89-28

Analytic properties of singular values and vectors

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ESAT-SISTA report 1989-28.

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Abstract

It is shown that the singular value and vector functions of a matrix with elements that are analytic functions of a real parameter, are analytic if the singular values functions are not ordered and allowed to become negative. In points of multiplicity larger than one, there is a preferred choice of basis in the left and right singular subspaces, which are the analytic continuations of the singular vector functions. We show how these preferred basis vectors and the slopes of the unordered singular value functions can be computed from a generalized eigenvalue problem. The first order terms of the expansions for the preferred basis vectors cannot be determined completely from a first order analysis. Several examples are given to illustrate the results.

1 Introduction

The analytic properties of singular values and vectors of a matrix, the elements of which are analytic functions of a real parameter, play an important role in many systems and control problems. Let us mention some examples:

- Many identification and estimation algorithms (see e.g. [3] for a nice survey) are based upon the singular values and vectors of a data matrix, which is possibly corrupted by additive noise. The output is a vector valued function of the singular values and vectors. If the derivatives of the singular vectors and values with respect to the data were available, the derivatives of these vector valued functions with respect to the data could be computed via the chain rule. In this way, it is possible in principle to investigate not only the numerical sensitivity, but also the statistical performance of these algorithms, especially for high signal-to-noise ratios. An illustration of this approach can be found in [7] [9].

- The fact that an isolated singular value of a rational matrix (a transfer function $H(j\omega)$ of a linear system) is analytic, is used in [5] to find a Taylor series expansion of the singular value functions via implicit differentiation of a characteristic equation. However, the i-th singular value of $H(j\omega)$ need not to be a differentiable function of ω at frequencies where its multiplicity is greater than one. It has also be shown recently [2] that near a local maximum, the i-th singular value of $H(jw)$ has a Lipschitz second derivative, but need not have a third derivative. As a direct consequence, the convergence rate of the algorithm in [2] for the computation of the H_∞ norm, is quadratic.

- A final example concerns optimization problems that occur in structural and control engineering [6] of the form $min_x \sigma_1(A(x))$ where $A(x) = A_0 + \sum_{i=1}^{m} x_k A_k$ is an affine matrix function of the real parameters x_k. Typically, the optimum of such a function occurs at a parameter point x where two or more singular values coalesce. In such a point, the objective function is not differentiable. Observe however that it is convex since the largest singular value of a matrix is a convex function of the matrix elements.

The conclusion is that in many situations of practical interest, the singular values functions are not analytic at all. It is the purpose of the present paper to clarify in some detail the analytic properties of singular values and vectors of a matrix, the elements of which are analytic functions of a real parameter. In section 2, we introduce the *Unordered-Unsigned Singular Value Decomposition* (**USVD**). We derive a universal local representation of the singular value functions. We also show that near a local maximum, a singular value need not to have a third derivative. In section 3, we define the notion of *preferred basis vectors* when two or more singular values coincide. This definition is an immediate consequence of the analyticity of the singular vector functions. In section 4, it is shown how the preferred basis vectors and the first order terms of their expansion as well as the slopes of the unordered singular value functions, can be computed from a generalized eigenvalue problem. In the case of multiplicity 1, the result parallels the classical Taylor series expansion approach. A similar approach can be followed for a higher order analysis.

2 The Unordered-Unsigned Singular Value Decomposition

Let A be a real or complex $m \times n$ matrix, the elements of which are analytic functions of a real parameter x. The analyticity of A in the neighborhood of a point x_0 implies the existence of a Taylor series:

$$A(x) = A(x_0) + A_1(x - x_0) + A_2(x - x_0)^2 + \dots \tag{1}$$

Let $(x - x_0) = \epsilon$ and define $A(x_0) = A_0$, then this can be represented as

$$A(\epsilon) = A_0 + A_1\epsilon + A_2\epsilon^2 + \dots \tag{2}$$

It is well known [4] that an isolated root of a polynomial whose coefficients depend analytically on a parameter, is analytic in some neighborhood of that nominal parameter. The non-zero singular values are the square roots of the non-zero eigenvalues of AA^*. Because the eigenvalues are the roots of the characteristic polynomial, it follows that isolated singular values, i.e. singular values of multiplicity 1, are real analytic functions of the parameter x in the neighborhood of x_0. There remains the important question of how the singular values behave at nominal points x_0, where they are not isolated. Clearly, when two singular value functions cross, or when one singular value becomes zero, they need not even be differentiable functions, let alone analytic. However, by reordening the singular value functions, and possibly allowing them to become negative, we can guarantee that these (reordered, unsigned) singular values are analytic, including at all points x where some singular value functions are not distinct. More precisely, we have

Theorem 1 The USVD: Unordered-Unsigned SVD
Let $A(x)$ be a (complex) $m \times n$ matrix, the elements of which are analytic functions of a

real parameter x. There are real analytic functions $f_i : \Re \rightarrow \Re, i = 1, \ldots, min(m,n)$ such that, for all $x \in \Re$,

$$\{\sigma_i(A(x)), i = 1, \ldots, min(m,n)\} = \{|f_i(x)|, i = 1, \ldots, min(m,n)\} \tag{3}$$

These functions f_i can be considered as *unordered, unsigned* singular values of $A(x)$. We shall refer to these functions as the *unordered, unsigned singular value functions.*
The theorem follows immediately from perturbation theory for normal operators (Theorems 1.10 [4, p.82] and Theorem 6.1 [4, p.139]).
The **USVD** allows us to give a universal local representation of the singular value functions [2]:

Corollary 1
Given any $x_0 \in \Re$ and $1 \leq i \leq min(m,n)$, there are two real analytic functions f_i^- and f_i^+ such that in a neighborhood of x_0

$$\sigma_i(A(x)) = \begin{cases} f_i^-(x), x \leq x_0 \\ f_i^+(x), x > x_0 \end{cases} \tag{4}$$

If the functions $A(x)$ are not necessarily analytic, but continuously differentiable, then, there exist $min(m,n)$ continuously differentiable functions $g_i(x), i = 1, \ldots, min(m,n)$ that represent the repeated singular values of $A(x)$ (see Theorem 6.8 in [4, p.141]). However, even if the elements of $A(x)$ are infinitely differentiable, it is possible that these functions $g_i(x)$ are even not twice differentiable. An example of a similar statement for eigenvalues, which can easily be adapted for the singular value case, can be found in [4, p.142]. Summarizing we can say that analyticity plays an essential role in Theorem 1.

The *maximal* singular value of an analytic matrix function plays an important role in a lot of applications. For instance, in linear system theory, for stable systems, the maximal singular value of the transfer function as a function of $j\omega$, where ω is $2\pi \times frequency$, is an important measure of robustness and sensitivity [1] [2]. In structural engineering, one is interested in the minimum of the maximum singular value [6].
The following result is an immediate consequence of Corollary 1:

Corollary 2
Let $\sigma_1(x)$ be the maximal singular value function of $A(x)$. Then, there are two real analytic functions f_1^+ and f_1^- such that

$$\sigma_1(x) = max(f_1^-(x), f_1^+(x)) \tag{5}$$

In other words, $f_1^-(x) \geq f_1^+(x)$ for $x < x_0$ and $f_1^-(x) \leq f_1^+(x)$ for $x > x_0$.

Let's now consider the behavior of $\sigma_1(x)$ in the neighborhood of a local maximum, occuring, say at x_M. Let f^- and f^+ be the real analytic functions corresponding to $\sigma_1(x)$ near x_M. Define $\epsilon = x - x_M$. If $f^- = f^+$, then obviously, $\sigma(\epsilon)$ is analytic at $\epsilon = 0$ or at $x = x_M$.

Let us consider the case that $f^- \neq f^+$ so that $\sigma_1(\epsilon)$ is *not* analytic at x_M. Of course, the values of f^- and f^+ agree at $\epsilon = 0$. Their first derivatives must be zero since we are in a local maximum. It is less obvious but true that their *second* derivatives at x_M must also agree. For if, say, $(f^-)''(x_M) > (f^+)''(x_M)$, then, in a neighborhood of x_M, we would have that $f^-(x_M) > f^+(x_M)$, except at x_M. This contradicts the assertion in corollary 2. Thus, the Taylor expansions of f^- and f^+ about x_M could disagree first at order three. More generally, the same argument shows that the Taylor expansions of f^- and f^+ about x_M disagree first at some *odd* order, in other words, for some $k \geq 1$:

$$(f^-)^{(j)}(x_M) = (f^+)^{(j)}(x_M) \quad , \quad j = 0, \ldots, 2k \tag{6}$$

$$(f^-)^{(2k+1)}(x_M) \neq (f^+)^{(2k+1)}(x_M) \tag{7}$$

which implies that the maximum singular value function has a continuous but not differentiable $2k$-th order derivative. We summarize these remarks in the following theorem:

Theorem 2
Suppose $\sigma_1(A(x))$ has a local maximum at x_M. Then, near x_M, it has a continuous second derivative. In fact:

$$\begin{aligned} \sigma_1(A(x)) &= \sigma_1(A(x_M)) - \alpha(x - x_M)^{2k} \\ &+ \begin{cases} \beta^+(x - x_M)^{2k+1} + o((x - x_M)^{2k+1}) & , \quad x \geq x_M \\ \beta^-(x - x_M)^{2k+1} + o((x - x_M)^{2k+1}) & , \quad x < x_M \end{cases} \end{aligned}$$

for some $k \geq 1$, $\alpha > 0$ and $\beta^- \leq \beta^+$.

Thus at a local maximum, the maximum singular value function is twice continuously differentiable but need not to have a third derivative as the following example shows:

Example 1: Consider the following analytic functions of $x \in \Re$:

$$\begin{aligned} f_1(x) &= \frac{x^2(3x^2 + 2)}{1 + 4x^4} \\ f_2(x) &= \frac{3 + 2x^2}{4 + x^4} \\ f_3(x) &= \frac{1}{16}(x + 1)^2 - \frac{1}{3} \end{aligned}$$

and define the 3×3 diagonal matrix $A(x)$ with diagonal elements $f_i(x), i = 1, 2, 3$. Let x_1, x_5, x_6, x_{10} be the real roots of the equation $f_1(x) = |f_3(x)|$. Let x_2, x_9 be real the roots of $f_2(x) = f_3(x)$, x_3, x_6 be the real roots of $f_3(x) = 0$ and x_4, x_7 be the real roots of $f_1(x) = f_2(x)$.

$$\begin{aligned} x_1 &= -5.198235774591117e + 00 & x_2 &= -3.784635123896212e + 00 \\ x_3 &= -3.309401076758503e + 00 & x_4 &= -1.000000000000000e + 00 \\ x_5 &= -3.810408695923720e - 01 & x_6 &= 3.262277419094032e - 01 \\ x_7 &= 1.000000000000000e + 00 & x_8 &= 1.309401076758503e + 00 \\ x_9 &= 2.401861053059173e + 00 & x_{10} &= 3.249967155162040e + 00 \end{aligned}$$

Figure 1: Largest and smallest singular value of example 1.

Figure 2: Unordered singular value functions

The following table summarizes the analytic properties of the ordered singular values $\sigma_1(x) \geq \sigma_2(x) \geq \sigma_3(x) \geq 0$ of $A(x)$ as a function of x as in Theorem 1 and Corollary 1.

x	$\sigma_1(x)$		$\sigma_2(x)$		$\sigma_3(x)$	
	f_1^-	f_1^+	f_2^-	f_2^+	f_3^-	f_3^+
$x_0 = x_1$	f_3	f_1	f_1	f_3	f_2	f_2
$x_0 = x_2$	f_1	f_1	f_3	f_2	f_2	f_3
$x_0 = x_3$	f_1	f_1	f_2	f_2	f_3	$-f_3$
$x_0 = -1$	f_1	f_2	f_2	f_1	$-f_3$	$-f_3$
$x_0 = x_5$	f_2	f_2	f_1	$-f_3$	$-f_3$	f_1
$x_0 = x_6$	f_2	f_2	$-f_3$	f_1	f_1	$-f_3$
$x_0 = 1$	f_2	f_1	f_1	f_2	$-f_3$	$-f_3$
$x_0 = x_8$	f_1	f_1	f_2	f_2	$-f_3$	f_3
$x_0 = x_9$	f_1	f_1	f_2	f_3	f_3	f_2
$x_0 = x_{10}$	f_1	f_3	f_3	f_1	f_2	f_2

The reader may wish to verify that for $x_0 = -1$ and $x_0 = -1$, one finds that $(f_1^-)(x_0) = (f_1^+)(x_0)$, $(f_1^-)'(x_0) = (f_1^+)'(x_0)$, $(f_1^-)''(x_0) = (f_1^+)''(x_0)$, $(f_1^-)'''(x_0) \neq (f_1^+)'''(x_0)$.

3 Analyticity of the singular vectors

The following result is an immediate consequence of the well known relation of the singular value decomposition of a matrix A with the symmetric eigenvalue problem for AA^* or A^*A:

Theorem 3
For each real x, let the matrices $U(x)$ and $V(x)$ contain the left and right singular vectors of the matrix $A(x)$, the elements of which depend analytically on x. Then, the orthonormal vectors of $U(x)$ and $V(x)$ can be chosen as analytic functions of x.

The existence of such an orthonormal basis for the left and right singular spaces, depending smoothly on x, is one of the most remarkable results of the analytic perturbation theory for symmetric operators. A proof can be found in [4, p.140].
We shall refer to the analytic functions of Theorem 3 as the *singular vector functions.*

It is easy to show that, up to a constant of magnitude one, singular vectors corresponding to a singular value of multiplicity one, are unique. If two or more singular values coincide, the corresponding singular vectors are not uniquely determined but the singular subspaces they generate (i.e. the null spaces of $A^*A - \sigma^2 I_n$ and $AA^* - \sigma^2 I_m$), are well determined. Now consider example 1 in the interval $-1 < x < x_6$. If $-1 < x < x_5$, the three singular values are distinct and the corresponding singular vectors are well determined up to a constant of unit magnitude. The same situation occurs for $x_5 < x < x_6$. For $x = x_5$ however, $\sigma_2(x_5) = \sigma_3(x_5)$ and the corresponding singular vectors are not uniquely determined. However, the null spaces of $A^*(x_5)A(x_5) - (\sigma_2(x_5))^2 I_3$ and $A(x_5)A^*(x_5) - (\sigma_2(x_5))^2 I_3$

are well determined. According to Theorem 3, it is possible to find vectors in these null spaces, such that the singular vector functions $u_2(x), u_3(x), v_2(x), v_3(x)$ are analytic, even for $x = x_5$. This means, that there exists a priviliged choice of basis in the null spaces of $A^*(x_5)A(x_5) - (\sigma_2(x_5))^2 I_3$ and $A(x_5)A^*(x_5) - (\sigma_2(x_5))^2 I_3$. We shall now define these preferred basis vectors and show in the next section how they can be computed.

Definition 1 Preferred basis vectors
Let the elements of $A(x)$ be analytic functions of x and assume that for $x = x_0$, $\sigma = \sigma(x_0)$ is a singular value of multiplicity r. Let $u_i(x)$ and $v_i(x)$, $i = 1, \ldots, r$ be the analytic left and right singular value functions of Theorem 3 corresponding to $\sigma_i(x)$. Then, the preferred basis vectors for the null space $A(x_0)A^*(x_0) - \sigma^2 I_m$ are $u_i(x_0), i = 1, \ldots r$ and the preferred basis vectors for the null space of $A^*(x_0)A(x_0) - \sigma^2 I_n$ are $v_i(x_0), i = 1, \ldots, r$.

The preferred left and right singular vectors corresponding to a singular value σ of multiplicity larger than one, are nothing else than the analytic continuation in the corresponding null spaces of $A^*A - \sigma^2 I_n$ and $AA^* - \sigma^2 I_m$ of the singular value functions of Theorem 3.

Note that once the assumption of analyticity is removed, the singular vectors have much less continuity than the singular values. An illustrative example of this is given in [4, p.128].

4 First order analysis

It will now be shown that the slopes of the unordered singular value functions of Theorem 1 and the preferred vector functions of Definition 1, can be computed from a generalized eigenvalue problem. Another result will be that the first order terms of the Taylor series expansion of these preferred basis vectors, cannot be determined uniquely from a first order analysis. Let u and v be preferred left and right singular vectors and σ the corresponding singular value of multiplicity r:

$$A_0 v = u\sigma \tag{8}$$
$$A_0^* u = v\sigma \tag{9}$$

Consider a first order perturbation of A_0 as $A_0 + A_1\epsilon$. Because of the analyticity of the unordered singular value and vector functions, the perturbed singular values and vectors will satisfy up to first order:

$$(A_0 + A_1\epsilon)(v + h\epsilon) = (u + g\epsilon)(\sigma + \lambda\epsilon) \tag{10}$$
$$(A_0 + A_1\epsilon)^*(u + g\epsilon) = (v + h\epsilon)(\sigma + \lambda\epsilon) \tag{11}$$

where λ is the slope of an unordered singular value function and g and h are the first order terms of the series expansion of the singular vector functions. Then we have:

Theorem 4

The preferred singular vectors of $A_0 + A_1\epsilon$ and their first order terms

Let σ be a singular value of multiplicity r of the $m \times n$ matrix A_0 with a singular value decomposition:

$$A_0 = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} \sigma I_r & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} V_1^* \\ V_2^* \end{pmatrix} \tag{12}$$

where U_1 and V_1 are arbitrary orthonormal matrices, the columns of which generate an orthonormal basis for the null spaces of $A_0 A_0^* - \sigma I_m$ and $A_0^* A_0 - \sigma I_n$.
Consider a first order perturbation of A_0 as $A_0 + A_1\epsilon$, $\epsilon \in \Re$, and define the matrices B_{ij}, $i, j = 1, 2$ as

$$B_{ij} = U_i^* A_1 V_j \tag{13}$$

There are two cases, $\sigma \neq 0$ and $\sigma = 0$:

Case 1: $\sigma \neq 0$:

Consider the eigenvalue problem:

$$\frac{(B_{11} + B_{11}^*)}{2} x_i = x_i \lambda_i \qquad i = 1, \ldots, r \tag{14}$$

where the eigenvectors are normalized such that $x_i^* x_j = \delta_{ij}$ (Kronecker delta).
Then:

- *The slopes of the r unordered singular value functions are given by the eigenvalues λ_i, $i = 1, \ldots, r$.*
- *The r preferred left and right singular vectors (u_i, v_i) are given by:*

$$u_i = U_1 x_i \tag{15}$$
$$v_i = V_1 x_i \tag{16}$$

- *The first order terms of the series expansion of the singular vector functions satisfy:*

$$g_i = U_1 g_1^i + U_2 g_2^i \tag{17}$$
$$h_i = V_1 h_1^i + V_2 h_2^i \tag{18}$$

where

$$g_2^i = (\sigma^2 I_{m-r} - \Sigma_2 \Sigma_2^t)^{-1} (B_{21}\sigma + \Sigma_2 B_{12}^*) x_i \tag{19}$$
$$h_2^i = (\sigma^2 I_{n-r} - \Sigma_2^t \Sigma_2)^{-1} (\Sigma_2^t B_{21} + \sigma B_{12}^*) x_i \tag{20}$$

and

$$g_1^i - h_1^i = \frac{(B_{11} - B_{11}^*)}{2\sigma} x_i \tag{21}$$

and

$$(g_1^j)^* x_i + x_j^* g_1^i = 0 \qquad i = 1, \ldots, r \tag{22}$$
$$(h_1^j)^* x_i + x_j^* h_1^i = 0 \qquad j = 1, \ldots, r \tag{23}$$

Case 2: $\sigma = 0$ **:**

Consider a singular value decomposition of B_{11}*:*

$$B_{11}y_i = x_i\lambda_i \tag{24}$$
$$B_{11}^*x_i = y_i\lambda_i \qquad i = 1,\ldots,r \tag{25}$$

Then:

- *The slopes of the* r *unordered singular value functions are given by the* r *singular values* $\lambda_i, i = 1,\ldots,r$.
- *The preferred left and right singular vectors are given by*

$$u_i = U_1x_i \tag{26}$$
$$v_i = V_1y_i \tag{27}$$

- *The first order terms of the series expansion of the singular vector functions satisfy:*

$$g_i = U_1g_1^i + U_2g_2^i \tag{28}$$
$$h_i = V_1h_1^i + V_2h_2^i \tag{29}$$

where

$$(\Sigma_2\Sigma_2^t)g_2^i = -\Sigma_2B_{12}^*x_i \tag{30}$$
$$(\Sigma_2^t\Sigma_2)h_2^i = -\Sigma_2^tB_{21}y_i \tag{31}$$

and

$$(g_1^j)^*x_i + x_j^*g_1^i = 0 \qquad i = 1,\ldots,r \tag{32}$$
$$(h_1^j)^*x_i + x_j^*h_1^i = 0 \qquad j = 1,\ldots,r \tag{33}$$

Proof: Up to first order, (10) and (11) must be satisfied. The equations in ϵ^0 reduce to (8)-(9). Equating the first order terms results in:

$$A_0h + A_1v = u\lambda + g\sigma \tag{34}$$
$$A_0^*g + A_1^*u = v\lambda + h\sigma \tag{35}$$

Now use the singular value decomposition of A_0 as in (12) to define

$$\begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} = \begin{pmatrix} U_1^* \\ U_2^* \end{pmatrix} A_1 \begin{pmatrix} V_1 & V_2 \end{pmatrix} \tag{36}$$

and

$$\begin{pmatrix} g_1 \\ g_2 \end{pmatrix} = \begin{pmatrix} U_1^*g \\ U_2^*g \end{pmatrix} \qquad \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} = \begin{pmatrix} V_1^*h \\ V_2^*h \end{pmatrix} \tag{37}$$

It is easy to show from (8)-(9) that

$$U_2^* u = 0 \qquad V_2^* v = 0 \tag{38}$$

Define also

$$x = U_1^* u \qquad y = V_1^* v \tag{39}$$

Then, equations (34) and (35) become:

$$\begin{pmatrix} \sigma I_r & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} + \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \begin{pmatrix} y \\ 0 \end{pmatrix} = \begin{pmatrix} x \\ 0 \end{pmatrix} \lambda + \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} \sigma \tag{40}$$

$$\begin{pmatrix} \sigma I_r & 0 \\ 0 & \Sigma_2^t \end{pmatrix} \begin{pmatrix} g_1 \\ g_2 \end{pmatrix} + \begin{pmatrix} B_{11}^* & B_{21}^* \\ B_{12}^* & B_{22}^* \end{pmatrix} \begin{pmatrix} x \\ 0 \end{pmatrix} = \begin{pmatrix} y \\ 0 \end{pmatrix} \lambda + \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \sigma \tag{41}$$

The expression for the case $\sigma = 0$ follows directly from these equations.
For $\sigma \neq 0$, it follows from (8)-(9) that

$$x = y \tag{42}$$

Using this equality in equations (40)-(41) gives the formulas of the Theorem. Equations (22)-(23) and (32)-(33) are normalizing conditions that express the fact that, up to first order, the r left and right singular vectors have norm 1 and are mutually orthonormal. □

Before we discuss the Theorem in some more detail, let's first introduce some notation. The $r \times r$ matrix X contains the r normalized eigenvectors ((14) for the case $\sigma \neq 0$) or left singular vectors ((25) for the case $\sigma = 0$). The $r \times r$ matrices G_1 and H_1 contain the vectors $g_1^i, h_1^i, i = 1, \ldots, r$ and the $r \times r$ matrices G_2 and H_2 contain the vectors $g_2^i, h_2^i, i = 1, \ldots, r$. Define Λ as the diagonal matrix $\Lambda = diag(\lambda_i)$ where $\lambda_i, i = 1, \ldots, r$ are either the eigenvalues (14) or singular values (25).

Let us now first discuss the case $\sigma \neq 0$. The conditions (21) between the first order terms in the expansion of $u(x)$ and $v(x)$ and the normalizing conditions (22)-(23) can be summarized as:

$$\frac{B_{11} - B_{11}^*}{2\sigma} X = G_1 - H_1 \tag{43}$$

$$G_1^* X + X^* G_1 = 0 \tag{44}$$

$$H_1^* X + X_1^* H_1 = 0 \tag{45}$$

Observe that these equations alone are not sufficient to determine uniquely the matrices G_1 and H_1. However, once G_1 is chosen such that it satisfies (44), H_1 is determined by equation (43). It can be verified that it will satisfy automatically (45). It is straightforward to show that the general solution to equation (44) can be written as:

$$G_1 = XC \tag{46}$$

where C is any skew-Hermitian matrix,

$$C^* = -C \tag{47}$$

In addition, the choice of C is restricted in the following sense: The norms of the columns of G_1 and H_1 have to be 'small', say, smaller than 1, so that the terms $U_1 g_1^i \epsilon$ and $V_1 h_1^i \epsilon$ remain first order terms in the expansion of the singular value functions.
The fact that the vectors of G_1 and H_1 are not uniquely determined by a first order analysis, can be explained from equations (10)-(11):

$$(A_0 + A_1\epsilon)(V_1 X + V_1 H_1 \epsilon + V_2 H_2 \epsilon) = (U_1 X + U_1 G_1 \epsilon + U_2 G_2 \epsilon)(\sigma I_r + \Lambda\epsilon) \tag{48}$$

$$(A_0^* + A_1^*\epsilon)(U_1 X + U_1 G_1 \epsilon + U_2 G_2 \epsilon) = (V_1 X + V_1 H_1 \epsilon + V_2 H_2 \epsilon)(\sigma I_r + \Lambda\epsilon) \tag{49}$$

These equations are satisfied, up to first order, for any choice of G_1, H_1 that satisfies (43).

Let us illustrate these claims with an example:

Example 2:

$$A_0 + A_1\epsilon = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 & 2 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \epsilon$$

where $\epsilon = 1e-010$.
A singular value decomposition for A_0 is obviously $A_0 = I_3 I_3 I_3^*$. Hence, $B_{11} = U_1^* A_1 V_1 = A_1$. The preferred basis vectors can be found by solving the eigenvalue problem (14), which gives the eigenvalues

$$\lambda_1 = 1.6916e+00 \qquad \lambda_2 = 8.5823e-01 \qquad \lambda_3 = -1.5498e+00$$

and eigenvectors

$$X = \begin{pmatrix} -6.5810e-01 & -2.4623e-01 & 7.1153e-01 \\ -4.7578e-01 & 8.6843e-01 & -1.3953e-01 \\ -5.8356e-01 & -4.3036e-01 & -6.8866e-01 \end{pmatrix}$$

The matrices G_1 and H_1 have to satisfy equations (44) and (45) and are related by (43):

$$G_1 - H_1 = \frac{B_{11} - B_{11}^*}{2\sigma} X = \begin{pmatrix} -5.2967e-01 & 2.1903e-01 & -4.1409e-01 \\ 3.2905e-01 & 1.2312e-01 & -3.5577e-01 \\ 3.2905e-01 & 1.2312e-01 & -3.5577e-01 \end{pmatrix}$$

It can be verified numerically that, up to first order:

$$A_0 + A_1\epsilon = (X + G_1\epsilon)(I_3 + \Lambda\epsilon)(X + H_1\epsilon)^t$$

for any choice of matrices G_1 and H_1 satisfying (43)-(45). For instance, one may choose $H_1 = 0$ and $G_1 = (B_{11} - B_{11}^*)X/(2\sigma)$. Note that

$$X(I_3 + \Lambda\epsilon)X^t \approx \begin{pmatrix} 1 & \epsilon/2 & 3\epsilon/2 \\ \epsilon/2 & 1+\epsilon & 0 \\ 3\epsilon/2 & 0 & 1 \end{pmatrix} \neq A_0 + A_1\epsilon$$

The reason is of course that this would correspond to a choice of $G_1 = H_1 = 0$, which violates equation (43).

The main conclusion for the case $\sigma \neq 0$ is that a first order analysis allows us to determine the preferred basis vectors in the left and right singular subspaces and the part of the first order terms in the expansion of these vectors, orthogonal to these subspaces. The slopes of the unordered singular value functions are the eigenvalues of a certain matrix.

In addition, note that:

- The matrix B_{22} plays no role whatsoever in a first order analysis. There are also some special cases. If the matrix B_{11} is Hermitian, then $G_1 = H_1$. If B_{11} is skew-Hermitian, $B_{11}^* = -B_{11}$, then, the eigenvalues (14) are all 0, hence, the singular values remain unchanged up to first order. In this case, the preferred basis cannot be determined from a first order analysis. Also the matrices G_1, H_1, G_2, H_2 are undetermined since they depend on the eigenvectors (14). Intuitively, this indeterminacy follows from the fact that the singular values themselves are not changed by the perturbation.

- The Theorem remains valid for an isolated singular value, i.e. when $r = 1$. In that case, we obtain a Taylor series expansion as can be found also in [9] and [10]. In this case, the vectors g_1 and h_1 only represent a modification of the norm of U_1 and V_1 (which are vectors now).

- Whenever σ is close to one of the diagonal elements of Σ_2, the norm of the vectors of G_2 and H_2 is large because of the appearance of the factors $\sigma^2 I_{m-r} - \Sigma_2\Sigma_2^t$ and $\sigma^2 I_{n-r} - \Sigma_2^t\Sigma_2$. The result is that the singular vectors become very sensitive to small perturbations. The sensitivity increases inversely proportional to the distance of σ to the singular values in Σ_2.

- Up to first order, (10) and (11) are equivalent to the following generalized eigenvalue problem:

$$\begin{pmatrix} -\sigma I_m & A_0 & 0 & 0 \\ A_0^* & -\sigma I_n & 0 & 0 \\ 0 & A_1 & -\sigma I_m & A_0 \\ A_1^* & 0 & A_0^* & -\sigma I_n \end{pmatrix} \begin{pmatrix} u \\ v \\ g \\ h \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ I_m & 0 & 0 & 0 \\ 0 & I_n & 0 & 0 \end{pmatrix} \begin{pmatrix} u \\ v \\ g \\ h \end{pmatrix} \lambda \qquad (50)$$

  Hence, the preferred basis vectors u and v and the vectors g, h can be found from the eigenvectors while the slopes of the unordered singular value functions are the eigenvalues of this pencil.

- The Theorem can also be used in the determination of the subgradient (see e.g. [8] for definition and properties) of the singular value functions, if these are convex. This is for instance the case for the maximal singular value of an affine matrix function $A_0 + A_1\epsilon$ where ϵ is real. As an example, consider the following problem:

  Example 3:

  For which values of x is the minimum over all ϵ of the maximal singular value of $A_0 + A_1(x)\epsilon$ equal to 1, where

  $$A(x,\epsilon) = A_0 + A_1\epsilon = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & x \\ x & 4 \end{pmatrix}\epsilon$$

  First, note that for $\epsilon = 0$, the maximal singular value is equal to 1, with multiplicity 2. The *ordered* singular value functions are not differentiable in $\epsilon = 0$, but the unordered singular value functions are. Because of the convexity of the maximal singular value as a function of ϵ, the subgradient $\delta\sigma_{max}$ of the maximal singular value function in $\epsilon = 0$ coincides with the real interval $[\lambda_1, \lambda_2]$ where λ_1 is the smallest and λ_2 is the largest slope of the unordered singular value functions.

  $$\delta\sigma_{max} = [\ \lambda_1\ ,\ \lambda_2\ ]$$

  The minimum of σ_{max} will be 1 iff $0 \in [\ \lambda_1\ ,\ \lambda_2\ ]$. Let's compute the subgradient of the maximal singular value for fixed x as a function of ϵ. It follows from Theorem 4 that the slopes λ_1 and λ_2 are the eigenvalues of

  $$(B_{11} + B_{11}^*)/2 = \begin{pmatrix} 1 & x \\ x & 4 \end{pmatrix}$$

  Hence

  $$\delta\sigma_{max} = [(5 - \sqrt{9 + 4x^2})/2, (5 + \sqrt{9 + 4x^2})/2]$$

  The minimum of σ_{max} is 1 if $0 \in \delta\sigma_{max}$ or if

  $$|x| \geq 2$$

If $\sigma = 0$, it is possible that one of the two matrices G_2 or H_2 cannot be determined from the first order analysis, namely if $\Sigma_2\Sigma_2^t$ or $\Sigma_2^t\Sigma_2$ is rank deficient which occurs if $m > n$ or $m < n$. Let us illustrate this with an example:

Example 4:

$$A_0 + A_1\epsilon = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 1 & 0 & 0 & 2 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 2 & 0 & 0 & 0 & 3 \end{pmatrix}\epsilon$$

Here $\Sigma_2 = (\ 3\ \ 0\ \ 0\ )$ and the matrices U_1, U_2, V_1, V_2 can be chosen as:

$$U_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} \quad U_2 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad V_1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \quad V_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

from which the matrices $B_{11}, B_{12}, B_{21}, B_{22}$ can easily be found. The matrix B_{11} has a singular value decomposition:

$$B_{11} = X\Lambda Y^* = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Hence, the slopes of the unordered singular value functions are 0 and 1. We easily find that

$$G_2 = -(\Sigma_2\Sigma_2^t)^{-1}\Sigma_2 B_{12}^* X = (\ 0\ \ -1/3\ )$$

The matrix H_2 has to satisfy $(\Sigma_2^t\Sigma_2)H_2 = -\Sigma_2^t B_{21} Y$ so that

$$H_2 = \begin{pmatrix} -2/3 & 0 \\ \star & \star \\ \star & \star \end{pmatrix}$$

where a '$\star$' represents an element that cannot be determined from a first order analysis.

A similar approach as that in Theorem 4 can be followed to obtain higher order results. For instance, for a second order analysis, consider the following equations which have to be satisfied up to second order:

$$(A_0 + A_1\epsilon + A_2\epsilon^2)(v + h_1\epsilon + h_2\epsilon^2) = (u + g_1\epsilon + g_2\epsilon^2)(\sigma + \lambda_1\epsilon + \lambda_2\epsilon^2) \qquad (51)$$

$$(A_0^* + A_1^*\epsilon + A_2^*\epsilon^2)(u + g_1\epsilon + g_2\epsilon^2) = (v + h_1\epsilon + h_2\epsilon^2)(\sigma + \lambda_1\epsilon + \lambda_2\epsilon^2) \qquad (52)$$

Comparison of zero-th, first and second order terms leads to the following generalized eigenvalue problem:

$$\begin{pmatrix} \sigma I_m & A_0 & 0 & 0 & 0 & 0 \\ A_0^* & \sigma I_n & 0 & 0 & 0 & 0 \\ 0 & A_1 & \sigma I_m & A_0 & 0 & 0 \\ A_1^* & 0 & A_0^* & -\sigma I_n & 0 & 0 \\ 0 & A_2 & \lambda_1 I_m & A_1 - \sigma I_m & A_0 & \\ A_2^* & 0 & A_1^* - \lambda_1 I_n & A_0^* & -\sigma I_n & \end{pmatrix} \begin{pmatrix} u \\ v \\ g_1 \\ h_1 \\ g_2 \\ h_2 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ I_m & 0 & 0 & 0 & 0 & 0 \\ 0 & I_n & 0 & 0 & 0 & 0 \\ I_m & 0 & 0 & 0 & 0 & 0 \\ 0 & I_n & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} u \\ v \\ g_1 \\ h_1 \\ g_2 \\ h_2 \end{pmatrix} \lambda_2 \qquad (53)$$

Obviously, for the solution of this generalized eigenvalue problem, we need the slopes λ_1 of the unordered singular value functions. There is an eigenvalue problem for each slope λ_1. The second order eigenvalues λ_2 could be used to determine if the unordered singular value functions are convex, a result which could for instance lead to the determination of the subgradients of the (ordered) singular value functions.

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