Numerical Analysis for Computing
COT 4501
Spring 2005
Midterm II Solutions

April 21, 2009

1. **[35 points] Newton Error Formula:** Let $f \in C^2(I)$ be given, for some interval $I \subset \mathcal{R}$, with $f(\alpha) = 0$ for some $\alpha \in I$. For a given $x_n \in I$, define

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}.$$

Then there exists a point ξ_n between α and x_n such that

$$(\alpha - x_{n+1}) = -\frac{1}{2}(\alpha - x_n)^2 \frac{f''(\xi_n)}{f'(x_n)}.$$

(a) **[5 points]** If $\xi_n \to \alpha$ and $x_n \to \alpha$ as $n \to \infty$, what does the ratio $R_n = \frac{\alpha - x_{n+1}}{(\alpha - x_n)^2}$ converge to?
The ratio $R_n = \frac{\alpha - x_{n+1}}{(\alpha - x_n)^2}$ converges to $\lim_{n\to\infty} R_n = -\frac{1}{2}\lim_{n\to\infty} \frac{f''(\xi_n)}{f'(x_n)} = -\frac{1}{2}\frac{f''(\alpha)}{f'(\alpha)}$.

(b) **[5 points]** Evaluate R_n (in the limiting case as $n \to \infty$) for $f(x) = 2e^{-\beta x} - 1$.
For $f(x) = 2e^{-\beta x} - 1$, $f'(x) = -2\beta e^{-\beta x}$ and $f''(x) = 2\beta^2 e^{-\beta x}$. Therefore, $\lim_{n\to\infty} R_n = -\frac{1}{2}\frac{f''(\alpha)}{f'(\alpha)} = \frac{\beta}{2}$.

(c) **[10 points]** The Newton Error Formula can be used to approximately "peek ahead" at the solution $f(\alpha) = 0$ when we are getting close to convergence. Imagine that you are executing Newton's method and are at time step n. You think you are somewhat close to the true answer. In order to get a better estimate $\hat{\alpha}(n)$ of the true answer α, you replace ξ_n by x_n in the Newton Error Formula to get an estimate $\hat{\alpha}(n)$. Using this approximation in the above Newton's Error Formula, find a solution for $\hat{\alpha}(n)$ in terms of $x_{n+1}, x_n, f''(x_n)$ and $f'(x_n)$.
You are asked to use the Newton Error Formula $[(\alpha - x_{n+1}) = -\frac{1}{2}(\alpha - x_n)^2 \frac{f''(\xi_n)}{f'(x_n)}]$ to find an approximate value $\hat{\alpha}(n)$ for the true root α by substituting x_n for the unknown ξ_n. Therefore

$$(\hat{\alpha}(n) - x_{n+1}) = -\frac{1}{2}(\hat{\alpha}(n) - x_n)^2 \frac{f''(x_n)}{f'(x_n)}.$$

Define $S_n = -\frac{1}{2}\frac{f''(x_n)}{f'(x_n)}$. Now

$$\begin{aligned}(\hat{\alpha}(n) - x_{n+1}) &= S_n(\hat{\alpha}(n) - x_n)^2 \\ &= S_n(\hat{\alpha}(n)^2 - 2\hat{\alpha}(n)x_n + x_n^2).\end{aligned}$$

Grouping terms, we get

$$S_n\hat{\alpha}(n)^2 - (2S_n x_n + 1)\hat{\alpha}(n) + (S_n x_n^2 + x_{n+1}) = 0.$$

This is a quadratic equation in $\hat{\alpha}(n)$. Solving for $\hat{\alpha}(n)$, we get

$$\begin{aligned}\hat{\alpha}(n) &= \frac{(2S_n x_n + 1) \pm \sqrt{(2S_n x_n + 1)^2 - 4S_n(S_n x_n^2 + x_{n+1})}}{2S_n} \\ &= \frac{(2S_n x_n + 1) \pm \sqrt{4S_n(x_n - x_{n+1}) + 1}}{2S_n}.\end{aligned}$$

Defining $T_n \stackrel{\text{def}}{=} \frac{f(x_n)}{f'(x_n)}$, we can rewrite the Newton update equation as

$$x_n - x_{n+1} = T_n$$

from which we get that

$$\hat{\alpha}(n) = \frac{(2S_n x_n + 1) \pm \sqrt{4S_n T_n + 1}}{2S_n}.$$

It is not clear at this point whether we should take the positive or negative root. It is also not clear whether $4S_nT_n + 1 \geq 0$. If the latter is not true, then the estimate $\hat{\alpha}(n)$ becomes complex which is unacceptable.

(d) **[5 points]** Do you think you can actually use the above method to "peek ahead" at the true solution in an actual application? Discuss.

There are two possible values of $\hat{\alpha}(n)$, one corresponding to the positive root and the other to the negative root. If both roots are real, they can both be tested by evaluating $f(\hat{\alpha}(n))$. If $|f(\hat{\alpha}(n))| < |f(x_{n+1})|$, we can use $\hat{\alpha}(n)$ instead of x_{n+1} and proceed with Newton's method.

(e) **[10 points]** Apply your solution for $\hat{\alpha}(n)$ to determine $|\alpha - \hat{\alpha}(n)|$ for $f(x) = 2e^{-\beta x} - 1$.

For $f(x) = 2e^{-\beta x} - 1$, $S_n = -\frac{1}{2}\frac{f''(x_n)}{f'(x_n)} = \frac{\beta}{2}$ and $T_n = \frac{f(x_n)}{f'(x_n)} = \frac{1-2e^{-\beta x_n}}{2\beta e^{-\beta x_n}}$. From this, we get that $4S_nT_n + 1 = \frac{1-2e^{-\beta x_n}}{e^{-\beta x_n}} + 1 = e^{\beta x_n} - 1 > 0$ provided $\beta x_n > 0$. The estimate $\hat{\alpha}(n)$ is

$$\hat{\alpha}(n) = \frac{\beta x_n + 1 \pm \sqrt{e^{\beta x_n} - 1}}{\beta} = x_n + \frac{1}{\beta} \pm \frac{1}{\beta}\sqrt{e^{\beta x_n} - 1}.$$

It is still unclear which root to take. The true value α corresponds to $f(\alpha) = 0 \Rightarrow 2e^{-\beta\alpha} - 1 = 0 \Rightarrow \alpha = \frac{1}{\beta}\log 2$. The error $|\alpha - \hat{\alpha}(n)| = |\frac{1}{\beta}\log 2 - x_n - \frac{1}{\beta} \mp \frac{1}{\beta}\sqrt{e^{\beta x_n} - 1}|$.

2. **[35 points] Lagrange Interpolation:** Consider the function $f_1(x) = |x|$. Since this function is not

differentiable at the origin, we replace it by $f_2(x) = \sqrt{x^2+\epsilon}$ for $\epsilon > 0$.

(a) **[5 points]** Use the Lagrange interpolation formula to construct a second order approximation $p_2(x)$ of $f_2(x)$ that is exact at $x = -1, 0, 1$.

$$p_2(x) = \sqrt{1+\epsilon}\frac{x(x-1)}{2} + \sqrt{1+\epsilon}\frac{x(x+1)}{2} - \sqrt{\epsilon}(x+1)(x-1) = x^2(\sqrt{1+\epsilon}-\sqrt{\epsilon}) + \sqrt{\epsilon}.$$

(b) **[5 points]** Use the Lagrange interpolation formula to construct a fourth order approximation $p_4(x)$ of $f_2(x)$ that is exact at $x = -2, -1, 0, 1, 2$. There is no need to evaluate the expressions.

$$\begin{aligned} p_4(x) &= \sqrt{4+\epsilon}\frac{x(x-1)(x+1)(x-2)}{24} + \sqrt{1+\epsilon}\frac{x(x-1)(x+2)(x-2)}{6} - \sqrt{1+\epsilon}\frac{x(x+1)(x+2)(x-2)}{6} \\ &\quad + \sqrt{4+\epsilon}\frac{x(x-1)(x+1)(x+2)}{24} + \sqrt{\epsilon}\frac{(x-1)(x+1)(x-2)(x+2)}{4}. \end{aligned}$$

(c) **[5 points]** What happens to the second order Lagrange interpolation formula $p_2(x)$ [for $f_2(x)$] as $\epsilon \to 0$? Note that $f_2(x) = |x|$ for $\epsilon = 0$.

$$\lim_{\epsilon \to 0} p_2(x) = \frac{x(x-1)}{2} + \frac{x(x+1)}{2} = x^2.$$

This is a bad approximation for $|x|$ since $|x|$ is linear and x^2 is quadratic.

(d) **[10 points]** Evaluate the error $e(x) = ||x| - p_2(x)|$ where $p_2(x)$ is the Lagrange interpolation formula [for $f_2(x)$]. For what value of x do you get the maximum error? [Please note that you are comparing $p_2(x)$ with the original function $f_1(x) = |x|$ and not $f_2(x) = \sqrt{x^2+\epsilon}$.]

$$e(x) = ||x| - p_2(x)| = ||x| - \sqrt{1+\epsilon}\frac{x(x-1)}{2} - \sqrt{1+\epsilon}\frac{x(x+1)}{2} + \sqrt{\epsilon}(x+1)(x-1)|.$$

Since both $|x|$ and $p_2(x)$ are symmetric, we restrict ourselves to $x \geq 0$. In order to find the maximum error, we take the difference

$$\begin{aligned} g(x) &= x - \sqrt{1+\epsilon}\frac{x(x-1)}{2} - \sqrt{1+\epsilon}\frac{x(x+1)}{2} + \sqrt{\epsilon}(x+1)(x-1) \\ &= x - \sqrt{1+\epsilon}x^2 + \sqrt{\epsilon}(x^2-1) \end{aligned}$$

and attempt to find its maximum or minimum by setting its derivative to zero and solving to get

$$\frac{dg(x)}{dx} = 0 \Rightarrow 1 - 2\sqrt{1+\epsilon}x + 2x\sqrt{\epsilon} = 0.$$

From this, we get

$$x = \frac{1}{2\sqrt{1+\epsilon}-\sqrt{\epsilon}}.$$

The value of $g(x)$ at $x = \frac{1}{2\sqrt{1+\epsilon}-\sqrt{\epsilon}}$ is

$$\begin{aligned} g(x) &= x - \sqrt{1+\epsilon}x^2 + \sqrt{\epsilon}(x^2-1) \\ &= x - (\sqrt{1+\epsilon} - \sqrt{\epsilon})x^2 - \sqrt{\epsilon} \\ &= \frac{1}{2\sqrt{1+\epsilon}-\sqrt{\epsilon}} - (\sqrt{1+\epsilon}-\sqrt{\epsilon})\frac{1}{[2\sqrt{1+\epsilon}-\sqrt{\epsilon}]^2} - \sqrt{\epsilon} \\ &= \frac{2\sqrt{1+\epsilon} - \sqrt{\epsilon} - \sqrt{1+\epsilon} + \sqrt{\epsilon} - \sqrt{\epsilon}[2\sqrt{1+\epsilon}-\sqrt{\epsilon}]^2}{[2\sqrt{1+\epsilon}-\sqrt{\epsilon}]^2} \\ &= \frac{\sqrt{1+\epsilon} - \sqrt{\epsilon}[4(1+\epsilon)+\epsilon - 4\sqrt{\epsilon(1+\epsilon}]}{[2\sqrt{1+\epsilon}-\sqrt{\epsilon}]^2} \\ &= \frac{(4\epsilon+1)\sqrt{1+\epsilon} - (4+5\epsilon)\sqrt{\epsilon}}{[2\sqrt{1+\epsilon}-\sqrt{\epsilon}]^2}. \end{aligned}$$

At $\epsilon = 0$, $g(x) = x - x^2 = \frac{1}{2} - (\frac{1}{2})^2 = \frac{1}{4}$. From symmetry arguments, we get the maximum error for $x = -\frac{1}{2\sqrt{1+\epsilon}-\sqrt{\epsilon}}$ as well. Note that this is valid only for x in the interval $[-1,1]$. Since that wasn't made explicit in the question, the worst error actually occurs for $x = \pm\infty$ since $e(x) = \infty$.

(e) **[10 points]** Evaluate the interpolation error $E(x) = f_2(x) - p_2(x)$ of the second order Lagrange interpolation formula at an arbitrary $x \in [-1,1]$? What happens at $\epsilon = 0$? Does the interpolation error formula still hold for $\epsilon = 0$? Discuss. [Please note that you are comparing $p_2(x)$ with $f_2(x) = \sqrt{x^2+\epsilon}$ and not the original function $f_1(x) = |x|$.]

$$E(x) = \sqrt{x^2+\epsilon} - \sqrt{1+\epsilon}\frac{x(x-1)}{2} - \sqrt{1+\epsilon}\frac{x(x+1)}{2} + \sqrt{\epsilon}(x+1)(x-1).$$

At $\epsilon = 0$, the error is

$$E(x) = |x| - x^2.$$

Assuming that the interpolation error formula holds, we get at $\epsilon = 0$,

$$\begin{aligned} f(x) - p_n(x) &= \frac{w_n(x)}{(n+1)!}f^{(n+1)}(\xi_x) \\ &= \frac{x(x-1)(x+1)}{6}f^{(3)}(\xi_x) \\ &= \frac{x(x-1)(x+1)}{6}[\frac{-3\xi_x}{(\xi_x^2+\epsilon)^{\frac{3}{2}}} + \frac{3\xi_x^3}{(\xi_x^2+\epsilon)^{\frac{5}{2}}}] \\ &= 0 \end{aligned}$$

for $\epsilon = 0$ because $[\frac{-3\xi_x}{(\xi_x^2+\epsilon)^{\frac{3}{2}}} + \frac{3\xi_x^3}{(\xi_x^2+\epsilon)^{\frac{5}{2}}}] = [-3\xi_x^2 + 3\xi_x^2] = 0$ at $\epsilon = 0$. This is obviously wrong since the error for $\epsilon = 0$ is $f(x) - p_2(x) = |x| - x^2 \neq 0$ for $x \neq 0$. The interpolation error formula does not hold because $\sqrt{x^2+\epsilon}$ is not C^3 for $\epsilon = 0$.

3. **[30 points] Modification to the Trapezoid rule:** The trapezoid rule for constructing an approx-

imation to the definite integral of a function $f(x)$ over the interval $[a, b]$ is based on constructing a first order Lagrange interpolation to the function $f(x)$ and then integrating the interpolant in the interval $[a, b]$ to get

$$T(f) = \frac{(b-a)}{2}(f(b) + f(a)).$$

(a) **[5 points]** Construct a first order Lagrange interpolation to an arbitrary function $f(x)$ which is exact at the points a and b.

$$p_1(x) = f(a)\frac{x-b}{a-b} + f(b)\frac{x-a}{b-a}.$$

(b) **[5 points]** Integrate the first order Lagrange interpolation of $f(x)$ over the interval $[a, b]$ and show that you get the above trapezoid rule.

$$\int_a^b p_1(x)dx = f(b)\frac{(b-a)}{2} - f(a)\frac{(a-b)}{2} = \frac{f(b) + f(a)}{2}(b-a).$$

(c) **[5 points]** Now you are given that $f(x) = x^2$. Do you think the trapezoid rule will be exact for $f(x) = x^2$? If not, what is the error of the trapezoid rule for the integral of $f(x) = x^2$ over the interval $[a, b]$.

$$\int_a^b x^2 dx = \frac{b^3 - a^3}{3}.$$

The trapezoid rule applied to $f(x) = x^2$ is

$$(b^2 + a^2)\frac{b-a}{2} = \frac{b^3 - a^3 + a^2 b - ab^2}{2}.$$

The error of the trapezoid rule is therefore

$$I(f) - T(f) = \frac{-b^3 + a^3 - 3a^2 b + 3ab^2}{6}.$$

(d) **[10 points]** How would you modify the trapezoid rule so that it is exact for the integral of $f(x) = x^2$ over the interval $[a, b]$?

The short answer is "Use Simpson's rule" which is exact not only for second order polynomials but third order polynomials as well. The long answer is that

$$\int_a^b x^2 dx = \frac{b^3 - a^3}{3} = \frac{(b^2 + ab + a^2)}{3}(b-a) = \frac{f(b) + \sqrt{f(b)f(a)} + f(a)}{3}(b-a).$$

(e) **[5 points]** Will your above modification to the trapezoid rule continue to be exact for integrals of first order polynomials $f(x) = \alpha x + \beta$ over the interval $[a, b]$? Discuss.

No. We can prove this by just taking $f(x) = x$.

$$\int_a^b x dx = \frac{b^2 - a^2}{2}$$

whereas the modified rule gives

$$\frac{b+\sqrt{ab}+a}{3}(b-a) \neq \frac{b^2-a^2}{2}.$$

Since $f(x) = x$ is not integrated correctly by our modified trapezoid rule, $f(x) = \alpha x + \beta$ will not be correctly integrated as well for a general α, β. Please note that if you specified Simpson's rule as the modification, then all first order polynomials will be perfectly integrated over the interval $[a, b]$.

List of Useful Formulae

Taylor series approximation: $f(x) = \sum_{i=0}^{n} \frac{(x-x_0)^i f^{(i)}(x_0)}{i!} + \frac{(x-x_0)^{(n+1)} f^{(n+1)}(\xi_{[x_0,x]})}{(n+1)!}$ with $\xi_{[x_0,x]}$ in the interval $[x_0, x]$.
Euler's method: Approximation of $y' = f(t, y)$ is $y_{n+1} = y_n + hf(t_n, y_n)$ with $y_0 = y(t_0)$.
Difference Approximations of Derivatives: $f'(x) = \frac{f(x+h)-f(x)}{h} - \frac{1}{2}hf''(\xi_{x,h})$, $f''(x) = \frac{f(x+h)-2f(x)+f(x-h)}{h^2} - \frac{1}{12}h^2 f''''(\xi_{x,h})$.
Linear Interpolation formula: $p_1(x) = \frac{x_1-x}{x_1-x_0} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1)$.
Bisection method: $|\alpha - x_n| \leq \left(\frac{1}{2}\right)^n (b-a)$ with the midpoint of the interval chosen at each step.
Newton's method: Iterative update to solve $f(x) = 0$ is $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$ with initial condition x_0.
Quadratic formula: Solution of $ax^2 + bx + c = 0$ is $x = \frac{-b\pm\sqrt{b^2-4ac}}{2a}$.
Lagrange interpolation formula: $p_n(x) = \sum_{k=0}^{n} f(x_k) L_k^{(n)}(x)$ where

$$L_i^{(n)}(x) = \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{x - x_k}{x_i - x_k}.$$

Trapezoid rule: $T(f) = \frac{1}{2}(b-a)(f(b) + f(a))$.
Simpson's rule: $S_2(f) = \frac{(b-a)}{6}(f(a) + 4f(c) + f(b))$ where $h = \frac{(b-a)}{2}$ and $c = \frac{(a+b)}{2}$.
Interpolation Error of Lagrange interpolation: Let $f \in C^{n+1}([a, b])$ and let the nodes $x_k \in [a, b]$ for $0 \leq k \leq n$. Then, for each $x \in [a, b]$, there is a $\xi_x \in [a, b]$ such that

$$f(x) - p_n(x) = \frac{w_n(x)}{(n+1)!} f^{(n+1)}(\xi_x),$$

where

$$w_n(x) = \prod_{k=0}^{n} (x - x_k).$$

Cubic difference: $(b^3 - a^3) = (b-a)(b^2 + ab + a^2)$.
Derivatives:

1. $f^{(0)}(x) = \sqrt{x^2 + \epsilon}$, $f^{(1)}(x) = \frac{x}{\sqrt{x^2+\epsilon}}$, $f^{(2)}(x) = \frac{1}{\sqrt{x^2+\epsilon}} - \frac{x^2}{(x^2+\epsilon)^{\frac{3}{2}}}$, $f^{(3)}(x) = \frac{-3x}{(x^2+\epsilon)^{\frac{3}{2}}} + \frac{3x^3}{(x^2+\epsilon)^{\frac{5}{2}}}$
2. $f^{(0)}(x) = 2e^{-\beta x} - 1$, $f^{(1)}(x) = -2\beta e^{-\beta x}$, $f^{(2)}(x) = 2\beta^2 e^{-\beta x}$.