Mathematics 373 Workshop 3 Solutions

Quadratic Convergence

Fall 2003

Introduction

Given a function $f(x)$, the solutions of $f(x) = 0$ can be found by iterating

$$N(x) = x - \frac{f(x)}{f'(x)}.$$

Such an iteration is called **Newton's method**. If x_∞ is a solution of $f(x) = 0$, then $N(x_\infty) = x_\infty$ and

$$N(x) - x_\infty = x - x_\infty - \frac{f(x) - f(x_\infty)}{f'(x)}.$$

If $f'(x)$ is bounded away from zero on an interval containing the x_n, a sequence defined by $x_{n+1} = N(x_n)$ converges to a value x_∞ and Taylor's formula based at x_n,

$$f(x_\infty) = f(x_n) + (x_\infty - x_n) f'(x_n) + \frac{f''(\xi)(x_\infty - x_n)^2}{2},$$

leads to

$$x_{n+1} - x_\infty = -\frac{f''(\xi)}{2 f'(x_n)} \left(x_n - x_\infty \right)^2$$

for some real number ξ between x_n and x_∞. This essentially doubles the number of correct decimal places at each step, as long as the initial value is close enough to x_∞.

Problem 1

Consider the function

$$h(x) = \frac{\sin x}{x} \qquad (0 < x \le \pi)$$

where we have restricted to an interval on which $h(x)$ decreases from 1 to 0. If we define $h(0) = 1$ and use the formula for other values, the function has derivatives of all orders, so we may speak of the value of derivatives of h at zero. Since $h(x)$ is a decreasing function, it has an inverse function that we will call k. The domain of k is $[0, 1]$ and k is defined by $k(y) = x$ if $h(x) = y$ and $0 \le x \le \pi$. Our task is to devise a process to compute $k(a)$ for any given $a \in [0, 1]$. This will be done by formulating this problem as a **rootfinding** problem that can be solved by Newton's method.

1a Statement

One way to find $k(a)$ is to set $f(x) = h(x) - a$. This has the advantage that there is a unique solution to $f(x) = 0$ for all $a \in [0, 1]$. It can be shown that $h''(x)$ increases from $-1/3$ at $x = 0$ to approximately $+0.203$ at $x = \pi$, so that $\left|h''(x)\right| \le 1/3$ for $0 \le x \le \pi$. Unfortunately, $h'(0)$ is zero, so there is a bound on the error only for x bounded away from zero. Find a bound on $1/\left|h'(x)\right|$ for $x \ge 0.3$

1a Solution The claims about the behavior of $h'(x)$ and $h''(x)$ are based on

$$f'(x) = h'(x) = \frac{\cos x}{x} - \frac{\sin x}{x^2}$$
$$f''(x) = h''(x) = -\frac{\sin x}{x} - \frac{2\cos x}{x^2} + \frac{2\sin x}{x^3}$$

For $0 < x$, $h'(x) < 0$ is equivalent to $\sin x > x\cos x$. For $x < \pi/2$, $\cos x > 0$ and this is equivalent to $\tan x > x$, which follows from the fact that $\tan x - x$ is zero at $x = 0$ and its derivative is always positive. For $\pi/2 < x < \pi$, we need $\tan x < x$, which follows from $\tan x < 0 < x$.

The study of $h''(x)$ is more complicated. It can be rewritten as

$$h''(x) = x^{-3}\big((2 - x^2)\sin x - 2x\cos x\big).$$

This can be studied by considering $\arctan\big(2x/(2 - x^2)\big)$ on various intervals.

So much for **background information** — here is what we needs to be done. Since $h''(x)$ increases from a negative value to a positive value, it is zero somewhere on our domain. Thus, $h'(x)$ is initially decreasing, then increasing. The minimum of $h'(x)$ is attained at an interior point and the maximum is attained at an endpoint. We have $h'(0.3) = -0.099102888$ and $h'(\pi) = -0.3183098861$, so the **maximum** is the **negative** value -0.099102888. The negative of this gives a lower bound on $\left|h'(x)\right|$ and the reciprocal of that — 10.09052330 — is the desired upper bound on $1/\left|h'(x)\right|$. Since only an **upper bound** is required, we can use the **more convenient** value of 10.1.

1b Statement Since $h(0.3) \approx 0.985$, Newton's method for $f(x)$ has a uniform error estimate for values of a smaller than this. If one starts with $x_0 = 2.081575978$ — the location of the inflection point — the sequence x_n always moves towards x_∞. Use this to give a bound on the number of steps required to compute $k(a)$ to 8 decimal places for all a with $0 \le a < 0.985$.

1b Solution To get a uniform error estimate on the error in Newton's method, we can use our upper bounds of ⅓ on $\left|f''(\xi)\right|$ and 10.1 on $\left|1/f'(x)\right|$ in our formula for $x_{n+1} - x_\infty$ to get

$$|x_{n+1} - x_\infty| < 1.7\,|x_n - x_\infty|^2\,,$$

where we have again rounded up to get a number that is easier to write.

This inequality may be rewritten as

$$1.7\,|x_{n+1} - x_\infty| < \big(1.7\,|x_n - x_\infty|\big)^2.$$

Induction on this shows that, if $1.7\,|x_0 - x_\infty| < k$, then $1.7\,|x_n - x_\infty| < k^{2^n}$ for all n. (The **basis** case $n = 0$ is the definition of k, and the step from n to $n+1$ follows from the displayed inequality.) This is only useful if $k < 1$, but we will show how to reduce the general case to this special case.

Before proving anything, we should find out what is true. It seems plausible that the extreme values of $a = 0$ and $a = h(0.3) \approx 0.985$ would take the largest number of steps. With $a = 0$, four steps are required: (start) 2.081575978, (step 1) 3.042386451, (step 2) 3.138766291, (step 3) 3.141590118, (step 4) 3.141592654, which agrees with π to more than 8 decimal places (the distance to π at the previous step was about 2.5×10^{-6}). With $a = h(0.3)$, six steps are required: (start) 2.081575978, (step 1) 0.783999428, (step 2) 0.4403481391, (step 3) .3217480269, (step 4) 0.3007207552, (step 5) 0.3000008468, (step 6) 0.2999999972 (the distance to 0.3 at the last step is about 3×10^{-9}). Roundoff error has made the last value appear to overshoot the target.

This empirical investigation is all that was expected at this stage. A careful error analysis is more difficult. The biggest danger is that this analysis will be **oversimplified**, leading to conclusions that are **too good to be true**. You should never put a **lot** of effort into an analysis to conclude that a **little** more computation is unnecessary. Error analysis should **overestimate** the error to give an **easy proof** that a **reasonable** effort will **surely** give an answer that meets specifications.

These calculations were done in Maple using the default precision of 10 decimal places. Repeating the calculation with extended precision reveals that the calculation of $h(0.3)$ gave a value that was slightly too large, so that the root was slightly smaller than expected.

Now, let's try to show that we reach the root to within 10^{-8} in at most 6 steps for any a. Our error estimate shows that this will be true if $k = 1.7\,|x_0 - x_\infty|$ satisfies $k^{2^6} < 10^{-8}$. Taking logarithms, this is equivalent to $64 \ln k < -8 \ln 10$. Thus $\ln k < -(\ln 10)/8$ or $k < 10^{-1/8} \approx 0.74989$. Taking this distance on either side of the value of x_0 that we decided to use in all cases shows that six steps suffice for $1.332 < x_\infty < 2.831$. This gives the desired accuracy in six steps for $0.108 < a < 0.729$

To extend these results, we note that the form of the function iterated in Newton's method shows that the result is an increasing function of a for each x (because $h'(x) < 0$). Thus, if a is outside the interval that we found, one step will take us at least as far as if a had been 0.108 or 0.729. The resulting values of x_1 are 2.795 (for small a) and 1.370 (for large a). Then, one needs to see how far one can get from here in **five** steps. The value of k is now determined by $32 \ln k < -8 \ln 10$, or $k < 10^{-1/4} \approx 0.56234$. Convergence is now guaranteed for $0.8074289988 < x_\infty$. The calculation of the right endpoint gave a value greater than that of the interval used to formulate the estimates, so we can only conclude validity for $0 \le a < 0.895$ (the latter value being a convenient **upward** rounding of $h(0.8074289988)$). Because of the cautious nature of the estimates, it may not be possible to use this approach to **prove** that six steps suffice in all cases. However, for large a, even if six steps won't give the answer to the required accuracy, **two** steps will lead to $x_2 < 0.89302$ and we have seen that we can solve all relevant equations in six steps from this point. The solution has thus been guaranteed in a total of **eight** steps.

1c Statement A simpler function is $f(x) = \sin x - ax$. This has the disadvantage that $f(0) = 0$, while we are always looking for the **other** place where $f(x) = 0$. Find a method that will guarantee that the Newton iteration determined by this function will converge to $k(a)$. Find a rule for choosing x_0 and bound on the number of steps of this iteration required to compute $k(a)$ to 8 decimal places for all a with $0 \le a < 0.985$.

1c Solution For all a, this $f(x)$ is concave downward between 0 and π with inflection points at both ends of this interval, and the maximum point lies between 0 and the desired root. A uniform method of solving the equation is to start with $x_0 = \pi$. Then, iterating the Newton function $x - f(x)/f'(x)$ gives a decreasing sequence that converges to the positive root of $f(x) = 0$. Again, we suspect that $a = 0.985$ will exhibit the slowest convergence. Calculating gives the sequence: $x_0 = 3.141592654$, $x_1 = 1.582666325$, $x_2 = 1.021914236$, $x_3 = 0.6906204033$, $x_4 = 0.4886790201$, $x_5 = 0.3721739656$, $x_6 = 0.3169948089$, $x_7 = 0.3018505633$, $x_8 = 0.3006856430$, $x_9 = 0.3006788963$.

Uniform estimates based on the error estimate for Newton's method are more difficult to find in this case because $\left|f'(x)\right|$ can be smaller than 0.03 for a near 0.985. With a uniform upper bound of $\left|f''(\xi)\right| \le 1$, we have

$$|x_{n+1} - x_\infty| < 16.82\,|x_n - x_\infty|^2\,,$$

$$16.82\,|x_{n+1} - x_\infty| < \big(16.82\,|x_n - x_\infty|\big)^2.$$

Thus, the benefits of quadratic convergence are seen only when very close to end of the computation. We also notice that there is little benefit in modest changes in the choice of x_0 like using $x_0 = \pi/2$ for $a > 2/\pi$, since one or two steps starting from $x_0 = \pi$ leads to smaller values.

Problem 2

Steffensen's method, which calls for forming $p_1 = g(p_0)$ and $p_2 = g(p_1)$, and then

$$p_* = p_0 - \frac{(p_1 - p_0)^2}{p_2 - 2p_1 + p_0}$$

is described as **accelerating convergence**.

2a Statement

Here is an example of the primary use of Steffensen's method. If a function $f(x)$ has a zero of multiplicity greater than 1, Newton's method is no longer quadratically convergent. Example 2 in section 2.4 investigates the Newton iteration constructed to find the root of

$$e^x - x - 1$$

at $x = 0$. This is a *toy example* — you know that the process should converge to zero. The example suggests **linear convergence**. Use Steffensen's method to produce a quadratically convergent iteration from the iteration of this example. (Note that the function being iterated is **not shown** in the text, so you will need to construct it.) **Show all intermediate steps** in the computation of the Newton function and the Steffensen function. The accuracy to which those quantities can be computed play a role in the behavior of these methods.

2a Solution

The first step is to find $N(x) = x - f(x)/f'(x)$ when $f(x) = e^x - x - 1$:

$$N(x) = x - \frac{e^x - x - 1}{e^x - 1}.$$

Computations should use $N(x)$ in the form shown, but analysis of its properties may use expressions that are algebraically equivalent. This allows L'Hôpital's rule to be used to show that

$$\lim_{x \to 0} \frac{N(x)}{x} = \frac{1}{2}$$

by writing

$$\frac{N(x)}{x} = \frac{xe^x - e^x + 1}{xe^x - x}.$$

(Actually, the use of Taylor's theorem on the numerator and denominator of this expression is more efficient:

$$\frac{N(x)}{x} = \frac{\frac{1}{2}x^2 + O(x^3)}{x^2 + O(x^3)}$$

where $O(x^3)$ stands for "terms of degree 3 or more").

Iterating this function gives values that agree with the table shown in the textbook, and the limit that was just calculated shows that $N(x) \sim x/2$, confirming the observation that this sequence appears to be linearly convergent to zero with ration $1/2$. As in the text, we start with $p_0 = 1$. The rows of the following table show p_0, p_1, p_2 from the application of $N(x)$, and each new row begins with the p_* computed from the triple on the row above.

p_0	p_1	p_2
1.	0.5819767070	0.3190550411
-0.126638558	-0.06198319467	-0.03067145206
-0.0012677701	-0.0006339729082	-0.0003168241544
8.25704×10^{-7}		

Iterating $N(x)$ would divide an entry by 2 to get the next entry in a row. The next Steffensen step may not be possible because the denominator will be so small that it will look like zero.

2b Statement If the goal is to get accuracy to with 10^{-6}, how many steps will be required using Newton's method, and how many steps using the accelerated method? What accuracy would be needed in each of these computations?

2b Solution In this case, Newton's method is only linearly convergent with ratio $1/2$, and we started at distance 1 form the root, so the distance to the root is 2^{-n} after n steps. To get $2^{-n} < 10^{-6}$ requires $-n \ln 2 < -6 \ln 10$ or $n > 6 \ln 10 / \ln 2 \approx 19.93156857$. Since n is an integer, it must be at least 20. A more precise error estimate might require a larger ratio, leading to a few more steps.

2c Statement Under some circumstances, Steffensen's method is able to turn a **divergent** process into a convergent one. Experiment with $g(x) = \cos(2x)$ and various choices of starting value.

2c Solution Start with $p_0 = 0$ and construct a table in the same format as in 2a.

p_0	p_1	p_2
0.	2.	-0.8322936730
0.8277642608	1.353047788	0.4320637532
1.018546929	1.049207144	0.9965172662
1.029825246	1.029937307	1.029745181
1.029866529	1.029866530	1.029866528
1.029866529		

End of Workshop 3