Multiple Roots

We study two classes of functions for which there is additional difficulty in calculating their zeros. The first of these are functions in which the desired zero has a multiplicity greater than 1. What does this mean?

Let α be a zero of the function f(x), and imagine writing it in the factored form

$$f(x) = (x - \alpha)^m \, h(x)$$

with some integer $m \geq 1$ and some continuous function h(x) for which $h(\alpha) \neq 0$. Then, we say that α is a root of f(x) = 0 with multiplicity m.

For example, the function

$$f(x) = e^{x^2} - 1$$

has x = 0 as a root of multiplicity with m = 2.

Define $$h(x) = \frac{e^{x^2} - 1}{x^2} \quad , \quad x \neq 0$$

$$h(x) = 1 \quad , \quad x = 0$$

Using MacLaurin series expansion, prove that $\lim_{x \to 0} h(x) = 1$

Thus, x = is a root of $f(x) = x^2 h(x) = 0$ with multiplicity m = 2

If the function f(x) is m-times differentiable around α, then we can differentiate

$$f(x) = (x - \alpha)^m h(x)$$

m times to obtain an equivalent formulation of what it means for the root to have multiplicity m.

For an example,

$$f(x) = (x - \alpha)^3 h(x)$$

$$f'(x) = 3 (x - \alpha)^2 h(x) + (x - \alpha)^3 h'(x) = (x - \alpha)^2 h_2(x)$$

$$f''(x) = (x - \alpha) h_3(x)$$

$$f(\alpha) = 0$$

$$f'(\alpha) = 0$$

$$f''(\alpha) = 0 \quad \rightarrow \quad x = \alpha \text{ is a simple root of } f''(x).$$

$$f'''(\alpha) \neq 0$$

In general, α is a zero of f(x) of multiplicity m if and only if

$$f(\alpha) = \dots = f^{(m-1)}(\alpha) = 0$$
$$f^{(m)}(\alpha) \neq 0$$

Difficulties with Multiple Roots

- Methods such as Newton's method and the secant method converge more slowly than for the case of a simple root;
- There is a large interval of uncertainty in the precise location of a multiple root on a computer or calculator.

We can regard Newton's method as a fixed-point iteration:

$$x_{n+1} = g(x_n) \quad , \quad g(x) = x - \frac{f(x)}{f'(x)}$$

Substitute $f(x) = (x - \alpha)^m \, h(x)$

$$g(x) = x - \frac{(x-\alpha)^m \, h(x)}{m\,(x-\alpha)^{m-1}\, h(x) + (x-\alpha)^m \, h'(x)}$$

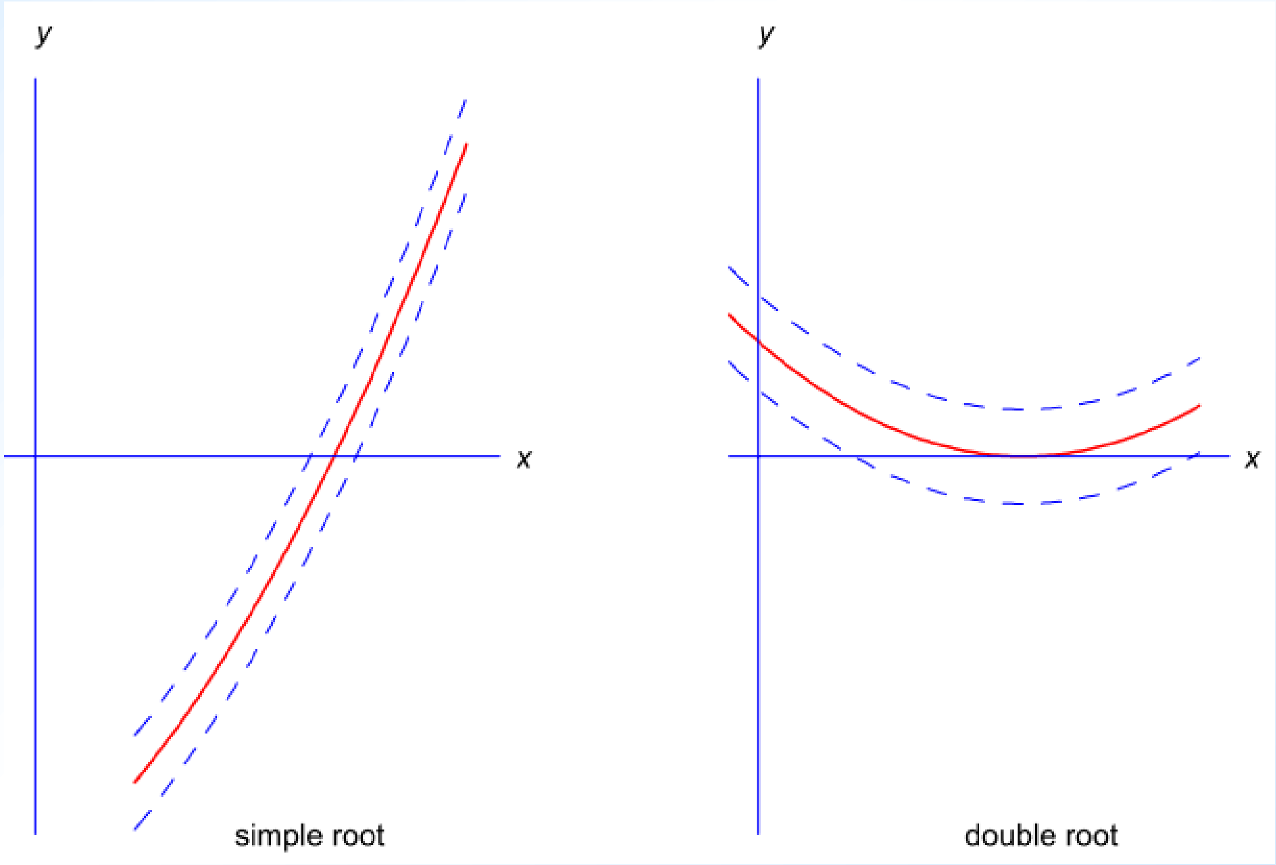
$$= x - \frac{(x-\alpha)\, h(x)}{m\, h(x) + (x-\alpha)\, h'(x)}$$

We may use this to show $g'(\alpha) = 1 - \frac{1}{m} = \frac{m-1}{m}$

For m > 1, this is nonzero, and therefore Newton's method is only linearly convergent. Similar results hold for the secand method.

Noise in Function Evaluation

In the following figures, the noise as measured by vertical distance is the same in both graphs.



Any root finding method to find a multiple root α that uses evaluation of f(x) is doomed to having a large interval of uncertainty as to the location of the root. If high accuracy is desired, then the only satisfactory solution is to reformulate the problem as a new problem F(x) = 0 in which α is a simple root of F . Then use a standard root finding method to calculate α.

It is important that the evaluation of F(x) not involve f(x) directly, as that is the source of the noise and the uncertainly.

In general, if we know the root α has multiplicity m > 1, then replace the problem by that of solving

$$f^{(m-1)}(x) = 0$$

since α is a simple root of this equation.

Example

Consider finding the roots of

$$f(x) = 2.7951 - 8.954\,x + 10.56\,x^2 - 5.4\,x^3 + x^4 = 0$$

This has one root to the right of 1. From an examination of the rate of linear convergence of Newton’s method applied to this function, one can guess with high probability that the multiplicity is m = 3. Then form exactly the second derivative

$$F(x) = f''(x) = 21.12 - 32.4\,x + 12\,x^2 = 0$$

Applying Newton’s method to this with a guess of x = 1 will lead to rapid convergence to α = 1.1.

Stability

Consider the polynomial

$$f(x) = x^7 - 28\,x^6 + 322\,x^5 - 1960\,x^4 + 6769\,x^3 - 3132\,x^2 + 13068\,x - 5040 = 0$$

This has the exact roots { 1, 2, 3, 4, 5, 6, 7 } .

Now consider the perturbed polynomial

$$F(x) = x^7 - 28.002\,x^6 + 322\,x^5 - 1960\,x^4 + 6769\,x^3 - 3132\,x^2 + 13068\,x - 5040 = 0$$

This is a relatively small change in one coefficient, of relative error $7.14\ 10^{-5}$.

What are the roots of $F(x) = 0$?

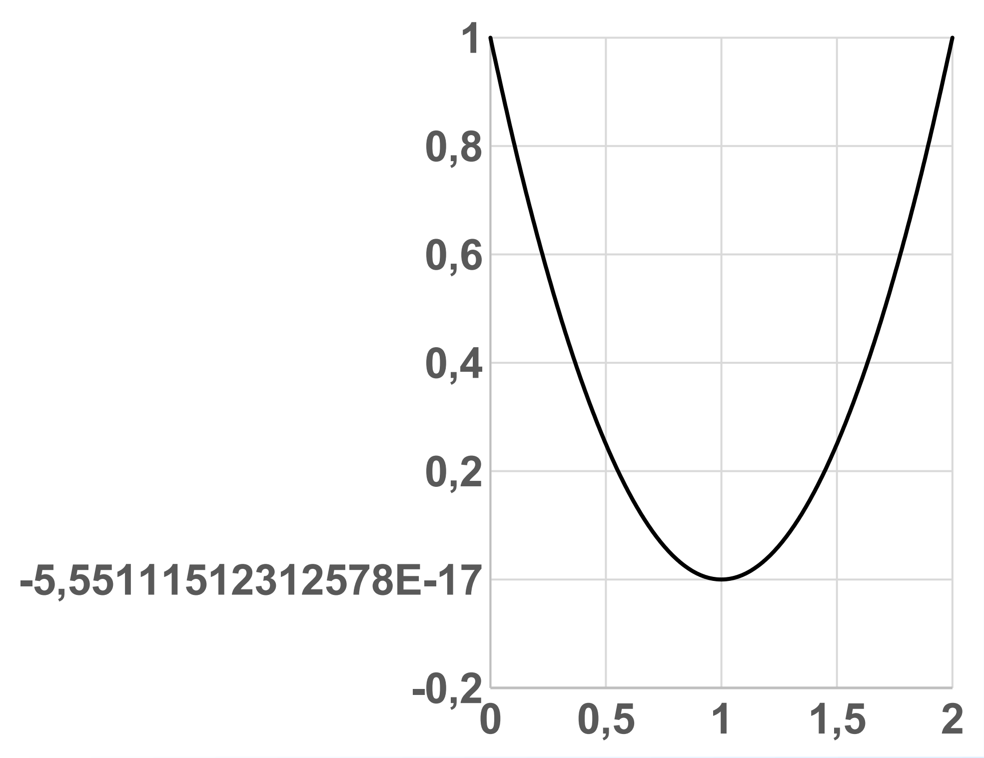
Root of f(x) = 0	Root of F(x) = 0	Error
1.0	1.0000028	-2.80E-06
2.0	1.9989382	1.10E-03
3.0	3.0331253	-0.033
4.0	3.8195692	0.18
5.0	5.4586758 + 0.5412578 i	-0.46 - 0.54 i
6.0	- 5.4586758 + 0.540122578 i	-0.46 + 0.54 i
7.0	7.2330128	-0.233

Why have some of the roots departed so radically from the original values? This phenomena goes under a variety of names. We sometimes say this is an example of an unstable or ill-conditioned root finding problem.

These words are often used in a casual manner, but they also have a very precise meaning in many areas of numerical analysis (and more generally, in all of mathematics).

Example

Find the roots of the equation $f(x) = x^2 - 2x + 1 = 0$



Newton-Raphson on f(x)

n	x_n	$f(x_n)$	$f'(x_n)$
0	1.1000000	0.01	0.2
1	1.0500000	0.0025	0.1
2	1.0250000	0.000625	0.05
3	1.0125000	0.00015625	0.025
4	1.0062500	3.9062E-05	0.0125
5	1.0031250	9.7656E-06	0.00625
6	1.0015625	2.4414E-06	0.003125
7	1.0007812	6.1035E-07	0.0015625
8	1.0003906	1.5259E-07	0.00078125
9	1.0001953	3.8147E-08	0.00039063
10	1.0000977	9.5367E-09	0.00019531