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THE ANALYTIC SVD: ON THE NON-GENERIC POINTS ON THE PATH*

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Abstract. A new technique for computing the Analytic SVD is proposed. The idea is to follow a branch of just one simple singular value and the corresponding left/right singular vector. Numerical computation may collapse at non-generic points; we will consider the case when the continuation gets stuck due to a nonzero multiple singular value. We interpret such a point as a singularity of the branch. We employ singularity theory in order to describe and classify this point. Since its codimension is one, we meet such a point "rarely."

Key words. SVD, ASVD, continuation, singularity theory.

AMS subject classifications. 65F15

1. Introduction. A singular value decomposition (SVD) of a real matrix $A \in \mathbb{R}^{m\times n}$, $m \geq n$, is a factorization $A = U\Sigma V^T$, where $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ are orthogonal matrices and $\Sigma = \mathrm{diag}(s_1, \ldots, s_n) \in \mathbb{R}^{m\times n}$. The values s_i, $i = 1, \ldots, n$, are called singular values. They may be defined to be nonnegative and to be arranged in nonincreasing order.

Let A depend smoothly on a parameter $t \in \mathbb{R}$, $t \in [a, b]$. The aim is to construct a path of SVDs

$$A(t) = U(t)\Sigma(t)V(t)^T, \tag{1.1}$$

where $U(t)$, $\Sigma(t)$ and $V(t)$ depend smoothly on $t \in [a, b]$. If A is a real analytic matrix function on $[a, b]$, then there exists an *Analytic Singular Value Decomposition* (ASVD) [1], a factorization (1.1) that *interpolates* the classical SVD defined at $t = a$, i.e.

- the factors $U(t)$, $V(t)$ and $\Sigma(t)$ are real analytic on $[a, b]$,
- for each $t \in [a, b]$, both $U(t) \in \mathbb{R}^{m\times m}$ and $V(t) \in \mathbb{R}^{n\times n}$ are orthogonal matrices, and $\Sigma(t) = \mathrm{diag}(s_1(t), \ldots, s_n(t)) \in \mathbb{R}^{m\times n}$ is a diagonal matrix,
- at $t = a$, the matrices $U(a)$, $\Sigma(a)$ and $V(a)$ are the factors of the classical SVD of the matrix $A(a)$.

The diagonal entries $s_i(t) \in \mathbb{R}$ of $\Sigma(t)$ are called *singular values*. Due to the requirement of smoothness, singular values may be negative, and their ordering may by arbitrary. Under certain assumptions, the ASVD may be uniquely determined by the factors at $t = a$. For theoretical background, see [9]. As far as the computation is concerned, an incremental technique is proposed in [1]. Given a point on the path, one computes a classical SVD for a neighboring parameter value. Next, one computes permutation matrices which link the classical SVD to the next point on the path. The procedure is approximative with a local error of order $O(h^2)$, where h is the step size.

An alternative technique for computing the ASVD is presented in [13]. A non-autonomous vector field $H : \mathbb{R} \times \mathbb{R}^N \to \mathbb{R}^N$ of large dimension $N = n + n^2 + m^2$ can be constructed in such a way that the solution of the initial value problem for the system $x' = H(t, x)$ is linked to the path of the ASVD. Moreover, [13] contributes to the analysis of *non-generic points* of the ASVD path; see [1]. These points could be, in fact, interpreted as singularities of the vector field $\mathbb{R}^N$. In [12], both approaches are compared.

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A continuation algorithm for computing the ASVD is presented in [7]. It follows a path of a few *selected* singular values and left/right singular vectors. It is appropriate for large sparse matrices. The continuation algorithm is of predictor-corrector type. The relevant predictor is based on the Euler method, hence on an ODE solver. In this respect, there is a link to [13]. Nevertheless, the Newton-type corrector guarantees the solution with prescribed precision.

The continuation may get stuck at points where a nonsimple singular value $s_i(t)$ appears for a particular parameter t and index i. In [1, 13], such points are called non-generic points of the path. They are related to branching of the singular value paths. The code in [7] incorporates extrapolation strategies in order to "jump over" such points.

In this paper, we investigate non-generic points. In Section 2, we give an example that motivated our research. Then we introduce a path-following method for continuation of a simple singular value and the corresponding left/right singular vector. In Section 4, we define and analyze a singularity on the path. Next, we perturb this singularity; see Section 5. We summarize our conclusions in Section 6. Finally, in Appendix A, we provide details of the expansions used in our asymptotic analysis.

2. Motivation. Let

$$A(t) = \begin{bmatrix} 1-t & 0 \\ 0 & 1+t \end{bmatrix};$$

see [1, Example 2]. The relevant ASVD, $A(t) = U(t)\Sigma(t)V(t)^T$, $-0.5 \le t \le 0.5$, can be computed explicitly:

$$U(t) = V(t) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}, \quad s_1(t) = 1-t, \quad s_2(t) = 1+t.$$

Obviously, $s_1(0) = s_2(0) = 1$ is a nonsimple (multiple) singular value of $A(0)$.

We will ask the following question: does the ASVD-path persist for an arbitrary sufficiently small perturbation? Let

$$A(t) = \begin{bmatrix} 1-t & 0 \\ 0 & 1+t \end{bmatrix} + \varepsilon \begin{bmatrix} 1/2 & 1 \\ -1/4 & -1 \end{bmatrix}. \tag{2.1}$$

Consider the relevant ASVD. This time, we compute it numerically using the techniques described in [7]. We show the results for the unperturbed and perturbed matrices in Figures 2.1 and 2.2, respectively. Notice that the branches in Figure 2.1 and in Figure 2.2 are qualitatively different. We observe a *sensitive dependence on the initial conditions* of the branches.

3. Continuation of a simple singular value.

3.1. Preliminaries. Let us recall the notion of a singular value of a matrix $A \in \mathbb{R}^{m\times n}$, $m \ge n$.

DEFINITION 3.1. *Let $s \in \mathbb{R}$. We say that s is a singular value of the matrix A if there exist $u \in \mathbb{R}^m$ and $v \in \mathbb{R}^n$ such that*

$$Av - su = 0, \quad A^T u - sv = 0, \quad \|u\| = \|v\| = 1. \tag{3.1}$$

The vectors v and u are called the right and the left singular vectors of the matrix A. Note that s is defined up to its sign: if the triplet (s, u, v) satisfies (3.1) then at least three more triplets

$$(s, -u, -v), \quad (-s, -u, v), \quad (-s, u, -v),$$

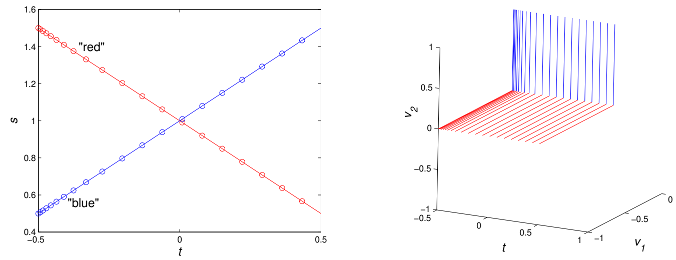

FIGURE 2.1. *Perturbation $\varepsilon = 0$. Left: Branches of singular values $s_1(t)$ and $s_2(t)$ in red and blue as functions of t. Right: The relevant right singular vectors in red and blue.*

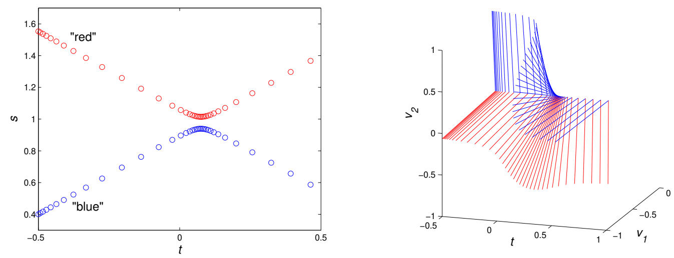

FIGURE 2.2. *Perturbation $\varepsilon = 0.1$. Left: Branches of singular values $s_1(t)$ and $s_2(t)$ in red and blue as functions of t. Right: The relevant right singular vectors in red and blue.*

can be interpreted as singular values and left and right singular vectors of A.

DEFINITION 3.2. *Let $s \in \mathbb{R}$. We say that s is a simple singular value of a matrix A if there exist $u \in \mathbb{R}^m$, $u \neq 0$, and $v \in \mathbb{R}^n$, $v \neq 0$, where*

$$(s, u, v), \quad (s, -u, -v), \quad (-s, -u, v), \quad (-s, u, -v)$$

are the only solutions to (3.1). A singular value s which is not simple is called a nonsimple (multiple) singular value.

REMARK 3.3. Let $s \neq 0$. Then s is a simple singular value of A if and only if s^2 is a simple eigenvalue of $A^T A$. In particular, $v \in \mathbb{R}^n$ and $u \in \mathbb{R}^m$ such that

$$A^T A v = s^2 v, \quad \|v\| = 1, \quad u = \frac{1}{s} A v$$

are the relevant right and left singular vectors of A.

REMARK 3.4. $s = 0$ is a simple singular value of A if and only if $m = n$ and $\dim \operatorname{Ker} A = 1$.

REMARK 3.5. Let s_i, s_j be simple singular values of A with $i \neq j$. Then $s_i \neq s_j$ and $s_i \neq -s_j$.

Let us recall the idea of [7]. The branches of *selected* singular values $s_i(t)$ and the corresponding left/right singular vectors $U_i(t) \in \mathbb{R}^m$, $V_i(t) \in \mathbb{R}^n$ are considered, i.e.,

$$A(t)V_i(t) = s_i(t)U_i(t), \quad A(t)^T U_i(t) = s_i(t)V_i(t), \tag{3.2}$$

$$U_i(t)^T U_i(t) = V_i(t)^T V_i(t) = 1, \tag{3.3}$$

for $t \in [a, b]$. The natural orthogonality conditions $U_i(t)^T U_j(t) = V_i(t)^T V_j(t) = 0$, $i \neq j$, $t \in [a, b]$, are added. For $p \leq n$, the selected singular values $S(t) = (s_1(t), \ldots, s_p(t)) \in \mathbb{R}^p$ and the corresponding left/right singular vectors $U(t) = [U_1(t), \ldots, U_p(t)] \in \mathbb{R}^{m \times p}$ and $V(t) = [V_1(t), \ldots, V_p(t)] \in \mathbb{R}^{n \times p}$ are followed for $t \in [a, b]$.

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3.2. The path of simple singular values. In this section, we consider the idea of path-following for *one* singular value and the corresponding left/right singular vectors. We expect the path to be locally a branch of $s_i(t)$, $U_i(t) \in \mathbb{R}^m$, $V_i(t) \in \mathbb{R}^n$, satisfying conditions (3.2) and (3.3) for $t \in [a, b]$.

We consider the ith branch, $1 \le i \le n$, namely, the branch which is initialized by $s_i(a)$, $U_i(a) \in \mathbb{R}^m$, $V_i(a) \in \mathbb{R}^n$, computed by the classical SVD [4]. Note that the SVD algorithm orders all singular values in descending order $s_1(a) \ge \cdots \ge s_i(a) \ge \cdots \ge s_n(a) \ge 0$. We assume that $s_i(a)$ is *simple*; see Remarks 3.3 and 3.4.

DEFINITION 3.6. *For a given $t \in [a, b]$ and $s \in \mathbb{R}$, let us set*

$$\mathcal{M}(t,s) \equiv \begin{bmatrix} -sI_m & A(t) \\ A^T(t) & -sI_n \end{bmatrix}, \tag{3.4}$$

where $I_m \in \mathbb{R}^{m\times m}$ and $I_n \in \mathbb{R}^{n\times n}$ are identities.

REMARK 3.7. Let $s \neq 0$, $t \in [a, b]$.

1. s is a singular value of $A(t)$ if and only if $\dim \operatorname{Ker} \mathcal{M}(t, s) \ge 1$.
2. s is a simple singular value of $A(t)$ if and only if $\dim \operatorname{Ker} \mathcal{M}(t, s) = 1$.

REMARK 3.8. Let $s \neq 0$, $t \in [a, b]$.

1. If $\mathcal{M}(t,s)\begin{bmatrix} u \\ v \end{bmatrix} = 0$ then $u^T u = v^T v$.
2. If in addition $\mathcal{M}(t,s)\begin{bmatrix} \tilde{u} \\ \tilde{v} \end{bmatrix} = 0$ then $u^T \tilde{u} = v^T \tilde{v}$.

Note that if $s_i(t) \neq 0$ then due to Remark 3.8 one of the scaling conditions (3.3) is *redundant*. This motivates the following definition.

DEFINITION 3.9. *Consider the mapping*

$$f : \mathbb{R} \times \mathbb{R}^{1+m+n} \longrightarrow \mathbb{R}^{1+m+n},$$
$$t \in \mathbb{R}, \quad x = (s, u, v) \in \mathbb{R}^1 \times \mathbb{R}^m \times \mathbb{R}^n \longmapsto f(t, x) \in \mathbb{R}^{1+m+n},$$

where

$$f(t,x) \equiv \begin{bmatrix} -su + A(t)v \\ A^T(t)u - sv \\ v^T v - 1 \end{bmatrix}. \tag{3.5}$$

As an alternative to (3.5) we will also use

$$f(t,x) \equiv \begin{bmatrix} -su + A(t)v \\ A^T(t)u - sv \\ u^T u + v^T v - 2 \end{bmatrix}. \tag{3.6}$$

The equation

$$f(t,x) = 0, \quad x = (s, u, v), \tag{3.7}$$

may locally define a branch $x(t) = (s(t), u(t), v(t)) \in \mathbb{R}^{1+m+n}$ of singular values $s(t)$ and left/right singular vectors $u(t)$ and $v(t)$. The branch is initialized at t^0, which plays the role of $t = a$. It is assumed that there exists $x^0 \in \mathbb{R}^{1+m+n}$ such that $f(t^0, x^0) = 0$. The initial condition $x^0 = (s^0, u^0, v^0) \in \mathbb{R}^{1+m+n}$ plays the role of already computed SVD factors $s_i(a) \in \mathbb{R}^1$, $U_i(a) \in \mathbb{R}^m$ and $V_i(a) \in \mathbb{R}^n$.

We solve (3.7) on an open interval $\mathcal{J}$ of parameters t such that $t^0 \in \mathcal{J}$.

THEOREM 3.10. *Consider* (3.5). *Let $(t^0, x^0) \in \mathcal{J} \times \mathbb{R}^{1+m+n}$, $x^0 = (s^0, u^0, v^0)$, be a root of $f(t^0, x^0) = 0$. Assume that $s^0 \neq 0$ is a simple singular value of $A(t^0)$. Then*

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there exists an open subinterval $\mathcal{I} \subset \mathcal{J}$ containing t^0 and a unique function $t \in \mathcal{I} \longmapsto x(t) \in \mathbb{R}^{1+m+n}$ such that $f(t, x(t)) = 0$ for all $t \in \mathcal{I}$ and that $x(t^0) = x^0$. Moreover, if $A \in C^k(\mathcal{I}, \mathbb{R}^{m\times n})$, $k \geq 1$, then $x \in C^k(\mathcal{I}, \mathbb{R}^{1+m+n})$. If $A \in C^\omega(\mathcal{I}, \mathbb{R}^{m\times n})$ then $x \in C^\omega(\mathcal{I}, \mathbb{R}^{1+m+n})$.

Proof. We will show that the assumptions imply that the partial differential f_x at the point (t^0, x^0) is a regular $(1 + m + n) \times (1 + m + n)$ matrix. Let $\delta x = (\delta s, \delta u, \delta v) \in \mathbb{R}^{1+m+n}$,

$$f_x(t^0, x^0)\, \delta x = \begin{bmatrix} -u^0 & -s^0 I_m & A(t^0) \\ -v^0 & A(t^0)^T & -s^0 I_n \\ 0 & 0_m^T & 2(v^0)^T \end{bmatrix} \begin{bmatrix} \delta s \\ \delta u \\ \delta v \end{bmatrix} = 0 \in \mathbb{R}^{1+m+n}. \tag{3.8}$$

This is equivalent to the system

$$\mathcal{M}(t^0, s^0) \begin{bmatrix} \delta u \\ \delta v \end{bmatrix} = \delta s \begin{bmatrix} u^0 \\ v^0 \end{bmatrix}, \quad (v^0)^T\, \delta v = 0. \tag{3.9}$$

Projecting the first equation on (u^0, v^0), and using the symmetry of the matrix $\mathcal{M}(t^0, s^0)$, yields

$$\begin{bmatrix} u^0 \\ v^0 \end{bmatrix}^T \mathcal{M}(t^0, s^0) \begin{bmatrix} \delta u \\ \delta v \end{bmatrix} = \begin{bmatrix} \delta u \\ \delta v \end{bmatrix}^T \mathcal{M}(t^0, s^0) \begin{bmatrix} u^0 \\ v^0 \end{bmatrix} = \delta s(\|u^0\|^2 + \|v^0\|^2). \tag{3.10}$$

By definition (3.5), $\mathcal{M}(t^0, s^0) \begin{bmatrix} u^0 \\ v^0 \end{bmatrix} = 0 \in \mathbb{R}^{m+n}$. Therefore, $\delta s = 0$.

Due to Remark 3.7 (2), there exists a constant c such that $\begin{bmatrix} \delta u \\ \delta v \end{bmatrix} = c \begin{bmatrix} u^0 \\ v^0 \end{bmatrix}$. The second condition in (3.9) implies that $c = 0$. Hence $\delta x = (\delta s, \delta u, \delta v) = 0$, which proves the claim.

Assuming that $A \in C^k(\mathcal{I}, \mathbb{R}^{m\times n})$, $k \geq 1$, the statement is a consequence of the Implicit Function Theorem; see, e.g., [6]. In case that $A \in C^\omega(\mathcal{I}, \mathbb{R}^{m\times n})$, i.e., when A is real analytic, the result again follows from the Implicit Function Theorem; see [10]. □

REMARK 3.11. The above statement also holds for the alternative scaling (3.6). The argument is similar.

The practical advantage of (3.7) is that we can use standard packages for continuation of an implicitly defined curve. In particular, we use the MATLAB toolbox MATCONT [3]. Path-following of the solution set of (3.7) via MATCONT is very robust. However, one has to be careful when interpreting the results. In particular, the lower bound for the step size, `MinStepsize`, should be chosen sufficiently small. We will comment on this observation in Section 6.

In order to illustrate the performance, we consider the same problem as in [7], namely, the homotopy

$$A(t) = t\,\mathrm{A2} + (1 - t)\,\mathrm{A1}, \quad t \in [0, 1], \tag{3.11}$$

where the matrices $\mathrm{A1} \equiv$ `well1033.mtx`, $\mathrm{A2} \equiv$ `illc1033.mtx` are taken from the Matrix Market [11]. Note that $\mathrm{A1}, \mathrm{A2} \in \mathbb{R}^{1033\times 320}$ are sparse and A1, A2 are well- and ill-conditioned, respectively. The aim is to continue the ten smallest singular values and corresponding left/right singular vectors of $A(t)$. The continuation is initialized at $t = 0$. The initial decomposition of A1 is computed via `svds`; see the MATLAB Function Reference.

The results of continuation are displayed in Figure 3.1. We run MATCONT ten times, once for each singular value. The branches do not cross. The computation complies with Theorem 3.10. Each curve is computed as a sequence of isolated points marked by circles; see the zoom on the right. The adaptive stepsize control refines the stepsize individually for each branch.

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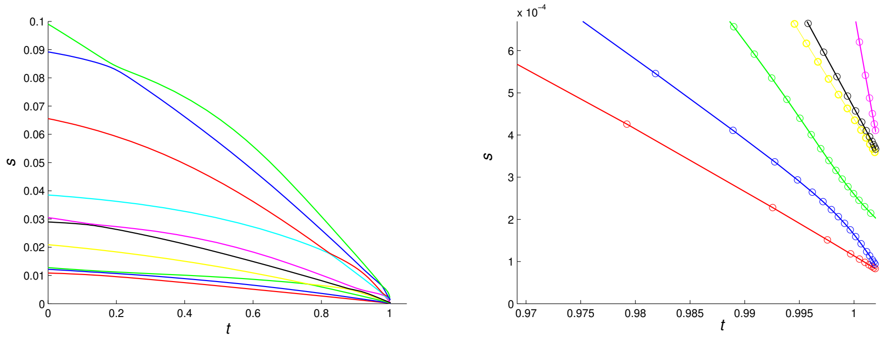

FIGURE 3.1. *Branches of singular values $s_{320}(t), \ldots, s_{310}(t)$ as functions of t. On the right: The relevant zooms.*

4. Singular point on the path. Let $f(t^0, x^0) = 0$, $x^0 = (s^0, u^0, v^0)$, $s^0 \neq 0$. Let us discuss the case when the assumptions of Theorem 3.10 do not hold; namely, assume that $s^0 \neq 0$ is a nonsimple (multiple) singular value of $A(t^0)$. Then we conclude that $\dim \operatorname{Ker} \mathcal{M}(t, s) \geq 2$; see Remark 3.7.

In particular, we will assume that $\dim \operatorname{Ker} \mathcal{M}(t^0, s^0) = 2$. Then, there exist $\delta u \in \mathbb{R}^m$, $\|\delta u\| = 1$, and $\delta v \in \mathbb{R}^n$, $\|\delta v\| = 1$, such that

$$\mathcal{M}(t^0, s^0) \begin{bmatrix} \delta u \\ \delta v \end{bmatrix} = 0, \quad (v^0)^T \, \delta v = 0.$$

Note that this implies $(u^0)^T \, \delta u = 0$. Computing $\operatorname{Ker} f_x(t^0, x^0)$, see (3.8)–(3.10), we conclude that $\dim \operatorname{Ker} f_x(t^0, s^0) = 1$ and

$$\operatorname{Ker} f_x(t^0, x^0) = \operatorname{span} \left\{ \begin{bmatrix} 0 \\ \delta u \\ \delta v \end{bmatrix} \right\}. \tag{4.1}$$

4.1. Dimensional reduction. Our aim is to analyze the singular root (t^0, x^0) of the parameter dependent equation (3.7). A standard technique is *Lyapunov-Schmidt reduction* [6]. We apply a version based on bordered matrices [5]. We assume that $\dim \operatorname{Ker} f_x(t^0, x^0) = 1$, i.e., the corank of the matrix $f_x(t^0, x^0)$ is one. Using the proper terminology, we deal with a $\operatorname{corank} = 1$ singularity.

The algorithm of the reduction is as follows. Let us fix vectors $B, C \in \mathbb{R}^{1+m+n}$. Find $\xi \in \mathbb{R}$, $\tau \in \mathbb{R}$, $\Delta x \in \mathbb{R}^{1+m+n}$ and $\varphi \in \mathbb{R}$ such that

$$f(t^0 + \tau, x^0 + \Delta x) + \varphi B = 0, \tag{4.2}$$

$$C^T \, \Delta x = \xi. \tag{4.3}$$

We define an operator related to the above equation:

$$\mathcal{F} : \mathbb{R} \times \mathbb{R} \times \mathbb{R}^{1+m+n} \times \mathbb{R} \to \mathbb{R}^{1+m+n} \times \mathbb{R},$$

$$\mathcal{F}(\tau, \xi, \Delta x, \varphi) \equiv \begin{bmatrix} f(t^0 + \tau, x^0 + \Delta x) + \varphi B \\ C^T \, \Delta x - \xi \end{bmatrix}. \tag{4.4}$$

Let us assume that

$$\det \begin{bmatrix} f_x(t^0, x^0) & B \\ C^T & 0 \end{bmatrix} \neq 0. \tag{4.5}$$

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It can be shown, see [5], that this assumption is satisfied for a generic choice of *bordering vectors* B and C. Nevertheless, later on we specify B and C.

Obviously, $(\xi, \tau, \Delta x, \varphi) = (0, 0, 0, 0) \in \mathbb{R} \times \mathbb{R} \times \mathbb{R}^{1+m+n} \times \mathbb{R}$ is a root of $\mathcal{F}$, i.e., $\mathcal{F}(0, 0, 0, 0) = 0$. The partial differential of $\mathcal{F}$ with respect to the variables Δx, φ, namely, the matrix $\mathcal{F}_{\Delta x,\varphi}(0, 0, 0, 0) \in \mathbb{R}^{(2+m+n)\times(2+m+n)}$, is regular at the origin $(0, 0, 0, 0)$ by the assumption (4.5). Due to the Implicit Function Theorem [6], the solution manifold of $\mathcal{F}(\xi, \tau, \Delta x, \varphi) = 0$ can be locally parameterized by τ and ξ; that is, there exist functions

$$\varphi = \varphi(\tau, \xi) \in \mathbb{R}, \quad \Delta x = \Delta x(\tau, \xi) \in \mathbb{R}^{1+m+n}, \tag{4.6}$$

such that $\mathcal{F}(\tau, \xi, \Delta x(\tau, \xi), \varphi(\tau, \xi)) = 0$ for all τ and ξ being small. From (4.2) and the fact that $B \neq 0$ due to (4.5), we conclude that

$$f(t^0 + \tau, x^0 + \Delta x(\tau, \xi)) = 0 \tag{4.7}$$

if and only if

$$\varphi(\tau, \xi) = 0. \tag{4.8}$$

The scalar equation (4.8) is called the *bifurcation equation*. There is a one-to-one link between the solution $(\tau, \xi) \in \mathbb{R}^2$ of the bifurcation equation (4.8) and the solution $(t, x) \in \mathbb{R} \times \mathbb{R}^{1+m+n}$ of the equation (3.7):

$$t = t^0 + \tau, \quad x = x^0 + \Delta x(\tau, \xi). \tag{4.9}$$

The statement has an obvious local meaning: it describes all roots of (3.7) in a neighborhood of (t^0, x^0).

As a rule, the solutions of the bifurcation equation can be approximated only numerically. The usual technique is

1. approximate the mapping $(\tau, \xi) \longmapsto \varphi(\tau, \xi)$ via its Taylor expansion at the origin,
2. solve a *truncated bifurcation equation*, i.e., the equation with truncated higher order terms.

The Taylor expansion reads

$$\varphi(\tau, \xi) = \varphi + \varphi_\tau \, \tau + \varphi_\xi \, \xi + \frac{1}{2}\varphi_{\tau\tau} \, \tau^2 + \varphi_{\xi\tau} \, \xi\tau + \frac{1}{2}\varphi_{\xi\xi} \, \xi^2 + \text{h.o.t.}\,, \tag{4.10}$$

where the partial derivatives of $\varphi = \varphi(\tau, \xi)$ are understood to be evaluated at the origin, e.g., $\varphi \equiv \varphi(0, 0)$ or $\varphi_{\xi\tau} \equiv \varphi_{\xi\tau}(0, 0)$. Note that $\varphi(0, 0) = 0$. The symbol h.o.t. denotes higher order terms.

We also need to expand

$$\Delta x(\tau, \xi) = \Delta x + \Delta x_\tau \, \tau + \Delta x_\xi \, \xi + \frac{1}{2}\Delta x_{\tau\tau} \, \tau^2 + \Delta x_{\xi\tau} \, \xi\tau + \frac{1}{2}\Delta x_{\xi\xi} \, \xi^2 + \text{h.o.t.}\,. \tag{4.11}$$

The partial derivatives of $\Delta x = \Delta x(\tau, \xi)$ are understood to be evaluated at the origin. This expansion is needed to approximate the link (4.9) between (4.8) and (3.7).

Computing the coefficients of both expansions (4.10) and (4.11) is a routine procedure; see [5, Section 6.2]. For example, the coefficients Δx_ξ, φ_ξ satisfy a linear system with the matrix from (4.5),

$$\begin{bmatrix} f_x(t^0, x^0) & B \\ C^T & 0 \end{bmatrix} \begin{bmatrix} \Delta x_\xi \\ \varphi_\xi \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

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The coefficients $\Delta x_{\xi\xi}$, $\varphi_{\xi\xi}$ are defined via a linear system with the same matrix,

$$\begin{bmatrix} f_x(t^0,x^0) & B \\ C^T & 0 \end{bmatrix} \begin{bmatrix} \Delta x_{\xi\xi} \\ \varphi_{\xi\xi} \end{bmatrix} = \begin{bmatrix} -f_{xx}(t^0,x^0)\,\Delta x_\xi\,\Delta x_\xi \\ 0 \end{bmatrix},$$

etc.

We considered the particular function f defined in (3.6). In our computation, we specified B and C as

$$B = \begin{bmatrix} \delta u \\ \delta v \\ 0 \end{bmatrix}, \quad C = \begin{bmatrix} 0 \\ \delta u \\ \delta v \end{bmatrix}. \tag{4.12}$$

Note that condition (4.5) is satisfied. Moreover, the computations are simplified. In Appendix A, we list Taylor coefficients of (4.10) and (4.11) up to the second order. The coefficients are computed by using the specific data of the problem: t^0, x^0, δu^0, δv^0, $A(t)$ and higher derivatives of $A(t)$ at t^0.

4.2. Bifurcation analysis. Let us analyze the bifurcation equation (4.8) in a neighborhood of the origin. Let us start with a heuristic. Due to (A.1), the bifurcation equation can be factored as

$$\varphi(\tau,\xi) = \tau\,\eta(\tau,\xi) = 0, \quad \eta(\tau,\xi) \equiv \varphi_\tau + \frac{1}{2}\varphi_{\tau\tau}\,\tau + \varphi_{\xi\tau}\,\xi + \text{h.o.t.}, \tag{4.13}$$

where h.o.t. are of second order. The solutions (τ,ξ) of (4.13) are linked to the solutions (t,x) of (3.7) via the transformation (4.9), where the increments $\Delta x(\tau,\xi)$ are expanded as

$$\Delta s(\tau,\xi) = \Delta s_\tau\,\tau + \frac{1}{2}\Delta s_{\tau\tau}\,\tau^2 + \Delta s_{\xi\tau}\,\xi\tau + \text{h.o.t.}, \tag{4.14}$$

$$\Delta u(\tau,\xi) = \Delta u_\tau\,\tau + \frac{1}{2}\delta u\,\xi - \frac{1}{8}u^0\,\xi^2 + \frac{1}{2}\Delta u_{\tau\tau}\,\tau^2 + \Delta u_{\xi\tau}\,\xi\tau + \text{h.o.t.}, \tag{4.15}$$

$$\Delta v(\tau,\xi) = \Delta v_\tau\,\tau + \frac{1}{2}\delta v\,\xi - \frac{1}{8}v^0\,\xi^2 + \frac{1}{2}\Delta v_{\tau\tau}\,\tau^2 + \Delta v_{\xi\tau}\,\xi\tau + \text{h.o.t.}. \tag{4.16}$$

Note that we exploited (A.12), (A.6), and (A.9). The h.o.t. are of third order.

Obviously, $\tau = 0$ is a trivial solution of (4.13). In case $\varphi_\tau \neq 0$, this is the only solution locally available. In what follows, let us consider the case $\varphi_\tau = 0$. We solve (4.13) on an open interval $\mathcal{J}$ of parameters t assuming that $t^0 \in \mathcal{J}$.

THEOREM 4.1. *Let $(t^0,x^0) \in \mathcal{J} \times \mathbb{R}^{1+m+n}$, $x^0 = (s^0,u^0,v^0)$ be a root of $f(t^0,x^0) = 0$. Let* $\dim \operatorname{Ker} f_x(t^0,x^0) = 1$*; that is, let $\delta u \in \mathbb{R}^m$, $\|\delta u\| = 1$, $\delta v \in \mathbb{R}^n$, $\|\delta v\| = 1$, be such that* (4.1) *holds. Assume that*

$$\varphi_\tau = 0, \quad \varphi_\tau \equiv \frac{1}{2}(\delta u)^T A'(t^0) v^0 + \frac{1}{2}(u^0)^T A'(t^0)\delta v, \tag{4.17}$$

$$\varphi_{\tau\tau} \neq 0. \tag{4.18}$$

For $\varphi_{\tau\tau}$, see (A.4)*. Let $A = A(t)$ be smooth, i.e., $A \in C^\omega(\mathcal{J},\mathbb{R}^{1+m+n})$. Then there exists an open subinterval $\mathcal{I} \subset \mathcal{J}$ containing t^0 and a unique function $t \in \mathcal{I} \longmapsto x(t) \in \mathbb{R}^{1+m+n}$, $x \in C^\omega(\mathcal{I},\mathbb{R}^{1+m+n})$, such that $f(t,x(t)) = 0$ for all $t \in \mathcal{I}$ with $x(t^0) = x^0$.*

Proof. By virtue of the factorization (4.13) we have to solve $\eta(\tau,\xi) = 0$ for τ and ξ. The assumption (4.18) makes it possible to apply the Implicit Function Theorem for real analytic functions [10]. □

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In order to introduce required terminology, let us briefly review Singularity Theory [5, Chapter 6]. Let $(t^0, x^0) \in \mathbb{R} \times \mathbb{R}^{1+m+n}$ be a root of f, i.e., $f(t^0, x^0) = 0$; see (3.6) in this particular context. If this root (t^0, x^0) satisfies the assumptions of Theorem 3.10, then we say that it is a *regular root*. If not, then (t^0, x^0) is said to be a *singular root*. In other words, (t^0, x^0) is a *singular point* of the mapping $f : \mathbb{R} \times \mathbb{R}^{1+m+n} \to \mathbb{R}^{1+m+n}$.

In Section 4.1 we have already mentioned the *codimension* of a singular point. Theorem 4.1 classifies $\mathrm{codim} = 1$ singular points. The codimension is not the only aspect of the classification. In Theorem 4.1 we require the equality (4.17) and the inequality (4.18). The former condition is called the *defining condition* and the latter one is the *nondegeneracy condition*. The number of defining conditions is called the *codimension*. Theorem 4.1 deals with a singular point of $\mathrm{codim} = 1$. The next item of the classification list, namely, a singular point of $\mathrm{codim} = 2$, would be defined by the conditions $\varphi_\tau = \varphi_{\tau\tau} = 0$ and the nondegeneracy condition $\varphi_{\tau\tau\tau} \neq 0$, etc.

With some abuse of language, we note the following:

REMARK 4.2. Equation (3.7) defines a path of parameter dependent *singular values* and corresponding left/right singular vectors. There are *singular points* on this path. One of them could be classified as $\mathrm{corank} = 1$, $\mathrm{codim} = 1$ singular point. This particular point (t^0, x^0), $x^0 = (s^0, u^0, v^0)$, is related to a nonsimple (multiple) singular value s^0.

PROPOSITION 4.3. *Let the assumptions of Theorem 4.1 be satisfied. Let (t^0, x^0) be a singular point of f of $\mathrm{corank} = 1$ and $\mathrm{codim} = 1$. Let $\delta u \in \mathbb{R}^m$, $\|\delta u\| = 1$, $\delta v \in \mathbb{R}^n$, $\|\delta v\| = 1$, span the kernel (4.1). Then the point $(t^0, y^0) \in \mathbb{R} \times \mathbb{R}^{1+m+n}$, $y^0 \equiv (s^0, \delta u, \delta v)$, is also a singular point of f of $\mathrm{corank} = 1$ and $\mathrm{codim} = 1$. Moreover, the Taylor expansion at (t^0, y^0) can be obtained from that at the point (t^0, x^0), i.e., from (4.13), (4.14)–(4.16). More precisely, let the coefficients of the Taylor expansion at (t^0, y^0) be marked by tilde, i.e., $\widetilde{\varphi}_\xi$, $\widetilde{\varphi}_\tau$, $\widetilde{\varphi}_{\xi\tau}$, $\widetilde{\varphi}_{\xi\tau}$, $\frac{\partial^j \widetilde{\varphi}}{\partial \xi^j}(0,0)$, and $\frac{\partial^j \widetilde{\Delta s}}{\partial \xi^j}(0,0)$. Then*

$$\widetilde{\varphi}_\tau = \varphi_\tau, \quad \widetilde{\varphi}_{\xi\tau} = -\varphi_{\xi\tau}, \quad \widetilde{\varphi}_{\tau\tau} = \varphi_{\tau\tau} \tag{4.19}$$

and

$$\widetilde{\varphi}_\xi = \widetilde{\varphi}_{\xi\xi} = \cdots = \frac{\partial^j \widetilde{\varphi}}{\partial \xi^j}(0,0) = \cdots = 0, \tag{4.20}$$

$$\widetilde{\Delta s}_\xi = \widetilde{\Delta s}_{\xi\xi} = \cdots = \frac{\partial^j \widetilde{\Delta s}}{\partial \xi^j}(0,0) = \cdots = 0 \tag{4.21}$$

for $j = 1, 2, \ldots$.

Proof. The statement concerning the singularity at (t^0, y^0) follows from the properties of the kernel of (3.4). The formulae (4.19)–(4.21) can be readily verified. Hence, the classification of (t^0, y^0) follows from the assumptions (4.17) and (4.18). □

As mentioned in Section 1, the paper [13] contains a detailed analysis of non-generic points on the path. It was noted that [13] attempts to track *all* singular values, i.e., to construct the path of $\Sigma(t)$, $U(t)$ and $V(t)$; see (1.1). Nevertheless, on the analytical level, one can speak about paths of singular values $s_j(t)$ and $s_k(t)$.

REMARK 4.4. In [13, Section 3], the author investigates "simple cross over of the paths." He proposed a set of defining conditions for this phenomenon. Nevertheless, he does not resolve this system *explicitly*. It is intuitively clear that this "simple cross over of the paths" should be the singular point treated in Theorem 4.1. In our analysis, we can point out computable constants (A.2) and (A.4) to decide about the case.

4.3. Example. We consider [13, Example 2]; see also [12, Example 1]. Let $A(t) \equiv U(t)S(t)U(t)$, $t \in \mathbb{R}$, where

$$S(t) = \operatorname{diag}\left(0.5 + t, 2 - t, 1 - t, t\right),$$

$$U(t) = \begin{bmatrix} c_1(t) & s_1(t) & 0 & 0 \\ -s_1(t) & c_1(t) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & c_2(t) & s_2(t) & 0 \\ 0 & -s_2(t) & c_2(t) & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & c_3(t) & s_3(t) \\ 0 & 0 & -s_3(t) & c_3(t) \end{bmatrix},$$

with $c_1(t) = \cos(t)$, $s_1(t) = \sin(t)$, $c_2(t) = \cos(1+t)$, $s_2(t) = \sin(1+t)$, $c_3(t) = \cos(2+t)$, $s_3(t) = \sin(2 + t)$. There are five singular points of all paths at $t = 0.25, 0.5, 0.75, 1, 1.5$. These are manifested as "simple cross over of the paths" or "simple cross overs" (in terms of [13]) related to particular pairs of paths; see Figure 4.1 on the left. Note that if $t = 1.5$, then $s_1(t) = -s_2(t) = 0.5$. Due to Remark 3.5, either $s_1(t)$ or $s_2(t)$ is nonsimple (actually, both of them are nonsimple).

We are able to continue *separate* branches of singular values and left/right singular vectors. Let us set $t = 0.1$, compute the classical SVD of $A(t) = U(t)\Sigma(t)V(t)^T$ and initialize the continuation at $(s_3(t), U_3(t), V_3(t))$, which are the third singular value and the third columns of $U(t)$ and $V(t)$ at $t = 0.1$. We actually continue a curve in $\mathbb{R} \times \mathbb{R}^{1+4+4}$. In Figure 4.1 and Figure 4.2, $s(t)$ and $v_4(t)$ are depicted in green. On this curve there are just two singular points, one at $t = 0.25$ and the other at $t = 0.75$.

Let us perform an asymptotic analysis of the former point. Using the notation of Theorem 4.1,

$$\begin{aligned} t^0 &= 0.25, & s^0 &= 0.7500, \\ u^0 &= [0.9689; -0.2474; 0.0000; -0.0000], & v^0 &= [0.9689; 0.0780; -0.1475; 0.1827], \\ \delta u &= [-0.1475; -0.5776; -0.1981; -0.7781], & \delta v &= [0; -0.9490; -0.1981; 0.2453]. \end{aligned}$$

The leading Taylor coefficients of $\varphi(\tau, \xi)$ and $\Delta s(\tau, \xi)$ are

$$\begin{aligned} &\varphi_{\tau\tau} = -1.6871, \quad \varphi_{\xi\tau} = 1, \\ &\Delta s_\tau = 1, \quad \Delta s_{\xi\tau} = 0, \quad \Delta s_{\tau\tau} = -1.2751 \times 10^{-8}. \end{aligned}$$

Similarly, we can compute the leading coefficients of $\Delta u(\tau, \xi) \in \mathbb{R}^4$ and $\Delta v(\tau, \xi) \in \mathbb{R}^4$.

Neglecting quadratic terms in (4.13), (4.14)–(4.16), we get a local approximation of the green branch being parameterized by τ. In particular, we set $\tau = -0.1 : 0.05 : 0.15$ (regularly spaced points on the interval $[-0.1, 0.15]$ with increment 0.05) and mark the resulting points by black diamonds; see the zooms in Figure 4.1 and Figure 4.2. Due to Proposition 4.3, we can get an asymptotic expansion of the blue branch for free.

5. An unfolding. Let

$$f : \mathbb{R} \times \mathbb{R}^{1+m+n} \times \mathbb{R} \to \mathbb{R}^{1+m+n},$$

$$t \in \mathbb{R}, \quad x = (s, u, v) \in \mathbb{R}^1 \times \mathbb{R}^m \times \mathbb{R}^n, \quad \varepsilon \in \mathbb{R} \longmapsto f(t, x, \varepsilon) \in \mathbb{R}^{1+m+n},$$

$$f(t, x, \varepsilon) \equiv \begin{bmatrix} -su + (A(t) + \varepsilon Z(t))v \\ (A(t) + \varepsilon Z(t))^T u - sv \\ u^T u + v^T v - 2 \end{bmatrix}. \tag{5.1}$$

The mapping (5.1) is an example of an *unfolding* of the mapping (3.6). It is required that $f(t, x, 0)$ via (5.1) complies with $f(t, x)$ via (3.6), which is obvious. For a fixed value of ε,

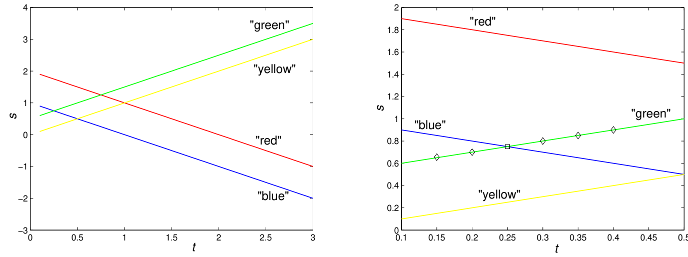

FIGURE 4.1. *Branches of singular values $s_1(t), \ldots, s_4(t)$ in red, blue, green, and yellow as functions of t. Zoomed: The singular point, marked as square, on the green branch. The approximations via asymptotic analysis are marked by diamonds.*

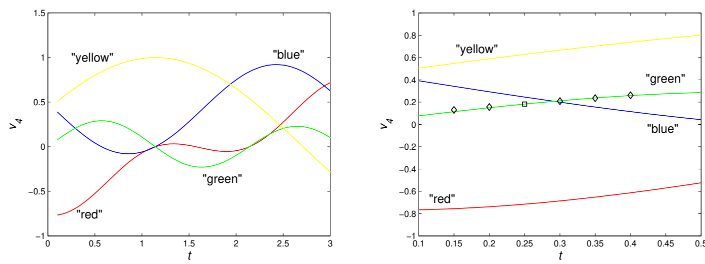

FIGURE 4.2. *Red, blue, green, and yellow branches of the ninth solution component, i.e., $v_4 = v_4(t)$. Zoomed: The relevant asymptotic analysis of the green branch.*

we consider the equation

$$f(t, x, \varepsilon) = 0, \quad x = (s, u, v), \tag{5.2}$$

for $t \in \mathbb{R}$ and $x \in \mathbb{R}^{1+m+n}$. The unfolding may also model an *imperfection* of the original mapping $f(t, x)$.

Let $(t^0, x^0, 0)$ be a singular point of the above f. Let this point satisfy the assumptions of Theorem 4.1. Our aim is to study solutions of (5.2) for a small fixed ε.

5.1. Dimensional reduction revisited. We adapt the dimensional reduction from Section 4.1 to the unfolding (5.1). Let us fix vectors $B \in \mathbb{R}^{1+m+n}$, $C \in \mathbb{R}^{1+m+n}$. Find $\xi \in \mathbb{R}$, $\tau \in \mathbb{R}$, $\varepsilon \in \mathbb{R}$, $\Delta x \in \mathbb{R}^{1+m+n}$ and $\varphi \in \mathbb{R}$ such that

$$f(t^0 + \tau, x^0 + \Delta x, \varepsilon) + \varphi B = 0, \tag{5.3}$$

$$C^T \Delta x = \xi. \tag{5.4}$$

Under the assumption (4.5), the solutions φ and Δx of (5.3) and (5.4) can be locally parameterized by τ, ξ, and ε, i.e.,

$$\varphi = \varphi(\tau, \xi, \varepsilon) \in \mathbb{R}, \quad \Delta x = \Delta x(\tau, \xi, \varepsilon) \in \mathbb{R}^{1+m+n}. \tag{5.5}$$

Using the same argument as in Section 4.1, we conclude that

$$f(t^0 + \tau, x^0 + \Delta x(\tau, \xi, \varepsilon),\ \varepsilon) = 0 \tag{5.6}$$

if and only if

$$\varphi(\tau, \xi, \varepsilon) = 0 \tag{5.7}$$

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for small τ, ξ and ε.

The aim is to compute Taylor expansions of the functions $\varphi(\tau, \xi, e\varepsilon)$ and $\Delta x(\tau, \xi, \varepsilon)$ at the origin in order to approximate solutions of (5.7) and (5.6). In Appendix A, we list the relevant Taylor coefficients up to second order. The bordering is chosen as in (4.12).

5.2. Imperfect bifurcation. Consider the expansions

$$\begin{aligned}\varphi(\tau,\xi,\varepsilon) =& \tau\left(\varphi_\tau + \frac{1}{2}\varphi_{\tau\tau}\,\tau + \varphi_{\xi\tau}\,\xi\right) \\ &+ \varepsilon\left(\varphi_\varepsilon + \varphi_{\xi\varepsilon}\,\xi + \varphi_{\tau\varepsilon}\,\tau + \frac{1}{2}\varphi_{\varepsilon\varepsilon}\,\varepsilon\right) + \text{h.o.t.}\end{aligned} \tag{5.8}$$

and

$$\begin{aligned}\Delta s(\tau,\xi,\varepsilon) =& \tau\left(\Delta s_\tau + \frac{1}{2}\Delta s_{\tau\tau}\,\tau + \Delta x_{\xi\tau}\,\xi\right) \\ &+ \varepsilon\left(\Delta s_\varepsilon + \Delta s_{\xi\varepsilon}\,\xi + \Delta s_{\tau\varepsilon}\,\tau + \frac{1}{2}\Delta s_{\varepsilon\varepsilon}\,\varepsilon\right) + \text{h.o.t.}\,,\end{aligned} \tag{5.9}$$

$$\begin{aligned}\Delta u(\tau,\xi,\varepsilon) =& \Delta u_\tau\,\tau + \frac{1}{2}\delta u\,\xi - \frac{1}{8}u^0\,\xi^2 + \frac{1}{2}\Delta u_{\tau\tau}\,\tau^2 + \Delta u_{\xi\tau}\;\xi\tau \\ &+ \varepsilon\left(\Delta u_\varepsilon + \Delta u_{\xi\varepsilon}\,\xi + \Delta u_{\tau\varepsilon}\,\tau + \frac{1}{2}\Delta u_{\varepsilon\varepsilon}\,\varepsilon\right) + \text{h.o.t.}\,,\end{aligned} \tag{5.10}$$

$$\begin{aligned}\Delta v(\tau,\xi,\varepsilon) =& \Delta v_\tau\,\tau + \frac{1}{2}\delta v\,\xi - \frac{1}{8}v^0\,\xi^2 + \frac{1}{2}\Delta v_{\tau\tau}\,\tau^2 + \Delta v_{\xi\tau}\;\xi\tau \\ &+ \varepsilon\left(\Delta v_\varepsilon + \Delta v_{\xi\varepsilon}\,\xi + \Delta v_{\tau\varepsilon}\,\tau + \frac{1}{2}\Delta v_{\varepsilon\varepsilon}\,\varepsilon\right) + \text{h.o.t.}\,.\end{aligned} \tag{5.11}$$

The h.o.t. are of third order.

Instead of (5.7), we solve the *truncated* bifurcation equation

$$\tau\left(\varphi_\tau + \frac{1}{2}\varphi_{\tau\tau}\,\tau + \varphi_{\xi\tau}\,\xi\right) + \varepsilon\left(\varphi_\varepsilon + \varphi_{\xi\varepsilon}\,\xi + \varphi_{\tau\varepsilon}\,\tau + \frac{1}{2}\varphi_{\varepsilon\varepsilon}\,\varepsilon\right) = 0 \tag{5.12}$$

for ξ and τ and fixed ε. If $\varphi_{\xi\varepsilon} \neq 0$, the solutions to (5.12) can be parameterized by τ.

Hence, given a small value of τ we compute $\xi = \xi(\tau)$ as a solution of the truncated bifurcation equation (5.12). Then we substitute this pair $(\tau, \xi(\tau))$ into the *truncated* version of (5.9)–(5.11). We get an approximation of the root of (5.6).

Let us consider the function (2.1) from Section 2 and set $\varepsilon = 0.1$. In Figure 2.2, in fact, the solution sets of (5.2) are depicted, namely, the solution components $t \longmapsto x_1(t) = s(t)$, $t \longmapsto x_4(t) = v_1(t)$ and $t \longmapsto x_5(t) = v_2(t)$ as $-0.5 \leq t \leq 0.5$, for both red and blue branches. In Figure 5.1, there are zooms of both red and blue branches showing the solution components $t \longmapsto s(t)$, on the left, and the components $t \longmapsto v_1(t)$, on the right. These solutions were computed numerically via path-following; see Section 3.2. Approximations via (5.12) and the truncated versions of (5.9)–(5.11) are marked by red and blue diamonds. They are reasonably accurate for small t.

5.3. Example continued. Let us consider $A(t)$ as in Example 4.3. We model an imperfection (5.1), $n = m = 4$. In particular, we set

$$\varepsilon = -0.1, \quad Z(t) \equiv \begin{bmatrix} 1.0 & -0.7 & 0.3 & -0.6 \\ 0.9 & 0.3 & -0.7 & 0.8 \\ 0.1 & 0.4 & -0.3 & 9.0 \\ -0.6 & 0.1 & 0.7 & -0.5 \end{bmatrix}.$$

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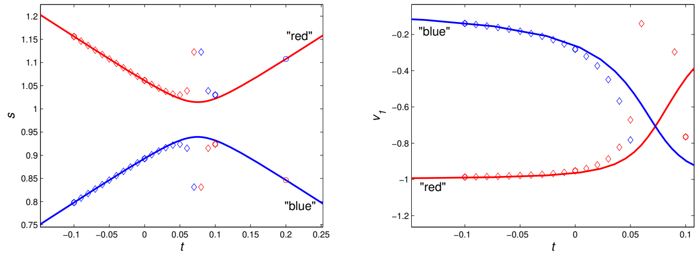

FIGURE 5.1. *Analysis of motivating example from Section 2, $\varepsilon = 0.1$: zooms of both red and blue branches, namely, the solution components $t \longmapsto s(t)$, $t \longmapsto v_1(t)$, compared with results of the truncated approximation marked by diamonds.*

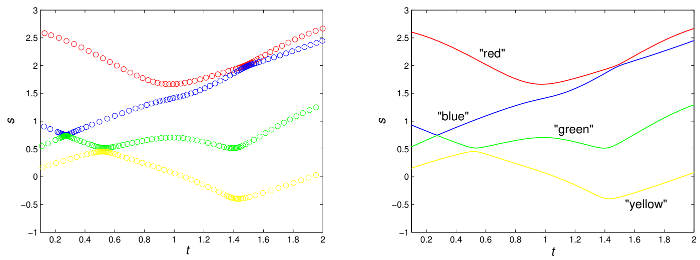

FIGURE 5.2. *Example from Section 5.3, $\varepsilon = -0.1$: Four perturbed branches of the analytic SVD, $t \longmapsto s(t)$. On the left: An illustration of the adaptive step length.*

We compute solutions of (5.2) for $t \geq 0.1$.

In Figure 5.2, there are four solution branches, namely, the first four components of s parameterized by t, $0.1 \leq t \leq 2$, colored by red, blue, green, and yellow. The initial conditions of these branches are the perturbations of the initial conditions from Example 4.3. Observe that the blue branch is close to the red one, and the green branch to the yellow one for $t \approx 1.5$ and $t \approx 0.5$, respectively.

We should have in mind our motivation, as illustrated in Figure 2.1 and Figure 2.2. The simple cross over branching *degenerates* to a touching of different branches like $\begin{smallmatrix}\cup\\\cap\end{smallmatrix}$. As far as the left/right singular vector paths are concerned, a perturbation implies twisting.

Coming back to the perturbed Example 5.3, namely, to the continuation of the blue and the green branches, we observed twists of left/right singular vectors for $t \approx 1.5$ and $t \approx 0.5$, respectively. In Figure 5.3, on the left, the (u_1, u_2)-solution components of the blue and red branches are shown near $t \approx 1.5$. The particular components twist. Similarly, in Figure 5.3, on the right, we depict the (u_2, u_3)-solution components of the green and yellow branches as $t \approx 0.5$. Again, there is a twist. Note that a similar observation can be made as the blue and green branches nearly touch for $t \approx 0.25$.

Comparing Figure 4.1 and Figure 5.2, we conclude that the global branching scenario may change dramatically under a perturbation.

6. Conclusions. We introduced a new path-following technique to follow simple singular values and the corresponding left/right singular vectors. We investigated singularities on the path; namely, we classified a singularity with $\mathrm{corank} = 1$ and $\mathrm{codim} = 1$. This singularity is related to “simple cross overs” (in terms of [13]). We also studied this singularity subject to a perturbation (an imperfection).

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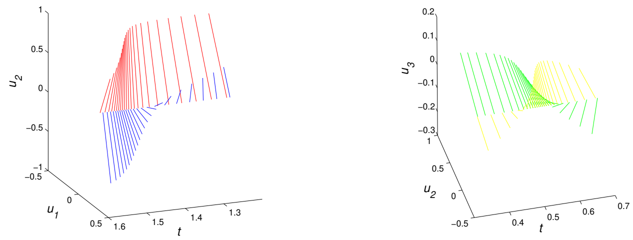

FIGURE 5.3. *The solution components. Left: The blue and red branches for* $t \approx 1.5$*. Right: The green and yellow branches for* $t \approx 0.5$*.*

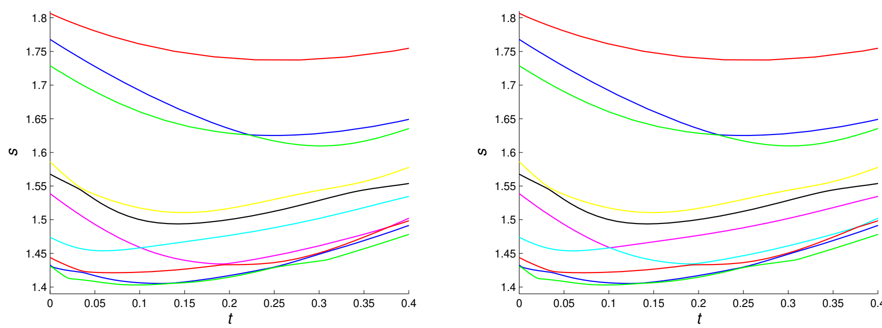

FIGURE 6.1. *Branches of singular values* $s_1(t), \ldots, s_{10}(t)$ *as functions of* $0 \le t \le 0.4$*. The branches* $s_6(t)$ *and* $s_7(t)$ *are in magenta and cyan. They cross on the left while they do not cross on the right. For the zoom, see Figure* 6.2.

These investigations try to support the claim that the aforementioned path-following technique works generically. Consider the homotopy (3.11) again. Let us compute the path of the ten largest singular values using MATCONT [3]. The result is summarized in Figure 6.1. The paths $s_6(t)$ and $s_7(t)$ intersect on the left. The Continuer was run under a default parameter setting (`InitStepsize` $= 0.01$, `MinStepsize` $= 10^{-5}$, `MaxStepsize` $= 0.1$). If we increase the precision (setting `InitStepsize` $= 0.001$, `MinStepsize` $= 10^{-6}$, `MaxStepsize` $= 0.01$) the relevant branches do not intersect, as shown in Figure 6.1 on the right. Figure 6.2 shows zooms of the mentioned branches computed with default (on the left) and the increased (on the right) precisions. The figure on the left suggests that the "crossing" is a numerical artifact. We refer to the magenta curve, i.e., the numerically computed branch $s_6(t)$. The cyan branch $s_7(t)$ (not shown there) exhibits similar zig-zag oscillations. The dotted cyan line is a trimmed curve $s_7(t)$ with removed oscillations.

Generically, parameter-dependent singular values do not change the ordering except if they change the sign. In a forthcoming paper we will investigate zero singular values subject to perturbations.

Appendix A. Details of Taylor expansions.

We review leading terms of the expansions (4.13), (4.14)–(4.16), and the imperfect versions (5.8), (5.9)–(5.11).

Note that the computation of these terms follows a routine chain rule procedure indicated at the end of Section 4.1. We take advantage of the structure of f_x and higher partial differentials of f.

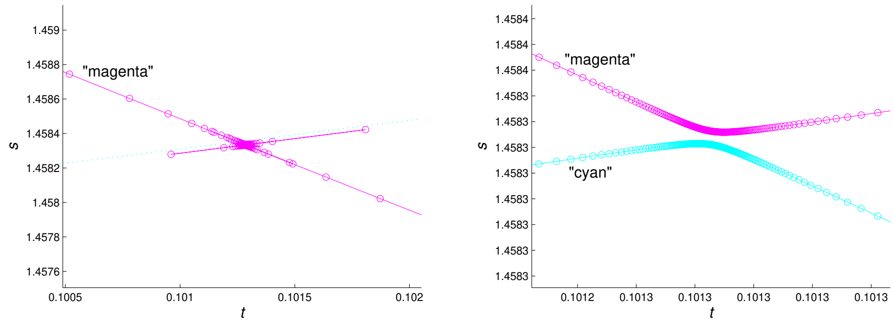

FIGURE 6.2. *Zooms: The crossing of the branches $s_6(t)$ and $s_7(t)$, shown in magenta and cyan, on the left of Figure 6.1 is actually a numerical artifact. If the precision is increased, then the numerically computed branches do not cross.*

The Taylor coefficients depend on the following data: u^0, v^0, δu^0, δv^0, $A(t)$, $A'(t)$, $A''(t)$ and higher derivatives of $A(t)$, and on $Z(t)$, $Z'(t)$ and higher derivatives of $Z(t)$. Note that $Z(t)$ is related to the unfolding (5.1).

Concerning (4.13):

$$\varphi_\xi = \varphi_{\xi\xi} = \cdots = \frac{\partial^j \varphi}{\partial \xi^j}(0,0) = \cdots = 0, \quad j = 1, 2, \ldots, \tag{A.1}$$

$$\varphi_\tau = -\frac{1}{2}(\delta u)^T A'(t^0) v^0 - \frac{1}{2}(u^0)^T A'(t^0)\delta v, \tag{A.2}$$

$$\varphi_{\xi\tau} = \frac{1}{2}\left((u^0)^T A'(t^0) v^0 - (\delta u)^T A'(t^0)\delta v\right), \tag{A.3}$$

$$\begin{aligned}\varphi_{\tau\tau} = &-\frac{1}{2}\left((\delta u)^T A''(t^0) v^0 + (u^0)^T A''(t^0)\delta v\right) \\ &- \left((\delta u)^T A'(t^0)\Delta v_\tau + (\Delta u_\tau)^T A'(t^0)\delta v\right),\end{aligned} \tag{A.4}$$

where

$$\begin{bmatrix}\Delta u_\tau \\ \Delta v_\tau\end{bmatrix} = -\mathcal{M}^+(t^0, s^0)\begin{bmatrix}A'(t^0)v^0 \\ A'(t^0)^T u^0\end{bmatrix}, \tag{A.5}$$

$\mathcal{M}(t^0, s^0)$ is defined in (3.4).

Concerning (4.14)–(4.16):

$$\Delta s_\xi = 0, \quad \Delta u_\xi = \frac{1}{2}\delta u, \quad \Delta v_\xi = \frac{1}{2}\delta v, \tag{A.6}$$

$$\Delta s_\tau = (u^0)^T A'(t^0) v^0, \quad \begin{bmatrix}\Delta u_\tau \\ \Delta v_\tau\end{bmatrix} = -\mathcal{M}^+(t^0, s^0)\begin{bmatrix}A'(t^0)v^0 \\ A'(t^0)^T u^0\end{bmatrix}, \tag{A.7}$$

$$\Delta s_{\xi\tau} = -\frac{1}{2}\varphi_\tau, \quad \begin{bmatrix}\Delta u_{\xi\tau} \\ \Delta v_{\xi\tau}\end{bmatrix} = -\frac{1}{2}\mathcal{M}^+(t^0, s^0)\begin{bmatrix}A'(t^0)\delta v \\ A'(t^0)^T \delta u\end{bmatrix}, \tag{A.8}$$

$$\Delta s_{\xi\xi} = 0, \quad \begin{bmatrix}\Delta u_{\xi\xi} \\ \Delta v_{\xi\xi}\end{bmatrix} = -\frac{1}{4}\begin{bmatrix}u^0 \\ v^0\end{bmatrix}, \tag{A.9}$$

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$$\Delta s_{\tau\tau} = (u^0)^T A''(t^0) v^0 + (u^0)^T A'(t^0) \Delta v_\tau + (\Delta u_\tau)^T A'(t^0) v^0, \tag{A.10}$$

$$\begin{aligned}
\begin{bmatrix} \Delta u_{\tau\tau} \\ \Delta v_{\tau\tau} \end{bmatrix} &= -\mathcal{M}^+(t^0, s^0) \begin{bmatrix} A''(t^0) v^0 \\ A''(t^0)^T u^0 \end{bmatrix} \\
&\quad -2\mathcal{M}^+(t^0, s^0) \begin{bmatrix} A'(t^0) \delta v_\tau \\ A'(t^0)^T \delta u_\tau \end{bmatrix} \\
&\quad -2(u^0)^T A'(t^0) v^0 \left(\mathcal{M}^+(t^0, s^0)\right)^2 \begin{bmatrix} A'(t^0) v^0 \\ A'(t^0)^T u^0 \end{bmatrix},
\end{aligned}$$

$$\Delta s_{\xi\xi\xi} = 0\,, \qquad \begin{bmatrix} \Delta u_{\xi\xi\xi} \\ \Delta v_{\xi\xi\xi} \end{bmatrix} = 0. \tag{A.11}$$

Moreover,

$$\Delta s_\xi = \Delta s_{\xi\xi} = \cdots = \frac{\partial^j \Delta s}{\partial \xi^j}(0,0) = \ldots \cdots = 0, \quad j = 1, 2, \ldots. \tag{A.12}$$

REMARK A.1. The formulae (A.1) and (A.12) can be verified by induction.

Concerning (5.9)–(5.11):

$$\varphi_\varepsilon = -\frac{1}{2}\left((\delta u)^T Z(t^0) v^0 + (u^0)^T Z(t^0) \delta v\right), \tag{A.13}$$

$$\varphi_{\xi\varepsilon} = \frac{1}{2}\left((u^0)^T Z(t^0) v^0 - (\delta u)^T Z(t^0) \delta v\right), \tag{A.14}$$

$$\varphi_{\varepsilon\varepsilon} = -(\delta u)^T Z(t^0) \Delta v_\varepsilon - (\Delta u_\varepsilon)^T Z(t^0) \delta v, \tag{A.15}$$

$$\begin{aligned}
\varphi_{\tau\varepsilon} &= -\frac{1}{2}\left((\delta u)^T A'(t^0) \Delta v_\varepsilon + (\delta v)^T (A'(t^0))^T \Delta u_\varepsilon\right) \\
&\quad -\frac{1}{2}\left((\delta u)^T Z'(t^0) v^0 + (\delta v)^T (Z'(t^0))^T u^0\right) \\
&\quad -\frac{1}{2}\left((\delta u)^T Z(t^0) \Delta v_\tau + (\delta v)^T (Z(t^0))^T \Delta u_\tau\right),
\end{aligned} \tag{A.16}$$

where Δu_τ, Δv_τ are defined by (A.5),

$$\begin{bmatrix} \Delta u_\varepsilon \\ \Delta v_\varepsilon \end{bmatrix} = -\mathcal{M}^+(t^0, s^0) \begin{bmatrix} Z(t^0) v^0 \\ Z^T(t^0) u^0 \end{bmatrix}. \tag{A.17}$$

$$\Delta s_\varepsilon = (u^0)^T Z(t^0) v^0, \tag{A.18}$$

$$\Delta s_{\xi\varepsilon} = \frac{1}{4}\left((u^0)^T Z(t^0) \delta v + (\delta u)^T Z(t^0) v^0\right), \tag{A.19}$$

$$\begin{bmatrix} \Delta u_{\xi\varepsilon} \\ \Delta v_{\xi\varepsilon} \end{bmatrix} = -\frac{1}{2}\mathcal{M}^+(t^0, s^0) \begin{bmatrix} Z(t^0) \delta v \\ Z^T(t^0) \delta u \end{bmatrix}, \tag{A.20}$$

$$\begin{aligned}
\Delta s_{\tau\varepsilon} &= \frac{1}{2}\left((u^0)^T A'(t^0) \Delta v_\varepsilon + (v^0)^T (A'(t^0))^T \Delta u_\varepsilon\right) \\
&\quad + \frac{1}{2}\left((\delta u)^T Z(t^0) \Delta v_\tau + (v^0)^T (Z(t^0))^T \Delta u_\tau\right) + (u^0)^T Z'(t^0) v^0,
\end{aligned} \tag{A.21}$$

$$\begin{bmatrix}\Delta u_{\tau\varepsilon}\\ \Delta v_{\tau\varepsilon}\end{bmatrix} = -\mathcal{M}^+(t^0,s^0)\begin{bmatrix}A'(t^0)\Delta v_\varepsilon\\ (A'(t^0))^T\Delta u_\varepsilon\end{bmatrix} - \mathcal{M}^+(t^0,s^0)\begin{bmatrix}Z'(t^0)v^0\\ (Z'(t^0))^T u^0\end{bmatrix}$$
$$+\Delta s_\tau \mathcal{M}^+(t^0,s^0)\begin{bmatrix}\Delta u_\varepsilon\\ \Delta v_\varepsilon\end{bmatrix} + \Delta s_\varepsilon \mathcal{M}^+(t^0,s^0)\begin{bmatrix}\Delta u_\tau\\ \Delta v_\tau\end{bmatrix}$$
$$-\mathcal{M}^+(t^0,s^0)\begin{bmatrix}Z(t^0)\Delta v_\tau\\ (Z(t^0))^T\Delta u_\tau\end{bmatrix}, \tag{A.22}$$

$$\Delta s_{\varepsilon\varepsilon} = (u^0)^T Z(t^0)\Delta v_\varepsilon + (\Delta u_\varepsilon)^T Z(t^0) v^0, \tag{A.23}$$

$$\begin{bmatrix}\Delta u_{\varepsilon\varepsilon}\\ \Delta v_{\varepsilon\varepsilon}\end{bmatrix} = 2\Delta s_\varepsilon \mathcal{M}^+(t^0,s^0)\begin{bmatrix}\Delta u_\varepsilon\\ \Delta v_\varepsilon\end{bmatrix} - 2\mathcal{M}^+(t^0,s^0)\begin{bmatrix}Z(t^0)\Delta v_\varepsilon\\ (Z(t^0))^T\Delta u_\varepsilon\end{bmatrix}. \tag{A.24}$$

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