Root-Finding

Lecture 3

Physics 200
Laboratory

Monday, February 14th, 2011

The fundamental question answered by this week's lab work will be: Given a function $F(x)$, find some/all of the values $\{x_i\}$ for which $F(x_i) = 0$. It's a modest goal, and we will use a simple method to solve the problem. But, as we shall see, there are a wide range of physical problems that have, at their heart, just such a question. We'll start in the simplest, polynomial setting, and work our way up to the "shooting" method.

3.1 Physical Problems

We'll set up some direct applications of root-finding with familiar physical examples, and then shift gears and define a numerical root-finding routine that can be used to solve a very different set of problems.

3.1.1 Orbital Motion

In two-dimensions, with a spherically symmetric potential (meaning here that $V(x, y, z) = V(r)$, a function of a single variable, $r \equiv \sqrt{x^2 + y^2 + z^2}$, the distance to the origin) we can use circular coordinates to write the total energy of a test particle moving under the influence of this potential as

$$E = \frac{1}{2} m \left(\dot{r}^2 + r^2 \dot{\phi}^2 \right) + V(r). \tag{3.1}$$

Conservation of momentum tells us that the z-component of angular momentum is conserved, with $L_z = (\mathbf{r} \times \mathbf{p})_z = m r^2 \dot{\phi}$, so we can rewrite the energy as:

$$E = \frac{1}{2}\, m\, \dot{r}^2 + \underbrace{\frac{1}{2}\,\frac{L_z^2}{m\, r^2} + V(r)}_{\equiv U(r)} \tag{3.2}$$

where $U(r)$ defines an "effective potential" – we have turned a two-dimensional problem into a one-dimensional problem for the coordinate r, and an effective potential that governs the motion in this setting.

Since we know the energy of the system in terms of r, we can invert (3.2) to get:

$$\dot{r}^2 = 2\,\frac{E - U(r)}{m} \equiv F(r). \tag{3.3}$$

Now we can ask for the "turning points" of orbital motion (if/when they exist), those points at which $\dot{r} = 0$ – the answer is provided by radial locations r_i for which:

$$F(r_i) = 0, \tag{3.4}$$

precisely the sort of root-finding problem of interest.

In cases like Newtonian gravity, where $V(r) \sim 1/r$, the resulting $F(r)$ is just a polynomial (in fact, quadratic), so we don't need any fancy numerical solutions. But for more complicated potentials, root-finding can be used efficiently to isolate, at least numerically, the zeroes of the function $F(r)$.

3.1.2 Area Minimization

Many "minimization" problems end in functions that require numerical root-finding. As a simple example of this type of problem, consider a surface connecting two rings of equal radii, R, separated a distance L as shown in Figure 3.1. We want to find the surface with *minimal* area – soap films find these minimal surfaces automatically, there the soap film is taking advantage of a minimal energy configuration, leading to a stable equilibrium.

The immediate goal is a function $s(z)$ that gives the radius of the surface as a function of height. We'll take $z = 0$ at the bottom ring, then $z = L$ is the height at the top ring. Our area expression follows from the azimuthal symmetry – for a platelet extending from z to $z + dz$ and going around an infinitesimal angle $d\phi$, the area is:

$$dA = s\, d\phi\, \sqrt{dz^2 + s'(z)^2\, dz^2}, \tag{3.5}$$

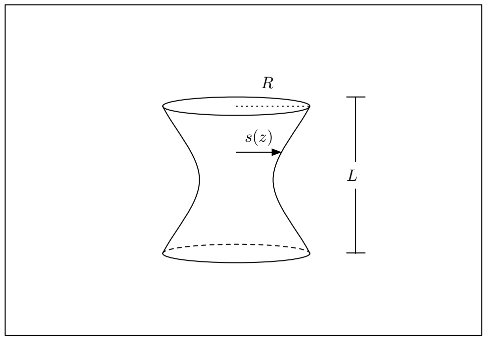

Figure 3.1: We want to find the function $s(z)$, the radius as a function of height, associated with a surface connecting two rings of radius R, separated a distance L, that has minimal surface area.

as can be seen in Figure 3.2.

If we integrate this expression for the area in both ϕ and z, we get the total area of the curve:

$$A = 2\,\pi \int_0^L s(z)\,\sqrt{1 + s'(z)^2}\,dz. \tag{3.6}$$

This formula is nice, but it proceeds from a *given* function of $s(z)$. There is a general method for taking such a functional (here A is a number that depends on the function $s(z)$, so A is itself a function of the function $s(z)$ – we call those functionals) and minimizing it – the result is an ODE for $s(z)$ that can be used to *find* $s(z)$[1]

When we carry out the minimization procedure in this problem, we get the following ODE, with appropriate boundary conditions:

$$1 + s'^2 - s\,s'' = 0 \qquad s(0) = R \qquad s(L) = R. \tag{3.7}$$

The general solution is:

$$s(z) = \alpha\,\cosh\left(\frac{z-\beta}{\alpha}\right), \tag{3.8}$$

for independent real constants α and β (with what dimensions?). Now for the $z = 0$ boundary, we have:

$$s(0) = \alpha\,\cosh\left(\frac{\beta}{\alpha}\right) = R \tag{3.9}$$

[1] This procedure will become familiar to you in classical mechanics, it is an application of variational calculus.

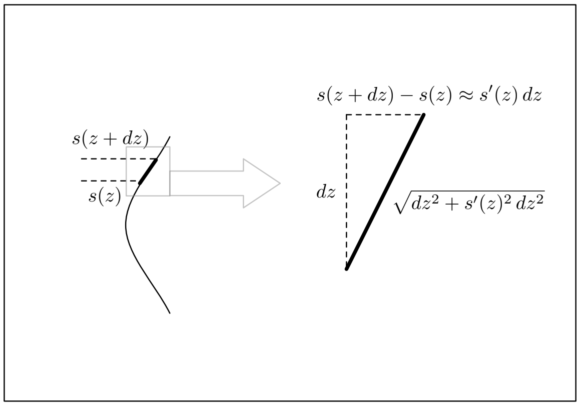

Figure 3.2: Calculating the infinitesimal hypotenuse for the platelet extending from $z \longrightarrow z+dz$ and going around an arc of $s(z)\,d\phi$.

and we must simultaneously solve:

$$s(L) = \alpha \cosh\left(\frac{L-\beta}{\alpha}\right) = R. \tag{3.10}$$

From the first equation, we can write $\beta = \alpha \cosh^{-1}\left(\frac{R}{\alpha}\right)$, and then the second equation becomes:

$$\alpha \cosh\left(\frac{L}{\alpha} - \cosh^{-1}\left(\frac{R}{\alpha}\right)\right) = R. \tag{3.11}$$

Define the function:

$$F(x) \equiv x \cosh\left(\frac{L}{x} - \cosh^{-1}\left(\frac{R}{x}\right)\right) - R \tag{3.12}$$

it is clear that we are interested in the roots, those define the final constant of integration for our solution: $F(\alpha)=0$. Note the importance of actually *plotting* $F(x)$ – not all functions $F(x)$ have roots.

3.2 Shooting

Another class of problems we can solve with an ability to solve for the roots of an arbitrary function are known as “shooting” problems. They come in a few different flavors – we’ll discuss a classic case, and the one that motivates the violent name first, then consider quantum mechanical applications.

3.2.1 Range

We have a cannon that can fire projectiles with speed v at an angle θ. Question: What angle θ should we use to force our cannon to hit a target a distance R away?

Here, we know the answer automatically – the trajectory of the slug is given by:

$$\begin{aligned} x(t) &= v \cos\theta \, t \\ y(t) &= v \sin\theta \, t - \frac{1}{2} g \, t^2, \end{aligned} \tag{3.13}$$

and we can solve for y as a function of x, since $t = \frac{x}{v \cos\theta}$, then

$$y(x) = \tan\theta \, x - \frac{1}{2} g \left(\frac{x}{v \cos\theta}\right)^2. \tag{3.14}$$

Now the range R is the location of x when $y = 0$, a root-finding issue, of course, but in this case, we can solve directly:

$$R = \frac{v^2}{g} \sin(2\,\theta) \longrightarrow \theta = \frac{1}{2} \sin^{-1}\left(\frac{R\,g}{v^2}\right). \tag{3.15}$$

Notice that one important element of this calculation was our ability to make the height, y, a function of x. We can do this pretty generically starting from Newton's second law – if $y(t) \equiv y(x(t))$, then $\frac{dy}{dt} = \frac{dy(x)}{dx}\frac{dx}{dt} = y'(x)\,v_x$, so that we take $\frac{d}{dt} \longrightarrow v_x \frac{d}{dx}$, then

$$\begin{aligned} F_x &= m\,v_x \frac{dv_x}{dx} \\ F_y &= m\,v_x \left[\frac{dv_x}{dx}\frac{dy}{dx} + v_x \frac{d^2y}{dx^2}\right] = F_x \frac{dy}{dx} + m\,v_x^2 \frac{d^2y}{dx^2}, \end{aligned} \tag{3.16}$$

and in this form, we can start with almost any force, and develop the ODE version of the range formula with height parametrized by x.

As a check, take $F_x = 0$, and $F_y = -m\,g$, then the above reads:

$$\frac{dv_x}{dx} = 0 \qquad y''(x) = -\frac{g}{v_x^2}, \tag{3.17}$$

and v_x is a constant, equal to $v \cos\theta$ for us, so

$$y''(x) = -\frac{g}{v^2 \cos^2\theta} \longrightarrow y(x) = \tan\theta \, x - \frac{1}{2} g \frac{x^2}{v^2 \cos^2\theta}, \tag{3.18}$$

as before. This time, the $\tan\theta$ term comes up naturally, since the x derivative is related to the time derivative at zero: $\dot{y}(0) = y'(0)v_x(0)$, and $v_x(0) = \dot{x}(0) = v\,\cos\theta$, so we have $\dot{y}(0) = y'(0)\,\dot{x}(0)$, and then $y'(0) = \dot{y}(0)/\dot{x}(0) = \tan\theta$.

Suppose, for fun, we try introducing wind-resistance, a drag term of the form: $\mathbf{F}_g = -\gamma\, v\, \mathbf{v}$. This gives us an additional force in both directions, and Newton's second law tells us that:

$$m\,\ddot{x} = -\gamma\,\sqrt{\dot{x}^2 + \dot{y}^2}\,\dot{x} \qquad m\,\ddot{y} = -m\,g - \gamma\,\sqrt{\dot{x}^2 + \dot{y}^2}\,\dot{y}, \tag{3.19}$$

from which we learn, using (3.16), that:

$$\begin{aligned} v_x'(x) &= -\frac{\gamma}{m}\,\sqrt{1 + y'(x)^2}\,v_x(x) \\ y''(x) &= -\frac{g}{v_x(x)^2}. \end{aligned} \tag{3.20}$$

There is no longer any simple answer, but we can still imagine solving this equation numerically; it is, after all, a second order ODE, and we have a method for solving those. Suppose we ask the same question, in this context: Given v, find θ so that a projectile hits a target a distance R away from the starting point. Our "initial conditions" are $v_x(0) = v\,\cos\theta$, and $v_y(0) = \tan\theta$ as always. Define the function: $\texttt{Verlet}(\theta)$ to be the numerical solution for $y(R)$ given an angle θ, then we have a function whose zero is precisely the correct θ, i.e. we want to find the roots of:

$$F(x) = \texttt{Verlet}(x), \tag{3.21}$$

those roots will be the values of x for which $y = 0$ at $x = R$. So we can define a numerical function of a single variable, and perform our (numerical) root-finding on that.

3.3 Quantum Mechanics

The time-independent Schrödinger equation governing $\psi(x)$ reads:

$$-\frac{\hbar^2}{2\,m}\,\psi''(x) + V(x)\,\psi(x) = E\,\psi(x), \tag{3.22}$$

where $\psi(x)$ is the "wavefunction" describing a particle of mass m moving under the influence of a potential $V(x)$ (in one dimension) with energy E.

We interpret $\psi(x)^* \psi(x)\, dx$ as the probability of finding the particle "near" the location x (i.e. in a window of width dx centered about x). From this point of view, it is clear that we must have:

$$\int_{-\infty}^{\infty} \psi(x)^* \psi(x)\, dx = 1, \tag{3.23}$$

i.e. the particle must be somewhere.

We can rewrite the above ODE to look more like Newton's second law, an equation we know how to solve numerically:

$$\frac{d^2\psi(x)}{dx^2} = -\frac{2\,m}{\hbar^2}\,(E - V(x))\,\psi(x). \tag{3.24}$$

While we're at it, we may as well nondimensionalize the above – let $x \equiv x_0\, q$ where q is dimensionless, then:

$$\frac{d^2\psi(q)}{dq^2} = -\left(\tilde{E} - \tilde{V}(q)\right)\psi(q) \qquad \tilde{E} \equiv \frac{2\,m\,x_0^2}{\hbar^2}\,E \qquad \tilde{V}(q) = \frac{2\,m\,x_0^2}{\hbar^2}\,V(q). \tag{3.25}$$

Associated with this ODE must be some boundary conditions. This is where the shooting method will play an important role. We typically provide boundary conditions that are physically motivated – like $\psi(\pm\infty) = 0$, so that the probability of finding a function out at spatial infinity is zero. On a computer, of course, we have to approximate infinity with some finite value, and in our non-dimensionalized variable q, the only requirement is that $q \gg 1$. For simplicity, we'll work on the half-line, so that we'll take $\psi(0) = 0$ and $\psi(q_\infty) = 0$ for some value q_∞ meant to capture the behavior at spatial infinity.

Now we can begin to see the problem – our second-order ODE solution method is Verlet, and it requires an initial value and initial derivative value, so $\psi(0)$ and $\psi'(0)$. We need to turn a boundary condition into an initial condition. In addition, we know that the ODE (3.25) says nothing about the magnitude of $\psi(x)$ – that magnitude is fixed separately through the condition (3.23), so if we set $\psi(0) = 0$, then $\psi'(0)$ is actually unconstrained – what is the variable that we can move around to correctly match the boundary conditions? Answer: E (or its dimensionless form, $\tilde{E}$).

Our problem, then, amounts to finding both $\psi(q)$ and E, in a particular setting. The way we will accomplish this functionally is to define `Verlet`$(\tilde{E})$

to be the function that gives the numerical value of $\psi(q_\infty)$ given a value of $\tilde{E}^2$. Then the function whose roots we want to find is:

$$F(x) = \texttt{Verlet}(x) \tag{3.26}$$

and those roots will tell us the *allowed energies of the system*. This is clearly a very different sort of physical system, and yet the solution to a variety of problems here boils down to finding the roots of a function $F(x)$.

Example: Particle in a box

For a particle constrained to the interior of a "one-dimensional square well", we have the potential:

$$V(x) = \begin{cases} \infty & x < 0 \text{ or } x > a \\ 0 & 0 < x < a \end{cases} \tag{3.27}$$

Take $x_0 = a$, then in terms of (3.25), we set $\tilde{V}(q) = 0$ for the interior, and require that $\psi(0) = \psi(1) = 0$. Now, we know the solution to the resulting second order ODE:

$$\psi''(q) = -\tilde{E}\,\psi(q) \longrightarrow \psi(q) = A\,\cos(\sqrt{\tilde{E}}\,q) + B\,\sin(\sqrt{\tilde{E}}\,q). \tag{3.28}$$

If we require that $\psi(0) = 0$, then we learn that $A = 0$. We are left with the second boundary condition, at $q = 1$:

$$\psi(1) = B\,\sin(\sqrt{\tilde{E}}) = 0 \tag{3.29}$$

and this could be true if $B = 0$, but then $\psi(q) = 0$, and we have a particle that is not in the box at all (nor outside it), i.e. no particle. Instead, we take:

$$\sqrt{\tilde{E}} = n\,\pi \longrightarrow \tilde{E} = n^2\,\pi^2. \tag{3.30}$$

The boundary condition here has imposed a requirement on the allowed energies of the system – $\sin(n\,\pi) = 0$ for integer n, so the only particle energies you can have inside the box come in discrete steps: $E = \frac{n^2\,\pi^2\,\hbar^2}{2\,m\,a^2}$ for integer n.

[2]What happened to $\psi'(0)$? The value of the derivative of $\psi(x)$ at zero is arbitrary, set externally, so all we need is to give it a non-zero value, say $\psi'(0) = 1$. Note that we have chosen the boundary conditions $\psi(0) = \psi(q_\infty) = 0$, but there are many cases in which $\psi(0)$ is, instead, a constant and $\psi'(0)$, say, is zero. In those cases, we set $\psi(0) = 1$, and our shooting method still proceeds in terms of $\tilde{E}$.

3.4 Bisection

Finally, we come to the relevant numerical method – we will use bisection to find a zero of a function $F(x)$ lying in between two initial points, x_ℓ and x_r. How do we know that there is a root between those two points? What if there is more than one root in there? The easiest thing to do is to plot $F(x)$, always an option, and see roughly where the zero crossings are. Then bookend a particular zero of interest, and hone in on it using the bisection routine.

Bisection itself is almost entirely defined by its name. We start with two locations, x_ℓ and x_r, we evaluate $F(x_\ell)$ and $F(x_r)$ – if a root lies between these two, then one will be positive, and the other negative. Now, we evaluate the function F at the midpoint $x_m \equiv \frac{1}{2}(x_\ell + x_r)$. If $F(x_m)$ has the same sign as $F(x_\ell)$, then the root lies between x_m and x_r – if $F(x_m)$ has the same sign as $F(x_r)$, then the root lies between x_ℓ and x_m. In either case, we update the labels x_ℓ and x_r appropriately, so that the root now lies in an interval half as large as the original one. We continue this process until $F(x_m)$ is as small as we want (set by some external tolerance $\epsilon \sim 10^{-12}$ or so). A schematic of the first few steps of the process is shown in Figure 3.3.

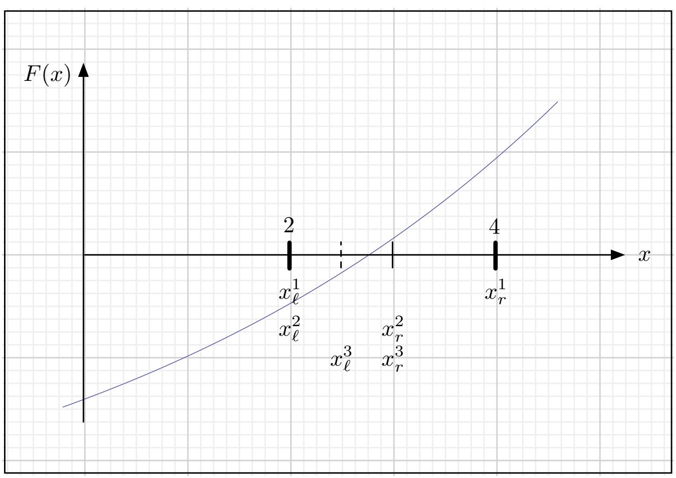

Figure 3.3: The successive bisections for the function $F(x)$. Here, x_ℓ^n and x_r^n refer to the left and right endpoints of the interval for the n^{th} iteration of the bisection.

Lab

In this lab, you will implement the bisection routine sketched in the notes. You can use either a `While` loop, or a recursive approach. The first problem should ensure that your routine is working properly. Don't forget, in all cases, to plot the function whose roots you are trying to find – that will allow you to successively bracket them for bisection honing. Use $g = 9.8$ m/s^2 as the constant associated with gravity near the surface of the earth.

Problem 3.1

Write your bisection function – it should take, as arguments, a function `F` (the function whose roots we are interested in), an initial bracketing, a pair `xl` and `xr`, and a tolerance `eps` that specifies how close to zero we should be before exiting. Try your bisection routine on

$$F(x) = x^3 - \pi\, x^2 - \sqrt{2}\, x + 5. \tag{3.31}$$

Find all three roots, using `eps`$= 10^{-8}$, and record your results below (show five digits):

Problem 3.2

Generate the range formula modified as follows (start from the solution (3.14)): We want the projectile to land on a hill whose height is given by $h(x)$ (a monotonically increasing function of x), a distance R away. Write the function $F(x)$ whose roots you must find in order to find the starting angle θ, given a muzzle speed v, below

Problem 3.3

Continuing with the above problem, find the angle θ given $v = 100$ m/s, and a target range of $R = 100$ m, use $h(x) = \frac{1}{1000}x^2$ as your height function, and write the angle θ you find below (use $\epsilon = 10^{-5}$ in your bisection of the function $F(x)$ you generated in the previous problem):

What happens if you instead set $v = 10$ m/s? What is your physical interpretation of this phenomenon?

Problem 3.4

Write a Verlet-based function that takes `Etilde` as input, solves (3.25) with $\tilde{V}(q) = 0$, $\psi(0) = 0$, $\psi'(0) = 1.0$, and returns the value $\psi(1)$. Call this function `VerletShoot`. What value does your function return when you send in `Etilde`$= .5$ using $N = 2000$ steps?

Problem 3.5

Use your function `VerletShoot`, together with your bisection routine for root-finding, to determine the first four energies $\tilde{E}$ consistent with the boundary condition $\psi(1) = 0$ with `eps`$= 10^{-9}$ (for the bisection routine), record those energies (five digits) below (check against the actual answer):