3]$ example and specially draw the attention on the value taken by $x_{5,3}$ (that should be $x_{5,3} = 15$). We already met with the usual SVD result,

**Ordinary SVD, Rank 1, nonrobust**

\[
X \approx AB' = \begin{pmatrix} 1.167 & 2.326 & 2.574 \\ 2.364 & 4.710 & 5.212 \\ 3.527 & 7.027 & 7.777 \\ 4.741 & 9.445 & 10.45 \\ 2.536 & 5.053 & 5.592 \end{pmatrix}
\]

Taking into account the limited precision of product components $A$ and $B$ adds little to the quality of the resulting approximation,

**Total SVD, Rank 1, nonrobust**

\[
X \approx AB' = \begin{pmatrix} 1.078 & 2.147 & 2.376 \\ 2.183 & 4.349 & 4.813 \\ 3.257 & 6.489 & 7.180 \\ 4.377 & 8.721 & 9.651 \\ 2.342 & 4.666 & 5.164 \end{pmatrix}
\]

However, becoming robust induces a major quality improvement,

**Ordinary SVD, Rank 1, robust : $k_3 = 1$**

\[
X \approx AB' = \begin{pmatrix} 1.005 & 2.000 & 2.983 \\ 2.018 & 4.016 & 5.989 \\ 3.012 & 5.995 & 8.941 \\ 4.018 & 7.997 & 11.93 \\ 5.021 & 9.995 & 14.91 \end{pmatrix}
\]

and this is even better when Total SVD is estimated,

**Total SVD, Rank 1, robust : $k_3 = 1$**

\[
X \approx AB' = \begin{pmatrix} 0.9990 & 1.989 & 2.987 \\ 2.009 & 3.999 & 6.006 \\ 2.998 & 5.969 & 8.963 \\ 4.034 & 8.032 & 12.06 \\ 5.020 & 9.995 & 15.01 \end{pmatrix}
\]

Thinking at biplot applications, we analyse the European Health and Fertility data treated at Section 5.1 of Croux et al (1993). It is their $[16 \times 9]$-Table 1 set and clearly it has columns of very different scalings,

\[
\text{European Data} = \begin{pmatrix} -0.1 & 48 & \ldots & 3440 & 6 \\ 1.8 & 50 & \ldots & 2716 & 7 \\ 0.2 & 47 & \ldots & 3593 & 6 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 1.9 & 49 & \ldots & 3218 & 8 \\ 0.5 & 51 & \ldots & 3499 & 7 \\ 0.2 & 48 & \ldots & 3421 & 5 \end{pmatrix}
\]
The scalings are so different that it makes little sense to act as if some homoscedasticity could be assumed. Hence, we transform the data set and the columns become centered and with variances 1,

\[
\text{European Data} = \begin{pmatrix}
-0.8778 & 0.26812 & \ldots & 0.43654 & -0.0768 \\
2.2616 & 1.4938 & \ldots & -2.2925 & 0.53751 \\
-0.3821 & -0.3447 & \ldots & 1.0132 & -0.0768 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
2.4268 & 0.88097 & \ldots & -0.4003 & 1.1518 \\
0.11359 & 2.1067 & \ldots & 0.65893 & 0.53751 \\
-0.3821 & 0.26812 & \ldots & 0.36492 & -0.6911 \\
\end{pmatrix}
\]

The treatment allocate a weight to each of the entries,

\[
\text{Total SVD Rank 2, robust : } k_3 = 1
\]

Weights =

\[
\begin{pmatrix}
0.95895 & 0.77783 & \ldots & 0.94071 & 0.98998 \\
0.27558 & 0.32983 & \ldots & 0.20418 & 1.00000 \\
0.79620 & 0.97667 & \ldots & 0.56217 & 1.00000 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
0.98847 & 0.99972 & \ldots & 0.99998 & 0.99144 \\
1.00000 & 0.21158 & \ldots & 0.65800 & 0.94428 \\
0.99977 & 0.96668 & \ldots & 0.93092 & 0.93200 \\
\end{pmatrix}
\]

and we do not observe any very small weight. We are entitled to say that no entry is clearly outlying. The 5 lowest weights are

| Weight     | Entry       | Country, Factor     |
|------------|-------------|---------------------|
| 0.18181    | (7, 9) H, baby underw. |         |
| 0.18522    | (2, 7) AL, inhab. doc. |         |
| 0.20418    | (2, 8) AL, calorie   |         |
| 0.20607    | (13, 3) SU, women %  |         |
| 0.21158    | (15, 2) YU, give birth|        |

Contrary to the observation of Croux et al (1993), we do not have to eliminate by down-weighting the full fourteenth row corresponding to Turkey; what properly fits with the Rank 2 decomposition, properly contributes to our estimation.

Of course, the situation becomes more extreme when we increase the level of robustness.

Now we clearly find outlying entries,

\[
\text{Total SVD Rank 2, robust : } k_3 = 0.5
\]

Weights =

\[
\begin{pmatrix}
0.16691 & 0.18247 & \ldots & 0.27318 & 0.25611 \\
0.04308 & 0.06851 & \ldots & 0.04143 & 0.60169 \\
0.26271 & 0.79319 & \ldots & 0.12728 & 0.99098 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
0.07989 & 0.99997 & \ldots & 0.99992 & 0.50327 \\
0.99110 & 0.04645 & \ldots & 0.14016 & 0.30331 \\
0.99951 & 0.16474 & \ldots & 0.38905 & 0.42217 \\
\end{pmatrix}
\]

and the above 5 low weights decrease,

| Weight     | Entry       | Country, Factor     |
|------------|-------------|---------------------|
| 0.03469    | (7, 9) H, baby underw. |         |
| 0.03422    | (2, 7) AL, inhab. doc. |         |
| 0.04143    | (2, 8) AL, calorie   |         |
| 0.03915    | (13, 3) SU, women %  |         |
| 0.04645    | (15, 2) YU, give birth|        |

As is ordinary in the field of robustness, the analyst must master the tools he uses. A complementary feature is how vary the eigenvalues of \( \Lambda = \text{diag}\{\lambda_1, \ldots, \lambda_p\} \) in the ordinary SVD of the approximation \( A B' \); this is reported at Table 3.
Table 3: Eigenvalues of $A B'$ for the European Health and Fertility data.

|                | Rank 1          | Rank 2          | Rank 3          |
|----------------|-----------------|-----------------|-----------------|
| Ordinary SVD   | 8.5194          | 8.5194          | 5.7931          |
| Total SVD      |                 |                 |                 |
| $k_3 = \infty$ | 7.5963          | 7.7213          | 4.7238          |
| $k_3 = 2.0$    | 7.4674          | 7.5167          | 4.5743          |
| $k_3 = 1.0$    | 7.3074          | 7.3593          | 4.0388          |
| $k_3 = 0.5$    | 7.2501          | 6.4301          | 3.1360          |

Numerical notes

1. The Gaussian numerical sample.

For a sample of size $m$, we represent the Gaussian distribution by its $m$ quantiles defined as follows: we generate the points $x_i$ such that

$$\left\{ \int_{-\infty}^{x_i} \phi(x) \, dx = \frac{i - 1/2}{m} \right\} , \quad \text{where} \quad \phi(x) = \exp^{-x^2/2} / \sqrt{2 \pi} .$$

2. Breakdown point $BP_a$ by Eq. (13).

We add $k$ points to a sample of the standard Gaussian, constructed as above by $m$ quantiles. The $k$ new points are located far away, namely at $x = 10^6$. Then, Offset$_a$ varies continuously with $k$ and we can evaluate $BP_a$ for any $a$ value. For numerical convenience, we take $a = \sigma_x$ and evaluate $BP_1$.

Clearly, the estimated $BP_a$ depends on the selected $a$-value. However, this dependence is very moderate. The curve $BP_a(a)$ is linear for small $a$ and, fairly suddenly, displays a sharp increase that defines a quasi-asymptote.

3. Asymptotic estimations. Consider an estimator $t = t(m)$ that depends on the sample size $m$ used to represent the standard Gaussian distribution. We assume the model

$$t(m) = t(\infty) + \frac{t_1}{m + t_2}$$

and expect the parameter $t_2$ to be small.

The three sample sizes $m = 100, 300, 900$ are used in the experiment. A model fit delivers the asymptotic value $t(\infty)$.

In the linear regression context of Eqs. (17), rather than implementing with respect to the two factors of the product $k_3 = k_1 \times k_2$, it is convenient to parametrize on $k_3$ and approximate $k_2$ by an expression such as

$$\ln k_2 \approx (0.4762 - 0.8465 \ln k_3 + 0.4554 \ln^2 k_3)/(1 - 0.3425 \ln k_3).$$

4. Covariance estimator, Eq. (16).

In addition to the approximation

$$\sum_{i=1}^{m} w_i^4 \left[ e_i d_i - S_i \hat{\beta} \right] \left[ e_i d_i - S_i \hat{\beta} \right]' \approx \sum_{i=1}^{m} w_i^4 \left[ s^2 d_i d_i' + (S_i \hat{\beta})(S_i \hat{\beta})' \right]$$

where $s^2 = \bar{e_i^2}$, we modified the scaling factor obtained by the infinitesimal jackknife, $N/(N - 1)$, into the $N/(N - p)$ familiar in ordinary linear regression. The above approximation and the latter modification have been supported by simulation runs with arbitrary weights and diagonal matrices $S_i$. The covariance estimator Eq. (16) tends to slightly overestimate the true covariance when the right term of $\left[ s^2 d_i d_i' + (S_i \hat{\beta})(S_i \hat{\beta})' \right]$ dominates the left one, on the average.
5. Computation of Total SVD by Eqs. (26).

The experimental estimation of the fixed point of Eqs. (26) has presented hazards. It sometimes occurs that the mapping contracts in a fairly small vicinity of the solution \( \{ A, \sigma^2(a_{i,k})_{i=1..m, k=1..p'}, B, s \} \). Eventually, we have been solving

\[
\{ \hat{A}, \hat{B} \} = \arg\min_{\{A,B\}} \left\{ \sum_{i=1}^{m} \sum_{j=1}^{n} \left[ (x_{ij} - a_i'b_j)^2 + t \left( a_i' \text{DiACov}(b_j) a_i + b_j' \text{DiACov}(a_i) b_j \right) \right] \right\}
\]

for a parameter \( t \) varied from \( t = 0 \) to \( t = 1 \). We apply a predictor-corrector method of continuation built around the fixed point algorithm.

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