Computational Physics – Lecture 12

(18 March 2020)

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4. You can use the chat window also.
5. 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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1. Euler's Method
2. Error analysis and optimum step size for Euler's Method
3. Taylor and Runge-Kutta Methods
4. Multi-dimensional differential equations
5. Simultaneous differential equations
6. Higher-order differential equations
7. Adaptive step-size control

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We want to see what these cases are, why they behave like this, and what can be done about them.

An example

Consider the initial value problem

$$y' = \lambda y, \tag{1}$$

where $\lambda < 0$ and $y(0) = \alpha$.

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But we are interested in getting this solution numerically.

(That is, we are interested in getting an *accurate numerical approximation* to this exact solution.)

Solve example problem using Euler's Method

Let us apply Euler's Method to our given initial value problem with mesh points

$$t_j = jh \qquad j = 0, 1, 2, \ldots, N, \tag{3}$$

where as usual

$$h = \frac{b-a}{N} \tag{4}$$

is the step size. (In our case a is 0 and b is some arbitrary positive real number.)

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What is the numerical approximation to the solution $y(t)$ according to this method?

Solve example problem using Euler's Method

Well, as we have studied before, the solution according to Euler's Method is

$$w_0 = \alpha \tag{5}$$

$$w_{j+1} = w_j + h \cdot f(w_j, t_j), \tag{6}$$

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or, written differently, we have

$$w_0 = \alpha \tag{9}$$

$$w_{j+1} = (1 + h\lambda) w_j. \tag{10}$$

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Is this an accurate approximation to the true solution?

We can answer than question by calculating the error. (We can do this for this example problem because we know the true solution.)

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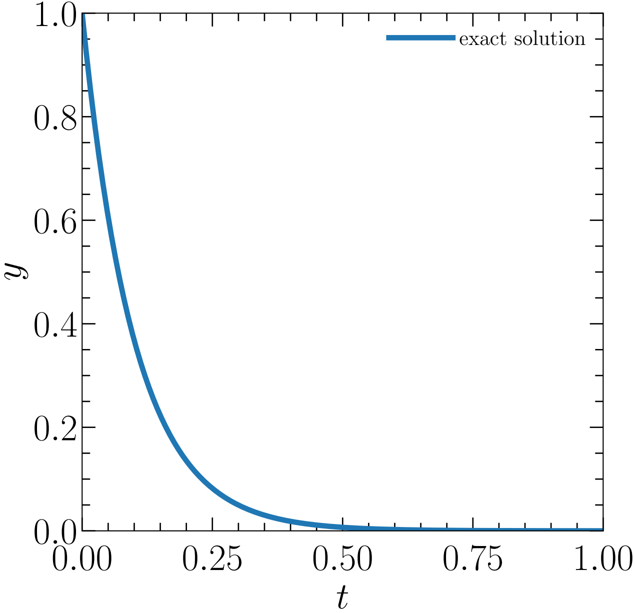
For other values of the step size h, Euler's Method will fail for this problem.

Demo: $y' = -10y$ with $y(0) = 1$



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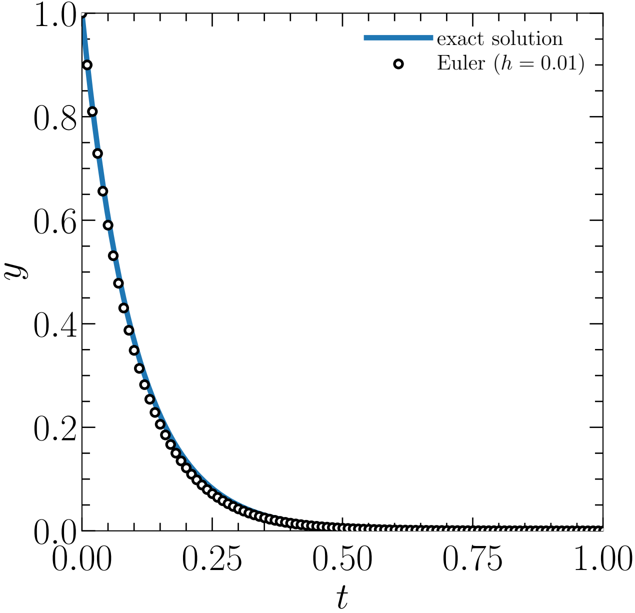

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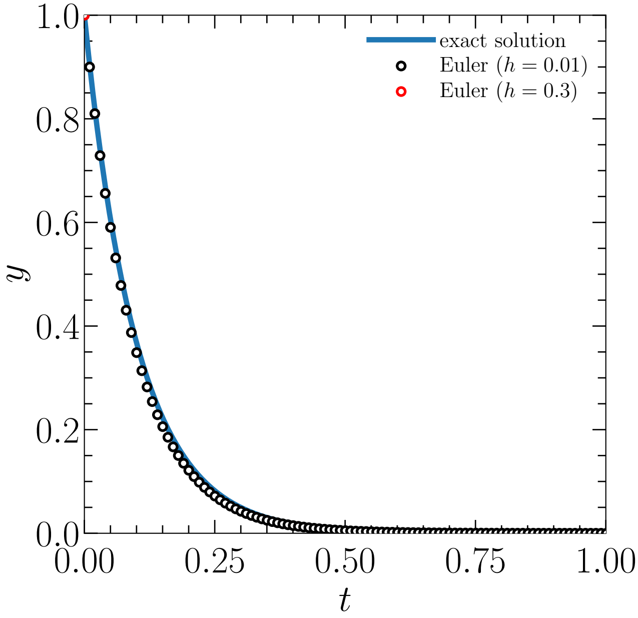

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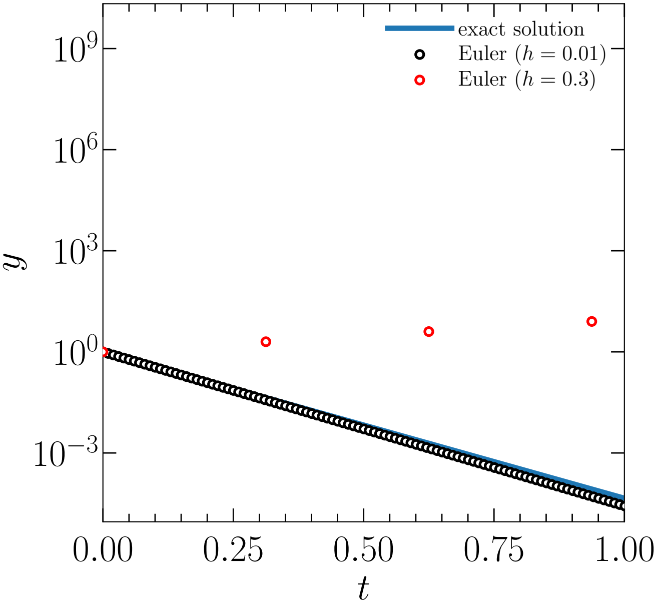

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In general, you get an expression of the form

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The error will grow without bounds if $|Q(h\lambda)| > 1$.

Try other methods?

For an nth-order Taylor Method, for example, you can see that our condition for accuracy becomes

$$\left|1 + h\lambda + \frac{1}{2}h^2\lambda^2 + \cdots + \frac{1}{n!}h^n\lambda^n\right| < 1. \tag{18}$$

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So how do we come up with a method that stays accurate at reasonable values of the step-size h?

A trick: Implicit integration

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So our job now is to come up with methods that have a large stability region.

We do this by means of a trick called implicit integration or backward integration.

Backward (or Implicit) Euler Method

We remember that the Euler method is given by

$$w_0 = \alpha \tag{19}$$

$$w_{j+1} = w_j + h \cdot f(w_j, t_j), \tag{20}$$

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This small change makes a big difference. It transforms our Euler method from being catastrophically inaccurate to being stable for any value of step size h.

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For our example problem, $y' = \lambda y$ with $\lambda < 0$, the implicit Euler method will give

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Luckily, solving for w_{j+1} is easy in this case.

Backward (or Implicit) Euler Method

The solution is

$$w_{j+1} = \frac{w_j}{1 - h\lambda} \tag{27}$$

or

$$w_{j+1} = \left(\frac{\alpha}{1 - h\lambda}\right)^{j+1}. \tag{28}$$

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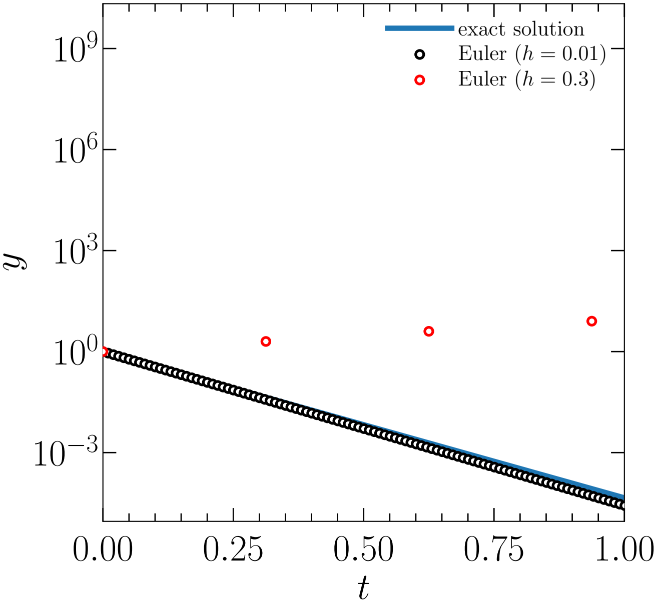
Now we see that that for $\lambda < 0$, the term $(1 - h\lambda)^{j+1}$ will be < 1 as long as $|1 - h\lambda| > 1$ so the error will now not grow catastrophically. We have expanded our region of stability by a large margin.

Demo: $y' = -10y$ with $y(0) = 1$



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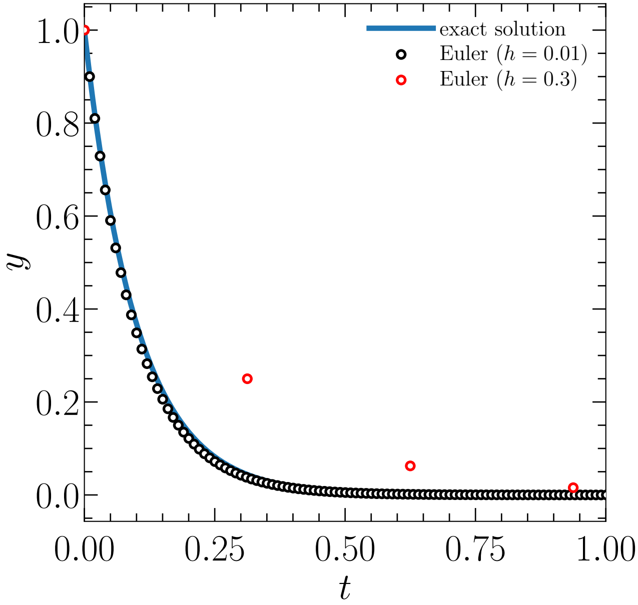

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If the differential equation is not linear, solving for w_{j+1} is hard. We will then have to use a root-finding method such as Newton-Raphson.

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But so what? Is all this relevant beyond our little example?

The answer is unfortunately yes. Implicit methods are useful in solving stiff differential equations, which unfortunately are quite common in physics.

What is a stiff differential equation?

Consider the system of equations

$$u_1' = 9u_1 + 24u_2 + 5\cos t - 13\sin t, \tag{29}$$

$$u_2' = -24u_1 - 51u_2 - 9\cos t + \frac{1}{3}\sin t, \tag{30}$$

with $u_1(0) = 4/3$ and $u_2(0) = 2/3$.

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with $u_1(0) = 4/3$ and $u_2(0) = 2/3$.

The unique solution to this system of equations is

$$u_1(t) = 2e^{-3t} - e^{-39t} + \frac{1}{3}\cos t \tag{31}$$

$$u_2(t) = -e^{-3t} + 2e^{-39t} - \frac{1}{3}\cos t. \tag{32}$$

What is a stiff differential equation?

We see that the solution has a decaying part or a *transient*, namely e^{-39t}. The solution want to move closer to

$$u_1(t) = \frac{1}{3}\cos t \tag{33}$$

$$u_2(t) = -\frac{1}{3}\cos t, \tag{34}$$

as soon as possible. That is why it is stiff.

What is a stiff differential equation?

t	$u_1(t)$ (exact)	$u_1(t)$ (RK4 $h = 0.1$)
0.1	1.793061	-2.645169
0.2	1.423901	-18.45158
0.3	1.131575	-87.47221
0.4	0.9094086	-934.0722
0.5	0.7387877	-1760.016
...	...	...

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In general, in a higher-order initial value problem, the unique solution can have such transient components.

This is the case, e.g., for equations describing an equilibrium between different processes (such as chemical reactions).

Exercise

Solve $y' = -30y$ with $0 \geq t \geq 1.5$ and $y(0) = \frac{1}{3}$

- Using Forward Euler with $h = 0.1$
- Using Backward Euler with $h = 0.1$
- Using Forward fourth-order Runge Kutta with $h = 0.1$

Make a plot showing these solutions and the exact solution.

Remember!

1. Get good sleep and nutrition
2. Keep yourself busy with work but avoid stress and anxiety
3. Maintain good hygiene