problem sheet 12

discussion: week of Monday, 15.1.2020

12.1. The *secant method* (i.e., Broyden's method in 1D) to find the zero x^* of $F(x) = 0$ is defined as follows given initial points x_0, x_1:

$$x_{n+1} = x_n - \frac{x_n - x_{n-1}}{F(x_n) - F(x_{n-1})} F(x_n), \qquad n = 1, 2, \ldots$$

(If $F(x_n) = F(x_{n-1})$ the difference quotient is formally replaced with $F'(x_n)$.) Sei nun $F(x) = 2 - x^2 - e^x$.

1. Compute, using Newton's method the positive zero x^* of F to machine precision.
2. Compute the zero x^* with the secant method. Set $x_1 = x_0 - \frac{F(x_0)}{F'(x_0)}$. Plot for $n \in \{1, \ldots, 8\}$ and $x_0 = 2.5$ the error $|x^* - x_n|$ versus the step number n. Also plot the *numerical convergence order* $p_n = \log(|x^* - x_{n+1}|)/\log(|x^* - x_n|)$ versus n. What convergence order do you observe?
3. Compare the *efficiency* of the secant method with that of the Newton method by comparing accuracy versus number of function evaluations. To that end, assume that a Newton step costs 3 function evaluations (this is realistic assuming that F' is approximated with a difference quotient) and plot achieved accuracy versus number of function evaluations. Which method is more efficient?

12.2. (Gerschgorin theorem) Let $\mathbf{A} \in \mathbb{C}^{n \times n}$. Show: for every eigenvalue λ of $\mathbf{A}$ there is an i such that $|\lambda - \mathbf{A}_{ii}| \leq \sum_{j \neq i} |\mathbf{A}_{ij}|$. Put differently: the spectrum of $\mathbf{A}$ is contained in the closed circles with centers $\mathbf{A}_{ii}$ and radii $r_i = \sum_{j \neq i} |\mathbf{A}_{ij}|$. *Hint:* Let $\mathbf{x}$ be eigenvector for λ. Consider i such that $|\mathbf{x}_i| \geq |\mathbf{x}_j|$.

12.3. Consider symmetric matrices.

a) How expensive is to bring a *symmetric* matrix to Hessenberg form? How expensive is then each QR-step?

12.4. **a)** Program the basic QR-method (i.e., without shift). Input is the matrix $\mathbf{A}$ and the number ℓ_{max} of QR-steps to be done. Output are the ℓ_{max} diagonals of the matrices of the QR method (i.e., the approximations to the eigenvalues).

b) Program the QR-method with the so-called Wilkinson shift and deflation. Input is the matrix $\mathbf{A}$. Output is the list of (approximate) eigenvalues as well as the number of QR steps needed. The Wilkinson shift μ is defined as follows: Let λ_1, λ_2 be the 2×2 matrix $\mathbf{A}([n-1; n], [n-1 : n])$ and $\mu \in \{\lambda_1, \lambda_2\}$ is the eigenvalue that closest to $\mathbf{A}(n, n)$. In `matlab`, you may use the routines `eig` (to compute the eigenvalues of 2×2 matrices), `qr` (to compute QR-factorizations), and `hess` to obtain a Hessenberg matrix. The criterion to determine whether deflation is possible is $|\mathbf{A}(n-1, n)| \leq \varepsilon \left[|\mathbf{A}(n-1, n)| + |\mathbf{A}(n, n)|\right]$ with $\varepsilon = 10^{-14}$.

c) Define the tridiagonal matrices

$$\mathbf{A}^{(n)} = a = \mathtt{diag}(2 * \mathtt{ones}(n, 1), 0) - \mathtt{diag}(\mathtt{ones}(n-1, 1), -1) - \mathtt{diag}(\mathtt{ones}(n-1, 1), 1);$$

with $n = 2^j$, $j = 2, \ldots, 10$. Consider the QR-method without shift. Plot the maximal error of the eigenvalues versus the iteration number ℓ for $n = 2^3$ and $n = 2^5$. What do you observe? *Hint:* you may use `eig` to compute the exact eigenvalues.

d) For the above matrices $\mathbf{A}^{(n)}$, plot (use `loglog`) the number of QR-steps needed versus the problem size n. What do you observe?