RAYLEIGH-SCHRÖDINGER PERTURBATION THEORY: PSEUDOINVERSE FORMULATION

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Dedicated to the memory of my parents:

Dorothy F. (Kelly) McCartin
and
James D. McCartin

for all of the sacrifices that they made for their children.

Lord Rayleigh

Erwin Schrödinger

PREFACE

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

Mathematically, we have a discretized Laplacian-type operator embodied in a real symmetric matrix which is subjected to a small symmetric perturbation due to some physical inhomogeneity. The Rayleigh-Schrödinger procedure produces approximations to the eigenvalues and eigenvectors of the perturbed matrix by a sequence of successively higher order corrections to the eigenvalues and eigenvectors of the unperturbed matrix.

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

This malady can be remedied by expressing the Rayleigh-Schrödinger procedure in terms of the Moore-Penrose pseudoinverse. This permits these corrections to be computed knowing only the eigenvectors of the unperturbed matrix 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 matrix factorization, elmination/back substitution and orthogonal projection. However, the formalism of the pseudoinverse provides a concise formulation of the procedure and permits ready analysis of theoretical properties of the algorithm.

The present book provides a complete and self-contained treatment of the Rayleigh-Schrödinger perturbation theory based upon such a pseudoinverse formulation. The theory is built up gradually and many numerical examples are included. The intent of this spiral approach is to provide the reader with ready access to this important technique without being deluged by a torrent of formulae. Some redundancy has been intentionally incorporated into the presentation so as to make the chapters individually accessible.

Chapter 1 provides historical background relative to this technique and also includes several examples of how such perturbed eigenvalue problems arise in Applied Mathematics. Chapter 2 presents a self-contained summary of the most important facts about pseudoinverses needed in subsequent chapters. Chapter 3 treats the symmetric eigenvalue problem, first for linear perturbations and then for general analytic perturbations. The theory is then extended in Chapter 4 to the symmetric definite generalized eigenvalue problem.

Finally, Chapter 5 presents a detailed application of the previously developed theory to the technologically important problem of the analysis of inhomogeneous acoustic waveguides. Specifically, the walls of a duct (such as a muffler) are heated thereby producing a temperature gradient within the waveguide. The consequent perturbations to the propagating acoustic pressure waves are then calculated by applying the Rayleigh-Schrödinger pseudoinverse technique to the resulting generalized eigenvalue problem. Of particular interest is that this approach allows one to study the so-called degenerate modes of the waveguide. Enough background material is provided so as to be accessible to a wide scientific audience.

The target audience for this book includes practicing Engineers, Scientists and Applied Mathematicians. Particular emphasis has been placed upon including enough background material to also make the book accessible to graduate students in these same fields. The goal of the book has been not only to provide its readership with an understanding of the theory but also to give an appreciation for the context of this method within the corpus of Techniques of Applied Mathematics as well as to include sufficient examples and applications for them to apply the method in their own work. For those readers interested in the theoretical underpinnings of this technique, a generalized version of Rellich's Spectral Perturbation Theorem is presented and proved in the Appendix.

Many thanks are due Bruce E. Deitz, Interlibrary Loan Coordinator at Kettering University, for his tireless efforts to track down many obscure, incomplete and frankly incorrect references. Also, I would like to warmly thank Dr. Ghasi R. Verma, Professor Emeritus of Mathematics at University of Rhode Island, specifically for introducing me to Perturbation Methods at a tender age and generally for giving me an appreciation for the Art of Applied Mathematics. Finally, I would be remiss if I did not express my sincere gratitude to my loving wife Barbara A. (Rowe) McCartin who has good-naturedly tolerated all of the endless hours spent on my mathematical research. As if that were not enough, she has faithfully illustrated all of my publications for the past fifteen years.

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Chapter 1

Introduction

1.1 Lord Rayleigh's Life and Times

G. G. Stokes [54, Chapter 7], Lord Kelvin [52], J. C. Maxwell [55] and Lord Rayleigh [107] may rightfully be said to form the Mount Rushmore of 19th Century British Mathematical Physicists. The connecting thread amongst these "Masters of Theory" [112] was their common training in the Cambridge school of mathematical physics. This school in turn was a natural outgrowth of the long tradition of mathematical excellence at Cambridge University [2]. Lord Rayleigh was closely connected to his three distinguished colleagues. Stokes was one of his teachers and he maintained life-long correspondences with both Kelvin and Maxwell.

Lord Rayleigh [8], [53], [107] lived the bulk of his professional life during the *Pax Britannica* of the Victorian Era (1837-1901). Despite the misnomer (England was in fact at war during every year of this period), Rayleigh's life was virtually untouched by hardship. Unlike most other Peers of the Realm, he chose the life of a gentleman-scientist (except for a brief stint as head of the Cavendish Laboratory) simply because of his love for mathematical physics. In this sense, he is perhaps the greatest amateur scientist of all time.

John William Strutt (1842-1919) was born and died on the family estate at Terling in Chelmsford, Essex and, being the oldest son, eventually became the third Baron Rayleigh of Terling Place. He was a sickly child who gave no early indication of his native mathematical talents. The first unambiguous indication of such talents was given when he enrolled at Trinity College at age 20 where he studied physics with Stokes and "mixed" mathematics under the great Mathematical Tripos coach E. J. Routh.

In 1865, he followed in Stokes' 1841 footsteps and became both Senior Wrangler and Smith's Prizeman. To appreciate the magnitude of this accomplishment, consider that Kelvin placed as Second Wrangler and tied for Smith's Prizeman in 1845 while Maxwell did the same in 1854 (both losing to and tying

Routh himself!). In 1866 he was made a Fellow of Trinity College.

In 1868, Rayleigh broke with tradition and, in place of the conventional post-graduation grand tour of the Continent, he instead traveled to the United States soon after the American Civil War and toured the newly reconstructed South. Already, his growing stature is reflected in the fact that he met with President Andrew Johnson at the White House on this trip.

His standing in the aristocracy was further enhanced when, in 1871, he married Eleanor Balfour whose uncle and brother both became Prime Minister. Six months later he contracted rheumatic fever and nearly perished. Afraid of the possible consequences of the harsh British winter on his frail health, he and his wife cruised the length of the Nile River on a house boat late in 1872. This journey is of great significance to the present narrative because it was at this time that he wrote, without access to library resources, a substantial portion of Volume I of his great treatise *The Theory of Sound* about which we will have more to say below.

Shortly after their return to England, his father died and they became Lord and Lady Rayleigh. This change in status required him to administer the family estate and consequently prompted them to move to Terling Place where a laboratory was constructed for his experimental investigations. Except for the period 1879-1884, this became his base of scientific operations. This hiatus was brought about by a confluence of events: An agricultural downturn significantly reduced their income from the estate and Maxwell's death left open the Cavendish Professorship at Cambridge. As a result, Rayleigh accepted this chair for five years and is credited during this period with greatly enhancing the experimental component of the physics instruction at Cambridge. During this period, he and his students determined a revised set of electrical standards.

When he returned to Terling, he brought with him a renewed zeal for experimental work. His crowning achievement in this arena was his isolation of argon from the atmosphere in 1895. Prior to this work, it was believed that air was composed of oxygen and nitrogen alone. This work eventually led to the discovery of other rare gases in the atmosphere. In 1904, he shared the Nobel Prize in Physics with Sir William Ramsay for this discovery. It is noteworthy that this experimental investigation, which spanned a period of more than three years years, began with a minute discrepancy between the results of two different methods of measuring atmospheric nitrogen and was successfully completed with what, by modern standards, would be considered primitive experimental equipment.

Of particular interest for the present study are Rayleigh's extensive theoretical and experimental researches into acoustics. He became interested in acoustics early on in his student days while reading Helmholtz' *On Sensations of Tone*. This study resulted in his 1870 paper on Helmholtz resonators which appeared in the Philosophical Transactions of the Royal Society. This was his fifth publication out of 446 which he published in his lifetime. It is the first of his papers on acoustics which were to eventually number 128 (the last of which he published in the final year of his life at the age of 76). These acoustical researches reached their apex with the publication of his monumental treatise *The Theory of Sound*: Volume I (1877/1894) and Volume II (1878/1896) which will be considered in more detail in the next section.

His return to Terling did not sever him from the scientific life of Britain. From 1887 to 1905, he was Professor of Natural Philosophy at the Royal Institution where he delivered an annual course of public lectures complete with experimental demonstrations. Beginning in 1896, he spent the next fifteen years as Scientific Adviser to Trinity House where he was involved in the construction and maintenance of lighthouses and buoys. From 1905-1908, he served as President of the Royal Society and from 1909 to his death in 1919 he was Chancellor of Cambridge University.

In addition to his Nobel Prize (1904), he received many awards and distinctions in recognition for his prodigious scientific achievements: FRS (1873), Royal Medal (1882), Copley Medal (1899), Order of Merit (1902), Rumford Medal (1914). Also, in his honor, Cambridge University instituted the Rayleigh Prize in 1911 and the Institute of Physics began awarding the Rayleigh Medal in 2008.

His name is immortalized in many scientific concepts: e.g., Rayleigh Scattering, Rayleigh Quotient, Rayleigh-Ritz Variational Procedure, Rayleigh's Principle, Rayleigh-Taylor instability, Rayleigh waves. In fact, many mathematical results which he originated are attributed to others. For example, the generalization of Plancharel's Theorem from Fourier series to Fourier transforms is due to Rayleigh [83, p. 78]. In retrospect, his scientific accomplishments reflect a most remarkable synthesis of theory and experiment, perhaps without peer in the annals of science.

1.2 Rayleigh's Perturbation Theory

Perturbation theory in its modern form originated in 1749 with Euler's memoir on the irregularities in the orbits of Jupiter and Saturn [69, p. 172]. This analysis was further refined by Laplace in the mid-1780s [38, p. 321] and reached its culmination in the 1860s with the lunar theory of Delaunay [115, p. 1058]. In the early 1870s, Rayleigh extended this work to a generalized procedure applicable to any oscillatory system with n degrees of freedom [88, pp. 172-175, p. 185]. A more detailed explication of his perturbation procedure appeared in Volume I of his *The Theory of Sound* of 1877.

How many mathematical treatises are still heavily cited more than a century after they are written? A few. For example, Gauss' *Disquisitiones Arithmeticae* is one such classic. How many mathematical treatises are able to communicate across centuries in a readable fashion that provides insight and inspires thought? Very few, indeed. Lord Rayleigh's *The Theory of Sound* is a paramount example. From its birth in the late 19th Century, it continues to illuminate the way for scholars of the early 21st Century intent upon mastering acoustics. To put this masterpiece in perspective, the following pioneering analysis comprises a mere 5 pages out of more than 500 pages in this monumental treatise!

Free undamped vibrations of a system with n degrees of freedom are the subject of Chapter IV of this scientific classic. Section 90 presents a general perturbation procedure while Section 91 concerns the application of this procedure to a vibrating string with mild longitudinal density variation. In this application, Rayleigh harkens back to Lagrange and models the continuous string as a discrete system with a large number of degrees of freedom unlike D'Alembert who studied the vibrating string with a continuum model based upon the wave equation. In the ensuing summary of this pathbreaking work, his analysis will be recast into more modern notation utilizing matrices, inner products, asymptotic notation and distributions.

1.2.1 The Unperturbed System

Rayleigh begins by expressing the potential and kinetic energies, respectively, of the unperturbed oscillating system in terms of generalized coordinates comprised of the normal modes of vibration [36]:

$$V^{(0)} = \frac{1}{2}\langle \phi^{(0)}, A_0\phi^{(0)}\rangle;\ T^{(0)} = \frac{1}{2}\langle \dot{\phi}^{(0)}, B_0\dot{\phi}^{(0)}\rangle, \tag{1.1}$$

where $\phi^{(0)} = [\phi_1^{(0)}, \phi_2^{(0)}, \dots, \phi_n^{(0)}]^T$ with $A_0 = \text{diag}(a_1, a_2, \dots, a_n)$ and positive $B_0 = \text{diag}(b_1, b_2, \dots, b_n)$. $\langle \cdot, \cdot \rangle$ denotes the standard Euclidean inner product.

Defining the Lagrangian

$$L^{(0)} = T^{(0)} - V^{(0)} = \frac{1}{2}\left[\langle \dot{\phi}^{(0)}, B_0\dot{\phi}^{(0)}\rangle - \langle \phi^{(0)}, A_0\phi^{(0)}\rangle\right], \tag{1.2}$$

Lagrange's equations of motion are

$$\frac{d}{dt}L^{(0)}_{\dot{\phi}_i^{(0)}} - L^{(0)}_{\phi_i^{(0)}} = 0\ (i = 1, \dots, n). \tag{1.3}$$

Since

$$\frac{d}{dt}L^{(0)}_{\dot{\phi}_i^{(0)}} = b_i\ddot{\phi}_i^{(0)};\ L^{(0)}_{\phi_i^{(0)}} = -a_i\phi_i^{(0)}, \tag{1.4}$$

the equations of motion become

$$b_i\ddot{\phi}_i^{(0)} + a_i\phi_i^{(0)} = 0\ (i = 1, \dots, n), \tag{1.5}$$

or, in matrix form,

$$B_0\ddot{\phi}^{(0)} + A_0\phi^{(0)} = 0. \tag{1.6}$$

The unperturbed normal modes are thereby seen to be

$$\phi_i^{(0)}(t) = c_i \cdot \sin(\omega_i^{(0)}t + \psi_i); \;\; [\omega_i^{(0)}]^2 := \frac{a_i}{b_i}. \tag{1.7}$$

Observe that $\lambda_i^{(0)} := [\omega_i^{(0)}]^2$ is a generalized eigenvalue of

$$A_0 x_i^{(0)} = \lambda_i^{(0)} B_0 x_i^{(0)}, \tag{1.8}$$

with corresponding generalized eigenvector $x_i^{(0)} = e_i$ where e_i is the ith column of the identity matrix. We assume that these generalized eigenvalues are all distinct, i.e. they are simple, and have been ordered: $\lambda_1^{(0)} < \lambda_2^{(0)} < \cdots < \lambda_n^{(0)}$.

1.2.2 The Perturbed System

Suppose now that the potential and kinetic energies of our mechanical system with n degrees of freedom undergo small perturbations:

$$A(\epsilon) = A_0 + \epsilon A_1; \;\; B(\epsilon) = B_0 + \epsilon B_1, \tag{1.9}$$

where ϵ is a small parameter, A is symmetric and B is symmetric positive definite. The determination of the perturbed natural angular frequencies $\omega_i(\epsilon) = \sqrt{\lambda_i(\epsilon)}$ and normal modes $\phi_i(t;\epsilon)$ requires the simultaneous diagonaliztion of $A(\epsilon)$ and $B(\epsilon)$ [23, pp. 42-44] which is equivalent to solving the generalized eigenvalue problem [78, pp. 396-399]:

$$A(\epsilon)x_i(\epsilon) = \lambda_i(\epsilon)B(\epsilon)x_i(\epsilon) \;\; (i = 1, \ldots, n). \tag{1.10}$$

The generalized eigenvectors $x_i(\epsilon)$ are the coordinate vectors of the perturbed normal modes $\phi_i(t;\epsilon)$ relative to the basis of unperturbed normal modes $\phi^{(0)}$.

Thus, the potential and kinetic energies, respectively, of the perturbed oscillating system in terms of generalized coordinates comprised of the perturbed normal modes of vibration may be expressed as [36]:

$$V = \frac{1}{2}\langle \phi, A\phi \rangle; \;\; T = \frac{1}{2}\langle \dot{\phi}, B\dot{\phi} \rangle, \tag{1.11}$$

where $\phi = [\phi_1, \phi_2, \ldots, \phi_n]^T$. The Lagrangian is then given by

$$L = T - V = \frac{1}{2}\left[\langle \dot{\phi}, B\dot{\phi} \rangle - \langle \phi, A\phi \rangle\right], \tag{1.12}$$

and Lagrange's equations of motion become

$$\frac{d}{dt}L_{\dot{\phi}_i} - L_{\phi_i} = 0 \ (i = 1, \ldots, n). \tag{1.13}$$

Since

$$\frac{d}{dt}L_{\dot{\phi}_i} = \sum_{j=1}^{n} b_{i,j}\ddot{\phi}_j; \ L_{\phi_i} = -\sum_{j=1}^{n} a_{i,j}\phi_j, \tag{1.14}$$

the equations of motion are

$$\sum_{j=1}^{n} b_{i,j}\ddot{\phi}_j + \sum_{j=1}^{n} a_{i,j}\phi_i = 0 \ (i = 1, \ldots, n), \tag{1.15}$$

or, in matrix form,

$$B\ddot{\phi} + A\phi = 0. \tag{1.16}$$

Since we are assuming that both the unperturbed and perturbed generalized eigenvalues are simple, both the generalized eigenvalues and eigenvectors may be expressed as power series in ϵ [23, p. 45]:

$$\lambda_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \lambda_i^{(k)}; \ x_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k x_i^{(k)} \ (i = 1, \ldots, n). \tag{1.17}$$

Substitution of the perturbation expansions, Equation (1.17), into the generalized eigenvalue problem, Equation (1.10), yields

$$\begin{aligned} & (A_0 - \lambda_i^{(0)} B_0)x_i^{(0)} + \epsilon\left[(A_0 - \lambda_i^{(0)} B_0)x_i^{(1)} + (A_1 - \lambda_i^{(0)} B_1 - \lambda_i^{(1)} B_0)x_i^{(0)}\right] \\ + \ & \epsilon^2\left[(A_0 - \lambda_i^{(0)} B_0)x_i^{(2)} + (A_1 - \lambda_i^{(0)} B_1 - \lambda_i^{(1)} B_0)x_i^{(1)} - (\lambda_i^{(1)} B_1 + \lambda_i^{(2)} B_0)x_i^{(0)}\right] \\ = \ & \vec{0}. \end{aligned} \tag{1.18}$$

Taking the inner product of Equation (1.18) with e_j $(j \neq i)$ and setting the coefficient of ϵ to zero produces

$$[x_i^{(1)}]_j = \frac{\lambda_i^{(0)} b_{j,i} - a_{j,i}}{b_j(\lambda_j^{(0)} - \lambda_i^{(0)})}, \tag{1.19}$$

where $[A_1]_{i,j} = a_{i,j}$ and $[B_1]_{i,j} = b_{i,j}$. Without loss of generality, we may set

$$[x_i^{(1)}]_i = 0, \tag{1.20}$$

since

$$x_i(\epsilon) = \begin{bmatrix} \epsilon[x_i^{(1)}]_1 \\ \vdots \\ 1+\epsilon[x_i^{(1)}]_i \\ \vdots \\ \epsilon[x_i^{(1)}]_n \end{bmatrix} + O(\epsilon^2) = (1+\epsilon[x_i^{(1)}]_i) \begin{bmatrix} \epsilon[x_i^{(1)}]_1 \\ \vdots \\ 1 \\ \vdots \\ \epsilon[x_i^{(1)}]_n \end{bmatrix} + O(\epsilon^2), \quad (1.21)$$

and generalized eigenvectors are only defined up to a scalar multiple.

Taking the inner product of Equation (1.18) with e_i and setting the coefficient of ϵ to zero produces

$$\lambda_i^{(1)} = \frac{a_{i,i} - \lambda_i^{(0)} b_{i,i}}{b_i}, \quad (1.22)$$

while setting the coefficient of ϵ^2 to zero produces

$$\lambda_i^{(2)} = -\frac{b_{i,i}(a_{i,i} - \lambda_i^{(0)} b_{i,i})}{b_i^2} - {\sum_j}' \frac{(a_{j,i} - \lambda_i^{(0)} b_{j,i})^2}{b_i b_j (\lambda_j^{(0)} - \lambda_i^{(0)})}, \quad (1.23)$$

where we have invoked Equation (1.19). ${\sum_j}'$ denotes summation over all values of j from 1 to n except for $j = i$.

Rayleigh thereby approximates the perturbed normal modes to first-order in ϵ and the perturbed natural frequencies to second-order in ϵ. An equivalent perturbation analysis may be performed using the governing differential equation rather than energy considerations [23, pp. 343-350]. This development is due to Schrödinger [101, 102] and is detailed in Section 1.4.

1.2.3 Example: The Nonuniform Vibrating String

Rayleigh next applies the perturbation approximations of Section 1.2.2 to the vibrations of a stretched spring with mild longitudinal density variation. The string itself is modeled as a discrete vibrating system with infinitely many degrees of freedom.

Specifically, consider a vibrating string with fixed endpoints (Figure 1.1) of length ℓ and density $\rho(x) = \rho_0 + \epsilon \cdot \rho_1(x)$. Then, the potential and kinetic energies are given, respectively, by (τ = tension, y = transverse displacement) [11, pp. 22-23]:

$$V = \frac{\tau}{2}\int_0^\ell \left(\frac{\partial y}{\partial x}\right)^2 dx; \; T = \frac{1}{2}\int_0^\ell \rho(x)\left(\frac{\partial y}{\partial t}\right)^2 dx. \quad (1.24)$$

Thus, the potential energy is unaltered by the nonuniform density so that $a_{i,j} = 0$.

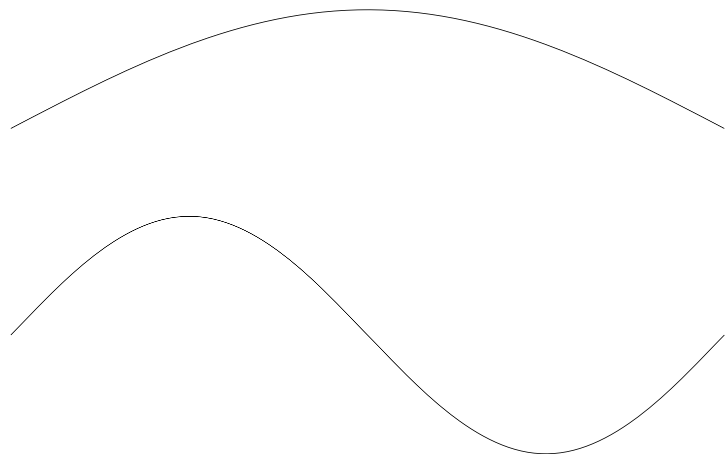

Figure 1.1: Vibrating String: Top = Fundamental, Bottom = First Overtone

The transverse displacement corresponding to the ith perturbed mode is

$$y_i(x,t;\epsilon) = \sin(\omega_i(\epsilon)t + \psi_i) \cdot \sum_{j=1}^{n} [x_i(\epsilon)]_j \sin\left(\frac{j\pi x}{\ell}\right). \tag{1.25}$$

Inserting ρ and y_i into the energy expressions, Equation (1.24), leads directly to:

$$a_i = \frac{i^2\pi^2\tau}{2\ell};\ b_i = \frac{1}{2}\ell\rho_0,\ b_{i,j} = \int_0^\ell \rho_1(x)\sin\left(\frac{i\pi x}{\ell}\right)\sin\left(\frac{j\pi x}{\ell}\right)\,dx. \tag{1.26}$$

Thus,

$$\lambda_i^{(0)} = \frac{a_i}{b_i} = \frac{\tau\pi^2 i^2}{\rho_0\ell^2} \Rightarrow \frac{\lambda_i^{(0)}}{\lambda_j^{(0)} - \lambda_i^{(0)}} = \frac{i^2}{j^2 - i^2}. \tag{1.27}$$

Therefore, substitution of Equations (1.26-1.27) into Equations (1.19-1.20) and Equations (1.22-1.23) yields

$$[x_i^{(1)}]_i = 0;\ [x_i^{(1)}]_j = \frac{i^2}{j^2 - i^2} \cdot \frac{2}{\ell\rho_0} \int_0^\ell \rho_1(x)\sin\left(\frac{i\pi x}{\ell}\right)\sin\left(\frac{j\pi x}{\ell}\right)\,dx\ (j \neq i), \tag{1.28}$$

and

$$\lambda_i(\epsilon) = \lambda_i^{(0)} \cdot \{1 - \epsilon \cdot \frac{2}{\ell\rho_0} \int_0^\ell \rho_1(x) \sin^2\left(\frac{i\pi x}{\ell}\right) dx$$
$$+\epsilon^2 \cdot [\left(\frac{2}{\ell\rho_0} \int_0^\ell \rho_1(x) \sin^2\left(\frac{i\pi x}{\ell}\right) dx\right)^2$$
$$-{\sum_j}' \frac{i^2}{j^2 - i^2} \cdot \left(\frac{2}{\ell\rho_0} \int_0^\ell \rho_1(x) \sin\left(\frac{i\pi x}{\ell}\right) \sin\left(\frac{j\pi x}{\ell}\right) dx\right)^2] + O(\epsilon^3)\}. \quad (1.29)$$

Rayleigh then employs the above analysis to calculate the displacement of the nodal point of the second mode, $i = 2$, (pictured in Figure 1.1: Bottom) which would be located at the midpoint of the string, $x = \frac{\ell}{2}$, if the density were uniform. He proceeds as follows.

For $x = \frac{\ell}{2} + \Delta x$, Equation (1.25) with $i = 2$ may be expanded in a Taylor series about $x = \frac{\ell}{2}$ [31, p. 146]:

$$y_2(\frac{\ell}{2} + \Delta x, t; \epsilon) = \{[\epsilon[x_2^{(1)}]_1 \sin(\frac{\pi}{2}) + \sin(\frac{2\pi}{2}) + \epsilon[x_2^{(1)}]_3 \sin(\frac{3\pi}{2}) + \cdots] + O(\epsilon^2)$$
$$+\Delta x \cdot \frac{\pi}{\ell}[\epsilon[x_2^{(1)}]_1 \cos(\frac{\pi}{2}) + \cos(\frac{2\pi}{2}) + \epsilon[x_2^{(1)}]_3 \cos(\frac{3\pi}{2}) + \cdots] + O(\Delta x \cdot \epsilon^2)$$
$$+O((\Delta x)^2)\} \cdot \sin(\omega_2(\epsilon)t + \psi_2), \quad (1.30)$$

or, upon simplification,

$$y_2(\frac{\ell}{2} + \Delta x, t; \epsilon) = \{\epsilon[[x_2^{(1)}]_1 - [x_2^{(1)}]_3 + \cdots] + O(\epsilon^2)$$
$$+\Delta x \cdot \frac{2\pi}{\ell}[-1 + \epsilon[x_2^{(1)}]_4 - \cdots] + O(\Delta x \cdot \epsilon^2)$$
$$+O((\Delta x)^2)\} \cdot \sin(\omega_2(\epsilon)t + \psi_2). \quad (1.31)$$

For a nodal point, $y_2 = 0$, so that

$$\Delta x = \epsilon \cdot \frac{\ell}{2\pi}\{[x_2^{(1)}]_1 - [x_2^{(1)}]_3 + \cdots\} + O(\epsilon^2 + \Delta x \cdot \epsilon^2 + (\Delta x)^2), \quad (1.32)$$

where, by Equation (1.28),

$$[x_2^{(1)}]_j = \frac{4}{j^2 - 4} \cdot \frac{2}{\ell\rho_0} \int_0^\ell \rho_1(x) \sin\left(\frac{2\pi x}{\ell}\right) \sin\left(\frac{j\pi x}{\ell}\right) dx \ (j \neq 2). \quad (1.33)$$

Next, suppose that the inhomogeneity in density is due to a small load, $\epsilon \cdot \rho_0\lambda$, located at $x = \frac{\ell}{4}$. I.e, $\rho_1(x) = \rho_0\lambda\delta(x - \frac{\ell}{4})$ where $\delta(x - \hat{x})$ is the

δ-function centered at $\hat{x}$ [34, p. 2]. Then, Equation (1.32) becomes:

$$\begin{aligned} \Delta x &\approx \epsilon \cdot \frac{2\lambda}{\pi\sqrt{2}} \left\{ \frac{2}{1^2-4} - \frac{2}{3^2-4} - \frac{2}{5^2-4} + \frac{2}{7^2-4} + \frac{2}{9^2-4} - \cdots \right\} \\ &= -\epsilon \cdot \frac{2\lambda}{\pi\sqrt{2}} \left\{ 1 + \frac{1}{3} - \frac{1}{5} - \frac{1}{7} + \frac{1}{9} + \frac{1}{11} \cdots \right\}. \end{aligned} \tag{1.34}$$

Invocation of the geometric series permits the recognition of the bracketed series in Equation (1.34) as none other than the definite integral:

$$\int_0^1 \frac{1+x^2}{1+x^4}\, dx. \tag{1.35}$$

This definite integral may be evaluated with the aid of [109, Art. 255, p. 227]:

$$\int_0^\infty \frac{x^{s-1}}{1+x^r}\, dx = \frac{\pi}{r \sin\left(\frac{s}{r}\cdot\pi\right)}. \tag{1.36}$$

Setting $r = 4$ and $s = 1, 3$ in Equation (1.36) produces

$$\int_0^\infty \frac{1+x^2}{1+x^4}\, dx = 2 \cdot \frac{\pi}{4\sin\left(\frac{\pi}{4}\right)}. \tag{1.37}$$

However,

$$\int_0^\infty \frac{1+x^2}{1+x^4}\, dx = \int_0^1 \frac{1+x^2}{1+x^4} + \int_1^\infty \frac{1+x^2}{1+x^4} = 2 \cdot \int_0^1 \frac{1+x^2}{1+x^4}\, dx. \tag{1.38}$$

Thus,

$$\int_0^1 \frac{1+x^2}{1+x^4}\, dx = \frac{1}{2} \cdot \int_0^\infty \frac{1+x^2}{1+x^4}\, dx = \frac{\pi}{4\sin\left(\frac{\pi}{4}\right)} = \frac{\pi\sqrt{2}}{4}. \tag{1.39}$$

Hence, by Equation (1.34),

$$\Delta x \approx -\epsilon \cdot \frac{2\lambda}{\pi\sqrt{2}} \cdot \frac{\pi\sqrt{2}}{4} = -\epsilon \cdot \frac{\lambda}{2}. \tag{1.40}$$

Finally, Rayleigh applies his perturbation procedure to the determination of the shifts of natural frequencies due to an inhomogeneity in density resulting from a small load, $\epsilon \cdot \rho_0 \lambda$, located at the midpoint of the string. I.e., $\rho_1(x) = \rho_0 \lambda \delta(x - \frac{\ell}{2})$.

In this case, Equation (1.26) becomes

$$b_i = \frac{1}{2}\ell\rho_0;\ b_{i,i} = \rho_0\lambda \sin^2\left(\frac{i\pi}{2}\right),\ b_{i,j} = \rho_0\lambda \sin\left(\frac{i\pi}{2}\right)\sin\left(\frac{j\pi}{2}\right)\ (j \neq i). \tag{1.41}$$

Thus, if i is even then $b_{i,i} = b_{j,i} = 0$ and Equation (1.29) becomes

$$\lambda_i(\epsilon) = \lambda_i^{(0)} + O(\epsilon^3), \tag{1.42}$$

while, if i is odd then Equation (1.29) becomes

$$\lambda_i(\epsilon) = \lambda_i^{(0)} \cdot \left\{ 1 - \epsilon \cdot \frac{2\lambda}{\ell} + \epsilon^2 \cdot \left(\frac{2\lambda}{\ell}\right)^2 \left[1 - \sum_j{}' \frac{i^2}{j^2 - i^2} \right] + O(\epsilon^3) \right\}, \tag{1.43}$$

where the summation extends over odd j other than i.

Specifically, if $i = 1$ (Figure 1.1: Top) then Equation (1.43) reduces to

$$\lambda_i(\epsilon) = \lambda_i^{(0)} \cdot \left\{ 1 - \epsilon \cdot \frac{2\lambda}{\ell} + \epsilon^2 \cdot \left(\frac{2\lambda}{\ell}\right)^2 \left[1 - \sum_{j=3,5,\ldots} \frac{1}{j^2 - 1} \right] + O(\epsilon^3) \right\}. \tag{1.44}$$

The sum of the series appearing in Equation (1.44) is [45, Series (367), p. 68]:

$$\sum_{j=3,5,\ldots} \frac{1}{j^2 - 1} = \frac{1}{4}, \tag{1.45}$$

so that

$$\lambda_i(\epsilon) = \lambda_i^{(0)} \cdot \left\{ 1 - \epsilon \cdot \frac{2\lambda}{\ell} + \epsilon^2 \cdot \frac{3\lambda^2}{\ell^2} + O(\epsilon^3) \right\}. \tag{1.46}$$

Thus, the perturbed fundamental frequency is given by:

$$\omega_1(\epsilon) = \sqrt{\lambda_1(\epsilon)} = \omega_1^{(0)} \cdot \left[1 - \epsilon \cdot \frac{\lambda}{\ell} + \epsilon^2 \cdot \left(\frac{\lambda}{\ell}\right)^2 + O\left(\left(\epsilon \cdot \frac{\lambda}{\ell} \right)^3 \right) \right], \tag{1.47}$$

where

$$\omega_1^{(0)} = \frac{\pi}{\ell} \cdot \sqrt{\frac{\tau}{\rho_0}};\ f_1^{(0)} = \frac{1}{2\pi} \cdot \omega_1^{(0)} = \frac{1}{2\ell} \cdot \sqrt{\frac{\tau}{\rho_0}}. \tag{1.48}$$

Although Lord Rayleigh played no direct role in the development of quantum mechanics, we will see in the ensuing sections that Erwin Schrödinger adapted and extended his perturbation procedure to the atomic realm. Furthermore, the well-known WKB approximation of quantum mechanics is a variation of Rayleigh's perturbation analysis by Wentzel [100, p. 178].

1.3 Erwin Schrödinger's Life and Times

Unlike Lord Rayleigh and despite their historical proximity, the backdrop for Erwin Schrödinger's life was one of the most tumultuous periods in human history [73]. Whereas Rayleigh lived a life virtually untouched by war or political upheaval, Schrödinger fought in World War I, was geographically displaced during World War II and never knew a life of tranquillity. Scientifically, while Rayleigh was equally at home in both the theoretical and experimental realms, all of Schrödinger's significant contributions were confined to theoretical investigations. If Lord Rayleigh was given to philosophical reflection then he left no record of it while Schrödinger put his psychobiological musings into words in *Mind and Matter* [103].

In their personal lives, Rayleigh and Schrödinger could not have been more unlike. Lord Rayleigh lived a retiring lifestyle cast in the rigid mold of Victorian respectability. In contrast, Schrödinger lived unconventionally with both he and his wife taking lovers outside of their marriage. She had a long term affair with the noted mathematician Hermann Weyl while he moved his mistress (the wife of a friend no less) into their home and sired a child by her. (Although, truth be told, such sexual peccadillos were not unheard of even in Victorian society: witness the lifestyle of Mary Anne Evans, a.k.a. author George Eliot [44]). By all accounts [73, p. 3], Schrödinger's creative impulse was inseparable from his considerable libido. (In this, he is reminiscent of Mozart's great librettist Lorenzo Da Ponte [28].) In his *Autobiographical Sketches* [103], he expressly avoids discussion of his "relationships with women" in order to preclude kindling gossip.

Erwin Schrödinger (1887-1961) was born in Vienna into a financially secure family. His father owned an oilcloth factory and was himself an accomplished botanist. Growing up, he was extremely close to and greatly influenced by his father. He was tutored at home until entering the Gymnasium in Vienna at age 11 where he excelled not only in mathematics and physics but also in classical studies and languages.

At age 19, he entered the University of Vienna where he studied mathematics under Wilhelm Wirtinger, experimental physics under Franz Exner and theoretical physics under Friedrich Hasenöhrl. Four years later, in 1910, he received his doctorate (roughly equivalent to an American Master's degree) under Hasenöhrl with a dissertation titled "On the conduction of electricity on the surface of instruments in moist air".

Immediately upon graduation, he underwent mandatory military training as an officer in the fortress artillery at Krakow. When he returned to Vienna the following year, he became Exner's laboratory assistant and he held this position until the beginning of World War I. During this period, he completed his Habilitation (roughly equivalent to an American Ph.D.) on "Studies on the

Kinetics of Dielectrics, the Melting Point, Pyro- and Piezo-Electricity" and became a Privat Dozent at the beginning of 1914.

Just as he had his foot on the first rung of the academic ladder, World War I broke out later that year and Schrödinger received his mobilization orders. He spent the period 1915-1916 fighting on the Italian front where he was awarded a citation for bravery in action. Remarkably, he was able to continue his scientific work during this period even managing to publish a pair of papers. In 1917, he was transferred back to Vienna for the remainder of the War in order to teach meteorology at a school for anti-aircraft officers and also to teach a laboratory course in physics at the University.

At the conclusion of the War to End All Wars, he resumed his research on optics at the University but not in a "tenure-track" capacity. His personal life underwent a sea change during this time. His father died in 1919 after falling on financially hard times and in 1920 he married Annemarie Bartel. He and his young bride then undertook a year of wandering while he held successive faculty positions at Jena, Stuttgart and Breslau.

In 1921, he was appointed to the faculty at Zurich where he was to stay until 1927. In addition to his work on color theory and statistical thermodynamics during this period, in 1925 he penned his *My View of the World* (published posthumously) where he detailed his belief in the ancient Indian Hindu philosophy of life (Vedanta). Seemingly without warning, his scientific creativity reached its apex.

Leaving his wife in Zurich, he spent Christmas of 1925 at the winter resort of Arosa with a "mystery lover" and spawned his greatest brainchild, wave mechanics. In the words of Hermann Weyl [73, p. 191]: Schrödinger "did his great work during a late erotic outburst in his life". This creative masterpiece was elaborated upon and published during 1926-1927 and will be studied in greater detail in the next section.

Immediately hailed for its pathbreaking nature, this work led to his appointment to succeed Max Planck in the chair of theoretical physics at the University of Berlin. However, due to the declining political situation in Germany, he packed up his wife and Hilde March (his pregnant mistress and wife of his friend and colleague Arthur March) and moved to Oxford in 1933. While in residence there, he shared the 1933 Nobel Prize in Physics with Dirac (Heisenberg was awarded the 1932 Prize) and Hilde gave birth to their daughter, Ruth. (Arthur, Hilde and Ruth March returned to Innsbruck in 1935.)

Homesick for Austria, he spent the years 1936-1938 in Graz. (Hilde and Ruth came to live with them in 1937.) However, the further eroding of the political climate led him to accept the invitation of Irish President Eamon de Valera to establish the Dublin Institute for Advanced Studies modeled after that in Princeton. Here he remained for the next 17 years. (Despite living with both Annemarie and Hilde, he fathered two more children with two different women during this period!)

Not wishing to return to Austria while still under Soviet occupation, it was not until 1956, at age 69, that Schrödinger finally accepted his own chair at the University of Vienna. Thus, he closed out his illustrious career where it had begun. He was the first recipient of a prize bearing his name from the Austrian Academy of Sciences and was also awarded the Austrian Medal for Arts and Science in 1957. That same year, he was accepted into the German Order *Pour le mérite*.

In addition to being granted honorary doctorates from a number of elite universities, he was named a member of many scientific societies, most notably the Pontifical Academy of Sciences, the Royal Society of London, the Prussian (later German) Academy of Sciences and the Austrian Academy of Sciences.

Despite Schrödinger's fascination with the submicroscopic world of quantum mechanics, he was also intimately concerned with "big picture" issues. This is never more evident than in his fascinating book *What is Life?* [103] (the prequel to *Mind and Matter*).

1.4 Schrödinger's Perturbation Theory

Just as 1905 was Einstein's *annus mirabilis* [80], 1926 was to prove to be the apex of Schrödinger's scientific creativity [73]. In six papers published during that year, he created wave mechanics from whole cloth. These *Meisterwerke* were embroidered by three more papers on this topic which appeared the following year. This creative outburst fundamentally altered our viewpoint of the submicroscopic world.

The nexus of the 1926 "Schrödinger six-pack" was the four-part series *Quantisierung als Eigenwertproblem* which appeared in the *Annalen der Physik*. Following [73] (which contains a synopsis of each of the papers on wave mechanics), we will refer to the individual parts as: Q1 (January), Q2 (February), Q3 (May), Q4 (June). Fortunately, all of Schrödinger's writings on wave mechanics are available in full as English translations [102].

A basic problem of the emerging quantum mechanics was to "explain" the observed discrete (as opposed to continuous) energy levels present at the submicroscopic level rather than to introduce them as an *ad hoc* assumption. Following de Broglie and Einstein, Schrödinger took as his inspiration the discrete natural modes of the vibrating string. Since these arose from an eigenvalue problem for the wave equation, he began to search for a wave equation for subatomic particles.

This he succeeded in doing in Q1 where he showed that his wave equation, which he derived using the Hamilton-Jacobi equation of classical mechanics, gave the correct quantization of the energy levels of the hydrogen atom. A second independent derivation based upon the Hamiltonian analogy between mechanics and optics appeared in Q2.

Sandwiched between Q2 and Q3, Schrödinger published two additional papers on wave mechanics. The first demonstrated how particle-like behavior could arise from his wave equation (wave-particle duality) thereby establishing a link between microscopic and macroscopic mechanics. The second showed that his wave mechanics was mathematically equivalent to the competing matrix mechanics of Heisenberg [19].

In Q3 [101, 102], which will be examined in further detail below, Schrödinger developed his extension of Rayleigh's perturbation theory and applied it to explain the Stark effect on the Balmer lines. Lastly, Q4 undertook the task of extending the wave mechanics of stationary systems developed in Q1-3 to systems changing in time. This extended theory was applicable to scattering, absorption and emission of radiation by atoms and molecules and forms the basis for all of chemical kinetics.

A survey of the resulting stationary perturbation theory is available in [26], while the generalization to nonstationary perturbation theory is considered in [56, Section 11.25]. Whereas Rayleigh's perturbation theory as described above employed an energy formulation, it is possible to utilize an alternative formulation directly in terms of the governing differential equation [32]. In fact, his example of the perturbed vibrating string may be so treated [77, Section 3.1.6]. This is precisely the approach taken by Schrödinger.

Just as Rayleigh's assumption of a large but finite number of degrees of freedom leads to the discrete Equation (1.16), the replacement of the differential operators in Schrödinger's formulation by finite-dimensional approximations (finite differences, finite elements etc.) also leads to the matrix generalized eigenvalue problem

$$Ax = \lambda Bx. \tag{1.49}$$

For this reason, after this introductory chapter, the Rayleigh-Schrödinger procedure will be formulated in terms of matrix perturbation theory. An interesting treatment of the limiting case of infinite-dimensional matrix perturbation theory appears in [5, Section 7.5] while [41, Section 1.6] considers the effect of a nonlinear perturbation to the linear problem Equation (1.49).

1.4.1 Ordinary Differential Equations

Schrödinger first considers the effects of a perturbation upon the spectrum of the self-adjoint Sturm-Liouville boundary value problem:

$$\frac{d}{dx}\left(p(x)\frac{dy^{(0)}}{dx}\right) - q(x)y^{(0)}(x) + \lambda^{(0)}\rho(x)y^{(0)}(x) = 0, \tag{1.50}$$

subject to the end-conditions:

$$y^{(0)}(a)\cos(\alpha) - p(a)\frac{dy^{(0)}}{dx}(a)\sin(\alpha) = 0, \tag{1.51}$$

$$y^{(0)}(b)\cos(\beta) - p(b)\frac{dy^{(0)}}{dx}(b)\sin(\beta) = 0; \tag{1.52}$$

where $p(x) > 0$, $p'(x)$, $q(x)$, $\rho(x) > 0$ are assumed continuous on $[a, b]$.

In this case, the eigenvalues, $\lambda_i^{(0)}$, are real and distinct, i. e. the problem is nondegenerate, and the eigenfunctions corresponding to distinct eigenvalues are ρ-orthogonal [21, pp. 211-214]:

$$\langle y_i^{(0)}(x), \rho(x) y_j^{(0)}(x)\rangle = \int_a^b \rho(x) y_i^{(0)}(x) y_j^{(0)}(x)\ dx = 0\ (i \neq j). \tag{1.53}$$

The case of periodic boundary conditions is excluded in order to avoid eigenvalues of multiplicity two while the restriction to a finite interval precludes the possibility of a continuous portion to the spectrum.

Introducing the linear operators:

$$A_0[y^{(0)}(x)] := -\frac{d}{dx}\left(p(x)\frac{dy^{(0)}}{dx}\right) + q(x)y^{(0)}(x);\ B_0[y^{(0)}(x)] := \rho(x)y^{(0)}(x), \tag{1.54}$$

Equation (1.50) may be recast as:

$$A_0[y_i^{(0)}(x)] = \lambda_i^{(0)} B_0[y_i^{(0)}(x)], \tag{1.55}$$

where $\{\lambda_i^{(0)}\}_{i=1}^{\infty}$ is the discrete spectrum and the corresponding eigenfunctions are $\{y_i^{(0)}(x)\}_{i=1}^{\infty}$ which are assumed to have been normalized so that:

$$\langle y_i^{(0)}(x), B_0[y_j^{(0)}(x)]\rangle = \int_a^b \rho(x) y_i^{(0)}(x) y_j^{(0)}(x)\ dx = \delta_{i,j}. \tag{1.56}$$

Furthermore, introduction of the linear operator:

$$A_1[y(x)] := r(x)y(x), \tag{1.57}$$

with $r(x)$ assumed continuous on $[a, b]$, permits consideration of the perturbed boundary value problem:

$$A[y_i(x,\epsilon)] = \lambda_i(\epsilon) B_0[y_i(x,\epsilon)];\ A[\cdot] := A_0[\cdot] + \epsilon A_1[\cdot] \tag{1.58}$$

under identical boundary conditions, where ϵ is a small parameter. Then, perturbation expansions:

$$\lambda_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \lambda_i^{(k)}; \ y_i(x,\epsilon) = \sum_{k=0}^{\infty} \epsilon^k y_i^{(k)}(x) \tag{1.59}$$

are sought for its corresponding eigenvalues and eigenfunctions, respectively.

Before proceeding any further, observe that if we approximate the above linear differential operators by, say, finite differences then the problem reduces to one of finite dimension with A_0 and A_1 replaced by symmetric matrices and B_0 by a symmetric positive-definite matrix. The same is true of the partial differential operators of the next section. This is precisely the subject of Section 4.1 of the present book with the choice $B_1 = 0$.

Inserting the perturbation expansions Equation (1.59) into the eigenvalue problem Equation (1.58) and equating the coefficients of ϵ yields [17, pp. 192-196]:

$$(A_0 - \lambda_i^{(0)} B_0)[y_i^{(1)}(x)] = -(A_1 - \lambda_i^{(1)} B_0)[y_i^{(0)}(x)]. \tag{1.60}$$

In order that Equation (1.60) may have a solution, it is necessary that its right-hand side be orthogonal to the null space of $(A_0 - \lambda_i^{(0)} B_0)$ [33, Theorem 1.5, pp. 44-46], i.e. to $y_i^{(0)}(x)$. Thus,

$$\lambda_i^{(1)} = \langle y_i^{(0)}(x), A_1[y_i^{(0)}(x)]\rangle = \int_a^b r(x)[y_i^{(0)}(x)]^2 \, dx. \tag{1.61}$$

It remains to find $y_i^{(1)}(x)$ from Equation (1.60) which may be accomplished as follows. By Equation (1.56), for $j \neq i$, Equation (1.60) implies that

$$\begin{aligned} \langle y_j^{(0)}(x), (A_0 - \lambda_i^{(0)} B_0)[y_i^{(1)}(x)]\rangle &= -\langle y_j^{(0)}(x), (A_1 - \lambda_i^{(1)} B_0)[y_i^{(0)}(x)]\rangle \\ &= -\langle y_j^{(0)}(x), A_1[y_i^{(0)}(x)]\rangle. \end{aligned} \tag{1.62}$$

The left-hand side of Equation (1.62) may now be rewritten as

$$\begin{aligned} &\langle y_j^{(0)}(x), A_0[y_i^{(1)}(x)]\rangle - \lambda_i^{(0)}\langle y_j^{(0)}(x), B_0[y_i^{(1)}(x)]\rangle = \\ &\langle A_0[y_j^{(0)}(x)], y_i^{(1)}(x)\rangle - \lambda_i^{(0)}\langle y_j^{(0)}(x), B_0[y_i^{(1)}(x)]\rangle = \\ &\lambda_j^{(0)}\langle B_0[y_j^{(0)}(x)], y_i^{(1)}(x)\rangle - \lambda_i^{(0)}\langle y_j^{(0)}(x), B_0[y_i^{(1)}(x)]\rangle = \\ &(\lambda_j^{(0)} - \lambda_i^{(0)})\langle y_j^{(0)}(x), B_0[y_i^{(1)}(x)]\rangle. \end{aligned} \tag{1.63}$$

Thus, Equation (1.62) becomes

$$(\lambda_i^{(0)} - \lambda_j^{(0)})\langle y_j^{(0)}(x), B_0[y_i^{(1)}(x)]\rangle = \langle y_j^{(0)}(x), A_1[y_i^{(0)}(x)]\rangle \tag{1.64}$$

and, since $\lambda_i^{(0)} \neq \lambda_j^{(0)}$ by nondegeneracy,

$$\langle y_j^{(0)}(x), B_0[y_i^{(1)}(x)]\rangle = \frac{\langle y_j^{(0)}(x), A_1[y_i^{(0)}(x)]\rangle}{\lambda_i^{(0)} - \lambda_j^{(0)}}. \tag{1.65}$$

Expanding in the eigenfunctions of the unperturbed problem yields:

$$y_i^{(1)}(x) = \sum_j \langle y_j^{(0)}(x), B_0[y_i^{(1)}(x)]\rangle y_j^{(0)}(x), \tag{1.66}$$

and, invoking the "intermediate normalization":

$$\langle y_i^{(0)}(x), B_0[y_i^{(1)}(x)]\rangle = 0, \tag{1.67}$$

finally produces, via Equation (1.65), the eigenfunction expansion:

$$\begin{aligned} y_i^{(1)}(x) &= \sum_{j \neq i} \frac{\langle y_j^{(0)}(x), A_1[y_i^{(0)}(x)]\rangle}{\lambda_i^{(0)} - \lambda_j^{(0)}} y_j^{(0)}(x) \\ &= \sum_{j \neq i} \frac{\int_a^b r(x) y_i^{(0)}(x) y_j^{(0)}(x)\ dx}{\lambda_i^{(0)} - \lambda_j^{(0)}} y_j^{(0)}(x). \end{aligned} \tag{1.68}$$

In summary, Equations (1.59), (1.61) and (1.68) jointly imply the first-order approximations to the eigenvalues:

$$\lambda_i \approx \lambda_i^{(0)} + \epsilon \cdot \int_a^b r(x)[y_i^{(0)}(x)]^2\ dx, \tag{1.69}$$

and the corresponding eigenfunctions:

$$y_i(x) \approx y_i^{(0)}(x) + \epsilon \cdot \sum_{j \neq i} \frac{\int_a^b r(x) y_i^{(0)}(x) y_j^{(0)}(x)\ dx}{\lambda_i^{(0)} - \lambda_j^{(0)}} y_j^{(0)}(x). \tag{1.70}$$

Schrödinger closes this portion of Q3 with the observation that this technique may be continued to yield higher-order corrections. However, it is important to note that Equation (1.70) requires knowledge of all of the unperturbed eigenfunctions and not just that corresponding to the eigenvalue being corrected. A procedure based upon the pseudoinverse is developed in Chapters 3 and 4 of the present book which obviates this need.

1.4.2 Partial Differential Equations

Schrödinger next extends the perturbation procedure to linear self-adjoint partial differential equations:

$$\mathcal{L}[u^{(0)}(x)] + \lambda^{(0)} \rho(x) u^{(0)}(x) = 0 \tag{1.71}$$

where $x := (x_1, \ldots, x_n) \in \mathcal{D}$, $\mathcal{L}[\cdot]$ is self-adjoint and $\rho(x) > 0$ is continuous on the domain $\mathcal{D}$.

The principal mathematical obstacle that must be overcome in this extension is rooted in the fact that, even for homogeneous Dirichlet, Neumann or Robin boundary conditions, there can appear eigenvalues, $\lambda^{(0)}$, of multiplicity $m > 1$ (i.e., degenerate eigenvalues). These typically arise from symmetry inherent in the boundary value problem (see Chapter 5 for an example).

Introducing the linear operators:

$$A_0[u^{(0)}(x)] := -\mathcal{L}[u^{(0)}(x)]; \;\; B_0[u^{(0)}(x)] := \rho(x)u^{(0)}(x), \tag{1.72}$$

Equation (1.71) may be recast as:

$$A_0[u_i^{(0)}(x)] = \lambda_i^{(0)} B_0[u_i^{(0)}(x)], \tag{1.73}$$

where the eigenfunctions have been B_0-orthonormalized so that:

$$\lambda_i^{(0)} \neq \lambda_j^{(0)} \Rightarrow \langle u_i^{(0)}(x), B_0[u_j^{(0)}(x)] \rangle = \int_{\mathcal{D}} \rho(x) u_i^{(0)}(x) u_j^{(0)}(x) \; dx = \delta_{i,j}. \tag{1.74}$$

Also, suppose now that $\lambda_i^{(0)}$ is an eigenvalue of exact multiplicity $m > 1$ with corresponding B_0-orthonormalized eigenfunctions:

$$u_{i,1}^{(0)}(x), u_{i,2}^{(0)}(x), \ldots, u_{i,m}^{(0)}(x). \tag{1.75}$$

Furthermore, introduction of the linear operator:

$$A_1[u(x)] := r(x)u(x), \tag{1.76}$$

with $r(x)$ assumed continuous on $\mathcal{D}$, permits consideration of the perturbed boundary value problem:

$$A[u_i(x,\epsilon)] = \lambda_i(\epsilon) B_0[u_i(x,\epsilon)]; \;\; A[\cdot] := A_0[\cdot] + \epsilon A_1[\cdot] \tag{1.77}$$

under identical boundary conditions, where ϵ is a small parameter. Then, perturbation expansions:

$$\lambda_{i,\mu}(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \lambda_{i,\mu}^{(k)}; \;\; u_{i,\mu}(x,\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \hat{u}_{i,\mu}^{(k)}(x) \;\; (\mu = 1, \ldots, m), \tag{1.78}$$

with $\lambda_{i,\mu}^{(0)} = \lambda_i^{(0)}$ $(\mu = 1, \ldots, m)$, are sought for its corresponding eigenvalues and eigenfunctions, respectively.

The new difficulty that confronts us is that we cannot necessarily select $\hat{u}_{i,\mu}^{(0)}(x) = u_{i,\mu}^{(0)}(x)$ $(\mu = 1, \ldots, m)$, since they must be chosen so that:

$$(A_0 - \lambda_i^{(0)} B_0)[\hat{u}_{i,\mu}^{(1)}(x)] = -(A_1 - \lambda_{i,\mu}^{(1)} B_0)[\hat{u}_{i,\mu}^{(0)}(x)] \tag{1.79}$$

(obtained by substituting the perturbation expansions Equation (1.78) into the eigenvalue problem Equation (1.77) and equating coefficients of ϵ) is solvable. I.e., $\hat{u}_{i,\mu}^{(0)}(x)$ must be selected so that the right-hand side of Equation (1.79) is orthogonal to the <u>entire</u> nullspace of $(A_0 - \lambda_i^{(0)} B_0)$ [33, Theorem 1.5, pp. 44-46], i.e. to $\{u_{i,\nu}^{(0)}(x)\}_{\nu=1}^{m}$.

Thus, we are required to determine appropriate linear combinations

$$\hat{u}_{i,\mu}^{(0)}(x) = a_1^{(\mu)} u_{i,1}^{(0)}(x) + a_2^{(\mu)} u_{i,2}^{(0)}(x) + \cdots + a_m^{(\mu)} u_{i,m}^{(0)}(x) \ (\mu = 1, \ldots, m) \quad (1.80)$$

so that, for each fixed μ,

$$\langle u_{i,\nu}^{(0)}(x), (A_1 - \lambda_{i,\mu}^{(1)} B_0) \hat{u}_{i,\mu}^{(0)}(x) \rangle = 0 \ (\nu = 1, \ldots, m). \quad (1.81)$$

Since we desire that $\{\hat{u}_{i,\mu}^{(0)}(x)\}_{\mu=1}^{m}$ likewise be B_0-orthonormal, we further require that

$$a_1^{(\mu)} a_1^{(\nu)} + a_2^{(\mu)} a_2^{(\nu)} + \cdots + a_m^{(\mu)} a_m^{(\nu)} = \delta_{\mu,\nu} \ (\mu, \nu = 1, \ldots, m). \quad (1.82)$$

Inserting Equation (1.80) into Equation (1.81) and invoking the B_0-orthonormality of $\{u_{i,\nu}^{(0)}(x)\}_{\nu=1}^{m}$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle u_{i,1}^{(0)}(x), A_1 u_{i,1}^{(0)}(x) \rangle & \cdots & \langle u_{i,1}^{(0)}(x), A_1 u_{i,m}^{(0)}(x) \rangle \\ \vdots & \ddots & \vdots \\ \langle u_{i,m}^{(0)}(x), A_1 u_{i,1}^{(0)}(x) \rangle & \cdots & \langle u_{i,m}^{(0)}(x), A_1 u_{i,m}^{(0)}(x) \rangle \end{bmatrix} \begin{bmatrix} a_1^{(\mu)} \\ \vdots \\ a_m^{(\mu)} \end{bmatrix} = \lambda_{i,\mu}^{(1)} \begin{bmatrix} a_1^{(\mu)} \\ \vdots \\ a_m^{(\mu)} \end{bmatrix}. \quad (1.83)$$

Thus, each $\lambda_{i,\mu}^{(1)}$ is an eigenvalue with corresponding eigenvector $[a_1^{(\mu)}, \ldots, a_m^{(\mu)}]^T$ of the matrix M defined by:

$$M_{\mu,\nu} := \langle u_{i,\mu}^{(0)}(x), A_1 u_{i,\nu}^{(0)}(x) \rangle = \int_{\mathcal{D}} r(x) u_{i,\mu}^{(0)}(x) u_{i,\nu}^{(0)}(x) \ dx \ (\mu, \nu = 1, \ldots, m). \quad (1.84)$$

Assuming that Equation (1.83) has distinct eigenvalues, the degeneracy of $\lambda_i^{(0)}$ is completely resolved at first-order and the analogue of Equation (1.69) with $y_i^{(0)}(x)$ replaced by $\hat{u}_{i,\mu}^{(0)}(x)$, as defined by Equation (1.80), provides the first-order corrections to the eigenvalues $\lambda_{i,\mu}^{(1)}$ $(\mu = 1, \ldots, m)$. However, the procedure for computing the first-order corrections to the eigenfunctions $\hat{u}_{i,\mu}^{(1)}(x)$ is complicated by the need to include the terms associated with $\hat{u}_{i,\nu}^{(0)}(x)$ $(\nu \neq \mu)$ in the eigenfunction expansion analogous to Equation (1.70) [17, pp. 200-202].

The coefficients of these additional terms must be chosen so that:

$$(A_0 - \lambda_i^{(0)} B_0)[\hat{u}_{i,\mu}^{(2)}(x)] = -(A_1 - \lambda_{i,\mu}^{(1)} B_0)[\hat{u}_{i,\mu}^{(1)}(x)] + \lambda_{i,\mu}^{(2)} B_0[\hat{u}_{i,\mu}^{(0)}(x)] \quad (1.85)$$

(obtained by substituting the perturbation expansions Equation (1.78) into the eigenvalue problem Equation (1.77) and equating coefficients of ϵ^2) is solvable. These difficulties are only exacerbated if Equation (1.83) itself has multiple eigenvalues and detailed consideration of such additional complications is deferred until Chapters 3 and 4 of the present book.

1.4.3 Example: The Stark Effect of the Hydrogen Atom

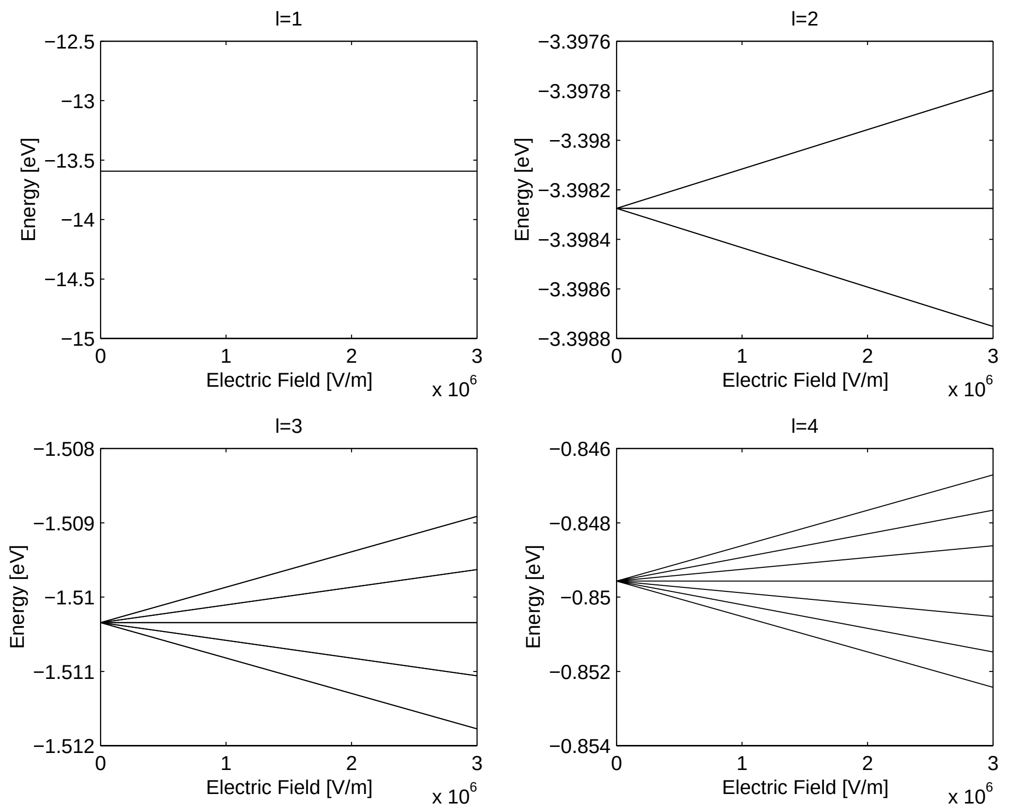

Figure 1.2: First-Order Stark Effect in Hydrogen

Quantum mechanics was born of necessity when it was realized that classical physical theory could not adequately explain the emission of radiation by the Rutherford model of the hydrogen atom [82, p. 27]. Indeed, classical mechanics and electromagnetic theory predicted that the emitted light should contain a wide range of frequencies rather than the observed sharply defined spectral lines (the Balmer lines).

Alternatively, the wave mechanics first proposed by Schrödinger in Q1 [102] assumed a governing wave equation (in Gaussian units)

$$\nabla^2\psi_l^{(0)} + \frac{8\pi^2 m}{h^2}(E_l^{(0)} + \frac{e^2}{r})\psi_l^{(0)} = 0 \ (l = 1, 2, \ldots,), \tag{1.86}$$

where m is the reduced mass of a hydrogen atom, e is the charge of an electron, h is Planck's constant, $r = x^2 + y^2 + z^2$, l are the principal quantum numbers and $E_l^{(0)}$ are the permitted energy levels (eigenvalues). The "meaning" of the corresponding wave functions (eigenfunctions), $\psi_l^{(0)}$, need not concern us.

The energy levels are given (in Gaussian units) by the Balmer formulas

$$E_l^{(0)} = -\frac{2\pi^2 me^4}{h^2 l^2} \ (l = 1, 2, \ldots), \tag{1.87}$$

each with multiplicity l^2, while analytical expressions (involving Legendre functions and Laguerre polynomials) for the corresponding wave functions, $\psi_l^{(0)}$, are available. The Balmer lines arise from transitions between energy levels with $l = 2$ and those with higher values of l. For example, the red H line is the result of the transition from $l = 2$, which is four-fold degenerate, to $l = 3$, which is nine-fold degenerate [73, p. 214].

The Stark effect refers to the experimentally observed shifting and splitting of the spectral lines due to an externally applied electric field. (The corresponding response of the spectral lines to an applied magnetic field is referred to as the Zeeman effect.) Schrödinger applied his degenerate perturbation theory as described above to derive the first-order Stark effect corrections to the unperturbed energy levels.

The inclusion of the potential energy corresponding to a static electric field with strength ϵ oriented in the positive z-direction yields the perturbed wave equation

$$\nabla^2\psi_l^{(0)} + \frac{8\pi^2 m}{h^2}(E_l^{(0)} + \frac{e^2}{r} - \epsilon \cdot ez)\psi_l^{(0)} = 0 \ (l = 1, 2, \ldots). \tag{1.88}$$

Under this small perturbation, each of the unperturbed energy levels, $E_l^{(0)}$ (of multiplicty l^2), bifurcates into the $2l-1$ first-order perturbed energy levels (in Gaussian units)

$$E_{l,k^*} = -\frac{2\pi^2 me^4}{h^2 l^2} - \epsilon \cdot \frac{3h^2 lk^*}{8\pi^2 me} \ (k^* = 0, \pm 1, \ldots, \pm(l-1)), \tag{1.89}$$

each with multiplicity $l - |k^*|$.

The first-order Stark effect is on prominent display in Figure 1.2 for the first four unperturbed energy levels (in SI units). Fortunately, the first-order corrections to the energy levels given by Equation (1.89) coincide with those given by the so-called Epstein formula for the Stark effect. This coincidence was an important certification of Schrödinger's perturbation procedure since the very existence of the requisite perturbation series was not rigorously established by Rellich until 1936 (see Appendix A).

Since its appearance in 1926, the Rayleigh-Schrödinger perturbation procedure as described in Q3 has been extended and applied to a variety of other problems in quantum mechanics as well as to physics in general. Indeed, its general utility in science and engineering is the *raison d'être* for the present book.

In retrospect, Schrödinger's treatment of nondegenerate problems was not essentially different from that of Rayleigh (a debt which is readily acknowledged in the second paragraph of Q3). Hence, his major contribution in this area was the insight into how to handle the degeneracies which naturally arise in the presence of symmetry. As such, this is one of those all too rare instances in the mathematical sciences where the names attached to an important principle are entirely appropriate.

1.5 Further Applications of Matrix Perturbation Theory

Thus far in this chapter, we have encountered two substantial applications of matrix perturbation theory (the nonuniform vibrating string and the Stark effect on the Balmer lines). Chapter 5 is devoted to a third such application of the Rayleigh-Schrödinger perturbation theory as developed in Chapters 3 an 4 (inhomogeneous acoustic waveguides). We conclude this introductory chapter by surveying two other important applications of matrix perturbation theory in engineering. Clearly, the intent is not to be exhaustive but merely to intimate the diverse nature of such applications. Many others are considered in [99, Chapter X].

1.5.1 Microwave Cavity Resonators

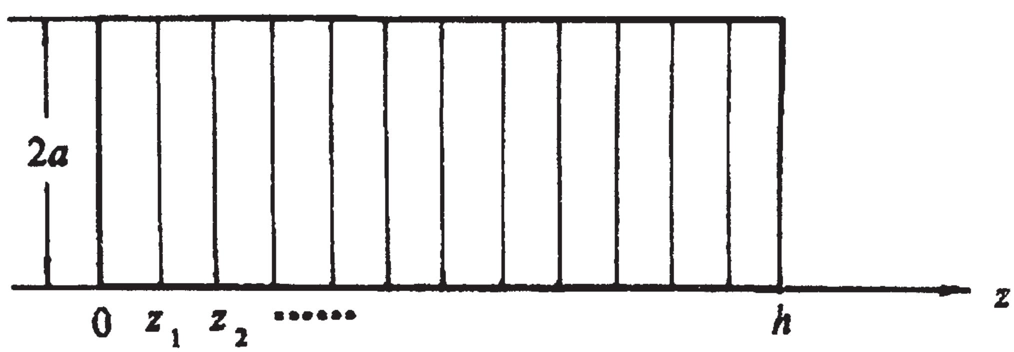

Figure 1.3: Cavity Resonator

The Rayleigh-Schrödinger perturbation procedure is of great utility throughout electrical engineering. As an example [25], consider a circular cavity resonator of radius a and length h as displayed in Figure 1.3. This is a metal enclosure that is used to store microwave (or, for that matter, acoustic) energy.

In the transverse cross-section of the cavity, the electromagnetic field modes coincide with those of the corresponding circular waveguide of radius a while the longitudinal component (i.e., the z-component), u, of the magnetic field for a TE-mode satisfies the two-point boundary value problem [46]:

$$\frac{d^2u}{dz^2} + (k_0^2 - k_c^2)u = 0 \ (0 < z < h); \ u(0) = 0 = u(h), \tag{1.90}$$

where k_0 is the desired resonant wave number and k_c is the cut-off wave number of a particular TE circular waveguide mode (and consequently a known function of a).

If we discretize Equation (1.90) by subdividing $0 \leq z \leq h$ into n equally spaced panels, as indicated in Figure 1.3, and approximate the differential operator using central differences [22] then we immediately arrive at the standard matrix eigenvalue problem:

$$Au = \lambda u; \ A := \text{tridiag}(-1/d^2, W/d^2, -1/d^2), \tag{1.91}$$

where $d = h/n$, $W = k_c^2 d^2 + 2$ and $\lambda = k_0^2$.

Following Cui and Liang [25], the Rayleigh-Schrödinger procedure may now be employed to study the variation of λ and u when the system is subjected to perturbations in a and h thereby producing the alteration $A(\epsilon) = A_0 + \epsilon \cdot A_1$:

$$\lambda(\epsilon) \approx \lambda^{(0)} + \epsilon \cdot \lambda^{(1)}; \; u(\epsilon) \approx u^{(0)} + \epsilon \cdot u^{(1)}. \tag{1.92}$$

For $n = 150$, they report that, when the variation of the geometric parameters is less than 10%, the error in the calculated first-order corrections is less than 1% while yielding an eight-fold increase in computational efficiency as opposed to directly solving the perturbed matrix eigenproblem Equation (1.91).

It should be pointed out that the above problem could be analytically solved in its entirety without recourse to a perturbation procedure. However, it was chosen precisely to illustrate the procedure in its simplest context. Such perturbation procedures may be readily adapted to more complicated problems, such as those involving small inhomogeneities within the cavity, where analytical treatment is not viable [111, p. 326-330].

1.5.2 Structural Dynamic Analysis

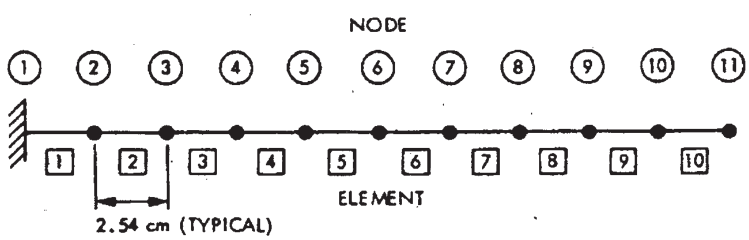

Figure 1.4: Cantilever Beam

The Rayleigh-Schrödinger perturbation procedure is of great utility throughout mechanical engineering. As an example [20], consider a cantilever beam which has been discretized into ten finite elements as displayed in Figure 1.4. The analysis of the vibration of the beam is thereby reduced to the study of the motion of a system of coupled oscillators located at the nodes.

If $x_i(t)$ denotes the vertical displacement of node i, while the beam is undergoing a free, undamped vibration, then the system of differential equations governing this basic problem of structural dynamics may be expressed as [108]:

$$M\ddot{x}(t) + Kx(t) = 0; \; x(t) := [x_2(t), \ldots, x_{11}(t)]^T, \tag{1.93}$$

where M is the symmetric, positive-definite mass matrix and K is the symmetric stiffness matrix.

Due to the linearity of this system of equations, this mechanical structure may be completely analyzed by seeking simple-harmonic motions which are in-phase with one another:

$$x(t) = e^{\imath\omega t} \cdot \phi, \tag{1.94}$$

thereby transforming Equation (1.93) into the matrix generalized eigenvalue problem:

$$K\phi = \lambda M\phi;\ \lambda := -\omega^2, \tag{1.95}$$

with natural angular frequencies ω and corresponding modal shapes ϕ.

Following Chen and Wada [20], the Rayleigh-Schrödinger procedure may now be employed to study the variation of λ and ϕ when the system is subjected to perturbations in the mass ($M(\epsilon) = M_0 + \epsilon \cdot M_1$) and stiffness ($K(\epsilon) = K_0 + \epsilon \cdot K_1$) matrices:

$$\lambda(\epsilon) \approx \lambda^{(0)} + \epsilon \cdot \lambda^{(1)};\ \phi(\epsilon) \approx \phi^{(0)} + \epsilon \cdot \phi^{(1)}. \tag{1.96}$$

They report that, when the variation of the structural parameters is such as to produce a change in ω of approximately 11% (on average), the error in the calculated first-order corrections is approximately 1.3%. They also consider the inclusion of damping but, as this leads to a quadratic eigenvalue problem, we refrain from considering this extension.

Chapter 2

The Moore-Penrose Pseudoinverse

2.1 History

The (unique) solution to the nonsingular system of linear equations

$$A^{n\times n}x^{n\times 1} = b^{n\times 1};\ \det(A) \neq 0 \tag{2.1}$$

is given by

$$x = A^{-1}b. \tag{2.2}$$

The (Moore-Penrose) pseudoinverse, $A^\dagger$, permits extension of the above to singular square and even rectangular coefficient matrices A [12].

This particular generalized inverse was first proposed by Moore in abstract form in 1920 [71] with details appearing only posthumously in 1935 [72]. It was rediscovered first by Bjerhammar in 1951 [9] and again independently by Penrose in 1955 [84, 85] who developed it in the form now commonly accepted. In what follows, we will simply refer to it as the pseudoinverse.

The pseudoinverse, $A^\dagger$, may be defined implicitly by:

Theorem 2.1.1 (Penrose Conditions). *Given $A \in \mathbb{R}^{m\times n}$, there exists a unique $A^\dagger \in \mathbb{R}^{n\times m}$ satisfying the four conditions:*

1. $AA^\dagger A = A$
2. $A^\dagger AA^\dagger = A^\dagger$
3. $(AA^\dagger)^T = AA^\dagger$
4. $(A^\dagger A)^T = A^\dagger A$

Both the existence and uniqueness portions of Theorem 2.1.1 will be proved in Section 2.6 where an explicit expression for $A^\dagger$ will be developed.

2.2 Matrix Theory Fundamentals

The reader is assumed to be familiar with the basic notions of linear algebra and matrix theory as presented in [3, 7, 43, 49, 50, 68, 78]. A particular favorite of the present author is [79] and the parenthetical numbers in the following (partial) list of prerequisite concepts refer to its page numbers.

- triangular matrix (2); transpose (13); symmetry (15); inverse (21)
- determinant (159); linear combination (179); (real) vector space (182)
- subspace (184); span (188); linear independence/dependence (190)
- basis (196); dimension (198); row/column space (211); rank (211)
- inner product (222); norm (223); orthogonality (224)
- orthogonal projection (226); Gram-Schmidt orthonormalization (229)
- null space (252); orthogonal complement (257); orthogonal matrix (305)

The following notation will be adhered to in the remainder of this chapter.

NOTATION	**DEFINITION**
$\mathbb{R}^n$	space of real column vectors with n rows
$\mathbb{R}^{m\times n}$	space of real matrices with m rows and n columns
$[A\|B]$	partitioned matrix
$< \cdot,\cdot >$	Euclidean inner product
$\|\|\cdot\|\|$	Euclidean norm
$\dim(S)$	dimension of S
$\mathcal{R}(A)/\mathcal{R}(A^T)/\mathcal{N}(A)$	column/row/null space of A
P_S^u	(orthogonal) projection of vector u onto subspace S
P_A	projection matrix onto column space of A
$S^\perp$	orthogonal complement of subspace S
$\sigma(A)$	spectrum of matrix A
e_k	k^{th} column of identity matrix I

Table 2.1: Notational Glossary

In the ensuing sections, we will have need to avail ourselves of the following elementary results.

Theorem 2.2.1 (Linear Systems). *Consider the linear system of equations* $A^{m\times n}x^{n\times 1} = b^{m\times 1}$.

1. *They are consistent iff* $b \in \mathcal{R}(A)$.

2. *They are consistent* $\forall\ b \in \mathbb{R}^m$ *iff* $\mathcal{R}(A) = \mathbb{R}^m$ *(so* $m \leq n$*).*

3. *There exists at most one solution* $\forall\ b \in \mathbb{R}^m$ *iff the column vectors of* A *are linearly independent, i.e. iff* $rank\,(A) = n$ $(\leq m)$.

Proof: This is a tautology based upon the definitions of the above terms. □

Corollary 2.2.1 (Nonsingular Matrices).

$m = n \Rightarrow A$ *is nonsingular iff the column vectors of* A *form a basis for* $\mathbb{R}^m$.

Theorem 2.2.2 (Solutions of Nonhomogeneous Systems). *If* x_p *is a particular solution of* $Ax = b$ *then any such solution is of the form* $x = x_p + x_h$ *where* x_h *is a solution to the corresponding homogeneous system* $Ax = 0$.

Proof: $A\underbrace{(x - x_p)}_{x_h} = Ax - Ax_p = b - b = 0$. $x_p + x_h = x_p + x - x_p = x$. □

2.3 Projection Matrices

Theorem 2.3.1 (Cross Product Matrix). *Define the cross product matrix* A^TA. *Then,* $\mathcal{N}(A^TA) = \mathcal{N}(A)$.

Proof:

- $x \in \mathcal{N}(A) \Rightarrow Ax = 0 \Rightarrow A^TAx = 0 \Rightarrow x \in \mathcal{N}(A^TA)$.

- $x \in \mathcal{N}(A^TA) \Rightarrow A^TAx = 0 \Rightarrow x^TA^TAx = 0 \Rightarrow ||Ax||^2 = 0 \Rightarrow Ax = 0 \Rightarrow x \in \mathcal{N}(A)$.

Thus, $\mathcal{N}(A^TA) = \mathcal{N}(A)$. □

Theorem 2.3.2 ($\mathbf{A^TA}$ Theorem). *If* $A \in \mathbb{R}^{m\times n}$ *has linearly independent columns (i.e.* $k := rank(A) = n$ $(\leq m)$*) then* A^TA *is square, symmetric and invertible.*

Proof:

- $\overbrace{A^T}^{n\times m}\overbrace{A}^{m\times n} \in \mathbb{R}^{n\times n}$.

- $(A^TA)^T = A^T(A^T)^T = A^TA$. (Note: $A^TA \neq AA^T$.)

- rank $(A) = n \Rightarrow \mathcal{N}(A) = \{0\} \Rightarrow \mathcal{N}(A^TA) = \{0\}$. Thus, the columns of A^TA are linearly independent and, since A^TA is square, A^TA is invertible. □

Corollary 2.3.1 (Normal Equations). *Suppose that* $Ax = b$*, where* $A \in \mathbb{R}^{m \times n}$*, and that the columns of* A *are linearly independent (*$\Rightarrow \text{rank}(A) = n \leq m$*). Then,*

$$\overbrace{A^T A}^{invertible}\; x = A^T b \text{ (normal equations)} \Rightarrow$$

$$x = (A^T A)^{-1} A^T b \text{ (``least squares'' solution).}$$

Theorem 2.3.3 (Projection onto a Subspace Spanned by Orthonormal Vectors). *Suppose that* V *is a subspace of* $\mathbb{R}^m$ *spanned by the orthonormal basis* $S := \{v_1, \ldots, v_n\}$ *(so that* $n \leq m$*) and* $v \in \mathbb{R}^m$*. Define* $Q^{m \times n} := [v_1|v_2|\cdots|v_n]$*. The orthogonal projection of the vector* v *onto the subspace* V *is given by:*

$$P_V^v = \overbrace{QQ^T}^{P^{m \times m}}\, v.$$

Proof:

$$\begin{aligned} P_V^v &= \langle v_1, v\rangle v_1 + \cdots + \langle v_n, v\rangle v_n \\ &= [v_1|\cdots|v_n] \begin{bmatrix} \langle v_1, v\rangle \\ \vdots \\ \langle v_n, v\rangle \end{bmatrix} \\ &= [v_1|\cdots|v_n] \begin{bmatrix} v_1^T \\ \hline \vdots \\ \hline v_n^T \end{bmatrix} v \\ &= QQ^T v = Pv. \end{aligned}$$

Note that $Q^T Q = I^{n \times n}$. $\square$

Example 2.3.1 (Projection onto Orthonormal Vectors).

$$Q := [v_1|v_2] = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{3} \\ -1/\sqrt{2} & 1/\sqrt{3} \\ 0 & 1/\sqrt{3} \end{bmatrix} \Rightarrow P := QQ^T = \begin{bmatrix} 5/6 & -1/6 & 2/6 \\ -1/6 & 5/6 & 2/6 \\ 2/6 & 2/6 & 2/6 \end{bmatrix}$$

$$v = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \Rightarrow Pv = \begin{bmatrix} 3/2 \\ 5/2 \\ 2 \end{bmatrix} = -\frac{1}{\sqrt{2}} v_1 + 2\sqrt{3} v_2$$

Theorem 2.3.4 (Properties of $\mathbf{P = QQ^T}$). $P^{m \times m} := QQ^T$ *where* $Q^T Q = I^{n \times n}$ *satisfies:*

1. $P^T = P$

2. $P^2 = P$ *(i.e. P is idempotent)*

3. $P(I - P) = (I - P)P = 0$

4. $(I - P)Q = 0$

5. $PQ = Q$

Proof:

1. $P^T = (QQ^T)^T = (Q^T)^T Q^T = QQ^T = P$

2. $P^2 = QQ^T QQ^T = QIQ^T = QQ^T = P$

3. $P - P^2 = P - P = 0$

4. $Q - PQ = Q - QQ^T Q = Q - IQ = Q - Q = 0$

5. $PQ = QQ^T Q = QI = Q$

□

Definition 2.3.1 (Projection Matrix). *$P \in \mathbb{R}^{m\times m}$ is a projection matrix if $(b - Pb)^T Pc = 0 \ \forall \ b, c \in \mathbb{R}^m$.*

Remark 2.3.1 (Rationale). *$b - Pb$ is the error in mapping b onto $\mathcal{R}(P)$, while any element of $\mathcal{R}(P)$ may be represented as Pc. So, if $b - Pb \ \perp Pc$ $\forall \ c \in \mathbb{R}^m$ then $Pb = P^b_{\mathcal{R}(P)}$.*

Theorem 2.3.5 (Projection Matrix Theorem). *$P \in \mathbb{R}^{m\times m}$ is a projection matrix iff*

1. $P = P^T$

2. $P^2 = P$

Proof:

- $(\Rightarrow)$ $P \in \mathbb{R}^{m\times m}$ is a projection matrix $\Rightarrow b^T Pc = b^T P^T Pc \ \forall \ b, c \in \mathbb{R}^m$. Let $b = e_i$ & $c = e_j$, then $P_{i,j} = (P^T P)_{i,j}$, so that $P = P^T P$. Thus, $P^T = P^T P = P \Rightarrow P = P^T P = P^2$.

- $(\Leftarrow)$ $P = P^T$ & $P^2 = P \Rightarrow (b - Pb)^T Pc = b^T (I - P)^T Pc = b^T (I - P^T) Pc$ $= b^T (P - P^T P)c = b^T (P - P^2)c = b^T (P - P)c = 0$.

□

Corollary 2.3.2. *By combining Theorem 2.3.4 with Theorem 2.3.5,* $P \in \mathbb{R}^{m\times m} = QQ^T$ *where* $Q^TQ = I^{n\times n}$ *is a projection matrix.*

Theorem 2.3.6 (Projection onto a Subspace Spanned by Independent Vectors). *Suppose that the columns of* $A^{m\times n}$ *are linearly independent (i.e.* $\mathrm{rank}\,(A) = n\ (\leq m)$*). Then,* $P^{m\times m} := A(A^TA)^{-1}A^T$ *is the projection matrix onto the column space of* A*,* $\mathcal{R}(A)$*.*

Proof: $Pb = A\left[(A^TA)^{-1}A^Tb\right] \in \mathcal{R}(A)$. It is a projection matrix since:

1. $P^T = \left[A(A^TA)^{-1}A^T\right]^T = A(A^TA)^{-1}A^T = P$,

2. $P^2 = A\underbrace{(A^TA)^{-1}A^TA}_{I}(A^TA)^{-1}A^T = A(A^TA)^{-1}A^T = P.$

□

Remark 2.3.2 (Column-Orthonormal Matrices). *If the columns of* $A^{m\times n}$ *are orthonormal then* $A = Q$ *where* $Q^TQ = I^{n\times n}$ *and* $P = Q(Q^TQ)^{-1}Q^T = QI^{-1}Q^T = QQ^T$*. I.e., Theorem 2.3.6 reduces to Theorem 2.3.3 in this case.*

Example 2.3.2 (Projection onto Independent Vectors).

$$A := [v_1|v_2] = \begin{bmatrix} 1 & 1 \\ -1 & 1 \\ 1 & 1 \end{bmatrix} \Rightarrow P := A(A^TA)^{-1}A^T = \begin{bmatrix} 1/2 & 0 & 1/2 \\ 0 & 1 & 0 \\ 1/2 & 0 & 1/2 \end{bmatrix}$$

$$v = \begin{bmatrix} 2 \\ 3 \\ 4 \end{bmatrix} \Rightarrow Pv = \begin{bmatrix} 3 \\ 3 \\ 3 \end{bmatrix} = 0v_1 + 3v_2$$

Remark 2.3.3 (Open Question). *If the columns of* A *are linearly dependent then how does one write down a projection matrix onto the column space of* A*,* $\mathcal{R}(A)$*? Observe that the formula* $P = A(A^TA)^{-1}A^T$ *is useless in this regard as* A^TA *is not invertible! (Since the columns of* A *are linearly dependent, Theorem 2.3.1 demands that* $\mathcal{N}(A^TA) = \mathcal{N}(A) \neq \{0\}$*.)*

2.4 QR Factorization

Before the Open Question can be answered, the QR factorization must be reviewed [29, 68, 79, 104, 105, 110].

Definition 2.4.1 (Gram-Schmidt Orthonormalization: Independent Vectors). *Consider the collection of linearly independent vectors* $\{v_1, \ldots, v_n\} \subset \mathbb{R}^m$ $(m \geq n)$*. The Gram-Schmidt procedure [79, pp. 229-232] may be applied to produce an orthonormal set of vectors* $\{w_1, \ldots, w_n\} \subset \mathbb{R}^m$ *with the same span as the original collection. This procedure (based upon subtracting off components via orthogonal projection) is embodied in the sequence of formulae:*

$$w_1 = v_1; \; q_1 = w_1 / \underbrace{||w_1||}_{r_{1,1}}$$

$$w_2 = v_2 - \overbrace{\langle v_2, q_1 \rangle}^{r_{1,2}} q_1; \; q_2 = w_2 / \underbrace{||w_2||}_{r_{2,2}}$$

$$w_3 = v_3 - \overbrace{\langle v_3, q_1 \rangle}^{r_{1,3}} q_1 - \overbrace{\langle v_3, q_2 \rangle}^{r_{2,3}} q_2; \; q_3 = w_3 / \underbrace{||w_3||}_{r_{3,3}}$$

$$\vdots$$

$$w_n = v_n - \overbrace{\langle v_n, q_1 \rangle}^{r_{1,n}} q_1 - \cdots - \overbrace{\langle v_n, q_{n-1} \rangle}^{r_{n-1,n}} q_{n-1}; \; q_n = w_n / \underbrace{||w_n||}_{r_{n,n}}$$

Definition 2.4.2 (QR Factorization: Independent Columns). *The above Gram-Schmidt formulae may be rearranged to read:*

$$v_1 = r_{1,1} \; q_1$$

$$v_2 = r_{1,2} \; q_1 + r_{2,2} \; q_2$$

$$v_3 = r_{1,3} \; q_1 + r_{2,3} \; q_2 + r_{3,3} \; q_3$$

$$\vdots$$

$$v_n = r_{1,n} \; q_1 + \cdots + r_{n,n} \; q_n$$

These equations may then be expressed in matrix form as

$$A^{m \times n} = Q^{m \times n} R^{n \times n}$$

where

$$A := [v_1 | \cdots | v_n]; \; Q := [q_1 | \cdots | q_n]; \; R_{i,j} = r_{i,j} \; (i \leq j).$$

Remark 2.4.1 (Remarks on Full Column Rank QR Factorization). *With $A = QR$ defined as above:*

- *R is upper triangular with positive diagonal elements.*
- *Q is column-orthonormal, i.e. $Q^T Q = I$.*
- *$rank\,(A) = rank\,(Q) = rank\,(R) = n$.*

Example 2.4.1 (QR: Independent Columns).

$$A := [v_1|v_2|v_3] = \begin{bmatrix} 1 & -1 & 4 \\ 1 & 4 & -2 \\ 1 & 4 & 2 \\ 1 & -1 & 0 \end{bmatrix} \Rightarrow$$

$$w_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \Rightarrow ||w_1|| = \overbrace{2}^{r_{1,1}} \Rightarrow q_1 = \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix}$$

$$w_2 = \begin{bmatrix} -1 \\ 4 \\ 4 \\ -1 \end{bmatrix} - \overbrace{3}^{r_{1,2}} \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix} = \begin{bmatrix} -5/2 \\ 5/2 \\ 5/2 \\ -5/2 \end{bmatrix} \Rightarrow ||w_2|| = \overbrace{5}^{r_{2,2}} \Rightarrow q_2 = \begin{bmatrix} -1/2 \\ 1/2 \\ 1/2 \\ -1/2 \end{bmatrix}$$

$$w_3 = \begin{bmatrix} 4 \\ -2 \\ 2 \\ 0 \end{bmatrix} - \overbrace{2}^{r_{1,3}} \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ 1/2 \end{bmatrix} - \overbrace{(-2)}^{r_{2,3}} \begin{bmatrix} -1/2 \\ 1/2 \\ 1/2 \\ -1/2 \end{bmatrix} = \begin{bmatrix} 2 \\ -2 \\ 2 \\ -2 \end{bmatrix} \Rightarrow$$

$$||w_3|| = \overbrace{4}^{r_{3,3}} \Rightarrow q_3 = \begin{bmatrix} 1/2 \\ -1/2 \\ 1/2 \\ -1/2 \end{bmatrix}$$

$$\Rightarrow QR = \begin{bmatrix} 1/2 & -1/2 & 1/2 \\ 1/2 & 1/2 & -1/2 \\ 1/2 & 1/2 & 1/2 \\ 1/2 & -1/2 & -1/2 \end{bmatrix} \begin{bmatrix} 2 & 3 & 2 \\ 0 & 5 & -2 \\ 0 & 0 & 4 \end{bmatrix}$$

Definition 2.4.3 (QR Factorization: Dependent Columns). *If $A^{m\times n}$ has $rank\,(A) = k < n$ then the (suitably modified) Gram-Schmidt procedure will produce $A = Q_0 R_0$ with some zero columns in Q_0 with matching zero rows in R_0. Deleting these zero columns and rows produces*

$$A^{m\times n} = Q^{m\times k} R^{k\times n}$$

where

- *R is upper triangular with positive leading elements in each row.*
- *Q is column-orthonormal, i.e. $Q^T Q = I^{k\times k}$.*
- *$rank\,(A) = rank\,(Q) = rank\,(R) = k$.*

Example 2.4.2 (QR: Dependent Columns).

$$A := [v_1|v_2|v_3|v_4] = \begin{bmatrix} 1 & 2 & 0 & -1 \\ 1 & -1 & 3 & 2 \\ 1 & -1 & 3 & 2 \\ -1 & 1 & -3 & 1 \end{bmatrix} \Rightarrow$$

$$w_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ -1 \end{bmatrix} \Rightarrow ||w_1|| = \overbrace{2}^{r_{1,1}} \Rightarrow q_1 = \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ -1/2 \end{bmatrix}$$

$$w_2 = \begin{bmatrix} 2 \\ -1 \\ -1 \\ 1 \end{bmatrix} - \overbrace{(-1/2)}^{r_{1,2}} \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ -1/2 \end{bmatrix} = \begin{bmatrix} 9/4 \\ -3/4 \\ -3/4 \\ 3/4 \end{bmatrix} \Rightarrow$$

$$||w_2|| = \overbrace{(3\sqrt{3}/2)}^{r_{2,2}} \Rightarrow q_2 = \begin{bmatrix} 3/2\sqrt{3} \\ -1/2\sqrt{3} \\ -1/2\sqrt{3} \\ 1/2\sqrt{3} \end{bmatrix}$$

$$w_3 = \begin{bmatrix} 0 \\ 3 \\ 3 \\ -3 \end{bmatrix} - \overbrace{9/2}^{r_{1,3}} \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ -1/2 \end{bmatrix} - \overbrace{(-3\sqrt{3}/2)}^{r_{2,3}} \begin{bmatrix} 3/2\sqrt{3} \\ -1/2\sqrt{3} \\ -1/2\sqrt{3} \\ 1/2\sqrt{3} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \Rightarrow$$

$$||w_3|| = \overbrace{0}^{r_{3,3}} \Rightarrow q_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$

$$w_4 = \begin{bmatrix} -1 \\ 2 \\ 2 \\ 1 \end{bmatrix} - \overbrace{1}^{r_{1,4}} \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \\ -1/2 \end{bmatrix} - \overbrace{(-\sqrt{3})}^{r_{2,4}} \begin{bmatrix} 3/2\sqrt{3} \\ -1/2\sqrt{3} \\ -1/2\sqrt{3} \\ 1/2\sqrt{3} \end{bmatrix} - \overbrace{0}^{r_{3,4}} \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 1 \\ 2 \end{bmatrix} \Rightarrow$$

$$||w_4|| = \overbrace{\sqrt{6}}^{r_{4,4}} \Rightarrow q_4 = \begin{bmatrix} 0 \\ 1/\sqrt{6} \\ 1/\sqrt{6} \\ 2/\sqrt{6} \end{bmatrix}$$

$$\Rightarrow Q_0 R_0 = \begin{bmatrix} 1/2 & 3/2\sqrt{3} & 0 & 0 \\ 1/2 & -1/2\sqrt{3} & 0 & 1/\sqrt{6} \\ 1/2 & -1/2\sqrt{3} & 0 & 1/\sqrt{6} \\ -1/2 & 1/2\sqrt{3} & 0 & 2/\sqrt{6} \end{bmatrix} \begin{bmatrix} 2 & -1/2 & 9/2 & 1 \\ 0 & 3\sqrt{3}/2 & -3\sqrt{3}/2 & -\sqrt{3} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{6} \end{bmatrix}$$

$$\Rightarrow QR = \begin{bmatrix} 1/2 & 3/2\sqrt{3} & 0 \\ 1/2 & -1/2\sqrt{3} & 1/\sqrt{6} \\ 1/2 & -1/2\sqrt{3} & 1/\sqrt{6} \\ -1/2 & 1/2\sqrt{3} & 2/\sqrt{6} \end{bmatrix} \begin{bmatrix} 2 & -1/2 & 9/2 & 1 \\ 0 & 3\sqrt{3}/2 & -3\sqrt{3}/2 & -\sqrt{3} \\ 0 & 0 & 0 & \sqrt{6} \end{bmatrix}$$

Remark 2.4.2 (QR Factorization: Summary). *If $A^{m\times n}$ has $rank\,(A) = k$ then*

$$A^{m\times n} = Q^{m\times k} R^{k\times n}$$

where $rank\,(A) = rank\,(Q) = rank\,(R) = k$.

We are now in a position to answer our Open Question (Remark 2.3.3).

Theorem 2.4.1 (Projection onto a Subspace Spanned by Dependent Vectors). *With A, Q and R as described above,*

$$A = QR \Rightarrow P_A = QQ^T,$$

where P_A is the projection matrix onto the column space of A, $\mathcal{R}(A)$.
Proof:

- $A = QR \Rightarrow \mathcal{R}(A) \subseteq \mathcal{R}(Q)$ since $Ax = Q(Rx)$.
- Since $\text{rank}\,(A) = \text{rank}\,(Q)$, their column spaces have the same dimension. Thus, $\mathcal{R}(A) = \mathcal{R}(Q)$.
- Hence, the columns of Q form an orthonormal basis for $\mathcal{R}(A)$ so that $P_A = QQ^T$.

□

Example 2.4.3 (Projection onto Dependent Vectors).

$$A = \begin{bmatrix} 1 & 2 & 0 & -1 \\ 1 & -1 & 3 & 2 \\ 1 & -1 & 3 & 2 \\ -1 & 1 & -3 & 1 \end{bmatrix} \Rightarrow$$

$$QR = \begin{bmatrix} 1/2 & 3/2\sqrt{3} & 0 \\ 1/2 & -1/2\sqrt{3} & 1/\sqrt{6} \\ 1/2 & -1/2\sqrt{3} & 1/\sqrt{6} \\ -1/2 & 1/2\sqrt{3} & 2/\sqrt{6} \end{bmatrix} \begin{bmatrix} 2 & -1/2 & 9/2 & 1 \\ 0 & 3\sqrt{3}/2 & -3\sqrt{3}/2 & -\sqrt{3} \\ 0 & 0 & 0 & \sqrt{6} \end{bmatrix} \Rightarrow$$

$$P_A = QQ^T = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 1/2 & 1/2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Remark 2.4.3 (MATLAB qr). *[39, pp. 113-114]; [70, pp. 147-149]*

If $\text{rank}\,(A^{m\times n}) = k$ then the MATLAB command:

$$[q, r] = qr(A)$$

produces the output:

$$q^{m\times m} = [Q^{m\times k} \mid Q_e^{m\times(m-k)}];\; r^{m\times n} = \left[\begin{array}{c} R^{k\times n} \\ \hline 0^{(m-k)\times n} \end{array} \right].$$

The columns of Q form an orthonormal basis for $\mathcal{R}(A)$ while those of the matrix of extra columns, Q_e, form an orthonormal basis for $\mathcal{R}(A)^{\perp}$. Thus,

$$Q = q(:, 1 : k);\; R = r(1 : k, :).$$

2.5 Least Squares Approximation

The QR factorization will now be employed to develop least squares approximations to linear systems of equations [10, 51, 79].

Definition 2.5.1 (Problem LS). *Given* $A \in \mathbb{R}^{m \times n}$*, with* $k = \text{ rank}\,(A) \leq \min\,(m, n)$*, and* $b \in \mathbb{R}^m$*, find* $x \in \mathbb{R}^n$ *minimizing the Euclidean length of the residual* $||r||_2 := ||b - Ax||_2$*.*

We will abbreviate Problem LS as:

$$Ax \cong b. \tag{2.3}$$

Definition 2.5.2 (Problem LS$_{\textbf{min}}$). *Given*

$$Ax \cong b:$$

- *If there is a* <u>*unique solution*</u>*, then find it.*
- *If there are* <u>*infinitely many solutions*</u>*, then find the one of minimum 2-norm.*
- *If there is* <u>*no solution*</u>*, then find an* x *that minimizes the 2-norm of the residual* $r := b - Ax$*. If this* x *is not uniquely defined, then find the one with minimal 2-norm.*

Definition 2.5.3 (LS Terminology). *Let* $A^{m \times n} x^{n \times 1} \cong b^{m \times 1}, \;\; \text{rank}\,(A) = k$*.*

- <u>*exactly determined*</u>*:* $m = n$
- <u>*overdetermined*</u>*:* $m > n$
- <u>*underdetermined*</u>*:* $m < n$
- <u>*full rank*</u>*:* $k = \min\,(m, n)$
- <u>*rank-deficient*</u>*:* $k < \min\,(m, n)$

Theorem 2.5.1 (LS Projection). *Any LS solution, i.e. any vector* x *minimizing* $||r|| := ||b - Ax||$*, must satisfy*

$$Ax = P^b_{\mathcal{R}(A)}.$$

Proof: Since $Ax \in \mathcal{R}(A)$, $||b - Ax||$ will be minimized iff $Ax = P^b_{\mathcal{R}(A)}$. □

Corollary 2.5.1. *Let* $A = QR$ *be the QR factorization of* A*. Then, any LS solution must satisfy*

$$Rx = Q^T b.$$

Proof: By Theorem 2.5.1, $Ax = P^b_{\mathcal{R}(A)} = P_A b$. But, $A = QR \Rightarrow P_A = QQ^T$ by Theorem 2.4.1. Thus, $QRx = QQ^T b \Rightarrow (Q^T Q)Rx = (Q^T Q)Q^T b \Rightarrow Rx = Q^T b$. □

Remark 2.5.1 (LS: Overdetermined Full Rank).

- Theorem 2.5.1 permits an alternative interpretation of Corollary 2.3.1. If $k := \text{rank}\,(A) = n < m$ then there is a unique "solution" to $A \cong b$ (either true or in the LS sense) and it may be found by projection as follows:

$$P_A = A(A^T A)^{-1} A^T \text{ (by Theorem 2.3.6)} \Rightarrow$$

$$Ax = A(A^T A)^{-1} A^T b \text{ (by Theorem 2.5.1)} \Rightarrow$$

$$A^T Ax = (A^T A)(A^T A)^{-1} A^T b \Rightarrow$$

$$A^T Ax = A^T b \text{ (normal equations).}$$

- By Theorem 2.3.2, $x = (A^T A)^{-1} A^T b$ (unique "solution").
- $A^T(b - Ax) = 0 \Rightarrow r \perp \mathcal{R}(A)$, i.e. $r \in \mathcal{R}(A)^\perp$.

Example 2.5.1 (LS: Overdetermined Full Rank).

$$A = \begin{bmatrix} 2 \\ 4 \end{bmatrix};\ b = \begin{bmatrix} 3 \\ 1 \end{bmatrix} \Rightarrow$$

$$A^T A = 20;\ A^T b = 10 \Rightarrow$$

$$x = (A^T A)^{-1} A^T b = \frac{1}{20} \cdot 10 = \frac{1}{2}$$

Definition 2.5.4 (Orthogonal Complement). *Let Y be a subspace of $\mathbb{R}^n$, then*

$$Y^\perp := \{x \in \mathbb{R}^n \mid \langle x, y \rangle = 0\ \forall\, y \in Y\}$$

is the <u>*orthogonal complement of Y*</u>.

Theorem 2.5.2 (Orthogonal Complement). *$Y^\perp$ is a subspace of $\mathbb{R}^n$.*

Proof:

- $0 \in Y^\perp$.
- $x \in Y^\perp,\ y \in Y,\ \alpha \in \mathbb{R} \Rightarrow \langle \alpha x, y\rangle = \alpha\langle x, y\rangle = 0 \Rightarrow \alpha x \in Y^\perp$.
- $x_1, x_2 \in Y^\perp,\ y \in Y \Rightarrow \langle x_1 + x_2, y\rangle = \langle x_1, y\rangle + \langle x_2, y\rangle = 0 + 0 = 0 \Rightarrow x_1 + x_2 \in Y^\perp$.

□

Theorem 2.5.3 (Fundamental Subspace Theorem). $A \in \mathbb{R}^{m\times n} \Rightarrow$

1. *The null space of A is the orthogonal complement of the row space of A, i.e. $\mathcal{N}(A) = [\mathcal{R}(A^T)]^\perp$.*
2. *The null space of A^T is the orthogonal complement of the column space of A, i.e. $\mathcal{N}(A^T) = [\mathcal{R}(A)]^\perp$.*

Proof:

1. - $\mathcal{N}(A) \subseteq [\mathcal{R}(A^T)]^\perp$: $\mathcal{N}(A) \perp \mathcal{R}(A^T)$ since $Ax = 0$ & $y = A^T z \Rightarrow$
   $$y^T x = (A^T z)^T x = z^T A x = z^T 0 = 0.$$
   - $[\mathcal{R}(A^T)]^\perp \subseteq \mathcal{N}(A)$: If $x \in [\mathcal{R}(A^T)]^\perp$ then x is $\perp$ to the rows of A
   $$\Rightarrow Ax = 0 \Rightarrow x \in \mathcal{N}(A).$$

   Thus, $\mathcal{N}(A) = [\mathcal{R}(A^T)]^\perp$.
2. Simply replace A by A^T in 1.

□

Theorem 2.5.4 (LS: Underdetermined Full Rank). *Let $k = m < n$, then*

1. $b \in \mathcal{R}(A)$.
2. $A^{m\times n} x^{n\times 1} = b^{m\times 1}$ *has ∞-many true solutions.*
3. *$\exists$ unique minimum norm true solution given by*
$$s = A^T (AA^T)^{-1} b.$$

Proof:

1. $k = m \Rightarrow \mathcal{R}(A) = \mathbb{R}^m \Rightarrow b \in \mathcal{R}(A)$.

2. By Theorem 2.2.1, there are ∞-many true solutions. By Theorem 2.2.2, any such solution is of the form $x = x_p + x_h$ (general solution) where $Ax_p = b$ (particular solution) and $Ax_h = 0$ (complementary solution), with x_p fixed and x_h an arbitrary element of $\mathcal{N}(A)$.

3. Clearly, any minimum norm solution, s, must satisfy $s \perp \mathcal{N}(A)$. By the Fundamental Subspace Theorem, Theorem 2.5.3, $s \in \mathcal{R}(A^T)$ so that $s = A^T t$. Thus,

$$As = b \Rightarrow AA^T t = b \Rightarrow t = (AA^T)^{-1} b \Rightarrow$$

   $\exists$ unique minimum norm true solution given by

$$s = A^T (AA^T)^{-1} b.$$

□

Remark 2.5.2 (LS: Underdetermined Full Rank).

- Since $k = m$, the rows of A are linearly independent so that the columns of A^T are linearly independent. By Theorem 2.3.2, $AA^T = (A^T)^T A^T$ is invertible so that the above formula for s is well-defined.

- We may calculate s as follows:

$$s = A^T (AA^T)^{-1} b \Rightarrow AA^T y = b \longmapsto [AA^T | b] \sim [I | y];\ x = A^T y.$$

Example 2.5.2 (LS: Underdetermined Full Rank).

$$x_1 + x_2 = 2 \Rightarrow A = [1\ 1];\ b = [2]$$

$$AA^T y = b \Rightarrow 2y = 2 \Rightarrow y = 1$$

$$\Rightarrow x = A^T y = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

is the (unique) solution of minimum 2-norm.

Theorem 2.5.5 (Least Squares Theorem). *Let $A^{m\times n} = Q^{m\times k} R^{k\times n}$ (all of rank k), with Q column-orthonormal (i.e. $Q^T Q = I^{k\times k}$) and R upper triangular (with positive leading elements in each row), then the unique minimum norm least squares solution to $Ax \cong b$ is given by $x = R^T (RR^T)^{-1} Q^T b$.*

Proof: By Corollary 2.5.1, any LS solution x must satisfy $Rx = Q^T b$.

- If $k = n$ then R is invertible and

$$x = R^{-1}Q^Tb = R^T(RR^T)^{-1}Q^Tb$$

is the unique LS solution.

- If $k < n$ then this system is underdetermined and of full rank so that, by Theorem 2.5.4,

$$x = R^T(RR^T)^{-1}Q^Tb$$

is the unique minimum norm LS solution.

□

Remark 2.5.3 (Using the Least Squares Theorem).

- If $k := \text{rank}\,(A) = n$ then it is easier to proceed as follows:

$$x = R^{-1}Q^Tb \Rightarrow Rx = Q^Tb \longmapsto [R|Q^Tb] \sim [I|x = R^{-1}Q^Tb].$$

- If $k := \text{rank}\,(A) < n$ then proceed as follows:

$$x = R^T(RR^T)^{-1}Q^Tb \Rightarrow RR^Ty = Q^Tb \longmapsto [RR^T|Q^Tb] \sim [I|y];\ x = R^Ty.$$

2.6 The Pseudoinverse

The Least Squares Theorem naturally leads to the concept of the (Moore-Penrose) pseudoinverse [1, 6, 12, 13, 14, 18, 76, 86, 106].

Definition 2.6.1 ((Moore-Penrose) Pseudoinverse). *Let $A^{m\times n} = Q^{m\times k}R^{k\times n}$ (all of rank k), with Q column-orthonormal (i.e. $Q^TQ = I^{k\times k}$) and R upper triangular (with positive leading elements in each row), then the (Moore-Penrose) pseudoinverse of A is $A^\dagger := R^T(RR^T)^{-1}Q^T$.*

Lemma 2.6.1 (Existence of Pseudoinverse). *There exists a matrix $A^\dagger \in \mathbb{R}^{n\times m}$ satisfying the four Penrose conditions (Theorem 2.1.1).*

Proof: We show that $A^\dagger$ as defined above satisfies the four Penrose conditions (Theorem 2.1.1).

1. $AA^\dagger A = [QR][R^T(RR^T)^{-1}Q^T][QR] =$
   $Q[(RR^T)(RR^T)^{-1}][Q^TQ]R = QR = A$

2. $A^\dagger AA^\dagger = [R^T(RR^T)^{-1}Q^T][QR][R^T(RR^T)^{-1}Q^T] =$
   $R^T(RR^T)^{-1}[Q^TQ][(RR^T)(RR^T)^{-1}]Q^T = R^T(RR^T)^{-1}Q^T = A^\dagger$

3. $(AA^\dagger)^T = (A^\dagger)^T A^T = [R^T(RR^T)^{-1}Q^T]^T[QR]^T =$
   $Q[(RR^T)^{-1}RR^T]Q^T = QQ^T = \underbrace{Q(R}_{A}\underbrace{R^T)(RR^T)^{-1}Q^T}_{A^\dagger} = AA^\dagger$

4. $(A^\dagger A)^T = A^T(A^\dagger)^T = [QR]^T[R^T(RR^T)^{-1}Q^T]^T =$
   $R^T[Q^TQ](RR^T)^{-1}R = \underbrace{R^T(RR^T)^{-1}[Q^T}_{A^\dagger}\underbrace{Q]R}_{A} = A^\dagger A$

□

Lemma 2.6.2 (Uniqueness of Pseudoinverse). *The pseudoinverse* $A^\dagger \in \mathbb{R}^{n\times m}$ *as defined above is the only* $n \times m$ *matrix satisfying the four Penrose conditions (Theorem 2.1.1).*

Proof: We show that there can be only one matrix satisfying the four Penrose conditions (Theorem 2.1.1). Suppose that $X^{n\times m}$ and $Y^{n\times m}$ both satisfy the Penrose conditions. Then:

- $X = XAX = (XA)^TX = A^TX^TX = (AYA)^TX^TX =$
  $(A^TY^T)(A^TX^T)X = YA(XAX) = YAX.$
- $Y = YAY = Y(AY)^T = YY^TA^T = YY^T(AXA)^T =$
  $Y(Y^TA^T)(X^TA^T) = (YAY)AX = YAX.$

Thus, $X = Y$. □

Proof of Theorem 2.1.1 (Penrose Conditions): Lemma 2.6.1 establishes existence and Lemma 2.6.2 establishes uniqueness of the (Moore-Penrose) pseudoinverse $A^\dagger \in \mathbb{R}^{n\times m}$. □

Remark 2.6.1 (Special Cases of Pseudoinverse).

1. Overdetermined Full Rank:

$$k = n < m \ (\Rightarrow \exists\, R^{-1}) \Rightarrow A^\dagger = (A^TA)^{-1}A^T :$$

$$(A^TA)^{-1}A^T = (R^TQ^TQR)^{-1}R^TQ^T = (R^TR)^{-1}R^TQ^T =$$

$$R^{-1}Q^T = R^T(RR^T)^{-1}Q^T = A^\dagger.$$

2. Underdetermined Full Rank:

$$k = m < n \ (\Rightarrow \exists\, (RR^T)^{-1}, Q^{-1} = Q^T) \Rightarrow A^\dagger = A^T(AA^T)^{-1} :$$

$$A^T(AA^T)^{-1} = R^TQ^T[Q(RR^T)Q^T]^{-1} = R^T(Q^TQ)(RR^T)^{-1}Q^T =$$

$$R^T(RR^T)^{-1}Q^T = A^\dagger.$$

Remark 2.6.2 (Properties of Pseudoinverse). *The pseudoinverse $A^\dagger$ shares the following properties with the matrix inverse A^{-1} [106, p.104]:*

- $(A^\dagger)^\dagger = A$
- $(A^T)^\dagger = (A^\dagger)^T$
- $rank\ (A) = rank\ (A^\dagger)\ \big(= rank\ (AA^\dagger) = rank\ (A^\dagger A)\big)$
- $(AA^T)^\dagger = (A^T)^\dagger A^\dagger;\ (A^T A)^\dagger = A^\dagger (A^T)^\dagger$
- $(AA^T)^\dagger AA^T = AA^\dagger;\ (A^T A)^\dagger A^T A = A^\dagger A$

Remark 2.6.3 (Non-Properties of Pseudoinverse). *The pseudoinverse $A^\dagger$ fails to share the following properties with the matrix inverse A^{-1} [106, p.105]:*

- $(AB)^\dagger \neq B^\dagger A^\dagger$
- $AA^\dagger \neq A^\dagger A$
- $(A^k)^\dagger \neq (A^\dagger)^k$
- $\lambda \neq 0 \in \sigma(A) \not\Rightarrow \lambda^{-1} \in \sigma(A^\dagger)$

Lemma 2.6.3 (Pseudoinverse: Projection Matrices).

1. $P_A = AA^\dagger$ is the projection matrix onto $\mathcal{R}(A)$.
2. $P_{A^T} = A^\dagger A$ is the projection matrix onto $\mathcal{R}(A^T)$.
3. $I - P_{A^T}$ is the projection matrix onto $\mathcal{N}(A)$.

Proof:

1. $AA^\dagger = Q[(RR^T)(RR^T)^{-1}]Q^T = QQ^T = P_A$.
2. $P_{A^T} = A^T(A^T)^\dagger = A^T(A^\dagger)^T = (A^\dagger A)^T = A^\dagger A$.
3. By Theorem 2.3.5, $P := I - P_{A^T} = I - A^\dagger A$ is a projection matrix since
   - $P^T = (I - A^\dagger A)^T = I - (A^\dagger A)^T = I - A^\dagger A = P$.
   - $P^2 = (I - A^\dagger A)^2 = I - 2A^\dagger A + A^\dagger(AA^\dagger A) = (I - A^\dagger A) = P$.

   But, $P = I - P_{A^T} = I - A^\dagger A$ is the projection matrix onto $\mathcal{N}(A)$ since:

   - $AP = A(I - A^\dagger A) = A - AA^\dagger A = A - A = 0$ so that P projects <u>into</u> $\mathcal{N}(A)$.
   - $Ax = 0 \Rightarrow Px = (I - A^\dagger A)x = x - A^\dagger Ax = x$ so that P projects <u>onto</u> $\mathcal{N}(A)$.

□

Lemma 2.6.4.

$$(A^\dagger)^T = (A^\dagger)^T A^\dagger A$$

Proof: $A^\dagger = R^T(RR^T)^{-1}Q^T \Rightarrow$

- $(A^\dagger)^T = Q(RR^T)^{-1}R$.
- $(A^\dagger)^T A^\dagger A = Q(RR^T)^{-1}[(RR^T)(RR^T)^{-1}](Q^T Q)R = Q(RR^T)^{-1}R$.

□

Theorem 2.6.1 (Penrose). *All solutions to Problem LS are of the form*

$$x = A^\dagger b + (I - P_{A^T})z$$

where z is arbitrary. Of all such solutions, $A^\dagger b$ has the smallest 2-norm, i.e. it is the unique solution to Problem LS_{min}.

Proof:

- By Theorem 2.5.1, any LS solution must satisfy $Ax = P_A b$. Since (by Part 1 of Lemma 2.6.3) $P_A b = (AA^\dagger)b = A(A^\dagger b)$, we have the particular solution $x_p := A^\dagger b$.
- Let the general LS solution be expressed as $x = x_p + x_h = A^\dagger b + x_h$.

  $$Ax_h = A(x - A^\dagger b) = Ax - AA^\dagger b = Ax - P_A b = 0.$$

  Thus, $x_h \in \mathcal{N}(A)$.
- By Part 3 of Lemma 2.6.3, $x_h = (I - P_{A^T})z$ where z is arbitrary.
- Consequently,

  $$x = A^\dagger b + (I - P_{A^T})z,$$

  where z is arbitrary.
- By Lemma 2.6.4, $A^\dagger b \perp (I - P_{A^T})z$:

  $$(A^\dagger b)^T (I - A^\dagger A)z = b^T (A^\dagger)^T (I - A^\dagger A)z = b^T[(A^\dagger)^T - (A^\dagger)^T A^\dagger A]z = 0.$$
- Therefore, by the Pythagorean Theorem,

  $$||x||^2 = ||A^\dagger b||^2 + ||(I - P_{A^T})z||^2$$

  which attains a minimum iff $(I - P_{A^T})z = 0$, i.e. iff $x = A^\dagger b$.

□

2.7 Linear Least Squares Examples

We may summarize the above results as follows [51, 79]:

Theorem 2.7.1 (Least Squares and the Pseudoinverse). *The unique minimum-norm least squares solution to* $A^{m\times n}x^{n\times 1} \cong b^{m\times 1}$ *where* $A^{m\times n} = Q^{m\times k}R^{k\times n}$ *(all of rank k), with Q column-orthonormal (i.e.* $Q^TQ = I^{k\times k}$*) and R upper triangular (with positive leading elements in each row), is given by* $x = A^\dagger b$ *where* $A^\dagger = R^T(RR^T)^{-1}Q^T$*. In the special case* $k = n$ *(i.e. full column rank), this simplifies to* $A^\dagger = R^{-1}Q^T$*.*

Corollary 2.7.1 (Residual Calculation).

$$Ax \cong b,\ r := b - Ax \Rightarrow ||r||^2 = ||b||^2 - ||Q^Tb||^2$$

Proof:

$$x = A^\dagger b + (I - P_{A^T})z \Rightarrow r = b - Ax = b - AA^\dagger b - \overbrace{A(I - P_{A^T})z}^{0} = (I - AA^\dagger)b$$

by Part 3 of Lemma 2.6.3. But, by Part 1 of Lemma 2.6.3 and Theorem 2.4.1, $AA^\dagger = QQ^T$. Thus,

$$r = (I - QQ^T)b \Rightarrow ||r||^2 = ||(I - QQ^T)b||^2 = b^T(I - QQ^T)^2b =$$

$$b^T(I - QQ^T)b = (b^Tb) - (b^TQ)(Q^Tb) = (b^Tb) - (Q^Tb)^T(Q^Tb) = ||b||^2 - ||Q^Tb||^2.$$

□

Remark 2.7.1 (Residual Calculation).

$$||r||^2 = ||b||^2 - ||Q^Tb||^2$$

permits the calculation of $||r||$ *<u>without</u> the need to pre-calculate r or, for that matter, x!*

Example 2.7.1 (Residual Calculation: Overdetermined Full Rank).

$$A = \begin{bmatrix} 2 & 1 \\ 1 & 1 \\ 2 & 1 \end{bmatrix};\ b = \begin{bmatrix} 12 \\ 6 \\ 18 \end{bmatrix} \notin \mathcal{R}(A) \Rightarrow QR = \begin{bmatrix} 2/3 & -\sqrt{2}/6 \\ 1/3 & 2\sqrt{2}/3 \\ 2/3 & -\sqrt{2}/6 \end{bmatrix} \begin{bmatrix} 3 & 5/3 \\ 0 & \sqrt{2}/3 \end{bmatrix}$$

$$\Rightarrow ||r||^2 = ||b||^2 - ||Q^Tb||^2 = 504 - 486 = 18$$

Check:

$$Rx = Q^T b \Rightarrow \begin{bmatrix} 3 & 5/3 \\ 0 & \sqrt{2}/3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 22 \\ -\sqrt{2} \end{bmatrix} \Rightarrow x = \begin{bmatrix} 9 \\ -3 \end{bmatrix}$$

$$\Rightarrow r = b - Ax = \begin{bmatrix} -3 \\ 0 \\ 3 \end{bmatrix} \Rightarrow ||r||^2 = 18 \;\surd$$

Remark 2.7.2 (LS Possibilities).

- $k < n \Rightarrow [RR^T | Q^T b] \sim [I | y = (RR^T)^{-1}(Q^T b)] \longmapsto x = R^T y$.
- $k = n \Rightarrow [R | Q^T b] \sim [I | x = R^{-1} Q^T b]$.
- $k = m \Rightarrow$ "true" solution (i.e. $||r|| = 0$).
- $k = n \Rightarrow$ unique "solution" (i.e. either true or LS).
- $k < n \Rightarrow \infty$-many "solutions" (i.e. either true or LS).

The six possibilities for Problem LS are summarized in Table 2.2. We next provide an example of each of these six cases.

PROBLEM LS	A) FULL RANK ($k = \min(m, n)$)	B) RANK-DEFICIENT ($k < \min(m, n)$)
1) EXACTLY DETERMINED ($m = n$)	$Ax = b$ $k = m = n$	$Ax \cong b$ $k < m = n$
2) OVERDETERMINED ($m > n$)	$Ax \cong b$ $k = n < m$	$Ax \cong b$ $k < n < m$
3) UNDERDETERMINED ($m < n$)	$Ax = b$ $k = m < n$	$Ax \cong b$ $k < m < n$

Table 2.2: Least Squares "Six-Pack" ($A \in \mathbb{R}^{m \times n},\ k = \operatorname{rank}(A) \le \min(m, n)$)

2.7.1 Example 1A: Exactly Determined, Full Rank

In this case, $k = m = n$, there is a unique, true solution (i.e. $||r|| = 0$) and $A^\dagger = A^{-1}$.

Example 2.7.2 (Case 1A).

$$\overbrace{\begin{bmatrix} 0 & 3 & 2 \\ 3 & 5 & 5 \\ 4 & 0 & 5 \end{bmatrix}}^{A} = \overbrace{\begin{bmatrix} 0 & 3/5 & 4/5 \\ 3/5 & 16/25 & -12/25 \\ 4/5 & -12/25 & 9/25 \end{bmatrix}}^{Q} \overbrace{\begin{bmatrix} 5 & 3 & 7 \\ 0 & 5 & 2 \\ 0 & 0 & 1 \end{bmatrix}}^{R}; \; b = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$Rx = Q^T b \Rightarrow \begin{bmatrix} 5 & 3 & 7 \\ 0 & 5 & 2 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 35/25 \\ 19/25 \\ 17/25 \end{bmatrix} \Rightarrow x = \begin{bmatrix} -3/5 \\ -3/25 \\ 17/25 \end{bmatrix}$$

$$||r||^2 = ||b||^2 - ||Q^T b||^2 = 3 - 3 = 0$$

2.7.2 Example 1B: Exactly Determined, Rank-Deficient

In this case, $k < m = n$,

- $b \in \mathcal{R}(A) \Rightarrow \infty$-many true solutions ($\exists$ unique minimum norm true solution),
- $b \notin \mathcal{R}(A) \Rightarrow \infty$-many LS solutions ($\exists$ unique minimum norm LS solution).

Example 2.7.3 (Case 1B).

$$\overbrace{\begin{bmatrix} 0 & 3 & 3 \\ 3 & 5 & 8 \\ 4 & 0 & 4 \end{bmatrix}}^{A} = \overbrace{\begin{bmatrix} 0 & 3/5 \\ 3/5 & 16/25 \\ 4/5 & -12/25 \end{bmatrix}}^{Q} \overbrace{\begin{bmatrix} 5 & 3 & 8 \\ 0 & 5 & 5 \end{bmatrix}}^{R}; \; b = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$RR^T y = Q^T b \Rightarrow \begin{bmatrix} 98 & 55 \\ 55 & 50 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 7/5 \\ 19/25 \end{bmatrix} \Rightarrow \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \frac{1}{46875} \cdot \begin{bmatrix} 705 \\ -63 \end{bmatrix}$$

$$x = R^T y = \frac{1}{46875} \cdot \begin{bmatrix} 5 & 0 \\ 3 & 5 \\ 8 & 5 \end{bmatrix} \begin{bmatrix} 705 \\ -63 \end{bmatrix} = \frac{1}{46875} \cdot \begin{bmatrix} 3525 \\ 1800 \\ 5325 \end{bmatrix} \approx \begin{bmatrix} .0752 \\ .0384 \\ .1136 \end{bmatrix}$$

$$||r||^2 = ||b||^2 - ||Q^T b||^2 \approx 3 - 2.5376 = .4624 \Rightarrow ||r|| \approx .68$$

2.7.3 Example 2A: Overdetermined, Full Rank

In this case, $k = n < m$, there is a unique "solution":

- $b \in \mathcal{R}(A) \Rightarrow \exists$ unique true solution,
- $b \notin \mathcal{R}(A) \Rightarrow \exists$ unique LS solution,

and $A^\dagger = (A^T A)^{-1} A^T$.

Example 2.7.4 (Case 2A).

$$\overbrace{\begin{bmatrix} 3 & 0 \\ 4 & 5 \\ 0 & 4 \end{bmatrix}}^{A} = \overbrace{\begin{bmatrix} 3/5 & -12/25 \\ 4/5 & 9/25 \\ 0 & 4/5 \end{bmatrix}}^{Q} \overbrace{\begin{bmatrix} 5 & 4 \\ 0 & 5 \end{bmatrix}}^{R}; \; b = \begin{bmatrix} 6 \\ 12 \\ 4 \end{bmatrix}$$

$$Rx = Q^T b \Rightarrow \begin{bmatrix} 5 & 4 \\ 0 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 66/5 \\ 116/25 \end{bmatrix} \Rightarrow x = \begin{bmatrix} 1186/625 \\ 116/125 \end{bmatrix} \approx \begin{bmatrix} 1.8976 \\ .928 \end{bmatrix}$$

$$||r||^2 = ||b||^2 - ||Q^T b||^2 \approx 196 - 195.7696 = .2304 \Rightarrow ||r|| \approx .48$$

2.7.4 Example 2B: Overdetermined, Rank-Deficient

In this case, $k < n < m$,

- $b \in \mathcal{R}(A) \Rightarrow \infty$-many true solutions ($\exists$ unique minimum norm true solution),
- $b \notin \mathcal{R}(A) \Rightarrow \infty$-many LS solutions ($\exists$ unique minimum norm LS solution).

Example 2.7.5 (Case 2B).

$$\overbrace{\begin{bmatrix} 3 & 6 \\ 4 & 8 \\ 0 & 0 \end{bmatrix}}^{A} = \overbrace{\begin{bmatrix} 3/5 \\ 4/5 \\ 0 \end{bmatrix}}^{Q} \overbrace{\begin{bmatrix} 5 & 10 \end{bmatrix}}^{R}; \; b = \begin{bmatrix} 6 \\ 12 \\ 4 \end{bmatrix}$$

$$RR^T y = Q^T b \Rightarrow 125 \cdot y = 66/5 \Rightarrow y = 66/625$$

$$x = R^T y = \frac{66}{625} \cdot \begin{bmatrix} 5 \\ 10 \end{bmatrix} = \frac{66}{125} \cdot \begin{bmatrix} 1 \\ 2 \end{bmatrix} \approx \begin{bmatrix} .528 \\ 1.056 \end{bmatrix}$$

$$||r||^2 = ||b||^2 - ||Q^T b||^2 \approx 196 - 174.24 = 21.76 \Rightarrow ||r|| \approx 4.6648$$

2.7.5 Example 3A: Underdetermined, Full Rank

In this case, $k = m < n$, $(k = m \Rightarrow \mathcal{R}(A) = \mathbb{R}^m \Rightarrow b \in \mathcal{R}(A))$:

- $b \in \mathcal{R}(A) \Rightarrow \infty$-many true solutions ($\exists$ unique minimum norm true solution),

and $A^\dagger = A^T(AA^T)^{-1}$.

Example 2.7.6 (Case 3A).

$$\overbrace{\begin{bmatrix} 3 & 4 & 0 \\ 0 & 5 & 4 \end{bmatrix}}^{A} = \overbrace{\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}}^{Q} \overbrace{\begin{bmatrix} 3 & 4 & 0 \\ 0 & 5 & 4 \end{bmatrix}}^{R}; \; b = \begin{bmatrix} 70 \\ 81 \end{bmatrix}$$

$$RR^Ty = Q^Tb \Rightarrow \begin{bmatrix} 25 & 20 \\ 20 & 41 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 70 \\ 81 \end{bmatrix} \Rightarrow \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 1 \end{bmatrix}$$

$$x = R^Ty = \begin{bmatrix} 3 & 0 \\ 4 & 5 \\ 0 & 4 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 6 \\ 13 \\ 4 \end{bmatrix}$$

$$||r||^2 = ||b||^2 - ||Q^Tb||^2 = ||b||^2 - ||b||^2 = 0$$

2.7.6 Example 3B: Underdetermined, Rank-Deficient

In this case, $k < m < n$,

- $b \in \mathcal{R}(A) \Rightarrow \infty$-many true solutions ($\exists$ unique minimum norm true solution),
- $b \notin \mathcal{R}(A) \Rightarrow \infty$-many LS solutions ($\exists$ unique minimum norm LS solution).

Example 2.7.7 (Case 3B).

$$\overbrace{\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}}^{A} = \overbrace{\begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}}^{Q} \overbrace{\begin{bmatrix} \sqrt{2} & \sqrt{2} & \sqrt{2} \end{bmatrix}}^{R}; \; b = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

$$RR^Ty = Q^Tb \Rightarrow 6 \cdot y = \frac{3}{\sqrt{2}} \Rightarrow y = \frac{1}{2\sqrt{2}}$$

$$x = R^Ty = \frac{1}{2\sqrt{2}} \cdot \begin{bmatrix} \sqrt{2} \\ \sqrt{2} \\ \sqrt{2} \end{bmatrix} = \begin{bmatrix} 1/2 \\ 1/2 \\ 1/2 \end{bmatrix}$$

$$||r||^2 = ||b||^2 - ||Q^Tb||^2 = 5 - 9/2 = 1/2 \Rightarrow ||r|| = 1/\sqrt{2} \approx 0.7071$$

Chapter 3

The Symmetric Eigenvalue Problem

In this chapter, a comprehensive treatment of Rayleigh-Schrödinger perturbation theory [87, 101] for the symmetric matrix eigenvalue problem is furnished with emphasis on the degenerate problem. Section 3.1 concerns linear perturbations [62]. 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.

Section 3.2 concerns analytic perturbations [63]. Again, the treatment is simply based upon the Moore-Penrose pseudoinverse thus constituting the natural generalization of the procedure for linear perturbation of the symmetric eigenvalue problem presented in Section 3.1. Along the way, we generalize the Dalgarno-Stewart identities [27] from linear to analytic matrix perturbations. The general procedure is illustrated by an extensive example.

3.1 Linear Perturbation

In Lord Rayleigh's investigation of vibrating strings with mild longitudinal density variation [87], a perturbation procedure was developed based upon the known analytical solution for a string of constant density. This technique was subsequently refined by Schrödinger [101] 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.

The difficulty with standard treatments of this procedure [17] 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 [42] only serves to exacerbate this difficulty.

This malady can be remedied by expressing the Rayleigh-Schrödinger procedure in terms of the Moore-Penrose pseudoinverse [106]. 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 QR-factorization and Gaussian elimination. 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 section is only concerned with real symmetric matrices, the existence of a complete set of orthonormal eigenvectors is assured [43, 81, 114]. The much more difficult case of defective matrices has been considered elsewhere [48]. Moreover, we only consider the computational aspects of this procedure. Existence of the relevant perturbation expansions has been rigorously established in [35, 47, 98].

3.1.1 Nondegenerate Case

Consider the eigenvalue problem

$$Ax_i = \lambda_i x_i \ (i = 1, \ldots, n), \tag{3.1}$$

where A is a real, symmetric, $n \times n$ matrix with distinct eigenvalues, λ_i ($i = 1, \ldots, n$), and, consequently, orthogonal eigenvectors, x_i ($i = 1, \ldots, n$). Furthermore (with $\epsilon \neq 0$ a sufficiently small real perturbation parameter),

$$A(\epsilon) = A_0 + \epsilon A_1, \tag{3.2}$$

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 [35, p. 92]. In this section, we consider the nondegenerate case where the unperturbed eigenvalues, $\lambda_i^{(0)}$ ($i = 1, \ldots, n$), are all distinct. Consideration of the degenerate case is deferred to the next section.

Under these assumptions, it is shown in [35, 47, 98] that the eigenvalues and eigenvectors of A possess the respective perturbation expansions

$$\lambda_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \lambda_i^{(k)};\ x_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k x_i^{(k)}\ (i = 1, \ldots, n). \tag{3.3}$$

for sufficiently small ϵ (see Appendix A). Clearly, the zeroth-order terms, $\{\lambda_i^{(0)};\ x_i^{(0)}\}$ $(i = 1, \ldots, n)$, are the eigenpairs of the unperturbed matrix, A_0. I.e.,

$$(A_0 - \lambda_i^{(0)} I) x_i^{(0)} = 0\ (i = 1, \ldots, n). \tag{3.4}$$

The unperturbed mutually orthogonal eigenvectors, $x_i^{(0)}$ $(i = 1, \ldots, n)$, are assumed to have been normalized to unity so that $\lambda_i^{(0)} = \langle x_i^{(0)}, A_0 x_i^{(0)} \rangle$.

Substitution of Equations (3.2) and (3.3) into Equation (3.1) yields the recurrence relation

$$(A_0 - \lambda_i^{(0)} I) x_i^{(k)} = -(A_1 - \lambda_i^{(1)} I) x_i^{(k-1)} + \sum_{j=0}^{k-2} \lambda_i^{(k-j)} x_i^{(j)}\ (k = 1, \ldots, \infty;\ i = 1, \ldots, n). \tag{3.5}$$

For fixed i, solvability of Equation (3.5) requires that its right hand side be orthogonal to $x_i^{(0)}$ for all k. Thus, the value of $x_i^{(j)}$ determines $\lambda_i^{(j+1)}$. Specifically,

$$\lambda_i^{(j+1)} = \langle x_i^{(0)}, A_1 x_i^{(j)} \rangle, \tag{3.6}$$

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

A beautiful result due to Dalgarno and Stewart [27], sometimes incorrectly attributed to Wigner in the physics literature [113, p. 5], says that much more is true: The value of the eigenvector correction $x_i^{(j)}$, in fact, determines the eigenvalue corrections 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

$$\begin{aligned} \lambda_i^{(k)} &= \langle x_i^{(0)}, (A_1 - \lambda_i^{(1)} I) x_i^{(k-1)} \rangle = \langle x_i^{(k-1)}, (A_1 - \lambda_i^{(1)} I) x_i^{(0)} \rangle \\ &= -\langle x_i^{(k-1)}, (A_0 - \lambda_i^{(0)} I) x_i^{(1)} \rangle = -\langle x_i^{(1)}, (A_0 - \lambda_i^{(0)} I) x_i^{(k-1)} \rangle \\ &= \langle x_i^{(1)}, (A_1 - \lambda_i^{(1)} I) x_i^{(k-2)} \rangle - \sum_{l=2}^{k-1} \lambda_i^{(l)} \langle x_i^{(1)}, x_i^{(k-1-l)} \rangle. \end{aligned} \tag{3.7}$$

Continuing in this fashion, we eventually arrive at, for odd $k = 2j+1$ ($j = 0, 1, \dots$),

$$\lambda_i^{(2j+1)} = \langle x_i^{(j)}, A_1 x_i^{(j)} \rangle - \sum_{\mu=0}^{j} \sum_{\nu=1}^{j} \lambda_i^{(2j+1-\mu-\nu)} \langle x_i^{(\nu)}, x_i^{(\mu)} \rangle. \tag{3.8}$$

while, for even $k = 2j$ ($j = 1, 2, \dots$),

$$\lambda_i^{(2j)} = \langle x_i^{(j-1)}, A_1 x_i^{(j)} \rangle - \sum_{\mu=0}^{j} \sum_{\nu=1}^{j-1} \lambda_i^{(2j-\mu-\nu)} \langle x_i^{(\nu)}, x_i^{(\mu)} \rangle. \tag{3.9}$$

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

The eigenfunction corrections are determined recursively from Equation (3.5) as

$$x_i^{(k)} = (A_0 - \lambda_i^{(0)} I)^{\dagger} [-(A_1 - \lambda_i^{(1)} I) x_i^{(k-1)} + \sum_{j=0}^{k-2} \lambda_i^{(k-j)} x_i^{(j)}] \; (k = 1, \dots, \infty;\; i = 1, \dots, n), \tag{3.10}$$

where $(A_0 - \lambda_i^{(0)} I)^{\dagger}$ denotes the Moore-Penrose pseudoinverse [106] of $(A_0 - \lambda_i^{(0)} I)$ and intermediate normalization has been employed.

Example 3.1.1. *Define*

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

Using MATLAB's Symbolic Toolbox, we find that

$$\lambda_1(\epsilon) = 1 - \frac{1}{2}\epsilon^2 - \frac{1}{8}\epsilon^3 + \frac{1}{4}\epsilon^4 + \frac{25}{128}\epsilon^5 + \cdots ,$$

$$\lambda_2(\epsilon) = 1 + 2\epsilon - \frac{1}{2}\epsilon^2 - \frac{7}{8}\epsilon^3 - \frac{5}{4}\epsilon^4 - \frac{153}{128}\epsilon^5 + \cdots ,$$

$$\lambda_3(\epsilon) = 2 + \epsilon^2 + \epsilon^3 + \epsilon^4 + \epsilon^5 + \cdots .$$

Applying the nondegenerate Rayleigh-Schrödinger procedure developed above to

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

we arrive at (using Equation (3.8) with $j = 0$)

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

Solving

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

produces

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

In turn, the Dalgarno-Stewart identities yield

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

and

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

Solving

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

produces

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

Again, the Dalgarno-Stewart identities yield

$$\lambda_3^{(4)} = \langle x_3^{(1)}, (A_1 - \lambda_3^{(1)} I) x_3^{(2)} \rangle - \lambda_3^{(2)} \langle x_3^{(1)}, x_3^{(1)} \rangle = 1,$$

and

$$\lambda_3^{(5)} = \langle x_3^{(2)}, (A_1 - \lambda_3^{(1)} I) x_3^{(2)} \rangle - 2\lambda_3^{(2)} \langle x_3^{(2)}, x_3^{(1)} \rangle - \lambda_3^{(3)} \langle x_3^{(1)}, x_3^{(1)} \rangle = 1.$$

3.1.2 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 [98, pp. 42-45] guarantees the existence of the perturbation expansions, Equation (3.3), only for certain special unperturbed eigenvectors.

These special unperturbed eigenvectors cannot be specified *a priori* but must instead emerge from the perturbation procedure itself (see Appendix A).

Furthermore, the higher order corrections to these special unperturbed eigenvectors are more stringently constrained than previously since they must be chosen so that Equation (3.5) is always solvable. I.e., they must be chosen so that the right hand side of Equation (3.5) 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

$$y_i^{(0)} = a_1^{(i)} x_1^{(0)} + a_2^{(i)} x_2^{(0)} + \cdots + a_m^{(i)} x_m^{(0)} \ (i = 1, \ldots, m) \tag{3.11}$$

so that the expansions, Equation (3.3), are valid with $x_i^{(k)}$ replaced by $y_i^{(k)}$. **In point of fact, the remainder of this section will assume that x_i has been replaced by y_i in Equations (3.3)-(3.10).** Moreover, the higher order eigenvector corrections, $y_i^{(k)}$, must be suitably determined. Since we desire that $\{y_i^{(0)}\}_{i=1}^m$ likewise be orthonormal, we require that

$$a_1^{(\mu)} a_1^{(\nu)} + a_2^{(\mu)} a_2^{(\nu)} + \cdots + a_m^{(\mu)} a_m^{(\nu)} = \delta_{\mu,\nu}. \tag{3.12}$$

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 begin by first 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.

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 Equation (3.5) 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,

$$\langle x_\mu^{(0)}, (A_1 - \lambda_i^{(1)} I) y_i^{(0)} \rangle = 0 \ (\mu = 1, \ldots, m). \tag{3.13}$$

Inserting Equation (3.11) and invoking the orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, A_1 x_1^{(0)} \rangle & \cdots & \langle x_1^{(0)}, A_1 x_m^{(0)} \rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, A_1 x_1^{(0)} \rangle & \cdots & \langle x_m^{(0)}, A_1 x_m^{(0)} \rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(1)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}. \tag{3.14}$$

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 Equation (3.12). These, in turn, may be used in concert with Equation (3.11) to yield the desired special unperturbed eigenvectors alluded to above.

Now that $\{y_i^{(0)}\}_{i=1}^m$ are fully determined, we have by Equation (3.6) the identities

$$\lambda_i^{(1)} = \langle y_i^{(0)}, A_1 y_i^{(0)} \rangle \ (i = 1, \ldots, m). \tag{3.15}$$

Furthermore, the combination of Equations (3.12) and (3.14) yield

$$\langle y_i^{(0)}, A_1 y_j^{(0)} \rangle = 0 \ (i \neq j). \tag{3.16}$$

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

Whenever Equation (3.5) is solvable, we will express its solution as

$$y_i^{(k)} = \hat{y}_i^{(k)} + \beta_{1,k}^{(i)} y_1^{(0)} + \beta_{2,k}^{(i)} y_2^{(0)} + \cdots + \beta_{m,k}^{(i)} y_m^{(0)} \ (i = 1, \ldots, m) \tag{3.17}$$

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 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 Equation (3.5) be solvable for $k \leftarrow k+1$ and $i = 1, \ldots, m$.

Since, by design, Equation (3.5) is solvable for $k = 1$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = \frac{\langle y_j^{(0)}, A_1 \hat{y}_i^{(k)} \rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+1)} \beta_{j,l}^{(i)}}{\lambda_i^{(1)} - \lambda_j^{(1)}} \ (i \neq j). \tag{3.18}$$

The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of Equation (3.5) for $k \leftarrow k+1$.

Example 3.1.2.

We resume with Example 3.1.1 and the first order degeneracy between $\lambda_1^{(0)}$ and $\lambda_2^{(0)}$. With the choice

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

we have

$$M = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix},$$

with eigenpairs

$$\lambda_1^{(1)} = 0,\ \begin{bmatrix} a_1^{(1)} \\ a_2^{(1)} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix};\ \lambda_2^{(1)} = 2,\ \begin{bmatrix} a_1^{(2)} \\ a_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}.$$

Availing ourselves of Equation (3.11), the special unperturbed eigenvectors are now fully determined as

$$y_1^{(0)} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{bmatrix};\ y_2^{(0)} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}.$$

Solving Equation (3.5) for $k = 1$,

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

produces

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

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 Equation (3.5) for $k = 2$,

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

thereby producing

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

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

$$\lambda_1^{(2)} = \langle y_1^{(0)}, A_1 y_1^{(1)} \rangle = -\frac{1}{2};\ \lambda_1^{(3)} = \langle y_1^{(1)}, (A_1 - \lambda_1^{(1)} I) y_1^{(1)} \rangle = -\frac{1}{8},$$

and

$$\lambda_2^{(2)} = \langle y_2^{(0)}, A_1 y_2^{(1)} \rangle = -\frac{1}{2};\ \lambda_2^{(3)} = \langle y_2^{(1)}, (A_1 - \lambda_2^{(1)} I) y_2^{(1)} \rangle = -\frac{7}{8}.$$

Solving Equation (3.5) for $k = 2$,

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

produces

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

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 Equation (3.5) for $k = 3$,

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

thereby fully determining

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

Subsequent application of the Dalgarno-Stewart identities yields

$$\lambda_1^{(4)} = \langle y_1^{(1)}, (A_1 - \lambda_1^{(1)} I) y_1^{(2)} \rangle - \lambda_1^{(2)} \langle y_1^{(1)}, y_1^{(1)} \rangle = \frac{1}{4},$$

$$\lambda_1^{(5)} = \langle y_1^{(2)}, (A_1 - \lambda_1^{(1)} I) y_1^{(2)} \rangle - 2\lambda_1^{(2)} \langle y_1^{(2)}, y_1^{(1)} \rangle - \lambda_1^{(3)} \langle y_1^{(1)}, y_1^{(1)} \rangle = \frac{25}{128},$$

and

$$\lambda_2^{(4)} = \langle y_2^{(1)}, (A_1 - \lambda_2^{(1)} I) y_2^{(2)} \rangle - \lambda_2^{(2)} \langle y_2^{(1)}, y_2^{(1)} \rangle = -\frac{5}{4},$$

$$\lambda_2^{(5)} = \langle y_2^{(2)}, (A_1 - \lambda_2^{(1)} I) y_2^{(2)} \rangle - 2\lambda_2^{(2)} \langle y_2^{(2)}, y_2^{(1)} \rangle - \lambda_2^{(3)} \langle y_2^{(1)}, y_2^{(1)} \rangle = -\frac{153}{128}.$$

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 $\lambda_i^{(2)}$ $(i = 1, \ldots, m)$ are all distinct. Thus, even though $\lambda^{(1)}$ is obtained as the only eigenvalue of Equation (3.14), $\{y_i^{(0)}\}_{i=1}^m$ are still indeterminate after enforcing solvability of Equation (3.5) for $k = 1$.

Hence, we will determine $\{\lambda_i^{(2)};\ y_i^{(0)}\}_{i=1}^m$ by insisting that Equation (3.5) be solvable for $k = 2$ and $i = 1, \ldots, m$. This requirement is equivalent to the condition that, for each fixed i,

$$\langle x_\mu^{(0)}, -(A_1 - \lambda^{(1)} I) y_i^{(1)} + \lambda_i^{(2)} y_i^{(0)} \rangle = 0 \ (\mu = 1, \ldots, m). \tag{3.19}$$

Inserting Equation (3.11) as well as Equation (3.17) with $k = 1$ and invoking the orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, M^{(2)} x_1^{(0)} \rangle & \cdots & \langle x_1^{(0)}, M^{(2)} x_m^{(0)} \rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, M^{(2)} x_1^{(0)} \rangle & \cdots & \langle x_m^{(0)}, M^{(2)} x_m^{(0)} \rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(2)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}, \tag{3.20}$$

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 $[a_1^{(i)}, \ldots, a_m^{(i)}]^T$ of the matrix M defined by $M_{\mu,\nu} = \langle x_\mu^{(0)}, M^{(2)} x_\nu^{(0)} \rangle$ $(\mu, \nu = 1, \ldots, m)$.

By assumption, the symmetric matrix M has m distinct real eigenvalues and hence orthonormal eigenvectors described by Equation (3.12). These, in turn, may be used in concert with Equation (3.11) 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 Equations (3.12) and (3.20) the identities

$$\langle y_i^{(0)}, M^{(2)} y_j^{(0)} \rangle = \lambda_i^{(2)} \cdot \delta_{i,j}. \tag{3.21}$$

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 Equation (3.17) are to be determined from the condition that Equation (3.5) be solvable for $k \leftarrow k + 2$ and $i = 1, \ldots, m$. Since, by design, Equation (3.5) is solvable for $k = 1, 2$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = \frac{\langle y_j^{(0)}, M^{(2)} \hat{y}_i^{(k)} \rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+2)} \beta_{j,l}^{(i)}}{\lambda_i^{(2)} - \lambda_j^{(2)}} \ (i \neq j). \tag{3.22}$$

The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of Equation (3.5) for $k \leftarrow k+2$.

Example 3.1.3. *Define*

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

Using MATLAB's Symbolic Toolbox, we find that

$$\lambda_1(\epsilon) = 1 + \epsilon \ ,$$

$$\lambda_2(\epsilon) = 1 + \epsilon - \frac{1}{2}\epsilon^2 - \frac{1}{4}\epsilon^3 + \frac{1}{8}\epsilon^5 + \cdots \ ,$$

$$\lambda_3(\epsilon) = 1 + \epsilon - \epsilon^2 - \epsilon^3 + 2\epsilon^5 + \cdots \ ,$$

$$\lambda_4(\epsilon) = 2 + \epsilon^2 + \epsilon^3 - 2\epsilon^5 + \cdots \ ,$$

$$\lambda_5(\epsilon) = 3 + \frac{1}{2}\epsilon^2 + \frac{1}{4}\epsilon^3 - \frac{1}{8}\epsilon^5 + \cdots \ .$$

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

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

we have from Equation (3.14), which enforces solvability of Equation (3.5) for $k = 1$,

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

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

Moving on to Equation (3.20), which enforces solvability of Equation (3.5) for $k = 2$, we have

$$M = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1/2 & 0 \\ 0 & 0 & 0 \end{bmatrix},$$

with eigenpairs: $\lambda_1^{(2)} = 0,\ \lambda_2^{(2)} = -\frac{1}{2},\ \lambda_3^{(2)} = -1$;

$$\begin{bmatrix} a_1^{(1)} \\ a_2^{(1)} \\ a_3^{(1)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix};\ \begin{bmatrix} a_1^{(2)} \\ a_2^{(2)} \\ a_3^{(2)} \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix};\ \begin{bmatrix} a_1^{(3)} \\ a_2^{(3)} \\ a_3^{(3)} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}.$$

Availing ourselves of Equation (3.11), the special unperturbed eigenvectors are now fully determined as

$$y_1^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{bmatrix};\ y_2^{(0)} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix};\ y_3^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Solving Equation (3.5) for $k = 1$,

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

produces

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

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

Solving Equation (3.5) for $k = 2$,

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

produces

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

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

We next enforce solvability of Equation (3.5) for $k = 3$,

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

thereby producing

$$y_1^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -1/2 \end{bmatrix}; \ y_3^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0 \end{bmatrix},$$

and

$$y_1^{(2)} = \begin{bmatrix} a_1 \\ b_1 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(2)} = \begin{bmatrix} a_2 \\ 0 \\ c_2 \\ 0 \\ -1/4 \end{bmatrix}; \ y_3^{(2)} = \begin{bmatrix} 0 \\ b_3 \\ c_3 \\ -1 \\ 0 \end{bmatrix}.$$

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

$$\lambda_1^{(3)} = \langle y_1^{(1)}, (A_1 - \lambda^{(1)} I) y_1^{(1)} \rangle = 0,$$

$$\lambda_2^{(3)} = \langle y_2^{(1)}, (A_1 - \lambda^{(1)} I) y_2^{(1)} \rangle = -\frac{1}{4},$$

and

$$\lambda_3^{(3)} = \langle y_3^{(1)}, (A_1 - \lambda^{(1)} I) y_3^{(1)} \rangle = -1.$$

Solving Equation (3.5) for $k = 3$,

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

produces

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

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 Equation (3.5) for $k = 4$,

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

thereby fully determining

$$y_1^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ -1/4 \end{bmatrix}; \ y_3^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \\ 0 \end{bmatrix}.$$

Subsequent application of the Dalgarno-Stewart identities yields

$$\lambda_1^{(4)} = \langle y_1^{(1)}, (A_1 - \lambda^{(1)} I) y_1^{(2)} \rangle - \lambda_1^{(2)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 0,$$

$$\lambda_1^{(5)} = \langle y_1^{(2)}, (A_1 - \lambda^{(1)} I) y_1^{(2)} \rangle - 2\lambda_1^{(2)} \langle y_1^{(2)}, y_1^{(1)} \rangle - \lambda_1^{(3)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 0,$$

and

$$\lambda_2^{(4)} = \langle y_2^{(1)}, (A_1 - \lambda^{(1)} I) y_2^{(2)} \rangle - \lambda_2^{(2)} \langle y_2^{(1)}, y_2^{(1)} \rangle = 0,$$

$$\lambda_2^{(5)} = \langle y_2^{(2)}, (A_1 - \lambda^{(1)} I) y_2^{(2)} \rangle - 2\lambda_2^{(2)} \langle y_2^{(2)}, y_2^{(1)} \rangle - \lambda_2^{(3)} \langle y_2^{(1)}, y_2^{(1)} \rangle = \frac{1}{8},$$

and

$$\lambda_3^{(4)} = \langle y_3^{(1)}, (A_1 - \lambda^{(1)} I) y_3^{(2)} \rangle - \lambda_3^{(2)} \langle y_3^{(1)}, y_3^{(1)} \rangle = 0,$$

$$\lambda_3^{(5)} = \langle y_3^{(2)}, (A_1 - \lambda^{(1)} I) y_3^{(2)} \rangle - 2\lambda_3^{(2)} \langle y_3^{(2)}, y_3^{(1)} \rangle - \lambda_3^{(3)} \langle y_3^{(1)}, y_3^{(1)} \rangle = 2.$$

Nth Order Degeneracy

We now consider the case of Nth order degeneracy which is characterized by the conditions $\lambda_1^{(j)} = \lambda_2^{(j)} = \cdots = \lambda_m^{(j)} = \lambda^{(j)}$ $(j = 0, \ldots, N-1)$ while $\lambda_i^{(N)}$ $(i = 1, \ldots, m)$ are all distinct. Thus, even though $\lambda^{(j)}$ $(j = 0, \ldots, N-1)$ are determinate, $\{y_i^{(0)}\}_{i=1}^m$ are still indeterminate after enforcing solvability of Equation (3.5) for $k = N - 1$.

Hence, we will determine $\{\lambda_i^{(N)}; \ y_i^{(0)}\}_{i=1}^m$ by insisting that Equation (3.5) be solvable for $k = N$ and $i = 1, \ldots, m$. This requirement is equivalent to the condition that, for each fixed i,

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

Inserting Equation (3.11) as well as Equation (3.17) with $k = 1, \ldots, N-1$ and invoking the orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

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

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

$$M^{(1)} = A_1, \quad (3.25)$$

$$M^{(2)} = (\lambda^{(1)} I - M^{(1)})(A_0 - \lambda^{(0)} I)^\dagger (A_1 - \lambda^{(1)} I), \quad (3.26)$$

$$M^{(3)} = (\lambda^{(2)} I - M^{(2)})(A_0 - \lambda^{(0)} I)^\dagger (A_1 - \lambda^{(1)} I) + \lambda^{(2)} (A_1 - \lambda^{(1)} I)(A_0 - \lambda^{(0)} I)^\dagger, \quad (3.27)$$

$$\begin{aligned} M^{(N)} = \; & (\lambda^{(N-1)} I - M^{(N-1)})(A_0 - \lambda^{(0)} I)^\dagger (A_1 - \lambda^{(1)} I) \\ & - \textstyle\sum_{l=2}^{N-3} \lambda^{(l)} (\lambda^{(N-l)} I - M^{(N-l)})(A_0 - \lambda^{(0)} I)^\dagger \\ & - \lambda^{(N-2)} [(A_1 - \lambda^{(1)} I)(A_0 - \lambda^{(0)} I)^\dagger (A_1 - \lambda^{(1)} I) + \lambda^{(2)} I](A_0 - \lambda^{(0)} I)^\dagger \\ & + \lambda^{(N-1)} (A_1 - \lambda^{(1)} I)(A_0 - \lambda^{(0)} I)^\dagger \; (N = 4, 5, \ldots). \quad (3.28) \end{aligned}$$

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 Equation (3.5) 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 Equation (3.12). These, in turn, may be used in concert with Equation (3.11) 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 Equations (3.12) and (3.24) the identities

$$\langle y_i^{(0)}, M^{(N)} y_j^{(0)} \rangle = \lambda_i^{(N)} \cdot \delta_{i,j}. \quad (3.29)$$

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 and second order degeneracies, $\beta_{j,k}^{(i)}$ $(i \neq j)$ of Equation (3.17) are to be determined from the condition that Equation (3.5) be solvable for $k \leftarrow k + N$ and $i = 1, \ldots, m$. Since, by design, Equation (3.5) is solvable for $k = 1, \ldots, N$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = \frac{\langle y_j^{(0)}, M^{(N)} \hat{y}_i^{(k)} \rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+N)} \beta_{j,l}^{(i)}}{\lambda_i^{(N)} - \lambda_j^{(N)}} \ (i \neq j). \tag{3.30}$$

The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of Equation (3.5) for $k \leftarrow k + N$.

Example 3.1.4. *Define*

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

Using MATLAB's Symbolic Toolbox, we find that

$$\lambda_1(\epsilon) = 1 + \epsilon - 2\epsilon^2 + 4\epsilon^4 + 0 \cdot \epsilon^5 + \cdots ,$$

$$\lambda_2(\epsilon) = 1 + \epsilon - 2\epsilon^2 - 2\epsilon^3 + 2\epsilon^4 + 10\epsilon^5 + \cdots ,$$

$$\lambda_3(\epsilon) = 2 + 2\epsilon^2 + 2\epsilon^3 - 2\epsilon^4 - 10\epsilon^5 + \cdots ,$$

$$\lambda_4(\epsilon) = 2 + \epsilon + 2\epsilon^2 - 4\epsilon^4 + 0 \cdot \epsilon^5 + \cdots .$$

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

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

we have from Equation (3.14), which enforces solvability of Equation (3.5) for $k = 1$,

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

with double eigenvalue $\lambda^{(1)} = 1$. Equation (3.20), which enforces solvability of Equation (3.5) for $k = 2$, yields

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

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

Moving on to Equation (3.24) with $N = 3$, which enforces solvability of Equation (3.5) for $k = 3$, we have

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

with eigenpairs

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

Availing ourselves of Equation (3.11), the special unperturbed eigenvectors are now fully determined as

$$y_1^{(0)} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(0)} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix}.$$

Solving Equation (3.5) for $k = 1$,

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

produces

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

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

Solving Equation (3.5) for $k = 2$,

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

produces

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

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

Solving Equation (3.5) for $k = 3$,

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

produces

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

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

We next enforce solvability of Equation (3.5) for $k = 4$,

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

thereby producing

$$y_1^{(1)} = \begin{bmatrix} 0 \\ 0 \\ -\sqrt{2} \\ 0 \end{bmatrix}; \ y_2^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -\sqrt{2} \end{bmatrix},$$

and

$$y_1^{(2)} = \begin{bmatrix} c \\ -c \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(2)} = \begin{bmatrix} d \\ d \\ 0 \\ -\sqrt{2} \end{bmatrix},$$

and

$$y_1^{(3)} = \begin{bmatrix} e \\ -e \\ 2\sqrt{2} \\ -2c \end{bmatrix}; \ y_2^{(3)} = \begin{bmatrix} f \\ f \\ -2d \\ \sqrt{2} \end{bmatrix}.$$

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 Equation (3.5) for $k = 4$,

$$(A_0 - \lambda^{(0)} I) y_i^{(4)} = -(A_1 - \lambda^{(1)} I) y_i^{(3)} + \lambda^{(2)} y_i^{(2)} + \lambda_i^{(3)} y_i^{(1)} + \lambda_i^{(4)} y_i^{(0)} \ (i = 1, 2),$$

produces

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

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

We now enforce solvability of Equation (3.5) for $k = 5$,

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

thereby fully determining

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

and further specifying

$$y_1^{(3)} = \begin{bmatrix} e \\ -e \\ 2\sqrt{2} \\ 0 \end{bmatrix};\ y_2^{(3)} = \begin{bmatrix} f \\ f \\ 0 \\ \sqrt{2} \end{bmatrix},$$

and

$$y_1^{(4)} = \begin{bmatrix} g \\ h \\ 0 \\ -2e \end{bmatrix};\ y_2^{(4)} = \begin{bmatrix} u \\ v \\ -2f \\ 5\sqrt{2} \end{bmatrix}.$$

Subsequent application of the Dalgarno-Stewart identities yields

$$\lambda_1^{(4)} = \langle y_1^{(1)}, (A_1 - \lambda^{(1)} I)y_1^{(2)} \rangle - \lambda_1^{(2)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 4,$$

$$\lambda_1^{(5)} = \langle y_1^{(2)}, (A_1 - \lambda^{(1)} I)y_1^{(2)} \rangle - 2\lambda_1^{(2)} \langle y_1^{(2)}, y_1^{(1)} \rangle - \lambda_1^{(3)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 0,$$

and

$$\lambda_2^{(4)} = \langle y_2^{(1)}, (A_1 - \lambda^{(1)} I)y_2^{(2)} \rangle - \lambda_2^{(2)} \langle y_2^{(1)}, y_2^{(1)} \rangle = 2,$$

$$\lambda_2^{(5)} = \langle y_2^{(2)}, (A_1 - \lambda^{(1)} I)y_2^{(2)} \rangle - 2\lambda_2^{(2)} \langle y_2^{(2)}, y_2^{(1)} \rangle - \lambda_2^{(3)} \langle y_2^{(1)}, y_2^{(1)} \rangle = 10.$$

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.

In the Rayleigh-Schrödinger procedure, whenever an eigenvalue branches by reduction in multiplicty at any order, one simply replaces the x_μ of Equation (3.24) 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 (3.30) 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 Equation (3.5) 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 Example 3.1.2 and Example 3.1.3 appearing in tandem.

Example 3.1.5. *Define*

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

Using MATLAB's Symbolic Toolbox, we find that

$$\lambda_1(\epsilon) = \epsilon\ ,$$

$$\lambda_2(\epsilon) = \epsilon - \epsilon^2 - \epsilon^3 + 2\epsilon^5 + \cdots\ ,$$

$$\lambda_3(\epsilon) = 0\ ,$$

$$\lambda_4(\epsilon) = 1 + \epsilon^2 + \epsilon^3 - 2\epsilon^5 + \cdots\ .$$

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

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

we have from Equation (3.14), which enforces solvability of Equation (3.5) for $k = 1$,

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

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

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

Introducing the new basis

$$z_1^{(0)} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix};\ z_2^{(0)} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix},$$

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

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

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

Solving Equation (3.5) for $k = 1$,

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

produces

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

Now, enforcing solvability of Equation (3.5) for $k = 2$,

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

we arrive at

$$M = \begin{bmatrix} -1/2 & -1/2 \\ -1/2 & -1/2 \end{bmatrix},$$

with eigenpairs

$$\lambda_1^{(2)} = 0, \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}; \ \lambda_2^{(2)} = -1, \begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \Rightarrow$$

$$y_1^{(0)} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

and

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

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 Equation (3.5) for $k = 2$,

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

produces

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

where we have invoked intermediate normalization.

We next enforce solvability of Equation (3.5) for $k = 3$,

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

thereby producing

$$y_1^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \end{bmatrix},$$

and

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

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

$$\lambda_1^{(3)} = \langle y_1^{(1)}, (A_1 - \lambda^{(1)} I) y_1^{(1)} \rangle = 0,$$

$$\lambda_2^{(3)} = \langle y_2^{(1)}, (A_1 - \lambda^{(1)} I) y_2^{(1)} \rangle = -1,$$

and

$$\lambda_3^{(3)} = \langle y_3^{(1)}, (A_1 - \lambda_3^{(1)} I) y_3^{(1)} \rangle = 0.$$

Solving Equation (3.5) for $k = 3$,

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

produces

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

where we have invoked intermediate normalization.

We now enforce solvability of Equation (3.5) for $k = 4$,

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

thereby fully determining

$$y_1^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix};\ y_2^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \end{bmatrix}.$$

Subsequent application of the Dalgarno-Stewart identities yields

$$\lambda_1^{(4)} = \langle y_1^{(1)}, (A_1 - \lambda^{(1)} I) y_1^{(2)} \rangle - \lambda_1^{(2)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 0,$$

$$\lambda_1^{(5)} = \langle y_1^{(2)}, (A_1 - \lambda^{(1)} I) y_1^{(2)} \rangle - 2\lambda_1^{(2)} \langle y_1^{(2)}, y_1^{(1)} \rangle - \lambda_1^{(3)} \langle y_1^{(1)}, y_1^{(1)} \rangle = 0,$$

and

$$\lambda_2^{(4)} = \langle y_2^{(1)}, (A_1 - \lambda^{(1)} I) y_2^{(2)} \rangle - \lambda_2^{(2)} \langle y_2^{(1)}, y_2^{(1)} \rangle = 0,$$

$$\lambda_2^{(5)} = \langle y_2^{(2)}, (A_1 - \lambda^{(1)} I) y_2^{(2)} \rangle - 2\lambda_2^{(2)} \langle y_2^{(2)}, y_2^{(1)} \rangle - \lambda_2^{(3)} \langle y_2^{(1)}, y_2^{(1)} \rangle = 2,$$

and

$$\lambda_3^{(4)} = \langle y_3^{(1)}, (A_1 - \lambda_3^{(1)} I) y_3^{(2)} \rangle - \lambda_3^{(2)} \langle y_3^{(1)}, y_3^{(1)} \rangle = 0,$$

$$\lambda_3^{(5)} = \langle y_3^{(2)}, (A_1 - \lambda_3^{(1)} I) y_3^{(2)} \rangle - 2\lambda_3^{(2)} \langle y_3^{(2)}, y_3^{(1)} \rangle - \lambda_3^{(3)} \langle y_3^{(1)}, y_3^{(1)} \rangle = 0.$$

3.2 Analytic Perturbation

A comprehensive treatment of linear Rayleigh-Schrödinger [87, 101] perturbation theory for the symmetric matrix eigenvalue problem based upon the Moore-Penrose pseudoinverse was provided in the previous section. It is the express intent of the present section to extend this technique to analytic perturbations of the symmetric eigenvalue problem. The origin of such problems in the analysis of electromechanical systems is discussed in [99].

Mathematically, we have a discretized differential operator embodied in a real symmetric matrix, A_0, which is subjected to a small symmetric perturbation due to physical inhomogeneities which is analytic in the small parameter ϵ, $A(\epsilon) = A_0 + \epsilon A_1 + \epsilon^2 A_2 + \cdots$. 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.

The difficulty with standard treatments of this procedure [17] 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 [42] only serves to exacerbate this difficulty.

This malady can be remedied by expressing the Rayleigh-Schrödinger procedure in terms of the Moore-Penrose pseudoinverse [106]. 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 QR-factorization and Gaussian elimination. 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 section is only concerned with the real symmetric case, the existence of a complete set of orthonormal eigenvectors is assured [43, 81, 114]. The much more difficult case of linear perturbation of defective matrices has been considered elsewhere [48]. Moreover, we only consider the computational aspects of this procedure. Existence of the relevant perturbation expansions has been rigorously established in [35, 47, 98].

3.2.1 Nondegenerate Case

Consider the eigenvalue problem

$$Ax_i = \lambda_i x_i \ (i = 1, \ldots, n), \tag{3.31}$$

where A is real, symmetric, $n \times n$ matrix with distinct eigenvalues, λ_i $(i = 1, \ldots, n)$. Under these assumptions the eigenvalues are real and the corresponding eigenvectors, x_i $(i = 1, \ldots, n)$, are guaranteed to be orthogonal [81, 99, 106].

Next (with $\epsilon \neq 0$ a sufficiently small real perturbation parameter), let

$$A(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k A_k, \tag{3.32}$$

where A_k $(k = 1, \ldots, \infty)$ are likewise real and symmetric but A_0 may now possess multiple eigenvalues (called degeneracies in the physics literature). The root cause of such degeneracy is typically the presence of some underlying symmetry. Any attempt to weaken the assumption on the eigenstructure of A leads to a Rayleigh-Schrödinger iteration that never terminates [35, p. 92]. In the remainder of this section, we consider the nondegenerate case where the unperturbed eigenvalues, $\lambda_i^{(0)}$ $(i = 1, \ldots, n)$, are all distinct. Consideration of the degenerate case is deferred to the next section.

Under the above assumptions, it is shown in [35, 47, 98] that the eigenvalues and eigenvectors of A possess the respective perturbation expansions,

$$\lambda_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \lambda_i^{(k)}; \ x_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k x_i^{(k)} \ (i = 1, \ldots, n), \tag{3.33}$$

for sufficiently small ϵ (see Appendix A). Clearly, the zeroth-order terms, $\{\lambda_i^{(0)};\ x_i^{(0)}\}$ $(i = 1, \ldots, n)$, are the eigenpairs of the unperturbed matrix A_0. I.e.,

$$(A_0 - \lambda_i^{(0)} I) x_i^{(0)} = 0 \ (i = 1, \ldots, n). \tag{3.34}$$

The unperturbed mutually orthogonal eigenvectors, $x_i^{(0)}$ $(i = 1, \ldots, n)$, are assumed to have been normalized to unity so that $\lambda_i^{(0)} = \langle x_i^{(0)}, A_0 x_i^{(0)} \rangle$.

Substitution of Equations (3.32) and (3.33) into Equation (3.31) yields the recurrence relation

$$(A_0 - \lambda_i^{(0)} I) x_i^{(k)} = -\sum_{j=0}^{k-1} (A_{k-j} - \lambda_i^{(k-j)} I) x_i^{(j)}, \tag{3.35}$$

for $(k = 1, \ldots, \infty;\ i = 1, \ldots, n)$. For fixed i, solvability of Equation (3.35) requires that its right hand side be orthogonal to $x_i^{(0)}$ for all k. Thus, the value of $x_i^{(j)}$ determines $\lambda_i^{(j+1)}$. Specifically,

$$\lambda_i^{(j+1)} = \sum_{l=0}^{j} \langle x_i^{(0)}, A_{j-l+1} x_i^{(l)} \rangle, \tag{3.36}$$

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

For linear matrix perturbations, $A = A_0 + \epsilon A_1$, a beautiful result due to Dalgarno and Stewart [27] (sometimes incorrectly attributed to Wigner in the physics literature [113, p. 5]) says that much more is true: The value of the eigenvector correction $x_i^{(j)}$, in fact, determines the eigenvalue corrections through $\lambda_i^{(2j+1)}$. For analytic matrix perturbations, Equation (3.32), this may be generalized via the following constructive procedure which heavily exploits the symmetry of A_k $(k = 1, \ldots, \infty)$.

We commence by observing that

$$\begin{aligned}
\lambda_i^{(k)} &= \langle x_i^{(0)}, (A_1 - \lambda_i^{(1)} I) x_i^{(k-1)} \rangle + \textstyle\sum_{l=0}^{k-2} \langle x_i^{(0)}, A_{k-l} x_i^{(l)} \rangle \\
&= \langle x_i^{(k-1)}, (A_1 - \lambda_i^{(1)} I) x_i^{(0)} \rangle + \textstyle\sum_{l=0}^{k-2} \langle x_i^{(0)}, A_{k-l} x_i^{(l)} \rangle \\
&= -\langle x_i^{(k-1)}, (A_0 - \lambda_i^{(0)} I) x_i^{(1)} \rangle + \textstyle\sum_{l=0}^{k-2} \langle x_i^{(0)}, A_{k-l} x_i^{(l)} \rangle \\
&= -\langle x_i^{(1)}, (A_0 - \lambda_i^{(0)} I) x_i^{(k-1)} \rangle + \textstyle\sum_{l=0}^{k-2} \langle x_i^{(0)}, A_{k-l} x_i^{(l)} \rangle \\
&= \langle x_i^{(1)}, (A_1 - \lambda_i^{(1)} I) x_i^{(k-2)} \rangle + \langle x_i^{(0)}, A_2 x_i^{(k-2)} \rangle \\
&\quad + \textstyle\sum_{l=0}^{k-3} [\langle x_i^{(1)}, (A_{k-l-1} - \lambda_i^{(k-l-1)} I) x_i^{(l)} \rangle + \langle x_i^{(0)}, A_{k-l} x_i^{(l)} \rangle].
\end{aligned} \tag{3.37}$$

Continuing in this fashion, we eventually arrive at, for odd $k = 2j + 1$ $(j = 0, 1, \ldots)$,

$$\lambda_i^{(2j+1)} = \sum_{\mu=0}^{j} [\langle x_i^{(0)}, A_{2j-\mu+1} x_i^{(\mu)} \rangle + \sum_{\nu=1}^{j} \langle x_i^{(\nu)}, (A_{2j-\mu-\nu+1} - \lambda_i^{(2j-\mu-\nu+1)} I) x_i^{(\mu)} \rangle]. \tag{3.38}$$

while, for even $k = 2j$ $(j = 1, 2, \dots)$,

$$\lambda_i^{(2j)} = \sum_{\mu=0}^{j} [\langle x_i^{(0)}, A_{2j-\mu} x_i^{(\mu)} \rangle + \sum_{\nu=1}^{j-1} \langle x_i^{(\nu)}, (A_{2j-\mu-\nu} - \lambda_i^{(2j-\mu-\nu)} I) x_i^{(\mu)} \rangle], \quad (3.39)$$

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

The eigenvector corrections are determined recursively from Equation (3.35) as

$$x_i^{(k)} = (A_0 - \lambda_i^{(0)} I)^{\dagger} [- \sum_{j=0}^{k-1} (A_{k-j} - \lambda_i^{(k-j)} I) x_i^{(j)}], \quad (3.40)$$

for $(k = 1, \dots, \infty;\ i = 1, \dots, n)$, where $(A_0 - \lambda_i^{(0)} I)^{\dagger}$ denotes the Moore-Penrose pseudoinverse [106] of $(A_0 - \lambda_i^{(0)} I)$ and intermediate normalization has been employed.

3.2.2 Degenerate Case

When the matrix 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 [98, pp. 42-45] guarantees the existence of the perturbation expansions, Equation (3.33), only for certain special unperturbed eigenvectors. These special unperturbed eigenvectors cannot be specified *a priori* but must instead emerge from the perturbation procedure itself (see Appendix A).

Furthermore, the higher order corrections to these special unperturbed eigenvectors are more stringently constrained than previously since they must be chosen so that Equation (3.35) is always solvable. I.e., they must be chosen so that the right hand side of Equation (3.35) 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 $x_1^{(0)}, x_2^{(0)}, \dots, x_m^{(0)}$. Then, we are required to determine appropriate linear combinations

$$y_i^{(0)} = a_1^{(i)} x_1^{(0)} + a_2^{(i)} x_2^{(0)} + \cdots + a_m^{(i)} x_m^{(0)}\ (i = 1, \dots, m) \quad (3.41)$$

so that the expansions, Equation (3.33), are valid with $x_i^{(k)}$ replaced by $y_i^{(k)}$. **In point of fact, the remainder of this section will assume that x_i has been replaced by y_i in Equations (3.33)-(3.40).** Moreover, the higher order eigenvector corrections, $y_i^{(k)}$, must be suitably determined. Since we desire that $\{y_i^{(0)}\}_{i=1}^m$ likewise be orthonormal, we require that

$$a_1^{(\mu)}a_1^{(\nu)} + a_2^{(\mu)}a_2^{(\nu)} + \cdots + a_m^{(\mu)}a_m^{(\nu)} = \delta_{\mu,\nu}. \tag{3.42}$$

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 begin by first 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 Nth order. 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. This seems preferable to presenting an impenetrable collection of opaque formulae.

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 Equation (3.35) 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,

$$\langle x_\mu^{(0)}, (A_1 - \lambda_i^{(1)} I) y_i^{(0)} \rangle = 0 \ (\mu = 1, \ldots, m). \tag{3.43}$$

Inserting Equation (3.41) and invoking the orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, A_1 x_1^{(0)} \rangle & \cdots & \langle x_1^{(0)}, A_1 x_m^{(0)} \rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, A_1 x_1^{(0)} \rangle & \cdots & \langle x_m^{(0)}, A_1 x_m^{(0)} \rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(1)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}. \tag{3.44}$$

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 Equation (3.42). These, in turn, may be used in concert with Equation (3.41) to yield the desired special unperturbed eigenvectors alluded to above.

Now that $\{y_i^{(0)}\}_{i=1}^m$ are fully determined, we have by Equation (3.36) the identities

$$\lambda_i^{(1)} = \langle y_i^{(0)}, M^{(1)} y_i^{(0)} \rangle \ (i = 1, \ldots, m). \tag{3.45}$$

Furthermore, the combination of Equations (3.42) and (3.44) yield

$$\langle y_i^{(0)}, M^{(1)} y_j^{(0)} \rangle = 0 \ (i \neq j). \tag{3.46}$$

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

Whenever Equation (3.35) is solvable, we will express its solution as

$$y_i^{(k)} = \hat{y}_i^{(k)} + \beta_{1,k}^{(i)} y_1^{(0)} + \beta_{2,k}^{(i)} y_2^{(0)} + \cdots + \beta_{m,k}^{(i)} y_m^{(0)} \ (i = 1, \ldots, m) \tag{3.47}$$

where $\hat{y}_i^{(k)} := (A_0 - \lambda^{(0)} I)^\dagger [-\sum_{j=0}^{k-1} (A_{k-j} - \lambda_i^{(k-j)} I) x_i^{(j)}]$ has no components in the $\{y_j^{(0)}\}_{j=1}^m$ directions. In 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 Equation (3.35) be solvable for $k \leftarrow k+1$ and $i = 1, \ldots, m$.

Since, by design, Equation (3.35) is solvable for $k = 1$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = \frac{\langle y_j^{(0)}, M^{(1)} \hat{y}_i^{(k)} \rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+1)} \beta_{j,l}^{(i)} + \sum_{l=0}^{k-1} \langle y_j^{(0)}, A_{k-l+1} y_i^{(l)} \rangle}{\lambda_i^{(1)} - \lambda_j^{(1)}} \ (i \neq j). \tag{3.48}$$

The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of Equation (3.35) for $k \leftarrow k+1$.

Nth Order Degeneracy

We now consider the case of Nth order degeneracy which is characterized by the conditions $\lambda_1^{(j)} = \lambda_2^{(j)} = \cdots = \lambda_m^{(j)} = \lambda^{(j)}$ $(j = 0, \ldots, N-1)$ while $\lambda_i^{(N)}$ $(i = 1, \ldots, m)$ are all distinct. Thus, even though $\lambda^{(j)}$ $(j = 0, \ldots, N-1)$ are determinate, $\{y_i^{(0)}\}_{i=1}^m$ are still indeterminate after enforcing solvability of Equation (3.35) for $k = N-1$.

Hence, we will determine $\{\lambda_i^{(N)};\ y_i^{(0)}\}_{i=1}^m$ by insisting that Equation (3.35) be solvable for $k = N$ and $i = 1, \ldots, m$. This requirement is equivalent to the condition that, for each fixed i,

$$\langle x_\mu^{(0)}, -(A_1 - \lambda^{(1)} I) y_i^{(N-1)} - \cdots - (A_N - \lambda^{(N)} I) y_i^{(0)} \rangle = 0 \ (\mu = 1, \ldots, m). \tag{3.49}$$

Inserting Equation (3.41) as well as Equation (3.47) with $k = 1, \ldots, N-1$ and invoking the orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, M^{(N)} x_1^{(0)} \rangle & \cdots & \langle x_1^{(0)}, M^{(N)} x_m^{(0)} \rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, M^{(N)} x_1^{(0)} \rangle & \cdots & \langle x_m^{(0)}, M^{(N)} x_m^{(0)} \rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(N)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}, \tag{3.50}$$

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

$$M^{(1)} = A_1, \tag{3.51}$$

$$M^{(N)} = (\lambda^{(N-1)}I - M^{(N-1)})(A_0 - \lambda^{(0)}I)^{\dagger}(A_1 - \lambda^{(1)}I)$$
$$-\sum_{l=2}^{N-1}(\lambda^{(N-l)}I - M^{(N-l)})(A_0 - \lambda^{(0)}I)^{\dagger}(A_l - \lambda^{(l)}I) + A_N$$
$$(N = 2, 3, \ldots). \tag{3.52}$$

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 Equation (3.35) 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 Equation (3.42). These, in turn, may be used in concert with Equation (3.41) 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 Equations (3.42) and (3.50) the identities

$$\langle y_i^{(0)}, M^{(N)} y_j^{(0)}\rangle = \lambda_i^{(N)} \cdot \delta_{i,j}. \tag{3.53}$$

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

Analogous to the cases of first order degeneracy, $\beta_{j,k}^{(i)}$ $(i \neq j)$ of Equation (3.47) are to be determined from the condition that Equation (3.35) be solvable for $k \leftarrow k + N$ and $i = 1, \ldots, m$. Since, by design, Equation (3.35) is solvable for $k = 1, \ldots, N$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = \frac{\langle y_j^{(0)}, M^{(N)} \hat{y}_i^{(k)}\rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+N)} \beta_{j,l}^{(i)} + \sum_{l=0}^{k+N-2} \langle y_j^{(0)}, A_{k-l+N} y_i^{(l)}\rangle}{\lambda_i^{(N)} - \lambda_j^{(N)}} \ (i \neq j). \tag{3.54}$$

The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of Equation (3.35) for $k \leftarrow k + N$.

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.

In the Rayleigh-Schrödinger procedure, whenever an eigenvalue branches by reduction in multiplicty at any order, one simply replaces the x_μ of Equation (3.50) 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 (3.54) 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 Equation (3.35) with $k \leftarrow k + N$.

We now present an example which illustrates the general procedure. This example features a simple (i.e. nondegenerate) eigenvalue together with a triple eigenvalue which branches into a single first order degenerate eigenvalue together with a pair of second order degenerate eigenvalues.

Example 3.2.1. *Define*

$$A(\epsilon) = \begin{bmatrix} \sin(\epsilon) & 0 & 0 & \sin(\epsilon) \\ 0 & \sin(\epsilon) & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \sin(\epsilon) & 0 & 0 & 1 \end{bmatrix} \Rightarrow$$

$$A_0 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \; A_1 = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix},$$

$$A_3 = \begin{bmatrix} -1/6 & 0 & 0 & -1/6 \\ 0 & -1/6 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1/6 & 0 & 0 & 0 \end{bmatrix}, \; A_5 = \begin{bmatrix} 1/120 & 0 & 0 & 1/120 \\ 0 & 1/120 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1/120 & 0 & 0 & 0 \end{bmatrix},$$

with $A_2 = A_4 = 0$.

Using MATLAB's Symbolic Toolbox, we find that

$$\lambda_1(\epsilon) = \epsilon - \frac{1}{6}\epsilon^3 + \frac{1}{120}\epsilon^5 - \cdots \;, \; \lambda_2(\epsilon) = \epsilon - \epsilon^2 - \frac{7}{6}\epsilon^3 + \frac{1}{3}\epsilon^4 + \frac{301}{120}\epsilon^5 + \cdots \;,$$

$$\lambda_3(\epsilon) = 0 \;, \; \lambda_4(\epsilon) = 1 + \epsilon^2 + \epsilon^3 - \frac{1}{3}\epsilon^4 - \frac{5}{2}\epsilon^5 + \cdots \;.$$

Applying the nondegenerate Rayleigh-Schrödinger procedure developed above to

$$\lambda_4^{(0)} = 1;\ x_4^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix},$$

we arrive at (using Equation (3.38) with $j = 0$)

$$\lambda_4^{(1)} = \langle x_4^{(0)}, A_1 x_4^{(0)} \rangle = 0.$$

Solving

$$(A_0 - \lambda_4^{(0)} I) x_4^{(1)} = -(A_1 - \lambda_4^{(1)} I) x_4^{(0)}$$

produces

$$x_4^{(1)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

where we have enforced the intermediate normalization $\langle x_4^{(1)}, x_4^{(0)} \rangle = 0$. In turn, the generalized Dalgarno-Stewart identities yield

$$\lambda_4^{(2)} = \langle x_4^{(0)}, A_2 x_4^{(0)} \rangle + \langle x_4^{(0)}, A_1 x_4^{(1)} \rangle = 1,$$

and

$$\lambda_4^{(3)} = \langle x_4^{(0)}, A_3 x_4^{(0)} \rangle + 2\langle x_4^{(0)}, A_2 x_4^{(1)} \rangle + \langle x_4^{(1)}, (A_1 - \lambda_4^{(1)} I) x_4^{(1)} \rangle = 1.$$

Solving

$$(A_0 - \lambda_4^{(0)} I) x_4^{(2)} = -(A_1 - \lambda_4^{(1)} I) x_4^{(1)} - (A_2 - \lambda_4^{(2)} I) x_4^{(0)}$$

produces

$$x_4^{(2)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

where we have enforced the intermediate normalization $\langle x_4^{(2)}, x_4^{(0)} \rangle = 0$. Again, the generalized Dalgarno-Stewart identities yield

$$\lambda_4^{(4)} = \langle x_4^{(0)}, A_4 x_4^{(0)} \rangle + 2\langle x_4^{(0)}, A_3 x_4^{(1)} \rangle + \langle x_4^{(1)}, (A_2 - \lambda_4^{(2)} I) x_4^{(1)} \rangle$$

$$+\langle x_4^{(1)}, (A_1 - \lambda_4^{(1)} I) x_4^{(2)} \rangle = -\frac{1}{3},$$

and

$$\lambda_4^{(5)} = \langle x_4^{(0)}, A_5 x_4^{(0)} \rangle + 2\langle x_4^{(0)}, A_4 x_4^{(1)} \rangle + 2\langle x_4^{(0)}, A_3 x_4^{(2)} \rangle$$

$$+\langle x_4^{(1)}, (A_3 - \lambda_4^{(3)} I) x_4^{(1)} \rangle + 2\langle x_4^{(2)}, (A_2 - \lambda_4^{(2)} I) x_4^{(1)} \rangle + \langle x_4^{(2)}, (A_1 - \lambda_4^{(1)} I) x_4^{(2)} \rangle = -\frac{5}{2}.$$

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

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

we have from Equation (3.44), which enforces solvability of Equation (3.35) for $k = 1$,

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

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

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

Introducing the new basis

$$z_1^{(0)} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix};\ z_2^{(0)} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \\ 0 \end{bmatrix},$$

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

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

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

Solving Equation (3.35) for $k = 1$,

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

produces

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

Now, enforcing solvability of Equation (3.35) for $k = 2$,

$$-(A_1 - \lambda_i^{(1)} I) y_i^{(1)} - (A_2 - \lambda_i^{(2)} I) y_i^{(0)} \perp \{z_1^{(0)}, z_2^{(0)}, y_3^{(0)}\} \ (i = 1, 2, 3),$$

we arrive at

$$M = \begin{bmatrix} -1/2 & -1/2 \\ -1/2 & -1/2 \end{bmatrix},$$

with eigenpairs

$$\lambda_1^{(2)} = 0, \ \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix}; \ \lambda_2^{(2)} = -1, \ \begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix} \Rightarrow$$

$$y_1^{(0)} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(0)} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

and

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

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 Equation (3.35) for $k = 2$,

$$(A_0 - \lambda^{(0)} I) y_i^{(2)} = -(A_1 - \lambda_i^{(1)} I) y_i^{(1)} - (A_2 - \lambda_i^{(2)} I) y_i^{(0)} \ (i = 1, 2, 3),$$

produces

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

where we have invoked intermediate normalization.

We next enforce solvability of Equation (3.35) for $k = 3$,

$$\langle y_j^{(0)}, -(A_1 - \lambda_i^{(1)} I) y_i^{(2)} - (A_2 - \lambda_i^{(2)} I) y_i^{(1)} - (A_3 - \lambda_i^{(3)} I) y_i^{(0)} \rangle = 0\ (i \neq j),$$

thereby producing

$$y_1^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix};\ y_2^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \end{bmatrix},$$

and

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

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

$$\lambda_1^{(3)} = -\frac{1}{6},\ \lambda_2^{(3)} = -\frac{7}{6},\ \lambda_3^{(3)} = 0.$$

Solving Equation (3.35) for $k = 3$,

$$(A_0 - \lambda^{(0)} I) y_i^{(3)} = -(A_1 - \lambda^{(1)} I) y_i^{(2)} - (A_2 - \lambda_i^{(2)} I) y_i^{(1)} - (A_3 - \lambda_i^{(3)} I) y_i^{(0)}\ (i = 1, 2),$$

produces

$$y_1^{(3)} = \begin{bmatrix} u_1 \\ 0 \\ w_1 \\ -a_1 \end{bmatrix};\ y_2^{(3)} = \begin{bmatrix} 0 \\ v_2 \\ w_2 \\ 1/6 \end{bmatrix},$$

where we have invoked intermediate normalization.

We now enforce solvability of Equation (3.35) for $k = 4$ $(i \neq j)$,

$$\langle y_j^{(0)}, -(A_1 - \lambda^{(1)} I) y_i^{(3)} - (A_2 - \lambda_i^{(2)} I) y_i^{(2)} - (A_3 - \lambda_i^{(3)} I) y_i^{(1)} - (A_4 - \lambda_i^{(4)} I) y_i^{(0)} \rangle = 0,$$

thereby fully determining

$$y_1^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix};\ y_2^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1 \end{bmatrix}.$$

Subsequent application of the generalized Dalgarno-Stewart identities yields

$$\lambda_1^{(4)} = 0,\ \lambda_1^{(5)} = \frac{1}{120},\ \lambda_2^{(4)} = \frac{1}{3},\ \lambda_2^{(5)} = \frac{301}{120},\ \lambda_3^{(4)} = 0,\ \lambda_3^{(5)} = 0.$$

Chapter 4

The Symmetric Definite Generalized Eigenvalue Problem

In this chapter, a comprehensive treatment of Rayleigh-Schrödinger perturbation theory for the symmetric definite generalized eigenvalue problem [87, 101] is furnished with emphasis on the degenerate problem. Section 4.1 concerns linear perturbations [64]. The treatment is simply based upon the Moore-Penrose pseudoinverse thus constituting the natural generalization of the procedure for the standard symmetric eigenvalue problem presented in Section 3.1. 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. Along the way, we generalize the Dalgarno-Stewart identities [27] from the standard to the generalized eigenvalue problem. The general procedure is illustrated by an extensive example.

Section 4.2 concerns analytic perturbations [65]. Again, the treatment is simply based upon the Moore-Penrose pseudoinverse thus constituting the natural generalization of the procedure for linear perturbation of the symmetric generalized eigenvalue problem presented in Section 4.1. Along the way, we generalize the Dalgarno-Stewart identities [27] from linear perturbation of the standard symmetric eigenvalue problem to analytic perturbation of the symmetric definite generalized eigenvalue problem. An extensive example illustrates the general procedure.

4.1 Linear Perturbation

A comprehensive treatment of Rayleigh-Schrödinger [87, 101] perturbation theory for the symmetric matrix eigenvalue problem based upon the Moore-Penrose pseudoinverse was provided in the previous chapter. It is the express intent of the present section to extend this technique to linear perturbation of the symmetric definite generalized eigenvalue problem. The origin of such problems in the analysis of electromechanical systems is discussed in [99].

Mathematically, we have a discretized differential operator embodied in a real symmetric matrix pair, (A_0, B_0) with B_0 positive definite, which is subjected to a small symmetric linear perturbation, $(A, B) = (A_0 + \epsilon A_1, B_0 + \epsilon B_1)$ with B also positive definite, due to physical inhomogeneities. The Rayleigh-Schrödinger procedure produces approximations to the eigenvalues and eigenvectors of (A, B) by a sequence of successively higher order corrections to the eigenvalues and eigenvectors of (A_0, B_0). Observe that $B_1 = 0$ permits reduction to the standard eigenvalue problem $(B^{-1}A_0 + \epsilon B^{-1}A_1, I)$. However, this destroys the very symmetry which is the linchpin of the Rayleigh-Schrödinger procedure.

The difficulty with standard treatments of this procedure [17] is that the eigenvector corrections are expressed in a form requiring the complete collection of eigenvectors of (A_0, B_0). For large matrices this is clearly an undesirable state of affairs. Consideration of the thorny issue of multiple eigenvalues of (A_0, B_0) [42] only serves to exacerbate this difficulty.

This malady can be remedied by expressing the Rayleigh-Schrödinger procedure in terms of the Moore-Penrose pseudoinverse [106]. This permits these corrections to be computed knowing only the eigenvectors of (A_0, B_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 QR-factorization and Gaussian elimination. 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 section is only concerned with the real symmetric definite case, the existence of a complete set of B-orthonormal eigenvectors is assured [43, 81, 114]. The much more difficult case of defective matrices has been considered in [48] for the standard eigenvalue problem. Moreover, we only consider the computational aspects of this procedure. Existence of the relevant perturbation expansions follows from the rigorous theory developed in [35, 47, 98] (see Appendix A).

4.1.1 Nondegenerate Case

Consider the generalized eigenvalue problem

$$Ax_i = \lambda_i B x_i \ (i = 1, \ldots, n), \tag{4.1}$$

where A and B are real, symmetric, $n \times n$ matrices and B is further assumed to be positive definite. We also assume that this matrix pair has distinct eigenvalues, λ_i $(i = 1, \ldots, n)$. Under these assumptions the eigenvalues are real and the corresponding eigenvectors, x_i $(i = 1, \ldots, n)$, are guaranteed to be B-orthogonal [81, 99, 106].

Next (with $\epsilon \neq 0$ a sufficiently small real perturbation parameter), let

$$A(\epsilon) = A_0 + \epsilon A_1;\ B(\epsilon) = B_0 + \epsilon B_1, \tag{4.2}$$

where, likewise, A_0 is real and symmetric and B_0 is real, symmetric and positive definite, except that now the matrix pair, (A_0, B_0), may possess multiple eigenvalues (called degeneracies in the physics literature). The root cause of such degeneracy is typically the presence of some underlying symmetry. Any attempt to weaken the assumption on the eigenstructure of (A, B) leads to a Rayleigh-Schrödinger iteration that never terminates [35, p. 92]. In the remainder of this section, we consider the nondegenerate case where the unperturbed eigenvalues, $\lambda_i^{(0)}$ $(i = 1, \ldots, n)$, are all distinct. Consideration of the degenerate case is deferred to the next section.

Under the above assumptions, it is shown in Appendix A that the eigenvalues and eigenvectors of (A, B) possess the respective perturbation expansions,

$$\lambda_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \lambda_i^{(k)};\ x_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k x_i^{(k)}\ (i = 1, \ldots, n), \tag{4.3}$$

for sufficiently small ϵ (see Appendix A). Using the Cholesky factorization, $B = LL^T$, this theory may be straightforwardly extended to accomodate arbitrary symmetric positive definite B [99]. Importantly, it is not necessary to actually calculate the Cholesky factorization of B in the computational procedure developed below. Clearly, the zeroth-order terms, $\{\lambda_i^{(0)};\ x_i^{(0)}\}$ $(i = 1, \ldots, n)$, are the eigenpairs of the unperturbed matrix pair, (A_0, B_0). I.e.,

$$(A_0 - \lambda_i^{(0)} B_0) x_i^{(0)} = 0\ (i = 1, \ldots, n). \tag{4.4}$$

The unperturbed mutually B_0-orthogonal eigenvectors, $x_i^{(0)}$ $(i = 1, \ldots, n)$, are assumed to have been B_0-normalized to unity so that $\lambda_i^{(0)} = \langle x_i^{(0)}, A_0 x_i^{(0)} \rangle$.

Substitution of Equations (4.2) and (4.3) into Equation (4.1) yields the recurrence relation

$$(A_0 - \lambda_i^{(0)} B_0) x_i^{(k)} = -(A_1 - \lambda_i^{(1)} B_0 - \lambda_i^{(0)} B_1) x_i^{(k-1)} + \sum_{j=0}^{k-2} (\lambda_i^{(k-j)} B_0 + \lambda_i^{(k-j-1)} B_1) x_i^{(j)}, \tag{4.5}$$

for $(k = 1, \ldots, \infty;\ i = 1, \ldots, n)$. For fixed i, solvability of Equation (4.5) requires that its right hand side be orthogonal to $x_i^{(0)}$ for all k. Thus, the value of $x_i^{(j)}$ determines $\lambda_i^{(j+1)}$. Specifically,

$$\lambda_i^{(j+1)} = \langle x_i^{(0)}, A_1 x_i^{(j)} \rangle - \sum_{l=0}^{j} \lambda_i^{(j-l)} \langle x_i^{(0)}, B_1 x_i^{(l)} \rangle, \tag{4.6}$$

where we have employed the so-called **intermediate normalization** that $x_i^{(k)}$ shall be chosen to be B_0-orthogonal to $x_i^{(0)}$ for $k = 1, \ldots, \infty$. This is equivalent to $\langle x_i^{(0)}, B_0 x_i(\epsilon)\rangle = 1$ and this normalization will be used throughout the remainder of this work.

For the standard eigenvalue problem, $B = I$, a beautiful result due to Dalgarno and Stewart [27] (sometimes incorrectly attributed to Wigner in the physics literature [113, p. 5]) says that much more is true: The value of the eigenvector correction $x_i^{(j)}$, in fact, determines the eigenvalue corrections through $\lambda_i^{(2j+1)}$. For the generalized eigenvalue problem, Equation (4.1), this may be generalized by the following constructive procedure which heavily exploits the symmetry of A_0, A_1, B_0, and B_1.

We commence by observing that

$$\begin{aligned}\lambda_i^{(k)} &= \langle x_i^{(0)}, (A_1 - \lambda_i^{(1)} B_0 - \lambda_i^{(0)} B_1) x_i^{(k-1)}\rangle - \textstyle\sum_{l=1}^{k-1} \lambda_i^{(l)} \langle x_i^{(0)}, B_1 x_i^{(k-l-1)}\rangle \\ &= \langle x_i^{(k-1)}, (A_1 - \lambda_i^{(1)} B_0 - \lambda_i^{(0)} B_1) x_i^{(0)}\rangle - \textstyle\sum_{l=1}^{k-1} \lambda_i^{(l)} \langle x_i^{(0)}, B_1 x_i^{(k-l-1)}\rangle \\ &= -\langle x_i^{(k-1)}, (A_0 - \lambda_i^{(0)} B_0) x_i^{(1)}\rangle - \textstyle\sum_{l=1}^{k-1} \lambda_i^{(l)} \langle x_i^{(0)}, B_1 x_i^{(k-l-1)}\rangle \\ &= -\langle x_i^{(1)}, (A_0 - \lambda_i^{(0)} B_0) x_i^{(k-1)}\rangle - \textstyle\sum_{l=1}^{k-1} \lambda_i^{(l)} \langle x_i^{(0)}, B_1 x_i^{(k-l-1)}\rangle \\ &= \langle x_i^{(1)}, (A_1 - \lambda_i^{(1)} B_0 - \lambda_i^{(0)} B_1) x_i^{(k-2)}\rangle - \lambda_i^{(1)} \langle x_i^{(0)}, B_1 x_i^{(k-2)}\rangle \\ &- \textstyle\sum_{l=2}^{k-1} [\langle x_i^{(1)}, (\lambda_i^{(l)} B_0 + \lambda_i^{(l-1)} B_1) x_i^{(k-l-1)}\rangle + \lambda_i^{(l)} \langle x_i^{(0)}, B_1 x_i^{(k-l-1)}\rangle]. \end{aligned} \tag{4.7}$$

Continuing in this fashion, we eventually arrive at, for odd $k = 2j + 1$ ($j = 0, 1, \ldots$),

$$\begin{aligned}\lambda_i^{(2j+1)} = \langle x_i^{(j)}, A_1 x_i^{(j)}\rangle - \sum_{\mu=0}^{j} [\lambda_i^{(2j-\mu)} \langle x_i^{(0)}, B_1 x_i^{(\mu)}\rangle \\ + \sum_{\nu=1}^{j} (\lambda_i^{(2j+1-\mu-\nu)} \langle x_i^{(\nu)}, B_0 x_i^{(\mu)}\rangle + \lambda_i^{(2j-\mu-\nu)} \langle x_i^{(\nu)}, B_1 x_i^{(\mu)}\rangle)], \end{aligned} \tag{4.8}$$

while, for even $k = 2j + 1$ ($j = 1, 2, \ldots$),

$$\begin{aligned}\lambda_i^{(2j)} = \langle x_i^{(j-1)}, A_1 x_i^{(j)}\rangle - \sum_{\mu=0}^{j} [\lambda_i^{(2j-1-\mu)} \langle x_i^{(0)}, B_1 x_i^{(\mu)}\rangle \\ + \sum_{\nu=1}^{j-1} (\lambda_i^{(2j-\mu-\nu)} \langle x_i^{(\nu)}, B_0 x_i^{(\mu)}\rangle + \lambda_i^{(2j-1-\mu-\nu)} \langle x_i^{(\nu)}, B_1 x_i^{(\mu)}\rangle)]. \end{aligned} \tag{4.9}$$

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

The eigenvector corrections are determined recursively from Equation (4.5) as

$$x_i^{(k)} = (A_0 - \lambda_i^{(0)} B_0)^\dagger [-(A_1 - \lambda_i^{(1)} B_0 - \lambda_i^{(0)} B_1) x_i^{(k-1)} + \sum_{j=0}^{k-2} (\lambda_i^{(k-j)} B_0 + \lambda_i^{(k-j-1)} B_1) x_i^{(j)}], \tag{4.10}$$

for $(k = 1, \ldots, \infty;\ i = 1, \ldots, n)$, where $(A_0 - \lambda_i^{(0)} B_0)^\dagger$ denotes the Moore-Penrose pseudoinverse [106] of $(A_0 - \lambda_i^{(0)} B_0)$ and intermediate normalization has been employed.

4.1.2 Degenerate Case

When the matrix pair (A_0, B_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, the Generalized Rellich's Theorem [98, pp. 42-45] (see Appendix A) guarantees the existence of the perturbation expansions, Equation (4.3), only for certain special unperturbed eigenvectors. These special unperturbed eigenvectors cannot be specified *a priori* but must instead emerge from the perturbation procedure itself (see Appendix A).

Furthermore, the higher order corrections to these special unperturbed eigenvectors are more stringently constrained than previously since they must be chosen so that Equation (4.5) is always solvable. I.e., they must be chosen so that the right hand side of Equation (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 B_0-orthonormal eigenvectors $x_1^{(0)}, x_2^{(0)}, \ldots, x_m^{(0)}$. Then, we are required to determine appropriate linear combinations

$$y_i^{(0)} = a_1^{(i)} x_1^{(0)} + a_2^{(i)} x_2^{(0)} + \cdots + a_m^{(i)} x_m^{(0)} \ (i = 1, \ldots, m) \tag{4.11}$$

so that the expansions, Equation (4.3), are valid with $x_i^{(k)}$ replaced by $y_i^{(k)}$. **In point of fact, the remainder of this section will assume that x_i has been replaced by y_i in Equations (4.3)-(4.10).** Moreover, the higher order eigenvector corrections, $y_i^{(k)}$, must be suitably determined. Since we desire that $\{y_i^{(0)}\}_{i=1}^m$ likewise be B_0-orthonormal, we require that

$$a_1^{(\mu)} a_1^{(\nu)} + a_2^{(\mu)} a_2^{(\nu)} + \cdots + a_m^{(\mu)} a_m^{(\nu)} = \delta_{\mu,\nu}. \tag{4.12}$$

Recall that we have assumed throughout that the perturbed matrix pair, $(A(\epsilon), B(\epsilon))$, 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 begin by first 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 Nth order. 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. This seems preferable to presenting an impenetrable collection of opaque formulae.

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 Equation (4.5) 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,

$$\langle x_\mu^{(0)}, (A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(0)} \rangle = 0 \ (\mu = 1, \ldots, m). \tag{4.13}$$

Inserting Equation (4.11) and invoking the B_0-orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, (A_1 - \lambda^{(0)} B_1) x_1^{(0)} \rangle & \cdots & \langle x_1^{(0)}, (A_1 - \lambda^{(0)} B_1) x_m^{(0)} \rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, (A_1 - \lambda^{(0)} B_1) x_1^{(0)} \rangle & \cdots & \langle x_m^{(0)}, (A_1 - \lambda^{(0)} B_1) x_m^{(0)} \rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(1)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}. \tag{4.14}$$

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 $M^{(1)} := A_1 - \lambda^{(0)} B_1$.

By assumption, the symmetric matrix M has m distinct real eigenvalues and hence orthonormal eigenvectors described by Equation (4.12). These, in turn, may be used in concert with Equation (4.11) to yield the desired special unperturbed eigenvectors alluded to above.

Now that $\{y_i^{(0)}\}_{i=1}^m$ are fully determined, we have by Equation (4.6) the identities

$$\lambda_i^{(1)} = \langle y_i^{(0)}, M^{(1)} y_i^{(0)} \rangle \ (i = 1, \ldots, m). \tag{4.15}$$

Furthermore, the combination of Equations (4.12) and (4.14) yield

$$\langle y_i^{(0)}, M^{(1)} y_j^{(0)} \rangle = 0 \ (i \neq j). \tag{4.16}$$

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

Whenever Equation (4.5) is solvable, we will express its solution as

$$y_i^{(k)} = \hat{y}_i^{(k)} + \beta_{1,k}^{(i)} y_1^{(0)} + \beta_{2,k}^{(i)} y_2^{(0)} + \cdots + \beta_{m,k}^{(i)} y_m^{(0)} \ (i = 1, \ldots, m) \tag{4.17}$$

where $\hat{y}_i^{(k)} := (A_0 - \lambda^{(0)} B_0)^\dagger [-(A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(k-1)} + \sum_{j=0}^{k-2} (\lambda_i^{(k-j)} B_0 + \lambda_i^{(k-j-1)} B_1) y_i^{(j)}]$ has no components in the $\{y_j^{(0)}\}_{j=1}^m$ directions. In 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 Equation (4.5) be solvable for $k \leftarrow k + 1$ and $i = 1, \ldots, m$.

Since, by design, Equation (4.5) is solvable for $k = 1$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = \frac{\langle y_j^{(0)}, M^{(1)} \hat{y}_i^{(k)} \rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+1)} \beta_{j,l}^{(i)} - \sum_{l=0}^{k-1} \lambda_i^{(k-l)} \langle y_j^{(0)}, B_1 y_i^{(l)} \rangle}{\lambda_i^{(1)} - \lambda_j^{(1)}} \ (i \neq j). \tag{4.18}$$

The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of Equation (4.5) for $k \leftarrow k + 1$.

Nth Order Degeneracy

We now consider the case of Nth order degeneracy which is characterized by the conditions $\lambda_1^{(j)} = \lambda_2^{(j)} = \cdots = \lambda_m^{(j)} = \lambda^{(j)}$ $(j = 0, \ldots, N - 1)$ while $\lambda_i^{(N)}$ $(i = 1, \ldots, m)$ are all distinct. Thus, even though $\lambda^{(j)}$ $(j = 0, \ldots, N - 1)$ are determinate, $\{y_i^{(0)}\}_{i=1}^m$ are still indeterminate after enforcing solvability of Equation (4.5) for $k = N - 1$.

Hence, we will determine $\{\lambda_i^{(N)};\ y_i^{(0)}\}_{i=1}^m$ by insisting that Equation (4.5) be solvable for $k = N$ and $i = 1, \ldots, m$. This requirement is equivalent to the condition that, for each fixed i,

$$\langle x_\mu^{(0)}, -(A_1 - \lambda^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(N-1)} + (\lambda^{(2)} B_0 + \lambda^{(1)} B_1) y_i^{(N-2)} + \cdots \\ + (\lambda_i^{(N)} B_0 + \lambda^{(N-1)} B_1) y_i^{(0)} \rangle = 0 \ (\mu = 1, \ldots, m). \tag{4.19}$$

Inserting Equation (4.11) as well as Equation (4.17) with $k = 1, \ldots, N - 1$ and invoking the B_0-orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, M^{(N)} x_1^{(0)} \rangle & \cdots & \langle x_1^{(0)}, M^{(N)} x_m^{(0)} \rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, M^{(N)} x_1^{(0)} \rangle & \cdots & \langle x_m^{(0)}, M^{(N)} x_m^{(0)} \rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(N)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}, \tag{4.20}$$

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

$$M^{(1)} = A_1 - \lambda^{(0)} B_1, \tag{4.21}$$

$$M^{(N)} = (\lambda^{(N-1)} B_0 - M^{(N-1)})(A_0 - \lambda^{(0)} B_0)^\dagger (A_1 - \lambda^{(1)} B_0 - \lambda^{(0)} B_1)$$
$$- \sum_{l=2}^{N-1} (\lambda^{(N-l)} B_0 - M^{(N-l)})(A_0 - \lambda^{(0)} B_0)^\dagger (\lambda^{(l)} B_0 + \lambda^{(l-1)} B_1) - \lambda^{(N-1)} B_1$$
$$(N = 2, 3, \ldots). \tag{4.22}$$

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 Equation (4.5) 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 Equation (4.12). These, in turn, may be used in concert with Equation (4.11) 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 Equations (4.12) and (4.20) the identities

$$\langle y_i^{(0)}, M^{(N)} y_j^{(0)} \rangle = \lambda_i^{(N)} \cdot \delta_{i,j}. \tag{4.23}$$

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

Analogous to the case of first order degeneracy, $\beta_{j,k}^{(i)}$ $(i \neq j)$ of Equation (4.17) are to be determined from the condition that Equation (4.5) be solvable for $k \leftarrow k + N$ and $i = 1, \ldots, m$. Since, by design, Equation (4.5) is solvable for $k = 1, \ldots, N$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = \frac{\langle y_j^{(0)}, M^{(N)} \hat{y}_i^{(k)} \rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+N)} \beta_{j,l}^{(i)} - \sum_{l=0}^{k+N-2} \lambda_i^{(k-l+N-1)} \langle y_j^{(0)}, B_1 y_i^{(l)} \rangle}{\lambda_i^{(N)} - \lambda_j^{(N)}}$$
$$(i \neq j). \tag{4.24}$$

The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of Equation (4.5) for $k \leftarrow k + N$.

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.

In the Rayleigh-Schrödinger procedure, whenever an eigenvalue branches by reduction in multiplicty at any order, one simply replaces the x_μ of Equation (4.20) by any convenient B_0-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 (4.24) 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 Equation (4.5) with $k \leftarrow k + N$.

We now present an example which illustrates the general procedure. This example features a simple (i.e. nondegenerate) eigenvalue together with a triple eigenvalue which branches into a single first order degenerate eigenvalue together with a pair of second order degenerate eigenvalues.

Example 4.1.1. *Define*

$$A_0 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix},\ A_1 = \begin{bmatrix} 5 & 3 & 0 & 3 \\ 3 & 5 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 \end{bmatrix};$$

$$B_0 = \begin{bmatrix} 5 & 3 & 0 & 0 \\ 3 & 5 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix},\ B_1 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Using MATLAB's Symbolic Toolbox, we find that

$$\lambda_1(\epsilon) = \epsilon\ ,\ \lambda_2(\epsilon) = \epsilon - \epsilon^2 - \epsilon^3 + 2\epsilon^5 + \cdots\ ,$$

$$\lambda_3(\epsilon) = 0\ ,\ \lambda_4(\epsilon) = 1 + \epsilon^2 + \epsilon^3 - 2\epsilon^5 + \cdots\ .$$

Applying the nondegenerate Rayleigh-Schrödinger procedure developed above to

$$\lambda_4^{(0)} = 1;\ x_4^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1/\sqrt{2} \end{bmatrix},$$

we arrive at (using Equation (4.8) with $j = 0$)

$$\lambda_4^{(1)} = \langle x_4^{(0)}, (A_1 - \lambda_4^{(0)} B_1) x_4^{(0)} \rangle = 0.$$

Solving

$$(A_0 - \lambda_4^{(0)} B_0) x_4^{(1)} = -(A_1 - \lambda_4^{(1)} B_0 - \lambda_4^{(0)} B_1) x_4^{(0)}$$

produces

$$x_4^{(1)} = \begin{bmatrix} 3/4\sqrt{2} \\ -1/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix},$$

where we have enforced the intermediate normalization $\langle x_4^{(1)}, B_0 x_4^{(0)} \rangle = 0$. In turn, the generalized Dalgarno-Stewart identities yield

$$\lambda_4^{(2)} = \langle x_4^{(0)}, (A_1 - \lambda_4^{(0)} B_1) x_4^{(1)} \rangle - \lambda_4^{(1)} \langle x_4^{(0)}, B_1 x_4^{(0)} \rangle = 1,$$

and

$$\lambda_4^{(3)} = \langle x_4^{(1)}, (A_1 - \lambda_4^{(1)} B_0 - \lambda_4^{(0)} B_1) x_4^{(1)} \rangle - 2\lambda_4^{(1)} \langle x_4^{(0)}, B_1 x_4^{(1)} \rangle - \lambda_4^{(2)} \langle x_4^{(0)}, B_1 x_4^{(0)} \rangle = 1.$$

Solving

$$(A_0 - \lambda_4^{(0)} B_0) x_4^{(2)} = -(A_1 - \lambda_4^{(1)} B_0 - \lambda_4^{(0)} B_1) x_4^{(1)} + (\lambda_4^{(2)} B_0 + \lambda_4^{(1)} B_1) x_4^{(0)}$$

produces

$$x_4^{(2)} = \begin{bmatrix} 3/4\sqrt{2} \\ -1/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix},$$

where we have enforced the intermediate normalization $\langle x_4^{(2)}, B_0 x_4^{(0)} \rangle = 0$. Again, the generalized Dalgarno-Stewart identities yield

$$\lambda_4^{(4)} = \langle x_4^{(1)}, (A_1 - \lambda_4^{(1)} B_0 - \lambda_4^{(0)} B_1) x_4^{(2)} \rangle - \lambda_4^{(2)} \langle x_4^{(1)}, B_0 x_4^{(1)} \rangle$$

$$-\lambda_4^{(1)} [\langle x_4^{(1)}, B_1 x_4^{(1)} \rangle + \langle x_4^{(0)}, B_1 x_4^{(2)} \rangle] - 2\lambda_4^{(2)} \langle x_4^{(1)}, B_1 x_4^{(0)} \rangle - \lambda_4^{(3)} \langle x_4^{(0)}, B_1 x_4^{(0)} \rangle = 0,$$

and

$$\lambda_4^{(5)} = \langle x_4^{(2)}, (A_1 - \lambda_4^{(1)} B_0 - \lambda_4^{(0)} B_1) x_4^{(2)} \rangle - 2\lambda_4^{(2)} \langle x_4^{(2)}, B_0 x_4^{(1)} \rangle - \lambda_4^{(3)} \langle x_4^{(1)}, B_0 x_4^{(1)} \rangle$$

$$-2\lambda_4^{(1)}\langle x_4^{(2)}, B_1 x_4^{(1)}\rangle - \lambda_4^{(2)}[\langle x_4^{(2)}, B_1 x_4^{(0)}\rangle\langle x_4^{(1)}, B_1 x_4^{(1)}\rangle + \langle x_4^{(0)}, B_1 x_4^{(2)}\rangle]$$

$$-2\lambda_4^{(3)}\langle x_4^{(1)}, B_1 x_4^{(0)}\rangle - \lambda_4^{(4)}\langle x_4^{(0)}, B_1 x_4^{(0)}\rangle = -2.$$

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

$$x_1^{(0)} = \begin{bmatrix} 3/4\sqrt{2} \\ -1/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix};\ x_2^{(0)} = \begin{bmatrix} -1/4\sqrt{2} \\ 3/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix};\ x_3^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1/\sqrt{2} \\ 0 \end{bmatrix},$$

we have from Equation (4.14), which enforces solvability of Equation (4.5) for $k = 1$,

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

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

$$\begin{bmatrix} a_1^{(3)} \\ a_2^{(3)} \\ a_3^{(3)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \Rightarrow y_3^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1/\sqrt{2} \\ 0 \end{bmatrix}.$$

Introducing the new basis

$$z_1^{(0)} = \begin{bmatrix} \sqrt{5}/4 \\ -3/4\sqrt{5} \\ 0 \\ 0 \end{bmatrix};\ z_2^{(0)} = \begin{bmatrix} 0 \\ 1/\sqrt{5} \\ 0 \\ 0 \end{bmatrix},$$

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

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

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

Solving Equation (4.5) for $k = 1$,

$$(A_0 - \lambda^{(0)} B_0) y_i^{(1)} = -(A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(0)}\ (i = 1, 2, 3),$$

produces

$$y_1^{(1)} = \begin{bmatrix} \alpha_1 \\ \beta_1 \\ \gamma_1 \\ -(3b_1^{(1)} + b_2^{(1)})/2\sqrt{5} \end{bmatrix}; \; y_2^{(1)} = \begin{bmatrix} \alpha_2 \\ \beta_2 \\ \gamma_2 \\ -(3b_1^{(2)} + b_2^{(2)})/2\sqrt{5} \end{bmatrix}; \; y_3^{(1)} = \begin{bmatrix} \alpha_3 \\ \beta_3 \\ \gamma_3 \\ 0 \end{bmatrix}.$$

Now, enforcing solvability of Equation (4.5) for $k = 2$,

$$-(A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(1)} + (\lambda_i^{(2)} B_0 + \lambda_i^{(1)} B_1) y_i^{(0)} \perp \{z_1^{(0)}, z_2^{(0)}, y_3^{(0)}\} \; (i = 1, 2, 3),$$

we arrive at

$$M = \begin{bmatrix} -9/10 & -3/10 \\ -3/10 & -1/10 \end{bmatrix},$$

with eigenpairs

$$\lambda_1^{(2)} = 0, \; \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{10} \\ -3/\sqrt{10} \end{bmatrix};$$

$$\lambda_2^{(2)} = -1, \; \begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \end{bmatrix} = \begin{bmatrix} 3/\sqrt{10} \\ 1/\sqrt{10} \end{bmatrix} \Rightarrow$$

$$y_1^{(0)} = \begin{bmatrix} 1/4\sqrt{2} \\ -3/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix}; \; y_2^{(0)} = \begin{bmatrix} 3/4\sqrt{2} \\ -1/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix},$$

and

$$y_1^{(1)} = \begin{bmatrix} -3\beta_1 \\ \beta_1 \\ 0 \\ 0 \end{bmatrix}; \; y_2^{(1)} = \begin{bmatrix} \alpha_2 \\ -3\alpha_2 \\ 0 \\ -1/\sqrt{2} \end{bmatrix}; \; y_3^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

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 Equation (4.5) for $k = 2$,

$$(A_0 - \lambda^{(0)} B_0) y_i^{(2)} = -(A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(1)} + (\lambda_i^{(2)} B_0 + \lambda_i^{(1)} B_1) y_i^{(0)} \; (i = 1, 2, 3),$$

produces

$$y_1^{(2)} = \begin{bmatrix} -3b_1 \\ b_1 \\ c_1 \\ 4\beta_1 \end{bmatrix}; \; y_2^{(2)} = \begin{bmatrix} a_2 \\ -3a_2 \\ c_2 \\ -1/\sqrt{2} \end{bmatrix}; \; y_3^{(2)} = \begin{bmatrix} a_3 \\ b_3 \\ 0 \\ 0 \end{bmatrix},$$

where we have invoked intermediate normalization.

We next enforce solvability of Equation (4.5) for $k = 3$ ($i \neq j$),

$$\langle y_j^{(0)}, -(A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(2)} + (\lambda_i^{(2)} B_0 + \lambda_i^{(1)} B_1) y_i^{(1)} + (\lambda_i^{(3)} B_0 + \lambda_i^{(2)} B_1) y_i^{(0)} \rangle = 0,$$

thereby producing

$$y_1^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \; y_2^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1/\sqrt{2} \end{bmatrix},$$

and

$$y_1^{(2)} = \begin{bmatrix} -3b_1 \\ b_1 \\ 0 \\ 0 \end{bmatrix}; \; y_2^{(2)} = \begin{bmatrix} a_2 \\ -3a_2 \\ 0 \\ -1/\sqrt{2} \end{bmatrix}; \; y_3^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

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

$$\lambda_1^{(3)} = 0, \; \lambda_2^{(3)} = -1, \; \lambda_3^{(3)} = 0.$$

Solving Equation (4.5) for $k = 3$,

$$\begin{aligned} (A_0 - \lambda^{(0)} B_0) y_i^{(3)} &= -(A_1 - \lambda^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(2)} + (\lambda_i^{(2)} B_0 + \lambda^{(1)} B_1) y_i^{(1)} \\ &\quad + (\lambda_i^{(3)} B_0 + \lambda_i^{(2)} B_1) y_i^{(0)} \; (i = 1, 2), \end{aligned}$$

produces

$$y_1^{(3)} = \begin{bmatrix} -3v_1 \\ v_1 \\ w_1 \\ 4b_1 \end{bmatrix}; \; y_2^{(3)} = \begin{bmatrix} u_2 \\ -3u_2 \\ w_2 \\ 0 \end{bmatrix},$$

where we have invoked intermediate normalization.

We now enforce solvability of Equation (4.5) for $k = 4$,

$$\langle y_j^{(0)}, -(A_1 - \lambda^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(3)} + (\lambda_i^{(2)} B_0 + \lambda^{(1))} B_1) y_i^{(2)}$$
$$+(\lambda_i^{(3)} B_0 + \lambda_i^{(2)} B_1) y_i^{(1)} + (\lambda_i^{(4)} B_0 + \lambda_i^{(3)} B_1) y_i^{(0)} \rangle = 0 \ (i \neq j),$$

thereby fully determining

$$y_1^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1/\sqrt{2} \end{bmatrix}.$$

Subsequent application of the generalized Dalgarno-Stewart identities yields

$$\lambda_1^{(4)} = 0, \ \lambda_1^{(5)} = 0, \ \lambda_2^{(4)} = 0, \ \lambda_2^{(5)} = 2, \ \lambda_3^{(4)} = 0, \ \lambda_3^{(5)} = 0.$$

4.2 Analytic Perturbation

A comprehensive treatment of linear Rayleigh-Schrödinger [87, 101] perturbation theory for the symmetric matrix eigenvalue problem based upon the Moore-Penrose pseudoinverse was provided in Section 3.1. The generalizations to analytic perturbation of the standard symmetric eigenvalue problem (Section 3.2) and to linear perturbation of the symmetric definite generalized eigenvalue problem (Section 4.1) have subsequently been treated. It is the express intent of the present section to provide the ultimate extension of this technique to analytic perturbation of the symmetric definite generalized eigenvalue problem. The origin of such problems in the analysis of electromechanical systems is discussed in [99].

Mathematically, we have a discretized differential operator embodied in a real symmetric matrix pair, (A_0, B_0) with B_0 positive definite, which is subjected to a small symmetric perturbation that is analytic in the small parameter ϵ, $(A(\epsilon), B(\epsilon)) = (A_0 + \epsilon A_1 + \epsilon^2 A_2 + \cdots, B_0 + \epsilon B_1 + \epsilon^2 B_2 + \cdots)$ with $B(\epsilon)$ also positive definite, due to physical inhomogeneities. The Rayleigh-Schrödinger procedure produces approximations to the eigenvalues and eigenvectors of (A, B) by a sequence of successively higher order corrections to the eigenvalues and eigenvectors of (A_0, B_0). Observe that $B(\epsilon) = B_0$ permits reduction to the standard eigenvalue problem $(B^{-1}A_0 + \epsilon B^{-1}A_1, I)$. However, this destroys the very symmetry which is the linchpin of the Rayleigh-Schrödinger procedure.

The difficulty with standard treatments of this procedure [17] is that the eigenvector corrections are expressed in a form requiring the complete collection of eigenvectors of (A_0, B_0). For large matrices this is clearly an undesirable state of affairs. Consideration of the thorny issue of multiple eigenvalues of (A_0, B_0) [42] only serves to exacerbate this difficulty.

This malady can be remedied by expressing the Rayleigh-Schrödinger procedure in terms of the Moore-Penrose pseudoinverse [106]. This permits these corrections to be computed knowing only the eigenvectors of (A_0, B_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 QR-factorization and Gaussian elimination. 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 section is only concerned with the real symmetric definite case, the existence of a complete set of B-orthonormal eigenvectors is assured [43, 81, 114]. The much more difficult case of defective matrices has been considered in [48] for the standard eigenvalue problem. Moreover, we only consider the computational aspects of this procedure. Existence of the relevant perturbation expansions follows from the rigorous theory developed in [4, 35, 47, 98] (see Appendix A).

4.2.1 Nondegenerate Case

Consider the generalized eigenvalue problem

$$Ax_i = \lambda_i B x_i \ (i = 1, \ldots, n), \tag{4.25}$$

where A and B are real, symmetric, $n \times n$ matrices and B is further assumed to be positive definite. We also assume that this matrix pair has distinct eigenvalues, λ_i $(i = 1, \ldots, n)$. Under these assumptions the eigenvalues are real and the corresponding eigenvectors, x_i $(i = 1, \ldots, n)$, are guaranteed to be B-orthogonal [81, 99, 106].

Next (with $\epsilon \neq 0$ a sufficiently small real perturbation parameter), let

$$A(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k A_k; \ \ B(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k B_k, \tag{4.26}$$

where, likewise, A_0 is real and symmetric and B_0 is real, symmetric and positive definite, except that now the matrix pair, (A_0, B_0), may possess multiple eigenvalues (called degeneracies in the physics literature). The root cause of such degeneracy is typically the presence of some underlying symmetry. Any attempt to weaken the assumption on the eigenstructure of (A, B) leads to a Rayleigh-Schrödinger iteration that never terminates [35, p. 92]. In the remainder of this section, we consider the nondegenerate case where the unperturbed eigenvalues, $\lambda_i^{(0)}$ $(i = 1, \ldots, n)$, are all distinct. Consideration of the degenerate case is deferred to the next section.

Under the above assumptions, it is shown in Appendix A that the eigenvalues and eigenvectors of (A, B) possess the respective perturbation expansions,

$$\lambda_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \lambda_i^{(k)}; \; x_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k x_i^{(k)} \; (i = 1, \ldots, n), \tag{4.27}$$

for sufficiently small ϵ (see Appendix A). Using the Cholesky factorization, $B = LL^T$, this theory may be straightforwardly extended to accomodate arbitrary symmetric positive definite B [99]. Importantly, it is not necessary to actually calculate the Cholesky factorization of B in the computational procedure developed below. Clearly, the zeroth-order terms, $\{\lambda_i^{(0)}; \; x_i^{(0)}\}$ $(i = 1, \ldots, n)$, are the eigenpairs of the unperturbed matrix pair, (A_0, B_0). I.e.,

$$(A_0 - \lambda_i^{(0)} B_0) x_i^{(0)} = 0 \; (i = 1, \ldots, n). \tag{4.28}$$

The unperturbed mutually B_0-orthogonal eigenvectors, $x_i^{(0)}$ $(i = 1, \ldots, n)$, are assumed to have been B_0-normalized to unity so that $\lambda_i^{(0)} = \langle x_i^{(0)}, A_0 x_i^{(0)} \rangle$.

Substitution of Equations (4.26) and (4.27) into Equation (4.25) yields the recurrence relation

$$(A_0 - \lambda_i^{(0)} B_0) x_i^{(k)} = - \sum_{j=0}^{k-1} (A_{k-j} - \sum_{l=0}^{k-j} \lambda_i^{(k-j-l)} B_l) x_i^{(j)}, \tag{4.29}$$

for $(k = 1, \ldots, \infty; \; i = 1, \ldots, n)$. For fixed i, solvability of Equation (4.29) requires that its right hand side be orthogonal to $x_i^{(0)}$ for all k. Thus, the value of $x_i^{(m)}$ determines $\lambda_i^{(m+1)}$. Specifically,

$$\lambda_i^{(m+1)} = \sum_{j=0}^{m} \langle x_i^{(0)}, (A_{m-j+1} - \sum_{l=1}^{m-j+1} \lambda_i^{(m-j-l+1)} B_l) x_i^{(j)} \rangle, \tag{4.30}$$

where we have employed the so-called **intermediate normalization** that $x_i^{(k)}$ shall be chosen to be B_0-orthogonal to $x_i^{(0)}$ for $k = 1, \ldots, \infty$. This is equivalent to $\langle x_i^{(0)}, B_0 x_i(\epsilon) \rangle = 1$ and this normalization will be used throughout the remainder of this work.

For linear perturbation, $A = A_0 + \epsilon A_1$, of the standard eigenvalue problem, $B = I$, a beautiful result due to Dalgarno and Stewart [27] (sometimes incorrectly attributed to Wigner in the physics literature [113, p. 5]) says that much more is true: The value of the eigenvector correction $x_i^{(m)}$, in fact, determines the eigenvalue corrections through $\lambda_i^{(2m+1)}$. For analytic perturbation of the generalized eigenvalue problem, Equation (4.26), this may be generalized by the following constructive procedure which heavily exploits the symmetry of A_k and B_k $(k = 0, \ldots, \infty)$.

We commence by observing that

$$\begin{aligned}
\lambda_i^{(k)} &= \langle x_i^{(0)}, (A_1 - \lambda_i^{(1)} B_0 - \lambda_i^{(0)} B_1) x_i^{(k-1)} \rangle \\
&+ \sum_{l=0}^{k-2} \langle x_i^{(0)}, (A_{k-l} - \sum_{m=1}^{k-l} \lambda_i^{(k-l-m)} B_m) x_i^{(l)} \rangle \\
&= \langle x_i^{(k-1)}, (A_1 - \lambda_i^{(1)} B_0 - \lambda_i^{(0)} B_1) x_i^{(0)} \rangle \\
&+ \sum_{l=0}^{k-2} \langle x_i^{(0)}, (A_{k-l} - \sum_{m=1}^{k-l} \lambda_i^{(k-l-m)} B_m) x_i^{(l)} \rangle \\
&= -\langle x_i^{(k-1)}, (A_0 - \lambda_i^{(0)} B_0) x_i^{(1)} \rangle \\
&+ \sum_{l=0}^{k-2} \langle x_i^{(0)}, (A_{k-l} - \sum_{m=1}^{k-l} \lambda_i^{(k-l-m)} B_m) x_i^{(l)} \rangle \\
&= -\langle x_i^{(1)}, (A_0 - \lambda_i^{(0)} B_0) x_i^{(k-1)} \rangle \\
&+ \sum_{l=0}^{k-2} \langle x_i^{(0)}, (A_{k-l} - \sum_{m=1}^{k-l} \lambda_i^{(k-l-m)} B_m) x_i^{(l)} \rangle,
\end{aligned}$$

so that

$$\begin{aligned}
\lambda_i^{(k)} &= \langle x_i^{(1)}, (A_1 - \lambda_i^{(1)} B_0 - \lambda_i^{(0)} B_1) x_i^{(k-2)} \rangle \\
&+ \langle x_i^{(0)}, (A_2 - \lambda_i^{(1)} B_1 - \lambda_i^{(0)} B_2) x_i^{(k-2)} \rangle \\
&+ \sum_{l=0}^{k-3} [\langle x_i^{(1)}, (A_{k-l-1} - \sum_{m=0}^{k-l-1} \lambda_i^{(k-l-m-1)} B_m) x_i^{(l)} \rangle \\
&\quad + \langle x_i^{(0)}, (A_{k-l} - \sum_{m=1}^{k-l} \lambda_i^{(k-l-m)} B_m) x_i^{(l)} \rangle]. \qquad (4.31)
\end{aligned}$$

Continuing in this fashion, we eventually arrive at, for odd $k = 2j+1$ ($j = 0, 1, \ldots$),

$$\begin{aligned}
\lambda_i^{(2j+1)} = \sum_{\mu=0}^{j} [\langle x_i^{(0)}, (A_{2j-\mu+1} - \sum_{\rho=1}^{2j-\mu+1} \lambda_i^{(2j-\mu-\rho+1)} B_\rho) x_i^{(\mu)} \rangle \\
+ \sum_{\nu=1}^{j} \langle x_i^{(\nu)}, (A_{2j-\mu-\nu+1} - \sum_{\sigma=0}^{2j-\mu-\nu+1} \lambda_i^{(2j-\mu-\nu-\sigma+1)} B_\sigma) x_i^{(\mu)} \rangle]. \qquad (4.32)
\end{aligned}$$

while, for even $k = 2j$ ($j = 1, 2, \ldots$),

$$\begin{aligned}
\lambda_i^{(2j)} = \sum_{\mu=0}^{j} [\langle x_i^{(0)}, (A_{2j-\mu} - \sum_{\rho=1}^{2j-\mu} \lambda_i^{(2j-\mu-\rho)} B_\rho) x_i^{(\mu)} \rangle \\
+ \sum_{\nu=1}^{j-1} \langle x_i^{(\nu)}, (A_{2j-\mu-\nu} - \sum_{\sigma=0}^{2j-\mu-\nu} \lambda_i^{(2j-\mu-\nu-\sigma)} B_\sigma) x_i^{(\mu)} \rangle], \qquad (4.33)
\end{aligned}$$

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

The eigenvector corrections are determined recursively from Equation (4.29) as

$$x_i^{(k)} = (A_0 - \lambda_i^{(0)} B_0)^\dagger [-\sum_{j=0}^{k-1} (A_{k-j} - \sum_{l=0}^{k-j} \lambda_i^{(k-j-l)} B_l) x_i^{(j)}], \tag{4.34}$$

for $(k = 1, \ldots, \infty;\ i = 1, \ldots, n)$, where $(A_0 - \lambda_i^{(0)} B_0)^\dagger$ denotes the Moore-Penrose pseudoinverse [106] of $(A_0 - \lambda_i^{(0)} B_0)$ and intermediate normalization has been employed.

4.2.2 Degenerate Case

When the matrix pair (A_0, B_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, the Generalized Rellich's Theorem [98, pp. 42-45] (see Appendix A) guarantees the existence of the perturbation expansions, Equation (4.27), only for certain special unperturbed eigenvectors. These special unperturbed eigenvectors cannot be specified *a priori* but must instead emerge from the perturbation procedure itself (see Appendix A).

Furthermore, the higher order corrections to these special unperturbed eigenvectors are more stringently constrained than previously since they must be chosen so that Equation (4.29) is always solvable. I.e., they must be chosen so that the right hand side of Equation (4.29) 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 B_0-orthonormal eigenvectors $x_1^{(0)}, x_2^{(0)}, \ldots, x_m^{(0)}$. Then, we are required to determine appropriate linear combinations

$$y_i^{(0)} = a_1^{(i)} x_1^{(0)} + a_2^{(i)} x_2^{(0)} + \cdots + a_m^{(i)} x_m^{(0)} \ (i = 1, \ldots, m) \tag{4.35}$$

so that the expansions, Equation (4.27), are valid with $x_i^{(k)}$ replaced by $y_i^{(k)}$. **In point of fact, the remainder of this section will assume that x_i has been replaced by y_i in Equations (4.27)-(4.34).** Moreover, the higher order eigenvector corrections, $y_i^{(k)}$, must be suitably determined. Since we desire that $\{y_i^{(0)}\}_{i=1}^m$ likewise be B_0-orthonormal, we require that

$$a_1^{(\mu)} a_1^{(\nu)} + a_2^{(\mu)} a_2^{(\nu)} + \cdots + a_m^{(\mu)} a_m^{(\nu)} = \delta_{\mu,\nu}. \tag{4.36}$$

Recall that we have assumed throughout that the perturbed matrix pair, $(A(\epsilon), B(\epsilon))$, 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 begin by first 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 Nth order. 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. This seems preferable to presenting an impenetrable collection of opaque formulae.

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 Equation (4.29) 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,

$$\langle x_\mu^{(0)}, (A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(0)} \rangle = 0 \ (\mu = 1,\ldots,m). \tag{4.37}$$

Inserting Equation (4.35) and invoking the B_0-orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, (A_1 - \lambda^{(0)} B_1) x_1^{(0)} \rangle & \cdots & \langle x_1^{(0)}, (A_1 - \lambda^{(0)} B_1) x_m^{(0)} \rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, (A_1 - \lambda^{(0)} B_1) x_1^{(0)} \rangle & \cdots & \langle x_m^{(0)}, (A_1 - \lambda^{(0)} B_1) x_m^{(0)} \rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(1)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}. \tag{4.38}$$

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 $M^{(1)} := A_1 - \lambda^{(0)} B_1$.

By assumption, the symmetric matrix M has m distinct real eigenvalues and hence orthonormal eigenvectors described by Equation (4.36). These, in turn, may be used in concert with Equation (4.35) to yield the desired special unperturbed eigenvectors alluded to above.

Now that $\{y_i^{(0)}\}_{i=1}^m$ are fully determined, we have by Equation (4.30) the identities

$$\lambda_i^{(1)} = \langle y_i^{(0)}, M^{(1)} y_i^{(0)} \rangle \ (i = 1,\ldots,m). \tag{4.39}$$

Furthermore, the combination of Equations (4.36) and (4.38) yield

$$\langle y_i^{(0)}, M^{(1)} y_j^{(0)} \rangle = 0 \ (i \neq j). \tag{4.40}$$

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

Whenever Equation (4.29) is solvable, we will express its solution as

$$y_i^{(k)} = \hat{y}_i^{(k)} + \beta_{1,k}^{(i)} y_1^{(0)} + \beta_{2,k}^{(i)} y_2^{(0)} + \cdots + \beta_{m,k}^{(i)} y_m^{(0)} \ (i = 1, \ldots, m) \tag{4.41}$$

where $\hat{y}_i^{(k)} := (A_0 - \lambda^{(0)} B_0)^{\dagger} [-\sum_{j=0}^{k-1} (A_{k-j} - \sum_{l=0}^{k-j} \lambda_i^{(k-j-l)} B_l) y_i^{(j)}]$ has no components in the $\{y_j^{(0)}\}_{j=1}^m$ directions. In 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 Equation (4.29) be solvable for $k \leftarrow k+1$ and $i = 1, \ldots, m$.

Since, by design, Equation (4.29) is solvable for $k = 1$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = [\langle y_j^{(0)}, M^{(1)} \hat{y}_i^{(k)} \rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+1)} \beta_{j,l}^{(i)}$$
$$+ \sum_{l=0}^{k-1} \langle y_j^{(0)}, (A_{k-l+1} - \sum_{r=1}^{k-l+1} \lambda_i^{(k-l-r+1)} B_r) y_i^{(l)} \rangle] / [\lambda_i^{(1)} - \lambda_j^{(1)}], \tag{4.42}$$

for $(i \neq j)$. The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of Equation (4.29) for $k \leftarrow k+1$.

Nth Order Degeneracy

We now consider the case of Nth order degeneracy which is characterized by the conditions $\lambda_1^{(j)} = \lambda_2^{(j)} = \cdots = \lambda_m^{(j)} = \lambda^{(j)}$ $(j = 0, \ldots, N-1)$ while $\lambda_i^{(N)}$ $(i = 1, \ldots, m)$ are all distinct. Thus, even though $\lambda^{(j)}$ $(j = 0, \ldots, N-1)$ are determinate, $\{y_i^{(0)}\}_{i=1}^m$ are still indeterminate after enforcing solvability of Equation (4.29) for $k = N-1$.

Hence, we will determine $\{\lambda_i^{(N)};\ y_i^{(0)}\}_{i=1}^m$ by insisting that Equation (4.29) be solvable for $k = N$ and $i = 1, \ldots, m$. This requirement is equivalent to the condition that, for each fixed i,

$$\langle x_\mu^{(0)}, -\sum_{j=0}^{N-1} (A_{N-j} - \sum_{l=0}^{N-j} \lambda_i^{(N-j-l)} B_l) y_i^{(j)} \rangle = 0 \ (\mu = 1, \ldots, m). \tag{4.43}$$

Inserting Equation (4.35) as well as Equation (4.41) with $k = 1, \ldots, N-1$ and invoking the B_0-orthonormality of $\{x_\mu^{(0)}\}_{\mu=1}^m$, we arrive at, in matrix form,

$$\begin{bmatrix} \langle x_1^{(0)}, M^{(N)} x_1^{(0)} \rangle & \cdots & \langle x_1^{(0)}, M^{(N)} x_m^{(0)} \rangle \\ \vdots & \ddots & \vdots \\ \langle x_m^{(0)}, M^{(N)} x_1^{(0)} \rangle & \cdots & \langle x_m^{(0)}, M^{(N)} x_m^{(0)} \rangle \end{bmatrix} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix} = \lambda_i^{(N)} \begin{bmatrix} a_1^{(i)} \\ \vdots \\ a_m^{(i)} \end{bmatrix}, \quad (4.44)$$

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

$$M^{(1)} = A_1 - \lambda^{(0)} B_1, \quad (4.45)$$

$$\begin{aligned} M^{(N)} = {} & (\lambda^{(N-1)} B_0 - M^{(N-1)})(A_0 - \lambda^{(0)} B_0)^\dagger (A_1 - \lambda^{(1)} B_0 - \lambda^{(0)} B_1) \\ & + \sum_{l=2}^{N-1} (\lambda^{(N-l)} B_0 - M^{(N-l)})(A_0 - \lambda^{(0)} B_0)^\dagger (A_l - \sum_{r=0}^{l} \lambda^{(l-r)} B_r) \quad (4.46) \\ & + (A_N - \sum_{s=1}^{N} \lambda^{(N-s)} B_s) \ (N = 2, 3, \ldots). \quad (4.47) \end{aligned}$$

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 Equation (4.29) 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 Equation (4.36). These, in turn, may be used in concert with Equation (4.35) 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 Equations (4.36) and (4.40) the identities

$$\langle y_i^{(0)}, M^{(N)} y_j^{(0)} \rangle = \lambda_i^{(N)} \cdot \delta_{i,j}. \quad (4.48)$$

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

Analogous to the case of first order degeneracy, $\beta_{j,k}^{(i)}$ $(i \neq j)$ of Equation (4.41) are to be determined from the condition that Equation (4.29) be solvable for $k \leftarrow k + N$ and $i = 1, \ldots, m$. Since, by design, Equation (4.29) is solvable for $k = 1, \ldots, N$, we may proceed recursively. After considerable algebraic manipulation, the end result is

$$\beta_{j,k}^{(i)} = [\langle y_j^{(0)}, M^{(N)} \hat{y}_i^{(k)} \rangle - \sum_{l=1}^{k-1} \lambda_i^{(k-l+N)} \beta_{j,l}^{(i)}$$
$$+ \sum_{l=0}^{k+N-2} \langle y_j^{(0)}, (A_{k-l+N} - \sum_{r=1}^{k-l+N} \lambda_i^{(k-l-r+N)} B_r) y_i^{(l)} \rangle] / [\lambda_i^{(1)} - \lambda_j^{(1)}], \qquad (4.49)$$

for $(i \neq j)$. The existence of this formula guarantees that each $y_i^{(k)}$ is uniquely determined by enforcing solvability of Equation (4.29) for $k \leftarrow k + N$.

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.

In the Rayleigh-Schrödinger procedure, whenever an eigenvalue branches by reduction in multiplicty at any order, one simply replaces the x_μ of Equation (4.44) by any convenient B_0-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 (4.49) 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 Equation (4.29) with $k \leftarrow k + N$.

We now present an example which illustrates the general procedure. This example features a simple (i.e. nondegenerate) eigenvalue together with a triple eigenvalue which branches into a single first order degenerate eigenvalue together with a pair of second order degenerate eigenvalues.

Example 4.2.1. *Define*

$$A(\epsilon) = \begin{bmatrix} 5\sin(\epsilon) & 3\sin(\epsilon) & 0 & 3\sin(\epsilon) \\ 3\sin(\epsilon) & 5\sin(\epsilon) & 0 & \sin(\epsilon) \\ 0 & 0 & 0 & 0 \\ 3\sin(\epsilon) & \sin(\epsilon) & 0 & 2 \end{bmatrix}, \quad B(\epsilon) = \begin{bmatrix} 5 & 3 & 0 & 0 \\ 3 & 5 & 0 & 0 \\ 0 & 0 & 2+2\sin(\epsilon) & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

$$\Rightarrow A_0 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}, \quad B_0 = \begin{bmatrix} 5 & 3 & 0 & 0 \\ 3 & 5 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix},$$

$$A_{2k-1} = \frac{(-1)^{k-1}}{(2k-1)!} \begin{bmatrix} 5 & 3 & 0 & 3 \\ 3 & 5 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 3 & 1 & 0 & 0 \end{bmatrix}, \ B_{2k-1} = \frac{(-1)^{k-1}}{(2k-1)!} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

with $A_{2k} = B_{2k} = 0$ $(k = 1, 2, \dots)$.

Using MATLAB's Symbolic Toolbox, we find that

$$\lambda_1(\epsilon) = \epsilon - \frac{1}{6}\epsilon^3 + \frac{1}{120}\epsilon^5 - \cdots \ , \ \lambda_2(\epsilon) = \epsilon - \epsilon^2 - \frac{7}{6}\epsilon^3 + \frac{1}{3}\epsilon^4 + \frac{301}{120}\epsilon^5 + \cdots \ ,$$

$$\lambda_3(\epsilon) = 0 \ , \ \lambda_4(\epsilon) = 1 + \epsilon^2 + \epsilon^3 - \frac{1}{3}\epsilon^4 - \frac{5}{2}\epsilon^5 + \cdots \ .$$

Applying the nondegenerate Rayleigh-Schrödinger procedure developed above to

$$\lambda_4^{(0)} = 1; \ x_4^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1/\sqrt{2} \end{bmatrix},$$

we arrive at (using Equation (4.32) with $j = 0$)

$$\lambda_4^{(1)} = \langle x_4^{(0)}, (A_1 - \lambda_4^{(0)} B_1) x_4^{(0)} \rangle = 0.$$

Solving

$$(A_0 - \lambda_4^{(0)} B_0) x_4^{(1)} = -(A_1 - \lambda_4^{(1)} B_0 - \lambda_4^{(0)} B_1) x_4^{(0)}$$

produces

$$x_4^{(1)} = \begin{bmatrix} 3/4\sqrt{2} \\ -1/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix},$$

where we have enforced the intermediate normalization $\langle x_4^{(1)}, B_0 x_4^{(0)} \rangle = 0$. In turn, the generalized Dalgarno-Stewart identities yield

$$\lambda_4^{(2)} = \langle x_4^{(0)}, (A_1 - \lambda_4^{(0)} B_1) x_4^{(1)} \rangle + \langle x_4^{(0)}, (A_2 - \lambda_4^{(1)} B_1 - \lambda_4^{(0)} B_2) x_4^{(0)} \rangle = 1,$$

and

$$\lambda_4^{(3)} = \langle x_4^{(1)}, (A_1 - \lambda_4^{(1)} B_0 - \lambda_4^{(0)} B_1) x_4^{(1)} \rangle + 2\langle x_4^{(0)}, (A_2 - \lambda_4^{(1)} B_1 - \lambda_4^{(0)} B_2) x_4^{(1)} \rangle$$

$$+\langle x_4^{(0)}, (A_3 - \lambda_4^{(2)} B_1 - \lambda_4^{(1)} B_2 - \lambda_4^{(0)} B_3) x_4^{(0)} \rangle = 1.$$

Solving

$$(A_0 - \lambda_4^{(0)} B_0) x_4^{(2)} = -(A_1 - \lambda_4^{(1)} B_0 - \lambda_4^{(0)} B_1) x_4^{(1)} - (A_2 - \lambda_4^{(2)} B_0 - \lambda_4^{(1)} B_1 - \lambda_4^{(0)} B_2) x_4^{(0)}$$

produces

$$x_4^{(2)} = \begin{bmatrix} 3/4\sqrt{2} \\ -1/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix},$$

where we have enforced the intermediate normalization $\langle x_4^{(2)}, B_0 x_4^{(0)} \rangle = 0$. Again, the generalized Dalgarno-Stewart identities yield

$$\lambda_4^{(4)} = \langle x_4^{(1)}, (A_1 - \lambda_4^{(1)} B_0 - \lambda_4^{(0)} B_1) x_4^{(2)} \rangle + \langle x_4^{(0)}, (A_2 - \lambda_4^{(1)} B_1 - \lambda_4^{(0)} B_2) x_4^{(2)} \rangle$$

$$+\langle x_4^{(1)}, (A_2 - \lambda_4^{(2)} B_0 - \lambda_4^{(1)} B_1 - \lambda_4^{(0)} B_2) x_4^{(1)} \rangle$$

$$+2\langle x_4^{(1)}, (A_3 - \lambda_4^{(3)} B_0 - \lambda_4^{(2)} B_1 - \lambda_4^{(1)} B_2 - \lambda_4^{(0)} B_3) x_4^{(1)} \rangle$$

$$+\langle x_4^{(0)}, (A_4 - \lambda_4^{(3)} B_1 - \lambda_4^{(2)} B_2 - \lambda_4^{(1)} B_3 - \lambda_4^{(0)} B_4) x_4^{(0)} \rangle = -\frac{1}{3},$$

and

$$\lambda_4^{(5)} = \langle x_4^{(2)}, (A_1 - \lambda_4^{(1)} B_0 - \lambda_4^{(0)} B_1) x_4^{(2)} \rangle + 2\langle x_4^{(2)}, (A_2 - \lambda_4^{(2)} B_0 - \lambda_4^{(1)} B_1 - \lambda_4^{(0)} B_2) x_4^{(1)} \rangle$$

$$+\langle x_4^{(1)}, (A_3 - \lambda_4^{(3)} B_0 - \lambda_4^{(2)} B_1 - \lambda_4^{(1)} B_2 - \lambda_4^{(0)} B_3) x_4^{(1)} \rangle$$

$$+2\langle x_4^{(2)}, (A_3 - \lambda_4^{(2)} B_1 - \lambda_4^{(1)} B_2 - \lambda_4^{(0)} B_3) x_4^{(0)} \rangle$$

$$+2\langle x_4^{(1)}, (A_4 - \lambda_4^{(4)} B_0 - \lambda_4^{(3)} B_1 - \lambda_4^{(2)} B_2 - \lambda_4^{(1)} B_3 - \lambda_4^{(0)} B_4) x_4^{(0)} \rangle$$

$$+\langle x_4^{(0)}, (A_5 - \lambda_4^{(4)} B_1 - \lambda_4^{(3)} B_2 - \lambda_4^{(2)} B_3 - \lambda_4^{(1)} B_4 - \lambda_4^{(0)} B_5) x_4^{(0)} \rangle = -\frac{5}{2},$$

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

$$x_1^{(0)} = \begin{bmatrix} 3/4\sqrt{2} \\ -1/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix};\ x_2^{(0)} = \begin{bmatrix} -1/4\sqrt{2} \\ 3/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix};\ x_3^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1/\sqrt{2} \\ 0 \end{bmatrix},$$

we have from Equation (4.38), which enforces solvability of Equation (4.29) for $k = 1$,

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

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

$$\begin{bmatrix} a_1^{(3)} \\ a_2^{(3)} \\ a_3^{(3)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \Rightarrow y_3^{(0)} = \begin{bmatrix} 0 \\ 0 \\ 1/\sqrt{2} \\ 0 \end{bmatrix}.$$

Introducing the new basis

$$z_1^{(0)} = \begin{bmatrix} \sqrt{5}/4 \\ -3/4\sqrt{5} \\ 0 \\ 0 \end{bmatrix};\ z_2^{(0)} = \begin{bmatrix} 0 \\ 1/\sqrt{5} \\ 0 \\ 0 \end{bmatrix},$$

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

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

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

Solving Equation (4.29) for $k = 1$,

$$(A_0 - \lambda^{(0)} B_0) y_i^{(1)} = -(A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(0)}\ (i = 1, 2, 3),$$

produces

$$y_1^{(1)} = \begin{bmatrix} \alpha_1 \\ \beta_1 \\ \gamma_1 \\ -(3b_1^{(1)} + b_2^{(1)})/2\sqrt{5} \end{bmatrix};\ y_2^{(1)} = \begin{bmatrix} \alpha_2 \\ \beta_2 \\ \gamma_2 \\ -(3b_1^{(2)} + b_2^{(2)})/2\sqrt{5} \end{bmatrix};\ y_3^{(1)} = \begin{bmatrix} \alpha_3 \\ \beta_3 \\ \gamma_3 \\ 0 \end{bmatrix}.$$

Now, enforcing solvability of Equation (4.29) for $k = 2$ $(i = 1, 2, 3)$,

$$-(A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(1)} - (A_2 - \lambda_i^{(2)} B_0 - \lambda_i^{(1)} B_1 - \lambda^{(0)} B_2) y_i^{(0)} \perp \{z_1^{(0)}, z_2^{(0)}, y_3^{(0)}\},$$

we arrive at

$$M = \begin{bmatrix} -9/10 & -3/10 \\ -3/10 & -1/10 \end{bmatrix},$$

with eigenpairs

$$\lambda_1^{(2)} = 0, \begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \end{bmatrix} = \begin{bmatrix} 1/\sqrt{10} \\ -3/\sqrt{10} \end{bmatrix}; \ \lambda_2^{(2)} = -1, \begin{bmatrix} b_1^{(2)} \\ b_2^{(2)} \end{bmatrix} = \begin{bmatrix} 3/\sqrt{10} \\ 1/\sqrt{10} \end{bmatrix}$$

$$\Rightarrow y_1^{(0)} = \begin{bmatrix} 1/4\sqrt{2} \\ -3/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(0)} = \begin{bmatrix} 3/4\sqrt{2} \\ -1/4\sqrt{2} \\ 0 \\ 0 \end{bmatrix};$$

$$y_1^{(1)} = \begin{bmatrix} -3\beta_1 \\ \beta_1 \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(1)} = \begin{bmatrix} \alpha_2 \\ -3\alpha_2 \\ 0 \\ -1/\sqrt{2} \end{bmatrix}; \ y_3^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix},$$

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 Equation (4.29) for $k = 2$ $(i = 1, 2, 3)$,

$$(A_0 - \lambda^{(0)} B_0) y_i^{(2)} = -(A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(1)} - (A_2 - \lambda_i^{(2)} B_0 - \lambda_i^{(1)} B_1 - \lambda^{(0)} B_2) y_i^{(0)},$$

produces

$$y_1^{(2)} = \begin{bmatrix} -3b_1 \\ b_1 \\ c_1 \\ 4\beta_1 \end{bmatrix}; \ y_2^{(2)} = \begin{bmatrix} a_2 \\ -3a_2 \\ c_2 \\ -1/\sqrt{2} \end{bmatrix}; \ y_3^{(2)} = \begin{bmatrix} a_3 \\ b_3 \\ 0 \\ 0 \end{bmatrix},$$

where we have invoked intermediate normalization.

We next enforce solvability of Equation (4.29) for $k = 3$,

$$\langle y_j^{(0)}, -(A_1 - \lambda_i^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(2)} - (A_2 - \lambda_i^{(2)} B_0 - \lambda_i^{(1)} B_1 - \lambda^{(0)} B_2) y_i^{(1)}$$

$$-(A_3 - \lambda_i^{(3)} B_0 - \lambda_i^{(2)} B_1 - \lambda_i^{(1)} B_2 - \lambda^{(0)} B_3) y_i^{(0)} \rangle = 0 \ (i \neq j),$$

thereby producing

$$y_1^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}; \ y_2^{(1)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1/\sqrt{2} \end{bmatrix};$$

$$y_1^{(2)} = \begin{bmatrix} -3b_1 \\ b_1 \\ 0 \\ 0 \end{bmatrix};\ y_2^{(2)} = \begin{bmatrix} a_2 \\ -3a_2 \\ 0 \\ -1/\sqrt{2} \end{bmatrix};\ y_3^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

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

$$\lambda_1^{(3)} = -\frac{1}{6},\ \lambda_2^{(3)} = -\frac{7}{6},\ \lambda_3^{(3)} = 0.$$

Solving Equation (4.29) for $k = 3$,

$$(A_0 - \lambda^{(0)} B_0) y_i^{(3)} = -(A_1 - \lambda^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(2)} - (A_2 - \lambda_i^{(2)} B_0 - \lambda^{(1)} B_1 - \lambda^{(0)} B_2) y_i^{(1)}$$

$$-(A_3 - \lambda_i^{(3)} B_0 - \lambda_i^{(2)} B_1 - \lambda^{(1)} B_2 - \lambda^{(0)} B_3) y_i^{(0)}\ (i = 1, 2),$$

produces

$$y_1^{(3)} = \begin{bmatrix} -3v_1 \\ v_1 \\ w_1 \\ 4b_1 \end{bmatrix};\ y_2^{(3)} = \begin{bmatrix} u_2 \\ -3u_2 \\ w_2 \\ 1/6\sqrt{2} \end{bmatrix},$$

where we have invoked intermediate normalization.

We now enforce solvability of Equation (4.29) for $k = 4$,

$$\langle y_j^{(0)}, -(A_1 - \lambda^{(1)} B_0 - \lambda^{(0)} B_1) y_i^{(3)} - (A_2 - \lambda_i^{(2)} B_0 - \lambda^{(1)} B_1 - \lambda^{(0)} B_2) y_i^{(2)}$$

$$-(A_3 - \lambda_i^{(3)} B_0 - \lambda_i^{(2)} B_1 - \lambda^{(1)} B_2 - \lambda^{(0)} B_3) y_i^{(1)}$$

$$-(A_4 - \lambda_i^{(4)} B_0 - \lambda_i^{(3)} B_1 - \lambda_i^{(2)} B_2 - \lambda^{(1)} B_3 - \lambda^{(0)} B_4) y_i^{(0)} \rangle = 0\ (i \neq j),$$

thereby fully determining

$$y_1^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix};\ y_2^{(2)} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -1/\sqrt{2} \end{bmatrix}.$$

Subsequent application of the generalized Dalgarno-Stewart identities yields

$$\lambda_1^{(4)} = 0,\ \lambda_1^{(5)} = \frac{1}{120},\ \lambda_2^{(4)} = \frac{1}{3},\ \lambda_2^{(5)} = \frac{301}{120},\ \lambda_3^{(4)} = 0,\ \lambda_3^{(5)} = 0.$$

Chapter 5

Application to Inhomogeneous Acoustic Waveguides

It is only fitting that this monograph should conclude by returning to the roots of the Rayleigh-Schrödinger perturbation procedure: Acoustics! Specifically, this chapter concerns itself with how the cut-off frequencies and modal shapes of cylindrical acoustic waveguides are altered by the presence of temperature gradients induced by an applied temperature distribution along the duct walls. A physical model is first formulated which incorporates an inhomogeneous sound speed as well as a density gradient. The associated mathematical model is then a generalized eigenproblem. This is then discretized via the Control Region Approximation (a finite difference scheme) yielding a generalized matrix eigenproblem. Under the assumption that the boundary temperature distribution is nearly constant, we apply the procedure of Rayleigh [87] and Schrödinger [101] to express the propagation constants and modal functions as perturbation series whose successive terms can be generated recursively. An addendum is included which outlines the modifications necessary for the correct treatment of degenerate modes [17]. The case of a rectangular duct with temperature variation in its cross-section is considered in detail. All numerical computations were performed using MATLAB©.

5.1 Physical Problem

The modal propagation characteristics of cylindrical acoustic waveguides (see Figure 5.1) at constant temperature have been investigated analytically for canonical duct cross-sections such as rectangular and circular [46] and numerically for general simply-connected cross-sections [57]. However, if there is a temperature variation across the duct then these analyses are inadequate. This is due to the inhomogeneous sound speed and density gradient induced by such a temperature distribution.

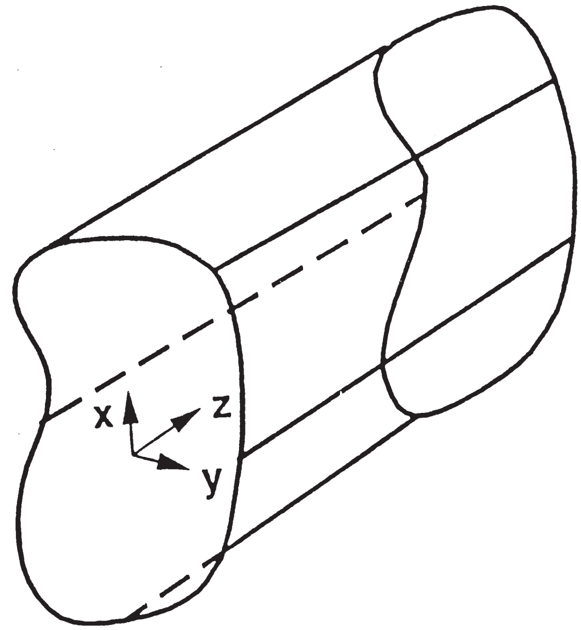

Figure 5.1: Acoustic Waveguide Cross-Section

Such temperature variations occur in the exhaust systems of vehicles [75] where the bottom portion of the waveguide is in direct contact with the ambient atmosphere while the upper portion is either near or in contact with the body of the vehicle which is at a different temperature. As will be shown, such an induced temperature perturbation across the waveguide can significantly alter the modal characteristics of the exhaust system with a consequent reduction in its overall effectiveness at suppressing selected acoustic frequencies.

In ocean acoustics [15], both depth and range dependent sound speeds are typically considered. Density gradients are usually ignored since the spatial scale of such variations is much larger than the wavelength of the acoustic disturbance. The same situation obtains in atmospheric propagation [16]. Unlike such ocean and atmospheric waveguides, the ducts and mufflers [75] under consideration in this chapter are fully enclosed and hence density gradients *must* be accounted for.

We commence with the formulation of a physical model which includes both an inhomogeneous sound speed and a density gradient across the duct. We will confine our attention to small perturbations of an isothermal ambient state. The corresponding mathematical model will involve a generalized Helmholtz operator whose eigenvalues (related to the cut-off frequencies) and eigenfunctions (modal shapes) are to be determined. This continuous problem is discretized via the Control Region Approximation [59, 66] (a finite difference procedure) resulting in a generalized matrix eigenvalue problem.

A perturbation procedure previously applied to uniform waveguides [58], invented by Rayleigh [87] in acoustics and developed by Schrödinger [101] in quantum mechanics, is invoked to produce perturbation expansions for the aforementioned eigenvalues and eigenvectors. In turn, this permits the development of analytical expressions for cut-off frequencies and modal shapes.

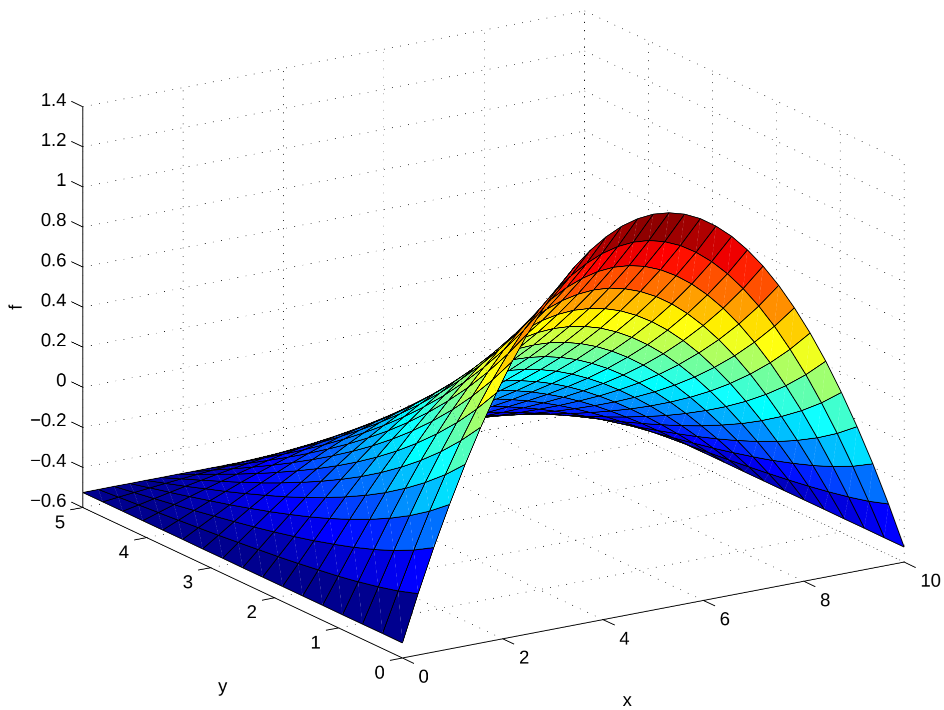

Figure 5.2: Temperature Perturbation Profile

This procedure is illustrated for the case of a rectangular duct with an applied parabolic temperature profile along its lower wall (see Figure 5.2). All numerical computations were performed using MATLAB©.

5.2 Mathematical Formulation

With reference to Figure 5.1, we consider the acoustic field within an infinitely long, hard-walled, cylindrical tube of general cross-section, Ω. The analysis of the propagation characteristics of such an acoustical waveguide typically proceeds by assuming a constant temperature throughout the undisturbed fluid.

However, in the present study, we permit a small steady-state temperature perturbation about the average cross-sectional temperature (see Figure 5.2)

$$\hat{T}(x,y;\epsilon) = \hat{T}_0[1 + \epsilon f(x,y)] \tag{5.1}$$

where $\int\int_\Omega f(x,y)\, dA = 0$ and ϵ is small.

This temperature perturbation is due to an applied steady-state temperature distribution along the walls of the duct

$$\Delta\hat{T} = 0 \ in \ \Omega; \ \hat{T} = T_{applied} \ on \ \partial\Omega \tag{5.2}$$

where, here as well as in the ensuing analysis, all differential operators are transverse to the longitudinal axis of the waveguide. Consequently, $\nabla(f^n) = nf^{n-1}(\nabla f)$ and $\Delta(f^n) = n(n-1)f^{n-2}(\nabla f \cdot \nabla f)$.

This small temperature variation across the duct will produce inhomogeneities in the background fluid density

$$\hat{\rho}(x,y;\epsilon) = \frac{1}{R} \cdot \frac{\hat{p}(\epsilon)}{\hat{T}(x,y;\epsilon)} = \frac{1}{R\hat{T}_0} \cdot \frac{\hat{p}(\epsilon)}{[1+\epsilon f(x,y)]} \tag{5.3}$$

and sound speed

$$c^2 = R\hat{T}(x,y;\epsilon) = c_0^2[1 + \epsilon f(x,y)]. \tag{5.4}$$

The self-consistent governing equation for the hard-walled acoustic pressure, p, with (angular) frequency ω and propagation constant β is [30]

$$\nabla \cdot (\frac{\hat{\rho}_0}{\hat{\rho}} \nabla p) + \frac{\hat{\rho}_0}{\hat{\rho}} (\frac{\omega^2}{c^2} - \beta^2) p - \frac{\hat{\rho}_0}{\hat{\rho}} \nabla \cdot (\frac{1}{\hat{\rho}} \nabla \hat{\rho}) p = 0 \ in \ \Omega; \ \frac{\partial p}{\partial n} = 0 \ on \ \partial\Omega \tag{5.5}$$

assuming that the fluid is at rest (the cut-off frequencies are unaltered by uniform flow down the tube [74]). In the above, hatted quantities refer to undisturbed background fluid quantities while $p(x,y,\epsilon)$ is the acoustic disturbance superimposed upon this background [30]. In what follows, it is important to preserve the self-adjointness of this boundary value problem.

5.3 Perturbation Procedure

Expansion of the pressure in a perturbation series in the small parameter ϵ

$$\hat{p}(\epsilon) = \sum_{n=0}^{\infty} \epsilon^n \hat{p}_n \tag{5.6}$$

induces a corresponding perturbation expansion for the density

$$\hat{\rho} = \hat{\rho}_0[1 + \epsilon(A_1 - f) + \epsilon^2(A_2 - A_1 f + f^2) + \epsilon^3(A_3 - A_2 f + A_1 f^2 - f^3) + \cdots] \tag{5.7}$$

where $\hat{\rho}_0 := \hat{p}_0/(R\hat{T}_0)$ and $A_n := \hat{p}_n/\hat{p}_0$.

By invoking conservation of mass, $M := \int\int_\Omega \hat{\rho}(x, y; \epsilon)\, dA$ must be independent of ϵ which together with $\int\int_\Omega f\, dA = 0$ implies that $A_1 = 0,\ A_2 = -(\int\int_\Omega f^2\, dA)/A_\Omega,\ A_3 = (\int\int_\Omega f^3\, dA)/A_\Omega$. Thus,

$$\hat{\rho} = \hat{\rho}_0[1 - \epsilon f + \epsilon^2(A_2 + f^2) + \epsilon^3(A_3 - A_2 f - f^3) + \cdots], \tag{5.8}$$

$$\frac{1}{\hat{\rho}} = \frac{1}{\hat{\rho}_0}[1 + \epsilon f - \epsilon^2 A_2 - \epsilon^3(A_2 f + A_3) + \cdots], \tag{5.9}$$

$$\nabla\hat{\rho} = \hat{\rho}_0[-\epsilon + \epsilon^2(2f) + \epsilon^3(-A_2 - 3f^2) + \cdots]\nabla f, \tag{5.10}$$

$$\frac{1}{c^2} = \frac{1}{c_0^2}[1 - \epsilon f + \epsilon^2 f^2 - \epsilon^3 f^3 + \cdots]. \tag{5.11}$$

Inserting these expansions into Equation (5.5) results in

$$\begin{aligned} \Delta p + \epsilon[\nabla\cdot(f\nabla p) - k_0^2 f p] - \epsilon^2[\alpha_2\Delta p + (\nabla f\cdot\nabla f)p] \\ +\epsilon^3[\alpha_3\Delta p + \alpha_2 f k_0^2 p - \alpha_2\nabla\cdot(f\nabla p) + (f\nabla f\cdot\nabla f)p] + \cdots \\ = \lambda p[1 + \epsilon f - \epsilon^2\alpha_2 + \epsilon^3(-\alpha_2 f + \alpha_3) + \cdots]\ in\ \Omega;\ \frac{\partial p}{\partial n} = 0\ on\ \partial\Omega. \end{aligned} \tag{5.12}$$

where the wave number is $k_0^2 := \omega^2/c_0^2$ and $\lambda := \beta^2 - k_0^2,\ \alpha_2 := A_2,\ \alpha_3 := -A_3$. It is interesting to note that the 3rd term of Equation (5.5) makes no $O(\epsilon)$ contribution and thus is of "higher order" than the 1st and 2nd terms.

5.4 Control Region Approximation

The Control Region Approximation [57, 59] is a generalized finite difference procedure that accomodates arbitrary geometries [67]. It involves discretization of conservation form expressions on Dirichlet/Delaunay tessellations (see below). This permits a straightforward application of relevant boundary conditions.

The first stage in the Control Region Approximation is the tessellation of the solution domain by Dirichlet regions associated with a pre-defined yet

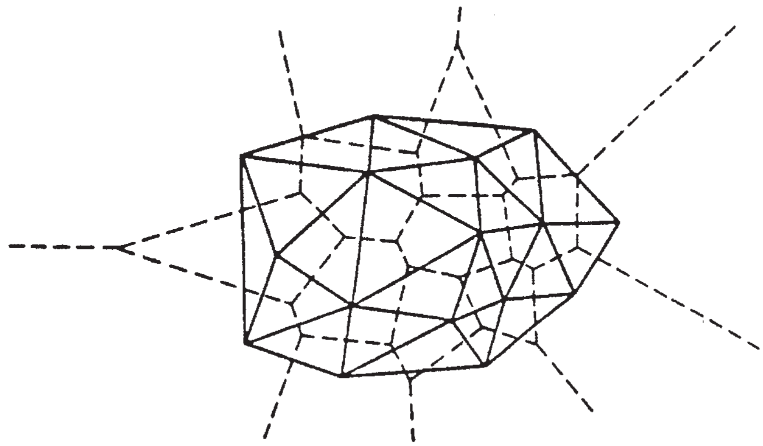

Figure 5.3: Dirichlet/Delaunay Tessellations

(virtually) arbitrary distribution of grid points. Denoting a generic grid point by P_i, we define its Dirichlet region as

$$D_i := \{P \ : \ ||P - P_i|| < ||P - P_j||, \ \forall j \neq i\}. \tag{5.13}$$

This is seen to be the convex polygon formed by the intersection of the half-spaces defined by the perpendicular bisectors of the straight line segments connecting P_i to P_j, $\forall j \neq i$. It is the natural control region to associate with P_i since it contains those and only those points which are closer to P_i than to any other grid point P_j.

If we construct the Dirichlet region surrounding each of the grid points, we obtain the Dirichlet tessellation of the plane which is shown dashed in Figure 5.3. There we have also connected by solid lines neighboring grid points which share an edge of their respective Dirichlet regions. This construction tessellates the convex hull of the grid points by so-called Delaunay triangles. The union of these triangles is referred to as the Delaunay tessellation. The grid point distribution is tailored so that the Delaunay triangle edges conform to $\partial\Omega$. It is essential to note that these two tessellations are dual to one another in the sense that corresponding edges of each are orthogonal.

With reference to Figure 5.4, we will exploit this duality in order to approximate the Dirichlet problem, Equation (5.2), for the temperature distribution at the point P_0. We first reformulate the problem by integrating over the

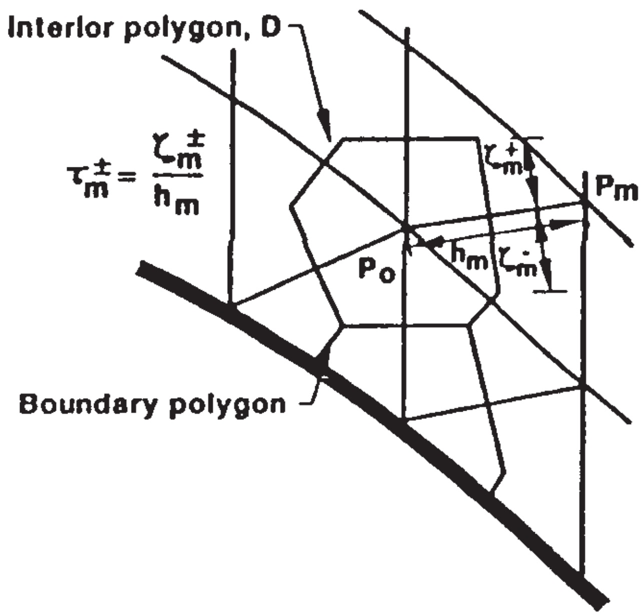

Figure 5.4: Control Region Approximation

control region, D, and applying the divergence theorem, resulting in:

$$\oint_{\partial D} \frac{\partial \hat{T}}{\partial \nu} \, d\sigma = 0, \tag{5.14}$$

where (ν, σ) are normal and tangential coordinates, respectively, around the periphery of D. The normal temperature flux, $\frac{\partial \hat{T}}{\partial \nu}$, may now be approximated by straightforward central differences [22] thereby yielding the Control Region Approximation:

$$\sum_m \tau_m \, (\hat{T}_m - \hat{T}_0) = 0, \tag{5.15}$$

where the index m ranges over the sides of D and $\tau_m := \tau_m^- + \tau_m^+$. Equation (5.15) for each interior grid point may be assembled in a (sparse) matrix equation which can then be solved for $\hat{T}(x, y)$ (with specified boundary values) and *ipso facto* for $f(x, y)$ from Equation (5.1).

It remains to discretize the homogeneous Neumann boundary value problem, Equation (5.12), for the acoustic pressure wave by the Control Region

Approximation. For this purpose we first rewrite it in the integral form:

$$\begin{aligned}
&\oint_{\partial D} \frac{\partial p}{\partial \nu}\, d\sigma + \epsilon[\oint_{\partial D} f \frac{\partial p}{\partial \nu}\, d\sigma - k_0^2 \int\int_D fp\, dA] \\
&-\epsilon^2[\alpha_2 \oint_{\partial D} \frac{\partial p}{\partial \nu}\, d\sigma + \int\int_D (\nabla f \cdot \nabla f) p\, dA] \\
&+\epsilon^3[\alpha_3 \oint_{\partial D} \frac{\partial p}{\partial \nu}\, d\sigma + \alpha_2 k_0^2 \int\int_D fp\, dA \\
&-\alpha_2 \oint_{\partial D} f \frac{\partial p}{\partial \nu}\, d\sigma + \int\int_D (f \nabla f \cdot \nabla f) p\, dA] + \cdots \\
&= \lambda[\int\int_D p\, dA + \epsilon \int\int_D fp\, dA - \epsilon^2 \alpha_2 \int\int_D p\, dA \\
&+\epsilon^3(-\alpha_2 \int\int_D fp\, dA + \alpha_3 \int\int_D p\, dA) + \cdots].
\end{aligned} \tag{5.16}$$

We then approximate each of the integral operators appearing in Equation (5.16) as follows:

$$\oint_{\partial D} \frac{\partial p}{\partial \nu}\, d\sigma \approx (Ap)_0 := \sum_m \tau_m\, (p_m - p_0), \tag{5.17}$$

$$\int\int_D p\, dA \approx (Bp)_0 := A_0\, p_0, \tag{5.18}$$

$$\oint_{\partial D} f \frac{\partial p}{\partial \nu}\, d\sigma \approx (Cp)_0 := \sum_m \tau_m\, \frac{f_0 + f_m}{2}\, (p_m - p_0), \tag{5.19}$$

$$\int\int_D fp\, dA \approx (D_0 p)_0 := f_0 A_0\, p_0, \tag{5.20}$$

$$\begin{aligned}
-\int\int_D (\nabla f \cdot \nabla f) p\, dA &= -\frac{1}{2} \int\int_D \Delta f^2\, dA = -\frac{1}{2} \oint_{\partial D} \frac{\partial f^2}{\partial \nu}\, d\sigma \\
&\approx (D_1 p)_0 := -\frac{p_0}{2} \cdot \sum_m \tau_m\, (f_m^2 - f_0^2),
\end{aligned} \tag{5.21}$$

$$\int\int_D (f \nabla f \cdot \nabla f) p\, dA \approx (D_2 p)_0 := \frac{f_0 p_0}{2} \cdot \sum_m \tau_m\, (f_m^2 - f_0^2), \tag{5.22}$$

where A_0 is the area of D (restricted to Ω, if necessary).

Also,

$$\alpha_2 = -\int\int_{\Omega} f^2 \; dA/A_{\Omega} \approx -\sum_k \; f_k^2 A_k / \sum_k \; A_k, \tag{5.23}$$

$$\alpha_3 = -\int\int_{\Omega} f^3 \; dA/A_{\Omega} \approx -\sum_k \; f_k^3 A_k / \sum_k \; A_k, \tag{5.24}$$

where the summations are over the entire Dirichlet grid.

The hard boundary condition, $\frac{\partial p}{\partial \nu} = 0$, is enforced by simply modifying any τ_m in Equations (5.17) and (5.19) corresponding to boundary edges. Because $\Delta f = 0$, the approximations of Equations (5.21) and (5.22) may be modified at the boundary using $\frac{1}{2}\frac{\partial f^2}{\partial \nu} = f\frac{\partial f}{\partial \nu}$ with $\frac{\partial f}{\partial \nu}$ then approximated as in Equations (5.14-5-15).

5.5 Generalized Eigenvalue Problem

Substitution of Equations (5.17-5.22) into Equation (5.16) yields the matrix generalized eigenvalue problem [114] $\hat{A}(\epsilon)p = \lambda\hat{B}(\epsilon)p$ with analytic perturbation which was extensively studied in Section 4.2:

$$\begin{aligned}[A + \epsilon(C - \beta^2 D_0) - \epsilon^2(\alpha_2 A - D_1) + \epsilon^3(\alpha_3 A + \alpha_2\beta^2 D_0 - \alpha_2 C + D_2) + \cdots]p \\ = \lambda[B - \epsilon^2\alpha_2 B + \epsilon^3\alpha_3 B + \cdots]p,\end{aligned} \tag{5.25}$$

where A is symmetric and nonpositive semidefinite, C is symmetric, B is positive and diagonal, while D_0, D_1 and D_2 are diagonal.

We next apply the perturbation procedure of Rayleigh [87] and Schrödinger [101], as described in [17] and developed in detail in Section 4.2, to construct expansions

$$\lambda(\epsilon) = \sum_{n=0}^{\infty} \epsilon^n \lambda_n; \; p(\epsilon) = \sum_{n=0}^{\infty} \epsilon^n p_n, \tag{5.26}$$

the convergence of which are studied in Appendix A.

Here, we assume that λ_0 is a simple eigenvalue with corresponding eigenvector p_0 for the unperturbed problem

$$Ap_0 = \lambda_0 B p_0 \tag{5.27}$$

which can be determined by the procedure of [57]. An eigenvalue of multiplicity m would entail an expansion in $\epsilon^{1/m}$ in the event of eigenvector deficiency [114]. As will be evident in what follows, our approximation scheme is greatly enhanced by the symmetry of $(\hat{A}(\epsilon), \hat{B}(\epsilon))$ which is inherited from that of A, B, C, D_0, D_1 and D_2 [47].

Inserting the expansions, Equation (5.26), into the eigenproblem, Equation (5.25), collecting terms, and equating coefficients of like powers of ϵ results in

$$(A - \lambda_0 B)p_0 = 0, \tag{5.28}$$

$$(A - \lambda_0 B)p_1 = \lambda_1 B p_0 - C p_0 + \beta^2 D_0 p_0, \tag{5.29}$$

$$(A - \lambda_0 B)p_2 = \lambda_2 B p_0 + \lambda_1 B p_1 - C p_1 - D_1 p_0 + \beta^2 D_0 p_1, \tag{5.30}$$

$$\begin{aligned}(A - \lambda_0 B)p_3 = \lambda_3 B p_0 + \lambda_2 B p_1 + \lambda_1 B p_2 - C p_2 + (\alpha_2 A - D_1 - \alpha_2 \lambda_0 B)p_1 \\ +(\alpha_2 C - D_2 - \alpha_2 \lambda_1 B)p_0 + \beta^2 (D_0 p_2 - \alpha_2 D_0 p_0),\end{aligned} \tag{5.31}$$

and so forth. Alternatively, we could have inserted the expansions, Equation (5.26), into the continuous Equation (5.5) and then discretized via the Control Region Approximation with the same end result, Equations (5.28-5.31).

Equation (5.28) together with the normalization $\langle p_0, B p_0 \rangle = 1$ yields $\lambda_0 = \langle p_0, A p_0 \rangle$. Note that $(A - \lambda_0 B)$ is singular (in fact, its nullity is 1 by assumption) and that the symmetry of A implies that the right hand side of Equation (5.29) must be orthogonal to p_0 producing

$$\lambda_1 = \hat{\lambda}_1 - \beta^2 \tilde{\lambda}_1; \; \hat{\lambda}_1 = \langle p_0, C p_0 \rangle, \; \tilde{\lambda}_1 = \langle p_0, D_0 p_0 \rangle. \tag{5.32}$$

Thus, the symmetry of A has produced λ_1 *without* calculating p_1. Since C is indefinite, λ_1 may be either positive or negative. As a result, this perturbation procedure provides neither lower nor upper bounds on the eigenvalues.

Next, employ the pseudoinverse to solve Equation (5.29) for p_1

$$\hat{p}_1 = -(A - \lambda_0 B)^{\dagger}(C - \beta^2 D_0 - \lambda_1 B)p_0; \; p_1 = -\langle \hat{p}_1, B p_0 \rangle p_0 + \hat{p}_1, \tag{5.33}$$

thus ensuring that $\langle p_1, B p_0 \rangle = 0$ for later convenience. However, the computation of the pseudoinverse may be avoided by instead performing the QR factorization of $(A-\lambda_0 B)$ and then employing it to produce the minimum-norm least-squares solution, $\hat{p}_1$, to this exactly determined rank-deficient system [78]. (Case 1B of Chapter 2 with deficiency in rank equal to eigenvalue multiplicity.) Again, define $p_1 := \hat{p}_1 - \langle \hat{p}_1, B p_0 \rangle p_0$ producing $\langle p_1, B p_0 \rangle = 0$ which simplifies subsequent computations.

The knowledge of p_1, together with the symmetry of A, permits the computation of *both* λ_2 and λ_3:

$$\lambda_2 = \hat{\lambda}_2 - \beta^2 \tilde{\lambda}_2; \;\; \lambda_3 = \hat{\lambda}_3 - \beta^2 \tilde{\lambda}_3, \tag{5.34}$$

$$\hat{\lambda}_2 = \langle p_0, Cp_1 + D_1 p_0 \rangle, \;\; \tilde{\lambda}_2 = \langle p_0, D_0 p_1 \rangle, \tag{5.35}$$

$$\hat{\lambda}_3 = \langle p_1, (C - \lambda_1 B) p_1 \rangle + \langle p_0, 2D_1 p_1 + D_2 p_0 \rangle, \;\; \tilde{\lambda}_3 = \langle p_1, D_0 p_1 \rangle. \tag{5.36}$$

In evaluating the required inner products, we benefit greatly from the sparsity of A and C and the diagonality of B, D_0, D_1, and D_2. Note that the computation of only a single pseudoinverse / QR factorization suffices to produce *all* of the modal corrections, p_n.

We can continue indefinitely in this fashion, with each succeeding term in the expansion for p producing the next two terms in the expansion for λ, as guaranteed by the generalized Dalgarno-Stewart identities, Equations (4.32-4.33). If we had reduced this to a standard eigenvalue problem through multiplication of Equation (5.25) by $[B - \cdots]^{-1}$, we would have destroyed the symmetry of the operators and sacrificed this substantial economy of computation. Observe that for a nondegenerate eigenvalue, p_0 does not depend upon β so that $\hat{\lambda}_1$ is frequency-independent.

When a mode is degenerate, the Rayleigh-Schrödinger procedure must be modified accordingly [17]. We illustrate this modification for the case of a double eigenvalue with degeneracy resolved at first-order. This occurs, for example, for the $(0,1)$ and $(2,0)$ modes of the rectangular waveguide of [60, 61]. For such a degenerate mode, p_0 now depends upon β so that $\hat{\lambda}_1$ is frequency-dependent.

In this case, we seek Rayleigh-Schrödinger expansions in the form

$$\lambda^{(i)}(\epsilon) = \lambda_0 + \sum_{n=1}^{\infty} \epsilon^n \lambda_n^{(i)}; \;\; p^{(i)}(\epsilon) = \sum_{n=0}^{\infty} \epsilon^n p_n^{(i)} \;\; (i = 1, 2). \tag{5.37}$$

Let $\{q_0^{(1)}, q_0^{(2)}\}$ be a B-orthonormal basis for the solution space of Equation (5.28) above. What is required is the determination of an appropriate linear combination of these generalized eigenvectors so that Equation (5.29) above will then be solvable.

Specifically, we seek a B-orthonormal pair of generalized eigenvectors

$$p_0^{(i)} = a_1^{(i)} q_0^{(1)} + a_2^{(i)} q_0^{(2)} \;\; (i = 1, 2). \tag{5.38}$$

This requires that $[a_1^{(i)}, \; a_2^{(i)}]^T$ be orthonormal eigenvectors, with corresponding eigenvalues $\lambda_1^{(i)}$, of the 2×2-matrix M with components

$$M_{i,j} = \langle q_0^{(i)}, (C - \beta^2 D_0) q_0^{(j)} \rangle. \tag{5.39}$$

Consequently, $\lambda_1^{(i)}$ $(i = 1, 2)$ are then given by Equation (5.32) above with p_0 replaced by $p_0^{(i)}$. For convenience, all subsequent $p_n^{(i)}$ $(n = 1, 2, \ldots)$ are chosen to be B-orthogonal to $p_0^{(i)}$ $(i = 1, 2)$.

Likewise, $p_1^{(i)}$ $(i = 1, 2)$ must be chosen so that Equation (5.30) above is then solvable. This is achieved by first solving Equation (5.29) above as

$$\hat{p}_1^{(i)} = -(A - \lambda_0 B)^\dagger (C - \beta^2 D_0 - \lambda_1^{(i)} B) p_0^{(i)} \ (i = 1, 2), \tag{5.40}$$

and then defining

$$p_1^{(i)} = k_1^{(i)} p_0^{(1)} + k_2^{(i)} p_0^{(2)} + \hat{p}_1^{(i)} \ (i = 1, 2); \ k_i^{(i)} = -\langle \hat{p}_1^{(i)}, B p_0^{(i)} \rangle = 0, \tag{5.41}$$

$$k_j^{(i)} = [\langle \hat{p}_1^{(i)}, (C - \beta^2 D_0) p_0^{(j)} \rangle + \langle p_0^{(j)}, D_1 p_0^{(i)} \rangle] / [\lambda_1^{(i)} - \lambda_1^{(j)}] \ (j \neq i). \tag{5.42}$$

Equations (5.34-5.36) are then used to determine $\lambda_2^{(i)}, \lambda_3^{(i)}$ $(i = 1, 2)$ with λ_1, p_0, p_1 replaced by $\lambda_1^{(i)}, p_0^{(i)}, p_1^{(i)}$, respectively.

For higher order degeneracy and/or degeneracy that is not fully resolved at first-order, similar but more complicated modifications (developed in Section 4.2) are necessary [17].

5.6 Numerical Example: Warmed / Cooled Rectangular Waveguide

With reference to Figure 5.5, we next apply the above numerical procedure to an analysis of the modal characteristics of the warmed/cooled rectangular duct with cross-section $\Omega = [0, a] \times [0, b]$. The exact eigenpair corresponding to the (p, q)-mode with constant temperature is [40]:

$$\left(\frac{\omega_c^2}{c_0^2} \right)_{p,q} = \left(\frac{p\pi}{a} \right)^2 + \left(\frac{q\pi}{b} \right)^2; \ p_{p,q}(x, y) = P \cdot \cos\left(\frac{p\pi}{a} \cdot x \right) \cos\left(\frac{q\pi}{b} \cdot y \right). \tag{5.43}$$

For this geometry and mesh, the Dirichlet regions are rectangles and the Control Region Approximation reduces to the familiar central difference approximation [22]. Also, exact expressions are available for the eigenvalues and eigenvectors of the discrete operator in the constant temperature case [40].

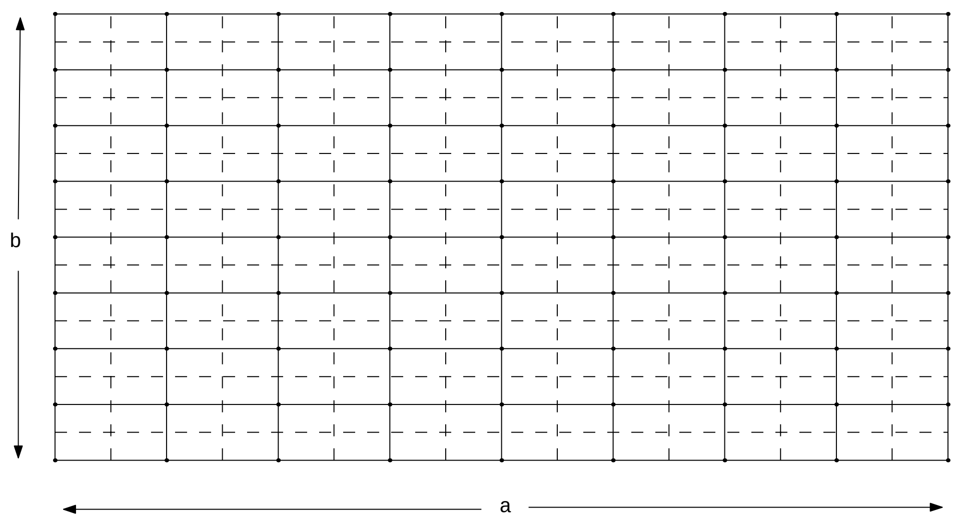

Figure 5.5: Rectangular Waveguide Cross-Section

Specifically, we now apply the above perturbation procedure to an analysis of the modal characteristics of a 10×5 rectangular duct with the lower wall subjected to the parabolic temperature profile

$$T_b = 1 + 16(\frac{x}{10})(1 - \frac{x}{10}) \tag{5.44}$$

while the other three walls are set to $T_b = 1$. (The hat has been dropped, hopefully without confusion.) We then solve $\Delta T = 0$ subject to this boundary condition, calculate $T_{avg} = \int\int_\Omega T(x,y)\, dA/A_\Omega$, and define

$$f(x,y) = \frac{T(x,y)}{T_{avg}} - 1 \tag{5.45}$$

which is displayed in Figure 5.2. A heated lower wall corresponds to positive warming ($\epsilon > 0$ in Equation (5.1)) while a cooled lower wall corresponds to negative warming ($\epsilon < 0$ in Equation (5.1)).

With these values of a and b, Equation (5.43) reveals the degeneracy between the $(0,1)$-mode and the $(2,0)$-mode in the constant temperature case. In general, Equations (5.38-5.39) imply that at cut-off, $\beta = 0$, $p_0^{(i)}$ $(i = 1,2)$ do not coincide with these two modes ($q_0^{(i)}$ $(i = 1,2)$) in the variable temperature case. However, these two modes of the rectangular waveguide are in fact C-orthogonal. This may be seen as follows.

By Equation (5.19),

$$\langle q_0^{(1)}, C q_0^{(2)} \rangle = \int\int_\Omega q_0^{(1)} \nabla \cdot (f \nabla q_0^{(2)})\; dA =$$

$$\oint_{\partial\Omega} q_0^{(1)} f \frac{\partial q_0^{(2)}}{\partial n}\; dl - \int\int_\Omega f(\nabla q_0^{(1)} \cdot \nabla q_0^{(2)})\; dA = 0,$$

since $\frac{\partial q_0^{(2)}}{\partial n} = 0$ along $\partial\Omega$ and $\nabla q_0^{(1)} \cdot \nabla q_0^{(2)} = 0$ by virtue of the fact that one mode is independent of x while the other mode is independent of y.

Thus, at cut-off, the matrix M of Equation (5.39) is diagonal and its eigenvectors are $\{[1\ 0]^T,\ [0\ 1]^T\}$ so that, by Equation (5.38), $p_0^{(i)}$ $(i = 1, 2)$ do, in fact, coincide with these modes of the constant temperature rectangular waveguide.

Substitution of Equation (5.45) into Equations (5.23-5.24) yields $\alpha_2 = -.210821$ and $\alpha_3 = -.088264$. In these and subsequent computations (performed using MATLAB©), a coarse 17×9 mesh and a fine 33×17 mesh were employed. These results were then enhanced using Richardson extrapolation [22] applied to the second-order accurate Control Region Approximation [67].

The cut-off frequencies are computed by setting to zero the expression for the dispersion relation, $\beta^2 = k_0^2 + \lambda$, thereby producing

$$\frac{\omega_c^2}{c_0^2} = -[\lambda_0 + \epsilon\hat{\lambda}_1 + \epsilon^2\hat{\lambda}_2 + \epsilon^3\hat{\lambda}_3 + O(\epsilon^4)]. \tag{5.46}$$

Table 5.1 displays the computed eigenvalue corrections at cut-off for the five lowest order modes. Figure 5.6 displays the cut-off frequencies for these same modes as ϵ varies. Figures 5.7-5.11 show, respectively, the unperturbed ($\epsilon = 0$) $(0,0)$-, $(1,0)$-, $(0,1)$-, $(2,0)$- and $(1,1)$-modes, together with these same modes at cut-off with a heated ($\epsilon = +1$) / cooled ($\epsilon = -1$) lower wall.

Collectively, these figures tell an intriguing tale. Firstly, the $(0,0)$-mode is no longer a plane wave in the presence of temperature variation. In addition, all variable-temperature modes possess a cut-off frequency so that, unlike the case of constant temperature, the duct cannot support any propagating modes at the lowest frequencies. Moreover, the presence of a temperature gradient alters all of the cut-off frequencies. In sharp contrast to the constant temperature case, the variable-temperature modal shapes are frequency-dependent. Lastly, the presence of a temperature gradient removes the modal degeneracy between the $(2,0)$- and $(0,1)$-modes that is prominent for constant temperature, although their curves cross for $\epsilon \approx .5$ thereby restoring this degeneracy. However, for ϵ this large, it might be prudent to compute $p_2^{(i)}$ $(i = 1, 2)$ from Equation (5.30) which would in turn produce $\hat{\lambda}_4^{(i)}, \hat{\lambda}_5^{(i)}$ $(i = 1, 2)$, and their inclusion in Equation (5.46) could once again remove this degeneracy [66].

Table 5.1: Computed Modal Eigenvalue Corrections ($\beta = 0$)

$Mode$	λ_0	$\hat{\lambda}_1$	$\hat{\lambda}_2$	$\hat{\lambda}_3$
$(0,0)$	0	0	$-.132332$	$.036847$
$(1,0)$	$-.098696$	$-.016542$	$-.114024$	$.030156$
$(0,1)$	$-.394778$	$.012651$	$-.110968$	$.070631$
$(2,0)$	$-.394778$	$-.015036$	$-.061933$	$.090678$
$(1,1)$	$-.493474$	$.055220$	$-.114566$	$.002713$

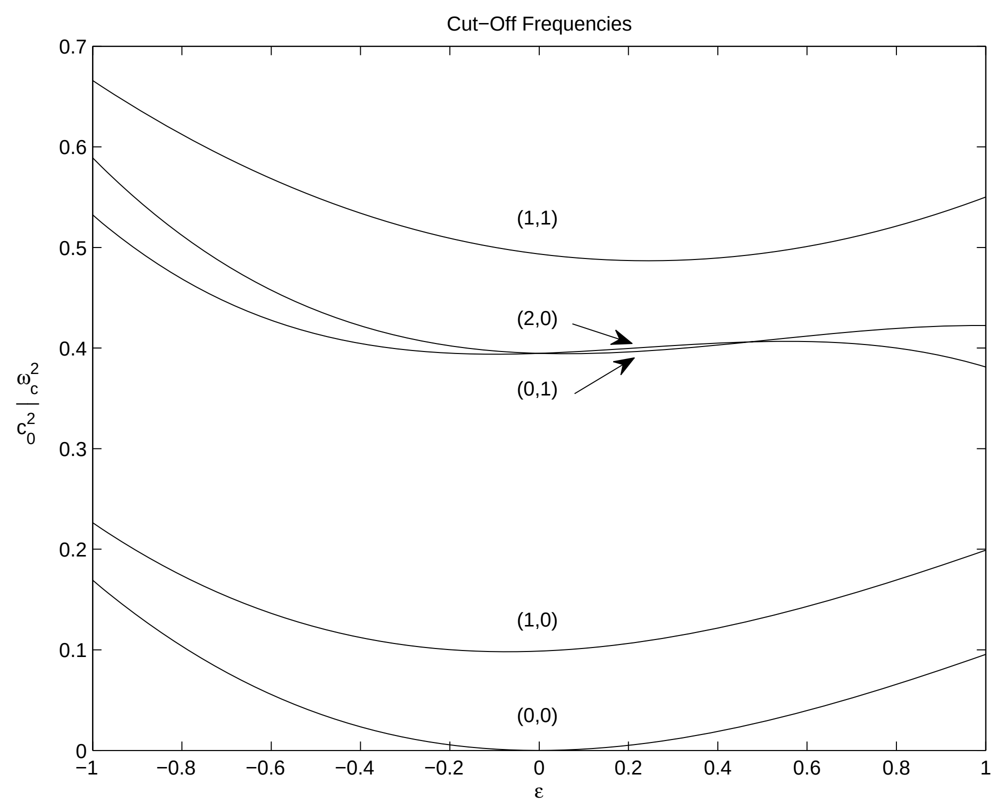

Figure 5.6: Cut-Off Frequencies versus Temperature Perturbation

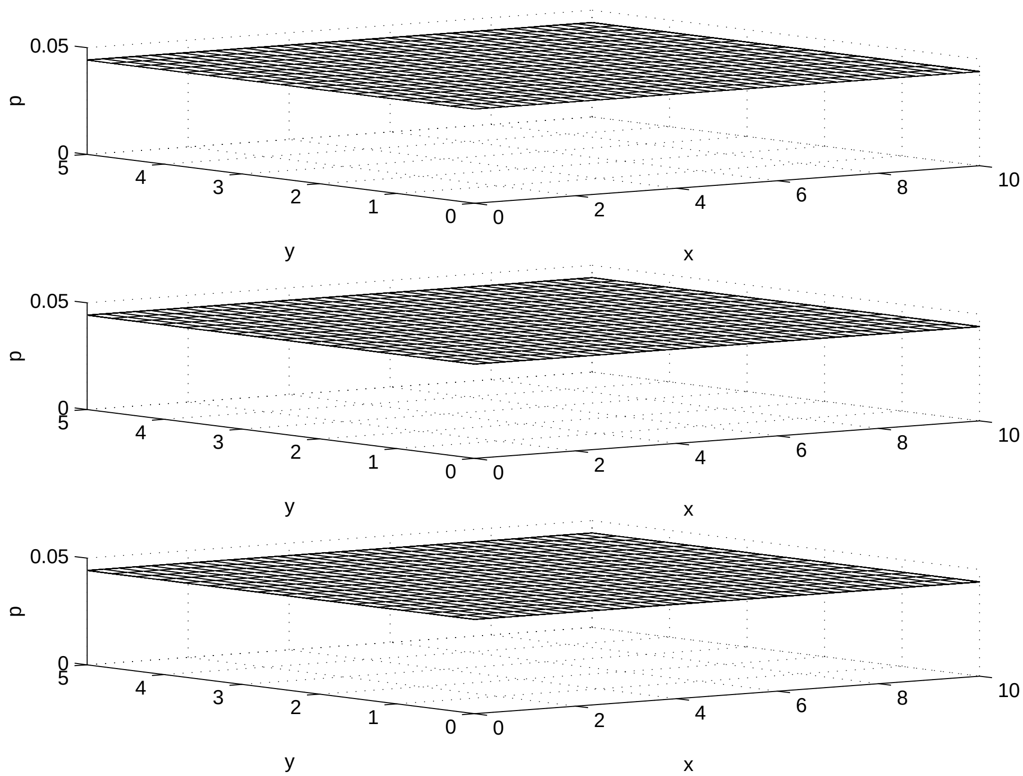

Figure 5.7: $(0, 0)$-Mode: $\epsilon = 0$; $\epsilon = +1$; $\epsilon = -1$

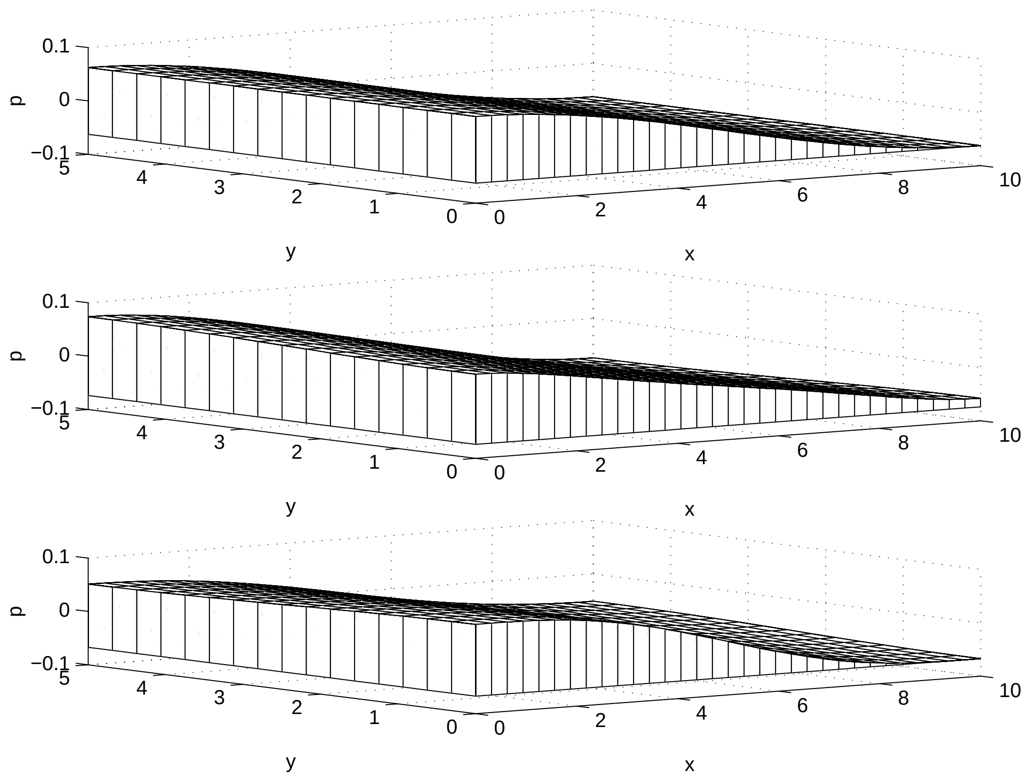

Figure 5.8: $(1, 0)$-Mode: $\epsilon = 0$; $\epsilon = +1$; $\epsilon = -1$

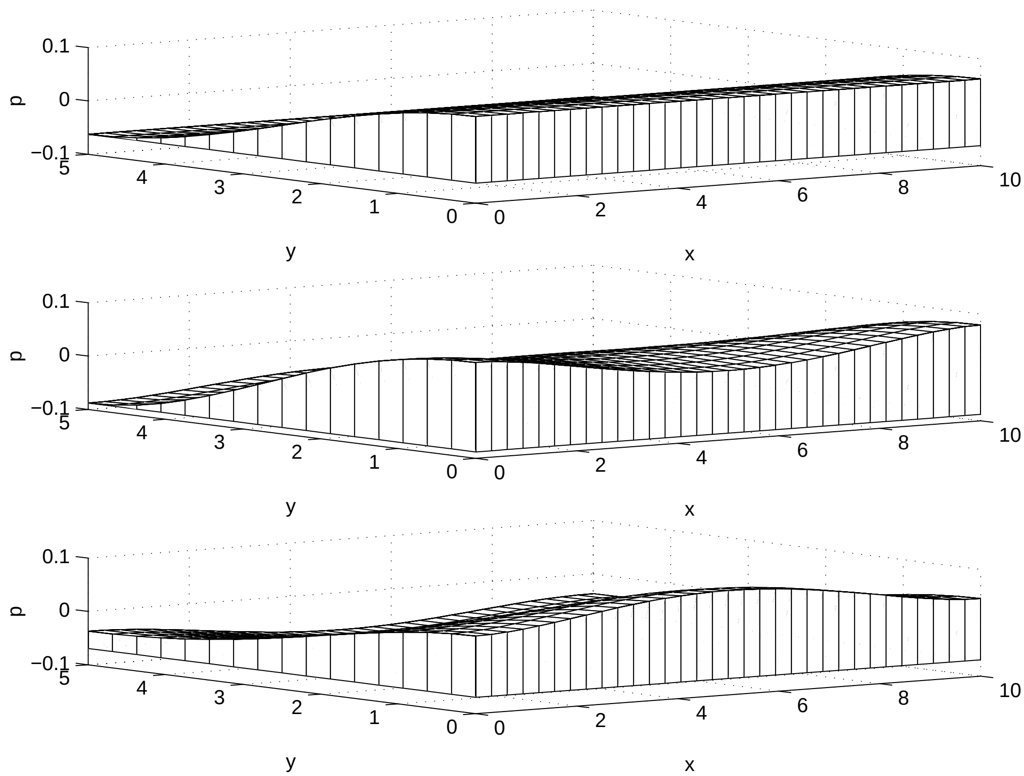

Figure 5.9: $(0, 1)$-Mode: $\epsilon = 0$; $\epsilon = +1$; $\epsilon = -1$

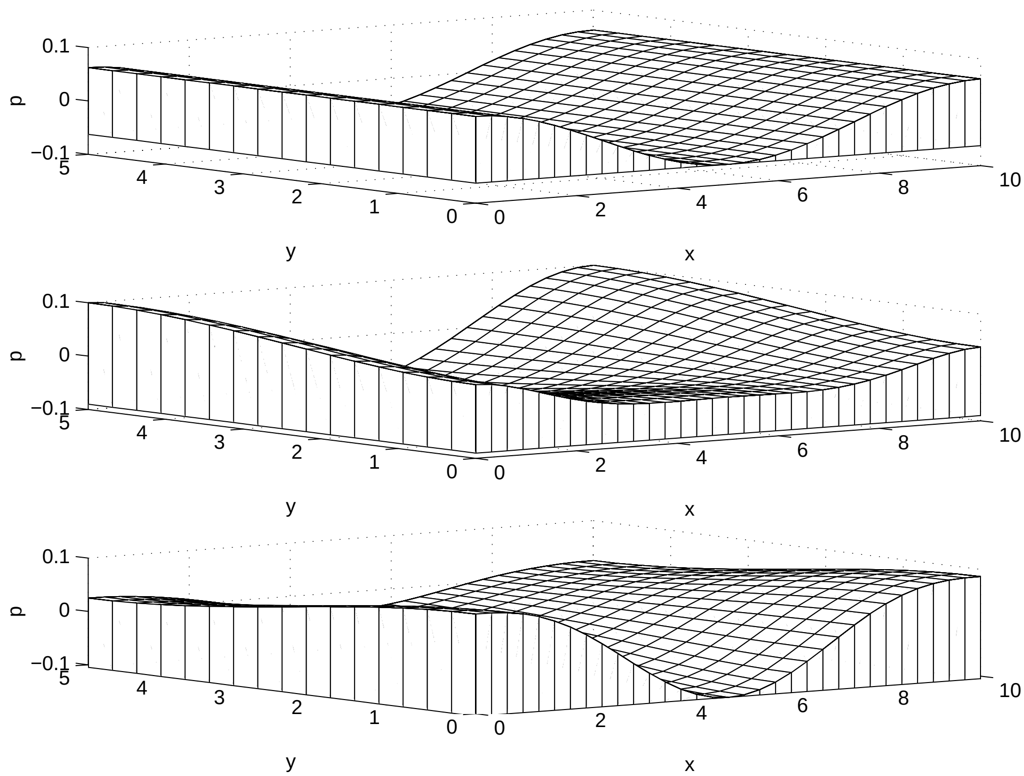

Figure 5.10: (2, 0)-Mode: $\epsilon = 0$; $\epsilon = +1$; $\epsilon = -1$

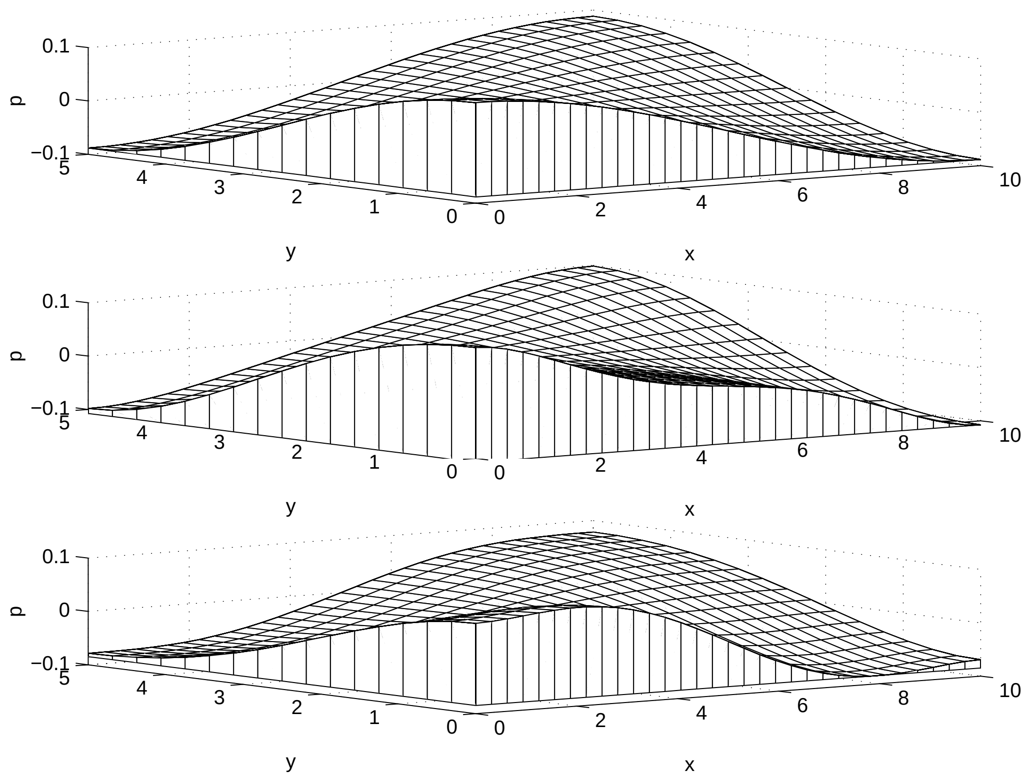

Figure 5.11: $(1, 1)$-Mode: $\epsilon = 0$; $\epsilon = +1$; $\epsilon = -1$

Chapter 6

Recapitulation

The practicing Applied Mathematician is frequently confronted with new problems that are "close" to old familiar problems for which either analytical or numerical solutions (or perhaps a hybrid of the two) have previously been derived. Many times it is possible to gain rudimentary information about the new problem by simply treating it as a small perturbation of the old one rather than attempting its full-blown analysis *ab initio*.

The preceding chapters have provided a thorough treatment of just such a perturbation method for approximating matrix (generalized) eigenvalue problems: the Rayleigh-Schrödinger perturbation procedure. The mathematical level of the presentation has been selected so as to make this important technique accessible to non-specialists in Applied Mathematics, Engineering and the Sciences. A spiral approach has been adopted in the development of the material that should foster understanding and make individual chapters reasonably independent.

An introductory chapter presented the origins of the procedure in the writings of Rayleigh and Schrödinger. While a more modern and consistent notation was adopted, the energy approach of Rayleigh and the differential equation approach of Schrödinger have been preserved. Yet, we have demonstrated that both approaches ultimately lead to (generalized) matrix eigenvalue problems and this is the form of the perturbation procedure that is further developed and applied in subsequent chapters. The description of the work of these Titans of Science was preceded by a summary of their respective life and times and was followed by a detailed description of the physical problems that led them to this method. This chapter concluded with representative applications of the matrix perturbation theory in electrical and mechanical engineering.

In preparation for the full development of the Rayleigh-Schrödinger perturbation procedure in later chapters, the next chapter was devoted to the Moore-Penrose pseudoinverse. After briefly tracing the history of this key concept, a list of basic concepts from linear algebra and matrix theory, together with a consistent notation, was presented and references to the literature were provided for those readers lacking in these prerequisites. These basic concepts became the cornerstone of an extensive development of projection matrices which in turn led to a self-contained treatment of QR factorization.

All of these tools of intermediate matrix theory were then brought to bear on the important practical problem of least squares approximation to linear systems of equations. It is here that the concept of the pseudoinverse naturally arose and this chapter included a substantial development of its theory and application to linear least squares. A comprehensive suite of numerical examples were included in order to make this chapter a stand-alone resource on this significant topic.

In succeeding chapters, a comprehensive, unified account of linear and analytic Rayleigh-Schrödinger perturbation theory for the symmetric matrix eigenvalue problem as well as the symmetric definite generalized eigenvalue problem has been provided. The cornerstone of this development was the Moore-Penrose pseudoinverse. Not only does such an 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 (generalized) eigenvectors of the unperturbed matrix (pair). Instead, we require only the unperturbed (generalized) eigenvectors corresponding to those (generalized) eigenvalues of interest. An important feature of the presentation was the generalization of the Dalgarno-Stewart identities from linear to analytic matrix perturbations and then to an arbitrary perturbation of the generalized eigenvalue problem. These results are new and made available here for the first time in book form.

The focal point of this investigation has been the degenerate case. In 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 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.

In the final chapter, we have presented a perturbation procedure for the modal characteristics of cylindrical acoustic waveguides in the presence of temperature gradients induced by an applied temperature distribution along the walls of the duct. Rather than simply making the sound speed spatially varying, as is done in atmospheric propagation and underwater acoustics, we have been careful to utilize a self-consistent physical model since we have dealt here with a fluid fully confined to a narrow region.

Great pains have been taken to preserve the self-adjointness inherent in the governing wave equation. This in turn leads to a symmetric definite generalized eigenvalue problem. As a consequence of this special care, we have been able to produce a third-order expression for the cut-off frequencies while only requiring a first-order correction to the propagating modes.

A detailed numerical example intended to intimate the broad possibilities offered by the resulting analytical expressions for cut-off frequencies and modal shapes has been presented. These include shifting of cut-off frequencies and shaping of modes. In point of fact, one could now pose the inverse problem: What boundary temperature distribution would produce prescribed cut-off frequencies?

The theoretical foundation of the Rayleigh-Schrödinger perturbation procedure for the symmetric matrix eigenvalue problem is Rellich's Spectral Perturbation Theorem. This important result establishes the existence of the perturbation expansions which are at the very heart of the method. The Appendix presents the generalization of Rellich's Theorem to the symmetric definite generalized eigenvalue problem. Both the explicit statement and the accompanying proof of the Generalized Spectral Perturbation Theorem are original and appear here in print for the first time.

Appendix A

Generalization of Rellich's Spectral Perturbation Theorem

Figure A.1: Franz Rellich

F. Rellich

$\Uparrow$

R. Courant

$\Uparrow$

D. Hilbert

$\Uparrow$

F. Lindemann

$\Uparrow$

F. Klein

$\Uparrow$

J. Plücker

$\Uparrow$

C. L. Gerling

$\Uparrow$

K. F. Gauss

Table A.1: Franz Rellich's "Family Tree"

As should be abundantly clear from the above table of dissertation advisors, Franz Rellich's mathematical pedigree was unquestionably elite. This outstanding Austrian-Italian mathematician was born in 1906 in Tramin (Tremeno) and, at the tender age of 18 years, he traveled to the Mathematisches Institut of the Georg-August-Universität in Göttingen for the completion of his formal mathematical studies. At this time, David Hilbert [89], although in the twilight of his distinguished career, was still an inspiration to his younger colleagues while his protégé Richard Courant [90] had ascended to the leadership of this pre-eminent international center of mathematical learning.

Rellich completed his dissertation under Courant in 1929 on the subject of *Generalization of Riemann's Integration Method for Differential Equations of n^{th} Order in Two Variables*. Although Rellich remained in Germany throughout World War II, he was dismissed from his teaching post at Göttingen by the Nazis only to return as the Director of its reconstituted Mathematisches Institut in 1946. Tragically, Rellich died in 1955 from a brain tumor.

This truly great mathematician left behind many "Rellich's Theorems" for posterity (e.g., [24, pp. 324-325]), but the one which particularly concerns us here had its genesis in a series of five pioneering papers which appeared in the *Mathematische Annalen* from 1936 to 1942 under the title *Störungstheorie der Spectralzerlegung* [91, 92, 93, 94, 95]. At the conclusion of World War II, he resumed publishing this pathbreaking work [96, 97].

When Courant transplanted the Mathematical Institute from Göttingen to New York, he brought with him the tradition of assigning to graduate students (and in some cases to junior faculty) the task of creating written records of the lectures by Herren Professors. Thus, Rellich's magnificent *Lectures on Perturbation Theory of Eigenvalue Problems*, delivered in the Fall of 1953 at the (Courant) Institute of Mathematical Sciences of New York University, were thereby transcribed and thus are still available today in English [98] for the enlightenment of future generations of aspiring mathematicians.

Rellich's Spectral Perturbation Theorem [98, pp. 42-43, Theorem 1] concerns the variation of the eigenvalues/eigenvectors of the symmetric eigenvalue problem under an analytic perturbation as studied in Chapter 3:

$$Ax_i = \lambda_i x_i \ (i = 1, \ldots, n); \ A(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k A_k. \tag{A.1}$$

This theorem established the existence of corresponding power series expansions for the eigenvalues/eigenvectors:

$$\lambda_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k \lambda_i^{(k)}; \ x_i(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k x_i^{(k)} \ (i = 1, \ldots, n), \tag{A.2}$$

convergent for sufficiently small $|\epsilon|$.

In the present appendix, this theorem is extended to analytic perturbation of the symmetric definite generalized eigenvalue problem as studied in Chapter 4:

$$Ax_i = \lambda_i Bx_i \ (i = 1, \ldots, n); \ A(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k A_k, \ B(\epsilon) = \sum_{k=0}^{\infty} \epsilon^k B_k. \tag{A.3}$$

At first sight, it seems that one could simply rewrite Equation (A3) as

$$B^{-1}Ax_i = \lambda_i x_i \ (i = 1, \ldots, n) \tag{A.4}$$

and then apply the Spectral Perturbation Theorem.

However, Rellich's proof of the Spectral Perturbation Theorem depends critically upon the symmetry of the coefficient matrix. But,

$$(B^{-1}A)^T = AB^{-1} \neq B^{-1}A, \tag{A.5}$$

unless it is possible to find a set of n linearly independent eigenvectors common to both A and B [78, p. 342, Ex. 10.42].

Hence, the extension of Rellich's Spectral Perturbation Theorem to the symmetric generalized eigenvalue problem requires a more elaborate proof. Fortunately, the gist of Rellich's ideas may be so extended in a relatively straightforward fashion. The details are as follows. (To the extent feasible, Rellich's notation will be utilized, although some minor modification has proven irresistible.)

Theorem A.1 (Generalized Eigenvalue Perturbation Theorem). *The generalized eigenvalues of the symmetric (definite) generalized eigenvalue problem, Equation (A3), where the power series for $A(\epsilon)$ and $B(\epsilon)$ are convergent for sufficiently small $|\epsilon|$, can be considered as power series in ϵ convergent for sufficiently small $|\epsilon|$.*

Proof: The generalized eigenvalues are precisely the roots of the characteristic polynomial

$$\kappa(A, B) := \det(A - \lambda B) = c_n\lambda^n + c_{n-1}\lambda^{n-1} + \cdots c_1\lambda + c_0,$$

where c_i ($i = 1, \ldots, n$) are power series in ϵ converging for sufficiently small $|\epsilon|$. In general, the roots of such a polynomial need not be regular analytic functions of ϵ for sufficiently small $|\epsilon|$. However, there always exists the Puiseux expansion [37, pp. 237-240, §99]: if $\lambda_0 = \lambda(0)$ is a root for $\epsilon = 0$ then the root $\lambda(\epsilon)$ may be written as a convergent (for sufficiently small $|\epsilon|$) power series in $\epsilon^{1/m}$ where m is the multiplicity of $\lambda_0 = \lambda(0)$. Since A is symmetric and B is symmetric positive definite, the roots of $\kappa(A, B)$ are all real [81, p. 345, Theorem 15.3.3].

This implies that in Puiseux's expansion of $\lambda(\epsilon)$,

$$\lambda(\epsilon) = \lambda_0 + d_1\epsilon^{1/m} + d_2\epsilon^{2/m} + \cdots,$$

only integral powers of ϵ may appear. To see this, let d_μ denote the first nonzero coefficient (i.e., $d_1 = \cdots = d_{\mu-1} = 0, d_\mu \neq 0$). Then,

$$d_\mu = \lim_{\epsilon \to 0^+} \frac{\lambda(\epsilon) - \lambda_0}{\epsilon^{\mu/m}}$$

is real because $\lambda(\epsilon)$ is real for real ϵ. Moreover,

$$(-1)^{\mu/m} \cdot d_\mu = \lim_{\epsilon \to 0^-} \frac{\lambda(\epsilon) - \lambda_0}{(-\epsilon)^{\mu/m}}$$

is also real. Hence, $(-1)^{\mu/m}$ is a real number so that μ must be a multiple of m. This argument may be continued to show that only integral powers of ϵ in the Puiseux expansion can have nonzero coefficients. □

Lemma A.1 (Singular Homogeneous System Perturbation Lemma).

Let $\Gamma(\epsilon) := [\gamma_{i,j}(\epsilon)]$ *be power series convergent in a neighborhood of* $\epsilon = 0$ *and let* $\det(\Gamma(\epsilon)) = 0$. *Then, there exist power series* $a(\epsilon) := [a_1(\epsilon), \ldots, a_n(\epsilon)]^T$ *convergent in a neighborhood of* $\epsilon = 0$*, such that* $\Gamma(\epsilon)a(\epsilon) = 0$ *and, for real* ϵ*,* $||a(\epsilon)||_B = 1$.

Proof: This result is proved using determinants in [98, pp. 40-42] with $||a(\epsilon)|| = 1$ which may readily be renormalized to $||a(\epsilon)||_B = 1$. □

Theorem A.2 (Generalized Eigenvector Perturbation Theorem). *Corresponding to the generalized eigenvalue*

$$\lambda(\epsilon) = a_0 + \epsilon a_1 + \cdots,$$

there exists a generalized eigenvector

$$u(\epsilon) = [u_1(\epsilon), \cdots, u_n(\epsilon)]^T$$

each of whose components $u_k(\epsilon)$ $(k = 1, \ldots, n)$ *is a power series in* ϵ *convergent for sufficiently small* $|\epsilon|$ *and which is normalized so that* $||u(\epsilon)||_B = 1$ *for real* ϵ *and* $|\epsilon|$ *sufficiently small.*

Proof: Simply apply the previous Lemma with $\Gamma(\epsilon) := A(\epsilon) - \lambda(\epsilon)B(\epsilon)$. □

Theorem A.3 (Generalized Spectral Perturbation Theorem). *Let $A(\epsilon)$ be symmetric and $B(\epsilon)$ be symmetric positive definite with both matrices expressible as power series in ϵ which are convergent for sufficiently small $|\epsilon|$. Suppose that $\lambda_0 := \lambda(0)$ is a generalized eigenvalue of $(A_0, B_0) := (A(0), B(0))$ of exact multiplicity $m \geq 1$ and suppose that the interval $(\lambda_0 - \delta_-, \lambda_0 + \delta_+)$, with positive numbers δ_- and δ_+, contains no generalized eigenvalue of (A_0, B_0) other than λ_0. Then, there exist power series,*

$$\lambda_1(\epsilon), \ldots, \lambda_m(\epsilon);\ \phi^{(1)}(\epsilon), \ldots, \phi^{(m)}(\epsilon),$$

all convergent in a neighborhood of $\epsilon = 0$, which satisfy the following conditions:

(1) The vector $\phi^{(\nu)}(\epsilon) := [f_1^{(\nu)}(\epsilon), \ldots, f_n^{(\nu)}(\epsilon)]^T$ is a generalized eigenvector of $(A(\epsilon), B(\epsilon))$ corresponding to the generalized eigenvalue $\lambda_\nu(\epsilon)$. I.e.,

$$A(\epsilon)\phi^{(\nu)}(\epsilon) = \lambda_\nu(\epsilon)B(\epsilon)\phi^{(\nu)}(\epsilon)\ (\nu = 1, \ldots, m).$$

Furthermore, $\lambda_\nu(0) = \lambda_0$ $(\nu = 1, \ldots, m)$ and for real ϵ these generalized eigenvectors are $B(\epsilon)$-orthonormal. I.e.,

$$\langle \phi^{(\nu)}(\epsilon), \phi^{(\mu)}(\epsilon)\rangle_{B(\epsilon)} = \langle \phi^{(\nu)}(\epsilon), B(\epsilon)\phi^{(\mu)}(\epsilon)\rangle = \delta_{\nu,\mu}\ (\nu, \mu = 1, \ldots, m).$$

(2) For each pair of positive numbers $(\delta'_- < \delta_-, \delta'_+ < \delta_+)$, there exists a positive number ρ such that the portion of the generalized spectrum of $(A(\epsilon), B(\epsilon))$ lying in the interval $(\lambda_0 - \delta'_-, \lambda_0 + \delta'_+)$ consists precisely of the points $\lambda_1(\epsilon), \ldots, \lambda_m(\epsilon)$ provided that $|\epsilon| < \rho$.

Proof:
(1) The first part of the theorem has already been proved in the case of $m = 1$. Proceeding inductively, assume that (1) is true in the case of multiplicity $m-1$ and then proceed to prove it for multiplicity m.

Theorems A.1 and A.2 ensure the existence, for real ϵ, of the generalized eigenpair $\{\lambda_1(\epsilon), \phi^{(1)}(\epsilon)\}$ such that

$$A(\epsilon)\phi^{(1)}(\epsilon) = \lambda_1(\epsilon)B(\epsilon)\phi^{(1)}(\epsilon); \; ||\phi^{(1)}(\epsilon)||_B = 1,$$

whose power series converge for sufficiently small $|\epsilon|$.

Define the linear operator $M(\epsilon)$ by

$$M(\epsilon)u := \langle u, B(\epsilon)\phi^{(1)}(\epsilon)\rangle B(\epsilon)\phi^{(1)}(\epsilon),$$

whose (symmetric) matrix representation is

$$M(\epsilon) = B(\epsilon)\phi^{(1)}(\epsilon)\phi^{(1)}(\epsilon)^T B(\epsilon).$$

Next, define the symmetric matrix

$$C(\epsilon) := A(\epsilon) - M(\epsilon),$$

with power series in ϵ convergent for sufficiently small $|\epsilon|$. Set $\psi_1 = \phi^{(1)}(0)$ and let $\psi_1, \psi_2, \ldots, \psi_m$ be a B-orthonormal set of generalized eigenvectors belonging to the generalized eigenvalue λ_0 of (A_0, B_0).

Thus, we have

$$C_0\psi_j = \lambda_0 B_0 \psi_j \; (j = 2, \ldots, m),$$

where $C_0 := C(0)$. Hence, λ_0 is a generalized eigenvalue of (C_0, B_0) of multiplicity at least $m - 1$. On the other hand, its multiplicity cannot exceed $m - 1$. Otherwise, there would exist an element ψ with $||\psi||_B = 1$ such that $C_0\psi = \lambda_0 B_0 \psi$ and $\langle \psi, \psi_j \rangle_B = 0$ $(j = 2, \ldots, m)$. Since $C_0\psi_1 = (\lambda_0 - 1)\psi_1$, it follows that $\langle \psi, \psi_1 \rangle_B = 0$ because ψ and ψ_1 are consequently generalized eigenvectors corresponding to distinct generalized eigenvalues of (C_0, B_0). Therefore, $\psi, \psi_1, \psi_2, \ldots, \psi_m$ are $m + 1$ linearly independent generalized eigenvectors of (A_0, B_0) corresponding to the generalized eigenvalue λ_0. But, this is impossible because the multiplicity of λ_0 as a generalized eigenvalue of (A_0, B_0) is exactly m so that the multiplicity of λ_0 as a generalized eigenvalue of (C_0, B_0) is exactly $m - 1$.

As a result, by the induction hypothesis, there exist power series

$$\lambda_\nu(\epsilon); \; \phi^{(\nu)}(\epsilon) \; (\nu = 2, \ldots, m),$$

convergent in a neighborhood of $\epsilon = 0$ which satisfy the relations

$$C(\epsilon)\phi^{(\nu)}(\epsilon) = \lambda_\nu(\epsilon)B(\epsilon)\phi^{(\nu)}(\epsilon) \; (\nu = 2, \ldots, m),$$

where, for real ϵ,

$$\langle \phi^{(\nu)}(\epsilon), \phi^{(\mu)}(\epsilon) \rangle_{B(\epsilon)} = \delta_{\nu,\mu} \ (\nu, \mu = 2, \ldots, m).$$

Moreover, we find that

$$A(\epsilon)\phi^{(1)}(\epsilon) = \lambda_1(\epsilon)B(\epsilon)\phi^{(1)}(\epsilon); \ C(\epsilon)\phi^{(1)}(\epsilon) = (\lambda_1(\epsilon) - 1)B(\epsilon)\phi^{(1)}(\epsilon).$$

For sufficiently small $|\epsilon|$, we certainly have $\lambda_\nu(\epsilon) \neq \lambda_1(\epsilon) - 1$ $(\nu = 2, \ldots, m)$, so that $\langle \phi^{(1)}(\epsilon), \phi^{(\nu)}(\epsilon) \rangle_{B(\epsilon)} = 0$ $(\nu = 2, \ldots, m)$.

Hence, we finally obtain

$$A(\epsilon)\phi^{(\nu)}(\epsilon) = C(\epsilon)\phi^{(\nu)}(\epsilon) + M(\epsilon)\phi^{(\nu)}(\epsilon) = \lambda_\nu(\epsilon)B(\epsilon)\phi^{(\nu)}(\epsilon) \ (\nu = 2, \ldots, m).$$

Thus, the first part of the theorem is proved.
(2) In exactly the same way, we can treat each generalized eigenvalue of (A_0, B_0) thereby obtaining n convergent power series which can be labeled $\lambda_1(\epsilon), \ldots, \lambda_n(\epsilon)$ and which for fixed ϵ comprise the entire generalized spectrum of $(A(\epsilon), B(\epsilon))$. The second part of the theorem is then an immediate consequence.
□

Remark A.1. *In Theorem A.1, the phrase "can be considered" has been chosen to indicate that a suitable arrangement of the eigenvalues $\lambda_1(\epsilon), \ldots, \lambda_n(\epsilon)$ must be made for the conclusion to be valid.*

Consider, for example,

Example A.1.

$$A(\epsilon) = \begin{bmatrix} \epsilon & 0 \\ 0 & -\epsilon \end{bmatrix}; \ B(\epsilon) = I,$$

which possesses eigenvalues $\lambda_1(\epsilon) = \epsilon$ and $\lambda_2(\epsilon) = -\epsilon$, evidently convergent power series. But, if they were to be arranged in order of magnitude then $\lambda^1(\epsilon) = -|\epsilon|$ and $\lambda^2(\epsilon) = |\epsilon|$ which are not regular analytic functions of ϵ near $\epsilon = 0$.

Remark A.2. *It is important to observe what Theorem A.3 does* **not** *claim. It is* **not** *true that if λ_0 is an unperturbed generalized eigenvalue of multiplicity m and if $\{\psi_1, \ldots, \psi_m\}$ is a B-orthonormal set of generalized eigenvectors of the unperturbed problem (A_0, B_0) corresponding to λ_0 then there exist generalized eigenvectors $\phi^{(\nu)}(\epsilon)$ $(\nu = 1, \ldots, m)$ which are convergent power series in ϵ and such that the vector equation*

$$\phi^{(\nu)}(\epsilon) = \psi_\nu + \epsilon \cdot \psi_\nu^1 + \epsilon^2 \cdot \psi_\nu^2 + \cdots$$

obtains. All that has been proved is that the $\phi^{(\nu)}(\epsilon)$ exist and that $\phi^{(\nu)}(0)$ $(\nu = 1, \ldots, m)$ are a B-orthonormal set of generalized eigenvectors of the unperturbed problem. In general, $\phi^{(\nu)}(0)$ cannot be prescribed in advance; the perturbation method itself must select them.

Consider, for example,

Example A.2.

$$A(\epsilon) = \begin{bmatrix} 1+\epsilon & 0 \\ 0 & 1-\epsilon \end{bmatrix}; B(\epsilon) = I.$$

For $\epsilon = 0$, every nonzero vector is an eigenvector. In particular, we may select $\psi_1 = [1/\sqrt{2}, 1/\sqrt{2}]^T$ and $\psi_2 = [-1/\sqrt{2}, 1/\sqrt{2}]^T$. For $\epsilon \neq 0$, the normalized eigenvectors are uniquely determined up to a factor of unit magnitude as $\phi^{(1)}(\epsilon) = [1, 0]^T$ and $\phi^{(2)}(\epsilon) = [0, 1]^T$, which are quite unrelated to ψ_1 and ψ_2.

Remark A.3. *If, as has been assumed throughout this book, $(A(\epsilon), B(\epsilon))$ has distinct generalized eigenvalues in a deleted neighborhood of $\epsilon = 0$ then the*

Rayleigh-Schrödinger perturbation procedure as developed in the previous chapters will yield power series expansions for the generalized eigenvalues and eigenvectors as guaranteed by the Generalized Rellich Spectral Perturbation Theorem. However, if $(A(\epsilon), B(\epsilon))$ *has a repeated eigenvalue in a neighborhood of* $\epsilon = 0$*, i.e. if the degeneracy is unresolved at any level of approximation, then the Rayleigh-Schrödinger perturbation procedure fails to terminate.*

Consider, for example,

Example A.3.

$$A(\epsilon) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \epsilon^2 & \epsilon(1-\epsilon) \\ 0 & \epsilon(1-\epsilon) & (1-\epsilon)^2 \end{bmatrix};\ B(\epsilon) = I,$$

which possesses eigenvalues

$$\lambda_1(\epsilon) = \lambda_2(\epsilon) = 0;\ \lambda_3(\epsilon) = 1 - 2\epsilon + 2\epsilon^2,$$

with corresponding eigenvectors

$$x_1(\epsilon) = \begin{bmatrix} \alpha_1(\epsilon) \\ \beta_1(\epsilon)\cdot(\epsilon-1) \\ \beta_1(\epsilon)\cdot\epsilon \end{bmatrix};\ x_2(\epsilon) = \begin{bmatrix} \alpha_2(\epsilon) \\ \beta_2(\epsilon)\cdot(\epsilon-1) \\ \beta_2(\epsilon)\cdot\epsilon \end{bmatrix};\ x_3(\epsilon) = \begin{bmatrix} 0 \\ \gamma(\epsilon)\cdot\epsilon \\ \gamma(\epsilon)\cdot(1-\epsilon) \end{bmatrix},$$

where the orthogonality of $\{x_1(\epsilon), x_2(\epsilon)\}$ *necessitates the restriction*

$$\alpha_1(\epsilon)\alpha_2(\epsilon) + \beta_1(\epsilon)\beta_2(\epsilon)(2\epsilon^2 - 2\epsilon + 1) = 0.$$

The Rayleigh-Schrödinger perturbation procedure successively yields $\lambda_1^{(k)} = 0 = \lambda_2^{(k)}$ $(k = 1, 2, \ldots, \infty)$ but, never terminating, it fails to determine $\{y_1^{(0)}, y_2^{(0)}\}$. In fact, *any* orthonormal pair of unperturbed eigenvectors corresponding to $\lambda = 0$ will suffice to generate corresponding eigenvector perturbation expansions. However, since they correspond to the same eigenvalue, orthogonality of $\{y_1(\epsilon), y_2(\epsilon)\}$ needs to be explicitly enforced.

Thus, in a practical sense, the Rayleigh-Schrödinger perturbation procedure fails in this case since it is unknown *a priori* that $\lambda_1^{(k)} = \lambda_2^{(k)}$ $(k = 1, 2, \ldots, \infty)$ so that the stage where eigenvector corrections are computed is never reached.

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