Numerical Solution of Partial Differential Equations

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Lecture 7

Example 1

Consider

$$
\begin{aligned}
-u''(x) + c\,u(x) = f(x), \qquad & x \in (0,1), \\
u(0) = 0, \quad & u(1) = 0,
\end{aligned}
$$

where $c \geq 0$ and $f \in C([0,1])$. The finite difference approximation of this boundary-value problem on the mesh $\{x_i : i = 0, \ldots, N\}$ of uniform spacing $h = 1/N$, with $N \geq 2$, and $x_i = ih$, $i = 0, \ldots, N$, is given by

$$
\begin{aligned}
-\frac{U_{i+1} - 2U_i + U_{i-1}}{h^2} + c\,U_i = f(x_i), \quad & i = 1, \ldots, N-1, \\
U_0 = 0, \quad & U_N = 0.
\end{aligned} \tag{1}
$$

In terms of matrix notation, this can be rewritten as the linear system:

$$
AU = F \tag{2}
$$

where A is an $(N-1) \times (N-1)$ symmetric tridiagonal matrix, with distinct positive eigenvalues Λ_k, $k = 1, \ldots, N-1$, $F = (f(x_1), \ldots, f(x_{N-1}))^{\mathrm{T}}$, and $U = (U_1, \ldots, U_{N-1})^{\mathrm{T}}$ is the associated vector of unknowns.

Example 2

Similarly, if one considers the elliptic boundary-value problem

$$\begin{aligned} -\Delta u + cu &= f(x, y) \qquad && \text{in } \Omega, \\ u &= 0 && \text{on } \Gamma := \partial\Omega, \end{aligned}$$

where $c \geq 0$ is a given real number and $f \in C(\overline{\Omega})$, whose finite difference approximation posed on a uniform mesh $\{(x_i, y_j) : i, j = 0, \ldots, N\}$ of spacing $h = 1/N$, $N \geq 2$, in the x and y directions, is

$$\begin{aligned} -\frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{h^2} - \frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{h^2} + c\, U_{i,j} &= f(x_i, y_j), \\ U_{i,j} &= 0 \end{aligned} \tag{3}$$

where, Γ_h is the set of mesh-points on Γ, then this, too, can be rewritten as a system of linear algebraic equations of the form $AU = F$, where now A is an $(N-1)^2 \times (N-1)^2$ symmetric matrix with positive eigenvalues, $\Lambda_{k,m}$, $k, m = 1, \ldots, N-1$.

Objective

We shall be interested in developing a simple iterative method for the approximate solution of systems of linear algebraic equations of the form

$$AU = F,$$

where $A \in \mathbb{R}^{M \times M}$ is a symmetric matrix with positive eigenvalues, which are contained in a nonempty closed interval $[\alpha, \beta]$, with $0 < \alpha < \beta$, $U \in \mathbb{R}^M$ is the vector of unknowns and $F \in \mathbb{R}^M$ is a given vector.

We consider the following iteration for the approximate solution of the linear system $AU = F$:

$$U^{(j+1)} := U^{(j)} - \tau(AU^{(j)} - F), \qquad j = 0, 1, \ldots, \tag{4}$$

where $U^{(0)} \in \mathbb{R}^M$ is a given initial guess, and $\tau > 0$ is a parameter to be chosen so as to ensure that the sequence of iterates $\{U^{(j)}\}_{j=0}^{\infty} \subset \mathbb{R}^M$ converges to $U \in \mathbb{R}^M$ as $j \to \infty$.

As $U = U - \tau(AU - F)$, by subtracting (4) from this equality we have that

$$\begin{aligned} U - U^{(j+1)} &= U - U^{(j)} - \tau A(U - U^{(j)}) \\ &= (I - \tau A)(U - U^{(j)}), \qquad j = 0, 1, \ldots, \end{aligned} \tag{5}$$

where $I \in \mathbb{R}^{M \times M}$ is the identity matrix. Hence,

$$U - U^{(j)} = (I - \tau A)^j (U - U^{(0)}), \qquad j = 1, 2, \ldots .$$

Recall that if $\|\cdot\|$ is a(ny) norm on $\mathbb{R}^M$, then the induced matrix norm is defined, for a matrix $B \in \mathbb{R}^{M\times M}$, by

$$\|B\| := \sup_{V\in\mathbb{R}^M\setminus\{0\}} \frac{\|BV\|}{\|V\|}.$$

Thus, $\|BV\| \leq \|B\|\|V\|$ for all $V \in \mathbb{R}^M$, and hence, by induction

$$\|B^j V\| \leq \|B\|^j \|V\|, \qquad j = 1, 2 \ldots$$

for all $V \in \mathbb{R}^M$.

Therefore, with $B := I - \tau A$ and $V := U - U^{(0)}$, we have that

$$\|U - U^{(j)}\| = \|(I - \tau A)^j (U - U^{(0)})\| \leq \|I - \tau A\|^j \|U - U^{(0)}\|. \tag{6}$$

We shall take $\|\cdot\|$ to be the Euclidean norm on $\mathbb{R}^M$:

$$\|V\| := \left(\sum_{i=1}^{M} V_i^2\right)^{1/2}, \qquad V = (V_1, \ldots, V_M)^{\mathrm{T}} \in \mathbb{R}^M.$$

Recall that a symmetric matrix $B \in \mathbb{R}^{M\times M}$ has real eigenvalues $\{\lambda_i\}_{i=1}^M$, and the associated set of orthonormal eigenvectors $\{e_i\}_{i=1}^M$ spans $\mathbb{R}^M$.

For any vector

$$V = \alpha_1 e_1 + \cdots + \alpha_M e_M,$$

expanded in terms of the eigenvectors of B, thanks to orthonormality:

$$\|V\| = \left(\sum_{i=1}^{M} \alpha_i^2 \right)^{1/2} \quad \text{and} \quad \|BV\| = \left(\sum_{i=1}^{M} \alpha_i^2 \lambda_i^2 \right)^{1/2}.$$

Clearly,

$$\|BV\| \leq \max_{i=1,\ldots,M} |\lambda_i| \, \|V\| \qquad \forall\, V \in \mathbb{R}^M,$$

and the inequality becomes an equality if V is the eigenvector of B associated with the largest in absolute value eigenvalue of B. Thus,

$$\|B\| = \max_{i=1,\ldots,M} |\lambda_i|,$$

where now $\| \cdot \|$ is the matrix norm induced by the Euclidean norm.

Returning to (6), $\|I - \tau A\|$ on the r.h.s. of (6) is therefore equal to the largest in absolute value eigenvalue of the symmetric matrix $I - \tau A$.

As the eigenvalues of A are assumed to belong to the interval $[\alpha, \beta]$, where $0 < \alpha < \beta$, and the parameter τ is by assumption positive, the eigenvalues of $I - \tau A$ are contained in the interval $[1 - \tau\beta, 1 - \tau\alpha]$. Thus,

$$\|I - \tau A\| \leq \max\{|1 - \tau\beta|,\ |1 - \tau\alpha|\}.$$

To ensure that the iterative method (4) converges as fast as possible, we shall choose τ so that: $\|I - \tau A\| < 1$ and $\|I - \tau A\|$ is as small as possible.

We shall therefore seek $\tau > 0$ s.t.

$$\min_{\tau>0} \max\{|1 - \tau\beta|,\ |1 - \tau\alpha|\} < 1.$$

As $0 < \alpha < \beta$, by plotting the continuous piecewise linear function

$$\tau \mapsto \max\{|1 - \tau\beta|, |1 - \tau\alpha|\}$$

for $\tau \in [0, \infty)$, we observe that it attains its minimum at $\tau = \frac{2}{\alpha+\beta}$ where $1 - \tau\beta = \tau\alpha - 1$. Thus,

$$\min_{\tau>0} \max\{|1-\tau\beta|, |1-\tau\alpha|\} = \max\{|1-\tau\beta|, |1-\tau\alpha|\}\big|_{\tau=\frac{2}{\alpha+\beta}} = \frac{\beta-\alpha}{\beta+\alpha} < 1.$$

Hence, the optimal choice of the parameter τ in the iterative method

$$U^{(j+1)} := U^{(j)} - \tau(AU^{(j)} - F), \qquad j = 0, 1, \ldots; \quad U^{(0)} \in \mathbb{R}^M,$$

for the approximate solution of the linear system $AU = F$ is

$$\tau = \frac{2}{\beta + \alpha},$$

where $[\alpha, \beta]$ is a closed subinterval of $(0, \infty)$ that contains all eigenvalues of the symmetric matrix $A \in \mathbb{R}^{M \times M}$. Furthermore,

$$\|U - U^{(j)}\| \leq \left(\frac{\beta - \alpha}{\beta + \alpha}\right)^j \|U - U^{(0)}\|, \qquad j = 1, 2, \ldots.$$

An alternative, computable bound on the iteration error

We note that by multiplying (5) by the matrix A and recalling that $AU = F$, one has that

$$F - AU^{(j+1)} = (I - \tau A)(F - AU^{(j)}),$$

and therefore, by proceeding as above,

$$\|F - AU^{(j)}\| \leq \|I - \tau A\|^{j} \|F - AU^{(0)}\| \leq \left(\frac{\beta - \alpha}{\beta + \alpha}\right)^{j} \|F - AU^{(0)}\|. \quad (7)$$

If α and β are available, because F, A and the initial guess $U^{(0)}$ are known, it is possible to quantify the number of iterations required to ensure that the Euclidean norm of the so-called residual $F - AU^{(j)}$ of the j-th iterate becomes smaller than a chosen tolerance $\mathtt{TOL} > 0$.

A sufficient condition for this is that the right-hand side of (7) is smaller than $\mathtt{TOL}$, which will hold as soon as

$$j > \log \frac{\|F - AU^{(0)}\|}{\mathtt{TOL}} \left[\log\left(\frac{\beta+\alpha}{\beta-\alpha}\right)\right]^{-1}. \tag{8}$$

We will show that for both examples of boundary-value problems stated at the beginning of the lecture

$$\frac{\beta-\alpha}{\beta+\alpha} = 1 - \mathrm{Const.}h^2$$

and therefore (because $\log(1 - \mathrm{Const.}h^2) \sim -\mathrm{Const.}h^2$ as $h \to 0$) the right-hand side of the inequality (8) is $\sim \mathrm{Const.}\, h^{-2}\log(1/\mathtt{TOL})$.

We see in particular that the smaller the value of the mesh-size h the larger the number of iterations j will need to be to ensure that

$$\|F - AU^{(j)}\| < \mathtt{TOL}.$$

Example 1

Consider the eigenvalue problem:

$$\begin{aligned} -u''(x) + c\,u(x) = \lambda u(x), \qquad & x \in (0,1), \\ u(0) = 0, \quad & u(1) = 0, \end{aligned}$$

where $c \geq 0$ is a real number.

A nontrivial solution $u(x) \not\equiv 0$ of this is called an eigenfunction, and the corresponding $\lambda \in \mathbb{C}$ for which such a nontrivial solution exists is called an eigenvalue. A simple calculation reveals that there is an infinite sequence of eigenfunctions u^k and eigenvalues λ_k, $k = 1, 2, \ldots,$ where

$$u^k(x) := \sin(k\pi x) \quad \text{and} \quad \lambda_k := c + k^2\pi^2, \qquad k = 1, 2, \ldots.$$

Clearly, $c + \pi^2 \leq \lambda_k$ for all $k = 1, 2, \ldots$, and $\lambda_k \to +\infty$ as $k \to +\infty$.

The finite difference approximation of this eigenvalue problem on the mesh $\{x_i : i = 0, \dots, N\}$ of uniform spacing $h = 1/N$, with $N \geq 2$, and $x_i = ih$, $i = 0, \dots, N$, is given by

$$-\frac{U_{i+1} - 2U_i + U_{i-1}}{h^2} + c\, U_i = \Lambda U_i, \quad i = 1, \dots, N-1,$$
$$U_0 = 0, \quad U_N = 0.$$

A simple calculation yields the nontrivial solution: $U_i := U^k(x_i)$ where

$$U^k(x) := \sin(k\pi x), \quad x \in \{x_0, x_1, \dots, x_N\} \quad \text{and} \quad \Lambda_k := c + \frac{4}{h^2}\sin^2\frac{k\pi h}{2}$$

for $k = 1, 2, \dots, N-1$.

This can be verified by inserting

$$U_i = U^k(x_i) = \sin(k\pi x_i) \quad \text{and} \quad U_{i\pm1} = U^k(x_{i\pm1}) = \sin(k\pi x_{i\pm1})$$

into the finite difference scheme and noting that

$$\sin(k\pi x_{i\pm1}) = \sin(k\pi(x_i \pm h)) = \sin(k\pi x_i)\cos(k\pi h) \pm \cos(k\pi x_i)\sin(k\pi h)$$

and

$$1 - \cos(k\pi h) = 2\sin^2\frac{k\pi h}{2}$$

for $k = 1, 2, \dots, N-1$ and $i = 1, 2, \dots, N-1$.

Using matrix notation the finite difference approximation of the eigenvalue problem can be written as

$$\begin{bmatrix} \frac{2}{h^2}+c & -\frac{1}{h^2} & & & \mathbf{0} \\ -\frac{1}{h^2} & \frac{2}{h^2}+c & -\frac{1}{h^2} & & \\ & \ddots & \ddots & \ddots & \\ & & -\frac{1}{h^2} & \frac{2}{h^2}+c & -\frac{1}{h^2} \\ \mathbf{0} & & & -\frac{1}{h^2} & \frac{2}{h^2}+c \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_{N-2} \\ U_{N-1} \end{bmatrix} = \Lambda \begin{bmatrix} U_1 \\ U_2 \\ \vdots \\ U_{N-2} \\ U_{N-1} \end{bmatrix},$$

or, more compactly, $AU = \Lambda U$, where A is the symmetric tridiagonal $(N-1)\times(N-1)$ matrix displayed above, and $U = (U_1, \dots, U_{N-1})^{\mathrm{T}}$ is a column vector of size $N-1$. The calculation performed above implies that the eigenvalues of the matrix A are

$$\Lambda_k = c + \frac{4}{h^2}\sin^2\frac{k\pi h}{2}, \qquad k = 1, 2, \dots, N-1$$

and the corresponding eigenvectors are, respectively,

$$(U^k(x_1), \dots, U^k(x_{N-1}))^{\mathrm{T}}, \qquad k = 1, \dots, N-1.$$

Clearly,

$$c + 8 \leq \Lambda_k \leq c + \frac{4}{h^2} \qquad \text{for all } k = 1, 2, \ldots, N-1.$$

The first of these inequalities follows by noting that

$$\Lambda_k \geq \Lambda_1 = c + \frac{4}{h^2} \sin^2 \frac{\pi h}{2} \qquad \text{for } k = 1, \ldots, N-1$$

and $\sin x \geq \frac{2\sqrt{2}}{\pi} x$ for $x \in [0, \frac{\pi}{4}]$ (recall that $h \in [0, \frac{1}{2}]$ because $N \geq 2$, whereby $0 < \frac{\pi h}{2} \leq \frac{\pi}{4}$).

The second inequality is the consequence of $0 \leq \sin^2 x \leq 1$ for all $x \in \mathbb{R}$.

Example 2

Exercise

Let $\Omega = (0,1)^2 \subset \mathbb{R}^2$*, and consider the problem*

$$\begin{aligned} -\Delta u + cu &= \lambda u \qquad && \text{in } \Omega, \\ u &= 0 && \text{on } \Gamma := \partial\Omega, \end{aligned}$$

where $c \geq 0$ *is a given real number.*

Find the eigenfunctions and the associated eigenvalues for the boundary-value problem, as well for its finite difference approximation on a mesh of uniform spacing $h = 1/N$ *in the* x *and* y *directions.*

Solution:

$u^{k,m}(x,y) = \sin(k\pi x)\sin(m\pi y), \quad \lambda_{k,m} = c+(k^2+m^2)\pi^2, \quad k,m = 1,2,\ldots.$

The finite difference approximation of this eigenvalue problem posed on a uniform mesh $\{(x_i, y_j) : i,j = 0,\ldots,N\}$ of spacing $h = 1/N$, $N \geq 2$, is:

$$-\frac{U_{i+1,j} - 2U_{i,j} + U_{i-1,j}}{h^2} - \frac{U_{i,j+1} - 2U_{i,j} + U_{i,j-1}}{h^2} + c\,U_{i,j} = \Lambda U_{i,j}, \qquad i,j = 1,\ldots,N-1,$$

$$U_{i,j} = 0 \qquad \text{for } (x_i, y_j) \in \Gamma_h,$$

where, Γ_h is the set of all mesh-points on $\Gamma = \partial\Omega$. This can be rewritten as an algebraic eigenvalue problem of the form $AU = \Lambda U$, where now A is a symmetric $(N-1)^2 \times (N-1)^2$ matrix with positive eigenvalues

$$\Lambda_{k,m} = c + \frac{4}{h^2}\left(\sin^2\frac{k\pi h}{2} + \sin^2\frac{m\pi h}{2}\right),$$

with $c + 16 \leq \Lambda_{k,m} \leq c + \frac{8}{h^2}$, and eigenvectors/(discrete) eigenfunctions $U_{i,j} = U^{k,m}(x_i, y_j)$, where

$$U^{k,m}(x,y) = \sin(k\pi x)\sin(m\pi y),$$

for $i,j = 1,\ldots,N-1$ and $k,m = 1,\ldots,N-1$. $\square$

Conclusions

In the case of the finite difference scheme (1), $\alpha = c + 8$ and $\beta = c + \frac{4}{h^2}$, while in the case of (3), $\alpha = c + 16$ and $\beta = c + \frac{8}{h^2}$. In both cases

$$\frac{\beta - \alpha}{\beta + \alpha} = 1 - \mathrm{Const.}\, h^2;$$

thus, while the sequence of iterates $\{U^{(j)}\}_{j=0}^{\infty}$ defined by the iterative method (4) is guaranteed to converge to the exact solution U of the linear system $AU = F$, the speed of convergence will deteriorate as $h \to 0$:

$$\|U - U^{(j)}\| \leq \left(\frac{\beta - \alpha}{\beta + \alpha}\right)^j \|U - U^{(0)}\|. \tag{9}$$