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Scientific Computing II
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Solutions to Examination in Scientific Computing

1. (a)

$$A = \begin{pmatrix} 1 & 0 & \cdots & 0 & -1 \\ -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -1 & 1 \end{pmatrix}$$

(b)

$$\begin{aligned} (FAv)_k &= \sum_{j=1}^{N} e^{2\pi ijk/N}(Av)_j \\ &= e^{2\pi ik/N}(v_1 - v_N) + \sum_{j=2}^{N} e^{2\pi ijk/N}(v_j - v_{j-1}) \\ &= \sum_{j=1}^{N} e^{2\pi ijk/N} v_j - \underbrace{\sum_{j=2}^{N+1} e^{2\pi ijk/N} v_{j-1}}_{\text{since } e^{2\pi i(N+1)k/N} = e^{2\pi ik} e^{2\pi ik/N} = e^{2\pi ik/N}} \\ &= \sum_{j=1}^{N} e^{2\pi ijk/N} v_j - \sum_{j=1}^{N} e^{2\pi i(j+1)k/N} v_j \\ &= (1 - e^{2\pi ik/N}) \sum_{j=1}^{N} e^{2\pi ijk/N} v_j \\ &= (1 - e^{2\pi ik/N})(Fv)_k. \end{aligned}$$

We see that

$$d_k = (1 - e^{2\pi ik/N}).$$

(c) By applying A to an eigenvector, we find

$$\begin{aligned} Av_j^{(k)} &= \begin{cases} e^{-2\pi ik/N} - e^{-2\pi ikN/N}, & j = 1, \\ e^{-2\pi ijk/N} - e^{-2\pi i(j-1)k/N}, & j = 2, \ldots, N, \end{cases} \\ &= \begin{cases} (1 - e^{2\pi ik/N})e^{-2\pi ik/N}, & j = 1, \\ (1 - e^{2\pi ik/N})e^{-2\pi ijk/N}, & j = 2, \ldots, N. \end{cases} \end{aligned}$$

And we see that

$$Av^{(k)} = (1 - e^{2\pi ik/N})v^{(k)}.$$

2. (a) Given the splitting $A = L + D + U$, where

$$L + U = \begin{pmatrix} 0 & N^2 & & \\ N^2 & 0 & N^2 & \\ & & \ddots & \\ & & N^2 & 0 \end{pmatrix} \quad \text{and} \quad D = \begin{pmatrix} -2N^2 & & \\ & \ddots & \\ & & -2N^2 \end{pmatrix}$$

the Jacobi method can be written $x^{k+1} = Mx^k + c$, with $M = -D^{-1}(L+U)$ and $c = D^{-1}b$. Here,

$$M = \begin{pmatrix} 0 & 1/2 & & \\ 1/2 & 0 & 1/2 & \\ & & \ddots & \\ & & 1/2 & 0 \end{pmatrix} \quad \text{and} \quad c = \begin{pmatrix} -1/2N^2 \\ -1/2N^2 \\ \vdots \\ -1/2N^2 \end{pmatrix}.$$

(b) Gershgorin gives only two different conditions on the eigenvalues of M, $|\lambda| \leq 1/2$ and $|\lambda| \leq 1$, so $\rho(M) \leq 1$. Since Jacobi converges if and only if $\rho(M) < 1$, the estimate cannot be used to prove convergence.

(c) Since the eigenvalues of A are real and negative, our task is to find the eigenvalue with smallest modulus, which can be computed by inverse iteration:

Choose x^0 arbitrary
For $k = 1, 2, \ldots$
  Solve $Ay^k = x^{k-1}$
  Let $x^k = y^k/||y^k||$

(d) Assuming the ordering $|\lambda_1| \leq |\lambda_2| \leq \ldots \leq |\lambda_{N-1}|$, and since the eigenvalues of A^{-1} are λ_k^{-1}, inverse iteration converges towards the eigenvector corresponding to λ_1, and the error behaves like

$$\left(\frac{\lambda_2^{-1}}{\lambda_1^{-1}}\right)^k \approx \left(\frac{\frac{1}{-4\pi^2}}{\frac{1}{-\pi^2}}\right)^k = \frac{1}{4^k}$$

3. Let $p(x) = a + bx + cx^2 + dx^3$.

(a) We use Legendre polynomials since they are orthogonal on the right interval. The approximation can be explicitly written as

$$p(x) = \sum_{i=0}^{3} \frac{(p_i, f)}{(p_i, p_i)} p_i$$

where

$$(p_i, f) = \int_{-1}^{1} p_i(x) f(x) dx = -\int_{-1}^{0} p_i(x) dx + \int_{0}^{1} p_i(x) dx.$$

The last equality holds due to the specific f in this problem. The following orthogonality relation holds for the Legendre polynomials,

$$(p_i, p_j) = \begin{cases} 0, & i \neq j, \\ \frac{2}{2i+1}, & i = j. \end{cases}$$

It is easy to see that

$$(p_0, f) = (p_2, f) = 0,$$

e.g by noting that those polynomials are even and that f is odd. The other scalar products are

$$(p_1, f) = -\int_{-1}^{0} x dx + \int_{0}^{1} x dx = 1,$$

and

$$(p_3, f) = -\int_{-1}^{0} \frac{5x^3 - 3x}{2} dx + \int_{0}^{1} \frac{5x^3 - 3x}{2} dx = -1/4.$$

The least squares approximation can now be written as

$$p(x) = \frac{1}{2/3} x + \frac{-1/4}{2/7} \frac{(5x^3 - 3x)}{2} = -\frac{35}{16} x^3 + \frac{45}{16} x,$$

so the answer is

$$a = 0, \quad b = \frac{45}{16}, \quad c = 0, \quad d = -\frac{35}{16}.$$

(b) Make the Ansatz

$$p(x) = \alpha p_0(x) + \beta p_1(x) + \gamma p_2(x) + \delta p_3(x)$$

and require the error $p - f$ to be orthogonal to p_i, $i = 0, \ldots, 3$, i.e $(\alpha p_0 + \beta p_1 + \gamma p_2 + \delta p_3 - f, p_i)$, $i = 0, \ldots, 3$. Using the orthogonality of the polynomials, we find that the normal equations are diagonal,

$$\begin{pmatrix} (p_0, p_0) & 0 & 0 & 0 \\ 0 & (p_1, p_1) & 0 & 0 \\ 0 & 0 & (p_2, p_2) & 0 \\ 0 & 0 & 0 & (p_3, p_3) \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} (p_0, f) \\ (p_1, f) \\ (p_2, f) \\ (p_3, f) \end{pmatrix}.$$

All entries are already computed, so we can equivalently write

$$\begin{pmatrix} 2/1 & 0 & 0 & 0 \\ 0 & 2/3 & 0 & 0 \\ 0 & 0 & 2/5 & 0 \\ 0 & 0 & 0 & 2/7 \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \gamma \\ \delta \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ -1/4 \end{pmatrix}.$$

4. (a) The discrete Fourier transform of the difference equation is

$$\begin{aligned} \frac{\hat{v}_m^{n+1} - \hat{v}_m^n}{k} =& \theta \frac{e^{2\pi i m/N} - 2 + e^{-2\pi i m/N}}{h^2} \hat{v}_m^{n+1} \\ &+ (1-\theta) \frac{e^{2\pi i m/N} - 2 + e^{-2\pi i m/N}}{h^2} \hat{v}_m^{n+1} \end{aligned}$$

for $m = 0, \ldots, N-1$, or, equivalently

$$\frac{\hat{v}_m^{n+1} - \hat{v}_m^n}{k} = \frac{2\cos(2\pi m/N) - 2}{h^2} (\theta\, \hat{v}_m^{n+1} + (1-\theta)\, \hat{v}_m^n).$$

Let $\alpha_m = -k\,(2\cos(2\pi m/N) - 2)/h^2$. Then the equation reads

$$(1 + \alpha_m \theta) \hat{v}_m^{n+1} = (1 - \alpha_m (1-\theta)) \hat{v}_m^n.$$

If $m = 0$, then $\alpha_0 = 0$, $\hat{v}_0^{n+1} = \hat{g}_0 \hat{v}_0^n$ where $\hat{g}_0 = 1$, and $|\hat{g}_0| \leq 1$.
If $m = 1, \ldots, N-1$, then $0 < \alpha_m \leq 4k/h^2$, and $\hat{v}_m^{n+1} = \hat{g}_m \hat{v}_m^n$, where

$$\hat{g}_m = \frac{1 - \alpha(1-\theta)}{1 + \alpha\theta} = \ldots = 1 - \frac{1}{\alpha^{-1} + \theta}.$$

Thus, $|\hat{g}_m| \leq 1$ if

$$-1 \leq 1 - \frac{1}{\alpha_m^{-1} + \theta} \leq 1 \quad \Leftrightarrow \quad 2 \geq \frac{1}{\alpha_m^{-1} + \theta} \geq 0$$

or, since $\alpha_m^{-1} + \theta > 0$,

$$\alpha_m^{-1} + \theta \geq \frac{1}{2}.$$

Since $\alpha_m^{-1} \geq h^2/4k > 0$ this is true for all $\theta \geq 1/2$.
If $\theta < 1/2$, the stability condition is

$$\frac{k}{h^2} \leq \frac{1}{2 - 4\theta}.$$

(b) A Taylor expansion gives the local truncation error

$$\begin{aligned}
&\frac{u(x,t+k) - u(x,t)}{k} - \\
&\quad - \theta \frac{u(x+h,t+k) - 2u(x,t+k) + u(x-h,t+k)}{h^2} \\
&\quad - (1-\theta) \frac{u(x+h,t) - 2u(x,t) + u(x-h,t)}{h^2} = \ldots = \\
&= u_t + \frac{k}{2}u_{tt} + \frac{k^2}{6}u_{ttt} + \ldots \\
&\quad - \theta \left(u_{xx} + k u_{xxt} + \frac{k^2}{2} u_{xxtt} + \ldots + \frac{h^2}{12} (u_{xxxx} + \ldots) + \ldots \right) \\
&\quad - (1-\theta) \left(u_{xx} + \frac{h^2}{12} u_{xxxx} + \ldots \right) \\
&= k(\frac{1}{2} - \theta) u_{xxt} + k^2 \left(\frac{1}{6} u_{ttt} - \frac{\theta}{2} u_{xxtt} \right) + \ldots - \frac{h^2}{12} u_{xxxx} + \ldots
\end{aligned}$$

since $u_t = u_{xx}$ and $u_{tt} = u_{xxt}$. If $\theta = 1/2$ the order of approximation is $(2,2)$. Otherwise, it's $(2,1)$.

(c) Consistent schemes are convergent if and only if they are stable, so the convergence condition is the same as the stability condition, i.e. the one given in (a).

5. (a) Let V be the space

$$V = \{v \mid v \in \mathrm{C}([0,1]), v' \text{ piecewise continuous}, v(0) = v(1) = 0\}.$$

If u solves the ODE and $v \in V$, it follows from integration by parts that

$$\begin{aligned}
\int_0^1 v(x) f(x)\,dx &= \int_0^1 v(x) u''(x)\,dx + a \int_0^1 v(x) u(x)\,dx \\
&= [v(x)u'(x)]_0^1 - \int_0^1 v'(x) u'(x)\,dx + a \int_0^1 v(x) u(x)\,dx
\end{aligned}$$

Since $v(0) = v(1) = 0$, the boundary terms vanish. The variational formulation is: Find $u \in V$ such that

$$-\int_0^1 v'(x) u'(x)\,dx + a \int_0^1 v(x) u(x)\,dx = \int_0^1 v(x) f(x)\,dx, \quad \forall v \in V.$$

(b) Let V_h be given by

$$V_h = \{v \mid v \in \mathrm{C}([0,1]), v \text{ linear on } [x_j, x_{j+1}], v(0) = v(1) = 0\},$$

where $x_j = jh$ and $h = 1/(N+1)$. The piecewise linear functions $\phi_j(x) \in V_h$, $j = 1, \ldots, N$, satisfying

$$\phi_j(x_i) = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

are a basis in V_h. Thus, any function u_h can be written

$$u_h(x) = \sum_{j=1}^{N} c_j \phi_j(x),$$

for some constants c_j. The FEM is given by: Find $u_h \in V_h$ such that

$$-\int_0^1 v_h'(x) u_h'(x)\, dx + a \int_0^1 v_h(x) u_h(x)\, dx = \int_0^1 v_h(x) f(x)\, dx, \; \forall v_h \in V_h,$$

or equivalently,

$$-\sum_{j=1}^{N} c_j \int_0^1 \phi_i'(x)\phi_j'(x)\, dx + \sum_{j=1}^{N} c_j\, a \int_0^1 \phi_i(x)\phi_j(x)\, dx = \int_0^1 \phi_i(x) f(x)\, dx,$$

for $i = 1, \ldots, N$.

(c) The FEM gives a large system of equations $Ac = b$, where

$$A_{i,j} = -\int_0^1 \phi_i'(x)\phi_j'(x)\, dx + a \int_0^1 \phi_i(x)\phi_j(x)\, dx$$

and

$$b_i = \int_0^1 \phi_i(x) f(x)\, dx.$$

Since $\phi_i(x) = 0$ when $x < x_{i-1}$ or $x > x_{i+1}$, the coefficients $A_{i,j}$ are different from zero only when $i = j$ or $i - j = \pm 1$. Then,

$$A_{j,j} = -\int_0^1 (\phi_j'(x))^2\, dx + a \int_0^1 (\phi_j(x))^2\, dx = \ldots = -\frac{2}{h} + a\frac{2h}{3},$$

$$A_{j+1,j} = -\int_0^1 \phi_j'(x)\phi_{j+1}'(x)\, dx + a \int_0^1 \phi_j(x)\phi_{j+1}(x)\, dx = \ldots = \frac{1}{h} + a\frac{h}{6},$$

and $A_{j,j+1} = A_{j+1,j}$. The elements of b are usually computed by numerical integration. The trapezoidal rule gives

$$b_i = \int_0^1 \phi_i(x) f(x)\, dx \approx h\frac{0 + f(x_i)}{2} + h\frac{f(x_i) + 0}{2} = hf(x_i).$$

(d) On a nonuniform grid, h is not constant. The hat functions $\phi_j(x)$ therefore have different "width" on different parts of the grid, and the integrals determining for example $A_{j,j+1}$ depends on j. Thus, A is no longer toeplitz. The vector b also changes.