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Graphical illustration of perturbed system of linear equations and computed number of condition via SDV

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Abstract

We observe conditionality as an indicator of the sensitivity of the numerical solution, when it comes to a particular problem, with small changes in input numerical data, i.e. we observe the sensitivity of the solution of the linear system $Ax = b$ with small changes in the values of the elements of the matrix A and (or) of the vector b. Number of condition indicates a relative change of the system solution when the matrix is perturbed. This number is computed in several ways, and we will determine this by the singular values of matrix (SVD). It is shown that ill-conditioned matrices are "almost singular". The correlation between the number of condition and the numerical rank of a matrix will be illustrated in the examples that are solved and graphically shown using the program package *Mathematica*.

Keywords: Perturbed system, number of condition of matrix, singular value decomposition, numerical rank, graphic illustration.

Introduction

In various applications in science and technology, it is rarely possible to compute the exact solution of the system of linear equations $Ax = b$, because, the formation of the system itself (calculate of the coefficients a_{ij} and vector b) and its solution on the computer cause certain errors.
Let A be a quadratic regular matrix, so there exists an inverse A^{-1} and is unique. Then the linear system $Ax = b$ has a unique solution $x = A^{-1}b$. Suppose we changed the right side of the system to $b + \delta b$, while the matrix A remained unchanged. Let $x + \delta x_b$ be the solution of such a system:

$$A(x+\delta x_b) = b+\delta b\ .$$

Since $Ax = b$, it follows that $A\delta x_b = \delta b$ respectively $\delta x_b = A^{-1}\delta b$. So we get a rating:

$$\|\delta x_b\| \le \|A^{-1}\|\|\delta b\|, \tag{1}$$

where equality valid for at least one vector δb. Also, from the relation $Ax = b$ follows:

$$\|b\| \le \|A\|\|x\|, \tag{2}$$

where equality valid for some vectors x and b. By multiplying the inequalities (1) and (2) and by dividing both sides with $\|x\|\|b\|$, we get:

$$\frac{\|\delta x_b\|}{\|x\|} \le \|A^{-1}\|\|A\|\frac{\|\delta b\|}{\|b\|}\ . \tag{3}$$

Similarly, we can change the matrix *A*, and leave the vector *b* unchanged. Let $x+\delta x_A$ be the solution of such a system:

$$\left(A+\delta A\right)\left(x+\delta x_A\right)=b .$$

In doing so, we assume that $\left\|\delta A\right\|$ is small enough and that the matrix $A+\delta A$ is regular. Derived analogously as for (3), we obtain:

$$\frac{\left\|\delta x_A\right\|}{\left\|x+\delta x_A\right\|}\le\left\|A^{-1}\right\|\left\|A\right\|\frac{\left\|\delta A\right\|}{\left\|A\right\|} . \tag{4}$$

The value of $\left\|A^{-1}\right\|\left\|A\right\|$, which appears in (3) and (4), is called the *condition number* of the matrix *A* (in relation to solving the system $Ax=b$) and denote with $\kappa(A)$. She shows how much the relative change in solution *x* is increased to the relative change the vector *b* in (3), or matrix *A* in (4). The value of $\kappa(A)$ depends on the norm applies, but for any norm it is valid $\kappa(A)\ge 1$.

Matrix *A* is *well-conditioned* if small changes in the vector *b* or matrix *A* results in small changes in solution *x*. From (3) and (4) we see it will this is valid when $\kappa(A)$ is close to 1. Contrary to this, the matrix *A* is *ill-conditioned* if small changes in vector *b* or matrix *A* lead to big changes in solution *x*, what will be fulfilled if $\kappa(A)$ is much greater than 1. By convention, $\kappa(A)=\infty$ when matrix *A* is singular.

In the case when both the matrix A and the vector b are simultaneously changed, we get the system:

$$\left(A+\delta A\right)\left(x+\delta x\right)=b+\delta b .$$

Assuming that δA is sufficiently small for to be validity $\left\|A^{-1}\delta A\right\| \le \left\|A^{-1}\right\|\left\|\delta A\right\|<1$, may be proved the following inequality:

$$\frac{\left\|\delta x\right\|}{\left\|x\right\|}\le\frac{\kappa(A)}{1-\kappa(A)\dfrac{\left\|\delta A\right\|}{\left\|A\right\|}}\left(\frac{\left\|\delta A\right\|}{\left\|A\right\|}+\frac{\left\|\delta b\right\|}{\left\|b\right\|}\right).$$

The value of $\dfrac{\kappa(A)}{1-\kappa(A)\dfrac{\left\|\delta A\right\|}{\left\|A\right\|}}$ is close to the condition number $\kappa(A)$ when $\left\|\delta A\right\|$ is sufficiently small.

Numerical representation in some examples

1. System of linear equations $Ax=b$, where $A=\begin{bmatrix}1.0000 & 2.0000\\ 1.0001 & 2.0000\end{bmatrix}$ and $b=\left[3.0000,\ 3.0001\right]^T$ has the exact solution $x=\left[1.0000,\ 1.0000\right]^T$. If vector *b* is perturbed for residual value $r=\left[0.0000,\ 0.0002\right]^T$, then the solution to the perturbed system:

$$\begin{bmatrix}1.0000 & 2.0000\\ 1.0001 & 2.0000\end{bmatrix}\begin{bmatrix}\tilde{x}_1\\ \tilde{x}_2\end{bmatrix}=\begin{bmatrix}0.0000\\ 3.0003\end{bmatrix}$$

will be

$$\tilde{x}=\begin{bmatrix}\tilde{x}_1\\ \tilde{x}_2\end{bmatrix}=\begin{bmatrix}3.0000\\ 0.0000\end{bmatrix}.$$

We see that the solution of the perturbed system totally changed. This change occurs because the inverse matrix is

$$A^{-1} = \begin{bmatrix} -10000.0 & 10000.0 \\ 5000.5 & -5000.0 \end{bmatrix},$$

and therefore the number of condition is

$$\kappa_\infty(A) = \left\|A^{-1}\right\|_\infty \left\|A\right\|_\infty = 2000.000 \cdot 3.0001 = 60002 .$$

This means that the matrix of system is *ill-conditioned*. In that case, in order to get the expected exact solution, we need to have a vector *b* with a certain accuracy.

2. There are a lot of matrices with the large number of condition. Typically example is the Hilbert matrix of order 4:

$$H_4 = \begin{bmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/5 \\ 1/3 & 1/4 & 1/5 & 1/6 \\ 1/4 & 1/5 & 1/6 & 1/7 \end{bmatrix},$$

which consists of conditioned number higher than 10000.

3. Consider the linear system $Ax = b$, where $A = \begin{bmatrix} 2.0 & 2.0 & 1.0 \\ 4.0 & -0.5 & 1.0 \\ -1.0 & -0.5 & 4.0 \end{bmatrix}$ and $b = \begin{bmatrix} 7.0 \\ 4.0 \\ 2.0 \end{bmatrix}$.

The exact solution of this system is $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.0 \\ 2.0 \\ 1.0 \end{bmatrix}$. In fig.1 shows three planes which is defined by the three equations of this system:

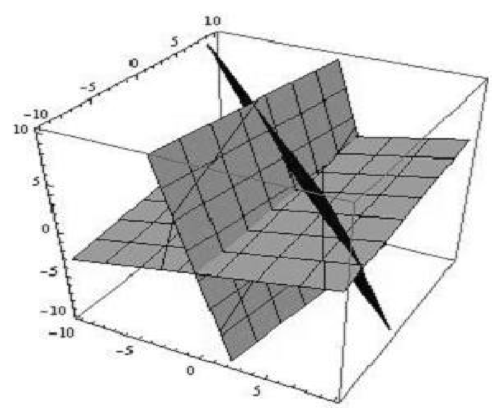

Fig. 1. Graphic representation of the system

Conditioned number of matrix *A* for the norm ∞ is:

$$\kappa_\infty(A) = 1.90295 .$$

It is seen that the given matrix *A* is well-conditioned. Because of the relation (3) we expect that small relative changes of the vector *b* will cause small relative changes of the vector *x*. This is confirmed by the graphical representation in fig.2. Vector *b* has been altered so that a normal random variable $\mathrm{N}\left(0,\sigma^2\right)$ is added to each of its components. Then for each thus obtained vector $b+\delta b$ we solve the system $A\left(x+\delta x_b\right) = b+\delta b$. In the

fig.2, on the left, shows the points which represent the relative change of the vector *b* and on the right are the points which represent the corresponding relative change of vector *x*.
From fig.2, we notice that "the crowd points" that represent these relative changes, are of similar size. This means that small relative changes in the vector *b* have indeed resulted in small relative changes in the vector *x*.

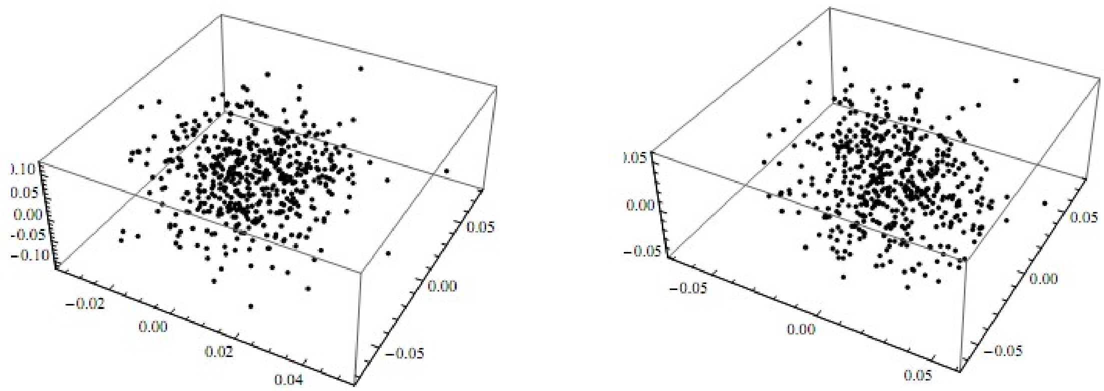

Fig. 2. Influence of relative change of vector *b* to relative change of solution *x*

4. Consider the following linear system $Ax = b$, where $A = \begin{bmatrix} 3.0 & 2.0 & 1.0 \\ 4.0 & -0.5 & 1.0 \\ 1.0 & -0.5 & 0.25 \end{bmatrix}$ and $b = \begin{bmatrix} 8.0 \\ 4.0 \\ 0.25 \end{bmatrix}$.

The exact solution of this system is again $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1.0 \\ 2.0 \\ 1.0 \end{bmatrix}$. In fig.3, we notice a small angle between one plane and the direction in which the other two planes are touched.

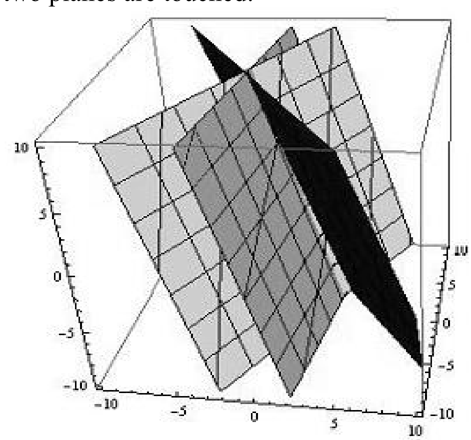

Fig. 3. Graphic representation of the system

This means that the rows of this matrix are almost linearly dependent. Indeed, if we do it the next combination of the first two rows:

$$-\frac{13}{9}\begin{bmatrix}3.0\\2.0\\1.0\end{bmatrix}+\frac{7}{19}\begin{bmatrix}4.0\\-0.5\\1.0\end{bmatrix}=\begin{bmatrix}1.0\\-0.5\\4/19\end{bmatrix}\approx\begin{bmatrix}1.0\\-0.5\\0.21\end{bmatrix},$$

we see that the result is slightly different from the last row of the matrix: [1.0, -0.5, 0.25].
We suspect that the matrix of system is ill-conditioned, which is confirmed by the computation: $\kappa_\infty(A)=232$.
Also, in fig.4 we notice that **small** relative changes in vector b result **in large** relative changes in solution x.

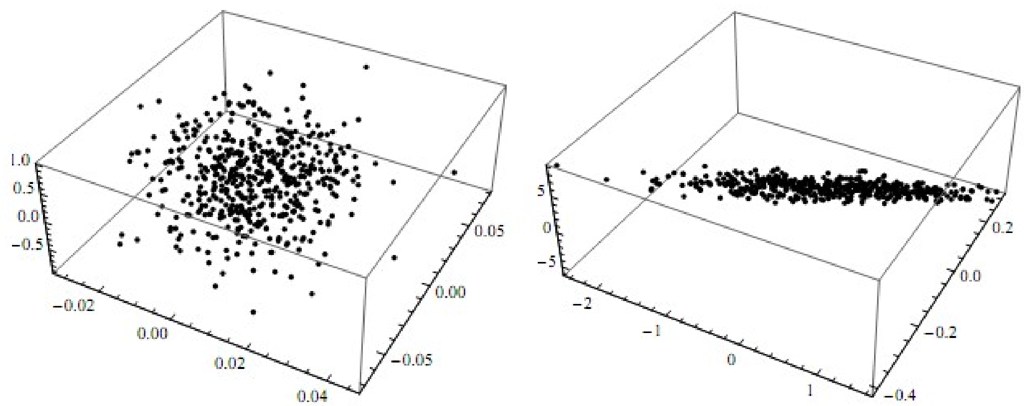

Fig. 4. Influence of relative change of vector b to relative change of solution x

We have seen that the matrix will be ill-conditioned if there are some of its rows almost linearly dependent.
Consequently, it can be concluded that the ill-conditioned matrix is "almost singular". Indeed, it is valid:

$$\min\left\{\frac{\|\Delta A\|}{\|A\|}:\quad (A+\Delta A)\ \text{-matricë singulare}\right\}=\frac{1}{\kappa_\infty(A)}.$$

Thus, the relative distance of the matrix A to the nearest singular matrix is exactly $\dfrac{1}{\kappa_\infty(A)}$.

What is the matrix too ill-conditioned, is closer to singularity.

Conditioned number of matrix via SVD
The fundamental theorem about the existence of decomposition (SVD) of a general matrix

Theorem1 (SVD):
Any $m\times n$ real matrix A can be decomposed as:

$$A=U\Sigma V^T=\begin{bmatrix}u_{11} & & u_{1m}\\ & \ddots & \\ u_{m1} & & u_{mm}\end{bmatrix}\begin{bmatrix}\sigma_1 & 0 & 0 & \cdots & 0\\ 0 & \cdots & & & \\ 0 & 0 & \sigma_r & \cdots & 0\\ 0 & 0 & 0 & \cdots & 0\\ 0 & 0 & 0 & \cdots & 0\end{bmatrix}_{m\times n}\begin{bmatrix}v_{11} & & v_{1n}\\ & \ddots & \\ v_{n1} & & v_{nn}\end{bmatrix}^T_{n\times n}$$

where U and V are orthogonal $m\times m$ and $n\times n$ matrices respectively, (i.e., $U^TU=I_m$ and $VV^T=I_n$), and Σ is an $m\times n$ diagonal matrix $\Sigma=\text{diag}(\sigma_1,\sigma_2,...,\sigma_r,0,...,0)$ with $\sigma_1 \ldots \sigma_2 \ldots \vdots \cdots \ldots \sigma_r > 0$ and $r=\text{rank}(A)$.

In the above, $\sigma_1, \sigma_2, ..., \sigma_r$ are the square roots of the eigenvalues of AA^T (or $A^T A$). They are called the *singular values* of A.

Singular values decomposition gives much information about the structure of matrix and one of these properties is the following:
Let be $U\Sigma V^T$ SVD of matrix $A \in \mathbb{R}^{m\times n}$ $(m \geq n)$, and $S = \{x \in \mathbb{R}^n : \|x\|_2 = 1\}$ unit sphere in $\mathbb{R}^n$. Then it is $A \cdot S = \{Ax : x \in \mathbb{R}^n \text{ and } \|x\|_2 = 1\}$ ellipsoid with a center at the origin of the $\mathbb{R}^m$ space and with the main poles $\sigma_i u_i$. The effect of matrix $A = U\Sigma V^T$ on the unit sphere is as follows: The orthogonal matrix V^T rotates the sphere, then the diagonal matrix Σ is stretched it and finally the other orthogonal matrix U is rotated again.

5. Consider the matrix of examples 3 and 4:

$$A_1 = \begin{bmatrix} 2.0 & 2.0 & 1.0 \\ 4.0 & -0.5 & 1.0 \\ -1.0 & -0.5 & 4.0 \end{bmatrix}, \qquad A_2 = \begin{bmatrix} 3.0 & 2.0 & 1.0 \\ 4.0 & -0.5 & 1.0 \\ 1.0 & -0.5 & 0.25 \end{bmatrix}.$$

By calculating the SVD of these matrices, we obtain that the singular values of the matrix A_1 are:

$$\sigma_1 = 4.71535, \qquad \sigma_2 = 4.14502, \qquad \sigma_3 = 2.02095,$$

while for matrix A_2 are:

$$\sigma_1 = 5.34839, \qquad \sigma_2 = 1.98897, \qquad \sigma_3 = 0.0352517.$$

Ellipsoids generated by the effect of the matrices A_1 and A_2 on the unit sphere *S*, is a graphical representation in fig.5.

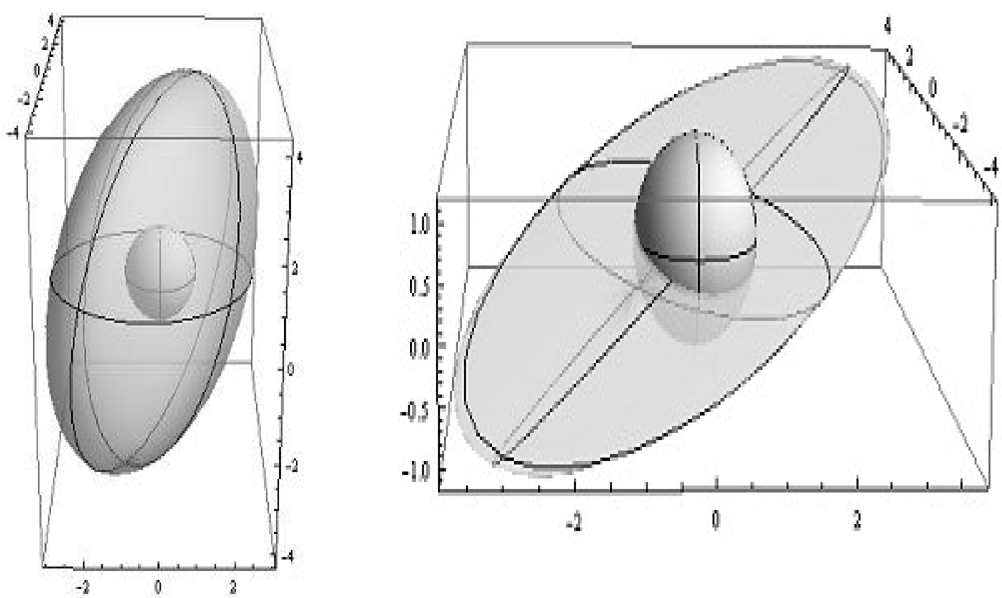

Fig. 5. Unit sphere *S* and ellipsoid A_1S, A_2S

Now, we remember of definition of matrix condition: $\kappa_\infty(A) = \|A^{-1}\|\|A\|$. For decomposed matrix *A*, namely $A = U\Sigma V^T$, we have $A^{-1} = V\Sigma^{-1}U^T$. This means that the singular value of a matrix A^{-1} is the reciprocal value of singular values of the matrix *A*. Therefore, the largest singular value of the matrix A^{-1} equals $\frac{1}{\sigma_n}$. Now, we have

$$\kappa_2(A) = \left\|A^{-1}\right\|_2 \left\|A\right\|_2 = \frac{\sigma_1}{\sigma_n},$$

It follows that the matrix *A* is increasingly ill-conditioned than soon as σ_n smaller.

*Theorem*2: Let $A \in \mathbb{R}^{m \times n}$ be a matrix of rank *r* with singular value decomposition $A = U \Sigma V^T$. Let $k < r$ and $A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T$, then it is:

$$\min_{rank(B)=k} \left\|A - B\right\|_2 = \left\|A - A_k\right\|_2 = \sigma_{k+1}.$$

The theorem states that the distance of matrix *A* (of rank *r*) to nearest matrix of rank *k* equals σ_{k+1} and that minimum is achieved in matrix A_k.

Considering the mentioned facts, the numerical rank r_ε can be defined as a number of singular values that are larger than a ε threshold:

$$\sigma_{r_\varepsilon} > \varepsilon > \sigma_{r_\varepsilon+1}.$$

Determining a numerical rank is relatively easy when there is a gap between large and small singular values. For example, some singular values of the matrix *A* the following:

$$\sigma_1 = 1.001, \qquad \sigma_2 = 0.498, \qquad \sigma_3 = 0.089, \qquad \sigma_4 = 10^{-2}, \qquad \sigma_5 = 10^{-5}.$$

If we take the threshold $\varepsilon = 10^{-3}$, the numerical rank of the matrix *A* will be 3, while for example $\varepsilon = 10^{-5}$ the numerical rank will be 4.

However, if singular values are:

$$\sigma_1 = 1.001, \qquad \sigma_2 = 10^{-3}, \qquad \sigma_3 = 10^{-4}, \qquad \sigma_4 = 10^{-5}, \qquad \sigma_5 = 10^{-6}$$

it is very difficult to determine the threshold, and thus the numerical rank. In general, numerical rank of matrix make sense to determine only when there is a clear gap between singular values.

6. Consider one ill-conditioned system $Ax = b$, where $A = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 5.0 & 2.0 & 7.0 \\ 6.0 & 4.0 & 9.999 \end{bmatrix}$ and $b = \begin{bmatrix} 14.0 \\ 30.0 \\ 43.997 \end{bmatrix}$.

The solution of the system is point $x = [1, 2, 3]^T$, although at first glance it seems that the solution is a straight line (see fig.6).

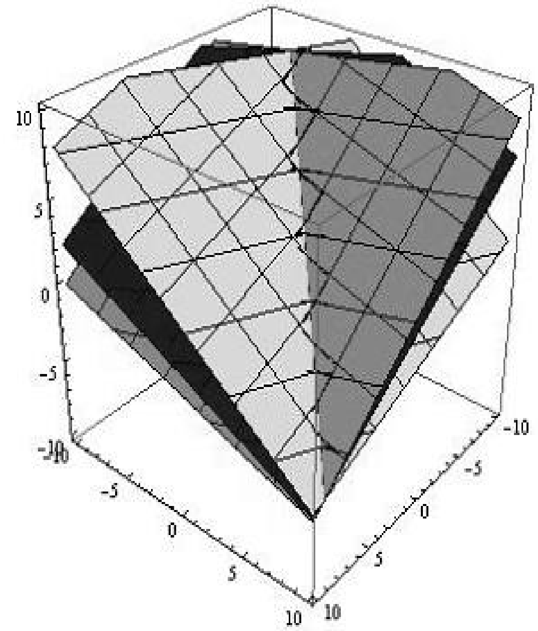

Fig. 6. Graphic representation of the system

It is obvious that this matrix is almost singular because its rows are almost linearly dependent. Therefore, its conditioned number even $\kappa_\infty(A) = 59997$. Let's observe its singular values:

$$\sigma_1 = 15.5434, \qquad \sigma_2 = 1.54398, \qquad \sigma_3 = 0.000333352 .$$

We see that σ_3 is of the order of 10^{-4} and could be neglected with the threshold for example $\varepsilon = 10^{-3}$. Then the numerical rank of the matrix A was 2. Also, σ_3 indicates that the matrix A is very close to the matrix rank 2. Although at first glance the closest matrix of rank 2 is exactly the matrix:

$$\tilde{A} = \begin{bmatrix} 1.0 & 2.0 & 3.0 \\ 5.0 & 2.0 & 7.0 \\ 6.0 & 4.0 & 10.0 \end{bmatrix},$$

still it is $\|\tilde{A} - A\|_2 = 0.001 > \sigma_3$.
Therefore, the nearest matrix of rank 2 is:

$$A_2 = U\Sigma_2 V^T = \begin{bmatrix} 1.00011 & 2.00011 & 2.99989 \\ 5.00011 & 2.00011 & 6.99989 \\ 5.99989 & 3.99989 & 9.99911 \end{bmatrix}$$

where is $\Sigma_2 = \operatorname{diag}(\sigma_1, \sigma_2, 0)$, because valid $\|A_2 - A\|_2 = 0.000333352 = \sigma_3$.

Conclusion:

By means of some specific examples we showed the relation between the number of conditions of a matrix and its numerical rank. For the full rank matrix *A*, its distance from the nearest non-singular matrix is equal to the highest singular value. On the other hand since the number of condition is $\kappa_2(A) = \frac{\sigma_1}{\sigma_n}$ it turns out that as σ_n is smaller, the matrix is getting ill-conditioned and closer to lower rank matrices. Also, if σ_n is sufficiently small, one can neglect with some threshold ε . Thus the numerical rank could be $n-1$. Thus, ill- conditioned matrices may have a numerical rank lower than the actual rank.