k	x_k	y_k	z_k
0	1.0	2.0	2.0
1	1.75	3.75	2.95
2	1.95	3.96875	2.98625
⋮	⋮	⋮	⋮
10	2.0	4.0	3.0

Table 3: Convergence of Jacobi iteration scheme to the solution value of $(x, y, z) = (2, 4, 3)$ from the initial guess $(x_0, y_0, z_0) = (1, 2, 2)$.

scheme which can be implemented in an effort to enhance convergence. It is also possible to use several previous iterations to achieve convergence. Krylov space methods [6] are often high end iterative techniques especially developed for rapid convergence. Included in these iteration schemes are conjugant gradient methods and generalized minimum residual methods which we will discuss and implement [6].

2.3 Eigenvalues, Eigenvectors, and Solvability

Another class of linear systems of equations which are of fundamental importance are known as eigenvalue problems. Unlike the system $\mathbf{Ax} = \mathbf{b}$ which has the single unknown vector $\vec{x}$, eigenvalue problems are of the form

$$\mathbf{Ax} = \lambda\mathbf{x} \tag{2.3.10}$$

which have the unknows $\mathbf{x}$ and λ. The values of λ are known as the *eigenvalues* and the corresponding $\mathbf{x}$ are the *eigenvectors*.

Eigenvalue problems often arise from differential equations. Specifically, we consider the example of a linear set of coupled differential equations

$$\frac{d\mathbf{y}}{dt} = \mathbf{Ay}\,. \tag{2.3.11}$$

By attempting a solution of the form

$$\mathbf{y} = \mathbf{x}\exp(\lambda t)\,, \tag{2.3.12}$$

where all the time-dependence is captured in the exponent, the resulting equation for $\mathbf{x}$ is

$$\mathbf{Ax} = \lambda\mathbf{x} \tag{2.3.13}$$

which is just the eigenvalue problem. Once the full set of eigenvalues and eigenvectors of this equation are found, the solution of the differential equation is written as

$$\vec{y} = c_1\mathbf{x}_1\exp(\lambda_1 t) + c_2\mathbf{x}_2\exp(\lambda_2 t) + \cdots + c_N\mathbf{x}_N\exp(\lambda_N t) \tag{2.3.14}$$

where N is the number of linearly independent solutions to the eigenvalue problem for the matrix $\mathbf{A}$ which is of size $N \times N$. Thus solving a linear system of differential equations relies on the solution of an associated eigenvalue problem.

The questions remains: how are the eigenvalues and eigenvectors found? To consider this problem, we rewrite the eigenvalue problem as

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{I}\mathbf{x} \tag{2.3.15}$$

where a multiplication by unity has been performed, i.e. $\mathbf{I}\mathbf{x} = \mathbf{x}$. Moving the right hand side to the left side of the equation gives

$$\mathbf{A}\mathbf{x} - \lambda\mathbf{I}\mathbf{x} = \mathbf{0}. \tag{2.3.16}$$

Factoring out the vector $\mathbf{x}$ then gives the desired result

$$(\mathbf{A} - \lambda\mathbf{I})\mathbf{x} = \mathbf{0}\,. \tag{2.3.17}$$

Two possibilities now exist.

Option I: The determinant of the matrix $(\mathbf{A}-\lambda\mathbf{I})$ is not zero. If this is true, the matrix is *nonsingular* and its inverse, $(\mathbf{A} - \lambda\mathbf{I})^{-1}$, can be found. The solution to the eigenvalue problem (2.3.17) is then

$$\mathbf{x} = (\mathbf{A} - \lambda\mathbf{I})^{-1}\mathbf{0} \tag{2.3.18}$$

which implies that

$$\mathbf{x} = \mathbf{0}\,. \tag{2.3.19}$$

This trivial solution could have been guessed from (2.3.17). However, it is not relevant as we require nontrivial solutions for $\mathbf{x}$.

Option II: The determinant of the matrix $(\mathbf{A} - \lambda\mathbf{I})$ is zero. If this is true, the matrix is *singular* and its inverse, $(\mathbf{A}-\lambda\mathbf{I})^{-1}$, cannot be found. Although there is no longer a guarantee that there is a solution, it is the only scenario which allows for the possibility of $\mathbf{x} \neq \mathbf{0}$. It is this condition which allows for the construction of eigenvalues and eigenvectors. Indeed, we choose the eigenvalues λ so that this condition holds and the matrix is singular.

To illustrate how the eigenvalues and eigenvectors are computed, an example is shown. Consider the matrix

$$\mathbf{A} = \begin{pmatrix} 1 & 3 \\ -1 & 5 \end{pmatrix} \tag{2.3.20}$$

This gives the eigenvalue problem

$$\mathbf{A} = \begin{pmatrix} 1 & 3 \\ -1 & 5 \end{pmatrix}\mathbf{x} = \lambda\mathbf{x} \tag{2.3.21}$$

which when manipulated to the form $(\mathbf{A}-\lambda\mathbf{I})\mathbf{x}=\mathbf{0}$ gives

$$\left[\begin{pmatrix} 1 & 3 \\ -1 & 5 \end{pmatrix} - \lambda\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right]\mathbf{x} = \begin{pmatrix} 1-\lambda & 3 \\ -1 & 5-\lambda \end{pmatrix}\mathbf{x} = 0\,. \tag{2.3.22}$$

We now require that the determinant is zero

$$\det\begin{vmatrix} 1-\lambda & 3 \\ -1 & 5-\lambda \end{vmatrix} = (1-\lambda)(5-\lambda)+3 = \lambda^2-6\lambda+8 = (\lambda-2)(\lambda-4) = 0 \tag{2.3.23}$$

which gives the two eigenvalues

$$\lambda = 2, 4\,. \tag{2.3.24}$$

The eigenvectors are then found from (2.3.22) as follows:

$$\lambda = 2: \quad \begin{pmatrix} 1-2 & 3 \\ -1 & 5-2 \end{pmatrix}\mathbf{x} = \begin{pmatrix} -1 & 3 \\ -1 & 3 \end{pmatrix}\mathbf{x} = 0\,. \tag{2.3.25}$$

Given that $\mathbf{x} = (x_1 \;\; x_2)^T$, this leads to the single equation

$$-x_1 + 3x_2 = 0 \tag{2.3.26}$$

This is an underdetermined system of equations. Thus we have freedom in choosing one of the values. Choosing $x_2 = 1$ gives $x_1 = 3$ and

$$\mathbf{x}_1 = \begin{pmatrix} 3 \\ 1 \end{pmatrix}\,. \tag{2.3.27}$$

The second eigenvector comes from (2.3.22) as follows:

$$\lambda = 4: \quad \begin{pmatrix} 1-4 & 3 \\ -1 & 5-4 \end{pmatrix}\mathbf{x} = \begin{pmatrix} -3 & 3 \\ -1 & 1 \end{pmatrix}\mathbf{x} = 0\,. \tag{2.3.28}$$

Given that $\mathbf{x} = (x_1 \;\; x_2)^T$, this leads to the single equation

$$-x_1 + x_2 = 0 \tag{2.3.29}$$

This is an underdetermined system of equations. Thus we have freedom in choosing one of the values. Choosing $x_2 = 1$ gives $x_1 = 1$ and

$$\mathbf{x}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}\,. \tag{2.3.30}$$

These results can be found from MATLAB by using the **eig** command. Specifically, the command structure

```
[V,D]=eig(A)
```

gives the matrix **V** containing the eigenvectors as columns and the matrix **D** whose diagonal elements are the corresponding eigenvalues.

Matrix Powers

Another important operation which can be performed with eigenvalue and eigenvectors is the evaluation of

$$\mathbf{A}^M \tag{2.3.31}$$

where M is a large integer. For large matrices $\mathbf{A}$, this operation is computationally expensive. However, knowing the eigenvalues and eigenvectors of of $\mathbf{A}$ allows for a significant ease in computational expense. Assuming we have all the eigenvalues and eigenvectors of $\mathbf{A}$, then

$$\begin{aligned}
\mathbf{A}\mathbf{x}_1 &= \lambda_1 \mathbf{x}_1 \\
\mathbf{A}\mathbf{x}_2 &= \lambda_2 \mathbf{x}_2 \\
&\vdots \\
\mathbf{A}\mathbf{x}_n &= \lambda_1 \mathbf{x}_n \, .
\end{aligned}$$

This collection of eigenvalues and eigenvectors gives the matrix system

$$\mathbf{A}\mathbf{S} = \mathbf{S}\boldsymbol{\Lambda} \tag{2.3.32}$$

where the columns of the matrix $\mathbf{S}$ are the eigenvectors of $\mathbf{A}$,

$$\mathbf{S} = (\mathbf{x}_1 \;\; \mathbf{x}_2 \;\; \cdots \;\; \mathbf{x}_n) \, , \tag{2.3.33a}$$

and $\boldsymbol{\Lambda}$ is a matrix whose diagonals are the corresponding eigenvalues

$$\boldsymbol{\Lambda} = \begin{pmatrix} \lambda_1 & 0 & \cdots & & 0 \\ 0 & \lambda_2 & 0 & \cdots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & & \cdots & 0 & \lambda_n \end{pmatrix} . \tag{2.3.34}$$

By multiplying (**??**)on the right by $\mathbf{S}^{-1}$, the matrix $\mathbf{A}$ can then be rewritten as

$$\mathbf{A} = \mathbf{S}\boldsymbol{\Lambda}\mathbf{S}^{-1} \, . \tag{2.3.35}$$

The final observation comes from

$$\mathbf{A}^2 = (\mathbf{S}\boldsymbol{\Lambda}\mathbf{S}^{-1})(\mathbf{S}\boldsymbol{\Lambda}\mathbf{S}^{-1}) = \mathbf{S}\boldsymbol{\Lambda}^2\mathbf{S}^{-1} \, . \tag{2.3.36}$$

This then generalizes to

$$\mathbf{A}^M = \mathbf{S}\boldsymbol{\Lambda}^M\mathbf{S}^{-1} \tag{2.3.37}$$

where the matrix $\boldsymbol{\Lambda}^M$ is easily calculated as

$$\boldsymbol{\Lambda}^M = \begin{pmatrix} \lambda_1^M & 0 & \cdots & & 0 \\ 0 & \lambda_2^M & 0 & \cdots & 0 \\ \vdots & & \ddots & & \vdots \\ 0 & & \cdots & 0 & \lambda_n^M \end{pmatrix} . \tag{2.3.38}$$

Since raising the diagonal terms to the M^{th} power is easily accomplished, the matrix $\mathbf{A}$ can then be easily calculated by multiplying the three matrices in (**??**)

Solvability and the Fredholm-Alternative Theorem

It is easy to ask under what conditions the system

$$\mathbf{Ax} = \mathbf{b} \tag{2.3.39}$$

can be solved. Aside from requiring the det$\mathbf{A} \neq 0$, we also have a solvability condition on $\mathbf{b}$. Consider the adjoint problem

$$\mathbf{A}^{\dagger}\mathbf{y} = 0 \tag{2.3.40}$$

where $\mathbf{A}^{\dagger} = \mathbf{A}^{*T}$ is the adjoint which is the transpose and complex conjugate of the matrix $\mathbf{A}$.

The definition of the adjoint is such that

$$\mathbf{yAx} = \mathbf{A}^{\dagger}\mathbf{yx}\,. \tag{2.3.41}$$

Since $\mathbf{Ax} = \mathbf{b}$, the left side of the equation reduces to $\mathbf{yb}$ while the right side reduces to $\mathbf{0}$ since $\mathbf{A}^{\dagger}\mathbf{y} = \mathbf{0}$. This then gives the condition

$$\mathbf{y} \cdot \mathbf{b} = \mathbf{0} \tag{2.3.42}$$

which is known as the *Fredholm-Alternative* theorem, or a *solvability* condition. In words, the equation states the in order for the system $\mathbf{Ax} = \mathbf{b}$ to be solvable, the right-hand side forcing $\mathbf{b}$ must be orthogonal to the null-space of the adjoint operator $\mathbf{A}^{\dagger}$.

3 Initial and Boundary Value Problems of Differential Equations

Our ultimate goal is to solve very general nonlinear partial differential equations of elliptic, hyperbolic, parabolic, or mixed type. However, a variety of basic techniques are required from the solutions of ordinary differential equations. By understanding the basic ideas for computationally solving initial and boundary value problems for differential equations, we can solve more complicated partial differential equations. The development of numerical solution techniques for initial and boundary value problems originates from the simple concept of the Taylor expansion. Thus the building blocks for scientific computing are rooted in concepts from freshman calculus. Implementation, however, often requires ingenuity, insight, and clever application of the basic principles.