Appendix 6B: Finding the Roots of a Function

If x^* is marginally stable, the second derivative f''(x) must be considered, and the trajectory approaches x^* with deviations from x^* inversely proportional to the square root of the number of iterations.

For the logistic map, the derivatives at the fixed points are, respectively,

$$f'(x=0) = \frac{d}{dx} [4rx(1-x)] \bigg|_{x=0} = 4r,$$
(6.73)

and

$$f'(x = x^*) = \frac{d}{dx} [4rx(1-x)] \bigg|_{x=1-1/4r} = 2 - 4r.$$
 (6.74)

It is straightforward to use (6.73) and (6.74) to find the range of r for which $x^* = 0$ and $x^* = 1 - 1/4r$ are stable.

If a trajectory has period two, then $f^{(2)}(x) = f(f(x))$ has two fixed points. If you are interested, you can solve for these fixed points analytically. As we found in Problem 6.2, these two fixed points become unstable at the same value of r. We can derive this property of the fixed points using the chain rule of differentiation:

$$\left. \frac{d}{dx} f^{(2)}(x) \right|_{x=x_0} = \left. \frac{d}{dx} f(f(x)) \right|_{x=x_0} = f'(f(x_0)) f'(x) \big|_{x=x_0}. \tag{6.75}$$

If we substitute $x_1 = f(x_0)$, we can write

$$\left. \frac{d}{dx} f(f(x)) \right|_{x=x_0} = f'(x_1) f'(x_0). \tag{6.76}$$

In the same way, we can show that

$$\left. \frac{d}{dx} f^{(2)}(x) \right|_{x=x_1} = f'(x_0) f'(x_1). \tag{6.77}$$

We see that if x_0 becomes unstable, then $|f^{(2)'}(x_0)| > 1$ as does $|f^{(2)'}(x_1)|$. Hence, x_1 is also unstable at the same value of r, and we conclude that both fixed points of $f^{(2)}(x)$ bifurcate at the same value of r, leading to an trajectory of period 4.

From (6.74) we see that $f'(x = x^*) = 0$ when r = 1/2 and $x^* = 1/2$. Such a fixed point is said to be superstable, because as we found in Problem 6.4, convergence to the fixed point is relatively rapid. Superstable trajectories occur whenever one of the fixed points is at $x^* = 1/2$.

APPENDIX 6B: FINDING THE ROOTS OF A FUNCTION

The roots of a function f(x) are the values of the variable x for which the function f(x) is zero. Even an apparently simple equation such as

$$f(x) = \tan x - x - c = 0,$$
 (6.78)

where c is a constant, cannot be solved analytically for x.

Regardless of the function and the approach to root finding, the first step should be to learn as much as possible about the function. For example, plotting the function will help us to determine the approximate locations of the roots.

Newton's (or the Newton-Raphson) method is based on replacing the function by the first two terms of the Taylor expansion of f(x) about the root x. If our initial guess for the root is x_0 , we can write $f(x) \approx f(x_0) + (x - x_0)f'(x_0)$. If we set f(x) equal to zero and solve for x, we find $x = x_0 - f(x_0)/f'(x_0)$. If we have made a good choice for x_0 , the resultant value of x should be closer to the root than x_0 . The general procedure is to calculate successive approximations as follows:

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}. (6.79)$$

If this series converges, it converges very quickly. However, if the initial guess is poor or if the function has closely spaced multiple roots, the series may not converge. The successive iterations of Newton's method is an another example of a map. Newton's method also works with complex functions as we will see in the following problem.

Problem 6.30 Cube roots

Consider the function $f(z) = z^3 - 1$, where z = x + iy, and $f'(z) = z^2$. Map the range of convergence of (6.79) in the region [-2 < x < 2, -2 < y < 2] in the complex plane. Color the starting z value red, green, or blue depending on the root to which the initial guess converges. If the trajectory does not converge, color the starting point black. For more insight add a mouse handler to your program so that if you click on your plot, the sequence of iterations starting from the point where you clicked will be shown.

The following problem discusses a situation that typically arises in courses on quantum mechanics.

Problem 6.31 Energy levels in a finite square well

The quantum mechanical energy levels in the one-dimensional finite square well can be found by solving the relation

$$\epsilon \tan \epsilon = \sqrt{\rho^2 - \epsilon^2},\tag{6.80}$$

where $\epsilon = \sqrt{mEa^2/2\hbar}$ and $\rho = \sqrt{mV_0a^2/2\hbar}$ are defined in terms of the particle mass m, the particle energy E, the width of the well a, and the depth of the well V_0 . The function ϵ tan ϵ has zeros at $\epsilon = 0, \pi, 2\pi, \ldots$ and asymptotes at $\epsilon = 0, \pi/2, 3\pi/2, 5\pi/2 \ldots$ The function $\sqrt{\rho - \epsilon^2}$ is a quarter circle of radius ρ . Write a program to plot these two functions with $\rho = 3$, and then use Newton's method to determine the roots of (6.80). Find the value of ρ and thus V_0 such that below this value there is only one energy level and above this value there is more than one. At what value of ρ do three energy levels first appear?

In Section 6.6 we introduced the bisection root-finding algorithm. This algorithm is implemented in the Root class in the numerics package. It can be used with any function.

Listing 6.6 The bisection method defined in the Root class in the numerics package.

public static double bisection(final Function f, double x1, double x2, final double tolerance) $\{$