PSEUDOINVERSE FORMULATION OF RAYLEIGH-SCHRÖDINGER PERTURBATION THEORY FOR THE SYMMETRIC MATRIX EIGENVALUE PROBLEM

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Received 20 March 2003

A comprehensive treatment of Rayleigh-Schrödinger perturbation theory for the symmetric matrix eigenvalue problem is furnished with emphasis on the degenerate problem. The treatment is simply based upon the Moore-Penrose pseudoinverse thus distinguishing it from alternative approaches in the literature. In addition to providing a concise matrix-theoretic formulation of this procedure, it also provides for the explicit determination of that stage of the algorithm where each higher-order eigenvector correction becomes fully determined. The theory is built up gradually with each successive stage appended with an illustrative example.

1. Introduction

In Rayleigh's investigation of vibrating strings with mild longitudinal density variation [9], a perturbation procedure was developed based upon the known analytical solution for a string of constant density. This technique was subsequently refined by Schrödinger [11] and applied to problems in quantum mechanics where it has become a mainstay of mathematical physics.

Mathematically, we have a discretized Laplacian-type operator embodied in a real symmetric matrix A_0, which is subjected to a small symmetric linear perturbation $A = A_0 + \epsilon A_1$, due to some physical inhomogeneity. The Rayleigh-Schrödinger procedure produces approximations to the eigenvalues and eigenvectors of A by a sequence of successively higher-order corrections to the eigenvalues and eigenvectors of A_0.

Journal of Applied Mathematics 2003:9 (2003) 459–485
2000 Mathematics Subject Classification: 15A18, 65F15
URL: http://dx.doi.org/10.1155/S1110757X03303092

The difficulty with standard treatments of this procedure [1] is that the eigenvector corrections are expressed in a form requiring the complete collection of eigenvectors of A_0. For large matrices, this is clearly an undesirable state of affairs. Consideration of the thorny issue of multiple eigenvalues of A_0 [4] only serves to exacerbate this difficulty.

This malady can be remedied by expressing the Rayleigh-Schrödinger procedure in terms of the Moore-Penrose pseudoinverse [12]. This permits these corrections to be computed knowing only the eigenvectors of A_0 corresponding to the eigenvalues of interest. In point of fact, the pseudoinverse need not be explicitly calculated since only pseudoinverse-vector products are required. In turn, these may be efficiently calculated by a combination of LU-factorization and orthogonal projections. However, the formalism of the pseudoinverse provides a concise formulation of the procedure and permits ready analysis of theoretical properties of the algorithm.

Since the present paper is only concerned with real symmetric matrices, the existence of a complete set of orthonormal eigenvectors is assured [5, 8, 13]. The much more difficult case for defective matrices has been considered elsewhere [7]. Moreover, we only consider the computational aspects of this procedure. Existence of the relevant perturbation expansions has been rigorously established in [3, 6, 10].

2. Nondegenerate case

Consider the eigenvalue problem

$$Ax_i = \lambda_i x_i \quad (i = 1,\dots,n), \tag{2.1}$$

where A is a real, symmetric, $n \times n$ matrix with distinct eigenvalues λ_i $(i = 1,\dots,n)$ and, consequently, orthogonal eigenvectors x_i $(i = 1,\dots,n)$. Furthermore,

$$A(\epsilon) = A_0 + \epsilon A_1, \tag{2.2}$$

where A_0 is likewise real and symmetric but may possess multiple eigenvalues (called degeneracies in the physics literature). Any attempt to drop the assumption on the eigenstructure of A leads to a Rayleigh-Schrödinger iteration that never terminates [3, page 92]. In this section, we consider the nondegenerate case where the unperturbed eigenvalues $\lambda_i^{(0)}$ $(i = 1,\dots,n)$ are all distinct. Consideration of the degenerate case is deferred to the next section.

Under these assumptions, it is shown in [3, 6, 10] that the eigenvalues and eigenvectors of A possess the respective perturbation expansions

$$\lambda_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \lambda_i^{(k)}, \quad x_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k x_i^{(k)} \quad (i = 1, \dots, n) \tag{2.3}$$

for sufficiently small ϵ. Clearly, the zeroth-order terms $\{\lambda_i^{(0)}; x_i^{(0)}\}$ $(i = 1, \dots, n)$ are the eigenpairs of the unperturbed matrix A_0. That is,

$$(A_0 - \lambda_i^{(0)} I) x_i^{(0)} = 0 \quad (i = 1, \dots, n). \tag{2.4}$$

The unperturbed mutually orthogonal eigenvectors $x_i^{(0)}$ $(i = 1, \dots, n)$ are assumed to have been normalized to unity.

Substitution of (2.2) and (2.3) into (2.1) yields the recurrence relation

$$\begin{aligned}(A_0 - \lambda_i^{(0)} I) x_i^{(k)} &= -(A_1 - \lambda_i^{(1)} I) x_i^{(k-1)} \\ &\quad + \sum_{j=0}^{k-2} \lambda_i^{(k-j)} x_i^{(j)} \quad (k = 1, \dots, \infty;\ i = 1, \dots, n).\end{aligned} \tag{2.5}$$

For fixed i, solvability of (2.5) requires that its right-hand side be orthogonal to $\{x_l^{(0)}\}_{l=1}^{n}$ for all k. Thus, the value of $x_i^{(j)}$ determines $\lambda_i^{(j+1)}$. Specifically,

$$\lambda_i^{(j+1)} = \langle x_i^{(0)}, A_1 x_i^{(j)} \rangle, \tag{2.6}$$

where we have employed the so-called *intermediate normalization* that $x_i^{(k)}$ will be chosen to be orthogonal to $x_i^{(0)}$ for $k = 1, \dots, \infty$. This is equivalent to $\langle x_i^{(0)}, x_i(\epsilon) \rangle = 1$ and this normalization will be used throughout the remainder of this paper.

A beautiful result due to Dalgarno and Stewart [2], sometimes incorrectly attributed to Wigner in the physics literature, says that much more is true: the value of the eigenvector correction $x_i^{(j)}$, in fact, determines the eigenvalues through $\lambda_i^{(2j+1)}$. Within the present framework, this may be established by the following constructive procedure which heavily exploits the symmetry of A_0 and A_1.

We commence by observing that

$$\begin{aligned}\lambda_i^{(k)} &= \langle x_i^{(0)}, (A_1 - \lambda_i^{(1)} I) x_i^{(k-1)} \rangle = \langle x_i^{(k-1)}, (A_1 - \lambda_i^{(1)} I) x_i^{(0)} \rangle \\ &= -\langle x_i^{(k-1)}, (A_0 - \lambda_i^{(0)} I) x_i^{(1)} \rangle = -\langle x_i^{(1)}, (A_0 - \lambda_i^{(0)} I) x_i^{(k-1)} \rangle \\ &= \langle x_i^{(1)}, (A_1 - \lambda_i^{(1)} I) x_i^{(k-2)} \rangle - \sum_{l=2}^{k-1} \lambda_i^{(l)} \langle x_i^{(1)}, x_i^{(k-1-l)} \rangle .\end{aligned} \tag{2.7}$$

Continuing in this fashion, we eventually arrive at, for even $k = 2j$,

$$\begin{aligned}\lambda_i^{(2j)} = {} & \langle x_i^{(j-1)}, (A_1 - \lambda_i^{(1)} I) x_i^{(j)} \rangle - \sum_{\mu=2}^{j-1} \lambda_i^{(\mu)} \sum_{\nu=j-\mu+1}^{j} \langle x_i^{(2j-\mu-\nu)}, x_i^{(\nu)} \rangle \\ & - \sum_{\mu=j}^{2j-2} \lambda_i^{(\mu)} \sum_{\nu=1}^{2j-\mu-1} \langle x_i^{(2j-\mu-\nu)}, x_i^{(\nu)} \rangle ,\end{aligned} \tag{2.8}$$

while, for odd $k = 2j+1$,

$$\begin{aligned}\lambda_i^{(2j+1)} = {} & \langle x_i^{(j)}, (A_1 - \lambda_i^{(1)} I) x_i^{(j)} \rangle - \sum_{\mu=2}^{j-1} \lambda_i^{(\mu)} \sum_{\nu=j-\mu+1}^{j} \langle x_i^{(2j-\mu-\nu+1)}, x_i^{(\nu)} \rangle \\ & - \sum_{\mu=j}^{2j-1} \lambda_i^{(\mu)} \sum_{\nu=1}^{2j-\mu} \langle x_i^{(2j-\mu-\nu+1)}, x_i^{(\nu)} \rangle .\end{aligned} \tag{2.9}$$

This important pair of equations will henceforth be referred to as the *Dalgarno-Stewart identities*.

The eigenfunction corrections are determined recursively from (2.5) as

$$x_i^{(k)} = (A_0 - \lambda_i^{(0)} I)^{\dagger} \left[-(A_1 - \lambda_i^{(1)} I) x_i^{(k-1)} + \sum_{j=0}^{k-2} \lambda_i^{(k-j)} x_i^{(j)} \right] \\ (k = 1, \ldots, \infty;\ i = 1, \ldots, n), \tag{2.10}$$

where $(A_0 - \lambda_i^{(0)} I)^{\dagger}$ denotes the Moore-Penrose pseudoinverse [12] of $(A_0 - \lambda_i^{(0)} I)$ and intermediate normalization has been employed.

Example 2.1. Define

$$A_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix}, \qquad A_1 = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}. \tag{2.11}$$

Using Matlab's Symbolic Toolbox, we find that

$$\begin{aligned}
\lambda_1(\epsilon) &= 1 - \frac{1}{2}\epsilon^2 - \frac{1}{8}\epsilon^3 + \frac{1}{4}\epsilon^4 + \frac{25}{128}\epsilon^5 + \cdots, \\
\lambda_2(\epsilon) &= 1 + 2\epsilon - \frac{1}{2}\epsilon^2 - \frac{7}{8}\epsilon^3 - \frac{5}{4}\epsilon^4 - \frac{153}{128}\epsilon^5 + \cdots, \\
\lambda_3(\epsilon) &= 2 + \epsilon^2 + \epsilon^3 + \epsilon^4 + \epsilon^5 + \cdots .
\end{aligned} \tag{2.12}$$

Applying the nondegenerate Rayleigh-Schrödinger procedure developed above to

$$\lambda_3^{(0)} = 2, \qquad x_3^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \tag{2.13}$$

we arrive at

$$\lambda_3^{(1)} = \langle x_3^{(0)}, A_1 x_3^{(0)} \rangle = 0. \tag{2.14}$$

Solving

$$(A_0 - \lambda_3^{(0)} I) x_3^{(1)} = -(A_1 - \lambda_3^{(1)} I) x_3^{(0)} \tag{2.15}$$

produces

$$x_3^{(1)} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}. \tag{2.16}$$

In turn, this produces

$$\lambda_3^{(2)} = \langle x_3^{(0)}, A_1 x_3^{(1)} \rangle = 1, \tag{2.17}$$

while the Dalgarno-Stewart identities yield

$$\lambda_3^{(3)} = \langle x_3^{(1)}, (A_1 - \lambda_3^{(1)} I) x_3^{(1)} \rangle = 1. \tag{2.18}$$

Solving

$$(A_0 - \lambda_3^{(0)} I) x_3^{(2)} = -(A_1 - \lambda_3^{(1)} I) x_3^{(1)} + \lambda_3^{(2)} x_3^{(0)} \tag{2.19}$$

produces

$$x_3^{(2)} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}. \tag{2.20}$$

Again, the Dalgarno-Stewart identities yield

$$\begin{aligned} \lambda_3^{(4)} &= \langle x_3^{(1)}, (A_1 - \lambda_3^{(1)} I) x_3^{(2)} \rangle - \lambda_3^{(2)} \langle x_3^{(1)}, x_3^{(1)} \rangle = 1, \\ \lambda_3^{(5)} &= \langle x_3^{(2)}, (A_1 - \lambda_3^{(1)} I) x_3^{(2)} \rangle - 2\lambda_3^{(2)} \langle x_3^{(2)}, x_3^{(1)} \rangle - \lambda_3^{(3)} \langle x_3^{(1)}, x_3^{(1)} \rangle = 1. \end{aligned} \tag{2.21}$$

3. Degenerate case

When A_0 possesses multiple eigenvalues (the so-called degenerate case), the above straightforward analysis for the nondegenerate case encounters serious complications. This is a consequence of the fact that, in this new case, Rellich's theorem [10, pages 42–45] guarantees the existence of the perturbation expansions (2.3) only for certain special unperturbed eigenvectors. These special unperturbed eigenvectors cannot be specified a priori but must instead emerge from the perturbation procedure itself.

Furthermore, the higher-order corrections to these special unperturbed eigenvectors are more stringently constrained than previously since they must be chosen so that (2.5) is always solvable. That is, they must be chosen so that the right-hand side of (2.5) is always orthogonal to the entire eigenspace associated with the multiple eigenvalue in question.

Thus, without any loss of generality, suppose that $\lambda_1^{(0)} = \lambda_2^{(0)} = \cdots = \lambda_m^{(0)} = \lambda^{(0)}$ is just such an eigenvalue of multiplicity m with corresponding known orthonormal eigenvectors $x_1^{(0)}, x_2^{(0)}, \ldots, x_m^{(0)}$. Then, we are required to determine appropriate linear combinations

$$y_i^{(0)} = a_1^{(i)} x_1^{(0)} + a_2^{(i)} x_2^{(0)} + \cdots + a_m^{(i)} x_m^{(0)} \quad (i = 1, \ldots, m) \tag{3.1}$$

so that the expansions (2.3) are valid with $x_i^{(k)}$ replaced by $y_i^{(k)}$. In point of fact, the remainder of this paper will assume that x_i has been replaced by y_i in (2.3)–(2.10). Moreover, the higher-order eigenvector corrections $y_i^{(k)}$ must be suitably determined. Since we would like $\{y_i^{(0)}\}_{i=1}^m$ to be likewise orthonormal, we require that

$$a_1^{(\mu)} a_1^{(\nu)} + a_2^{(\mu)} a_2^{(\nu)} + \cdots + a_m^{(\mu)} a_m^{(\nu)} = \delta_{\mu,\nu}. \tag{3.2}$$

Recall that we have assumed throughout that the perturbed matrix $A(\epsilon)$ itself has distinct eigenvalues, so that eventually all such degeneracies will be fully resolved. What significantly complicates matters is that it is not known beforehand at what stages portions of the degeneracy will be resolved.

In order to bring order to a potentially calamitous situation, we will first begin by considering the case where the degeneracy is fully resolved at first order. Only then do we move on to study the case where the degeneracy is completely and simultaneously resolved at second order. This will pave the way for the treatment of Nth order degeneracy resolution. Finally, we will have laid sufficient groundwork to permit treatment of the most general case of mixed degeneracy where resolution occurs across several different orders. Each stage in this process will be concluded with an illustrative example. This seems preferable to presenting an impenetrable collection of opaque formulae.

3.1. First-order degeneracy

We first dispense with the case of first-order degeneracy wherein $\lambda_i^{(1)}$ $(i = 1,\ldots,m)$ are all distinct. In this event, we determine $\{\lambda_i^{(1)}; y_i^{(0)}\}_{i=1}^m$ by insisting that (2.5) be solvable for $k = 1$ and $i = 1,\ldots,m$. In order for this to obtain, it is both necessary and sufficient that, for each fixed i,

$$\langle x_\mu^{(0)}, (A_1 - \lambda_i^{(1)} I) y_i^{(0)} \rangle = 0 \quad (\mu = 1,\ldots,m). \tag{3.3}$$

Inserting (3.1) and invoking the orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, A_1 x_1^{(0)} \rangle & \cdots & \langle x_1^{(0)}, A_1 x_m^{(0)} \rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, A_1 x_1^{(0)} \rangle & \cdots & \langle x_m^{(0)}, A_1 x_m^{(0)} \rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(1)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}. \tag{3.4}$$

Thus, each $\lambda_i^{(1)}$ is an eigenvalue with corresponding eigenvector $[a_1^{(i)},\ldots, a_m^{(i)}]^T$ of the matrix M defined by $M_{\mu,\nu} = \langle x_\mu^{(0)}, M^{(1)} x_\nu^{(0)} \rangle$ $(\mu,\nu = 1,\ldots,m)$, where $M^{(1)} := A_1$.

By assumption, the symmetric matrix M has m distinct real eigenvalues and hence orthonormal eigenvectors described by (3.2). These, in turn, may be used in concert with (3.1) to yield the desired special unperturbed eigenvectors alluded to above.

Now that $\{y_i^{(0)}\}_{i=1}^m$ are fully determined, we have by (2.6) the identities

$$\lambda_i^{(1)} = \langle y_i^{(0)}, A_1 y_i^{(0)} \rangle \quad (i = 1,\ldots,m). \tag{3.5}$$

Furthermore, the combination of (3.2) and (3.4) yields

$$\langle y_i^{(0)}, A_1 y_j^{(0)} \rangle = 0 \quad (i \neq j). \tag{3.6}$$

The remaining eigenvalue corrections $\lambda_i^{(k)}$ $(k \geq 2)$ may be obtained from the Dalgarno-Stewart identities.

Whenever (2.5) is solvable, we will express its solution as

$$y_i^{(k)} = \hat{y}_i^{(k)} + \beta_{1,k}^{(i)} y_1^{(0)} + \beta_{2,k}^{(i)} y_2^{(0)} + \cdots + \beta_{m,k}^{(i)} y_m^{(0)} \quad (i = 1, \ldots, m), \tag{3.7}$$

where $\hat{y}_i^{(k)} := (A_0 - \lambda^{(0)} I)^{\dagger}[-(A_1 - \lambda_i^{(1)} I) y_i^{(k-1)} + \sum_{j=0}^{k-2} \lambda_i^{(k-j)} y_i^{(j)}]$ has no components in the $\{y_j^{(0)}\}_{j=1}^{m}$ directions. In the light of intermediate normalization, we have $\beta_{i,k}^{(i)} = 0$ $(i = 1, \ldots, m)$. Furthermore, $\beta_{j,k}^{(i)}$ $(i \neq j)$ are to be determined from the condition that (2.5) be solvable for $k \leftarrow k+1$ and $i = 1, \ldots, m$.

Since, by design, (2.5) is solvable for $k = 1$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = \frac{\langle y_j^{(0)}, A_1 \hat{y}_i^{(k)} \rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+1)} \beta_{j,l}^{(i)}}{\lambda_i^{(1)} - \lambda_j^{(1)}} \quad (i \neq j). \tag{3.8}$$

The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of (2.5) for $k \leftarrow k+1$.

Example 3.1. We resume with Example 2.1 and the first-order degeneracy between $\lambda_1^{(0)}$ and $\lambda_2^{(0)}$. With the choice

$$x_1^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \qquad x_2^{(0)} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \tag{3.9}$$

we have

$$M = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \tag{3.10}$$

with eigenpairs

$$\lambda_1^{(1)} = 0, \quad \begin{bmatrix} a_1^{(1)} \\ a_2^{(1)} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}, \qquad \lambda_2^{(1)} = 2, \quad \begin{bmatrix} a_1^{(2)} \\ a_2^{(2)} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}. \tag{3.11}$$

Availing ourselves of (3.1), the special unperturbed eigenvectors are now fully determined as

$$y_1^{(0)} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}, \qquad y_2^{(0)} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \end{bmatrix}. \tag{3.12}$$

Solving (2.5), for $k = 1$,

$$(A_0 - \lambda^{(0)} I) y_i^{(1)} = -(A_1 - \lambda_i^{(1)} I) y_i^{(0)} \quad (i = 1, 2), \tag{3.13}$$

produces

$$y_1^{(1)} = \begin{bmatrix} a \\ a \\ -\frac{1}{\sqrt{2}} \end{bmatrix}, \qquad y_2^{(1)} = \begin{bmatrix} b \\ -b \\ -\frac{1}{\sqrt{2}} \end{bmatrix}, \tag{3.14}$$

where we have invoked intermediate normalization. Observe that, unlike the nondegenerate case, $y_i^{(1)}$ $(i = 1, 2)$ are not yet fully determined.

We next enforce solvability of (2.5) for $k = 2$:

$$\langle y_j^{(0)}, -(A_1 - \lambda_i^{(1)} I) y_i^{(1)} + \lambda_i^{(2)} y_i^{(0)} \rangle = 0 \quad (i \neq j), \tag{3.15}$$

thereby producing

$$y_1^{(1)} = \begin{bmatrix} \frac{1}{4\sqrt{2}} \\ \frac{1}{4\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}, \qquad y_2^{(1)} = \begin{bmatrix} -\frac{1}{4\sqrt{2}} \\ \frac{1}{4\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}. \tag{3.16}$$

With $y_i^{(1)}$ $(i = 1, 2)$ now fully determined, the Dalgarno-Stewart identities yield

$$\begin{aligned} \lambda_1^{(2)} &= \langle y_1^{(0)}, A_1 y_1^{(1)} \rangle = -\frac{1}{2}; \qquad & \lambda_1^{(3)} &= \langle y_1^{(1)}, (A_1 - \lambda_1^{(1)} I) y_1^{(1)} \rangle = -\frac{1}{8}, \\ \lambda_2^{(2)} &= \langle y_2^{(0)}, A_1 y_2^{(1)} \rangle = -\frac{1}{2}; \qquad & \lambda_2^{(3)} &= \langle y_2^{(1)}, (A_1 - \lambda_2^{(1)} I) y_2^{(1)} \rangle = -\frac{7}{8}. \end{aligned} \tag{3.17}$$

Solving (2.5), for $k=2$,

$$(A_0-\lambda^{(0)}I)y_i^{(2)}=-(A_1-\lambda_i^{(1)}I)y_i^{(1)}+\lambda_i^{(2)}y_i^{(0)}\quad(i=1,2),\tag{3.18}$$

produces

$$y_1^{(2)}=\begin{bmatrix}c\\c\\-\frac{1}{4\sqrt{2}}\end{bmatrix},\qquad y_2^{(2)}=\begin{bmatrix}d\\-d\\-\frac{7}{4\sqrt{2}}\end{bmatrix},\tag{3.19}$$

where we have again invoked intermediate normalization. Once again observe that, unlike the nondegenerate case, $y_i^{(2)}$ $(i=1,2)$ are not yet fully determined.

We now enforce solvability of (2.5) for $k=3$:

$$\langle y_j^{(0)},-(A_1-\lambda_i^{(1)}I)y_i^{(2)}+\lambda_i^{(2)}y_i^{(1)}+\lambda_i^{(3)}y_i^{(0)}\rangle=0\quad(i\neq j),\tag{3.20}$$

thereby fully determining

$$y_1^{(2)}=\begin{bmatrix}0\\0\\-\frac{1}{4\sqrt{2}}\end{bmatrix},\qquad y_2^{(2)}=\begin{bmatrix}-\frac{1}{2\sqrt{2}}\\\frac{1}{2\sqrt{2}}\\-\frac{7}{4\sqrt{2}}\end{bmatrix}.\tag{3.21}$$

Subsequent application of the Dalgarno-Stewart identities yields

$$\begin{aligned}
\lambda_1^{(4)}&=\langle y_1^{(1)},(A_1-\lambda_1^{(1)}I)y_1^{(2)}\rangle-\lambda_1^{(2)}\langle y_1^{(1)},y_1^{(1)}\rangle=\frac{1}{4},\\
\lambda_1^{(5)}&=\langle y_1^{(2)},(A_1-\lambda_1^{(1)}I)y_1^{(2)}\rangle-2\lambda_1^{(2)}\langle y_1^{(2)},y_1^{(1)}\rangle-\lambda_1^{(3)}\langle y_1^{(1)},y_1^{(1)}\rangle=\frac{25}{128},\\
\lambda_2^{(4)}&=\langle y_2^{(1)},(A_1-\lambda_2^{(1)}I)y_2^{(2)}\rangle-\lambda_2^{(2)}\langle y_2^{(1)},y_2^{(1)}\rangle=-\frac{5}{4},\\
\lambda_2^{(5)}&=\langle y_2^{(2)},(A_1-\lambda_2^{(1)}I)y_2^{(2)}\rangle-2\lambda_2^{(2)}\langle y_2^{(2)},y_2^{(1)}\rangle-\lambda_2^{(3)}\langle y_2^{(1)},y_2^{(1)}\rangle=-\frac{153}{128}.
\end{aligned}\tag{3.22}$$

3.2. Second-order degeneracy

We next consider the case of second-order degeneracy which is characterized by the conditions $\lambda_1^{(0)}=\lambda_2^{(0)}=\cdots=\lambda_m^{(0)}=\lambda^{(0)}$ and $\lambda_1^{(1)}=\lambda_2^{(1)}=\cdots=\lambda_m^{(1)}=\lambda^{(1)}$, while $\lambda_i^{(2)}$ $(i=1,\dots,m)$ are all distinct. Thus, even though $\lambda^{(1)}$

is obtained as the only eigenvalue of (3.4), $\{y_i^{(0)}\}_{i=1}^m$ are still indeterminate after enforcing solvability of (2.5) for $k=1$.

Hence, we will determine $\{\lambda_i^{(2)}; y_i^{(0)}\}_{i=1}^m$ by insisting that (2.5) be solvable for $k=2$ and $i=1,\dots,m$. This requirement is equivalent to the condition that, for each fixed i,

$$\langle x_\mu^{(0)}, -(A_1-\lambda^{(1)}I)y_i^{(1)}+\lambda_i^{(2)}y_i^{(0)}\rangle = 0 \quad (\mu=1,\dots,m). \tag{3.23}$$

Inserting (3.1) as well as (3.7) with $k=1$ and invoking the orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, M^{(2)}x_1^{(0)}\rangle & \cdots & \langle x_1^{(0)}, M^{(2)}x_m^{(0)}\rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, M^{(2)}x_1^{(0)}\rangle & \cdots & \langle x_m^{(0)}, M^{(2)}x_m^{(0)}\rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(2)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}, \tag{3.24}$$

where $M^{(2)} := -(A_1-\lambda^{(1)}I)(A_0-\lambda^{(0)}I)^\dagger(A_1-\lambda^{(1)}I)$. Thus, each $\lambda_i^{(2)}$ is an eigenvalue with corresponding eigenvector $[a_1^{(i)},\dots,a_m^{(i)}]^T$ of the matrix M defined by $M_{\mu,\nu}=\langle x_\mu^{(0)}, M^{(2)}x_\nu^{(0)}\rangle$ $(\mu,\nu=1,\dots,m)$.

By assumption, the symmetric matrix M has m distinct real eigenvalues and hence orthonormal eigenvectors described by (3.2). These, in turn, may be used in concert with (3.1) to yield the desired special unperturbed eigenvectors alluded to above.

Now that $\{y_i^{(0)}\}_{i=1}^m$ are fully determined, we have by the combination of (3.2) and (3.24) the identities

$$\langle y_i^{(0)}, M^{(2)}y_j^{(0)}\rangle = \lambda_i^{(2)}\cdot\delta_{i,j}. \tag{3.25}$$

The remaining eigenvalue corrections $\lambda_i^{(k)}$ $(k\geq 3)$ may be obtained from the Dalgarno-Stewart identities.

Analogous to the case of first-order degeneracy, $\beta_{j,k}^{(i)}$ $(i\neq j)$ of (3.7) are to be determined from the condition that (2.5) be solvable for $k\leftarrow k+2$ and $i=1,\dots,m$. Since, by design, (2.5) is solvable for $k=1,2$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = \frac{\langle y_j^{(0)}, M^{(2)}\hat{y}_i^{(k)}\rangle - \sum_{l=1}^{k-1}\lambda_i^{(k-l+2)}\beta_{j,l}^{(i)}}{\lambda_i^{(2)}-\lambda_j^{(2)}} \quad (i\neq j). \tag{3.26}$$

The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of (2.5) for $k \leftarrow k+2$.

Example 3.2. Define

$$A_0 = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 & 3 \end{bmatrix}, \qquad A_1 = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \end{bmatrix}. \tag{3.27}$$

Using Matlab's Symbolic Toolbox, we find that

$$\begin{aligned} \lambda_1(\epsilon) &= 1 + \epsilon, \\ \lambda_2(\epsilon) &= 1 + \epsilon - \frac{1}{2}\epsilon^2 - \frac{1}{4}\epsilon^3 + \frac{1}{8}\epsilon^5 + \cdots, \\ \lambda_3(\epsilon) &= 1 + \epsilon - \epsilon^2 - \epsilon^3 + 2\epsilon^5 + \cdots, \\ \lambda_4(\epsilon) &= 2 + \epsilon^2 + \epsilon^3 - 2\epsilon^5 + \cdots, \\ \lambda_5(\epsilon) &= 3 + \frac{1}{2}\epsilon^2 + \frac{1}{4}\epsilon^3 - \frac{1}{8}\epsilon^5 + \cdots. \end{aligned} \tag{3.28}$$

We focus on the second-order degeneracy amongst $\lambda_1^{(0)} = \lambda_2^{(0)} = \lambda_3^{(0)} = \lambda^{(0)} = 1$. With the choice

$$x_1^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \qquad x_2^{(0)} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \qquad x_3^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \tag{3.29}$$

we have from (3.4), which enforces solvability of (2.5) for $k = 1$,

$$M = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{3.30}$$

with triple eigenvalue $\lambda^{(1)} = 1$.

Moving on to (3.24), which enforces solvability of (2.5) for $k = 2$, we have

$$M = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{3.31}$$

with eigenpairs

$$\lambda_1^{(2)} = 0, \quad \begin{bmatrix} a_1^{(1)} \\ a_2^{(1)} \\ a_3^{(1)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix};$$
$$\lambda_2^{(2)} = -\frac{1}{2}, \quad \begin{bmatrix} a_1^{(2)} \\ a_2^{(2)} \\ a_3^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}; \tag{3.32}$$
$$\lambda_3^{(2)} = -1, \quad \begin{bmatrix} a_1^{(3)} \\ a_2^{(3)} \\ a_3^{(3)} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}.$$

Availing ourselves of (3.1), the special unperturbed eigenvectors are now fully determined as

$$y_1^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \quad y_2^{(0)} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad y_3^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}. \tag{3.33}$$

Solving (2.5), for $k = 1$,

$$(A_0 - \lambda^{(0)} I) y_i^{(1)} = -(A_1 - \lambda^{(1)} I) y_i^{(0)} \quad (i = 1,2,3), \tag{3.34}$$

produces

$$y_1^{(1)} = \begin{bmatrix} \alpha_1 \\ \beta_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \quad y_2^{(1)} = \begin{bmatrix} \alpha_2 \\ 0 \\ \gamma_2 \\ 0 \\ -\frac{1}{2} \end{bmatrix}, \quad y_3^{(1)} = \begin{bmatrix} 0 \\ \beta_3 \\ \gamma_3 \\ -1 \\ 0 \end{bmatrix}, \tag{3.35}$$

where we have invoked intermediate normalization. Observe that $y_i^{(1)}$ $(i = 1,2,3)$ are not yet fully determined.

Solving (2.5), for $k = 2$,

$$(A_0 - \lambda^{(0)} I) y_i^{(2)} = -(A_1 - \lambda^{(1)} I) y_i^{(1)} + \lambda_i^{(2)} y_i^{(0)} \quad (i = 1,2,3), \tag{3.36}$$

produces

$$y_1^{(2)} = \begin{bmatrix} a_1 \\ b_1 \\ 0 \\ -\alpha_1 \\ -\frac{\beta_1}{2} \end{bmatrix}, \qquad y_2^{(2)} = \begin{bmatrix} a_2 \\ 0 \\ c_2 \\ -\alpha_2 \\ -\frac{1}{4} \end{bmatrix}, \qquad y_3^{(2)} = \begin{bmatrix} 0 \\ b_3 \\ c_3 \\ -1 \\ -\frac{\beta_3}{2} \end{bmatrix}, \tag{3.37}$$

where we have invoked intermediate normalization. Likewise, $y_i^{(2)}$ ($i = 1,2,3$) are not yet fully determined.

We next enforce solvability of (2.5) for $k = 3$:

$$\langle y_j^{(0)}, -(A_1 - \lambda^{(1)} I) y_i^{(2)} + \lambda_i^{(2)} y_i^{(1)} + \lambda_i^{(3)} y_i^{(0)} \rangle = 0 \quad (i \neq j), \tag{3.38}$$

thereby producing

$$\begin{gathered} y_1^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \qquad y_2^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -\frac{1}{2} \end{bmatrix}; \qquad y_3^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0 \end{bmatrix}, \\ y_1^{(2)} = \begin{bmatrix} a_1 \\ b_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \qquad y_2^{(2)} = \begin{bmatrix} a_2 \\ 0 \\ c_2 \\ 0 \\ -\frac{1}{4} \end{bmatrix}; \qquad y_3^{(2)} = \begin{bmatrix} 0 \\ b_3 \\ c_3 \\ -1 \\ 0 \end{bmatrix}. \end{gathered} \tag{3.39}$$

With $y_i^{(1)}$ ($i = 1,2,3$) now fully determined, the Dalgarno-Stewart identities yield

$$\begin{aligned} \lambda_1^{(3)} &= \langle y_1^{(1)}, (A_1 - \lambda^{(1)} I) y_1^{(1)} \rangle = 0, \\ \lambda_2^{(3)} &= \langle y_2^{(1)}, (A_1 - \lambda^{(1)} I) y_2^{(1)} \rangle = -\frac{1}{4}, \\ \lambda_3^{(3)} &= \langle y_3^{(1)}, (A_1 - \lambda^{(1)} I) y_3^{(1)} \rangle = -1. \end{aligned} \tag{3.40}$$

Solving (2.5), for $k = 3$,

$$\begin{aligned} (A_0 - \lambda^{(0)} I) y_i^{(3)} = &-(A_1 - \lambda^{(1)} I) y_i^{(2)} \\ &+ \lambda_i^{(2)} y_i^{(1)} + \lambda_i^{(3)} y_i^{(0)} \quad (i = 1,2,3), \end{aligned} \tag{3.41}$$

produces

$$y_1^{(3)} = \begin{bmatrix} u_1 \\ v_1 \\ 0 \\ -a_1 \\ -\dfrac{b_1}{2} \end{bmatrix}, \qquad y_2^{(3)} = \begin{bmatrix} u_2 \\ 0 \\ w_2 \\ -a_2 \\ 0 \end{bmatrix}, \qquad y_3^{(3)} = \begin{bmatrix} 0 \\ v_3 \\ w_3 \\ 0 \\ -\dfrac{b_3}{2} \end{bmatrix}, \tag{3.42}$$

where we have invoked intermediate normalization. As before, $y_i^{(3)}$ ($i = 1,2,3$) are not yet fully determined.

We now enforce solvability of (2.5) for $k = 4$:

$$\langle y_j^{(0)}, -(A_1 - \lambda^{(1)} I) y_i^{(3)} + \lambda_i^{(2)} y_i^{(2)} + \lambda_i^{(3)} y_i^{(1)} + \lambda_i^{(4)} y_i^{(0)} \rangle = 0 \quad (i \neq j), \tag{3.43}$$

thereby fully determining

$$y_1^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \qquad y_2^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -\dfrac{1}{4} \end{bmatrix}, \qquad y_3^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0 \end{bmatrix}. \tag{3.44}$$

Subsequent application of the Dalgarno-Stewart identities yields

$$\begin{aligned}
\lambda_1^{(4)} &= \langle y_1^{(1)}, (A_1 - \lambda^{(1)} I) y_1^{(2)} \rangle - \lambda_1^{(2)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 0, \\
\lambda_1^{(5)} &= \langle y_1^{(2)}, (A_1 - \lambda^{(1)} I) y_1^{(2)} \rangle - 2\lambda_1^{(2)} \langle y_1^{(2)}, y_1^{(1)} \rangle - \lambda_1^{(3)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 0, \\
\lambda_2^{(4)} &= \langle y_2^{(1)}, (A_1 - \lambda^{(1)} I) y_2^{(2)} \rangle - \lambda_2^{(2)} \langle y_2^{(1)}, y_2^{(1)} \rangle = 0, \\
\lambda_2^{(5)} &= \langle y_2^{(2)}, (A_1 - \lambda^{(1)} I) y_2^{(2)} \rangle - 2\lambda_2^{(2)} \langle y_2^{(2)}, y_2^{(1)} \rangle - \lambda_2^{(3)} \langle y_2^{(1)}, y_2^{(1)} \rangle = \frac{1}{8}, \\
\lambda_3^{(4)} &= \langle y_3^{(1)}, (A_1 - \lambda^{(1)} I) y_3^{(2)} \rangle - \lambda_3^{(2)} \langle y_3^{(1)}, y_3^{(1)} \rangle = 0, \\
\lambda_3^{(5)} &= \langle y_3^{(2)}, (A_1 - \lambda^{(1)} I) y_3^{(2)} \rangle - 2\lambda_3^{(2)} \langle y_3^{(2)}, y_3^{(1)} \rangle - \lambda_3^{(3)} \langle y_3^{(1)}, y_3^{(1)} \rangle = 2.
\end{aligned} \tag{3.45}$$

3.3. *N th order degeneracy*

We now consider the case of Nth order degeneracy which is characterized by the conditions $\lambda_1^{(j)} = \lambda_2^{(j)} = \cdots = \lambda_m^{(j)} = \lambda^{(j)}$ ($j = 0, \dots, N-1$), while $\lambda_i^{(N)}$ ($i = 1, \dots, m$) are all distinct. Thus, even though $\lambda^{(j)}$ ($j = 0, \dots, N-1$)

are determinate, $\{y_i^{(0)}\}_{i=1}^m$ are still indeterminate after enforcing solvability of (2.5) for $k = N - 1$.

Hence, we will determine $\{\lambda_i^{(N)}; y_i^{(0)}\}_{i=1}^m$ by insisting that (2.5) be solvable for $k = N$ and $i = 1, \ldots, m$. This requirement is equivalent to the condition that, for each fixed i,

$$\langle x_\mu^{(0)}, -(A_1 - \lambda^{(1)} I) y_i^{(N-1)} + \lambda^{(2)} y_i^{(N-2)} + \cdots + \lambda_i^{(N)} y_i^{(0)} \rangle = 0 \quad (\mu = 1, \ldots, m). \tag{3.46}$$

Inserting (3.1) as well as (3.7) with $k = 1, \ldots, N-1$ and invoking the orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, M^{(N)} x_1^{(0)} \rangle & \cdots & \langle x_1^{(0)}, M^{(N)} x_m^{(0)} \rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, M^{(N)} x_1^{(0)} \rangle & \cdots & \langle x_m^{(0)}, M^{(N)} x_m^{(0)} \rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(N)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}, \tag{3.47}$$

where $M^{(N)}$ is specified by the recurrence relation

$$\begin{aligned} M^{(1)} &= A_1, \\ M^{(2)} &= (\lambda^{(1)} I - M^{(1)})(A_0 - \lambda^{(0)} I)^\dagger (A_1 - \lambda^{(1)} I), \\ M^{(3)} &= (\lambda^{(2)} I - M^{(2)})(A_0 - \lambda^{(0)} I)^\dagger (A_1 - \lambda^{(1)} I) \\ &\quad + \lambda^{(2)} (A_1 - \lambda^{(1)} I)(A_0 - \lambda^{(0)} I)^\dagger, \\ M^{(N)} &= (\lambda^{(N-1)} I - M^{(N-1)})(A_0 - \lambda^{(0)} I)^\dagger (A_1 - \lambda^{(1)} I) \\ &\quad - \sum_{l=2}^{N-3} \lambda^{(l)} (\lambda^{(N-l)} I - M^{(N-l)})(A_0 - \lambda^{(0)} I)^\dagger \\ &\quad - \lambda^{(N-2)} [(A_1 - \lambda^{(1)} I)(A_0 - \lambda^{(0)} I)^\dagger (A_1 - \lambda^{(1)} I) + \lambda^{(2)} I](A_0 - \lambda^{(0)} I)^\dagger \\ &\quad + \lambda^{(N-1)} (A_1 - \lambda^{(1)} I)(A_0 - \lambda^{(0)} I)^\dagger \quad (N = 4, 5, \ldots). \end{aligned} \tag{3.48}$$

Thus, each $\lambda_i^{(N)}$ is an eigenvalue with corresponding eigenvector $[a_1^{(i)}, \ldots, a_m^{(i)}]^T$ of the matrix M defined by $M_{\mu,\nu} = \langle x_\mu^{(0)}, M^{(N)} x_\nu^{(0)} \rangle$ ($\mu, \nu = 1, \ldots, m$). It is important to note that, while this recurrence relation guarantees that $\{\lambda_i^{(N)}; y_i^{(0)}\}_{i=1}^m$ are well defined by enforcing solvability of (2.5) for $k = N$, $M^{(N)}$ need not be explicitly computed.

By assumption, the symmetric matrix M has m distinct real eigenvalues and hence orthonormal eigenvectors described by (3.2). These, in turn, may be used in concert with (3.1) to yield the desired special unperturbed eigenvectors alluded to above.

Now that $\{y_i^{(0)}\}_{i=1}^{m}$ are fully determined, we have by the combination of (3.2) and (3.47) the identities

$$\langle y_i^{(0)}, M^{(N)} y_j^{(0)} \rangle = \lambda_i^{(N)} \cdot \delta_{i,j}. \tag{3.49}$$

The remaining eigenvalue corrections $\lambda_i^{(k)}$ $(k \geq N+1)$ may be obtained from the Dalgarno-Stewart identities.

Analogous to the cases of first-order and second-order degeneracies, $\beta_{j,k}^{(i)}$ $(i \neq j)$ of (3.7) are to be determined from the condition that (2.5) be solvable for $k \leftarrow k+N$ and $i = 1, \ldots, m$. Since, by design, (2.5) is solvable for $k = 1, \ldots, N$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = \frac{\langle y_j^{(0)}, M^{(N)} \hat{y}_i^{(k)} \rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+N)} \beta_{j,l}^{(i)}}{\lambda_i^{(N)} - \lambda_j^{(N)}} \quad (i \neq j). \tag{3.50}$$

The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of (2.5) for $k \leftarrow k+N$.

Example 3.3. Define

$$A_0 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}, \qquad A_1 = \begin{bmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & -1 \\ 1 & 1 & 1 & 0 \\ 1 & -1 & 0 & 0 \end{bmatrix}. \tag{3.51}$$

Using Matlab's Symbolic Toolbox, we find that

$$\begin{aligned} \lambda_1(\epsilon) &= 1 + \epsilon - 2\epsilon^2 + 4\epsilon^4 + 0 \cdot \epsilon^5 + \cdots, \\ \lambda_2(\epsilon) &= 1 + \epsilon - 2\epsilon^2 - 2\epsilon^3 + 2\epsilon^4 + 10\epsilon^5 + \cdots, \\ \lambda_3(\epsilon) &= 2 + 2\epsilon^2 + 2\epsilon^3 - 2\epsilon^4 - 10\epsilon^5 + \cdots, \\ \lambda_4(\epsilon) &= 2 + \epsilon + 2\epsilon^2 - 4\epsilon^4 + 0 \cdot \epsilon^5 + \cdots. \end{aligned} \tag{3.52}$$

We focus on the third-order degeneracy amongst $\lambda_1^{(0)} = \lambda_2^{(0)} = \lambda^{(0)} = 1$. With the choice

$$x_1^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \qquad x_2^{(0)} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \tag{3.53}$$

we have from (3.4), which enforces solvability of (2.5) for $k = 1$,

$$M = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{3.54}$$

with double eigenvalue $\lambda^{(1)} = 1$. Equation (3.24), which enforces solvability of (2.5) for $k = 2$, yields

$$M = \begin{bmatrix} -2 & 0 \\ 0 & -2 \end{bmatrix} \tag{3.55}$$

with double eigenvalue $\lambda^{(2)} = -2$.

Moving on to (3.47) with $N = 3$, which enforces solvability of (2.5) for $k = 3$, we have

$$M = \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \tag{3.56}$$

with eigenpairs

$$\lambda_1^{(3)} = 0, \quad \begin{bmatrix} a_1^{(1)} \\ a_2^{(1)} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}; \qquad \lambda_2^{(3)} = -2, \quad \begin{bmatrix} a_1^{(2)} \\ a_2^{(2)} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}. \tag{3.57}$$

Availing ourselves of (3.1), the special unperturbed eigenvectors are now fully determined as

$$y_1^{(0)} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \\ 0 \end{bmatrix}, \qquad y_2^{(0)} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \\ 0 \end{bmatrix}. \tag{3.58}$$

Solving (2.5), for $k = 1$,

$$(A_0 - \lambda^{(0)} I) y_i^{(1)} = -(A_1 - \lambda^{(1)} I) y_i^{(0)} \quad (i = 1,2), \tag{3.59}$$

produces

$$y_1^{(1)} = \begin{bmatrix} a \\ -a \\ -\sqrt{2} \\ 0 \end{bmatrix}, \qquad y_2^{(1)} = \begin{bmatrix} b \\ b \\ 0 \\ -\sqrt{2} \end{bmatrix}, \tag{3.60}$$

where we have invoked intermediate normalization. Observe that $y_i^{(1)}$ $(i = 1,2)$ are not yet fully determined.

Solving (2.5), for $k = 2$,

$$(A_0 - \lambda^{(0)} I) y_i^{(2)} = -(A_1 - \lambda^{(1)} I) y_i^{(1)} + \lambda^{(2)} y_i^{(0)} \quad (i = 1,2), \tag{3.61}$$

produces

$$y_1^{(2)} = \begin{bmatrix} c \\ -c \\ 0 \\ -2a \end{bmatrix}, \qquad y_2^{(2)} = \begin{bmatrix} d \\ d \\ -2b \\ -\sqrt{2} \end{bmatrix}, \tag{3.62}$$

where we have invoked intermediate normalization. Likewise, $y_i^{(2)}$ $(i = 1,2)$ are not yet fully determined.

Solving (2.5), for $k = 3$,

$$(A_0 - \lambda^{(0)} I) y_i^{(3)} = -(A_1 - \lambda^{(1)} I) y_i^{(2)} + \lambda^{(2)} y_i^{(1)} + \lambda_i^{(3)} y_i^{(0)} \quad (i = 1,2), \tag{3.63}$$

produces

$$y_1^{(3)} = \begin{bmatrix} e \\ -e \\ 2\sqrt{2} \\ -2c - 2a \end{bmatrix}, \qquad y_2^{(3)} = \begin{bmatrix} f \\ f \\ -2d \\ \sqrt{2} \end{bmatrix}, \tag{3.64}$$

where we have invoked intermediate normalization. Likewise, $y_i^{(3)}$ $(i = 1,2)$ are not yet fully determined.

We next enforce solvability of (2.5) for $k = 4$:

$$\langle y_j^{(0)}, -(A_1 - \lambda^{(1)} I) y_i^{(3)} + \lambda^{(2)} y_i^{(2)} + \lambda_i^{(3)} y_i^{(1)} + \lambda_i^{(4)} y_i^{(0)} \rangle = 0 \quad (i \neq j), \tag{3.65}$$

thereby producing

$$y_1^{(1)} = \begin{bmatrix} 0 \\ 0 \\ -\sqrt{2} \\ 0 \end{bmatrix}; \qquad y_2^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -\sqrt{2} \end{bmatrix},$$
$$y_1^{(2)} = \begin{bmatrix} c \\ -c \\ 0 \\ 0 \end{bmatrix}; \qquad y_2^{(2)} = \begin{bmatrix} d \\ d \\ 0 \\ -\sqrt{2} \end{bmatrix}, \tag{3.66}$$
$$y_1^{(3)} = \begin{bmatrix} e \\ -e \\ 2\sqrt{2} \\ -2c \end{bmatrix}; \qquad y_2^{(3)} = \begin{bmatrix} f \\ f \\ -2d \\ \sqrt{2} \end{bmatrix}.$$

Observe that $y_i^{(1)}$ $(i = 1,2)$ are now fully determined, while $y_i^{(2)}$ $(i = 1,2)$ and $y_i^{(3)}$ $(i = 1,2)$ are not yet completely specified.

Solving (2.5), for $k = 4$,

$$\begin{aligned}(A_0 - \lambda^{(0)} I) y_i^{(4)} = &-(A_1 - \lambda^{(1)} I) y_i^{(3)} + \lambda^{(2)} y_i^{(2)} \\ &+ \lambda_i^{(3)} y_i^{(1)} + \lambda_i^{(4)} y_i^{(0)} \quad (i = 1,2),\end{aligned} \tag{3.67}$$

produces

$$y_1^{(4)} = \begin{bmatrix} g \\ h \\ 0 \\ -2e - 2c \end{bmatrix}, \qquad y_2^{(4)} = \begin{bmatrix} u \\ v \\ -2f \\ 5\sqrt{2} \end{bmatrix}, \tag{3.68}$$

where we have invoked intermediate normalization. As before, $y_i^{(4)}$ $(i = 1,2)$ are not yet fully determined.

We now enforce solvability of (2.5) for $k = 5$:

$$\langle y_j^{(0)}, -(A_1 - \lambda^{(1)} I) y_i^{(4)} + \lambda^{(2)} y_i^{(3)} + \lambda_i^{(3)} y_i^{(2)} + \lambda_i^{(4)} y_i^{(1)} + \lambda_i^{(5)} y_i^{(0)} \rangle = 0 \quad (i \neq j), \tag{3.69}$$

thereby fully determining

$$y_1^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \qquad y_2^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -\sqrt{2} \end{bmatrix} \tag{3.70}$$

and further specifying

$$\begin{gathered} y_1^{(3)} = \begin{bmatrix} e \\ -e \\ 2\sqrt{2} \\ 0 \end{bmatrix}, \qquad y_2^{(3)} = \begin{bmatrix} f \\ f \\ 0 \\ \sqrt{2} \end{bmatrix}, \\ y_1^{(4)} = \begin{bmatrix} g \\ h \\ 0 \\ -2e \end{bmatrix}, \qquad y_2^{(4)} = \begin{bmatrix} u \\ v \\ -2f \\ 5\sqrt{2} \end{bmatrix}. \end{gathered} \tag{3.71}$$

Subsequent application of the Dalgarno-Stewart identities yields

$$\begin{aligned} \lambda_1^{(4)} &= \langle y_1^{(1)}, (A_1 - \lambda^{(1)} I) y_1^{(2)} \rangle - \lambda_1^{(2)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 4, \\ \lambda_1^{(5)} &= \langle y_1^{(2)}, (A_1 - \lambda^{(1)} I) y_1^{(2)} \rangle - 2\lambda_1^{(2)} \langle y_1^{(2)}, y_1^{(1)} \rangle - \lambda_1^{(3)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 0, \\ \lambda_2^{(4)} &= \langle y_2^{(1)}, (A_1 - \lambda^{(1)} I) y_2^{(2)} \rangle - \lambda_2^{(2)} \langle y_2^{(1)}, y_2^{(1)} \rangle = 2, \\ \lambda_2^{(5)} &= \langle y_2^{(2)}, (A_1 - \lambda^{(1)} I) y_2^{(2)} \rangle - 2\lambda_2^{(2)} \langle y_2^{(2)}, y_2^{(1)} \rangle - \lambda_2^{(3)} \langle y_2^{(1)}, y_2^{(1)} \rangle = 10. \end{aligned} \tag{3.72}$$

3.4. Mixed degeneracy

Finally, we arrive at the most general case of mixed degeneracy wherein a degeneracy (multiple eigenvalue) is partially resolved at more than a single order. The analysis expounded upon in the previous sections comprises the core of the procedure for the complete resolution of mixed degeneracy. The following modifications suffice.

During the Rayleigh-Schrödinger procedure, whenever an eigenvalue branches by reduction in multiplicity at any order, one simply replaces the x_μ of (3.47) by any convenient orthonormal basis z_μ for the reduced eigenspace. Of course, this new basis is composed of some a priori unknown linear combination of the original basis. Equation (3.50) will still be valid where N is the order of correction where the degeneracy between λ_i and λ_j is resolved. Thus, in general, if λ_i is degenerate to Nth order, then $y_i^{(k)}$ will be fully determined by enforcing the solvability of (2.5) with $k \leftarrow k + N$.

We now present a final example which illustrates this general procedure. This example features a triple eigenvalue which branches into a single first-order degenerate eigenvalue, together with a pair of second-order degenerate eigenvalues. Hence, we observe features of both Examples 3.1 and 3.2 appearing in tandem.

Example 3.4. Define

$$A_0 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \qquad A_1 = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}. \tag{3.73}$$

Using Matlab's Symbolic Toolbox, we find that

$$\begin{aligned} \lambda_1(\epsilon) &= \epsilon, \\ \lambda_2(\epsilon) &= \epsilon - \epsilon^2 - \epsilon^3 + 2\epsilon^5 + \cdots, \\ \lambda_3(\epsilon) &= 0, \\ \lambda_4(\epsilon) &= 1 + \epsilon^2 + \epsilon^3 - 2\epsilon^5 + \cdots. \end{aligned} \tag{3.74}$$

We focus on the mixed degeneracy amongst $\lambda_1^{(0)} = \lambda_2^{(0)} = \lambda_3^{(0)} = \lambda^{(0)} = 0$. With the choice

$$x_1^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \qquad x_2^{(0)} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \qquad x_3^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \tag{3.75}$$

we have from (3.4), which enforces solvability of (2.5) for $k = 1$,

$$M = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{3.76}$$

with eigenvalues $\lambda_1^{(1)} = \lambda_2^{(1)} = \lambda^{(1)} = 1$, $\lambda_3^{(1)} = 0$.

Thus, $y_1^{(0)}$ and $y_2^{(0)}$ are indeterminate, while

$$\begin{bmatrix} a_1^{(3)} \\ a_2^{(3)} \\ a_3^{(3)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \Longrightarrow y_3^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}. \tag{3.77}$$

Introducing the new basis

$$z_1^{(0)} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \\ 0 \end{bmatrix}, \qquad z_2^{(0)} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \\ 0 \\ 0 \end{bmatrix}, \tag{3.78}$$

we now seek $y_1^{(0)}$ and $y_2^{(0)}$ in the form

$$y_1^{(0)} = b_1^{(1)} z_1^{(0)} + b_2^{(1)} z_2^{(0)}, \qquad y_2^{(0)} = b_1^{(2)} z_1^{(0)} + b_2^{(2)} z_2^{(0)}, \tag{3.79}$$

with orthonormal $\{[b_1^{(1)}, b_2^{(1)}]^T, [b_1^{(2)}, b_2^{(2)}]^T\}$.

Solving (2.5), for $k = 1$,

$$(A_0 - \lambda^{(0)} I) y_i^{(1)} = -(A_1 - \lambda_i^{(1)} I) y_i^{(0)} \quad (i = 1, 2, 3), \tag{3.80}$$

produces

$$y_1^{(1)} = \begin{bmatrix} \alpha_1 \\ \beta_1 \\ \gamma_1 \\ -\frac{(b_1^{(1)} + b_2^{(1)})}{\sqrt{2}} \end{bmatrix}, \quad y_2^{(1)} = \begin{bmatrix} \alpha_2 \\ \beta_2 \\ \gamma_2 \\ -\frac{(b_1^{(2)} + b_2^{(2)})}{\sqrt{2}} \end{bmatrix}, \quad y_3^{(1)} = \begin{bmatrix} \alpha_3 \\ \beta_3 \\ \gamma_3 \\ 0 \end{bmatrix}. \tag{3.81}$$

Now, enforcing solvability of (2.5), for $k = 2$,

$$-(A_1 - \lambda_i^{(1)} I) y_i^{(1)} + \lambda_i^{(2)} y_i^{(0)} \perp \{z_1^{(0)}, z_2^{(0)}, y_3^{(0)}\} \quad (i = 1, 2, 3), \tag{3.82}$$

we arrive at

$$M = \begin{bmatrix} -\frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & -\frac{1}{2} \end{bmatrix}, \tag{3.83}$$

with eigenpairs

$$\lambda_1^{(2)} = 0, \quad \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix};$$

$$\lambda_2^{(2)} = -1, \quad \begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \Longrightarrow y_1^{(0)} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}; \qquad y_2^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \tag{3.84}$$

$$y_1^{(1)} = \begin{bmatrix} \alpha_1 \\ \beta_1 \\ 0 \\ 0 \end{bmatrix}; \qquad y_2^{(1)} = \begin{bmatrix} \alpha_2 \\ \beta_2 \\ 0 \\ -1 \end{bmatrix}; \qquad y_3^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

as well as $\lambda_3^{(2)} = 0$, where we have invoked intermediate normalization. Observe that $y_1^{(1)}$ and $y_2^{(1)}$ have not yet been fully determined, while $y_3^{(1)}$ has indeed been completely specified.

Solving (2.5), for $k = 2$,

$$(A_0 - \lambda^{(0)} I) y_i^{(2)} = -(A_1 - \lambda_i^{(1)} I) y_i^{(1)} + \lambda_i^{(2)} y_i^{(0)} \quad (i = 1, 2, 3), \tag{3.85}$$

produces

$$y_1^{(2)} = \begin{bmatrix} a_1 \\ 0 \\ c_1 \\ -\alpha_1 \end{bmatrix}, \qquad y_2^{(2)} = \begin{bmatrix} 0 \\ b_2 \\ c_2 \\ -1 \end{bmatrix}, \qquad y_3^{(2)} = \begin{bmatrix} a_3 \\ b_3 \\ 0 \\ 0 \end{bmatrix}, \tag{3.86}$$

where we have invoked intermediate normalization.

We next enforce solvability of (2.5) for $k = 3$:

$$\langle y_j^{(0)}, -(A_1 - \lambda_i^{(1)} I) y_i^{(2)} + \lambda_i^{(2)} y_i^{(1)} + \lambda_i^{(3)} y_i^{(0)} \rangle = 0 \quad (i \neq j), \tag{3.87}$$

thereby producing

$$y_1^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \qquad y_2^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \end{bmatrix},$$
$$y_1^{(2)} = \begin{bmatrix} a_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \qquad y_2^{(2)} = \begin{bmatrix} 0 \\ b_2 \\ 0 \\ -1 \end{bmatrix}; \qquad y_3^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}. \tag{3.88}$$

With $y_i^{(1)}$ $(i = 1,2,3)$ now fully determined, the Dalgarno-Stewart identities yield

$$\begin{aligned} \lambda_1^{(3)} &= \langle y_1^{(1)}, (A_1 - \lambda^{(1)} I) y_1^{(1)} \rangle = 0, \\ \lambda_2^{(3)} &= \langle y_2^{(1)}, (A_1 - \lambda^{(1)} I) y_2^{(1)} \rangle = -1, \\ \lambda_3^{(3)} &= \langle y_3^{(1)}, (A_1 - \lambda_3^{(1)} I) y_3^{(1)} \rangle = 0. \end{aligned} \tag{3.89}$$

Solving (2.5), for $k = 3$,

$$(A_0 - \lambda^{(0)} I) y_i^{(3)} = -(A_1 - \lambda^{(1)} I) y_i^{(2)} + \lambda_i^{(2)} y_i^{(1)} + \lambda_i^{(3)} y_i^{(0)} \quad (i = 1,2), \tag{3.90}$$

produces

$$y_1^{(3)} = \begin{bmatrix} u_1 \\ 0 \\ w_1 \\ -a_1 \end{bmatrix}, \qquad y_2^{(3)} = \begin{bmatrix} 0 \\ v_2 \\ w_2 \\ 0 \end{bmatrix}, \tag{3.91}$$

where we have invoked intermediate normalization.

We now enforce solvability of (2.5) for $k = 4$:

$$\langle y_j^{(0)}, -(A_1 - \lambda^{(1)} I) y_i^{(3)} + \lambda_i^{(2)} y_i^{(2)} + \lambda_i^{(3)} y_i^{(1)} + \lambda_i^{(4)} y_i^{(0)} \rangle = 0 \quad (i \neq j), \tag{3.92}$$

thereby fully determining

$$y_1^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \qquad y_2^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \end{bmatrix}. \tag{3.93}$$

Subsequent application of the Dalgarno-Stewart identities yields

$$\begin{aligned}
\lambda_1^{(4)} &= \langle y_1^{(1)}, (A_1 - \lambda^{(1)} I) y_1^{(2)} \rangle - \lambda_1^{(2)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 0, \\
\lambda_1^{(5)} &= \langle y_1^{(2)}, (A_1 - \lambda^{(1)} I) y_1^{(2)} \rangle - 2\lambda_1^{(2)} \langle y_1^{(2)}, y_1^{(1)} \rangle - \lambda_1^{(3)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 0, \\
\lambda_2^{(4)} &= \langle y_2^{(1)}, (A_1 - \lambda^{(1)} I) y_2^{(2)} \rangle - \lambda_2^{(2)} \langle y_2^{(1)}, y_2^{(1)} \rangle = 0, \\
\lambda_2^{(5)} &= \langle y_2^{(2)}, (A_1 - \lambda^{(1)} I) y_2^{(2)} \rangle - 2\lambda_2^{(2)} \langle y_2^{(2)}, y_2^{(1)} \rangle - \lambda_2^{(3)} \langle y_2^{(1)}, y_2^{(1)} \rangle = 2, \\
\lambda_3^{(4)} &= \langle y_3^{(1)}, (A_1 - \lambda_3^{(1)} I) y_3^{(2)} \rangle - \lambda_3^{(2)} \langle y_3^{(1)}, y_3^{(1)} \rangle = 0, \\
\lambda_3^{(5)} &= \langle y_3^{(2)}, (A_1 - \lambda_3^{(1)} I) y_3^{(2)} \rangle - 2\lambda_3^{(2)} \langle y_3^{(2)}, y_3^{(1)} \rangle - \lambda_3^{(3)} \langle y_3^{(1)}, y_3^{(1)} \rangle = 0.
\end{aligned} \tag{3.94}$$

4. Conclusion

In this paper, we have endeavored to provide a comprehensive and unified account of the Rayleigh-Schrödinger perturbation theory for the symmetric matrix eigenvalue problem. The cornerstone of our development has been the Moore-Penrose pseudoinverse. Not only does this approach permit a direct analysis of the properties of this procedure but it also obviates the need of alternative approaches for the computation of all of the eigenvectors of the unperturbed matrix. Instead, we only require the unperturbed eigenvectors corresponding to those eigenvalues of interest.

The focal point of this investigation has been the degenerate case. In the light of the inherent complexity of this topic, we have built up the theory gradually with the expectation that the reader would thence not be swept away in a torrent of formulae. At each stage, we have attempted to make the subject more accessible by a judicious choice of an illustrative example. (Observe that all of the examples were worked through *without* explicit computation of the pseudoinverse.) Hopefully, these efforts have met with a modicum of success.

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