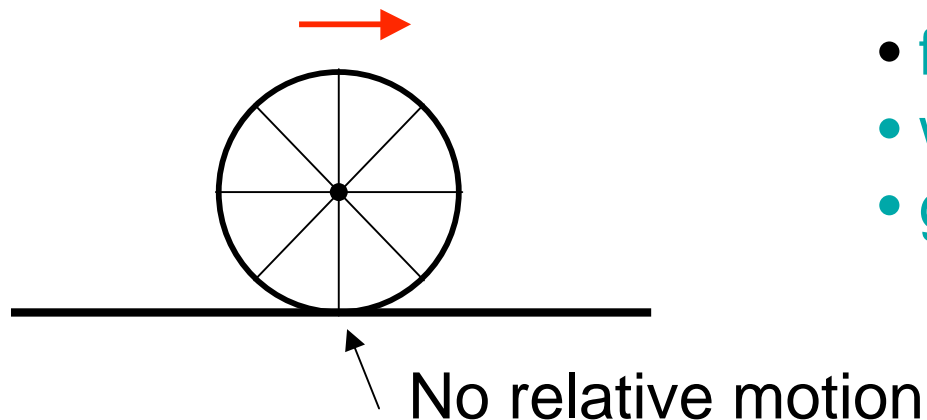


Ordinary Differential Equations

In this lecture, we will look at different options for coding simple differential equations. Start by considering bicycle riding as an example.

Why does a bicycle move forward ? Friction between the wheel and the ground. We will assume no relative motion (no sliding or slipping), so no energy lost there.



Sources of energy loss:

- friction among parts
- wind resistance
- gravity (if going uphill)

Bicycle Riding

Assuming flat terrain and no friction or wind resistance:

$$\frac{F}{m} = \frac{dv}{dt}$$

F is force provided by rider

m is mass of bicycle + rider

F is difficult to determine. Easier to work with power. Elite riders can produce a steady 400W for an extended period (1 hour or so).

$$P = \frac{dE}{dt}$$

E is the (kinetic) energy = $1/2mv^2$

P is the power provided by the rider = $mv dv/dt$

Bicycle Riding

We assume P is a constant (not good approximation when first get started, but once moving this is better).

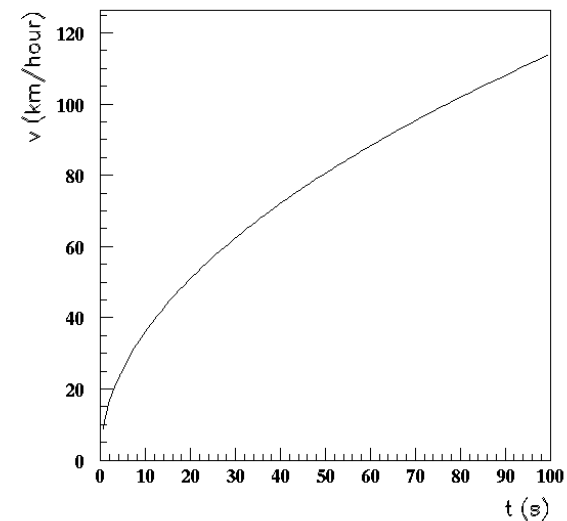
$$P = mv\dot{v} \quad \text{or} \quad \frac{dv}{dt} = \frac{P}{mv}$$

can write

$$v dv = \frac{P}{m} dt \quad \text{integrating yields} \quad \frac{1}{2}(v^2 - v_0^2) = \frac{P}{m}(t - t_0)$$

$$\text{setting } t_0 = 0, \text{ we have } v = \sqrt{\frac{2Pt}{m} + v_0^2}$$

Result is clearly nonsense - need friction and wind resistance !



Bicycle Riding

Let's see how we can code this. On the computer, we go back to the definition of the derivative as a limit of a ratio of differences:

$$\frac{dv}{dt} = \lim_{\delta t \rightarrow 0} \frac{v(t + \delta t) - v(t)}{\delta t} \approx \frac{v(t + \Delta t) - v(t)}{\Delta t}$$

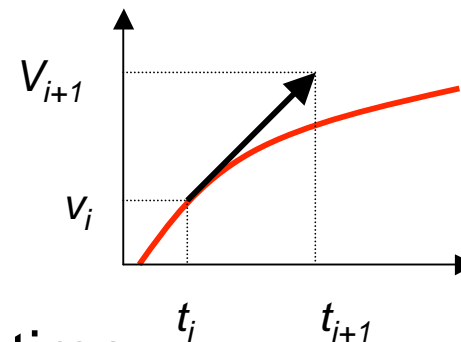
where Δt is the (usually constant) step size used in the computer

If we take $v(t = 0) = v_0$ and use the notation $v_i = v(i\Delta t)$, then

$$v_{i+1} = v_i + f(v, t)\Delta t, \quad \text{where } f(v, t) = \frac{dv}{dt}$$

In our example:

$$v_{i+1} \approx v_i + \frac{P}{mv_i} \Delta t$$



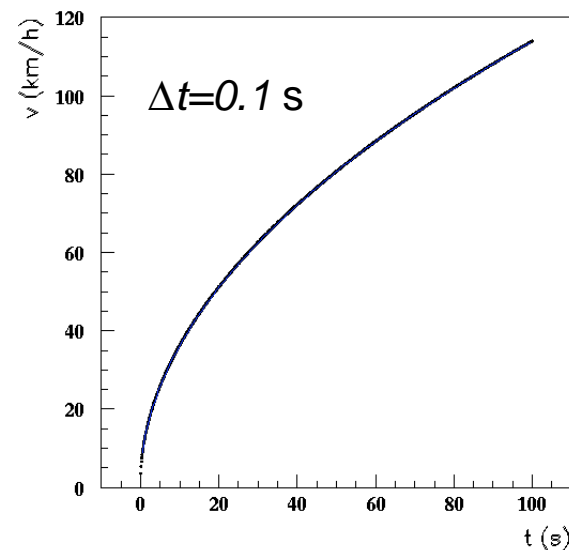
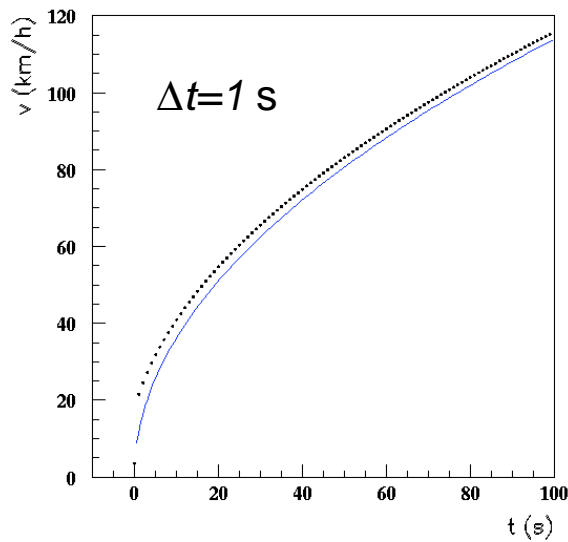
Use slope at t_i to estimate v at later time.

Bicycle Rider

Looking at the previous diagram, probably some thoughts arise:

- The smaller the time step, the better the approximation (but then the amount of computer time will go up as $T/\Delta t$)
- Maybe there are better ways to approximate the best slope for the time interval. We will look into this later.

Forging ahead with this simple algorithm (Called Euler algorithm):



Bicycle Rider

Let's now add some friction and air resistance. At large enough speed, we can approximate the drag force as:

$$F_{drag} \approx -Bv^2$$

We ignore friction in the bike - it is usually a small effect compared to air resistance. The coefficient B can be broken down as follows:

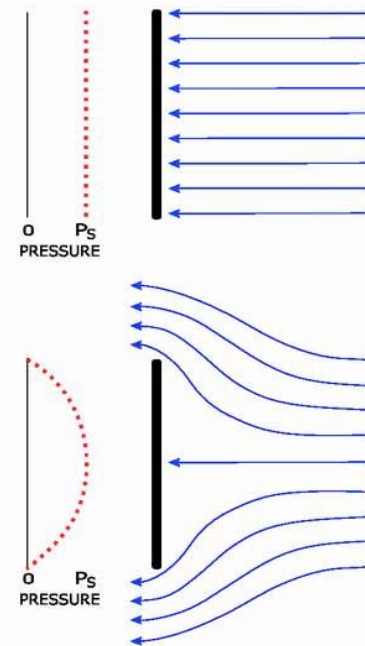
$$B = \frac{1}{2} C \rho A \quad \text{where}$$

C is the 'drag coefficient' - number not too far from 1

ρ is the density of air

A is the effective frontal area

Typical bike riding, $C=0.9$



Bicycle Rider

Let's add this drag force to our equations:

$$F_{drag} = m \frac{dv}{dt}, \quad \text{or} \quad \Delta v = \frac{F_{drag}}{m} \Delta t$$

Putting this together with our previous expression

$$\Delta v = \frac{P}{mv} \Delta t + \frac{F_{drag}}{m} \Delta t, \quad \text{or, on the computer}$$

$$v_{i+1} = v_i + \frac{P}{mv_i} \Delta t - \frac{C \rho A v_i^2}{2m} \Delta t$$

We take the following values:

$$A = 0.33 \text{ m}^2$$

$$C = 0.9$$

$$m = 80 \text{ kg (racer+bike)}$$

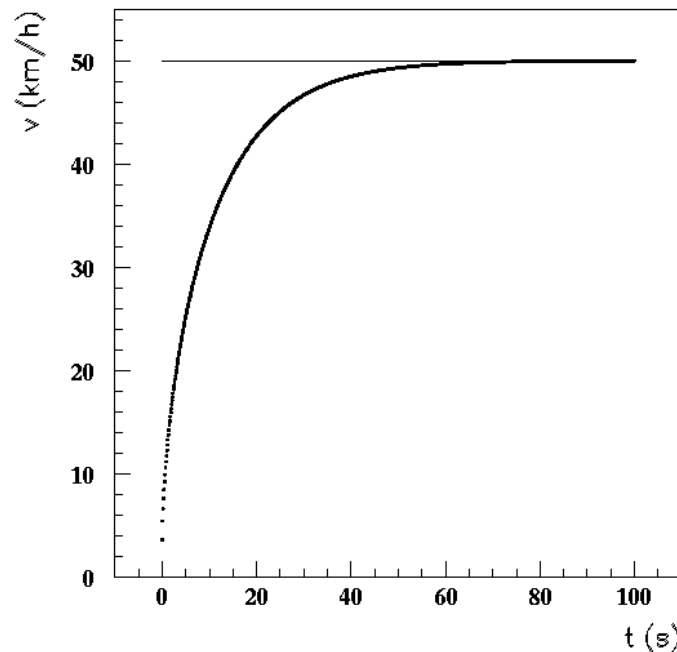
$$\rho = 1 \frac{\text{kg}}{\text{m}^3}$$

Bicycle Rider

We can solve for the equilibrium speed by setting the derivative to zero:

$$0 = \frac{P}{mv} - \frac{C\rho Av^2}{2m} \Rightarrow v^3 = \frac{2P}{C\rho A} \Rightarrow v = 13.9 \frac{\text{m}}{\text{s}} = 50 \frac{\text{km}}{\text{h}}$$

Compare to numerical solution with Euler algorithm:



Terminal velocity is 50 km/h. This is very close to actual max speeds achieved by professional riders.

Error in Numerical Differentiation

To **estimate** the error from the algorithm to calculate the derivative numerically, we compare to a Taylor series expansion:

$$\begin{aligned}\frac{f(x+h) - f(x)}{h} &= \frac{f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \dots - f(x)}{h} \\ &= f'(x) + \frac{h}{2}f''(x) + \dots\end{aligned}$$

When we replace $f'(x) \rightarrow \frac{f(x+h) - f(x)}{h}$

We make an error of about $hf''(x)$

Assuming that h is small so that each term in the series is much smaller than the previous one.

Error in Numerical Differentiation

How does this compare with the round-off error of the computer ?

$$\left| \frac{\overline{\Delta f}}{\Delta x} - \frac{\Delta f}{\Delta x} \right| \leq \left| \frac{\Delta f}{\Delta x} \right| 3\varepsilon + \left| \frac{f(x)}{h} \right| 2\varepsilon$$

See Scherer Lecture notes

So: want minimum h to minimize algorithm error, but small h can lead to large rounding error (they accumulate). Optimal value when errors comparable:

$$\frac{h}{2} f''(x) = \left| \frac{f(x)}{h} \right| 2\varepsilon$$

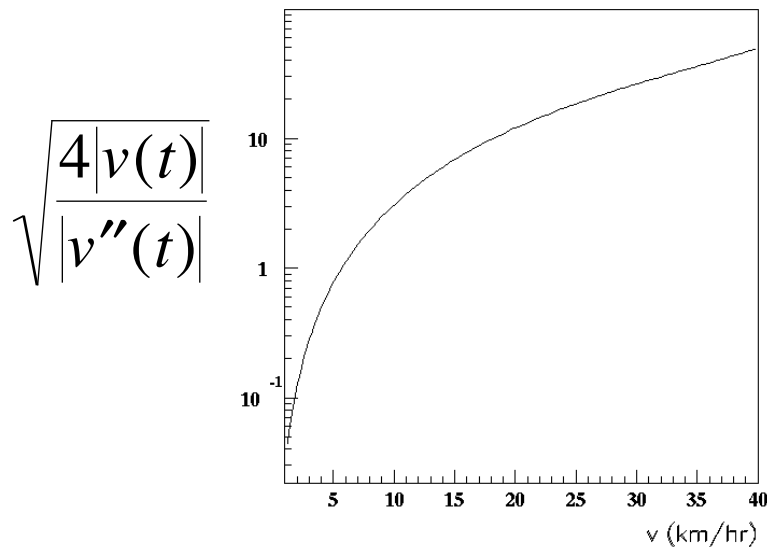
Bicycle Rider Example

For our bicycle riding example :

$$\frac{dv}{dt} = \frac{P}{mv} - \frac{C\rho Av^2}{2m}$$

$$\frac{d^2v}{dt^2} = -\left(\frac{P}{mv^2} + \frac{C\rho Av}{m}\right)\frac{dv}{dt} = -\frac{P^2}{m^2v^3} - \frac{PC\rho A}{2m^2} + \frac{C^2\rho^2 A^2v^3}{2m^2}$$

Condition on previous page yields: $\Delta t^2 = 4\varepsilon \frac{|v(t)|}{|v''(t)|}$



At small v , want $\Delta t \leq \sqrt{\varepsilon}$

At large v , can be much larger

(Because $v'' \rightarrow 0$)

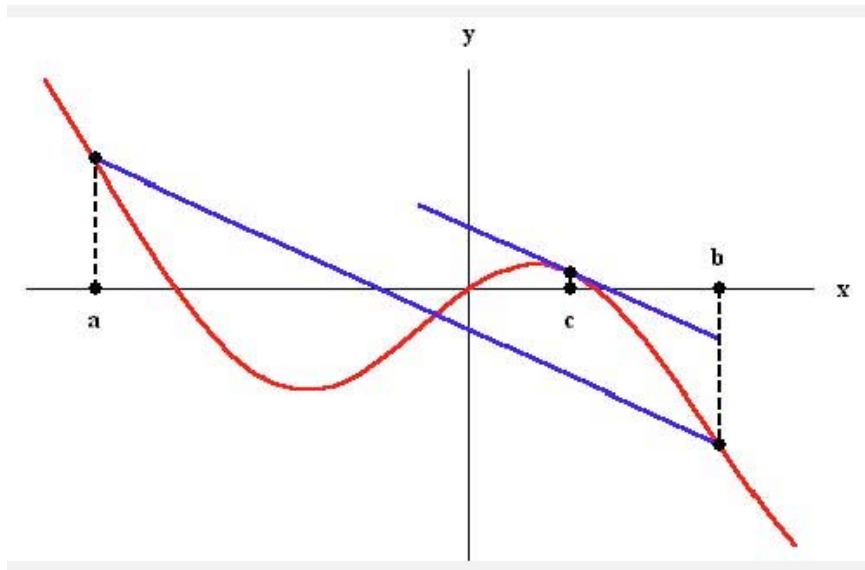
$$\Delta t = \sqrt{\varepsilon} = 3 \cdot 10^{-4} \text{ for single precision,}$$

$$10^{-8} \text{ double precision}$$

More on Derivatives

We now look into different approaches to code derivatives. We use the Mean Value Theorem for guidance:

In calculus, the mean value theorem states, roughly, that given a section of a smooth curve, there is a point on that section at which the derivative (slope) of the curve is equal to the "average" derivative of the section. It is used to prove theorems that make global conclusions about a function on an interval starting from local hypotheses about derivatives at points of the interval. (Wikipedia)



Derivative at c is same as average derivative from a to b

How does this guide us ?

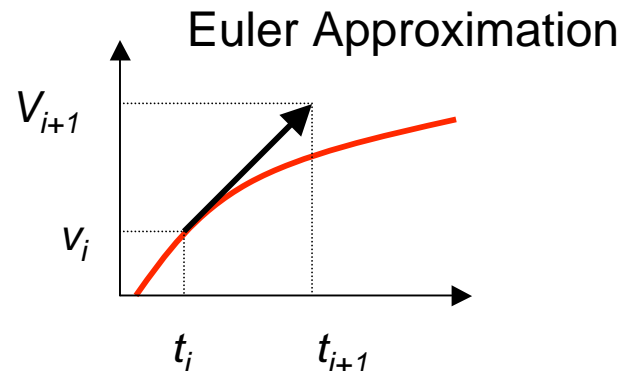
Mean Value Theorem

Note that replacing $dt \rightarrow \Delta t$ is equivalent to integration

$$\Delta x = \int_{t_1}^{t_2} \frac{dx}{dt} dt = x(t_2) - x(t_1)$$

We can state the Mean Value Theorem as

$$x(t + \Delta t) = x(t) + \left. \frac{dx}{dt} \right|_{t_m} \Delta t \quad \text{where } t_m \text{ is between } t_1, t_2$$



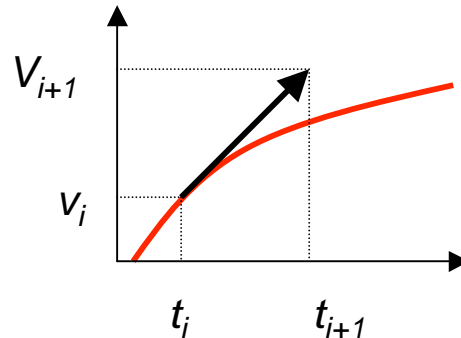
In the Euler approximation, $t_m = t_1$

$$\text{Error} \propto \frac{d^2 x}{dt^2}$$

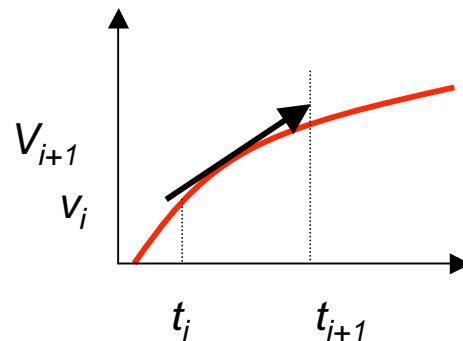
Look at some alternative choices

More on Derivatives

If we look at what we have done, basically, we estimate the derivative over the interval Δt with the derivative at the start of the interval.



We can do better by trying to find an average derivative:



We look at options for finding this average derivative

Runge-Kutta Method

2nd order Runge-Kutta construction:

$$x(t + \Delta t) = x(t) + f(x', t')\Delta t \quad \text{where} \quad \frac{dx}{dt} = f(x, t)$$

$$x' = x(t) + \frac{1}{2} f(x(t), t)\Delta t \quad t' = t + \frac{1}{2} \Delta t$$

so, $\left. \frac{dx}{dt} \right|_{t_m}$ is approximated by $f(x', t')$ where

t' is at the middle of the time interval, and

x' is the Euler approximation for x at the midpoint

To see the accuracy of a particular method, we compare to a Taylor series expansion:

$$x(t + \Delta t) = x(t) + \frac{dx}{dt} \Delta t + \frac{1}{2} \frac{d^2x}{dt^2} (\Delta t)^2 + \frac{1}{6} \frac{d^3x}{dt^3} (\Delta t)^3 + \dots = \sum_{n=0}^{\infty} \frac{x^{(n)}(t)}{n!} (\Delta t)^n$$

Runge-Kutta Method

Taylor Series:
$$x(t + \Delta t) = x(t) + \frac{dx}{dt} \Delta t + \frac{1}{2} \frac{d^2x}{dt^2} (\Delta t)^2 + \frac{1}{6} \frac{d^3x}{dt^3} (\Delta t)^3 + \dots$$

The Euler Method is of $O(\Delta t)$, because that is highest order term

2nd order R-K:
$$x(t + \Delta t) = x(t) + f(x', t') \Delta t = x(t) + \frac{dx'}{dt'} \Delta t$$

$$dx' = dx + \frac{1}{2} \frac{\partial f(x, t)}{\partial x} dx \Delta t + \frac{1}{2} \frac{\partial f(x, t)}{\partial t} dt \Delta t$$

$$dt' = dt$$

so,

$$\begin{aligned} x(t + \Delta t) &= x(t) + \left[\frac{dx}{dt} + \frac{1}{2} \frac{\partial f(x, t)}{\partial x} \frac{dx}{dt} \Delta t + \frac{1}{2} \frac{\partial f(x, t)}{\partial t} \Delta t \right] \Delta t \\ &= x(t) + \frac{dx}{dt} \Delta t + \frac{1}{2} \frac{d^2x}{dt^2} (\Delta t)^2 \quad O(\Delta t)^2 \end{aligned}$$

Runge-Kutta Method

Let's try it out on the bike riding example:

$$\frac{dv}{dt} = f(v, t) = \frac{P}{mv} - \frac{C\rho Av^2}{2m}$$

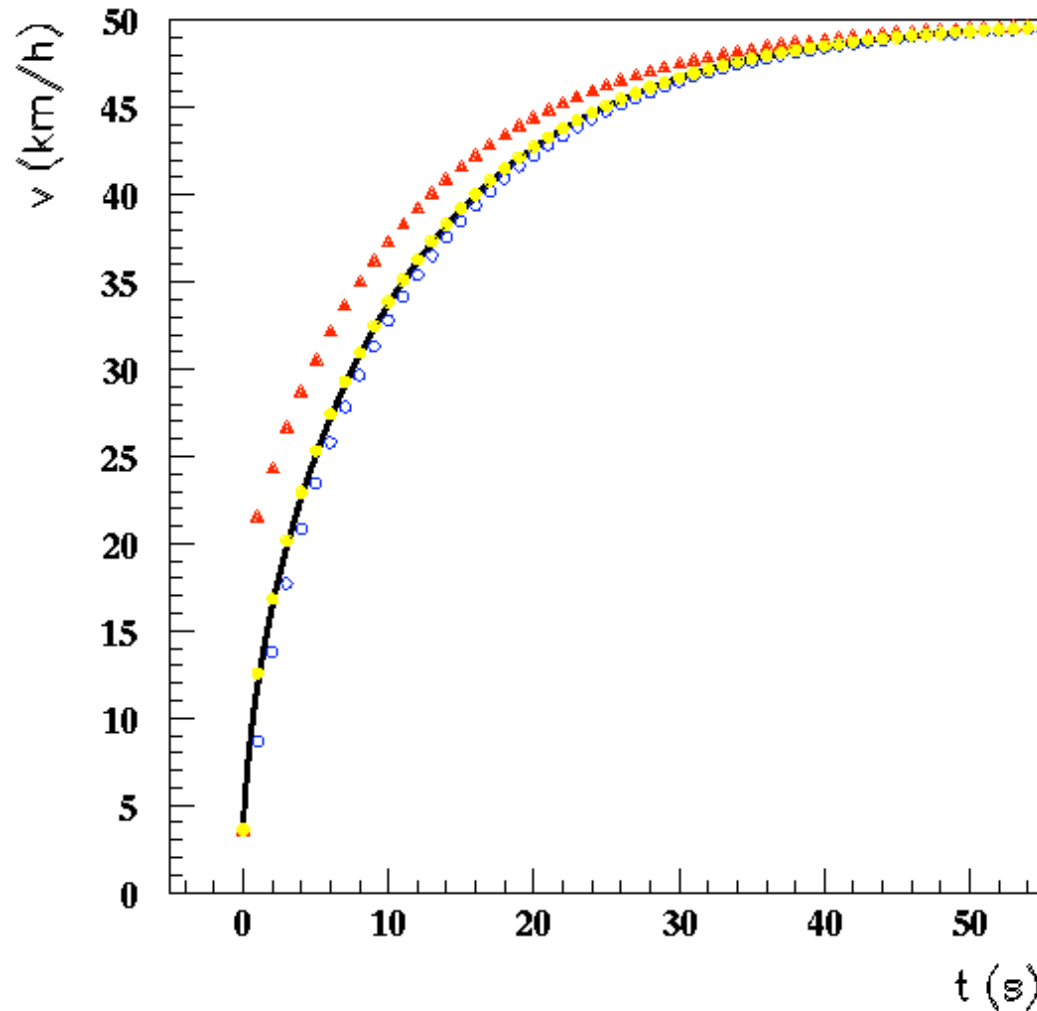
$$v(t + \Delta t) = v(t) + f(v', t')\Delta t$$

$$v' = v(t) + \frac{1}{2} f(v, t)\Delta t = v(t) + \frac{1}{2} \left[\frac{P}{mv} - \frac{C\rho Av^2}{2m} \right] \Delta t$$

$$t' = t + \frac{1}{2} \Delta t$$

$$v(t + \Delta t) = v(t) + \left[\frac{p}{mv'} - \frac{C\rho Av'^2}{2m} \right] \Delta t$$

Runge-Kutta Method



For this comparison, we take the same time step in all methods (1s).

- Exact
- ▲ Euler method
- 2nd order Runge-Kutta
- 4th order Runge-Kutta



Runge-Kutta Method

4th order Runge-Kutta:

$$x(t + \Delta t) = x(t) + \frac{1}{6} [f(x'_1, t'_1) + 2f(x'_2, t'_2) + 2f(x'_3, t'_3) + f(x'_4, t'_4)] \Delta t$$

with

$$x'_1 = x(t)$$

$$t'_1 = t$$

$$x'_2 = x(t) + \frac{1}{2} f(x'_1, t'_1) \Delta t$$

$$t'_2 = t + \frac{1}{2} \Delta t$$

$$x'_3 = x(t) + \frac{1}{2} f(x'_2, t'_2) \Delta t$$

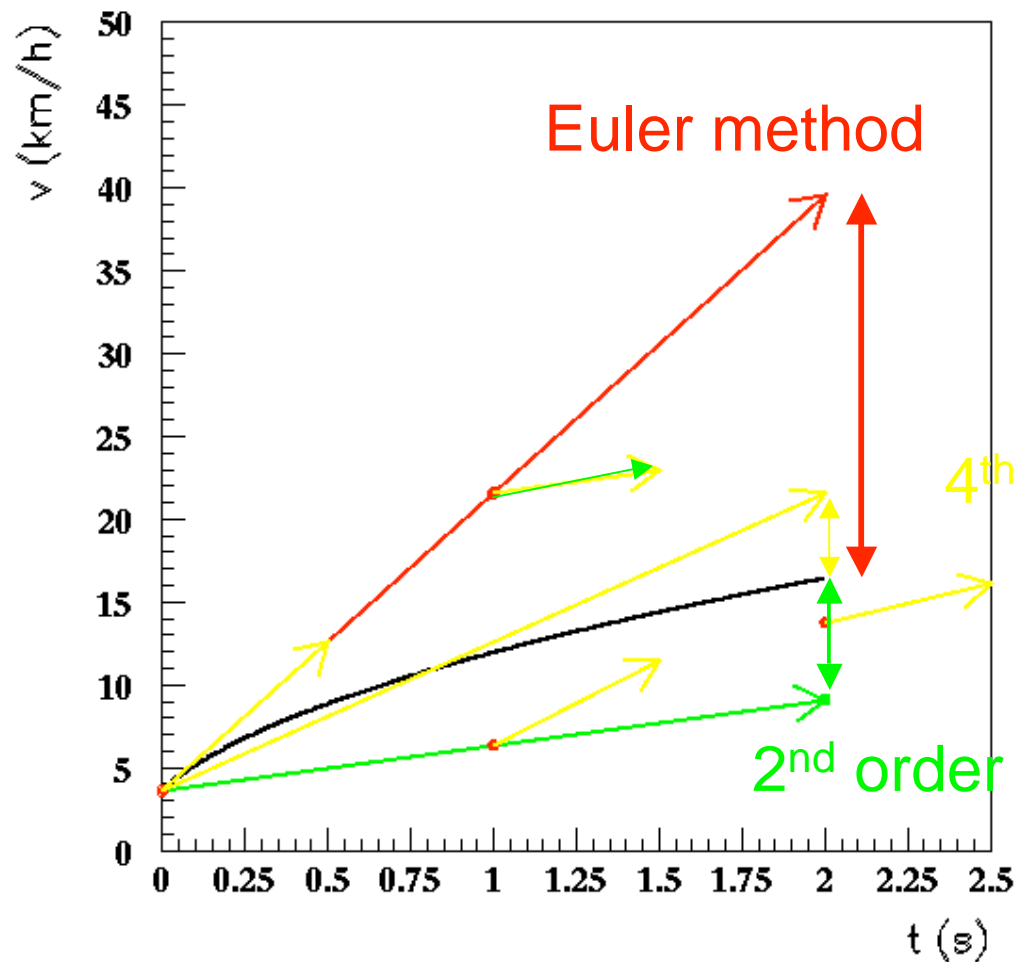
$$t'_3 = t + \frac{1}{2} \Delta t$$

$$x'_4 = x(t) + \frac{1}{2} f(x'_3, t'_3) \Delta t$$

$$t'_4 = t + \Delta t$$

Good to $(\Delta t)^4$

Graphical Representation



Take big time step (2s) to see effect of algorithm clearly

4th order R-K
True curve

2nd order R-K

Centered Difference Method (Verlet)

The Euler & R-K methods 'look forward' to try to estimate x at a later t . Can also symmetrize, in that we look forward and backward:

$$\frac{dx}{dt} \approx \frac{x(t + \Delta t/2) - x(t - \Delta t/2)}{\Delta t} \quad \text{Centered Difference Method}$$

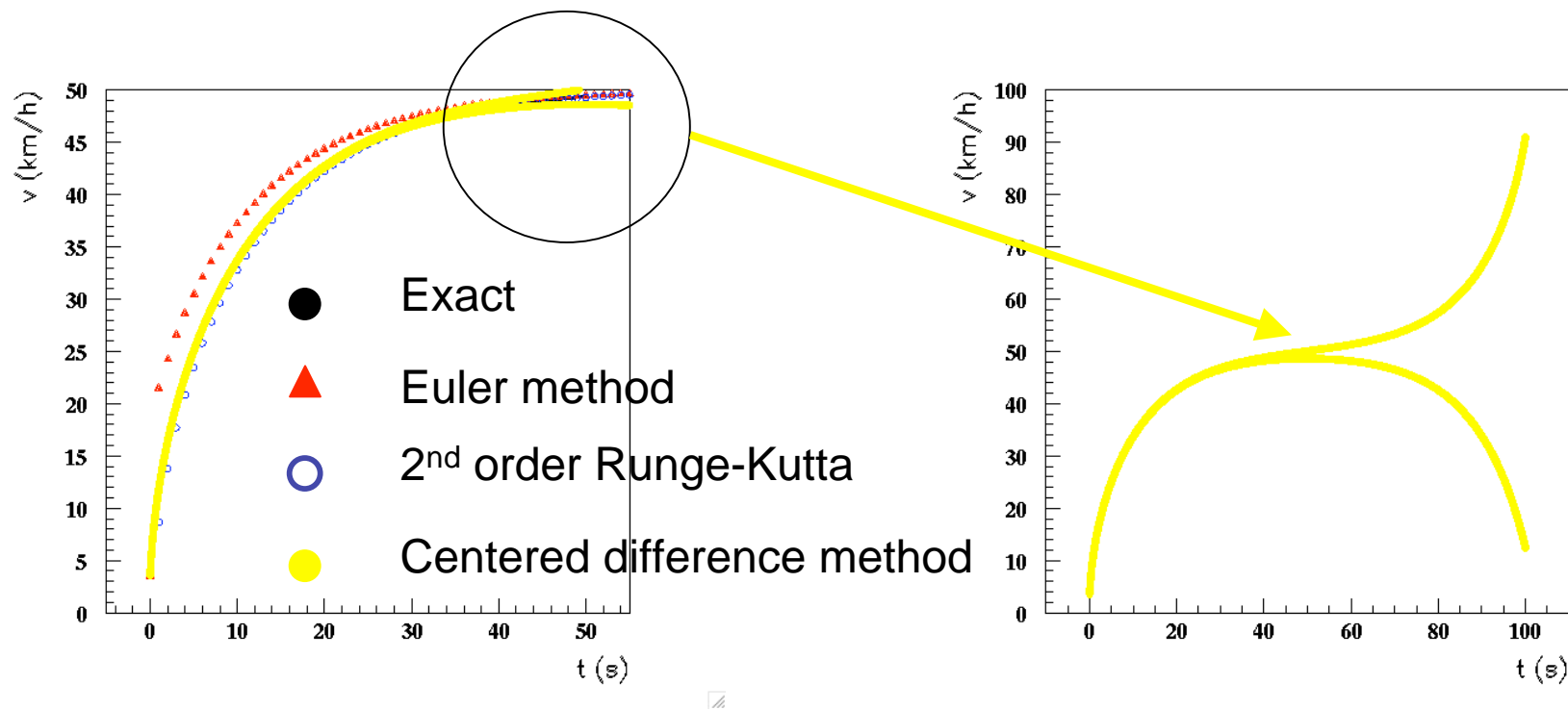
$$\begin{aligned} \frac{x(t + \Delta t/2) - x(t - \Delta t/2)}{\Delta t} &= \frac{x(t) + x' \Delta t/2 + \frac{1}{2} x'' (\Delta t/2)^2 + \dots - \left[x(t) - x' \Delta t/2 + \frac{1}{2} x'' (\Delta t/2)^2 - \dots \right]}{\Delta t} \\ &\approx \frac{\frac{dx}{dt} \Delta t + \frac{1}{24} \frac{d^3 x}{dt^3} (\Delta t)^3}{\Delta t} = \frac{dx}{dt} + \frac{1}{24} \frac{d^3 x}{dt^3} (\Delta t)^2 \end{aligned}$$

$$x(t + \Delta t) = x(t - \Delta t) + 2f(x, t)\Delta t \quad \text{with redefinition of } \Delta t$$

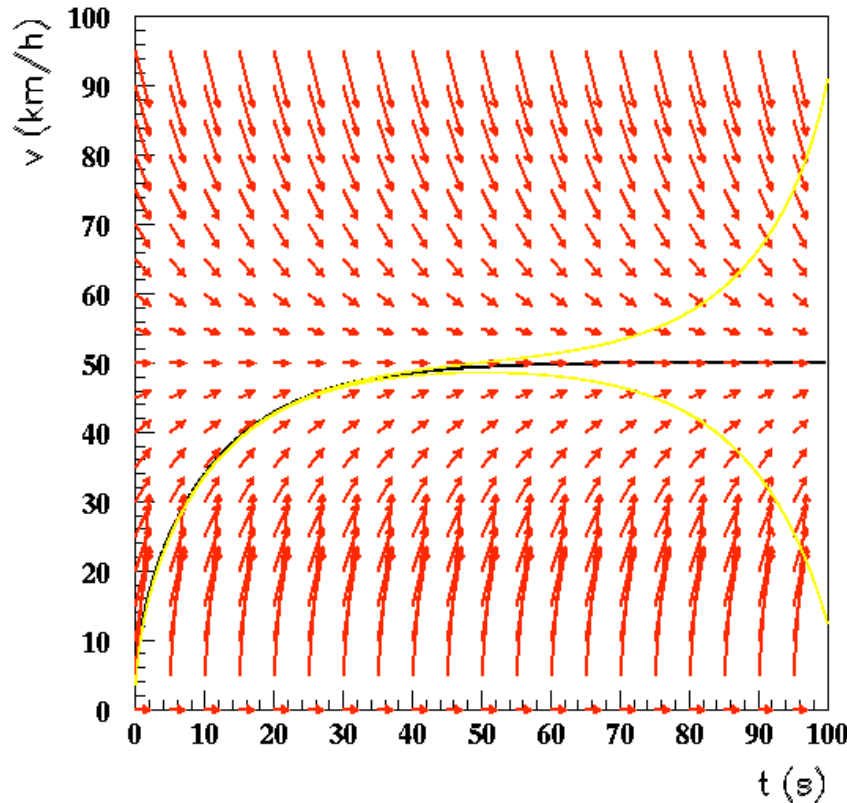
i.e., good to $O(\Delta t)^2$. Optimal step width from $\frac{(\Delta t)^2}{24} |f'''(x)| = |f(x)| \frac{2\varepsilon}{\Delta t}$

Centered Difference Method

Practical issue with this method is - how to get started ? To evaluate x_1 , need not only x_0 but also x_{-1} . Use Euler method or R-K to get x_1 , then can proceed.



Graphical Representation



Red arrows show the derivative dv/dt at a particular v .

Centered difference unstable because:

$$v_{i+2} = v_i + 2 \frac{dv_{i+1}}{dt} \Delta t$$

▮
If $v_i > v_{eq}$, and $v_{i+1} < v_{eq}$ then $\frac{dv_{i+1}}{dt} > 0$

Similarly for $v_i < v_{eq}$

Extrapolation Methods

Extrapolation Methods (Romberg):

Here, we try to guess the true value of the derivative by taking smaller and smaller step sizes and extrapolating to zero step size.

Define $D_0 = D(\Delta t)$, $D_1 = D\left(\frac{\Delta t}{2}\right)$, ...

Fit polynomial $p(\Delta t) = a + b\Delta t + c(\Delta t)^2 + \dots$ to $D(\Delta t)$

Estimate $D_\infty = a$

Example: extrapolated centered difference method:

$$D_i(h) = \frac{x(t+h) - x(t-h)}{2h} \quad h = \left(\frac{\Delta t}{2^i}\right)$$

Exercises

1. Work out the terminal velocity for a bicyclist when not travelling on flat terrain (assume a 10% slope, which is quite steep), and compare to the Euler and 4th order Runge-Kutta approaches. Investigate the effect of different step sizes.
2. Steadily diminish the step size in the example of the bicyclist travelling on flat terrain with air resistance until you find no further improvement (compare to the analytic result). Compare your final step size with expression on P.10.