Scientific Computation Comprehensive Examination Practice Questions

Answer the following questions explaining all steps that lead to a solution. Partial credit will be awarded for presenting a viable solution strategy. No credit will be given to computations presented without motivation. Your goal is to present skill in formulating precise mahtematical statements, and demonstrate understanding of theoretical material.

1. State the conditions on $g(x)$ that ensure third-order convergence to the root r of the equation $f(x)=0$ for the sequence defined by $x_{n+1}=F(x_n)$, $F(x)=x+f(x)g(x)$.

   SOLUTION. At $x=r$, $f(r)=0$, $F(r)=r$, hence r is a fixed point of F. Express error $e_{n+1}=x_{n+1}-r$ in terms of $e_n=x_n-r$, using Taylor series

$$e_{n+1}=F(x_n)-F(r)=F(r)+F'(r)e_n+\frac{1}{2}F''(r)e_n^2+\frac{1}{6}F'''(r)e_n^3-F(r)+\mathcal{O}(e_n^4),$$

   assuming $F\in C^3$ over interval containing all iterates $\{x_n\}_{n\in\mathbb{N}}$. Third-order, $e_{n+1}=\mathcal{O}(e_n^3)$, convergence is achieved if

$$F'(r)=1+f'(r)g(r)+f(r)g'(r)=0\Rightarrow g(r)=-1/f'(r), \text{and}$$

$$F''(r)=f''(r)g(r)+2f'(r)g'(r)+f(r)g''(r)=0\Rightarrow g'(r)=\frac{1}{2}\frac{f''(r)}{[f'(r)]^2}.$$

2. State an algorithm that requires $\mathcal{O}(n^2)$ operations to compute the QR decomposition of $\boldsymbol{A}=\boldsymbol{R}+\boldsymbol{u}\boldsymbol{v}^T$, with R an upper triangular matrix.

   SOLUTION. The triangular matrix $\boldsymbol{R}$ has QR factorization $\boldsymbol{R}=\boldsymbol{I}\boldsymbol{R}$, and is modified by a rank-1 update $\boldsymbol{u}\boldsymbol{v}^T=(\ v_1\boldsymbol{u}\ \ v_2\boldsymbol{u}\ \ \ldots\ \ v_n\boldsymbol{u}\ )$. Write $\boldsymbol{A}=\boldsymbol{I}(\boldsymbol{R}+\boldsymbol{u}\boldsymbol{v}^T)=\boldsymbol{Q}_1\boldsymbol{R}_1$, and let $\boldsymbol{H}$ be an orthogonal matrix that transforms $\boldsymbol{u}$ into $\boldsymbol{e}_1$. $\boldsymbol{H}\boldsymbol{u}=\|u\|\boldsymbol{e}_1$. Compute

$$\boldsymbol{H}\boldsymbol{A}=\boldsymbol{H}\boldsymbol{R}+\|\boldsymbol{u}\|\,\boldsymbol{e}_1\boldsymbol{v}^T.$$

   Recall that Givens rotations are the preferred orthogonal transformation matrices used to preserve existing structure in a matrix. Construct $\boldsymbol{H}$ as a succession of Givens rotations to preserve as much of the structure of $\boldsymbol{R}$ as possible

$$\boldsymbol{H}=\boldsymbol{G}_1\ldots\boldsymbol{G}_{n-1}$$

$$\boldsymbol{G}_{n-k}=\begin{pmatrix} \boldsymbol{I}_{n-1-k} & & & \\ & \cos\theta_{n-k} & \sin\theta_{n-k} & \\ & -\sin\theta_{n-k} & \cos\theta_{n-k} & \\ & & & \boldsymbol{I}_{k-1} \end{pmatrix}, k=1,\ldots,n-1$$

$$\boldsymbol{w}^{(0)}=\boldsymbol{u}, \boldsymbol{w}^{(k)}=\boldsymbol{G}_{n-k}\ldots\boldsymbol{G}_{n-1}\boldsymbol{u}, k=1,2,\ldots,n-1$$

$$-\sin\theta_{n-k}\,w_{n-k}^{(k-1)}+\cos\theta_{n-k}\,w_{n-k+1}^{(k-1)}=0\Rightarrow\tan\theta_{n-k}=\frac{w_{n-k+1}^{(k-1)}}{w_{n-k}^{(k-1)}},$$

with operation count $\mathcal{O}(n^2)$.

The matrix $\boldsymbol{H}\boldsymbol{R}$ is Hessenberg, and $\|\boldsymbol{u}\|\,\boldsymbol{e}_1\boldsymbol{v}^T$ is zero except for the first row, hence $\boldsymbol{H}\boldsymbol{A}=\boldsymbol{H}\boldsymbol{R}+\|\boldsymbol{u}\|\,\boldsymbol{e}_1\boldsymbol{v}^T$ is Hessenberg. Use Givens rotations to reduce $\boldsymbol{H}\boldsymbol{A}$ to upper triangular form

$$\boldsymbol{G}_{n-1}'\ldots\boldsymbol{G}_1'\boldsymbol{H}\boldsymbol{A}=\boldsymbol{R}\Rightarrow\boldsymbol{A}=\boldsymbol{H}^T\boldsymbol{G}_1'^T\ldots\boldsymbol{G}_{n-1}'^T\boldsymbol{R}=\boldsymbol{Q}_1\,\boldsymbol{R}_1,$$

again with operation count $\mathcal{O}(n^2)$.

3.

a) Determine the order of convergence of the sequence

$$S_n=\frac{1}{2}\sum_{j=0}^{n-1}(f_j+f_{j+1})(g_{j+1}-g_j), \tag{1}$$

to the integral

$$I(f,g)=\int_0^1 f(x)\,g'(x)\,\mathrm{d}x,$$

with $h=1/n$, $n\in\mathbb{N}$, $f_j\equiv f(jh)$, $g_j\equiv g(jh)$.

SOLUTION. With $x_j=jh$, $x=(j+\xi)h$, $\mathrm{d}x=h\,\mathrm{d}\xi$ use Taylor series expansion on $[x_j,x_{j+1}]$ to evaluate.

$$I_j=\int_{jh}^{(j+1)h} f(x)\,g'(x)\,\mathrm{d}x=h\int_0^1 f(jh+\xi h)\,g'(jh+\xi h)\,\mathrm{d}\xi=$$
$$h\int_0^1\left[f_j+\xi h f_j'+\frac{1}{2}(\xi h)^2 f_j''+\mathcal{O}(h^3)\right]\left[g_j'+\xi h g_j''+\frac{1}{2}(\xi h)^2 g_j'''+\mathcal{O}(h^3)\right]\mathrm{d}\xi=$$
$$f_j g_j' h+\frac{1}{2}(f_j'g_j'+f_jg_j'')h^2+\frac{1}{3}\left(\frac{1}{2}f_j''g_j'+f_j'g_j''+\frac{1}{2}f_jg_j'''\right)h^3+\mathcal{O}(h^4).$$

(note: powers of h equal sum of differentiation order are a useful check).

Taylor series expand the approximation over $[x_j,x_{j+1}]$

$$Q_j=\frac{1}{2}(f_j+f_{j+1})(g_{j+1}-g_j)=\frac{1}{2}\left(2f_j+f_j'h+f_j''\frac{h^2}{2}+\mathcal{O}(h^3)\right)\left(g_j'h+g_j''\frac{h^2}{2}+\mathcal{O}(h^3)\right)$$
$$=f_j g_j' h+\frac{1}{2}(f_j'g_j'+f_jg_j'')h^2+\frac{1}{2}\left(\frac{1}{3}f_jg_j'''+\frac{1}{2}f_j'g_j''+\frac{1}{2}f_j''g_j'\right)h^3+\mathcal{O}(h^4).$$

The error is

$$e_j=Q_j-I_j=\mathcal{O}(h^3),$$

and the error over the entire interval is $e=Q-I\leqslant n\max_{0\leqslant j\leqslant n-1}|e_j|=\mathcal{O}(h^2)$

b) Use quadrature rule (1) to provide approximation S_2 of

$$J=\int_0^1\frac{e^x}{\sqrt{1-x^2}}\,\mathrm{d}x,$$

and estimate the error $e_2 = |S_2 - J|$.

Solution. From (a) identify: $f(x) = e^x$, $g(x) = \arcsin(x)$. Compute

$$S_1 = \frac{1}{2}(f_0 + f_1)(g_1 - g_0) = \frac{1}{2}(1+e)\left(\frac{\pi}{2} - 0\right) = \frac{\pi}{4}(1+e)$$

$$S_2 = \frac{1}{2}[(f_0 + f_1)(g_1 - g_0) + (f_1 + f_2)(g_2 - g_2)] = \frac{1}{2}\left[(1+\sqrt{e})\frac{\pi}{6} + (\sqrt{e} + e)\frac{\pi}{3}\right] \Rightarrow$$

$$S_2 = \frac{\pi}{12}(1+\sqrt{e})(1+2\sqrt{e}).$$

Assume $S_1 = J + Ah_1^3 = J + A$, $S_2 = J + Ah_2^3 = J + A/8$, and find

$$A \cong \frac{8}{7}(S_1 - S_2) \Rightarrow e_2 \cong \frac{1}{7}(S_1 - S_2)$$