MATH3511/6111 Scientific Computing
Semester 1, 2022 — Linda Stals (MSI)

Assignment 5 (MATH3511 non-HPO)
Due date: 9am Monday 23 May (Week 12)

Please show all relevant working and present your solutions clearly: do not expect full marks for a correct answer without working, or where your reasoning is hard to follow.

Question 1 (6 marks)**.** Consider the solution of $A\boldsymbol{x} = \boldsymbol{b}$ where A is symmetric. We are going to study the convergence rate of the Gauss-Seidel method. Recall that we write A in the form $A = D + L + L^T = M + L^T$. ($U = L^T$ as A is symmetric). Furthermore we have the error matrix $E = I - M^{-1}A$ as show on Slide 18 of the Iterative Linear Solvers notes.

Define the quadratic form $Q(\boldsymbol{x})$ as $Q(\boldsymbol{x}) = \boldsymbol{x}^T A\boldsymbol{x}$.

(a) Show that
$$Q(E\boldsymbol{x}) = Q(\boldsymbol{x}) - \boldsymbol{y}^T D\boldsymbol{y},$$
where $\boldsymbol{y} = M^{-1}A\boldsymbol{x}$.

Hint: Firstly show $Q(E\boldsymbol{x}) = \boldsymbol{x}^T A\boldsymbol{x} - \boldsymbol{y}^T A\boldsymbol{x} - \boldsymbol{x}^T A\boldsymbol{y} + \boldsymbol{y}^T A\boldsymbol{y}$ *and then use* $-M - M^T + A = -D$ *to complete the proof.*

(b) Similarly, show that
$$Q(\boldsymbol{e}^{k+1}) = Q(\boldsymbol{e}^k) - (\boldsymbol{y}^k)^T D\boldsymbol{y}^k,$$
where $\boldsymbol{y}^k = M^{-1}A\boldsymbol{e}^k$.

(c) From the previous result deduce that, if A is a nonsingular, symmetric matrix with positive diagonal elements and if the Gauss-Seidel method converges for any $\boldsymbol{x}^k$, then A must be positive definite.

Question 2 (4 marks)**.** Prove that, in the method of steepest descent for solving linear system $A\boldsymbol{y} = \boldsymbol{b}$ with A being symmetric and positive definite, $\boldsymbol{y}_{k+1} - \boldsymbol{y}_k$ and $\boldsymbol{y}_{k+2} - \boldsymbol{y}_{k+1}$ are orthogonal, i.e. $(\boldsymbol{y}_{k+2} - \boldsymbol{y}_{k+1})^T(\boldsymbol{y}_{k+1} - \boldsymbol{y}_k) = 0$ for all $k \geq 0$.

Hint: consider $\boldsymbol{d}_{k+1}^T\boldsymbol{d}_k$.

Question 3 (6 marks)**.** Let $\boldsymbol{x} = [x_0, x_1, \cdots, x_{n-1}]^T$ be a vector of length n whose Discrete Fourier Transformation (DFT) is given by $\hat{\boldsymbol{x}} = [\hat{x}_0, \hat{x}_1, \cdots, \hat{x}_{n-1}]^T$. Consider $\boldsymbol{y} = [y_0, y_1, \cdots, y_{2n-1}]^T$ with $y_k = x_k$ for $0 \leq k \leq n-1$ and $y_k = 0$ for $n \leq k \leq 2n-1$. Show that

$$\hat{y}_k = \begin{cases} \hat{x}_{k/2} & \text{, if } k \text{ is even} \\ \frac{2}{n}\sum_{m=0}^{n-1} \hat{x}_m / (1 - e^{i\frac{\pi(2m-k)}{n}}) & \text{, if } k \text{ is odd} \end{cases}.$$

Question 4 (4 marks)**.** Solve the ordinary differential equation

$$x'(t) = 10x(t) + 11t - 5t^2 - 1,$$

with initial value $x(0) = 0$ and $0 \leq t \leq 3$. Implement the fourth-order Runge-Kutta method with $h = 2^{-8}$ in Python. Plot the numerical solution and the exact solution $t^2/2 - t$. Verify that the solution of the same differential equation with initial value $x(0) = \epsilon$ is $\epsilon e^{10t} + t^2/2 - t$ and thus account for the discrepancy between the numerical and exact solutions of the original problem.