Solutions to Examination in Scientific Computing

1. a)

$$\|A\|_1 = \max_j \sum_{i=1}^n |a_{ij}| = \max(4, 11, 18) = 18,$$

$$\|A\|_\infty = \max_i \sum_{j=1}^n |a_{ij}| = \max(10, 12, 11) = 12.$$

b)

$$\begin{vmatrix} 2-\lambda & 8 \\ 6 & 9-\lambda \end{vmatrix} = (2-\lambda)(9-\lambda) - 48 = 0 \Rightarrow$$

$$18 - 9\lambda - 2\lambda + \lambda^2 - 48 = \lambda^2 - 11\lambda - 30 = 0 \Rightarrow$$

$$\lambda_{1,2} = \frac{11 \pm \sqrt{241}}{2} \Rightarrow \rho(B) = \max(\lambda_1, \lambda_2) = \frac{11 + \sqrt{241}}{2}.$$

c) A Householder-matrix has the form $P = I - 2ww^T$ where w is a vector such that $w^T w = 1$. $P^T = (I - 2ww^T)^T = I^T - 2(ww^T)^T = I - 2(w^T)^T w^T = I - 2ww^T$.

2. a) A direct method such as Gaussian elimination causes much "fill-in" when the coefficient-matrix A is large and sparse. Fill-in means that areas with elements equal to 0 are filled in with non-zeros, i.e. we have to store a lot more information in the computer memory. An *iterative method* however, is based on matrix-vector multiplication which means that there won't be any fill-in in the areas that are equal to 0. Hence, we save a lot of computer memory by using an iterative method.

b)

$$B = D - L - U,$$

$$D = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 5 \end{pmatrix}, \quad -L = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix}, \quad -U = \begin{pmatrix} 0 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}.$$

$$u^{k+1} = D^{-1}(L+U)u^k + D^{-1}b \Rightarrow$$

$$u^1 = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 5 \end{pmatrix}^{-1} \left(\begin{pmatrix} 0 & -1 & -1 \\ -1 & 0 & -1 \\ -1 & -1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} \right) = \begin{pmatrix} -0.2 \\ 0.0 \\ 0.2 \end{pmatrix}$$

c) Since B is strictly diagonally dominant the iteration will converge.

3. a) $\tilde{e}_1 = \sin(2\pi t)$ and $\tilde{e}_2 = \cos(2\pi t)$ are already orthogonal. In order to have an ON-basis we just need to normalize them.

$$(\tilde{e}_1, \tilde{e}_1) = \sum_{i=0}^4 \sin^2\left(\frac{2\pi i}{5}\right) = \frac{5}{2}$$

$$(\tilde{e}_2, \tilde{e}_2) = \sum_{i=0}^4 \cos^2\left(\frac{2\pi i}{5}\right) = \frac{5}{2}$$

Hence an ON-basis is formed by $e_1 = \sqrt{\frac{2}{5}} \sin(2\pi t)$ and $e_2 = \sqrt{\frac{2}{5}} \cos(2\pi t)$.

b) The least squares projection of the data unto M is given by $g^* = (y, e_1)e_1 + (y, e_2)e_2$.

$$(y, e_1) = \sqrt{\frac{2}{5}}(-3\sin(0) + 0\sin(0.4\pi) + 3\sin(0.8\pi) + 1.8\sin(1.2\pi) - 1.8\sin(1.6\pi))$$
$$\approx 1.5288$$

$$(y, e_2) = \sqrt{\frac{2}{5}}(-3\cos(0) + 0\cos(0.4\pi) + 3\cos(0.8\pi) + 1.8\cos(1.2\pi) - 1.8\cos(1.6\pi))$$
$$\approx -4.7052$$

The final answer is then $g^* = (y, e_1)e_1 + (y, e_2)e_2 \approx 0.9669\sin(2\pi t) - 2.9758\cos(2\pi t)$.

c) The equations are given by $y_i = a_1\sin(2\pi t_i) + a_2\cos(2\pi t_i)$, leading to the system $Ax = b$, where

$$A = \begin{bmatrix} \sin(0) & \cos(0) \\ \sin(0.4\pi) & \cos(0.4\pi) \\ \sin(0.8\pi) & \cos(0.8\pi) \\ \sin(1.2\pi) & \cos(1.2\pi) \\ \sin(1.6\pi) & \cos(1.6\pi) \end{bmatrix}, \quad x = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}, \quad b = \begin{bmatrix} -3 \\ 0 \\ 3 \\ 1.8 \\ -1.8 \end{bmatrix}$$

d) A QR-factorization can be computed through for example Householder transformations or by the Gram-Scmidt orthogonalization method applied to the columns of A.

When the factorization $A = QR$ is known, the normal equations $A^T Ax = A^T b$ can be rewritten as $Rx = Q^T b$. This is now a square linear system and furthermore, R is upper triangular. Hence, the system can be solved through backward substitution.

4. a) The eigenvalues are distinct if either the row circles or the column circles are non-overlapping. The circles are centerad at a_{ii}, that is at 1, 2, and 3. They are non-overlapping if the sum of the radii of two adjacent circles is less than 1 (the distance between the centers). Let r_1, r_2, and r_3 be the radii of the row circles and c_1, c_2 and c_3 of the column circles. We have

$$\begin{array}{llll} r_1 &= |a| + 0.3, & c_1 &= |b| + 0.2, \\ r_2 &= 0.5, & c_2 &= 0.4, \\ r_3 &= |b| + 0.1, & c_3 &= |a| + 0.3, \end{array}$$

For the row circles, $r_1 + r_2 < 1$ and $r_2 + r_3 < 1$ lead to $|a| < 0.2$ and $|b| < 0.4$. The conditions $c_1 + c_2 < 1$ and $c_2 + c_3 < 1$ lead to $|a| < 0.3$ and $|b| < 0.4$. Accordingly, the best possible bound through Gershgorin circles is $|a| < 0.3$ and $|b| < 0.4$.

b) The error of the power method depends on the ratio of the eigenvalue with the largest modulus and the eigenvalue with the next to largest modulus. In this case, the error is proportional to

$$\left(\frac{\lambda_2}{\lambda_3}\right)^k \approx \left(\frac{2}{3}\right)^k,$$

where k is the number of iterations. To get an error less than 10^{-5} we would (approximately) need

$$\left(\frac{2}{3}\right)^k < 10^{-5} \quad \Leftrightarrow \quad k > \frac{\log 10^{-5}}{\log(2/3)} \approx 28.4.$$

That is, we would need about 29 iterations to reach the desired accuracy.

c) By first shifting the matrix to $B = A - 2I$ we make the eigenvalue with the desired eigenvector have the smallest modulus. Then we apply inverse iteration to B (the power method on B^{-1}) to compute the eigenvector.

5. a) The Fourier series of u_j^n is

$$u_j^n = \sum_{\ell=0}^{N-1} c_\ell^n \exp(i2\pi\ell jh).$$

For one term $c_\ell^n \exp(i2\pi\ell jh)$ in the series we have

$$c_\ell^{n+1} \exp(i2\pi\ell jh)$$
$$= c_\ell^n \exp(i2\pi\ell jh)(1 - 0.5akh^{-1}(\exp(i2\pi\ell h) - \exp(-i2\pi\ell h))).$$

Then with $r = ah^{-1}k$, c_ℓ^n satisfies

$$c_\ell^{n+1} = (1 - 0.5r(\exp(i2\pi\ell h) - \exp(-i2\pi\ell h)))c_\ell^n$$
$$= (1 - ri\sin(2\pi\ell h))c_\ell^n = Qc_\ell^n.$$

For stability, $|Q| \leq 1$ which is possible only if $r = 0$, i.e. $a = 0$.

b) The recursion formula for the Fourier coefficient is

$$c_\ell^{n+1} = (1 - r(\exp(i2\pi\ell h) - 1))c_\ell^n$$
$$= (1 + r - r\cos(2\pi\ell h) - ri\sin(2\pi\ell h))c_\ell^n = Qc_\ell^n.$$

For stability, we have $|Q| \leq 1$, i.e.

$$|Q|^2 = (1 + r - r\cos(2\pi\ell h))^2 + r^2\sin(2\pi\ell h)^2$$
$$= 1 + r^2 + r^2\cos(2\pi\ell h)^2 + 2r - 2r\cos(2\pi\ell h) - 2r^2\cos(2\pi\ell h) + r^2\sin(2\pi\ell h)^2$$
$$= 1 + 2r(r + 1)(1 - \cos(2\pi\ell h)).$$

Since $0 \leq 1 - \cos(2\pi\ell h) \leq 2$ the strictest bound on r is when $\cos(2\pi\ell h) = -1$. The minimum of $f(r) = 1 + 4r(r + 1)$ is at $r = -0.5$ and $f(-0.5) = 0$ and $f(r) = 1$ at $r = 0$ and $r = -1$. Hence, for stability $-1 \leq r \leq 0$ or

$$-h/k \leq a \leq 0.$$