A sorting algorithm for complex eigenvalues

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Abstract

We present SPEC-RE, a new algorithm to sort complex eigenvalues, generated as the solutions to algebraic equations, whose coefficients are analytic functions of one or many, possibly complex parameters. The fact that the eigenvalues are analytic functions of the parameters, with atmost algebraic singularities, is used in formulating the algorithm. Several examples are presented to demonstrate the efficacy of the method; simple examples where other methods fail are also presented. The algorithm is likely to be useful in several problems of physics and engineering that require identification and sorting of eigenmodes.

1 Introduction

Linear stability analysis is ubiquitous in physics and engineering and basic to such analysis is computation of spectral maps i.e identifying eigenmodes as a function of the system parameters.

There are two broad approaches to producing such eigenmodes. The first one, which considers the parameter variations as perturbations and then computes the new eigenvalues as responses to these perturbations, has a long history dating back to Jacobi in the middle of the nineteenth century. Since then, a variety of methods like power methods and invariant subspace methods have been developed. A nice recent review of some of these methods is [6]. Starting with the original system eigenvalues, the various algorithms provide means to compute first-order eigenvalue sensitivities which are then used in a rapidly convergent iterative method to produce new eigenvalues corresponding to the parameter change. Some applications of this approach are [1], [5] and [11]. We call this the ‘tracing’ approach. Note that the eigenmodes are produced automatically in course of the tracing. The second approach is to solve the so-called dispersion relation (DR) for a range of parameter values and then to sort the already determined eigenvalues, at different values of the relevant parameter. Though this is mathematically simpler, it seems to have been explored relatively less; some publications, in fluid mechanics ([8], [10]) and electromagnetics ([2]) use this approach. We call this the ‘sorting’ approach. The ‘sorting’ approach is the approach to use if one is interested in identifying a few (typically 10-20) eigenmodes over a large range of parameter values for moderate sized matrix systems (typically $N < 5000$) whereas the ‘tracing’ approach has to be the preferred one if the goal is to generate very few (typically 1-2) eigenmodes for a limited range of parameter values, but for large matrix systems (typically $N > 5000$).

For real problems, the DR is rarely known in closed form; it exists as the outcome of a matrix eigenvalue problem and is only numerically known (NDR). Solution of such NDR is not really a problem; indeed fast and accurate numerical implementations (for example in LAPACK) exist and work well, in general. However, these algorithms only produce the eigenvalues for a given set of parameters; changing the parameters produces a new set of eigenvalues with no clarity on which of these eigenvalues belong together to say form a ‘mode’. 

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1 The terms ‘modal maps,’ ‘eigenvalue trajectories’ and ‘eigenpaths’ will also be used to denote these maps.
This would not be a major problem if the eigenvalues stay far apart and could be traced separately; this is in
general not the case because multiple roots are inevitable for such systems. In the neighbourhood of such roots,
the eigenvalue trajectories can tangle and cross and the task of determining which eigenvalue belongs to which
trajectory can become quite difficult.

The spectral maps for a given system are indispensable in solving initial / boundary value problems involving
that system. An understanding of the topography specified by these maps as signified by the knowledge of
critical points of the map like saddles and branch points is crucial to a correct solution of such problems. The
absence of a reliable method to sort the eigenmodes correctly has hampered a proper investigation of these
problems; for example, in the stability of fluid flows, very often only the least stable mode has been pursued
instead of a detailed study of the modal structure. The situation is described extensively in [10].

Crossing of the eigenvalue trajectories (equivalently collision of the eigenvalues) is the main obstacle in a
successful sorting of the eigenvalues. There are a variety of crossings that have been detailed in literature; we
describe some of these below (we use $\alpha$ and $\omega$ to denote the variable parameter and the eigenvalue respectively)
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1. False crossing C1. The trajectories, when plotted in the $\omega$ plane, appear to cross i.e. there exist points
in the $\omega$ plane such that $\omega_m(\alpha_l) = \omega_n(\alpha_k)$ with $\alpha_l \neq \alpha_k$. These are false crossings. In stability problems,
where the focus is often on the least stable mode, crossings in imaginary parts i.e. $\text{Im}[\omega_m(\alpha)] = \text{Im}[\omega_n(\alpha)]$
lead to ambiguous definition of various modes. However, unless the real parts also coincide at the same
$\alpha$, these are obviously false crossings.

2. True crossing. When the above mentioned $\alpha_l = \alpha_k$, we have a true crossing and the eigenvalues are
degenerate ([7]). However, there are two cases to distinguish -

   (a) The non-defective case C2. A full complement of eigenvectors exists i.e the geometric multiplicity of
the repeated eigenvalue equals its algebraic multiplicity.
   (b) The defective case C3. The geometric multiplicity is less than the algebraic multiplicity. A full
complement of independent eigenvectors does not exist and generalised eigenvectors have to be used
obtain a full complement. Two further subcases can be distinguished -

      i. The analytic case C3A. The eigenvalues are analytic functions of the parameter.
      ii. The non-analytic case C3B. The eigenvalues are non-analytic functions of the parameter; in
particular, they have branch points (BPs).

3. Avoided crossing C4. The eigenvalues come very close but do not actually collide. Avoided crossings can
be ‘broad’ or ‘sharp’; the latter case is the same as case C3B. Avoided crossings are of importance in
the study of chemical reaction mechanisms and in quantum mechanics, especially to an understanding of
quantum chaos.

Many approaches to sort eigenvalues exist in literature. We list some of these below -

1. Ascending / descending order of their real or imaginary parts (S1).
2. Absolute value (S2).
3. Nearest neighbour (S3).
4. A combination of nearest neighbouring eigenvalue and nearest neighbouring eigenvector (S4).

S1 is the simplest to use and is reliable if the eigenvalue trajectories are far apart. However, S1 fails even at false
crossings C1. Examples are given in [8] and [10] which consider stability problems in fluid mechanics. S2 and S3
negotiate the false crossings most of the time but can fail sometimes (for example when the crossing point is on
the real line) and at true crossings. S4, which is used in some of the Open Source subroutines (eigenshuffle.m,
eigenshuffle.py [2, 4]) is successful more widely but can fail at certain types of C3 crossings. We will provide
examples of these failures in Sec 3.
Figure 1: Schematic to explain mode sorting around a BP $\alpha_b$ by the algorithm SPEC-RE.

In this paper, we present a simple method to sort eigenmodes from eigenvalues that have been produced from an eigenvalue solver. The only assumption is that the dispersion relation is an analytic function of its parameters. The eigenvalues are sorted, based on their imaginary parts, at an initial point. From these, the neighbouring values of each mode are obtained by using the Cauchy – Riemann equations. This works in general because the eigenmodes are analytic and in particular at false collisions and true collisions of type C2 and C3A. Even though the C-R criterion cannot be employed at branch points (for e.g. a double root in the $\omega$ plane), the algorithm can still educe such critical points. The mode-sorting algorithm is explained in more detail in Sec. 2. We demonstrate the method on three problems in Sec. 3. We use the algorithm to sort the temporal even Orr-Sommerfeld (OS) modes that arise in a stability analysis of Couette flow in 3.1. In 3.2, we apply the algorithm to sort the jumbled eigenvalues in a model problem involving a cube-root branch point. Finally, we sort the eigenpaths of two low dimensional matrices in 3.3 and 3.4 and show how some currently available methods fail to produce the correct eigenpaths.

2 Mode sorting

2.1 The algorithm

SPEC-RE (Sorting Procedure for Eigenvalues based on Cauchy - Riemann Equations) is based on a well-known result of function theory for polynomials\(^2\) whose coefficients are analytic functions of a parameter. Thus, the eigenvalue $\omega_j$ is an analytic function of the complex wavenumber $\alpha$ except at isolated branch points. At any such point of analyticity $\alpha = \alpha_p$, the quantity

$$F = \left| \frac{\partial \text{Re}(\omega_j)}{\partial \alpha_r} - \frac{\partial \text{Im}(\omega_j)}{\partial \alpha_i} \right| + \left| \frac{\partial \text{Re}(\omega_j)}{\partial \alpha_i} + \frac{\partial \text{Im}(\omega_j)}{\partial \alpha_r} \right|$$

has to be negligible since Cauchy-Riemann conditions for analytic functions have to be satisfied. In what follows, this quantity $F(\omega_j; \alpha_p)$ is called the CR residue.

The primary task of SPEC-RE is to sort each eigenvalue of the spectrum from a given initial point in the $\alpha$ plane by minimization of the CR residue at the points of analyticity. The algorithm makes use of the negation of the CR criterion at the branch points rather than prescribing a ‘method’ to identify branch points. The primary feature of the algorithm, for analytic points, is described in 2.2; how the algorithm can educe non-analytic points like branch points is explained in 2.3 and 2.4.

2.2 Computation of analytic traces

The computational domain is a rectangular patch in the $\alpha$ plane with edges parallel to the axes. The grid points are equally spaced along both the axes; however, the grid size in these directions may be different. The sorting

\(^2\)This is often the case for physical problems.
\(^3\) The roots of such polynomials are then analytic functions of the same parameter with only algebraic singularities (p.64, [7]).
algorithm is implemented on a 4-point stencil of this grid (dashed line in figure 1(a)); at any given pivot point \( \alpha_{n,m} = (\alpha_r, \alpha_i) \) the stencil consists of the neighbouring points \( \alpha_{n-1,m} = (\alpha_r - \delta \alpha_r, \alpha_i) \), \( \alpha_{n+1,m} = (\alpha_r + \delta \alpha_r, \alpha_i) \) and \( \alpha_{n,m+1} = (\alpha_r, \alpha_i + \delta \alpha_i) \). Given a particular eigenvalue \( \omega_j \) at \( \alpha_{n,m} \), the algorithm is designed to pick one (and only one) of the eigenvalues from the spectrum at two neighbouring points \( \alpha_{n+1,m} \) and \( \alpha_{n,m+1} \) such that the CR condition at \( \alpha_{n,m} \) is satisfied. Equivalently, the relevant complex derivatives at \( \alpha_{n,m} \) must make the CR residue \( F \) to be negligible. In the numerical procedure, these derivatives are replaced by the central and forward differences

\[
\frac{\partial \omega_j}{\partial \alpha_r} = \frac{\omega_j(\alpha_{n+1,m}) - \omega_j(\alpha_{n-1,m})}{2 \delta \alpha_r}, \quad l = 1, 2, 3, ...
\]

\[
\frac{\partial \omega_j}{\partial \alpha_i} = \frac{\omega_k(\alpha_{n,m+1}) - \omega_j(\alpha_{n,m})}{i \delta \alpha_i}, \quad k = 1, 2, 3, ...
\]

The CR residue \( F(\omega_j; \alpha_{n,m}) \) is defined using these central-forward differences and is actually a set of numbers \( F_{lk}(\omega_j; \alpha_{n,m}); \ l = 1, 2, 3, ..., k = 1, 2, 3, ... \). The indices \( k_p \) and \( l_p \) that correspond to the minimum of these numbers for a given \( j \), which is expected to be a negligible quantity, are picked. As the analyticity condition for \( \omega_j \) at \( \alpha_{n,m} \) is numerically satisfied between \( \omega_j, \omega_{l_p} \) and \( \omega_{k_p} \), all three \( \omega \)'s belong to the same analytic function. In other words,

\[
\omega_j(\alpha_{n+1,m}) = \omega_{l_p}, \quad (a)
\]

\[
\omega_j(\alpha_{n,m+1}) = \omega_{k_p}. \quad (b)
\]

The pivot point can then be moved to one of the two adjacent points either in the horizontal direction or the vertical direction and the sorting procedure can be repeated for the new stencil. Hence, starting from an initial point \( \alpha_0 \), the sorting procedure picks one and only one value from the spectrum at each grid point and assigns it to the \( j \)-th collection so that an analytic function \( \omega_j(\alpha) \) is constructed, on the entire rectangular patch in the \( \alpha \)-plane.

2.3 Sweep direction

In a horizontal sweep, the pivot point \( \alpha_{n,m} \) moves along the direction of increasing \( Re(\alpha) \), keeping \( Im(\alpha) \) constant. After reaching the right-most point of the grid, the pivot point is moved to \( \alpha_{1,m+1} \). Further computations are performed on stencils containing \( \alpha_{n,m+1}, \alpha_{n+1,m+1} \) and \( \alpha_{n,m+2} \) starting from \( n = 1 \). It may be noted that the eigenvalues at this level have already been sorted from the computation at the \( m \)-th level, as shown in equation (b). Hence, using the eigenvalues at the \( m+1 \)-st level, either (i) \( \omega_j \) at the \( m+2 \)-nd level may be sorted, or (ii) re-sorting may be done afresh at the \( m+1 \)-st level. Method (ii) will not produce any new arrangement of eigenvalues at the \( m+1 \)-st level unless a branch point lies between the \( m \)-th and the \( m+1 \)-st levels. Eduction of a branch cut along the sweep direction (horizontal) by Method (ii) will be explained in the following subsection.

The sweep direction is not rigidly fixed. A vertical sweep, for instance, will produce a different modal map, with vertical branch cuts. One could indeed sweep even along any family of parametric curves; the C-R equations would then have to be satisfied in the appropriate coordinates.

2.4 Mode sorting around a branch point

Assume that there exists a branch point between \( \omega_j \) and \( \omega_{j+k} \) located in the box formed by the \( m \)-th, \( m+1 \)-st, \( n \)-th and \( n+1 \)-st lines as shown in figure 1 (i.e. \( \omega_j(\alpha) \) and \( \omega_{j+k}(\alpha) \) intersect at some \( \alpha_b \)). By design, the sorting algorithm produces an analytic \( \omega_j \) not only up to the \( m \)-th line, but also upto the point \( \alpha_{n+1,m+1} \) on the \( m+1 \)-st line. At the stencil formed by \( \alpha_{n+1,m}, \alpha_{n+2,m} \) and \( \alpha_{n+1,m+1} \), application of CR condition forces analyticity of \( \omega_j \) at both edges of the stencil and hence, does not allow the BC to cut the \( \alpha_{n+1,m} - \alpha_{n+1,m+1} \) edge. The forcing of analyticity on the lower and left edges of the box by the previous stencil leads to the BC cutting the \( \alpha_{n,m+1} - \alpha_{n+1,m+1} \) edge, as shown in figure 1(a). If further computations were to be done using Method (i) to sort eigenvalues at the \( m+2 \)-nd level, application of the CR condition for the stencil at \( \alpha_{n,m+1} \) will be erroneous due to the aforementioned non-analyticity at the \( \alpha_{n,m+1} - \alpha_{n+1,m+1} \) edge. By Method (ii),

\[\text{Re-sorting leads to a re-arrangement of the eigenvalues, but, the re-arrangement may be the same as the existing one.}\]
Figure 2: Temporal maps (Example 3.1) of the region $R = [0, 0.5] \times [0, 0.5]$ in the $\alpha$ plane. a) mode 1 b) mode 2 c) mode 3 d) mode 4. The red circles indicate starting points of the trajectories. ‘C’ and ‘D’ indicate cusps and double roots respectively.

$\omega_j$ values along that line are rearranged and analytic sorting between $\omega_j(\alpha_{n,m+1})$ and $\omega_j(\alpha_{n+1,m+1})$ is ensured. Analyticity along this edge forces non-analyticity of $\omega_j$ along the $\alpha_{n+1,m} - \alpha_{n+1,m+1}$ edge, which is equivalent to the BC being horizontal in that grid box as shown in figure 1(b). By continuation of the horizontal sweep at the $m+1$-st level, a horizontal BC evolves naturally. A vertical sweep, together with the application of Method (ii) in the vertical direction would produce a vertical BC. It should, in principle, be possible to modify the algorithm to obtain a branch cut along a suitable complex curve from the branch point by allowing non-analyticity at suitable edges of the stencils while sweeping. Such an improvement will be useful in situations when some points in the $\alpha-$plane are needed to be retained in an analytic region. However, it is not done here.

3 Results & Discussion

We now present some results obtained using SPEC-RE in a few problems. We start with a well-known problem from fluid mechanics.

3.1 Sorting of modes in a physical problem

The Orr - Sommerfeld (OS) equation is the basic equation of linear stability analysis of parallel shear flows and is given by

$$[i\alpha U(D^2 - k^2) - i\alpha D^2 U - \frac{1}{Re} (D^2 - k^2)^2]v = i\omega(D^2 - k^2)v$$

(1)

where $U(y)$ is the base streaming flow, $\alpha$ is the streamwise wavenumber, $k^2 = \alpha^2 + \beta^2$ where $\beta$ is the spanwise wavenumber, $D$ is differentiation wrt $y$, $Re$ is the Reynolds number and $\omega$ the frequency. $v$ is the normal perturbation velocity.
For a given $U(y)$, a Chebyshev discretisation of Eq.(1) results in a NDR which can then be solved for either $\alpha$ or $\omega$. We solve for $\omega$ and sort the temporal eigenvalues, into temporal eigenmodes for the Couette flow $U(y) = y, y \in [1-1,1], \beta = 0$ is assumed. We show in figure 2, the maps of the region $R = [0,0.5] \times [-0.5,0.5]$ (in the $\alpha$ plane) for the lowest four OS modes. The maps are analytic at almost all points, the only exceptional points being those at which branching occurs. It is easy to see that basing the sorting on the real or imaginary parts of $\omega$ will fail. Even other methods suggested in [10] fail, as detailed there (figure 1 of that paper), though this has not been shown here.

3.2 A model problem with a higher order branch point

The previous example elucidated square-root branch points. The sorting algorithm, in general, can also elucidate higher order branch points. In this section, the applicability of SPEC-RE around a cube root branch point is demonstrated. Here, the $\omega_j, j = 1, 2, 3$ are the three branches of the complex function (which can be thought as a factor in a characteristic polynomial) $f(z) = z^{1/3}$. The grid size is chosen as $(\delta\alpha, \delta\alpha) = (5e^{-4}, 5e^{-4})$. The three sets of $\omega$s are randomly jumbled at every point in the $\alpha$ plane, as shown in figure 3, and then read by the sorting program. The three sets of sorted values under a horizontal sweep are shown in different colors in figure 4.

3.3 2 × 2 normal and non-normal matrices

For the next example, we use two simple $2 \times 2$ matrices, given by

$$A_1 = \begin{bmatrix} \alpha & 0 \\ 0 & 1 - \alpha \end{bmatrix}, \quad A_2 = \begin{bmatrix} \alpha & 0 \\ \epsilon & 1 - \alpha \end{bmatrix},$$

where $\alpha \in [0,1]$ and $\epsilon$ is a fixed positive number. Note that $A_1$ is normal whereas $A_2$ is non-normal; they have the same eigenvalues $\omega_1 = \alpha$ and $\omega_2 = 1 - \alpha$ however. Sort $S_3$ fails to produce $\omega_1$ and $\omega_2$ for both $A_1$ and $A_2$. Sort $S_4$ produces the correct eigenpath for $A_1$ but fails for $A_2$. SPEC-RE produces the correct sort in both cases. The correct eigenpaths and the mis-sorted ones are shown in figure 5, for $\epsilon = 0.1$. $A_2$ has defective eigenvalues, and consequently a generalised eigenvector, at $\alpha = 0.5$; $S_4$ which makes use of both eigenvalue and eigenvector distance fails to sort correctly. In general, $S_4$ is expected to fail in such defective situations. This leads us to our last example involving a $5 \times 5$ matrix.
3.4 A $5 \times 5$ matrix with defective eigenvalues

Consider the $5 \times 5$ matrix whose non-zero elements are given by

\[
B(1, 1) = \alpha(1 + i) + \alpha^2, \quad B(2, 2) = \alpha(-\cos \theta_1 + i \sin \theta_1) + \alpha^2, \quad B(3, 3) = \alpha(-\cos \theta_2 + i \sin \theta_2) + \alpha^3,
\]

\[
B(4, 4) = \alpha(\cos \theta_3 - i \sin \theta_3) + \alpha^4, \quad B(5, 5) = \alpha(\cos \theta_4 + i \sin \theta_4) + \alpha^5,
\]

and $B(2, 1) = B(3, 2) = B(4, 3) = B(5, 4) = 0.1$.

$\theta_1 = 3\pi/20, \theta_2 = 11\pi/20, \theta_3 = 7\pi/20, \theta_4 = \pi/20$ and $B(i, i)$ have been chosen to produce a quintuple eigenvalue of 0 at $\alpha = 0, \alpha \in [-1, 1]$. The results of sorting by eigenshuffle and by the current algorithm SPEC-RE are shown in figure 6(a,b) respectively. The starting eigenvalues, for $\alpha = -1$ are marked with a star in fig 6(a) and the end eigenvalues, for $\alpha = 1$ are marked with a circle in fig 6(b). $S_4$ jumbles the eigenvalues at the defective point (fig 6(a)), so that the green curve continues as red, the blue as black, the black as magenta, the red as blue and finally the magenta as green. SPEC-RE maintains the correct eigenvalue positions for the entire $\alpha$ range (fig 6(b)).

The last two examples show how true crossings can be misinterpreted as avoided crossings (of the sharp kind) if the sorting is not proper. This could lead to a wrong inference of eigenstate exchange when none exists. In systems which allow both C3A and C3B type crossings, this could lead to misidentification of eigenmodes.
Figure 6: Eigenmodes of the $5 \times 5$ matrix $B$ of Example 3.4. The parameter $\alpha \in [-1, 1]$. Sorting scheme $S_4$ produces the eigenpaths in (a). Clearly, there is a mix-up of the modes beyond the quintuple root $\alpha = 0$. SPEC-RE produces the five correct eigenpaths in (b). The five eigenvalues at $\alpha = -1$ are marked with a star in (a) and at $\alpha = 1$ by a circle in (b).

Figure 7: Use of an L stencil in Example 3.4 results in missing eigenmodes beyond the quintuply degenerate eigenvalue at zero.

leading to wrong conclusions.

For the application of this algorithm, the initial sorting point should be a point where all eigenvalues are simple. The C-R equations involve first order derivatives in two directions; a numerical implementation could, in principle use finite differences of any order. For sorting at the point next to the initial one, we use a 3-point L stencil (forward differences in both directions) and 4-point T stencils (central difference in the sweep direction and forward in the other) for the subsequent grid points. The T stencil is found to be necessary as the L stencil can result in improper sorting under certain circumstances, for example, if a grid point corresponds to a multiple eigenvalue. In the latter case, the same mode can be picked multiple times since the mode is chosen based on the forward difference, which involves the multiple eigenvalue, at which grid point the modes are indistinguishable. A T stencil avoids this by including an upstream value as well, by using a central difference. Usage of an L stencil in Example 3.4 results in the wrong eigenmodes shown in figure 7.

4 Conclusion

An algorithm SPEC-RE, based on the analytic structure of the dispersion relation, has been devised to sort complex eigenvalues into modal families. The method makes full use of the fact that the eigenvalues are analytic functions of the parameters, something that the methods currently in existence do not. Collisions of
eigenvalues, whether false or true, are handled easily unlike say in [10]. The method can be easily extended to multi-parameter mode sorting, with the C-R criterion being applied with respect to one parameter at a time, with all other parameters kept fixed. Even generalised eigenvalue problems of polynomial type are amenable to this method because these can be transformed to linear eigenvalue problems which standard routines can solve. This algorithm can be even used to sort numbers that are not necessarily eigenvalues, as long as they are obtained by an analytic process, for e.g. they could be roots of a transcendental equation.

Acknowledgments

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