CPSC 542G Assignment 1

Due Thursday, Feb. 15, 2018

1. Given a sufficiently smooth function $f(x)$, consider the approximation to the first derivative
$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}.$$
   (a) Using Taylor expansions, show that this is a valid approximation, with a truncation error of $\mathcal{O}(h^2)$.
   (b) Derive a bound on the total computational error (truncation and rounding combined) and find the value for h for which the bound is minimized.
   (c) Generate a graph similar to Figure 1.3 in the book, for $f(x_0) = \sin(x_0)$ for $x = 1.2$. Explain the reasons for the difference between the results for the approximation in this question and Figure 1.3.

2. Consider the following equation, defined for $x > 0$:
$$x + \ln x = 0 \ .$$
   (a) Show analytically that there is exactly one root, $0 < x^* < \infty$.
   (b) Plot a graph of the function on the interval $[0.1, 1]$.
   (c) As you can see from the graph, the root is between 0.5 and 0.6. Write MATLAB routines for finding the root, using
      i. the bisection method, with the initial interval $[0.5, 0.6]$. Explain why this choice of the initial interval is valid.
      ii. a linearly convergent fixed point iteration, with $x_0 = 0.5$. Show that the conditions of the fixed point theorem (for the function you selected) are satisfied.
      iii. Newton's method, with $x_0 = 0.5$.
      iv. the secant method, with $x_{-1} = 0.5$ and $x_0 = 0.6$.

   For each of the methods:

   - Use $|x_k - x_{k-1}| < 10^{-10}$ as a convergence criterion.
   - Print out the iterates and show the progress in the number of correct decimal digits throughout the iteration.

- Explain the convergence behavior and how it matches theoretical expectations.

3. The function

$$f(x) = \alpha \cosh(x/4) - x$$

has two roots for $\alpha = 2$ and none for $\alpha = 10$. Is there an α for which there is precisely one root? If yes then find such an α and the corresponding root; if not then justify.

4. Use Newton's method to solve a discretized version of the differential equation

$$y'' = -(y')^2 - y + \ln x, \quad 1 \le x \le 2, \quad y(1) = 0, \quad y(2) = \ln 2.$$

The discretization on a uniform mesh can be

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \left(\frac{y_{i+1} - y_{i-1}}{2h}\right)^2 + y_i = \ln(1 + ih), \qquad i = 1, 2, \ldots, n.$$

The actual solution of this problem is $y(x) = \ln x$. Compare your numerical results to the solution $y(x)$ for $n = 8,\ 16,\ 32$ and 64. Make observations regarding the convergence behavior of Newton's method in terms of the iterations and the mesh size, as well as the solution error.

5. Consider the nonlinear problem

$$-(u_{xx} + u_{yy}) - e^u = 0,$$

defined in the unit square with homogenous Dirichlet boundary conditions. This problem has two solutions.

   (a) Using a discretization on a uniform grid with step size $h = 2^{-7}$, find approximations for the two solution functions. Use Newton's method with appropriate initial guesses and solve the resulting linear system directly (i.e., using `backslash`). Denote by n the number of unknowns. Plot the two solutions and display their scaled norms $\|\mathbf{u}\|_2/\sqrt{n}$ as well as $\|\exp(\mathbf{u})\|_\infty$. How many iterations does it take Newton's method to converge?

   (b) Repeat the process, this time using an appropriate Krylov subspace method of your choice for solving the linear system.

6. The $n \times n$ matrix A is said to be in *Hessenberg* or *upper Hessenberg* form if all its elements below the first sub-diagonal are zero, so that

$$a_{ij} = 0, \quad i > j + 1.$$

Consider the LU decomposition of an upper Hessenberg matrix, assuming that no pivoting is needed: $A = LU$.

(a) Provide an efficient algorithm for this LU decomposition (do not worry about questions of memory access and vectorization).

(b) What is the sparsity structure of the resulting matrix L (i.e., where are its nonzeros)?

(c) How many operations (to a leading order) does it take to solve a linear system $A\mathbf{x} = \mathbf{b}$ where A is upper Hessenberg?

(d) Suppose now that partial pivoting is applied. What are the sparsity patterns of the factors of A?

7. Consider the Helmholtz equation

$$-(u_{xx} + u_{yy}) - \omega^2 u = g(x, y),$$

defined in the unit square with homogenous Dirichlet boundary conditions.

(a) Suppose this problem is discretized on a uniform grid with step size $h = 1/(N+1)$ using a 5-point scheme as in Example 7.1 of the book plus an additional term. Write down the resulting difference method.

(b) Call the resulting matrix A. Find a value ω_c such that for $\omega^2 < \omega_c^2$ and h arbitrarily small, A is still positive definite, but for $\omega^2 > \omega_c^2$ the positive definiteness is lost.

(c) Solve the problem for $\omega = 1$ and $\omega = 10$ for $N = 2^7 - 1$ using an appropriate preconditioned Krylov subspace method of your choice, or a multigrid method. Use `tol` = 1.e-6. Verify that the last residual norm is below `tol` and tell us how many iterations it took to get there.