COMS30017
COMPUTATIONAL NEUROSCIENCE

LECTURE: INTRODUCTION TO NUMERICAL SOLUTIONS OF DIFFERENTIAL EQUATIONS

Dr. Rahul Gupta
xv20319@bristol.ac.uk

Intended learning outcomes

- Why do we need computer-based numerical algorithms of solving ODEs?

- Some basic methods of numerically solving ODEs

- Some important tips for applying the numerical solution of ODEs in practice

Why do we need Numerical Solutions of the ODEs

- In the previous lecture we saw how to solve an easy ODE analytically.

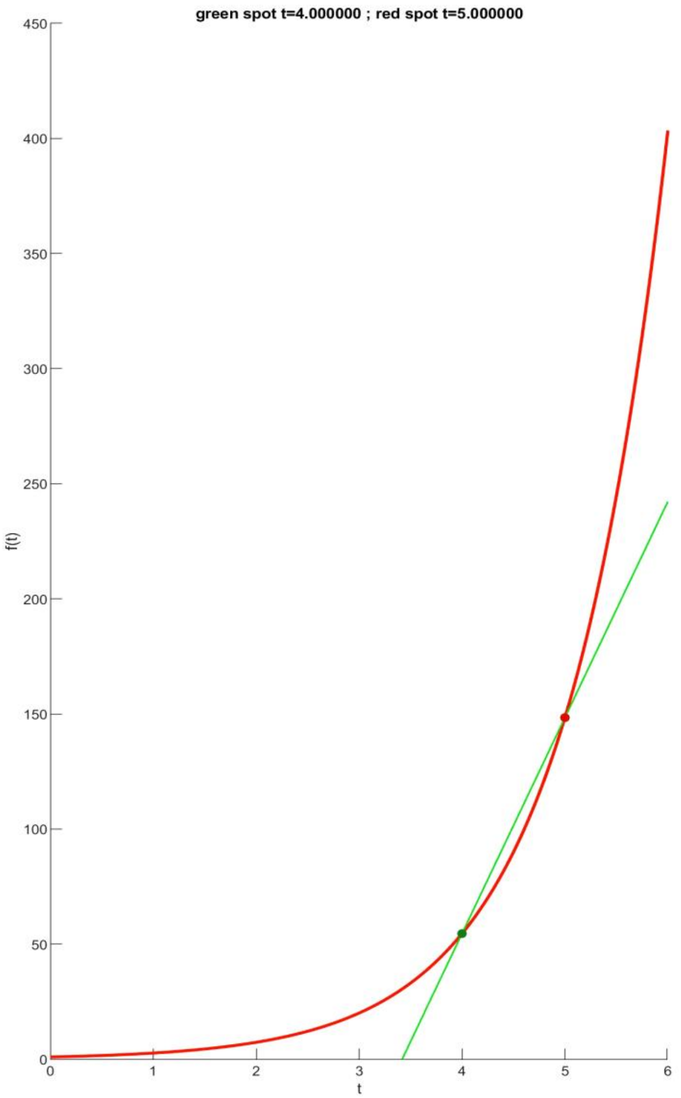
- However for almost any interesting differential equation model of a real-world system, we just can’t solve them analytically, perhaps because
  - : - the function is nonlinear.
  - : - we don’t know $g(t)$ analytically.

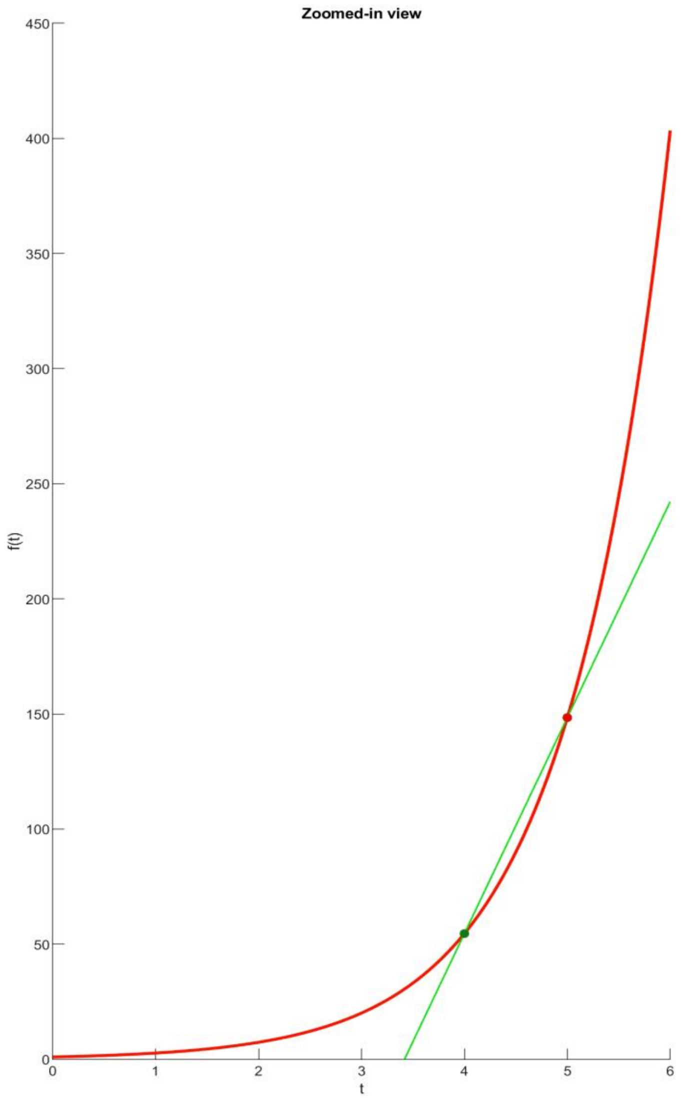
- Do we give up? No! Instead we use computers to approximate the solution function as a series of numbers.

- Most of the algorithms work iteratively

- There are many algorithms for doing this which vary in complexity, accuracy, and computational expense. Which algorithm performs best varies on a case-by-case basis.

Functions $f(t)$ and their Differentials $\frac{df}{dt}(t)$

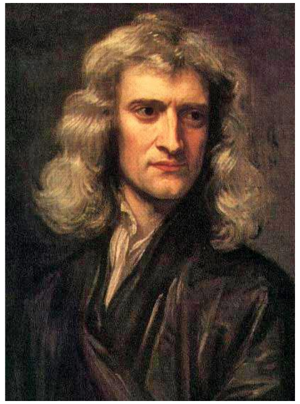




Nonlinear_becomes_linear.avi

Isaac Newton

*wikipedia



$$f(t) = e^t$$

$$\frac{df}{dt}(t) = \lim_{h \to 0} \frac{f(t+h) - f(t)}{h}$$

$$\frac{df}{dt}(t) = \ e^t$$

Instantaneous slope at $t = 4$

!! For an extremely small interval around t = 4, the differential at t = 4 very well approximate the function.

Taylor series for $f(t)$ and Taylor approximation

Brook Taylor

*wikipedia

If a function f(t) is infinitely differentiable at a point $t=t_0$, Taylor series provides a power-series representation of the function at any other point t based on its derivatives at $t=t_0$

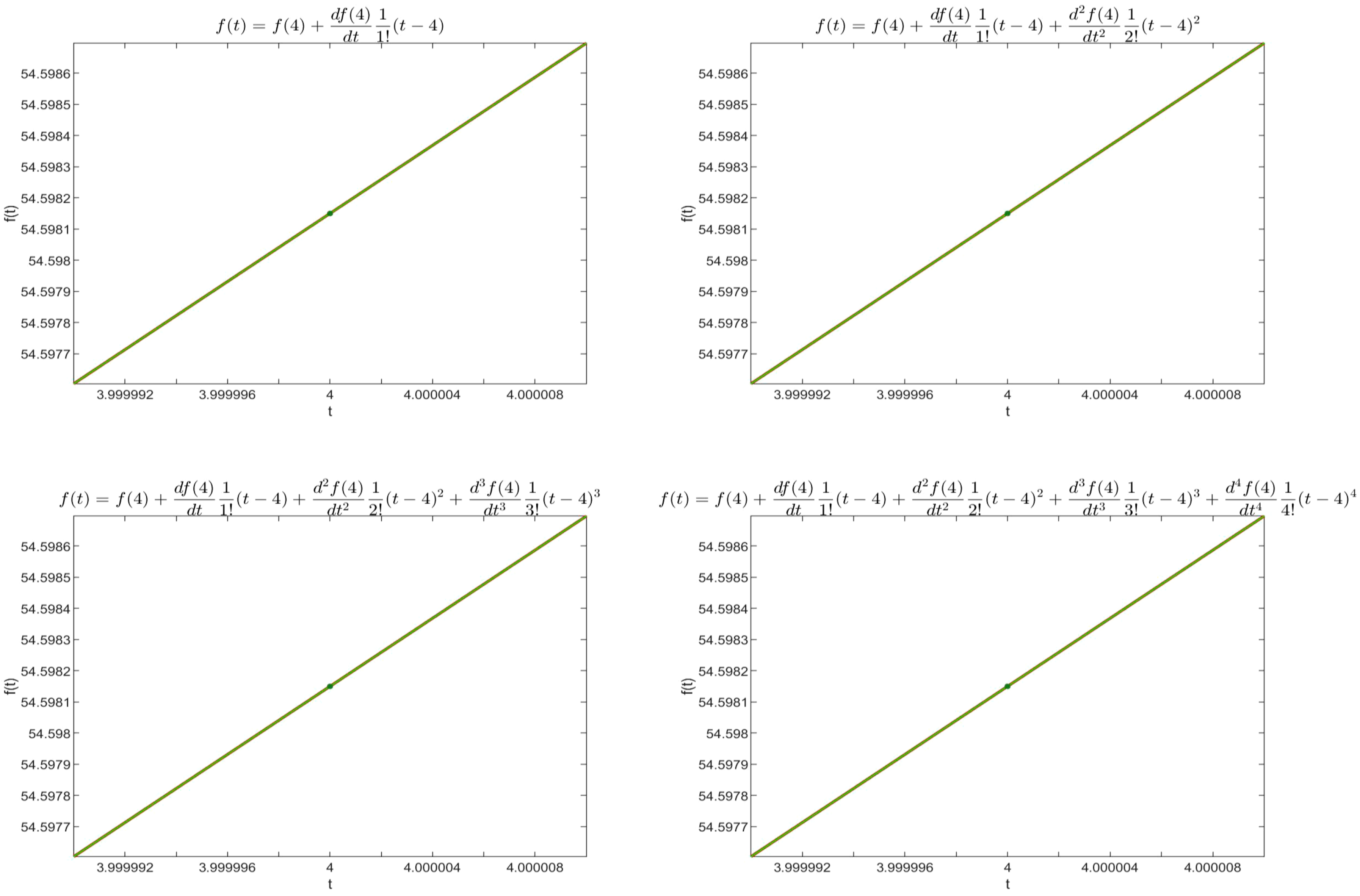
$$f(t) = \sum_{n=0}^{\infty} \frac{d^n f}{dt^n}(t_0)\frac{(t-t_0)^n}{n!}$$

It is typically used to approximate a function local to some point of interest, by truncating the series after a small number of terms:

$$f(t) \approx f(t_0) + \frac{1}{1!}\frac{df}{dt}(t-t_0) + \frac{1}{2!}\frac{d^2f}{dt^2}(t-t_0)^2 + \frac{1}{3!}\frac{d^3f}{dt^3}(t-t_0)^3$$

In this case, the error of the approximation is of order 4 truncation.

Taylor approximation for $f(t) = e^t$ around $t_0 = 4$



Taylor_fits_better.avi

Euler's Method for Numerically Solving ODEs

Leonhard Euler

*wikipedia

It is the most straightforward and simplest method of numerically solving ODEs.

It relies on the basic idea that, if $f(t)$ and $\frac{df}{dt}$ is known at t, the $f(t+\Delta t)$ at the next time-step $t+\Delta t$ can be linearly estimated using the tangent line at t defined by the differential $\frac{df}{dt}$:

$$f(t+\Delta t) = f(t) + \Delta t\left(\frac{df}{dt}(t)\right)$$

This strictly requires that Δt is sufficiently small enough for the linear tangent approximation to work in the neighbourhood of the point t

$$\underbrace{f(t+\Delta t) = f(t) + \frac{df(t)}{dt}\frac{\Delta t}{1!}} + \underbrace{\frac{d^2 f(t)}{dt^2}\frac{\Delta t^2}{2!} + \frac{d^3 f(t)}{dt^3}\frac{\Delta t^3}{3!} + \frac{d^4 f(t)}{dt^4}\frac{\Delta t^4}{4!} + \cdots}$$

Linear approximation

$y = mx + c$

- Collapses to negligible when Δt is extremely small
- Error of approximation is $\mathcal{O}(\Delta t^2)$

Given the IVP:

$$\frac{dx}{dt} = f(x,t), \qquad x(t_0) = x_0$$

Recursive Algorithm:

$$x(t_0) = x_0, \qquad f(x_0, t_0)$$

$$\Downarrow$$

$$x(t_0 + \Delta t) = x(t_0) + \Delta t f(x_0, t_0)$$

$$\Downarrow$$

$$x(t_0 + 2\Delta t) = x(t_0 + \Delta t) + \Delta t f(x(t_0 + \Delta t), t_0 + \Delta t)$$

$$\Downarrow$$

$$x(t_0 + 3\Delta t) = x(t_0 + 2\Delta t) + \Delta t f(x(t_0 + 2\Delta t), t_0 + 2\Delta t)$$

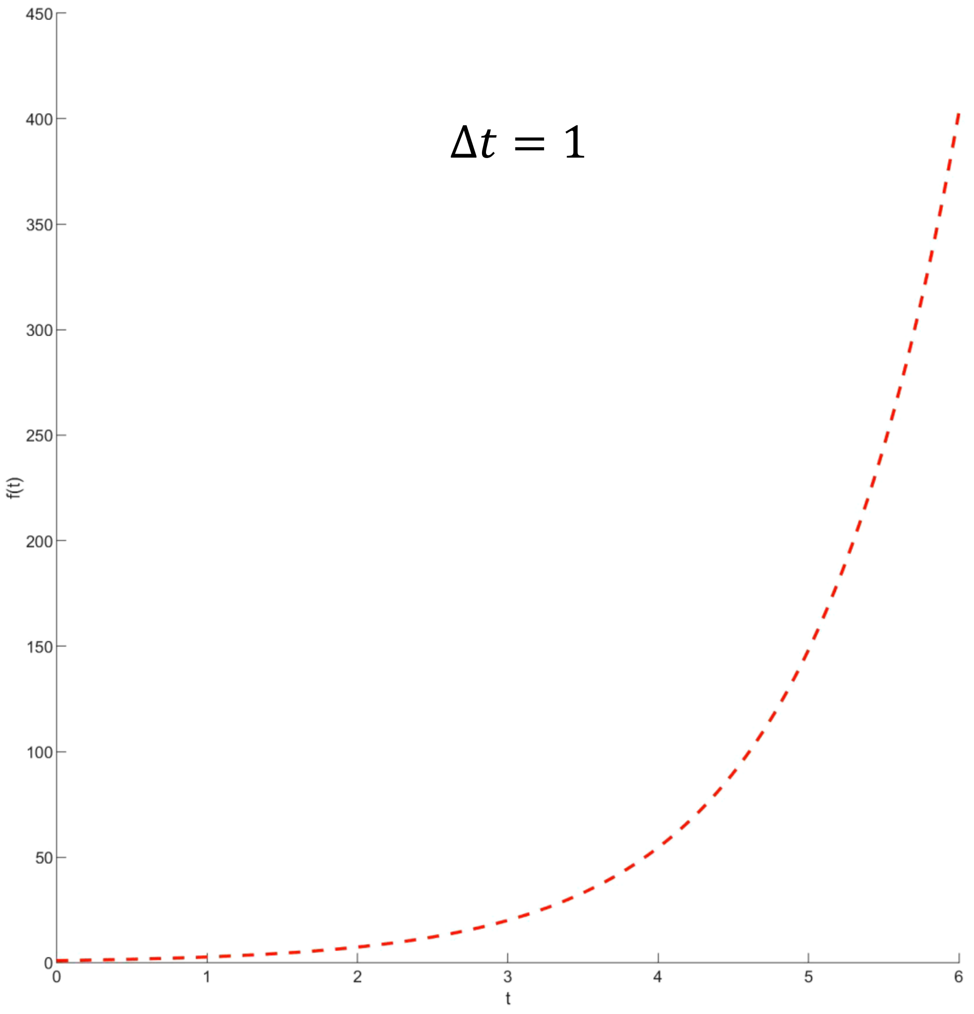
$$\Downarrow$$

$$\Downarrow$$

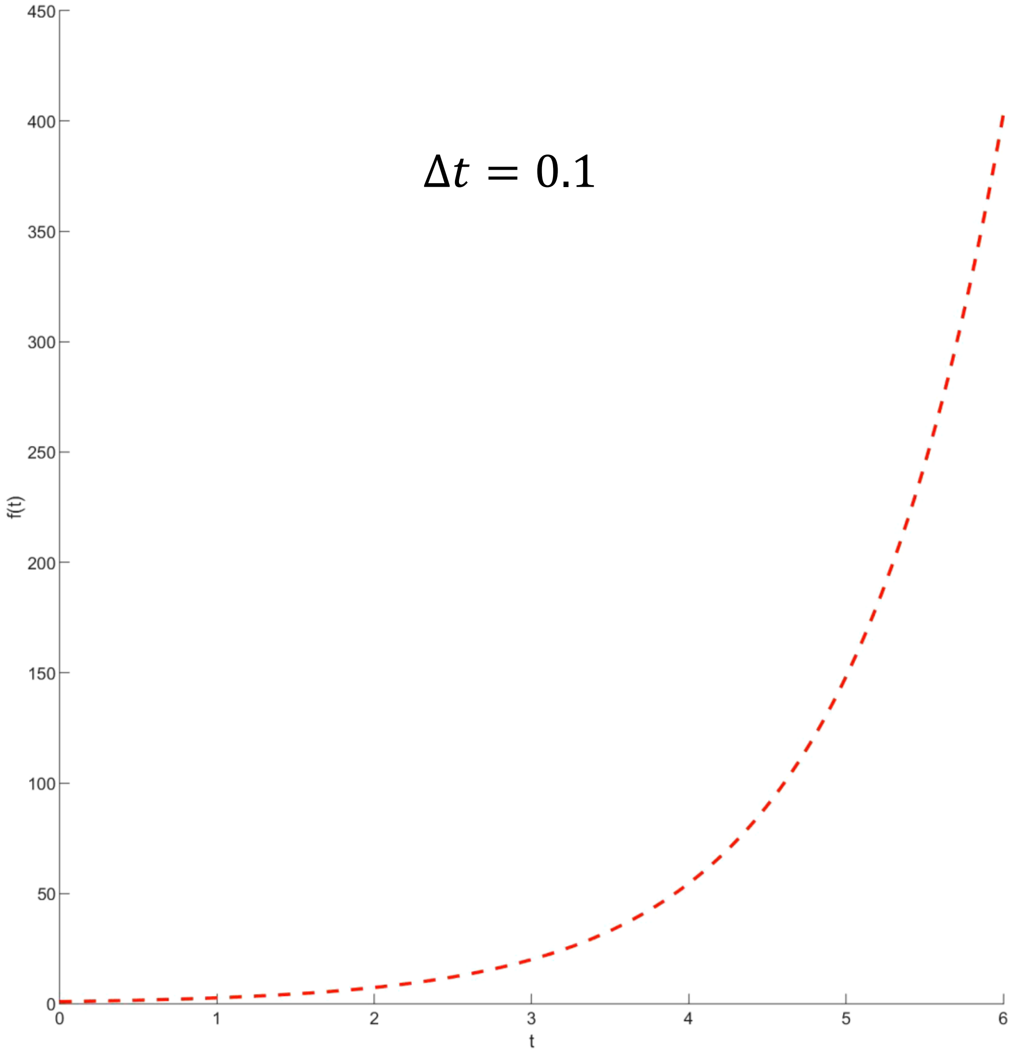
$$\Downarrow$$

$$x(t_0 + n\Delta t) = x(t_0 + (n-1)\Delta t) + \Delta t f(x(t_0 + (n-1)\Delta t), t_0 + (n-1)\Delta t)$$

$\frac{dx}{dt}(t) = x(t)$, starting at $t = 0$ **Analytical Solution** $\rightarrow$ $x(t) = e^t$



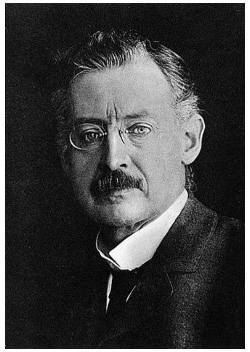
Euler_does_poor.avi



Euler_does_better.avi

!!Larger is the Δt, poorer is the approximation of the original function or solution by the numerical solution

Runge-Kutta Method for Numerically Solving ODEs



Carl Runge

*wikipedia

Martin Kutta

*wikipedia

Runge-Kutta (RK) method is a family of methods with different orders. RK4 is the most popular member

Recursive Algorithm:

1. Given the IVP: $\frac{dx}{dt} = f(x,t),\ x(t_0) = x_0$

2. Choose a step-size Δt

3. Compute $k_1 = f(x_0, t_0)$ and move to the new point $t_0 + \frac{\Delta t}{2}$ from the original point t_0 with slope k_1, yielding $x\left(t_0 + \frac{\Delta t}{2}\right) = x_0 + k_1\frac{\Delta t}{2}$

4. Now, compute $k_2 = f\left(x\left(t_0 + \frac{\Delta t}{2}\right), t_0 + \frac{\Delta t}{2}\right)$ and again move to the point $t_0 + \frac{\Delta t}{2}$ from the original point t_0 but with slope k_2, yielding a different $x\left(t_0 + \frac{\Delta t}{2}\right) = x_0 + k_2\frac{\Delta t}{2}$

5. Compute $k_3 = f\left(x\left(t_0 + \frac{\Delta t}{2}\right), t_0 + \frac{\Delta t}{2}\right)$, but using $x\left(t_0 + \frac{\Delta t}{2}\right)$ obtained in step 4.

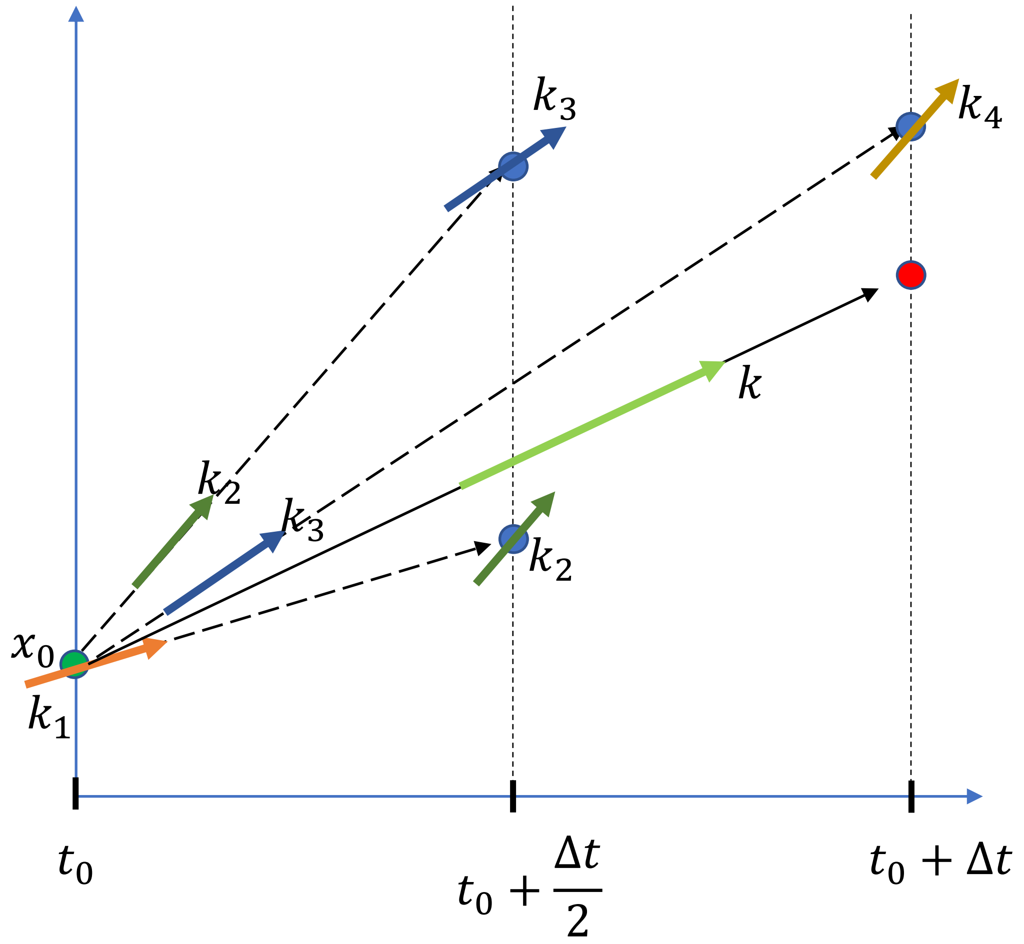
6. Now, move to the point $t_0 + \Delta t$ from the original point t_0 with slope k_3, yielding $x(t_0 + \Delta t) = x_0 + k_3 \Delta t$

7. Compute $k_4 = f(x(t_0 + \Delta t), t_0 + \Delta t)$

8. Obtain the average slope $k = \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$

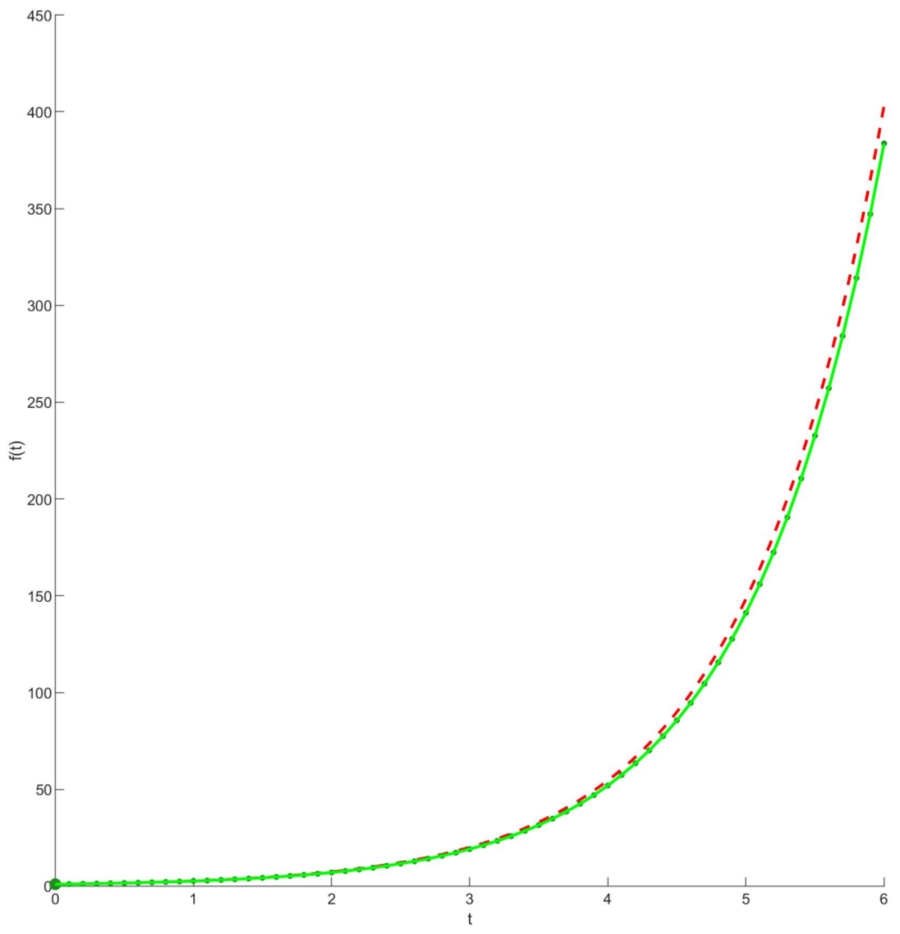
9. Make the final conclusive jump from the original point t_0 to the point $t_0 + \Delta t$, with $x(t_0 + \Delta t) = x_0 + k\Delta t$

A crude geometric depiction of RK4 Method

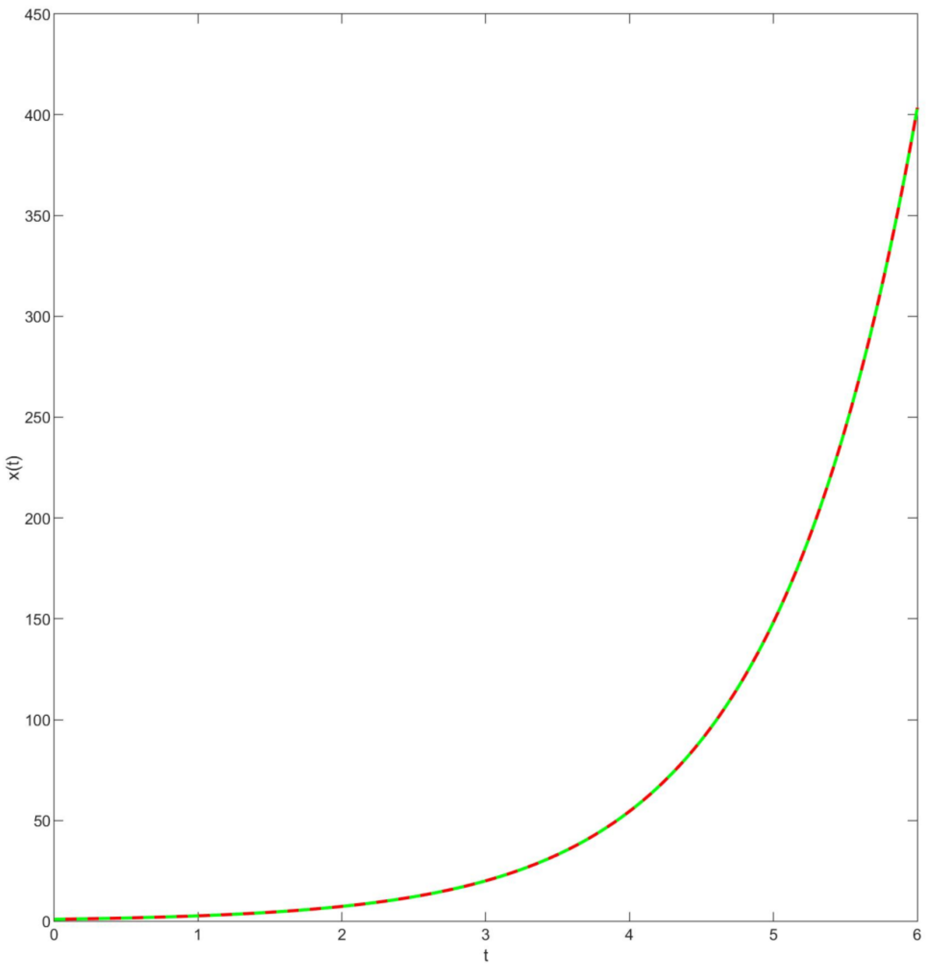


Better Accuracy: RK4 vs Euler Methods

Euler method, $\Delta t = 0.1$



RK4, $\Delta t = 0.1$



Euler vs RK in practise

- Both Euler and Runge-Kutta are widely used in practise.

- Because of its simplicity, Euler is especially common for quick-and-dirty models when people want to manually code something. You will use it in your coursework.

- Coding Runge-Kutta is more involved (usually though we just use a DE solver package that someone else has written in a black-box way).

- As you might guess Runge-Kutta is also computationally more expensive than Euler, per timestep.

- However RK's gain in accuracy over Euler usually more than offsets the increased computation time. This means that with Runge-Kutta we can get away with bigger timesteps, making it more efficient than Euler overall.