Computational Physics
Lecture 14 – Solving Boundary Value Problems

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Slides available from https://bb.imperial.ac.uk/

Goals

The point of this lecture is to teach you to

- Properly identify boundary value problems
- Set them up as root-finding problems
- Solve them using the shooting method
- Identify which problems are most amenable to shooting, and which ones are not.

Outline

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Setting up the problem

Any Nth order ordinary differential equation can be recast as a coupled set of N first order ODEs

$$
\begin{aligned}
y'(x) &= y_1(x, y) \\
y_1'(x) &= y_2(x, y, y_1) \\
&\cdots \\
y_{N-2}'(x) &= y_{N-1}(x, y, y_1, y_2, .., y_{N-2}) \\
y_{N-1}'(x) &= F(x, y, y_1, y_2, .., y_{N-2}, y_{N-1})
\end{aligned}
\tag{1}
$$

Note that not every set of N first order ODEs can necessarily be written as an neat *Nth* order ODE

Setting up the problem

Most general problem is to solve any system of N first order ODEs

We can rewrite these as

$$\frac{\mathrm{d}y_i}{\mathrm{d}x}(x) = f_i(x, \vec{y}(x)) \quad (2)$$

where $i = 0..N-1$ and each f_i may individually depend on the full vector $\vec{y} = (y_0, y_1, ..y_{N-1})$

Types of Boundary Conditions

1. $\vec{y}(x_s) = y_{\text{start}}$
   - Function and all derivatives are defined at some x_s
   - All that remains is to evolve the system forwards and/or backwards from x_s to get $\vec{y}(x)$ for all x of interest

These are **Initial Value Problems** – covered two lectures ago

Types of Boundary Conditions

2. Some components of $\vec{y}$ may be specified at one x_s, others at one (or more) other value(s) of x
    - Some components may not be specified anywhere
    - Some may be specified at multiple values of x
    - In general we just require that there are N unique constraints

These are **Boundary Value Problems**

Types of Boundary Conditions

3. Some other more complicated auxiliary condition must be satisfied
   - some combination of values might be fixed at one boundary, e.g.
     $$y_1(0) + y_2^3(0) = A$$
   - or a combination of values at different places, e.g.
     $$y_1(2) + 5y_2(10) = B$$
   - or some non-local condition might exist, e.g.
     $$\max[y_1(x)] = C$$

These are also examples of **Boundary Value Problems** – today's topic.

Outline

1. Quick Recap – Problem and Solution Classes
2. Solution methods for BVPs
   - The shooting method
   - Shooting to an interior point

Outline

The shooting method

The problem

- You have N differential equations, with N-dimensional solution vector $\vec{y}(x)$.
- You have N constraints on $\vec{y}$.
- Those constraints need to be applied at more than one value of x.

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The shooting method

Solution

1. Choose the x_s where the *most* constraints (n_1 of them) are defined
2. Apply them at x_s
3. Guess the remaining $n_2 \equiv N - n_1$ components of $\vec{y}(x_s)$
4. Propagate the system from x_s to other x_o at which remaining constraints are defined
5. Compare the propagated $\vec{y}(x_o)$ to the n_2 other constraints
6. If (when) they don't agree, repeat the process with different guesses

A concrete example

We have 2 coupled first order ODEs

- $y_1(x) \equiv y(x)$ and $y_2(x) \equiv y'(x)$
- We know $y(x_s)$ and $y(x_o)$ but not $y'(x_s)$ nor $y'(x_o)$

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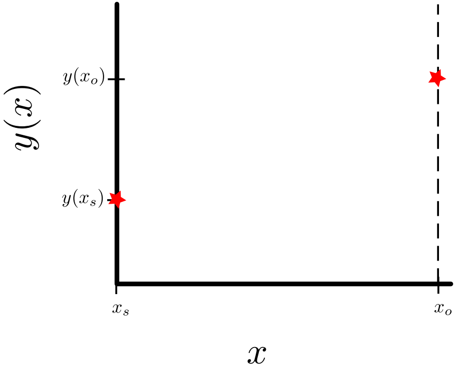

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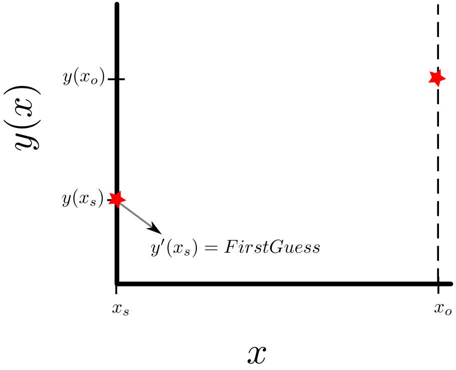

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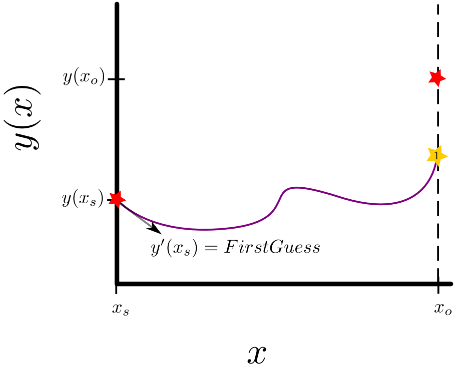

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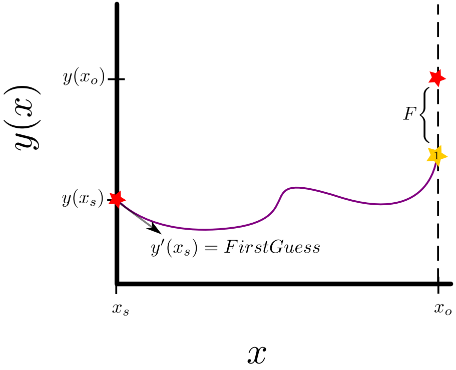

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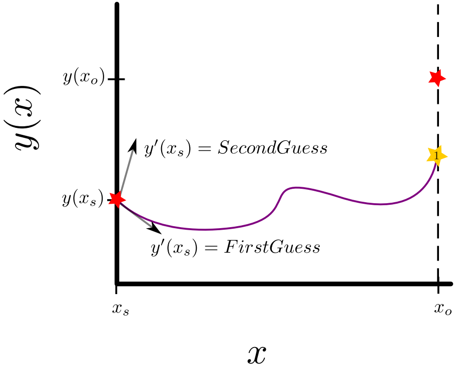

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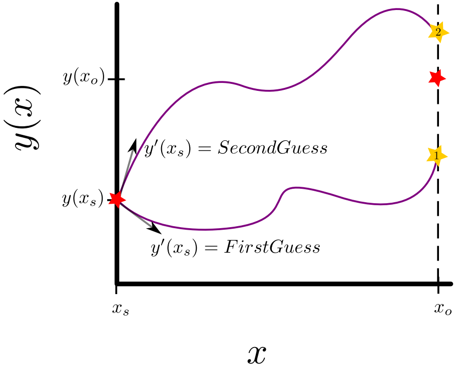
6. If your results at $x = x_o$ bracket the known value, start zooming in



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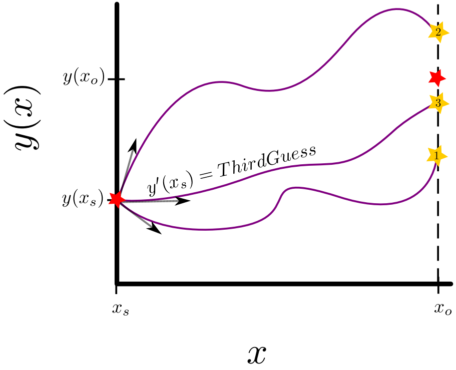

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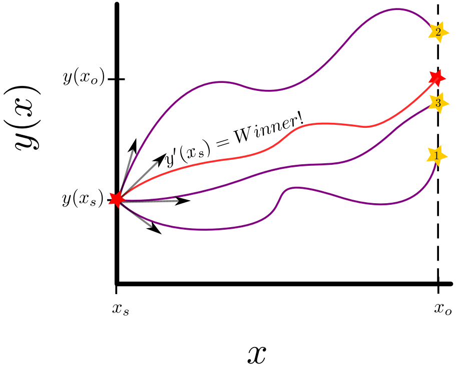

What? Bracketing? I know what this is. . .

BVPs are essentially IVPs wrapped in a root-finding problem

- To solve the IVP, you need to specify an N-dimensional $\vec{y}(x_s)$
- You know n_1 of these components from your BCs at x_s
- $\implies$ you have $n_2 = N - n_1$ unknowns to find
- You have n_2 equations to solve for these n_2 unknowns – these just come from the n_2 other BCs at x_o
- At the simplest level, these equations can be just

$$\vec{F} \equiv \begin{bmatrix} \hat{y}_{n_1}(x_o) \\ \vdots \\ \hat{y}_{N-2}(x_o) \\ \hat{y}_{N-1}(x_o) \end{bmatrix} - \begin{bmatrix} y_{n_1}(x_o) \\ \vdots \\ y_{N-2}(x_o) \\ y_{N-1}(x_o) \end{bmatrix} = \vec{0}, \tag{3}$$

where $\hat{y}_i$ are the solutions to the IVP at $x = x_o$ and y_i are the target values (i.e. the BCs).

Outline

Shoot first, ask questions later...

Shooting may fail due to (or cause?*) interior pathologies

- Bad guesses for $\vec{y}(x_s)$ might cause $\vec{y}$ to hit a singular point between x_s and x_o
- Your numerical approximations around $x = x_o$ may only be stable for a small range of y about the known BC value
  - $\rightarrow$ it is safe to integrate *out of* the BC, but not *into* it

Or, you may just have multiple x_o

- i.e. your BCs are defined at ≥ 3 different x values: x_s, x_{o1}, x_{o2}, etc.

* yes, that is a joke. hah.

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- integrate from both boundaries
- try to match solutions in the middle somewhere

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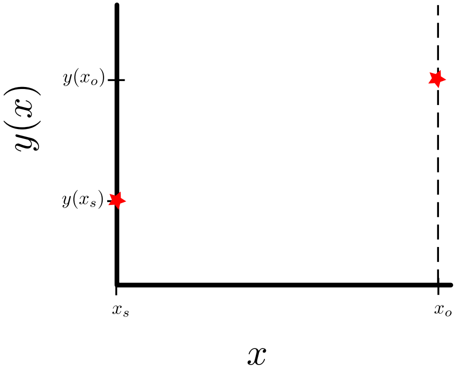

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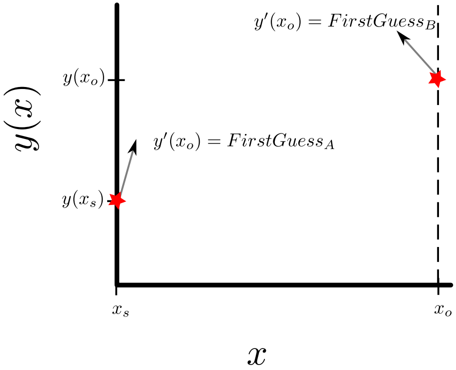

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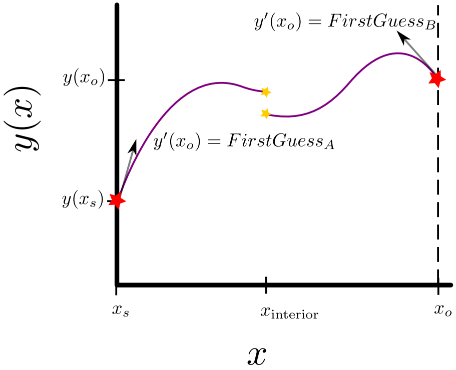

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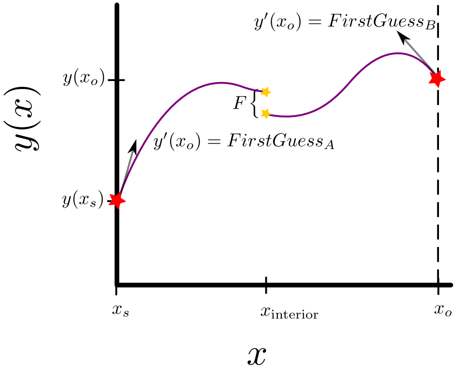

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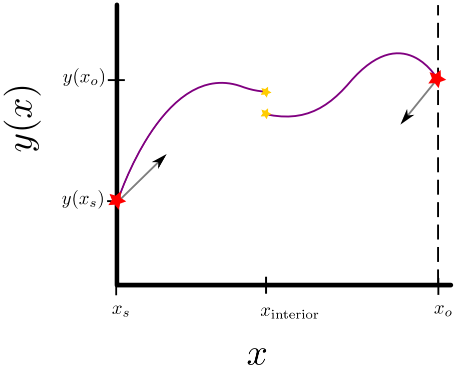

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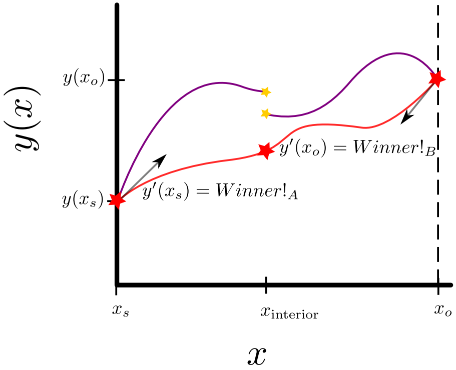
5. Make some more guesses
6. Keep guessing until whole $\vec{y}$ agrees at $x = x_{\text{interior}}$



Notice that in this example we must

- choose **2** derivatives:

$$y'(x_s) \quad \text{and} \quad y'(x_o)$$

- match the result in **2** quantities at the interior point:

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Actually an N-dimensional root-finding problem (instead of n_2-dimensional)

$\Longrightarrow$ often much harder than shooting boundary-to-boundary

So. . .

. . . this means solving an awful lot of IVPs.

And having to do multi-dimensional root-finding. . .

$\implies$ not usually just a simple afternoon's programming.

But – reasonably doable for many not-too-complicated problems.

Sometimes it totally fails

- Surface traversed by the root-finder is too messy
- or the appropriate starting values can't be located
- $\implies$ roots never get found

At that stage it is time to look further afield – relaxation and matrix methods are usually the next port of call.

(Stellar evolution is a classic example.)

Housekeeping

- Tuesday (last examinable lecture): PDEs
- Feedback: what do you want to see in the revision lecture?