Computational Methods Assignment 8 - Root Finding

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1 Bisection

A bisection method was written to determine the roots of an arbitrary function, given two initial points which are required to bracket the root. The bracketing region is successively halved so that it always contains the root, and iterates until either the function at the most recently found point it zero, or the size of the bracketed region has shrunk within a given tolerance. This was applied to the cubic spline interpolating function, with a tolerance of $\epsilon = 10^{-8}$ and chosen to have initial points that were found graphically as good starting points which would bracket either roots. The two roots of the interpolating function were found to be $x_1 = 2.06531359$ and $x_2 = 2.78071972$.

2 Brent's Method

2(a) Next, Brent's method was implemented into a class and used with the same parameters (starting values and tolerance) to determine the roots of the cubic interpolation function. Firstly, in the case that $a = c$ i.e. two of the points required (not the best guess) are the same, the inverse quadratic interpolation cannot be used as this required 3 points. The result of the inverse quadratic interpolation is that the value of x for which the inverse parabola is zero, is:

$$
\begin{aligned}
&x = b + \frac{P}{Q} \\
&P = S\left[T(R-T)(c-b) - (1-R)(b-a)\right], \;\; Q = (R-1)(S-1)(T-1) \\
&S = f(b)/f(a), \;\; R = f(b)/f(c), \;\; T = f(a)/f(c)
\end{aligned}
$$

In the limit that $c \to a$ and hence $T \to 1$, this becomes:

$$
\begin{aligned}
\lim_{c\to a}\frac{P}{Q} &= \left(\lim_{c\to a}\frac{S}{S-1}\right)\lim_{c\to a}\frac{T(R-T)(c-b)-(1-R)(b-a)}{(R-1)(T-1)} \\
&= \left(\lim_{c\to a}\frac{S}{(S-1)(R-1)}\right)\left[\left(\lim_{c\to a}(R-T)\right)\left(\lim_{c\to a}\frac{T(c-b)}{T-1}\right) - \lim_{c\to a}\frac{(R-1)(a-b)}{T-1}\right] \\
&= \left(\lim_{c\to a}\frac{S(R-1)}{(S-1)(R-1)}\right)\left[\left(\lim_{c\to a}(c-b)\right)\left(\lim_{c\to a}\frac{T}{T-1}\right) - \lim_{c\to a}\frac{a-b}{T-1}\right] = \frac{S(a-b)}{S-1}\left(\lim_{c\to a}\frac{T-1}{T-1}\right) \\
&= \frac{S(a-b)}{S-1} = \frac{f(b)}{f(a)}\frac{a-b}{f(b)/f(a)-1} = -f(b)\frac{b-a}{f(b)-f(a)} \\
&\implies x = b - f(b)\frac{b-a}{f(b)-(fa)}
\end{aligned}
$$

This collapsed result is known as the secant method, a finite difference equivalent of the Newton-Raphson method for root finding, which is essentially a linear interpolation.

2(b, c) Brent's method applied to the interpolating function (from assignment 2) and from the same initial bracketing points the roots were found as $x_1 = 2.06531359$ and $x_2 = 2.78071972$, the same as the bisection method. See code for explanatory comments on the steps.

	Bisection	Brent
Root 1 value	2.06531359	2.06531359
Root 1 iterations	24	6
Root 2 value	2.78071972	2.78071972
Root 2 iterations	23	6

Table 1: Comparison of Brent's method and the bisection method in determining the roots of the interpolation function.

2(d) The comparison between Brent's method and bisection method are shown in table 1. This was obtained with an initial bracketing for the first root of $[x_{min}, x_{max}] = [2.0, 2.25]$ and a bracketing for the second root of $[x_{min}, x_{max}] = [2.75, 2.9]$. This shows that Brent's method achieves the same precision and result as the bisection method with approximated 4 times less the number of iterations required. This is because the bisection method converges linearly whilst Brent's method combines different methods as is expected to converge at a higher rate.
2(e) Bracketing a root of a continuous function with two points whose function values have opposite is essential since the intermediate value theorem gives that there must be a root in the interval. If bracketing the root is not ensured, that is, the function has the same sign at either sides of the interval, doesn't guarantee that there *isn't* any roots in the interval, but makes it difficult if not impossible for a method to converge towards it in a minimal number of iterations. Also, bracketing is useful to tell the program running the algorithm if the method has overshot the root by determining the sign and ensuring the root has been bracketed. Initial bracketing is especially important in Brent's method because the method relies heavily on inverse quadratic interpolation (provided the conditions are met). This applies similarly to the linear interpolation of the root in the secant method, which will occur if the algorithm is only initially given two points. The interpolating method cannot determine what lies outside the interpolating region accurately. Additionally, the condition of Brent's method that the addition to the next best guess, P/Q, must satisfy $|P/Q| \leq 3|b-c|/4$, which means that if the interpolation or secant method gives an answer sufficientlly outside the bounds, a bisection method is triggered, and this means that the root can never be found, since bisection will only ever halve the interval.
2(f) Brent's method requires that if the absolute value of the inversely quadratic interpolated addition (to the current best guess of the root) is larger than three quarters of the absolute interval between the contrapoint and the current best guess (before the addition). This is because if the addition to the current best guess is beyond this, the quadratic is not a good approximation to the function near these points i.e. the function would be too steep from the estimated root point and the contra point. This comes from the limiting case if the inverse parabola was 'centred' (the bottom of the parabola if looked at in a rotated $y - x$ plaane) on the contra point c, and it was required by the algorithm that the current best guess b was closer to $f(x) = 0$ than the c i.e. $|f(b)| \leq |f(c)|$. This would mean that the amount the inverse parabola changes from the c to the root is $f(c)^2$ and the distance between that and b is $|b-c| \equiv d = (|f(b)|+|f(c)|)^2 \leq (2|f(c)|)^2 = 4|f(c)|^2$, hence

$$|f(c)|^2 \geq \frac{1}{4}d, \ \Rightarrow d - |f(c)|^2 \leq d - \frac{d}{4}, \ \Rightarrow d - |f(c)|^2 = \left|\frac{P}{Q}\right| \leq \frac{3d}{4} = \frac{3|b-c|}{4}$$

This is the limiting case and any other situation for which the parabola is considered a good fit, has an addition to the best guess which is less than this, so this condition must be fulfilled.