Problem Sheet 3 – Computational Tools

1. Use **LU** decomposition to solve the simultaneous equations

$$\begin{pmatrix} 4 & 1 & 1 \\ 1 & 2 & 3 \\ 1 & 3 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 7 \\ 8 \\ 8 \end{pmatrix}; \qquad \begin{pmatrix} 1 & 3 & 1 \\ 3 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 5 \\ 3 \end{pmatrix}.$$

2. This question is all about solving the matrix equation:

$$\begin{pmatrix} 4 & 2 \\ 2 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 8 \\ 3 \end{pmatrix}$$

using relaxation schemes. I have deliberately chosen the same example I solved on the lectures by exact methods, to give $x_1 = 2.25, x_2 = -0.5$

(a) Write down the Richardson iteration matrix $\mathbf{J}$ for this problem. Perform two iterations of the basic Richardson scheme by hand, for the starting guess $x_1^{(0)} = 2, x_2^{(0)} = -1$.

(b) Calculate the eigenvalues of $\mathbf{J}$ and use them to explain why the scheme in (a) failed.

(c) Use the fact that $(\mathbf{A}/a)\mathbf{x} = \mathbf{b}/a$ to define a modified Richardson matrix. Show that the eigenvalues of this matrix are

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

Hence find the value of a for which the modified Richardson scheme will converge most rapidly, and estimate the rate of convergence. Repeat the two iterations [from the same starting guess] of part (a) using your optimal iteration matrix. Calculate the residual error $\epsilon = |\mathbf{x} - \mathbf{x}^{(\mathbf{exact})}|$ at each step (using the known exact solution).

(d) Outline briefly how the Gauss-Seidel method, and Successive Over-Relaxation (SOR) may be used to improve the convergence rate of the modified Richardson iteration scheme. Apply each of these methods to the problem here, using the same starting guess as before, and performing at least 2 iterations in each case. Calculate the residual error at each iteration. Comment on your answers.

3. This question is all about finding the eigenvalues and eigenvectors of the matrix

$$\mathbf{A} = \begin{pmatrix} 10 & 3 \\ 3 & 2 \end{pmatrix}.$$

(a) First a bit of maths. Solve the secular equation $|\mathbf{A} - \lambda\mathbf{I}| = 0$ to show that the eigenvalues of $\mathbf{A}$ are $\lambda_1 = 11$, $\lambda_2 = 1$. Use these to show that the corresponding eigenvectors are

$$\mathbf{x}_1 = \frac{1}{\sqrt{10}}\begin{pmatrix} 3 \\ 1 \end{pmatrix} \approx \begin{pmatrix} 0.95 \\ 0.32 \end{pmatrix}; \qquad \mathbf{x}_2 = \frac{1}{\sqrt{10}}\begin{pmatrix} -1 \\ 3 \end{pmatrix} \approx \begin{pmatrix} -0.32 \\ 0.95 \end{pmatrix}.$$

(b) Now try to find the largest by modulus eigenvalue ($\lambda_1 = 11$) and the corresponding eigenvector by the power method. Start with the initial guess

$$x_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

and make two iterations. At each iteration calculate the estimated eigenvalue. Compare your results with the exact analytical result in part (a).

(c) Finally, try to find the second eigenvalue ($\lambda_2 = 1$) by the power method (inverse iterations), as the closest eigenvalue to $\lambda_0 = 2$. Use the same initial guess as in part (b), and make two iterations.

4. This question is about numerical calculation of periodic solutions of the nonlinear oscillator equation:

$$\frac{d^2x}{dt^2} + \omega_0^2 x + x^3 = 0$$

(this is the so-called Duffing oscillator equation).

To find a periodic solution with period T, $x(t+T) = x(t)$, you can solve the above equation as a Boundary Value Problem with the following boundary conditions:

$$\frac{dx}{dt}(t=0) = 0 \,, \qquad x(T/4) = 0$$

(a) Discretize the equation on the interval $(0, T/4)$ using N-point grid, applying the boundary conditions. What is the value of the time step a? What values of t your first grid point ($j = 1$) and your last grid point ($j = N$) correspond to? Write down the resulting equations for: (i) a generic grid point j, away from any boundaries; (ii) the first grid point $j = 1$; (iii) the last grid point $j = N$.

(b) Explain why the problem you formulated in part (a) cannot be solved by linear algebra methods. Suggest a suitable numerical method to solve this problem. Outline briefly how it works, and what do you need to set it up and run on a computer.

Optional Extra-Curricular activities

1. The common method of finding all eigenvalues and eigenvectors of a matrix is via diagonalization. Consider the eigen-value problem discussed in Q3. To diagonalise $\mathbf{A}$ computationally, a similarity transformation matrix $\mathbf{S}$ is found, such that $\mathbf{A}' = \mathbf{S}^{-1}\mathbf{A}\mathbf{S}$ becomes diagonal. This is usually done by using row transformations to nudge $\mathbf{A}$ toward diagonal form. Here we will do the job in one go. Since $\mathbf{A}$ is real symmetric, we must have $\mathbf{S}^{-1} = \mathbf{S}^T$, the transpose of $\mathbf{S}$. A 2×2 matrix satisfying this constraint is

$$\mathbf{S} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix},$$

which you might recognise as the transformation matrix for rotation by the angle θ about the origin. (You might like to show that this is the natural way to write down a matrix whose transpose is its inverse, starting from a general 2×2 real matrix.) Use this matrix to derive an expression for $\mathbf{A}'$ for the particular $\mathbf{A}$ in this question. Find the value of θ which makes $\mathbf{A}'$ diagonal. Hence find the eigenvalues of $\mathbf{A}$. (You should be able to express all your terms using double angle formulae; you may find sketching a "345" right-angled triangle will help too. In particular, in a '345' right-angle triangle with adjacent 4, opposite 3 and hypotenuse 5, you have $\cos(\alpha) = 4/5$ and $\sin(\alpha) = 3/5$.) Finally, use $\mathbf{S}$ to find the eigenvectors of $\mathbf{A}$.

2. Investigate the problem in Q4 numerically. For this:

   (a) Solve the Duffing equation numerically as the initial value problem, using initial conditions $x(t = 0) = A$, $dx/dt(t = 0) = 0$, where A is a variable amplitude. Use the fourth-order Runge-Kutta method for integration. Integrate over a sufficiently long time interval to observe several oscillations. Observe that the period changes, as you change A. Is there a limit, where you know a solution analytically? How would you test this in your numerical scheme?

   (b) Now you can implement numerically the scheme you suggested in Q4(b), and try to find periodic solutions. Compare your results with the results of your numerical integration in part (a).