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Scientific Computing II/NV2
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Solutions to Examination in Scientific Computing

1. (a) $\|Ax\|_2 = x^H A^H Ax$. Since A is unitary we have $A^H A = I$ and hence $\|Ax\|_2 = x^H x = \|x\|_2$.

   (b) A Hermitian $\Leftrightarrow A^H = A$. Thus $A^H A = AA^H$, i.e. A is normal.

   (c) A and B are similar if $A = CBC^{-1}$ for some nonsingular matrix C.

$$Ax = \lambda x$$

$$\Leftrightarrow$$

$$C^{-1}Ax = \lambda C^{-1}x$$

$$\Leftrightarrow$$

$$\underbrace{C^{-1}AC}_{B}\underbrace{C^{-1}x}_{y} = \lambda \underbrace{C^{-1}x}_{y}$$

$$\Leftrightarrow$$

$$By = \lambda y$$

   where $y = C^{-1}x$, i.e. B has eigenvalues λ and eigenvectors $C^{-1}x$ where λ are eigenvalues and x are eigenvectors of A.

   (d)
   - Poisson $u_{xx} + u_{yy} = f$, $0 - 1^2 = -1 < 0$, $\Rightarrow$ elliptic.
   - Wave equation $u_{tt} - c^2 u_{xx} = 0$, $0 - 1 \cdot (-c^2) = c^2 > 0$, $\Rightarrow$ hyperbolic.

2. (a) Use Gersgorin discs: the eigenvalues λ of A are located in the union of the discs with center c_i

$$|\lambda - c_i| \leq \textstyle\sum_{j=1, j\neq i}^{2n} |a_{ij}| \quad , \quad i = 1, \ldots, 2n.$$

   From A we get

$$\textstyle\sum_{j=1, j\neq i}^{2n} |a_{ij}| = 0.1 \quad , \quad i = 1 \text{ or } i = 2n,$$

$$\textstyle\sum_{j=1, j\neq i}^{2n} |a_{ij}| = 0.2 \quad , \quad i = 2, \ldots, 2n-1,$$

$$c_i = -n + i - 1 \quad , \quad i = 1, \ldots, 2n.$$

   Since the radius of the discs all differ by at least 1 and the radius of the discs are at most 0.2 the discs are all isolated. $2n$ isolated discs $\Rightarrow$ $2n$ distinct eigenvalues. Since A is symmetric all eigenvalues are on the real axis.

   (b) Shift A with e.g. nI and use the power method on $B = A + nI$ which gives $\lambda + n$. The obtained λ is the largest eigenvalue of A since $\lambda + n$ corresponds to the eigenvalue of B with largest modulus. Since $Bx = (A + nI)x = (\lambda + n)x$ the correct eigenvector is obtained.

   (c) Shift A with e.g. $-nI$ and use power method on $B = A - nI$. Argumentation as above.

(d) Use inverse iteration on A. The eigenvalue μ closest to the origin corresponds to the eigenvalue μ^{-1} of A^{-1} with largest modulus. Since $Ax = \mu x \Leftrightarrow \underbrace{A^{-1}A}_{I}x = \mu A^{-x} \Leftrightarrow \mu^{-1}x = A^{-1}x$ the correct eigenvector is obtained.
Remark: Other solutions using the power method and the inverse method with different shifts are possible to (b)-(d). Some of them also have better convergence properties than the solutions suggested above.

3. (a) (v_1, v_2) is a basis in M where $v_1 = 1$, $v_2 = x$. Determine an ON-basis (e_1, e_2) using Gram-Schmidt:

$$\begin{aligned}
&\|v_1\| = \sqrt{\textstyle\sum_{i=0}^{2} 1^2} = \sqrt{3} \Rightarrow e_1 = \tfrac{1}{\sqrt{3}}\\
&w_2 = v_2 - (v_2, e_1)e_1 = x - \left(\textstyle\sum_{i=0}^{2} i\tfrac{1}{\sqrt{3}}\right)\tfrac{1}{\sqrt{3}} =\\
&x - \left(\tfrac{0}{\sqrt{3}} + \tfrac{1}{\sqrt{3}} + \tfrac{2}{\sqrt{3}}\right)\tfrac{1}{\sqrt{3}} = x - 1\\
&\|w_2\| = \sqrt{\textstyle\sum_{i=0}^{2} (i-2)^2} = \sqrt{(-1)^2 + 0^2 + 1^2} = \sqrt{2} \Rightarrow e_2 = \tfrac{x-1}{\sqrt{2}}
\end{aligned}$$

(b)

$$g^* = (f, e_1)e_1 + (f, e_2)e_2$$

$$\begin{aligned}
(f, e_1) &= \textstyle\sum_{i=0}^{2} i^3 \tfrac{1}{\sqrt{3}} = (0 + 1 + 8)\tfrac{1}{\sqrt{3}} = 3\sqrt{3}\\
(f, e_2) &= \textstyle\sum_{i=0}^{2} i^3 \tfrac{i-1}{\sqrt{2}} = (0 + 0 + 8)\tfrac{1}{\sqrt{2}} = 4\sqrt{2}
\end{aligned}$$

Thus $g^* = 3\sqrt{3}\frac{1}{\sqrt{3}} + 4\sqrt{2}\frac{x-1}{\sqrt{2}} = 3 + 4(x-1) = 4x - 1$.

(c) $f - g^* = x^3 - 4x + 1$ is orthogonal to M if $(f - g^*, e_i) = 0$, $i = 1, 2$.

$$\begin{aligned}
(f - g^*, e_1) &= \textstyle\sum_{i=0}^{2} \left(i^3 - 4i + 1\right)\tfrac{1}{\sqrt{3}} =\\
&= (0 - 0 + 1 + 1 - 4 + 1 + 8 - 8 + 1)\tfrac{1}{\sqrt{3}} = 0\\
(f - g^*, e_2) &= \textstyle\sum_{i=0}^{2} \left(i^3 - 4i + 1\right)\tfrac{i-1}{\sqrt{2}} =\\
&= ((0 - 0 + 1)\cdot(-1) + (1 - 4 + 1)\cdot 0 + (8 - 8 + 1)\cdot 1)\tfrac{1}{\sqrt{2}} = 0
\end{aligned}$$

(d) $g = \alpha e_2 + \beta e_2 \Rightarrow f - g = x^3 - \alpha\left(\frac{x-1}{\sqrt{2}}\right) - \beta\frac{1}{\sqrt{3}}$. Define $\bar{\alpha} = \frac{\alpha}{\sqrt{2}}$, $\bar{\beta} = \frac{\beta}{\sqrt{3}}$ yielding $f - g = x^3 - \bar{\alpha}x + \bar{\alpha} - \bar{\beta}$. From $F = \|f - g\|$ we get

$$F^2 = \left(0^3 - \bar{\alpha}\cdot 0 + \bar{\alpha} - \bar{\beta}\right)^2 + \left(1^3 - \bar{\alpha}\cdot 1 + \bar{\alpha} - \bar{\beta}\right)^2 + \left(2^3 - \bar{\alpha}\cdot 2 + \bar{\alpha} - \bar{\beta}\right)^2.$$

$$\begin{aligned}
\tfrac{\partial F^2}{\partial \alpha} &= 4\bar{\alpha} - 16 \Rightarrow \bar{\alpha}^* = 4\\
\tfrac{\partial F^2}{\partial \beta} &= 6\bar{\beta} - 18 \Rightarrow \bar{\beta}^* = 3
\end{aligned}$$

Since $\frac{\partial^2 F^2}{\partial \alpha^2} = 4 > 0$ and $\frac{\partial^2 F^2}{\partial \beta^2} = 6 > 0$, $\bar{\alpha}^*$ and $\bar{\beta}^*$ minimizes F. From this we conclude that $g^* = 4\sqrt{2}e_2 + 3\sqrt{3}e_1 = 4x - 4 + 3 = 4x - 1$.

4. (a) Use the energy method to get

$$\tfrac{d}{dt}\|u\|^2 = \tfrac{d}{dt}\int_0^1 u^2 dx = \int_0^1 2uu_t dx = [\text{Use the PDE}] =$$

$$= -\int_0^1 2uu_x dx = -\int_0^1 \tfrac{d}{dx}(u^2) dx = -\left[u^2\right]_0^1 = -u^2(1,t) + u^2(0,t) = 0,$$

where we have used the periodic boundary conditions in the last equality. Hence $\frac{d}{dt}\|u\|^2 = 0$ and $\|u\| = \|f\|$.

(b) A Taylor-expansion around (x_j, t_n) yields

$$\begin{aligned} u(x_j, t_{n+1}) &= u + ku_t + \tfrac{k^2}{2}u_{tt} + \mathcal{O}(k^3), \\ u(x_{j-1}, t_n) &= u - hu_x + \tfrac{h^2}{2}u_{xx} + \mathcal{O}(h^3), \end{aligned}$$

where u denotes $u(x_j, t_n)$ etc. The local truncation error φ is then given by

$$\begin{aligned} &\varphi = \tfrac{u(x_j,t_{n+1})-u(x_j,t_n)}{k} + \tfrac{u(x_{j+1},t_n)-u(x_j,t_n)}{h} = \\ &u_t + \tfrac{k}{2}u_{tt} + \mathcal{O}(k^2) + u_x - \tfrac{h}{2}u_{xx} + \mathcal{O}(h^2) = \\ &[u_t + u_x = 0] = \tfrac{k}{2}u_{tt} - \tfrac{h}{2}u_{xx} + \mathcal{O}(k^2) + \mathcal{O}(h^2). \end{aligned}$$

Hence, $\lim_{h,k\to 0}\varphi = 0$, i.e. the difference approximation is consistent.

(c) Using that every grid function v of periodicity 1 can be approximated by a finite Fourier series

$$v_j^n = \tfrac{1}{N}\textstyle\sum_{m=0}^{N-1}\hat{v}_m^n e^{2\pi ijm/N}, \quad \text{where} \quad \hat{v}_m^n = \textstyle\sum_{j=0}^{N-1} v_j^n e^{-2\pi ijm/N},$$

we get the following transformed equation

$$\hat{v}_m^{n+1} = \left(1 - \frac{k}{h}\left(1 - e^{-2\pi im/N}\right)\right)\hat{v}_m^n = \left(1 - \frac{k}{h} + \frac{k}{h}\left(\cos\theta - i\sin\theta\right)\right) = \hat{g}_m\hat{v}_m^n.$$

$$|\hat{g}_m|^2 = \left(1 + \frac{k}{h}\left(\cos\theta - 1\right)\right)^2 + \frac{k^2}{h^2}\sin^2\theta = \ldots = 1 + \underbrace{\frac{2k}{h}}_{\geq 0}\left(1 - \frac{k}{h}\right)\underbrace{(\cos\theta - 1)}_{\leq 0}$$

where $\theta = \frac{2\pi m}{N}$. If $\frac{k}{h} \leq 1$ we get that $\left(1 - \frac{k}{h}\right) \geq 0$ and hence $|\hat{g}_m|^2 \leq 1$ which is necessary and sufficient for stability.

(d) A consistent finite difference approximation of a well-posed PDE is convergent if it is stable. From above we conclude that the difference approximation converges if $\frac{k}{h} \leq 1$.

5. Start by assuming the opposite, i.e. that v assumes its maximum at some inner point (i_0, j_0) and that $v_{i_0,j_0} = M$ where M is larger than all values on the boundary. From the difference equation it follows that

$$v_{i,j} = \frac{1}{4}\left(v_{i+1,j} + v_{i-1,j} + v_{i,j+1} + v_{i,j-1}\right),$$

i.e., $v_{i,j}$ is the mean value of its neighbouring points. Hence, v_{i_0,j_0} is smaller than or equal to its largest neighbour. On the other hand $v_{i_0,j_0} = M$ is larger than or equal to its neighbouring points, i.e. all the neighbouring points must also equal M. By repeating the argument, $v = M$ everywhere, including boundary points, which is a contradiction. Hence, v must assume its maximum on the boundary.