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APPLICATION OF THE SINGULAR VALUE DECOMPOSITION TO THE NUMERICAL COMPUTATION OF THE COEFFICIENTS OF AMPLITUDE EQUATIONS AND NORMAL FORMS

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The Fredholm alternative is a standard procedure by which one generates the coefficients of amplitude equations and normal forms. The alternative requires that the inhomogeneous terms in the underlying system of differential equations, which contain the unknown coefficients, be orthogonal to the independent eigenvectors spanning the null space of the adjoint system of differential equations. The numerical computation of the adjoint eigenvectors and their application to solvability is frequently difficult and inefficient. Typically the underlying system of the inhomogeneous differential equation is discretized and solved as an inhomogeneous matrix-valued eigenvalue problem. We find that the solvability conditions which lead to values of the unknown coefficients are conveniently and economically computed by application of the singular value decomposition directly to the matrix formulation, avoiding completely the computation of an adjoint system of differential equations.

1. Singular value decomposition

The singular value decomposition (SVD) is one of the most important decompositions in matrix algebra and is widely used for statistics and for solving least squares problems (see Businger and Golub [2], Golub and van Loan [5]). The decomposition theorem can be stated as follows: each and every $M \times N$ complex-valued matrix $\boldsymbol{T}$ can be reduced to diagonal form by unitary transformations $\boldsymbol{U}$ and $\boldsymbol{V}$,

$$\boldsymbol{T} = \boldsymbol{U}\,\mathrm{diag}[\sigma_1, \sigma_2, \ldots, \sigma_N]\,\boldsymbol{V}^H, \tag{1.1}$$

where $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_N \geqslant 0$ are real-valued scalars, called the singular values of $\boldsymbol{T}$. Here $\boldsymbol{U}$ is an $M \times N$ column orthonormal matrix, $\boldsymbol{V}$ an $N \times N$ unitary matrix and $\boldsymbol{V}^H$ is the Hermitian transpose of $\boldsymbol{V}$. The columns of $\boldsymbol{U}$ and $\boldsymbol{V}$ are called the left and right singular vectors of $\boldsymbol{T}$ respectively.

When $M = N$, $\boldsymbol{T}$ is a square matrix and

$$\boldsymbol{U}\boldsymbol{U}^H = \boldsymbol{U}^H\boldsymbol{U} = \boldsymbol{I}, \tag{1.2}$$

$$\boldsymbol{V}\boldsymbol{V}^H = \boldsymbol{V}^H\boldsymbol{V} = \boldsymbol{I}. \tag{1.3}$$

Consider the generalized matrix eigenvalue problem

$$(\boldsymbol{A} - c\boldsymbol{B})\boldsymbol{x} = 0, \tag{1.4}$$

where $\boldsymbol{A}$ and $\boldsymbol{B}$ are both square $N \times N$ complex matrices. Assume that c is a semisimple eigenvalue of (1.4) with algebraic and geometric multiplicity K. Then applying SVD to the matrix $\boldsymbol{A} - c\boldsymbol{B}$, we get

$$\boldsymbol{A} - c\boldsymbol{B} = \boldsymbol{U}\,\mathrm{diag}[\sigma_1, \sigma_2, \ldots, \sigma_{N-K}, 0, 0, \ldots, 0]\,\boldsymbol{V}^H, \tag{1.5}$$

where $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_{N-K} > 0$ are real constants [10]. Let

$$\boldsymbol{U} = [\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_{N-K}, \boldsymbol{u}_{N-K+1}, \ldots, \boldsymbol{u}_N], \tag{1.6}$$

$$\boldsymbol{V} = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_{N-K}, \boldsymbol{v}_{N-K+1}, \ldots, \boldsymbol{v}_N], \tag{1.7}$$

where $\boldsymbol{u}_j$ and $\boldsymbol{v}_j$, $j = 1, \ldots, N$, are the column vectors of matrices $\boldsymbol{U}$ and $\boldsymbol{V}$ respectively. From (1.4) and (1.5) we see that $\mathrm{diag}[\sigma_1, \sigma_2, \ldots, \sigma_{N-K}, 0, 0, \ldots, 0]\,\boldsymbol{y} = 0$, where $\boldsymbol{V}^H\boldsymbol{x} = \boldsymbol{y}$ and $\boldsymbol{x}$ is the eigenvector corresponding to the eigenvalue c. Therefore we have

$$\boldsymbol{V}^H\boldsymbol{x} = \boldsymbol{y} = [0, 0, \ldots, 0, y_{N-K+1}, \ldots, y_N], \tag{1.8}$$

where $y_{N-K+1}, \ldots, y_N$ are K arbitrary constants. Then $\boldsymbol{x} = \boldsymbol{V}\boldsymbol{y}$ is an eigenvector of $\boldsymbol{A} - c\boldsymbol{B}$. We find, in this way, that the column vectors $\boldsymbol{v}_j$, $j = N - K + 1, \ldots, N$, are the K independent eigenvectors corresponding to c, normalized with

$$\boldsymbol{v}_j^* \boldsymbol{v}_j^{\mathrm{T}} = 1, \quad j = N - K + 1, \ldots, N,$$

where superscript $*$ denotes the complex conjugate and superscript T transpose. Similarly the column vectors $\boldsymbol{u}_j$, $j = N - K + 1, \ldots, N$, are the K independent eigenvectors of the problem adjoint to (1.4):

$$(\boldsymbol{A} - c\boldsymbol{B})^H \boldsymbol{x} = 0. \tag{1.9}$$

They are the corresponding adjoint eigenvectors, normalized with

$$\boldsymbol{u}_j^* \boldsymbol{u}_j^{\mathrm{T}} = 1, \quad j = N - K + 1, \ldots, N.$$

The application of SVD to solve the inhomogeneous system of algebraic equations

$$(\boldsymbol{A} - c\boldsymbol{B})\boldsymbol{x} = \boldsymbol{f} \tag{1.10}$$

is straightforward. Suppose c is a semisimple eigenvalue of (1.4) of multiplicity K. We use SVD to decompose $\boldsymbol{A} - c\boldsymbol{B}$ in the form (1.5). We then compute

$$\mathrm{diag}[\sigma_1, \sigma_2, \ldots, \sigma_{N-K}, 0, 0, \ldots, 0]\,\boldsymbol{V}^H\boldsymbol{x} = \boldsymbol{U}^H\boldsymbol{f}. \tag{1.11}$$

The last K components of the vector on the left of (1.11) are identically zero and so must be those on the right. This defines the Fredholm alternative, the solvability conditions

$$\boldsymbol{u}_j^* \boldsymbol{f}^{\mathrm{T}} = 0, \quad j = N - K + 1, \ldots, N, \tag{1.12}$$

for the inhomogeneous matrix problem (1.10). The conditions (1.12) are necessary and sufficient for solvability of the inhomogeneous problem (1.10) in $\mathbb{C}$ when c is an eigenvalue of $\boldsymbol{A}$ relative to $\boldsymbol{B}$.

The solution to the inhomogeneous equation (1.10) is given by

$$\boldsymbol{x} = \boldsymbol{V}_{\mathrm{s}}\boldsymbol{g} + \sum_{j=N-K+1}^{N} \beta_j \boldsymbol{v}_j, \tag{1.13}$$

where the $N \times (N-K)$ matrix V_s is given by

$$V_s = [v_1, v_2, \ldots, v_{N-K}],$$

with $v_1, v_2, \ldots, v_{N-K}$ given by (1.7) and the vector g has $N-K$ components given by

$$g = [\sigma_1^{-1} u_1^* f^T, \sigma_2^{-1} u_2^* f^T, \ldots, \sigma_{N-K}^{-1} u_{N-K}^* f^T],$$

where the u_j are those given by (1.6). The β_j are constants and can be determined by K normalization conditions.

The solvability conditions (1.12) are easy to compute, if we remember that u_j, $j = N-K+1, \ldots, N$, are the corresponding K independent adjoint eigenvectors of (1.4). An efficient computer program for computing everything we need for the application of SVD to bifurcation problems is given in the paper by Businger and Golub [2], or one can use LINPACK routine CSVDC.

2. Applications to bifurcation theory

The problem is to find a numerical solution of

$$\mathscr{L}(c)\psi = f, \tag{2.1}$$

where f is a given vector depending on some unknown parameters, $\mathscr{L}(c)$ is a linear operator (think of a system of PDEs), c is a semisimple eigenvalue of multiplicity K and u is an eigenvector:

$$\mathscr{L}(c)u = 0. \tag{2.2}$$

We assume that the discretization of (2.1) and (2.2) leads to the matrix problems (1.10) and (1.4) respectively and then apply SVD.

There are various ways to compute bifurcating solutions, direct computation of steady or time-periodic bifurcating solutions or, more generally, the computation of amplitude equations, the normal forms which determine the dynamics of the bifurcating solutions. The bifurcation parameters and the coefficients for the amplitude equations can be determined by formulas expressing the requirements of the Fredholm alternative. These formulas involve many unit operations, explicit calculation of the adjoint, and integration over the flow domain of a multiplicative composition of eigenfunctions and adjoint eigenfunctions. These operations usually cannot be carried out analytically and numerical computations are necessary. For simple problems this procedure may not require too much work, but for new problems and complicated problems, like those which arise in two-fluid dynamics, this conventional procedure for enforcing solvability is a difficult and demanding one. For example, it took Blennerhassett [1] more than two pages just to write down the adjoint differential system and solvability condition. The conventional procedure works with the differential system explicitly, first deriving the analytic formulas, then discretizing them into matrix forms. The traditional method is mathematically beautiful, but not practical for numerical computations.

Increasingly, people who compute bifurcation numerically do not follow the conventional procedure. They work entirely in the matrix formulations generated by the initial discretization. SVD is a natural and practical method to carry out these numerical computations. The input needed to carry out this method is the matrix eigenvalue problem that we need to compute anyway, even using the traditional method. As far as we know, we are the first to apply SVD to the computation of bifurcation parameters, like the coefficients of the Ginzburg–Landau equation. A restricted application of SVD to numerical solution of bifurcation problems was made by Langford [6] who studied two-point boundary value problems. He proposed an algorithm converting a two-point boundary value problem to an initial value problem plus a best least squares problem, which is capable of handling a point of bifurcation. He solved the best least squares problem by applying SVD. However, the solvability condition was still enforced by evaluating a complicated integral involving the adjoint eigenvector.

We have been using SVD to compute the coefficients of the Ginzburg–Landau equation for the nonlinear evolution of interfacial waves arising from axisymmetric perturbations of core-annular flow of two fluids studied in the linearized case by Preziosi, Chen and Joseph [7] and Chen, Bai and Joseph [3]. We have applied SVD to the simpler problem of weakly nonlinear stability analysis of plane Poiseuille flow. Stewartson and Stuart [9] gave a heuristic derivation of the formulas required to compute coefficients of the Ginzburg–Landau equation. Their computations and all others used the theoretical formulas for the coefficients, requiring analytical followed by numerical computations of the adjoint and solvability conditions.

The conventional algorithm for computing is as follows:

Step 1. Derive the perturbation equations by analysis.

Step 2. Derive the adjoint eigenvalue problem by analysis. This is straightforward in the Stewartson–Stuart problem, but is very complicated for two-fluid problems.

Step 3. Form the solvability integrals expressing the Fredholm alternative by analysis. Certain constants are determined by these integrals.

Step 4. Discretize the eigenvalue problem. In the Stewartson–Stuart problem we must solve the eigenvalue problem for the Orr–Sommerfeld equation in the matrix form

$$(\boldsymbol{A} - c\boldsymbol{B})\psi_{11} = 0, \tag{2.3}$$

where $c = c_r + \mathrm{i}c_i$ is supposed to be a simple eigenvalue and $c_i = 0$ at criticality.

Step 5. Solve (2.3) for the eigenvalues. Find the critical eigenvalue, the marginally stable solution for which the largest eigenvalue has a growth rate $\sigma = -\mathrm{i}c_i\alpha = 0$, where α is a wave number.

Step 6. Solve (2.3) for the eigenvector ψ_{11} at criticality.

Step 7. Discretize the adjoint eigenvalue problem and compute the adjoint eigenvector.

Step 8. At first order we must invert the discretized problem at criticality

$$(\boldsymbol{A} - c_r\boldsymbol{B})\psi_{12} = \boldsymbol{f}(\psi_{11}, c_g), \tag{2.4}$$

where c_g is the group velocity at criticality.

Step 9. Evaluate c_g by carrying out a numerical integration of the solvability integral.

Step 10. Compute ψ_{12} by Gaussian elimination.

Step 11. Compute the mean flow distortion ψ_{02}, caused by the perturbation ψ_{11}.

Step 12. Compute the second harmonic ψ_{22}, generated by the fundamental mode.

Step 13. The Ginzburg–Landau equation, together with the coefficients, can be obtained by computing the solvability integrals for the inhomogeneous discretized problem

$$(\boldsymbol{A} - c_r\boldsymbol{B})\psi_{13} = \frac{\partial A}{\partial \tau} f_1 + \frac{\partial^2 A}{\partial \xi^2} f_2 + A f_3 + |A|^2 A f_4. \tag{2.5}$$

The solution procedure for SVD is much simpler, many steps are automatic and many are not needed. Steps 2, 3, 6, 7, 9, 10 and 13 may be omitted or are automatic.

In using SVD, we first do Steps 1 and 4, finding eigenvalues c and the critical eigenvalue $c = c_r$. Now we apply the SVD algorithm (1.5) to compute $\sigma_1, \sigma_2, \ldots, \sigma_{N-1}$, $\boldsymbol{U}$ and $\boldsymbol{V}$. We next invert (2.4) using SVD. We can find c_g automatically from (1.12). ψ_{12} is given automatically by (1.13). ψ_{02} and ψ_{22} can be computed by using Gaussian eliminations. Then we can get f_1, f_2, f_3, f_4 in (2.5). The Ginzburg–Landau coefficients may now be determined automatically again using (1.12).

It is clear from the above comparison that SVD is a neater procedure than the conventional one. It is completely self-contained and entirely numerical after Step 1. Since this procedure involves fewer numerical approximations we expect less roundoff errors. Apart from the increased efficiency and accuracy, the numerical recipes are standard and easy to implement, giving the method psychological as well as real advantages.

A further comparison of the conventional and SVD methods can be made in terms of the number of unit operations, the flop count for the matrix algorithms (see [5, Chapters 6, 7]). At the University of Minnesota, we typically use the QZ algorithm to solve matrix eigenvalue problems. The flop count for the QZ algorithm for solving (2.3) in Step 5 is

$$20N^3 + 13N^2,$$

where $\boldsymbol{A}$ and $\boldsymbol{B}$ are $N \times N$ matrices. The flop count for the SVD algorithm in (1.5) is $\frac{32}{3}N^3$. The total flop count for the computation of bifurcation parameters using SVD is about

$$\left(20 + \tfrac{32}{3}\right)N^3 + 13N^2.$$

For the conventional procedure, if the QZ algorithm is also used for the computation of the eigenvector and adjoint eigenvector, $2 \times (\frac{23}{2}N^3 + 8N^2)$ operations are needed. The solution of Step 10 by Gaussian elimination takes $\frac{1}{3}N^3$ operations. This gives a total flop count of

$$\left(43 + \tfrac{1}{3}\right)N^3 + 29N^2$$

for the conventional method, using QZ throughout, and it is much higher than using SVD.

The QZ algorithm for computing the eigenvectors when the eigenvalue is known is less efficient than the inverse iteration method, with a flop count about $\frac{2}{3}N^3$. The total flop count for the conventional method using QZ and inverse iteration is

$$\left(20 + \tfrac{5}{3}\right)N^3 + 13N^2,$$

lower than using SVD.

Our comparison of flop counts hugely underestimates the advantages of the self-contained, totally numerical method based on SVD.

In the application of SVD to the plane Poiseuille flow, we discretized the Orr–Sommerfeld equation by a pseudospectral Chebychev method with fifty collocation points. We compared our SVD calculation of the coefficients in the scaled Ginzburg–Landau equation

$$\frac{\partial A}{\partial \tau} - a_2 \frac{\partial^2 A}{\partial \xi^2} = \frac{d_1}{d_{1r}} A + \kappa |A|^2 A, \quad d_{1r} = \mathrm{Re}(d_1),$$

with values obtained by Reynolds and Potter [8] (RP) and Davey, Hocking and Stewartson [4] (DHS) using the conventional method. We note that the value a_2 was computed incorrectly by

Table 1
Comparison of the coefficients of the Ginzburg–Landau equation for plane Poiseuille flow ($\alpha_c = 1.02055$, $\mathscr{R}_c = 5772.22$)

	RP, DHS	Present
c_g	0.383	0.383098912
d_1	$(0.168 + i0.811)\ 10^{-5}$	$(0.1682592671 + i0.8112758976)\ 10^{-5}$
a_2	$0.187 + i0.0275$	$0.186701701 + i0.02746400111$
κ	$30.8 - i173$	$30.9434352 - i172.826053$

Stewartson and Stuart [9], and was later corrected by Davey, Hocking and Stewartson [4]. The comparison is displayed in Table 1.

3. Conclusion

The singular value decomposition appears to be the method of choice for the numerical computation of the coefficients in the amplitude equations which describe the slow evolution of bifurcating solution. It is straight forward, easy to implement, stable and reliable.

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