Computational Physics – Lecture 13

(30 March 2020)

Housekeeping

Remember Zoom etiquette:

1. You are welcome to turn on your video, but keeping it off will conserve your bandwidth.
2. Mute your microphone unless you are speaking to me or the class.
3. There are two ways of saying something: (a) click on the "Raise Hand" button and start speaking when I address you, or (b) type a message in the chat window to the class or privately to me.
4. I am recording this lecture, so you can catch up if you end up having to leave due to a technical problem.

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But we have exclusively focussed on *initial value problems* alone. In physics, many ordinary differential equations arise as *boundary value problems*.

Today's plan

In today's class, we want to learn how to solve boundary value problems using computers.

An example

Consider the boundary value problem

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -g, \tag{1}$$

where $g > 0$ is a constant and the boundary conditions are given as

$$x = 0 \text{ at } t = 0, \tag{2}$$

$$x = 0 \text{ at } t = t_1, \tag{3}$$

where $t_1 > 0$ is a constant.

Cannot solve this using our methods

Let's say we want to solve this problem using the Euler method. How do we proceed?

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As we have seen before, we begin by converting our second-order ODE to two simultaneous first-order ODEs, given by

$$\frac{\mathrm{d}v}{\mathrm{d}t} = -g, \text{ and} \tag{4}$$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = v, \tag{5}$$

where we have introduced a new quantity v.

Cannot solve this using our methods

We can cast our system of equations

$$\frac{\mathrm{d}v}{\mathrm{d}t} = -g, \text{ and} \tag{6}$$
$$\frac{\mathrm{d}x}{\mathrm{d}t} = v, \tag{7}$$

as

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{f}(\mathbf{r}, t), \tag{8}$$

where

$$\mathbf{r} = \begin{bmatrix} v \\ x \end{bmatrix}, \tag{9}$$

and

$$\mathbf{f}(\mathbf{r}, t) = \begin{bmatrix} -g \\ v(t) \end{bmatrix}. \tag{10}$$

Cannot solve this using our methods

Euler's method with step size h will now give us

$$\mathbf{w}_0 = ? \tag{11}$$

$$\mathbf{w}_{j+1} = \mathbf{w}_j + h \cdot \mathbf{f}(\mathbf{w}_j, t_j), \tag{12}$$

where we do not have the information that should replace the question mark.

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So we cannot apply our methods to boundary value problems.

This makes boundary value problems much harder to solve than initial value problems.

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Before learning some methods in detail, we should understand the idea behind these two types of method. Fortunately, this is quite straightforward.

Let us understand this in the context of our example problem.

Shooting methods of solving boundary value problems

In the case of our example problem, we happen to know the solution analytically. It is given by

$$x(t) = \frac{-gt^2}{2} + \frac{gt_1 t}{2}, \tag{13}$$

where g and t_1 are our given constants.

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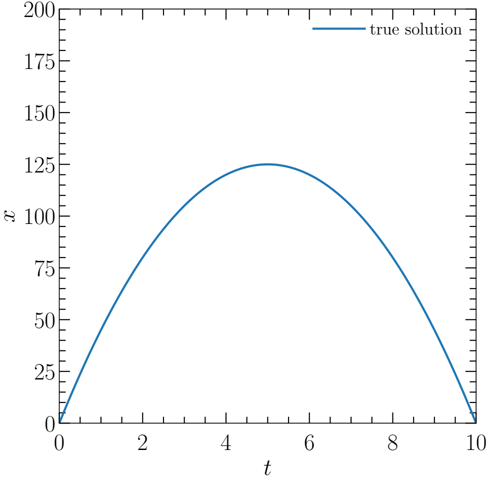
$$x(t) = \frac{-gt^2}{2} + \frac{gt_1 t}{2}, \tag{13}$$

where g and t_1 are our given constants.

(Notice that $\mathrm{d}x/\mathrm{d}t = -gt + gt_1/2$ so $\mathrm{d}^2x/\mathrm{d}t^2 = -g$. Also, $x(0) = 0$ and $x(t_1) = 0$. So this *is* our solution.)

Shooting methods of solving boundary value problems

Here is how the solution looks like for $g = 10$ and $t_1 = 10$:



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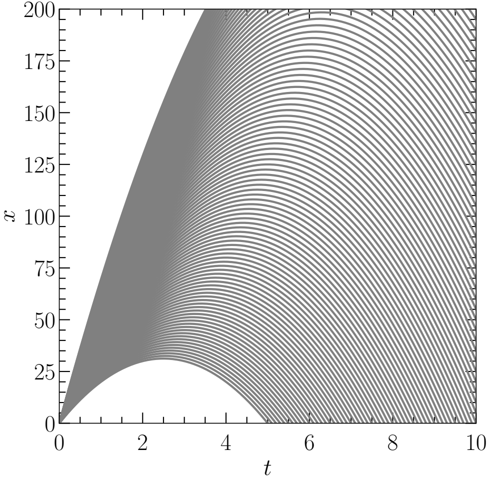
So shooting methods say:

- just assume various initial values of v,
- solve these *initial value problems* using your usual methods, and then
- choose the solution that satisfies the boundary value of x.

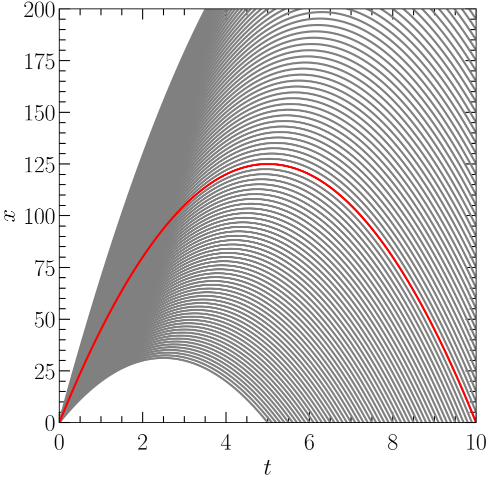
Shooting methods of solving boundary value problems

In our case, the initial value of x is specified. (It is 0.) If we choose a range of initial values on v and solve the resultant *initial value problem* using the fourth-order Runge-Kutta method, we get (for $g = 10$ and $t_1 = 10$)



Shooting methods of solving boundary value problems

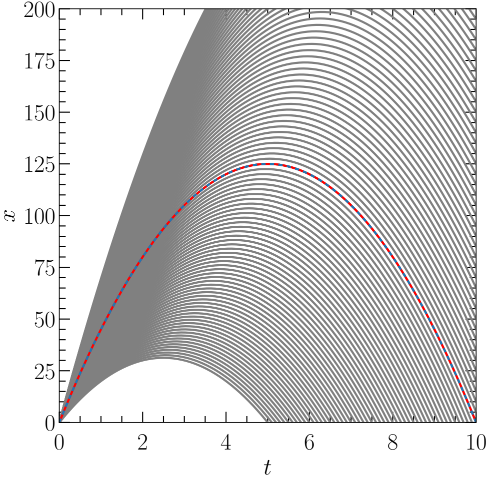
These solutions have different values at $t = t_1$. We now find the solution that is closest to our boundary value $x(t_1) = 0$. We get



(Red curve is the solution reported by the shooting method.)

Shooting methods of solving boundary value problems

Comparing with our true solution tells us that this is a good approximation:



(Red curve is the solution reported by the shooting method. Dashed blue curve is the true solution. They agree.)

Relaxation methods of solving boundary value problems

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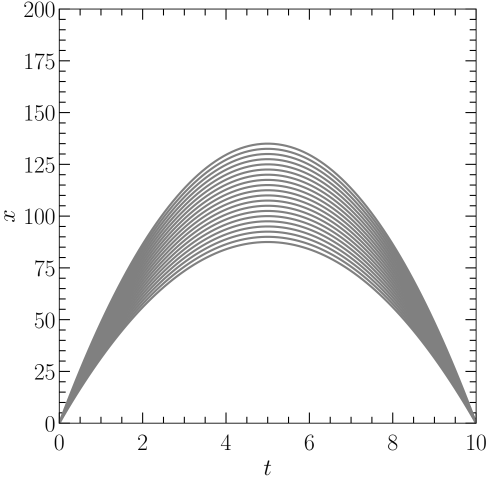
Relaxation methods of solving boundary value problems

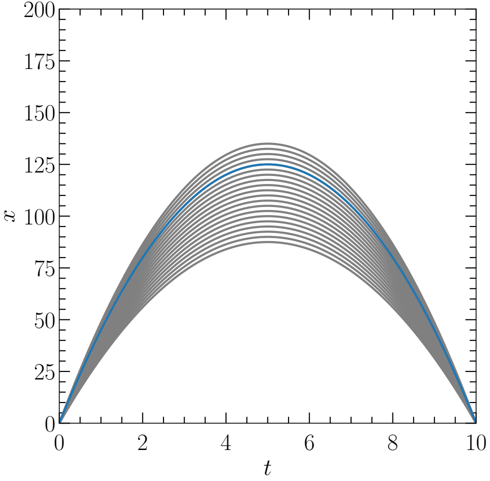
For example, here is a family of functions satisfying our given boundary conditions:



These functions do *not* satisfy our ODE!

Relaxation methods of solving boundary value problems

The function that is closest to satisfying our ODE is our result:



Relaxation methods of solving boundary value problems

The `solve_bvp` function in SciPy's `scipy.integrate` module solves boundary value problems using a type of relaxation method.

Shooting method

Consider the boundary value problem

$$y'' = f(x, y, y'), \tag{14}$$

with $a \geq x \geq b$, $y(a) = \alpha$, and $y(b) = \beta$.

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To solve this problem, we construct a family of initial value problems

$$y'' = f(x, y, y'), \tag{15}$$

with $a \geq x \geq b$, $y(a) = \alpha$, and $y'(a) = t$, and choose $t = t_k$ such that

$$\lim_{k \to \infty} y(b, t_k) = y(b) = \beta \tag{16}$$

Shooting method

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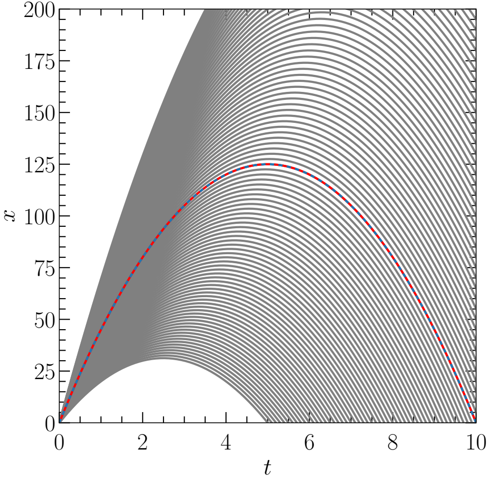
Examples of such iterative procedures are the bisection method, the secant method, or the Newton-Raphson method.

Shooting method

The result will look something like:



Shooting method

Write a Python code to implement our shooting method for the boundary value problem we considered before:

$$\frac{\mathrm{d}^2 x}{\mathrm{d}t^2} = -g, \tag{18}$$

where $g = 10$ and the boundary conditions are given as

$$x = 0 \text{ at } t = 0, \tag{19}$$

$$x = 0 \text{ at } t = t_1, \tag{20}$$

where $t_1 = 10$. Make a figure to show your intermediate solutions, the final solution, and the exact solution.

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How does that work?

Relaxation method

We start with a guess solution $x_0 = 1$ and plug it into the RHS of our equation to get

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Now we repeat the process and get

$$x_2 = 2 - e^{-1.632} \approx 1.804, \tag{23}$$

and so on to get a sequence of x's.

Relaxation method

If I quickly do a few more steps in Python, I get:

1.6321205588285577
1.8044854658474119
1.8354408939220457
1.8404568553435368
1.8412551139114340
1.8413817828128696
1.8414018735357267
1.8414050598547234
1.8414055651879888
1.8414056453310121
So we are converging to the true solution.

Relaxation method

What is happening here is that for a general equation $x = f(x)$ with a true solution x^*, if our guess is x then our updated value is

$$x' = f(x) = f(x^*) + (x - x^*)f'(x^*) + \dots . \tag{24}$$

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We have also used similar relaxation ideas in linear algebra in the context of the Jacobi and Gauss-Seidel techniques. (There, we also manipulated the relaxation concept to achieve over-relaxation.)

Relaxation method

Now, suppose we have a boundary value problem

$$y'' = f(x, y, y') \text{ for } a \geq x \geq b, \tag{26}$$

with $y(a) = \alpha$ and $y(b) = \beta$.

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We then discretise the derivatives to write

$$\begin{aligned} &\frac{y(x_{i+1}) - 2y(x_i) + y(x_{i-1})}{h^2} + \mathcal{O}(h^4) \\ &\qquad = f\left(x_i, y(x_i), \frac{y(x_{i+1}) - y(x_{i-1})}{2h} + \mathcal{O}(h^2)\right) \end{aligned} \tag{27}$$

Relaxation method

Now we can forget the higher-order terms and write $w_0 = \alpha$, $w_{N+1} = \beta$, and

$$\frac{w_{i+1} - 2w_i + w_{i-1}}{h^2} - f\left(x_i, w_i, \frac{w_{i+1} - w_{i-1}}{2h}\right) = 0. \qquad (28)$$

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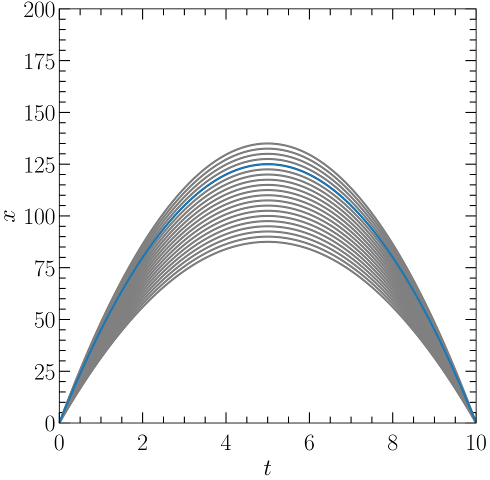
If f is linear, this is a system of linear equations that you can solve using the Jacobi or Gauss-Seidel methods.

Relaxation method

This will result in a sequence of solutions that will converge to the true solution:



Relaxation method

You can implement a relaxation method in your assignment. For the moment, try solving our projectile motion problem using `solve_bvp`.

ODE Wrap-up

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Here is what we have learnt:

1. Euler's Method
2. Error analysis and optimum step size for Euler's Method
3. Taylor and Runge-Kutta Methods
4. ODEs over infinite domains
5. Simultaneous differential equations
6. Higher-order differential equations
7. Adaptive step-size control
8. Backward integration for stiff problems
9. Boundary value problems

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But these methods can be often complex and unnecessary. You can go far with what we learnt.

Still: Keep an open mind. Keep adding methods to your toolbox. Use good libraries.