1 MATH661 - Homeworks 7 and 8 (combined)

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The final homework of the course is meant to aid in final examination preparation. You are asked to carefully read the following solutions to problems representative of those you can expect on the final. (honor system grading applied, 8 course grade points awarded *ex officio*). ror the final 8 homework grade points choose any 4 problems from the Mathematics Department Scientific Computation Comprehensive examination (http://math.unc.edu/for-grad-students/past-exams) and present solutions.

1.1 Final examination preparation

1. Newton's method for solving the nonlinear equation $f(x)=0$, $f\colon \mathbb{R}\to\mathbb{R}$, $f\in C^2(\mathbb{R})$ is obtained from a linear Hermite approximant based upon the data x_n, $f_n=f(x_n)$, $f_n'=f'(x_n)$. Generalize the approach to a quadratic Hermite approximant based upon data x_n, f_n, f_n', $f_n''=f''(x_n)$.

   Solution. From a Taylor series, the approximant is

$$g(x)=f_n+s\,f_n'+\frac{s^2}{2}f_n''$$

   with $s=x-x_n$. Setting $g(x_{n+1})=0$ gives roots

$$s_{1,2}=\frac{-f_n'\pm\sqrt{(f_n')^2-2f_n''f_n}}{f_n''},$$

   leading to

$$x_{n+1}^{(1,2)}=x_n-\frac{f_n'}{f_n''}\left[1\mp\sqrt{1-2\frac{f_nf_n''}{(f_n')^2}}\right].$$

   The method should revert to the Newton iteration

$$x_{n+1}=x_n-\frac{f_n}{f_n'}$$

   when $f_n''=0$, which implies choice of the following root

$$x_{n+1}=x_n-\frac{f_n'}{f_n''}\left[1-\sqrt{1-2\frac{f_n''}{f_n'}\cdot\frac{f_n}{f_n'}}\right],$$

   such that

$$\lim_{a\to 0}\frac{1}{a}\left(1-\sqrt{1-2\frac{a\,f_n}{(f_n')^2}}\right)=\lim_{a\to 0}\frac{1-\left(1-\frac{a\,f_n}{(f_n')^2}+\mathcal{O}(a^2)\right)}{a}=\frac{f_n}{(f_n')^2}.$$

2. Consider the algorithm of successive parabolas

$$x_{n+1}=x_n-\frac{f_n'}{f_n''}\left[1-\sqrt{1-2\frac{f_n''}{f_n'}\cdot\frac{f_n}{f_n'}}\right],$$

to solve the nonlinear equation $f(x)=0$, $f\in C^2(\mathbb{R})$. Determine the order of convergence of the method.

Solution. The algorithm can be written as the simple iteration

$$x=G(x), G(x)=x-\frac{f'}{f''}\left[1-\sqrt{1-2\frac{f}{f'}\cdot\frac{f''}{f'}}\right],$$

and the root r, the value for which $f(x)=0$ is a fixed point of the iteration, $r=G(r)$

Error analysis: Introduce error $e_{n+1}=x_{n+1}-r$ and compute

$$e_{n+1}=G(x_n)-G(r)=G'(r)e_n+\frac{1}{2}G''(r)e_n^2+\frac{1}{6}G'''(r)e_n^3+\ldots$$

If $G^{(q-1)}(r)=0$, $G^{(q)}(r)\neq 0$, the method is of order q since $e_{n+1}=\mathcal{O}(e_n^q)$. Computation of derivatives is aided by intermediate notation. Let $u(x)=f(x)/f'(x)$, $v(x)=f'(x)/f''(x)$, $w(x)=f''(x)/f'''(x)$, with

$$u'=\frac{(f')^2-ff''}{(f')^2}=1-\frac{u}{v}$$

$$v'=\frac{(f'')^2-f'f'''}{(f'')^2}=1-\frac{f'}{f''}\cdot\frac{f'''}{f''}=1-\frac{v}{w}$$

$$G(x)=x-v\left(1-\sqrt{1-2u/v}\right)$$

Note that $f(r)=0\Rightarrow u(r)=0$ (assuming $f'(r)\neq 0$)

Compute

$$\begin{aligned}G'(x) &= 1-v'\left(1-\sqrt{1-2u/v}\right)-\frac{u'v-uv'}{v\sqrt{1-2u/v}}\\ &= 1-\left(1-\frac{v}{w}\right)\left(1-\sqrt{1-\frac{2u}{v}}\right)-\frac{(v-u)v-u(1-v/w)}{v\sqrt{1-2u/v}}\end{aligned}$$

which becomes at $x=r$ (where $u(r)=0$)

$$G'(r)=1-u'=1-\left(1-\frac{u}{v}\right)=0,$$

so the algorithm is at least second order, $e_{n+1}=\mathcal{O}(e_n^2)$ if $v\neq 0, w\neq 0\Leftrightarrow f'(r)\neq 0, f''(r)\neq 0$. Compute $G''(r)$ (simplify computations by setting $u(r)=0$ as soon as it appears) to obtain

$$G''(r)=-\frac{(u')^2}{v}-u''=-\frac{1}{v}\left(1-\frac{u}{v}\right)^2+\frac{u'v-uv'}{v^2}=-\frac{1}{v}+\left(1-\frac{u}{v}\right)\frac{1}{v}=0,$$

so the method is at least third order.

3. Determine the order of convergence of Newton's method to find a root of $f(x)=0$ at a multiple root.

   Solution. Simplify computations by choosing origin such that the multiple root is $r=0$, and $(p>1)$, $f(x)=x^p g(x)$, $g(0)\neq 0$. Newton's method written as a simple iteration is

$$x_{n+1}=G(x_n), G(x)=x-\frac{f(x)}{f'(x)}=x-\frac{x^p g(x)}{px^{p-1}g(x)+x^p g'(x)}=x-\frac{xg(x)}{pg(x)+xg'(x)}.$$

The error $e_{n+1} = x_{n+1} - r$ is related to error $e_n = x_n - r$ by

$$e_{n+1} = G(x_n) - G(r) = G'(0)e_n + \mathcal{O}(e_n^2).$$

Compute

$$G'(x) = 1 - \frac{(g + xg')(pg + xg') - xg\,(pg' + g' + xg'')}{(pg + xg')^2}$$

Note that as $x \to 0$

$$G'(0) = 1 - \lim_{x \to 0} \frac{pg^2}{(pg)^2} = 1 - \frac{1}{p} \neq 0, \text{for } p > 1,$$

so Newton's method is at best first-order convergent at a multiple root, if $|G'(x)| < 1$ in a neighborhood of r.

4. Consider the nonlinear system

$$x^2 + y^2 = 218$$

$$x^3 + y^3 = 2540$$

Refine the initial approximation $(x_0, y_0) = (5, 10)$ by carrying out a Newton iteration.

Solution. The system can be written as $F(X) = 0$ with

$$X = \left(\begin{array}{c} x \\ y \end{array}\right), F(X) = \left(\begin{array}{c} x^2 + y^2 - 218 \\ x^3 + y^3 - 2540 \end{array}\right)$$

and Newton's iteration can is

$$F'(X_n)(X_{n+1} - X_n) = -F(X_n)$$

with the Jacobian

$$F'(X) = \left(\begin{array}{cc} 2x & 2y \\ 3x^2 & 3y^2 \end{array}\right).$$

Carry out Newton iteration $F'(X_0)(X_1 - X_0) = -F(X_0)$

$$\left(\begin{array}{cc} 10 & 20 \\ 75 & 300 \end{array}\right)\Delta X = -\left(\begin{array}{c} -93 \\ -1415 \end{array}\right) = \left(\begin{array}{c} 93 \\ 1415 \end{array}\right)$$

with solution

$$\Delta X = \left(\begin{array}{c} x_1 \\ y_1 \end{array}\right) - \left(\begin{array}{c} x_0 \\ y_0 \end{array}\right) = \left(\begin{array}{c} -4/15 \\ 287/60 \end{array}\right) \Rightarrow \left(\begin{array}{c} x_1 \\ y_1 \end{array}\right) = \left(\begin{array}{c} 71/15 \\ 887/60 \end{array}\right).$$

5. Show that the two-step method

$$y_{n+1} = 2y_{n-1} - y_n + h\left(\frac{5}{2}y_n' + \frac{1}{2}y_{n-1}'\right) \tag{1}$$

for solving the IVP $y' = f(t, y)$ is of order 2, but unstable.

Solution. The method is of the form

$$\sum_{k=0}^{r} \alpha_k\, y_{n+k} = h\sum_{k=0}^{r} \beta_k\, f_{n+k} = h\sum_{k=0}^{r} \beta_k\, y'_{n+k},$$

with $r=2$, $\alpha_2=1$, $\alpha_1=1$, $\alpha_0=-2$, $\beta_2=0$, $\beta_1=5/2$, $\beta_0=1/2$. Taylor series expansion around the point (t_n, y_n) leads to

$$\left(\sum_{k=0}^{r} \alpha_k\right) y(t_n) + h\left(\sum_{k=0}^{r} k\alpha_k\right) y'(t_n) + \ldots + \frac{h^p}{p!}\left(\sum_{k=0}^{r} k^p\,\alpha_k\right) y^{(p)}(t_n) + \ldots =$$

$$h\left(\sum_{k=0}^{r} \beta_k\right) y'(t_n) + h^2\left(\sum_{k=0}^{r} k\beta_k\right) y''(t_n) + \ldots + \frac{h^p}{(p-1)!}\left(\sum_{k=0}^{r} k^{p-1}\,\beta_k\right) y_n^{(p)} + \ldots$$

This of the form

$$c_0 y(t_n) + c_1 h y'(t_n) + c_2 h^2\, y''(t_n) + \ldots + c_p h^p y^{(p)}(t_n) + \ldots = 0,$$

with the coefficient of h^p

$$c_0 = \left(\sum_{k=0}^{r} \alpha_k\right), c_p = \sum_{k=0}^{r}\left(\frac{k^p}{p!}\alpha_k - \frac{k^{p-1}}{(p-1)!}\beta_k\right), p > 1$$

For a method to be of order p we must have $c_0 = c_1 = \ldots = c_p = 0$. For (1)

$$c_0 = \alpha_0 + \alpha_1 + \alpha_2 = -2 + 1 + 1 \checkmark$$

$$c_1 = (\alpha_1 + 2\alpha_2) - (\beta_0 + \beta_1) = (1+2) - \left(\frac{5}{2} + \frac{1}{2}\right) = 0 \checkmark$$

$$c_2 = \frac{1}{2}(\alpha_1 + 4\alpha_2) - (\beta_1) = \frac{1}{2}(1+4) - \frac{5}{2} = 0 \checkmark$$

so the scheme is second order. For the scheme to be stable the roots of the characteristic polynomial $\rho(z) = \sum_{k=0}^{r} \alpha_k\, z^k = z^2 + z - 2$ must be less than 1 in absolute value. This does not hold since $\rho(z)$ has roots $z_1 = 1$, $z_2 = -2$ with $|z_2| > 1$.

6. Derive a method to solve the IVP $y' = f(y)$ based upon a quadratic interpolation of y' at t_{n+1}, t_n, t_{n-1}.

   Solution. Integration from t_{n-1} to t_{n+1} gives

$$\int_{t_{n-1}}^{t_{n+1}} y'(t)\mathrm{d}t = y(t_{n+1}) - y(t_{n-1}) = \int_{t_{n-1}}^{t_{n+1}} f\,\mathrm{d}t$$

   A quadratic interpolation of $y' = f$ based on data $\{(t_{n-1}, f_{n-1}), (t_n, f_n), (t_{n+1}, f_{n+1})\}$ is

$$\tilde{f}(t) = \frac{f_{n+1} - 2f_n + f_{n-1}}{2h^2}(t - t_n)^2 + \frac{f_{n+1} - f_{n-1}}{2h}(t - t_n) + f_n$$

   with integral

$$\int_{t_{n-1}}^{t_{n+1}} \tilde{f}(t)\,\mathrm{d}t = \frac{h}{3}(f_{n+1} + f_n + f_{n-1})$$

giving the algorithm

$$y_{n+1} = y_{n-1} + \frac{h}{3}(f_{n+1} + f_n + f_{n-1})$$

7. Solve the difference equation

$$u_{n+1} = u_n + c^2(u_{n-1} - u_{n-2})$$

$u_0 = 0, u_1 = 1,\ u_2 = 0.$

Solution. Increase indices to $u_{n+3} = u_{n+2} + c(u_{n+1} - u_n)$. The characteristic equation is

$$r^3 - r^2 - cr + c = 0$$

with solutions $r_1 = 1$,$r_{2,3} = \pm c$, and the solution is

$$u_n = a_1 r_1^n + a_2 r_2^n + a_3 r_3^n = a_1 + a_2 c^n + (-1)^n a_3 c^n.$$

Apply initial conditions

$$0 = a_1 + a_2 + a_3$$

$$1 = a_1 + c a_2 - c a_3$$

$$-1 = a_1 + c^2 a_2 + c^2 a_3$$

with solution $a_1 = 0,\ a_2 = 1/(2c),\ a_3 = -1/(2c)$, so the solution is

$$u_n = \frac{c^{n-1}}{2}(1 - (-1)^n).$$

8. Convert the problem

$$y''' + 4y'' + 5y' + 2y = -4\sin t$$

into a system of first-order ODEs and derive the linear system obtained by appyling the backward Euler scheme $Y_{n+1} = Y_n + hF(Y_{n+1})$.

Solution. Introduce $u = y'$, $v = u' = y''$, and obtain the system

$$Y' = \frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} y \\ u \\ v \end{pmatrix} = F(Y) = \begin{pmatrix} u \\ v \\ -4\sin t - 4v - 5u - 2y \end{pmatrix} = A\begin{pmatrix} y \\ u \\ v \end{pmatrix} + b(t)$$

with

$$A = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -2 & -5 & -4 \end{pmatrix}, b(t) = \begin{pmatrix} 0 \\ 0 \\ -4\sin t \end{pmatrix}$$

Applying backward Euler leads to

$$Y_{n+1} = Y_n + hAY_{n+1} + hb(t_{n+1}) \Leftrightarrow (I - hA)Y_{n+1} = Y_n + hb_{n+1}$$

solved by LU factorization of $I - hA$ at beginning of iterations and backsubstitution with rhs $Y_n + hb_{n+1}$ at each iteration.

1.2 Additional questions

Choose from http://math.unc.edu/for-grad-students/past-exams, state year, problem number, 2 points each.