

Locating coalescing singular values of large two-parameter matrices

Luca Dieci^{a,*}, M. Grazia Gasparo^b, Alessandra Papini^b, Alessandro Pugliese^c

^a School of Mathematics, Georgia Institute of Technology, Atlanta, GA 30332, USA

^b Dep. Energetica S. Stecco, Univ. of Florence, via C. Lombroso 6/17, 50134 Florence, Italy

^c Dip. Matematica, Univ. of Bari, Via Orabona 4, 70125 Italy

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Abstract

Consider a matrix valued function $A(x) \in \mathbb{R}^{m \times n}$, $m \geq n$, smoothly depending on parameters $x \in \Omega \subset \mathbb{R}^2$, where Ω is simply connected and bounded. We consider a technique to locate parameter values where some of the q dominant ($q \leq n$) singular values of A coalesce, in the specific case when A is large and $m > n \gg q$.

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Notation. An $m \times n$ real matrix is indicated with $A \in \mathbb{R}^{m \times n}$. We always consider the 2-norm for vectors and matrices. A matrix valued function $A: \mathbb{R} \rightarrow \mathbb{R}^{m \times n}$, continuous with its first l derivatives ($l \geq 0$), is indicated as $A \in \mathcal{C}^l(\mathbb{R}, \mathbb{R}^{m \times n})$. If $l=0$, we also simply write $A \in \mathcal{C}$. If $A \in \mathcal{C}^l(\mathbb{R}, \mathbb{R}^{m \times n})$ is periodic of (minimal) period $\tau > 0$, we write it as $A \in \mathcal{C}_\tau^l(\mathbb{R}, \mathbb{R}^{m \times n})$. With $\Omega \subset \mathbb{R}^2$ we indicate an open and bounded simply connected planar region, and $x = (x_1, x_2)$ will be coordinates in Ω . For a function $A(x)$, $x \in \Omega$, we will write $A \in \mathcal{C}^l(\Omega, \mathbb{R}^{m \times n})$ as appropriate.

1. Introduction

Consider a matrix $A \in \mathbb{R}^{m \times n}$, $m \geq n$. Recall that the – reduced – SVD (Singular Value Decomposition) of A is the decomposition

$$A = U \Sigma V^T,$$

where $U \in \mathbb{R}^{m \times n}$ is orthonormal ($U^T U = I_n$), $V \in \mathbb{R}^{n \times n}$ is orthogonal, and $\Sigma \in \mathbb{R}^{n \times n}$ is the diagonal matrix of the singular values: $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$, $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n \geq 0$. The SVD of a matrix is one of the most useful decompositions in linear algebra: the rank of A , as well as orthogonal representations for fundamental subspaces associated with A can be nicely retrieved from the factors of the SVD; see [5].

An important application of the SVD is that it is easy to obtain from it the best approximation (in the 2-norm) to the matrix A among matrices of a given rank. Namely, if $A = U \Sigma V^T$, and $\sigma_1 \geq \dots \geq \sigma_q > \sigma_{q+1} \geq \dots \geq \sigma_n$, then the best approximation of rank q to A is given by $U^{(q)} \Sigma^{(q)} (V^{(q)})^T$, where $U^{(q)} = U(:, 1:q)$, $V^{(q)} = V(:, 1:q)$ and

* Corresponding author.

E-mail addresses: dieci@math.gatech.edu (L. Dieci), mariagrazia.gasparo@unifi.it (M.G. Gasparo), alessandra.papini@unifi.it (A. Papini), pugliese@dm.uniba.it (A. Pugliese).

$\Sigma^{(q)} = \Sigma(1 : q, 1 : q)$. In particular, if all singular values are distinct, the SVD at once allows to obtain the complete set of best approximations of rank $q = 1, 2, \dots$, and associated projections. Indeed, we notice that lack of uniqueness of the best approximation ensues when singular values coalesce. Amongst the multitude of applications where the best approximation problem finds a use, we recall image compression [8,10,12].

Naturally, a general matrix $A \in \mathbb{R}^{m \times n}$, is expected to have distinct singular values, in that (if not) an arbitrary small perturbation of it will do. In fact, more is true. A fundamental result of von Neumann and Wigner, known as the n on-crossing rule (see [14]), implies that having a pair of coalescing singular values is a co-dimension-2 phenomenon. In other words, when we consider matrix valued functions, we should not expect a function of one parameter to have coalescing singular values, whereas we should expect a function of 2 parameters to have coalescing singular values.

Example 1.1. Suppose we have matrices, $A_0, A_1, \dots, A_N$, corresponding to snapshots taken at different times from 0 to T , and we build a function $A(t)$, $t \in [0, T]$, by interpolation. Then, we should expect there being a smoothly varying best approximation of any desired rank, in that all singular values should be distinct.

Motivated by the previous discussion, in this work we focus on the problem of locating, and accurately approximating, coalescing points for singular values of a smooth function A depending on two parameters: $A \in C^l(\Omega, \mathbb{R}^{m \times n})$. We recall (e.g., see [4,7]) that one cannot expect to have a (globally) smooth SVD in a region containing coalescing points. Also, we emphasize that, generically, we expect to have coalescing singular values at isolated points in parameter space, and the phenomenon should not be destroyed under perturbation (though the point x where the coalescing occurs may of course change). A coalescing is now a bifurcation point for the best approximation problem of a certain rank (e.g., if the 10th and 11th singular values coalesce, there is no smoothly varying best approximation of rank 10).

Example 1.2. Suppose we have a sequence of matrices, A_{ij} , $i = 1, \dots, m$, $j = 1, \dots, n$, $m \geq n$, encoding photos taken at different latitude (x_1) and longitude (x_2), and we build a function $A(x_1, x_2)$ by 2-d interpolation in $R := \{(x_1, x_2) : a \leq x_1 \leq b, c \leq x_2 \leq d\}$. Then, we should not expect to have a unique best approximation in R of rank k , for all $k = 1, \dots, n$.

Besides the best approximation problem, coalescing points of singular values (or, more simply, eigenvalues of symmetric matrices) have several other applications; we cite here works in structural engineering [11,13], as well as works in molecular systems [1,14,15].

In [4], we gave theoretical results on coalescing singular values of square matrix valued functions in two parameters. Our theoretical results have been of localization type: to guarantee that inside a certain closed region there is a coalescing point. These results lend themselves very naturally to algorithms to localize coalescing points, algorithms which we begun studying in [3]. As it will be reviewed later on, the workhorse of these algorithms is a 1-dimensional solver which finds a smooth SVD along a closed path; in [3] we used a solver which is very similar to the one we use in the present work.

In this work, we continue our algorithmic study to locate coalescing points, but our emphasis here is on large (and typically sparse) functions A , and on locating coalescing points only for the first q singular values. To fix ideas, we can think of $A \in \mathbb{R}^{m \times n}$ with m and n in the order of thousands, but q only on the order of tens.

A plan of the paper is as follows. In Section 2, we give theoretical results which adapt those of [4] to the present situation. In the same section, we discuss the necessary algorithmic extensions with respect to the works [2,3], to deal with the problem at hand. In Section 3, we show the performance of our method on a few examples.

2. Theoretical and algorithmic extensions

In this section we extend both the theoretical results of [4] and the algorithmic approaches of [2,3] which were all based on the 1-d continuation of a complete SVD for a square valued function.

2.1. Theoretical results

We now give two results, which will be used to localize coalescing points. These results are an adaptation to the case of rectangular matrices of results in [4] relative to the case of square matrices. The notation used is from [4], to which we refer for further details. The first result is the extension of [4, Theorem 3.6].

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