Solutions to Examination in Scientific Computing

1. (a) \( Ax = \lambda x \Rightarrow A^{-1}Ax = \lambda A^{-1}x \Rightarrow \lambda^{-1}x = A^{-1}x. \) Hence, \( \lambda^{-1} \) is an eigenvalue to \( A^{-1} \) with eigenvector \( x \).

(b) A Taylor-expansion around \( x_j \) and denote \( u(x_j) \) by \( u \) etc., yields

\[
u(x_j \pm h) = u(x_j) \pm hu_x + \frac{h^2}{2}u_{xx} \pm \frac{h^3}{6}u_{xxx} \pm \frac{h^4}{24}u_{xxxx} + \mathcal{O}(h^5)
\]

\[
u(x_{j+1}) - 2u(x_j) + \nu(x_{j-1}) = \frac{h^2}{2} \left((1 - 2 + 1)u_x + (\frac{h^2}{2} + \frac{h^2}{2})u_{xx} + (\frac{h^3}{6} - \frac{h^3}{6})u_{xxx} + \frac{h^4}{24}u_{xxxx} + \mathcal{O}(h^5)\right) = u_{xx} + \mathcal{O}(h^2).
\]

(c) \( ||Qx||_2^2 = (Qx)^H(Qx) = x^HQ^HQx. \) But since \( Q \) is unitary we have that \( Q^HQ = I \) and \( ||Qx||_2^2 = x^Hx = ||x||_2^2 \Rightarrow ||Qx||_2 = ||x||_2. \)

2. (a) Gersgorin’s discs, row-version

- Disc 1, \( |\lambda - 8| \leq 0.1 + 0.2 = 0.3. \)
- Disc 2, \( |\lambda - 6| \leq 0.2 + 0.3 = 0.5. \)
- Disc 3, \( |\lambda - 10| \leq 0.5 + 0.5 = 1.0. \)

Three disjoint discs \( \Rightarrow \) one eigenvalue in each.

(b) The code is an implementation of the Power method. The resulting number 10.0888... is the eigenvalue to \( A \) with largest magnitude, i.e. the eigenvalue in Disc 3.

(c) The convergence rate depends on the quotient between the two eigenvalues with largest magnitude, i.e. the eigenvalue in Disc 1 (\( \lambda_2 \)) and the eigenvalue in Disc 3 (\( \lambda_3 \)). In the worst case \( \lambda_2 = 8.3 \) we have

\[
\frac{|\lambda_2 - \lambda_1|}{\lambda_1} \approx \frac{8.3}{10.0888} = 0.82. \]

A way to achieve better convergence is to use shift with \( \sigma \) and compute the eigenvalues \( \tilde{\lambda}_i \) of \( A - \sigma I \). Use for instance \( \sigma = \frac{5.5 + 8.3}{2} = 6.9, \Rightarrow \) the two eigenvalues with smallest magnitude fulfill \( |\tilde{\lambda}_2,3| \leq 1.4 \). Hence \( \frac{|\lambda_2 - \lambda_1|}{\lambda_1} \approx \frac{1.4}{3.1888} = 0.31 < 0.82. \)

Another possibility is to shift with \( \sigma = 10 \) and employ the inverse power method.

3. (a) Use the energy-method and define the norm \( ||u(\cdot, t)||^2 = \int_0^1 u^2(x, t)dx. \) Then

\[
\frac{d}{dt} ||u(\cdot, t)||^2 = \frac{d}{dt} \int_0^1 u^2(x, t)dx = 2 \int_0^1 uu_tdx = [u_t = u_{xx}]
\]

\[
2 \int_0^1 uu_{xx}dx = [\text{part. int.}] = 2[uu_x]_0^1 - \int_0^1 u_x^2 = 0 - \int_0^1 u_x^2 \leq 0.
\]

Thus, \( ||u(\cdot, t)|| \leq ||f|| \Rightarrow \) the solution depends continuously on given data. Since we have assumed a unique solution, the PDE is well-posed.
(b) Use Fourier technique and replace \( u^n_j \rightarrow \hat{u}^n_\omega e^{i2\pi \omega x_j} \) \( \Rightarrow \)

\[
\frac{\hat{u}^{n+1}_\omega - \hat{u}^n_\omega}{\Delta t} = \hat{u}^{n+1}_\omega e^{i2\pi \omega x_j} e^{i2\pi h} - 2 + e^{-i2\pi \omega h}.
\]

Rearranging gives

\[
\hat{u}^{n+1}_\omega \left( 1 + a_\omega \frac{2\Delta t}{h^2} \right) = \hat{u}^n_\omega,
\]

where \( a_\omega = 1 - \cos (2\pi \omega h) \). The finite difference scheme is unconditionally stable if \( \hat{u}^{n+1}_\omega \leq \hat{u}^n_\omega \) which in this case is true if \( 1 + a_\omega \frac{2\Delta t}{h^2} \geq 1 \). But since \( a_\omega \geq 0 \) and \( \Delta t \geq 0 \) it is clear that \( \hat{u}^{n+1}_\omega \leq \hat{u}^n_\omega \).

(c) The number of non-zero elements has increased due to fill-in from the factorization. This might cause problems with computer memory if the matrix \( A \) is large. One way to avoid fill-in is to use an iterative method to solve the system of equations instead.

4.

5.

\[
A \begin{pmatrix} a \\ b \end{pmatrix} = y,
\]

where

\[
A = \begin{pmatrix}
1 & 10.0 \\
1 & 10.2 \\
1 & 10.4 \\
1 & 10.6 \\
1 & 10.8 \\
1 & 11.0
\end{pmatrix}, \quad
y = \begin{pmatrix}
0.5 \\
1.0 \\
2.5 \\
4.5 \\
6.5 \\
8.0
\end{pmatrix}.
\]

The normal equations \( A^T A \begin{pmatrix} a \\ b \end{pmatrix} = A^T b \) reads

\[
\begin{pmatrix}
6 & 63 \\
63 & 662.2
\end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix}
23 \\
247.1
\end{pmatrix}.
\]

\( \Rightarrow \)

\[
\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix}
-80.166 \\
8
\end{pmatrix}.
\]

\( \Rightarrow \)

\[
y = 8x - 80.2
\]

6.

\[
A \begin{pmatrix} \beta \\ \alpha \end{pmatrix} = \ln y,
\]

where

\[
A = \begin{pmatrix}
1 & 10.0 \\
1 & 10.2 \\
1 & 10.4 \\
1 & 10.6 \\
1 & 10.8 \\
1 & 11.0
\end{pmatrix}, \quad
\ln y = \begin{pmatrix}
-0.6931 \\
0 \\
0.9163 \\
1.5041 \\
1.8718 \\
2.0794
\end{pmatrix},
\]

and \( \alpha = \ln C \) The normal equations \( A^T A \begin{pmatrix} \beta \\ \alpha \end{pmatrix} = A^T \ln y \)
reads\[
\begin{pmatrix}
6 & 63 \\
63 & 662.2
\end{pmatrix}
\begin{pmatrix}
\beta \\
\alpha
\end{pmatrix} = \begin{pmatrix}
5.678 \\
61.63
\end{pmatrix}.
\]
\[\Rightarrow \begin{pmatrix}
\beta \\
\alpha
\end{pmatrix} = \begin{pmatrix}
-29.15 \\
2.867
\end{pmatrix}.
\]
\[\Rightarrow y = e^{-29.15 + 2.867x}.
\]

7. (a) Let $V$ be the space
\[V = \{ v \mid v \text{ cont on } [0, 1], v' \text{ piecewise cont on } [0, 1], v(0) = v(1) = 0 \}.
\]
If $u$ solves the ODE and $v \in V$, it follows from integration by parts that
\[\int_0^1 v(x)f(x) \, dx = \int_0^1 v(x)u''(x) \, dx
\]
\[= [v(x)u'(x)]_0^1 - \int_0^1 v'(x)u'(x) \, dx
\]
Since $v(0) = v(1) = 0$, the boundary terms vanish. The variational formulation is: Find $u \in V$ such that
\[-\int_0^1 v'(x)u'(x) \, dx = \int_0^1 v(x)f(x) \, dx, \quad \forall v \in V.
\]

(b) The Discrete Fourier Transform $\hat{u} = W_N u$, where $W_N$ is a Fourier matrix of size $N \times N$ can be accomplished through the (Inverse) Fast Fourier Transform (FFT). The basic idea behind the algorithm is that the multiplication can be split into two multiplications $y_1 = W_{N/2} x_1$ and $y_2 = W_{N/2} x_2$, where $y_i, x_i$ are vectors of size $N/2$. The final result $\hat{u}$ is then obtained through a combination of $y_1$ and $y_2$. The splitting is repeated recursively until the length of the vectors is 1. The total number of arithmetic operations required is $O(N \log_2 N)$. 