Problem Sheet 3 - Answers

1. As we know that the top row of $\mathbf{U}$ is the same as the top row of $\mathbf{A}$, we can start with

$$\mathbf{A} = \begin{pmatrix} 4 & 1 & 1 \\ 1 & 2 & 3 \\ 1 & 3 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{pmatrix} \begin{pmatrix} 4 & 1 & 1 \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}.$$

To complete the $\mathbf{LU}$ decomposition of $\mathbf{A}$ we expand the product one element at a time, working through the rows of $\mathbf{A}$ in increasing order (so 2, then 3), and for each row, working from left to right (column 1, then 2 then 3). From row 2 we get

$$1 = 4\ell_{21} \to \ell_{21} = \frac{1}{4} \qquad 2 = \frac{1}{4} + u_{22} \to u_{22} = \frac{7}{4}; \qquad 3 = \frac{1}{4} + u_{23} \to u_{23} = \frac{11}{4},$$

and from row 3

$$1 = 4\ell_{31} \to \ell_{31} = \frac{1}{4} \quad 3 = \frac{1}{4} + \frac{7}{4}\ell_{32} \to \ell_{32} = \frac{11}{7}; \quad 1 = \frac{1}{4} + \frac{11}{4}\frac{11}{7} + u_{33} \to u_{33} = -\frac{25}{7}.$$

Now we have our decomposition $\mathbf{A} = \mathbf{LU}$:

$$\mathbf{A} = \begin{pmatrix} 4 & 1 & 1 \\ 1 & 2 & 3 \\ 1 & 3 & 1 \end{pmatrix} = \mathbf{LU} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{4} & 1 & 0 \\ \frac{1}{4} & \frac{11}{7} & 1 \end{pmatrix} \begin{pmatrix} 4 & 1 & 1 \\ 0 & \frac{7}{4} & \frac{11}{4} \\ 0 & 0 & -\frac{25}{7} \end{pmatrix}.$$

Now we can start solving the equations. First we write $\mathbf{Ly} = \mathbf{b}$:

$$\mathbf{Ly} = \mathbf{b} \to \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{4} & 1 & 0 \\ \frac{1}{4} & \frac{11}{7} & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 8 \\ 8 \end{pmatrix},$$

which we solve for $\mathbf{y}$ by forward substitution:

$$y_1 = 7; \qquad \frac{7}{4} + y_2 = 8 \to y_2 = \frac{25}{4}; \qquad \frac{7}{4} + \frac{275}{28} + y_3 = 8 \to y_3 = -\frac{25}{7}.$$

Finally, we write

$$\mathbf{Ux} = \mathbf{y} \to \begin{pmatrix} 4 & 1 & 1 \\ 0 & \frac{7}{4} & \frac{11}{4} \\ 0 & 0 & -\frac{25}{7} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ \frac{25}{4} \\ -\frac{25}{7} \end{pmatrix},$$

which we solve for $\mathbf{x}$ by back substitution:

$$x_3 = 1; \qquad 7x_2 + 11 = 25 \to x_2 = 2; \qquad 4x_1 + 1 + 2 = 7 \to x_1 = 1.$$

For the second example, we have

$$\mathbf{A} = \begin{pmatrix} 1 & 3 & 1 \\ 3 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ 1 & \frac{3}{7} & 1 \end{pmatrix} \begin{pmatrix} 1 & 3 & 1 \\ 0 & -7 & -3 \\ 0 & 0 & \frac{9}{7} \end{pmatrix} \to \mathbf{y} = \begin{pmatrix} 6 \\ -13 \\ \frac{18}{7} \end{pmatrix} \to \mathbf{x} = \begin{pmatrix} 1 \\ 1 \\ 2 \end{pmatrix}.$$

2. (a) For the simple Richardson scheme, the iteration matrix is:

$$\mathbf{J} = \mathbf{I} - \mathbf{A} = \begin{pmatrix} -3 & -2 \\ -2 & -2 \end{pmatrix}$$

Perform two iterations starting with $\mathbf{x}_0 = [2, -1]^T$:

$$\mathbf{x}_1 = \begin{pmatrix} -3 & -2 \\ -2 & -2 \end{pmatrix} \begin{pmatrix} 2 \\ -1 \end{pmatrix} + \begin{pmatrix} 8 \\ 3 \end{pmatrix} = \begin{pmatrix} 4 \\ 1 \end{pmatrix},$$

$$\mathbf{x}_2 = \begin{pmatrix} -3 & -2 \\ -2 & -2 \end{pmatrix} \begin{pmatrix} 4 \\ 1 \end{pmatrix} + \begin{pmatrix} 8 \\ 3 \end{pmatrix} = \begin{pmatrix} -6 \\ -7 \end{pmatrix},$$

Does not converge!

(b) Keeping in mind that we will need to calculate spectrum of a modified Richardson matrix later, it is useful to do this exercise for a general symmetric 2×2 matrix:

$$\mathbf{M} = \begin{pmatrix} p & q \\ q & r \end{pmatrix}$$

Solve $|\mathbf{M} - \lambda \mathbf{I}| = 0$:

$$\lambda_{1,2} = \frac{1}{2}\left[p + r \pm \sqrt{(p+r)^2 - 4pr + 4q^2}\right]$$

For $\mathbf{J}$ we have $p = -3$, $q = -2$, $r = -2$, hence:

$$\lambda_{1,2} = \frac{1}{2}\left[-5 \pm \sqrt{17}\right]$$

The spectral radius of $\mathbf{J}$ is:

$$\rho = \left|\frac{1}{2}\left[-5 - \sqrt{17}\right]\right| \approx 4.56 > 1$$

Therefore iterations diverge, as we observed in part (a).

(c) For the modified Richardson scheme, the iteration matrix is:

$$\mathbf{J} = \mathbf{I} - \frac{\mathbf{1}}{\mathbf{a}}\mathbf{A} = \begin{pmatrix} 1 - \frac{4}{a} & -\frac{2}{a} \\ -\frac{2}{a} & 1 - \frac{3}{a} \end{pmatrix}$$

Using the earlier derived formula for the eigenvalues with $p = 1 - 4/a$, $q = -2/a$, $r = 1 - 3/a$ gives

$$\lambda_{1,2} = 1 - \frac{1}{2a}\left[7 \pm \sqrt{17}\right]$$

At any a the greater of $|\lambda_1|$ and $|\lambda_2|$ defines the spectral radius. Figure below shows the behaviour of $|\lambda_{1,2}|$ as a is varying.
Fastest convergence will occur when $|\lambda_1| = |\lambda_2|$, which gives:

$$1 - \frac{1}{2a}\left[7 + \sqrt{17}\right] = -1 + \frac{1}{2a}\left[7 - \sqrt{17}\right]$$

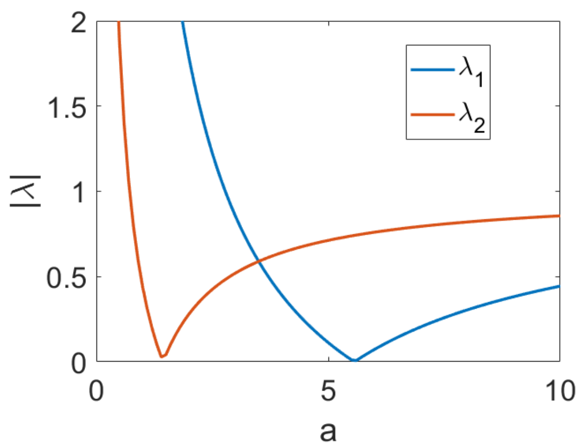

Figure 1: Eigenvalues of the modified Richardson iteration matrix, $|\lambda_1|$ and $|\lambda_2|$, as functions of a.

Hence the best convergence occurs for $a_0 = 7/2$. The corresponding rate of convergence is:

$$\rho(a_0) = \frac{\sqrt{17}}{7} \approx 0.589$$

At a_0 the iteration matrix is:

$$\mathbf{J} = \begin{pmatrix} -\frac{1}{7} & -\frac{4}{7} \\ -\frac{4}{7} & \frac{1}{7} \end{pmatrix}$$

And the vector $\mathbf{c} = (1/a)\mathbf{b}$ in the iteration formula is:

$$\mathbf{c} = \begin{pmatrix} \frac{16}{7} \\ \frac{6}{7} \end{pmatrix}$$

Make two iterations:

$$\mathbf{x}_1 = \begin{pmatrix} -\frac{1}{7} & -\frac{4}{7} \\ -\frac{4}{7} & \frac{1}{7} \end{pmatrix} \begin{pmatrix} 2 \\ -1 \end{pmatrix} + \begin{pmatrix} \frac{16}{7} \\ \frac{6}{7} \end{pmatrix} = \frac{1}{7} \begin{pmatrix} 18 \\ -3 \end{pmatrix} \approx \begin{pmatrix} 2.571 \\ -0.429 \end{pmatrix} ,$$

$$\mathbf{x}_2 = \begin{pmatrix} -\frac{1}{7} & -\frac{4}{7} \\ -\frac{4}{7} & \frac{1}{7} \end{pmatrix} \frac{1}{7} \begin{pmatrix} 18 \\ -3 \end{pmatrix} + \begin{pmatrix} \frac{16}{7} \\ \frac{6}{7} \end{pmatrix} = \frac{1}{49} \begin{pmatrix} 106 \\ -33 \end{pmatrix} \approx \begin{pmatrix} 2.163 \\ -0.673 \end{pmatrix} ,$$

Error at each step:

$$\epsilon_0 = |x_0 - x^{(exact)}| = \sqrt{(2 - 2.25)^2 + (-1 + 0.5)^2} \approx 0.56$$

$$\epsilon_1 = |x_1 - x^{(exact)}| = \sqrt{(2.571 - 2.25)^2 + (-0.429 + 0.5)^2} \approx 0.33$$

$$\epsilon_2 = |x_2 - x^{(exact)}| = \sqrt{(2.163 - 2.25)^2 + (-0.673 + 0.5)^2} \approx 0.19$$

Observe that $\epsilon_1/\epsilon_0 \approx 0.59$ and $\epsilon_2/\epsilon_1 \approx 0.58$ - which is consistent with the spectral radius calculations.

(d) GS and SOR schemes both require a converging iterative scheme to start with. We shall use the modified Richardson scheme from the previous part.

GS iterations

(For your exam answer, you would need to add more comments)

First iteration: calculate the first component of x_1

$$x_{11} = (-1/7) \cdot 2 + (-4/7) \cdot (-1) + 16/7 = 18/7 \approx 2.571$$

and then use this for calculation of the second component

$$x_{12} = (-4/7) \cdot 2.571 + (1/7) \cdot (-1) + 6/7 \approx -0.755$$

And therefore:

$$x_1 \approx \begin{pmatrix} 2.571 \\ -0.755 \end{pmatrix}, \qquad \epsilon_1 \approx 0.41$$

Proceed with the second iteration in a similar way:

$$x_{21} = (-1/7) \cdot 2.571 + (-4/7) \cdot (-0.755) + 16/7 = 18/7 \approx 2.350$$

$$x_{22} = (-4/7) \cdot 2.350 + (1/7) \cdot (-0.755) + 6/7 \approx -0.629$$

And therefore:

$$x_2 \approx \begin{pmatrix} 2.350 \\ -0.629 \end{pmatrix}, \qquad \epsilon_2 \approx 0.16$$

From the first two iterations, it is not apparent that GS gives you any improvement over the original modified Richardson scheme. But if you carry on with the iterations, you should be able to see that the convergence is better.

SOR iterations

For SOR scheme we need to select the relaxation parameter $1 < \omega < 2$. Let's select $w = 1.5$ and see how it works. Again, I will be using the modified Richardons iteration scheme as the "base" iteration. But you could implement SOR on top of GS in a similar way.

First iteration:

$$x_1^{(SOR)} = \omega x_1^{(R)} + (1 - \omega) x_0 = 1.5 \begin{pmatrix} 2.571 \\ -0.429 \end{pmatrix} - 0.5 \begin{pmatrix} 2 \\ -1 \end{pmatrix} \approx \begin{pmatrix} 2.857 \\ -0.144 \end{pmatrix}$$

The corresponding error is: $\epsilon_1 \approx 0.70$.

Second iteration:

$$x_2^{(R)} = \begin{pmatrix} -\frac{1}{7} & -\frac{4}{7} \\ -\frac{4}{7} & \frac{1}{7} \end{pmatrix} \begin{pmatrix} 2.857 \\ -0.144 \end{pmatrix} + \begin{pmatrix} \frac{16}{7} \\ \frac{6}{7} \end{pmatrix} \approx \begin{pmatrix} 1.960 \\ -0.796 \end{pmatrix},$$

$$x_2^{(SOR)} = \omega x_2^{(R)} + (1 - \omega) x_1 = 1.5 \begin{pmatrix} 1.960 \\ -0.796 \end{pmatrix} - 0.5 \begin{pmatrix} 2.857 \\ -0.144 \end{pmatrix} \approx \begin{pmatrix} 1.512 \\ -1.122 \end{pmatrix}$$

The corresponding error is: $\epsilon_2 \approx 0.97$. Using a large relaxation parameter at the start of iterations is not a very good idea!

3. (a) The secular equation is a 2×2 determinant, which can be expanded to give $(10-\lambda)(2-\lambda)-9=0$. This is a quadratic equation with two solutions; $\lambda = 11$ and $\lambda = 1$. We choose to label these $\lambda_1 = 11$, $\lambda_2 = 1$.

   To find the corresponding eigenvector, we substitute each λ_i into $\mathbf{A}\mathbf{x}_i = \lambda_i \mathbf{x}_i$, then normalise, to get the (orthonormal) eigenvectors shown in the question.

   (b) Using the algorithm provided on the lecture:

   1st iteration:

$$x_2' = \begin{pmatrix} 10 & 3 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 13 \\ 5 \end{pmatrix}$$

   Estimate the eigenvalue:

$$\lambda = x_2' \cdot x_1 = 18$$

   And the eigenvector:

$$x_2 = x_2'/|x_2'| = \frac{1}{\sqrt{194}} \begin{pmatrix} 13 \\ 5 \end{pmatrix} \approx \begin{pmatrix} 0.93 \\ 0.36 \end{pmatrix}$$

   Note: The eigenvalue estimate is still quite far from the true value, but the eigenvector is already very close to the true one... And this is only after one iteration!

   2nd iteration:

$$x_3' = \begin{pmatrix} 10 & 3 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} 0.93 \\ 0.36 \end{pmatrix} = \begin{pmatrix} 10.38 \\ 3.51 \end{pmatrix}$$

   Estimate the eigenvalue:

$$\lambda = x_3' \cdot x_2 \approx 10.92$$

   And the eigenvector:

$$x_3 = x_3'/|x_3'| \approx \begin{pmatrix} 0.95 \\ 0.32 \end{pmatrix}$$

   Note: After two iterations, we are very close to the exact values. Can you see why the convergence is so good in this case?

   (c) Again, we follow the procedure described on the lecture. First we need to find the iteration matrix:

$$\hat{J} = \left(\hat{A} - \lambda_0 \hat{I}\right)^{-1} = \begin{pmatrix} 8 & 3 \\ 3 & 0 \end{pmatrix}^{-1} = \frac{1}{-9} \begin{pmatrix} 0 & -3 \\ -3 & 8 \end{pmatrix} = \begin{pmatrix} 0 & 1/3 \\ 1/3 & -8/9 \end{pmatrix}$$

   Now, proceed with the iterations.

   1st iteration:

$$x_2' = \begin{pmatrix} 0 & 1/3 \\ 1/3 & -8/9 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1/3 \\ -5/9 \end{pmatrix}$$

   Estimate the eigenvalue:

$$\lambda = 2 + \frac{1}{x_2' \cdot x_1} = -2.5$$

And the eigenvector:

$$x_2 = x_2'/|x_2'| \approx \begin{pmatrix} 0.51 \\ -0.86 \end{pmatrix}$$

2nd iteration:

$$x_3' = \begin{pmatrix} 0 & 1/3 \\ 1/3 & -8/9 \end{pmatrix} \begin{pmatrix} 0.51 \\ -0.86 \end{pmatrix} \approx \begin{pmatrix} -0.29 \\ 0.93 \end{pmatrix}$$

Estimate the eigenvalue:

$$\lambda = 2 + \frac{1}{x_3' \cdot x_2} \approx 0.94$$

And the eigenvector:

$$x_3 = x_3'/|x_3'| \approx \begin{pmatrix} -0.29 \\ 0.96 \end{pmatrix}$$

Note: again, after just a couple of iterations, we are very close to the true eigenvalue and eigenvector.

4. (a) We have Dirichlet boundary condition at $t = T/4$, and therefore we should not include this point in the grid (as we know the value of the function at that point!) On the other end, at $t = 0$, we have a Neumann boundary condition, which fixes the derivative, but the function itself is unknown at this point. Hence $t = 0$ should be included in the grid.

   And thus, our N-point grid starts at $t = 0$ (this is $j = 1$ point) and ends at $T/4 - a$ (this is $j = N$ point). It is easy to see that $a = T/(4a)$ in this case.

   Using CDA approximation for the second derivative, for a generic point away from any boundaries, we have:

$$(x_{j+1} + x_{j-1} - 2x_j) + a^2\omega_0^2 x_j + a^2 x_j^3 = 0$$

   For $j = 1$ the above equation requires the value of $x_{j-1} = x_0$ (corresponding to $t = -a$), which does not exist in our grid. We should apply the Neumann boundary condition:

$$\frac{dx}{dt}(t = 0) = 0 \qquad => \qquad \frac{x_2 - x_0}{2a} = 0 \qquad => \qquad x_0 = x_2$$

   Hence for $j = 1$:

$$2\,(x_2 - x_1) + a^2\omega_0^2 x_1 + a^2 x_1^3 = 0$$

   For $j = N$ the generic equation requires the value of $x_{j+1} = x_{N+1}$ (corresponding to $t = T/4$), which does not exist in our grid. But it is fixed by the Dirichlet condition: $x(t = T/4) = 0$. Hence for $j = N$ the equation is:

$$(x_{N-1} - 2x_N) + a^2\omega_0^2 x_N + a^2 x_N^3 = 0$$

   (b) Here we deal with a set of **nonlinear** equations (because of the x_j^3 term), hence linear algebra tools are not applicable in this case. The equations can be solved by iterations, e.g. using Newton-Raphson iterations. See the lecture slides for a similar example and details.

Optional Extra-Curricular activities

1. From the question we know that, for some value of θ the following is true:

$$\mathbf{S}^{-1}\mathbf{A}\mathbf{S} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} 10 & 3 \\ 3 & 2 \end{pmatrix} \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} = \mathbf{A}' = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix}.$$

Multiplying out the matrices gives

$$\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} = \begin{pmatrix} 2 + 8\cos^2\theta + 6\sin\theta\cos\theta & 3(\cos^2\theta - \sin^2\theta) - 8\sin\theta\cos\theta \\ 3(\cos^2\theta - \sin^2\theta) - 8\sin\theta\cos\theta & 2 + 8\sin^2\theta - 6\sin\theta\cos\theta \end{pmatrix}.$$

We can find θ from either of the off-diagonal elements. Using the trig identities $\cos^2\theta - \sin^2\theta = \cos 2\theta$, and $2\sin\theta\cos\theta = \sin 2\theta$, the off-diagonal elements are telling us that $3\cos 2\theta = 4\sin 2\theta$. If we wished we could solve this equation for $\theta = \tan^{-1}(\frac{3}{4})$, but we don't need to. 2θ is the angle of a "'345" right-angled triangle with adjacent 4, opposite 3 and hypoteneuse 5. This means $\cos 2\theta = \frac{4}{5}$ and $\sin 2\theta = \frac{3}{5}$, which is all we need. Armed with the extra identities $2\cos^2\theta = 1 + \cos 2\theta$ and $2\sin^2\theta = 1 - \cos 2\theta$, we can calculate the eigenvalues:

$$\lambda_1 = 2 + 8\cos^2\theta + 6\sin\theta\cos\theta = 2 + 4(1 + \frac{4}{5}) + 3\frac{3}{5} = 11$$

and

$$\lambda_2 = 2 + 8\sin^2\theta - 6\sin\theta\cos\theta = 2 + 4(1 - \frac{4}{5}) - 3\frac{3}{5} = 1.$$

We can read the eigenvectors of $\mathbf{A}$ from the columns of $\mathbf{S} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$, for which will need to know $\cos\theta$ and $\sin\theta$. Note that $2\cos^2\theta = 1 + \cos 2\theta = \frac{9}{5}$, so $\cos\theta = \frac{3}{\sqrt{10}}$. Then $\sin\theta = \frac{1}{\sqrt{10}}$ and

$$\mathbf{S} = \frac{1}{\sqrt{10}} \begin{pmatrix} 3 & -1 \\ 1 & 3 \end{pmatrix} \to \mathbf{x}_1 = \frac{1}{\sqrt{10}} \begin{pmatrix} 3 \\ 1 \end{pmatrix}; \quad \mathbf{x}_2 = \frac{1}{\sqrt{10}} \begin{pmatrix} -1 \\ 3 \end{pmatrix}.$$

[To show that $\mathbf{S}$ has the form it does, first let $\mathbf{S} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$, where all the entries are real. Since $\mathbf{S}^{-1} = \mathbf{S}^T$, we can write

$$\begin{pmatrix} a & c \\ b & d \end{pmatrix} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}.$$

This can only be true if $a = d$, $b = -c$, and $ad - bc$ $(= |\mathbf{S}|) = 1$. We therefore have that $\mathbf{S} = \begin{pmatrix} a & b \\ -b & a \end{pmatrix}$, with $|\mathbf{S}| = a^2 + b^2 = 1$. The natural parameterisation that satifies these conditions uses an angle. If, for example we let $a = \cos\theta$; then $a^2 + b^2 = 1$ means $b = \sin\theta$, and we have the form shown.]