Convergence and Stability

Partial Differential Equations

J Robert Buchanan

Department of Mathematics

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Objectives

In this lesson we will:

- develop formulas for and properties of eigenvalues and eigenvectors of tridiagonal matrices, and
- explore the stability properties of iterative methods for solving the heat, wave, and Poisson's equations.

Eigensystems of Tridiagonal Matrices

Lemma

Suppose A is an $(n-1)\times(n-1)$ tridiagonal matrix of the form

$$A = \begin{bmatrix} a & b & 0 & \cdots & 0 & 0 & 0 \\ c & a & b & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & c & a & b \\ 0 & 0 & 0 & \cdots & 0 & c & a \end{bmatrix}$$

with real or complex entries. If $b\,c \neq 0$ then the eigenvalues of A are

$$\lambda_j = a + 2b\sqrt{\frac{c}{b}}\cos\frac{j\pi}{n},$$

with corresponding eigenvectors

$$\mathbf{v}_j = \left(\left(\frac{c}{b}\right)^{1/2}\sin\frac{j\pi}{n},\ldots,\left(\frac{c}{b}\right)^{(n-1)/2}\sin\frac{(n-1)j\pi}{n}\right)^T,$$

for $j = 1, 2, \ldots, n-1$.

Eigensystems of Block-Structured Matrices

Theorem

Let matrix A be an $NM \times NM$ matrix written in block form as

$$A = \begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,M} \\ A_{2,1} & A_{2,2} & \cdots & A_{2,M} \\ \vdots & \vdots & & \vdots \\ A_{M,1} & A_{M,2} & \cdots & A_{M,M} \end{bmatrix}.$$

Suppose each block $A_{i,j}$ is an $N \times N$ matrix and all the matrices $A_{i,j}$ have a set of N linearly independent eigenvectors $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_N\}$ in common. Then the eigenvalues of matrix A are the eigenvalues of the matrices

$$\Lambda_k = \begin{bmatrix} \lambda_{1,1}^{(k)} & \lambda_{1,2}^{(k)} & \cdots & \lambda_{1,M}^{(k)} \\ \lambda_{2,1}^{(k)} & \lambda_{2,2}^{(k)} & \cdots & \lambda_{2,M}^{(k)} \\ \vdots & \vdots & & \vdots \\ \lambda_{M,1}^{(k)} & \lambda_{M,2}^{(k)} & \cdots & \lambda_{M,M}^{(k)} \end{bmatrix} \quad \text{for } k = 1, 2, \ldots, N,$$

where $\lambda_{i,j}^{(k)}$ is the eigenvalue of $A_{i,j}$ corresponding to the common eigenvector $\mathbf{v}_k$.

Stability

- An algorithm (such as a finite difference scheme) is **stable** if small changes in the input data result in proportionately small changes in the output data.
- If an algorithm is not stable, then it is labeled **unstable**.
- If e_0 is the error present in the data and e_n is the error after n subsequent calculations, then the growth rate of the error is **linear** if $e_n \propto n\, e_0$ and the growth rate of the error is **exponential** if $e_n \propto \gamma^n e_0$ for some $\gamma > 1$.

Sources of Error

There are three primary types of error: truncation error, measurement error, and rounding error.

- Truncation error is due to the use of a finite number of terms taken from a Taylor series to develop the approximations to various derivatives and derivative operators used in the partial differential equations.
- Measurement error comes from approximations used to set the initial and boundary conditions of an initial boundary value problem.
- Round-off errors result from the machine arithmetic used by computing devices.

Even if measurement errors are eliminated, truncation error and rounding error will still be present.

Heat Equation

Recall the explicit scheme for approximating the solution to the heat/diffusion equation.

$$\mathbf{u}^{(j+1)} = A(r)\,\mathbf{u}^{(j)}$$

$$\begin{bmatrix} u_1^{j+1} \\ u_2^{j+1} \\ u_3^{j+1} \\ \vdots \\ u_{N-2}^{j+1} \\ u_{N-1}^{j+1} \end{bmatrix} = \begin{bmatrix} 1-2r & r & 0 & \cdots & 0 & 0 \\ r & 1-2r & r & \cdots & 0 & 0 \\ 0 & r & 1-2r & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1-2r & r \\ 0 & 0 & 0 & \cdots & r & 1-2r \end{bmatrix} \begin{bmatrix} u_1^{j} \\ u_2^{j} \\ u_3^{j} \\ \vdots \\ u_{N-2}^{j} \\ u_{N-1}^{j} \end{bmatrix}.$$

Matrix $A(r)$ is real, tridiagonal, and symmetric, thus the eigenvalues are all distinct and the eigenvectors form a basis for the vector space $\mathbb{R}^{N-1}$.

Heat Equation

Suppose after the completion of the calculation of $\mathbf{u}^{(j)}$, the vector can be expressed as $\mathbf{u}^{(j)} = \hat{\mathbf{u}}^{(j)} + \mathbf{e}^{(0)}$ where $\hat{\mathbf{u}}^{(j)}$ is the exact solution of the finite difference equations. The error in the calculation of $\mathbf{u}^{(j)}$ is therefore $\mathbf{e}^{(0)}$.

After n additional time steps forward

$$\begin{aligned}
\mathbf{u}^{(j+n)} &= (A(r))^n \mathbf{u}^{(j)} \\
\hat{\mathbf{u}}^{(j+n)} + \mathbf{e}^{(n)} &= (A(r))^n (\hat{\mathbf{u}}^{(j)} + \mathbf{e}^{(0)}) \\
\mathbf{e}^{(n)} &= (A(r))^n \mathbf{e}^{(0)}.
\end{aligned}$$

Since the eigenvectors of $A(r)$ form a basis for $\mathbb{R}^{N-1}$ then there exist constants $c_1, c_2, \ldots, c_{N-1}$ such that $\mathbf{e}^{(0)} = c_1\mathbf{v}_1 + c_2\mathbf{v}_2 + \cdots + c_{N-1}\mathbf{v}_{N-1}$.

$$\mathbf{e}^{(n)} = (A(r))^n \sum_{k=1}^{N-1} c_k \mathbf{v}_k = \sum_{k=1}^{N-1} c_k \lambda_k^n \mathbf{v}_k.$$

Heat Equation

The explicit finite difference scheme for the heat equation is stable if $|\lambda_k| \leq 1$ for $k = 1, 2, \ldots, N-1$.

$$\lambda_k = 1 - 2r + 2r\cos\frac{k\pi}{N} = 1 - 4r\sin^2\frac{k\pi}{2N}$$

and $|\lambda_k| \leq 1$ if $r \leq 1/2$. Thus the explicit finite difference scheme given in is stable if $r \leq 1/2$ and unstable for $r > 1/2$.

Crank-Nicolson Scheme

The implicit Crank-Nicolson scheme expressed is

$$\mathbf{u}^{(j+1)} = (A(r))^{-1} A(-r)\, \mathbf{u}^{(j)}.$$

By the Lemma the eigenvalues of $A(r)$ are

$$\lambda_k = 2(1+r) - 2r\cos\frac{k\pi}{N} = 2 + 4r\sin^2\frac{k\pi}{2N} \text{ for } k = 1, 2, \ldots, N-1,$$

while the eigenvalues of $A(-r)$ are

$$\mu_k = 2(1-r) + 2r\cos\frac{k\pi}{N} = 2 - 4r\sin^2\frac{k\pi}{2N} \text{ for } k = 1, 2, \ldots, N-1.$$

Matrices $A(r)$ and $A(-r)$ share the same set of eigenvectors

$$\mathbf{v}_k = \left(\sin\frac{k\pi}{N}, \ldots, \sin\frac{(N-1)k\pi}{N}\right)^T.$$

Crank-Nicolson Scheme

- If λ is an eigenvalue of an invertible square matrix A with corresponding eigenvector $\mathbf{v}$ then $1/\lambda$ is an eigenvalue of A^{-1} with the same eigenvector $\mathbf{v}$.
- If $\mathbf{v}$ is an eigenvector of matrix A corresponding to eigenvalue λ and also an eigenvector of matrix B corresponding to eigenvalue μ then $\mathbf{v}$ is an eigenvector of matrix $A\,B$ corresponding to eigenvalue $\lambda\,\mu$.
- The Crank-Nicolson finite difference scheme is stable for all $r > 0$ since for $k = 1, 2, \ldots, N-1$ the eigenvalues of $(A(r))^{-1}A(-r)$ all have magnitudes bounded by 1,

$$\left|\frac{\mu_k}{\lambda_k}\right| = \left|\frac{2 - 4r\sin^2\frac{k\pi}{2N}}{2 + 4r\sin^2\frac{k\pi}{2N}}\right| \leq 1.$$

Wave Equation

Recall the $O(k^2) + O(h^2)$ explicit scheme for approximating solutions to the wave equation.

$$u_i^{j+1} = r^2 u_{i+1}^j + 2(1 - r^2)u_i^j + r^2 u_{i-1}^j - u_i^{j-1}.$$

Suppose the solution u_i^j for $i = 1, 2, \dots, N - 1$ and $j = 1, 2, \dots$ is a product solution of the form $u_i^j = X_i T_j$. Substitute the product solution into the finite difference scheme divide both sides by $X_i T_j$ produce

$$X_i T_{j+1} = r^2 X_{i+1} T_j + 2(1 - r^2) X_i T_j + r^2 X_{i-1} T_j - X_i T_{j-1}$$

$$\frac{T_{j+1}}{T_j} + \frac{T_{j-1}}{T_j} = r^2 \frac{X_{i+1}}{X_i} + 2(1 - r^2) + r^2 \frac{X_{i-1}}{X_i}.$$

Wave Equation

$$\frac{T_{j+1}}{T_j} + \frac{T_{j-1}}{T_j} = r^2 \frac{X_{i+1}}{X_i} + 2(1 - r^2) + r^2 \frac{X_{i-1}}{X_i}$$

The left-hand side of the equation above depends only on the index j while the right-hand side depends on the index i and therefore the left- and right-hand sides must be constant with respect to i and j. The constant will be denoted as λ.

Thus two difference equations are implied:

$$r^2 X_{i-1} + [2(1 - r^2) - \lambda] X_i + r^2 X_{i+1} = 0 \text{ for } i = 1, \ldots, N - 1$$

$$T_{j-1} - \lambda T_j + T_{j+1} = 0 \text{ for } j = 1, 2, \ldots.$$

Wave Equation

$$r^2 X_{i-1} + [2(1-r^2) - \lambda] X_i + r^2 X_{i+1} = 0$$

This is a discrete boundary value problem with boundary conditions $X_0 = X_N = 0$ (assuming homogeneous Dirichlet boundary conditions). Hence the values of λ are:

$$\lambda_k = 2(1-r^2) + 2r^2 \cos\frac{k\pi}{N} = 2 - 4r^2 \sin^2\frac{k\pi}{2N}$$

and $X_i = \sin(ik\pi/N)$ for $i = 0, 1, \ldots, N$.

Wave Equation

$$T_{j-1} - \lambda T_j + T_{j+1} = 0$$

This is an initial value problem. Assume the initial conditions T_0 and T_1 are known, then

$$T_{j-1} - \lambda_k T_j + T_{j+1} = 0$$

for $j = 1, 2, \ldots$. If $T_j = s^j$ then

$$0 = s^{j-1} - \lambda_k s^j + s^{j+1} \iff s^2 - \lambda_k s + 1 = 0.$$

Solving this quadratic equation implies s takes on the value

$$s_1 = \frac{1}{2}\left(\lambda_k - \sqrt{\lambda_k^2 - 4}\right) \text{ or } s_2 = \frac{1}{2}\left(\lambda_k + \sqrt{\lambda_k^2 - 4}\right).$$

Wave Equation

By the Principle of Superposition the general solution is $T_j = \alpha\, s_1^j + \beta\, s_2^j$ where α and β are arbitrary constants. Let α_k and β_k be the solutions to the simultaneous equations

$$T_0 = \alpha_k + \beta_k$$
$$T_1 = \alpha_k s_1 + \beta_k s_2.$$

The product solution u_i^j can be written as

$$u_i^j = \sum_{k=1}^{N-1} \left(\alpha_k s_1^j + \beta_k s_2^j\right) \sin \frac{ik\pi}{N}.$$

The finite difference scheme is stable whenever u_i^j remains bounded for all j. This condition is met if and only if $|s_1| \leq 1$ and $|s_2| \leq 1$. If $\lambda_k^2 \leq 4$ then s_1 and s_2 are complex conjugates and

$$|s_i|^2 = s_1 s_2 = \frac{1}{4}\left(\lambda_k^2 - (\lambda_k^2 - 4)\right) = 1.$$

If $\lambda_k^2 > 4$ then $\lambda_k < -2$ in which case $|s_1| > 1$. A necessary and sufficient condition for the finite difference scheme to be stable is that $-2 \leq \lambda_k \leq 2$. This inequality is equivalent to having $r = k/h \leq 1$.

Poisson's Equation

- In matrix/vector form the iterative methods can be expressed as the iterative equation $\mathbf{u}^{(k+1)} = T\,\mathbf{u}^{(k)} + \mathbf{b}$.
- The vector $\mathbf{b}$ encompasses the boundary conditions for a Laplace or Poisson problem and, in the case of a Poisson problem, the nonhomogeneous function on the right-hand side of the equation.
- The matrix T will be one of T_J, T_{GS}, or T_{SOR}.
- Let $\hat{\mathbf{u}}$ be the exact solution of the linear system, then $\hat{\mathbf{u}} = T\,\hat{\mathbf{u}} + \mathbf{b}$.
- Define the error vector of the kth iterate as $\mathbf{e}^{(k)} = \mathbf{u}^{(k)} - \hat{\mathbf{u}}$, then

$$\begin{aligned} \hat{\mathbf{u}} + \mathbf{e}^{(k+1)} &= T(\hat{\mathbf{u}} + \mathbf{e}^{(k)}) + \mathbf{b} \\ \mathbf{e}^{(k+1)} &= T\mathbf{e}^{(k)} \end{aligned}$$

- Let the expression $\rho(T)$ denotes the spectral radius (eigenvalue of largest magnitude) of matrix T.

Jacobi and Gauss-Seidel Convergence

Theorem

If $\hat{\mathbf{u}} = T\,\hat{\mathbf{u}} + \mathbf{b}$ *then the iterates* $\mathbf{u}^{(k)} = T\,\mathbf{u}^{(k-1)} + \mathbf{b}$ *for* $k = 1, 2, \ldots$ *converge to* $\hat{\mathbf{u}}$ *for any choice of* $\mathbf{u}^{(0)}$ *if and only if* $\rho(T) < 1$*.*

Remark: one method for establishing that all the eigenvalues of a matrix lie within the unit circle in the complex plane is to demonstrate that $\|T\|_2 < 1$.

Jacobi Convergence

Theorem

If A is an $n \times n$ strictly diagonally dominant or irreducibly diagonally dominant matrix and $\mathbf{b}$ is an $n \times 1$ vector, then the Jacobi iterative method converges to the solution of $A\mathbf{u} = \mathbf{b}$ for any choice of initial estimate $\mathbf{u}^{(0)}$.

Gauss-Seidel Convergence

Theorem

If A is an $n \times n$ strictly diagonally dominant or irreducibly diagonally dominant matrix and $\mathbf{b}$ is an $n \times 1$ vector, then the Gauss-Seidel iterative method converges to the solution of $A\mathbf{u} = \mathbf{b}$ for any choice of initial estimate $\mathbf{u}^{(0)}$.

Successive Over-Relaxation Convergence

Theorem

If $A\mathbf{u} = \mathbf{b}$ is a linear system of equations with $a_{ii} \neq 0$ for $i = 1, 2, \ldots, n$, the successive over-relaxation method converges to the solution $\mathbf{u}$ for an arbitrary initial estimate $\mathbf{u}^{(0)}$ only if $0 < \omega < 2$.

Successive Over-Relaxation Convergence

Theorem

If $A\mathbf{u} = \mathbf{b}$ *is a linear system of equations with* $a_{ii} \neq 0$ *for* $i = 1, 2, \ldots, n$*, the successive over-relaxation method converges to the solution* $\mathbf{u}$ *for an arbitrary initial estimate* $\mathbf{u}^{(0)}$ *only if* $0 < \omega < 2$*.*

If matrix A is positive definite, the condition in the previous theorem is also sufficient.

Theorem (Ostrowski-Reich)

Let $A\mathbf{u} = \mathbf{b}$ *be a linear system of equations where* A *is a positive definite matrix. The successive over-relaxation method converges to the solution* $\mathbf{u}$ *for an arbitrary initial estimate* $\mathbf{u}^{(0)}$ *if and only if* $0 < \omega < 2$*.*

Remarks

- The matrices of the finite difference approximation methods for Laplace's or Poisson's equation are all positive definite and therefore the successive over-relaxation iterative method will converge.
- The optimal choice for the successive over-relaxation parameter ω is the one which minimizes the magnitude of the largest magnitude eigenvalue of T_{SOR}. The optimal value of ω is

$$\omega^* = \frac{2}{1 + \sqrt{1 - |\lambda|^2}}$$

  where λ is the eigenvalue of $A^{-1}(L + U)$ with the largest magnitude.