<u>**Computational Methods**</u> (PHYS 2030)

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Schedule: Lecture: MWF 11:30-12:30 (CLH M)

Website: http://www.yorku.ca/cberge/2030W2018.html

York University
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Lecture 6

The KEPLER problem is certainly one of the most important problems in the history of physics and natural sciences in general. We will study this problem for several reasons: (i) it is a nice demonstration of the applicability of the methods introduced in the previous chapters, (ii) important concepts of the numerical treatment of ordinary differential equations can be introduced quite naturally, and (iii) it allows to revisit some of the most important aspects of classical mechanics.

The final differential equations, which have to be solved are of the form

$$\dot{\varphi} = \frac{|\ell|}{\mu\rho^2}, \tag{4.1}$$

and

$$\dot{\rho} = \pm\sqrt{\frac{2}{\mu}\left(E - U(\rho) - \frac{|\ell|^2}{2\mu\rho^2}\right)}, \tag{4.2}$$

Stickler & Schachinger (2014)

$$\dot{y}_n = f(y_n, t_n). \tag{5.7}$$

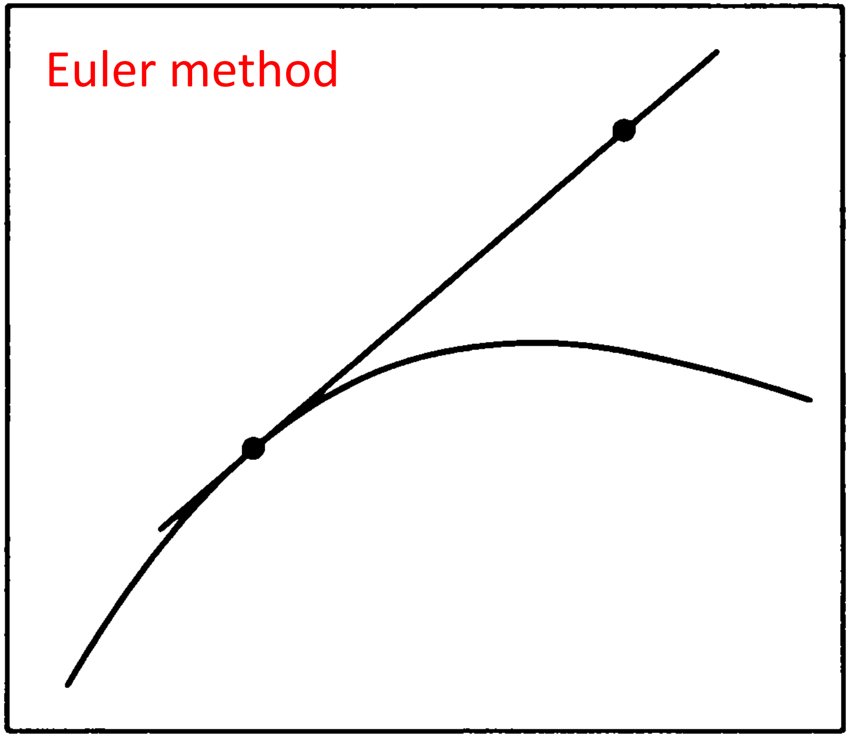
Integrating both sides of (5.7) over the interval $[t_n, t_{n+1}]$ gives

$$y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} \mathrm{d}t' f[y(t'), t']. \tag{5.8}$$

Applying the forward rectangular rule (3.9) to Eq. (5.8) yields

$$y_{n+1} = y_n + f(y_n, t_n)\Delta t + \mathcal{O}(\Delta t^2), \tag{5.9}$$

which is the explicit EULER method we encountered already in Sect. 4.3. This method is also referred to as the *forward* EULER *method* . In accordance to the forward rectangular rule, the leading term of the error of this method is proportional to Δt^2 as was pointed out in Sect. 3.2.



$$y'(x) = f(x, y).$$

$$y(x) = y(x_0) + (x - x_0)y'(x_0) + \frac{(x - x_0)^2}{2!}y''(x_0) + \cdots.$$

$$y(x) \approx y(x_0) + (x - x_0)y'(x_0).$$

Devries (1994)

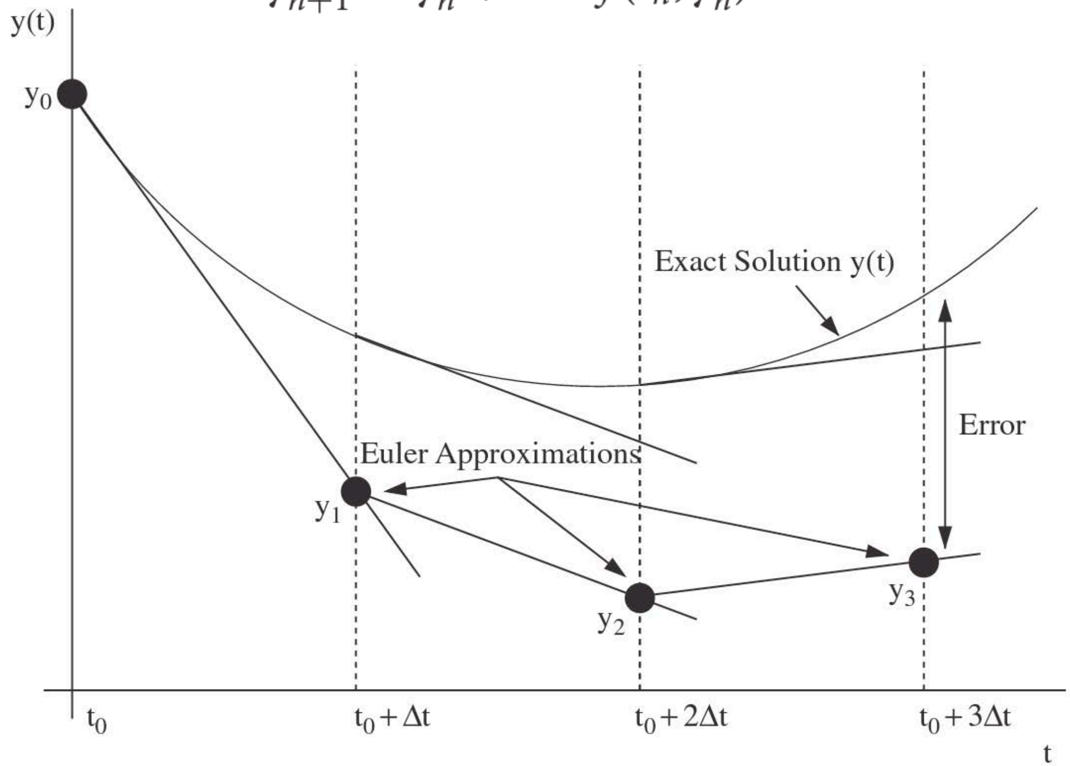
Starting point: Euler's method

Idea: Since equations tell us how things change, numerically integrate to find solution(s)

$$\frac{d\mathbf{y}}{dt} = f(t, \mathbf{y})$$

$$\frac{d\mathbf{y}}{dt} = f(t, \mathbf{y}) \quad \Rightarrow \quad \frac{\mathbf{y}_{n+1} - \mathbf{y}_n}{\Delta t} \approx f(t_n, \mathbf{y}_n).$$

$$\mathbf{y}_{n+1} = \mathbf{y}_n + \Delta t \cdot f(t_n, \mathbf{y}_n).$$



→ Note that while we can propagate a solution forward (or backward), there can be some associated ***error***

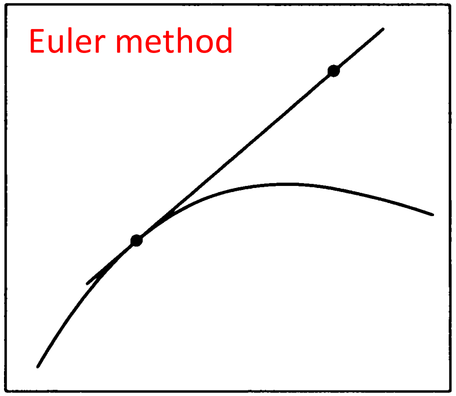
Kutz (2013)

Improved Euler's method?

$$y'(x) = f(x, y).$$

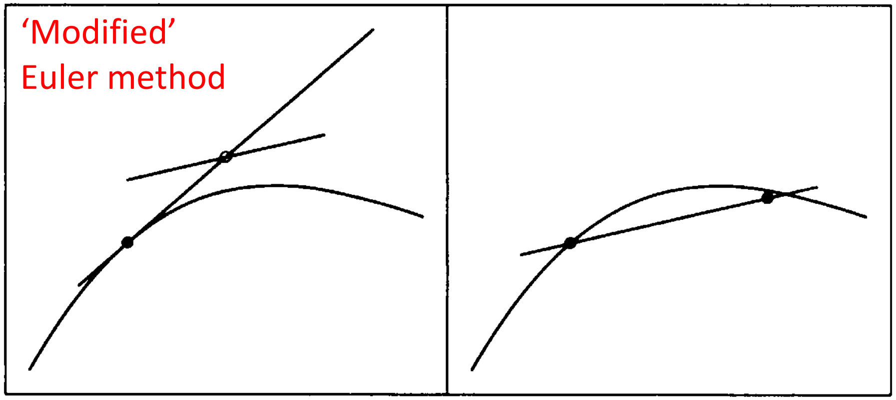
- Can we 'guess' the solution at a mid-point?

$$x_{mid} = x_0 + \frac{h}{2} \qquad y(x_{mid}) = y_0 + \frac{h}{2}y_0' = y_0 + \frac{h}{2}f_0$$



$$y(x_0 + h) = y(x_0) + hf\left(x_{mid}, y_{mid}\right)$$

$$y(x) \approx y(x_0) + (x - x_0)y'(x_0).$$



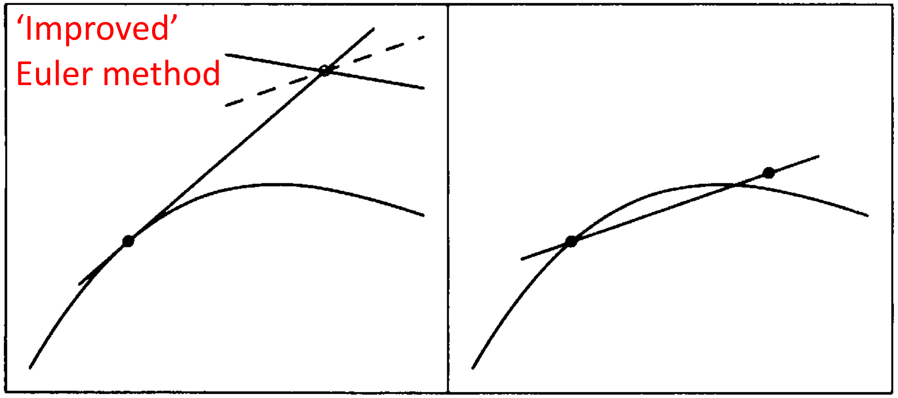
- Change in the associated error?
- How does this differ from changing our step-size?

$$f(x_{mid}, y_{mid}) = y'(x_{mid}) \approx \frac{y(x_0 + h) - y(x_0)}{h}$$

Devries (1994)

<u>Improved Euler's method?</u>

- What if we tried to use a *mean* value of the derivative?



$$y(x_0 + h) = y(x_0) + h\frac{f_0 + f(x_0 + h, y_0 + hf_0)}{2}$$

```matlab
% York U PHYS 2030  (09.15.14)
% use improved Euler method to solve the following differential equation
% f'(x)= f^2 + 1
% which has the solution f(x)= tan(x)

clear
% ***********************
% User Inputs
stepsize= 0.01;
f0= 0.0;   % initial condition at xI [i.e. f(xI)]
xI= 0;  % boundary conditions
xF= pi/2;

% ***********************

F(1)= f0;  %initialize first value
k=1;  % counter
for i=xI:stepsize:xF
 if i == xI
  F(k)= f0;
 else
  F(k)= F(k-1) + stepsize* (F(k-1)^2 + 1);  % first calculate f at this step
  nextstep= (F(k) + stepsize*F(k))^2 + 1;   % use that to get it at the subsequent step
  % now use these two to effectively average what f is over this interval
  F(k)= F(k-1) + (stepsize/2) * (F(k-1)^2 + 1 + nextstep);
 end
 x(k)= i;  % keep track of x for plotting
 k= k+ 1;  % increment counter
end

% visualize
figure(1); clf;
plot(x,F, 'o--','LineWidth',2); grid on;    hold on
xlabel('x');    ylabel('f(x)')
title('Solution to df/dx= f^2 +1 using improved Euler method')

% plot analytic solution
sol= tan(x);
plot(x,sol, 'r.-')
legend('Numeric solution', 'True solution', 0); axis([0 pi/2 0 100])
```

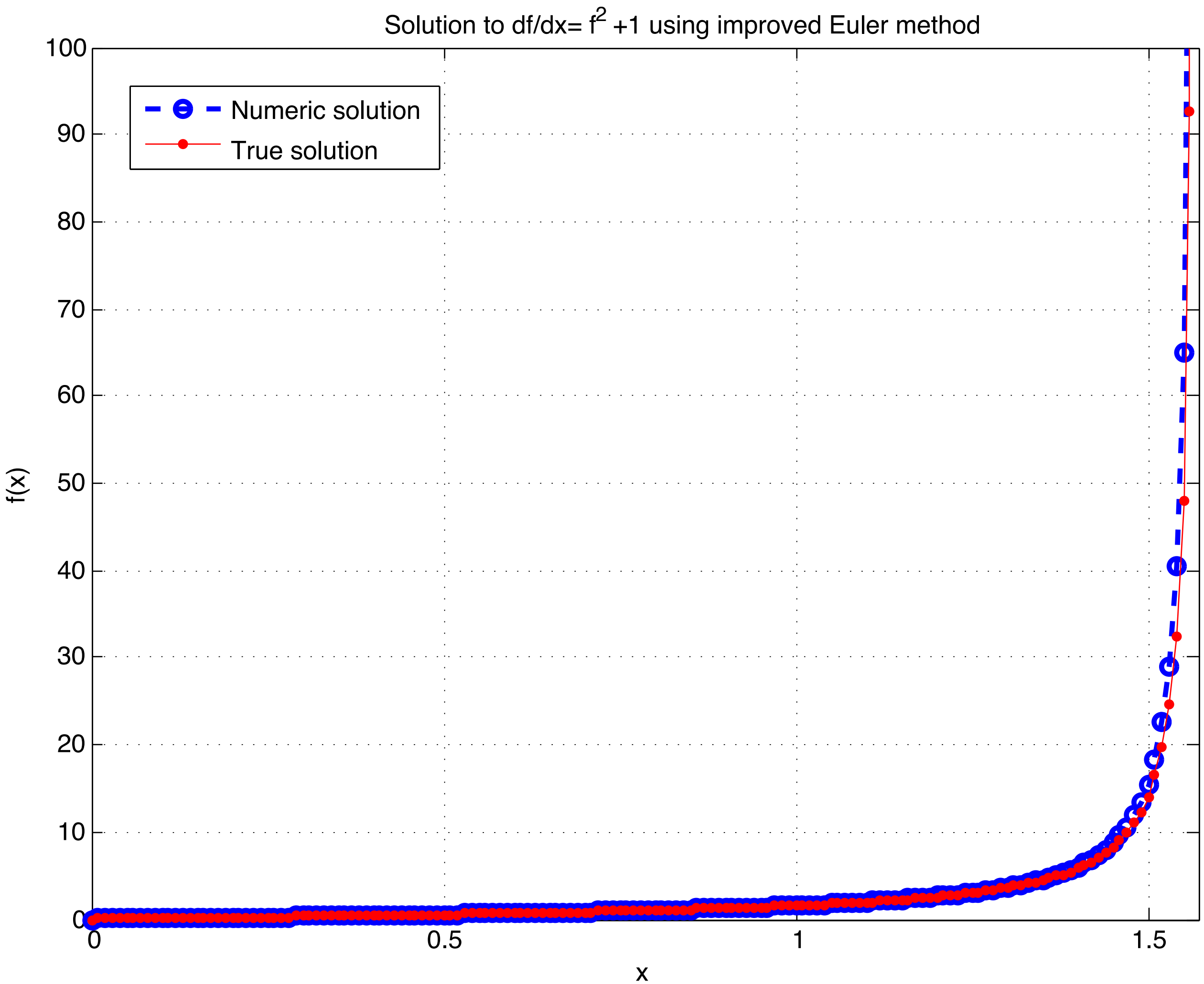
$$\frac{df}{dx} = f^2 + 1$$

Extra calculations along the way lead to 'improved' Euler's method

$$y(x_0 + h) = y(x_0) + h\frac{f_0 + f(x_0 + h, y_0 + hf_0)}{2}$$

Think about how/where this 'recipe' is being included

ODEeulerEX4.m



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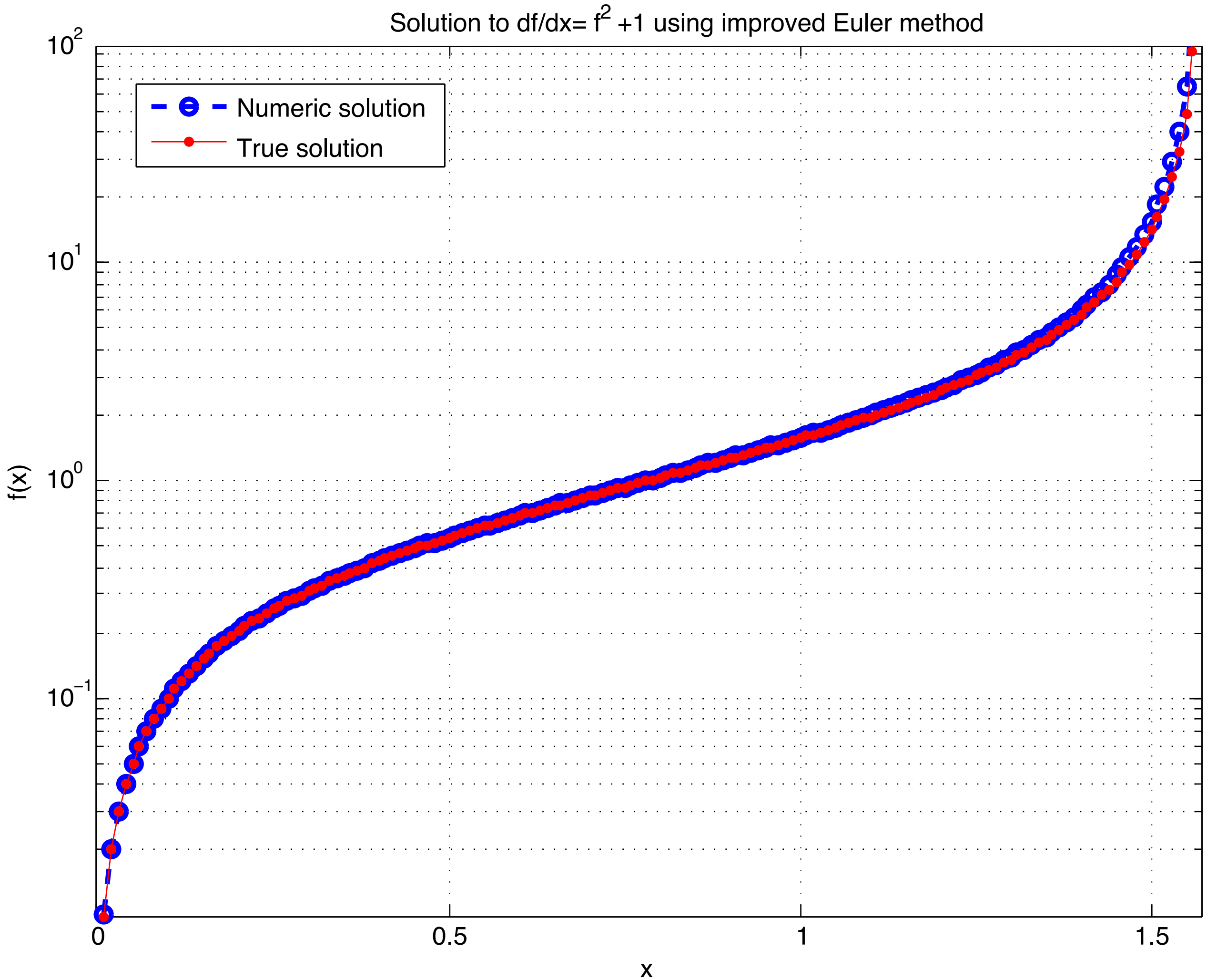
set(gca,'YScale','log');
```



Higher order methods

- Question: How can we know what the higher order derivatives are, since the ODE only tells us the first derivative?

$$y'(x) = f(x, y)$$

Taylor series

$$y(x) = y(x_0) + y'(x_0)(x - x_0) + \frac{y''(x_0)}{2!}(x - x_0)^2 + \frac{y^{(3)}(x_0)}{3!}(x - x_0)^3 + \cdots$$

Since we know $y'(x)$, we can determine higher order derivatives with a little work

$$\begin{aligned} y''(x) &= \frac{\partial}{\partial x} f(x,y) + \frac{dy}{dx}\frac{\partial}{\partial y} f(x,y) \\ &= \frac{\partial}{\partial x} f(x,y) + f(x,y)\frac{\partial}{\partial y} f(x,y) \end{aligned}$$

This gets messy quickly, but at least up to 2nd order, we have:

$$\begin{aligned} y(x) = y_0 + (x - x_0) f(x_0, y_0) &+ \frac{(x-x_0)^2}{2!}\left[\frac{\partial f(x_0,y_0)}{\partial x} + f(x_0,y_0)\frac{\partial f(x_0,y_0)}{\partial y}\right] \\ &+ \frac{(x-x_0)^3}{3!} y'''(\xi), \end{aligned}$$

Devries (1994)

Runge-Kutta (RK)

- RK methods characterized by expressing solution in terms of derivative evaluated for different arguments (various Euler methods being a subset of this)

- In contrast to Taylor series solutions, which rely of successively higher order derivatives all evaluated at the same argument

- Question: How well does Euler's method and a Taylor series solution match up?

general form for all Euler method solutions

$$y(x_0+h) = y(x_0) + h[\alpha f(x_0,y_0) + \beta f(x_0+\gamma h, y_0+\delta h f_0)]$$

Taylor series expansion for function of two variables

$$f(x,y) = f(x_0,y_0) + (x-x_0)\frac{\partial f(x_0,y_0)}{\partial x} + (y-y_0)\frac{\partial f(x_0,y_0)}{\partial y}$$
$$+ \frac{(x-x_0)^2}{2}\frac{\partial^2 f(\xi,\eta)}{\partial x^2} + (x-x_0)(y-y_0)\frac{\partial^2 f(\xi,\eta)}{\partial x \partial y}$$
$$+ \frac{(y-y_0)^2}{2}\frac{\partial^2 f(\xi,\eta)}{\partial y^2} + \cdots,$$

where $x_0 \le \xi \le x$ and $y_0 \le \eta \le y$

Devries (1994)

Runge-Kutta (RK)

Use last expression to expand general Euler equation

$$y(x) = y_0 + h\alpha f(x_0, y_0) + h\beta\left[f(x_0,y_0) + h\gamma\frac{\partial f(x_0,y_0)}{\partial x} + h\delta f(x_0,y_0)\frac{\partial f(x_0,y_0)}{\partial y} + O(h^2)\right]$$

$$= y_0 + h(\alpha+\beta)f(x_0,y_0) + h^2\beta\left[\gamma\frac{\partial f(x_0,y_0)}{\partial x} + \delta f(x_0,y_0)\frac{\partial f(x_0,y_0)}{\partial y}\right] + O(h^3)$$

Agrees with Taylor series

$$y(x) = y_0 + (x-x_0)f(x_0,y_0) + \frac{(x-x_0)^2}{2!}\left[\frac{\partial f(x_0,y_0)}{\partial x} + f(x_0,y_0)\frac{\partial f(x_0,y_0)}{\partial y}\right] + \frac{(x-x_0)^3}{3!}y'''(\xi),$$

if $\alpha+\beta=1,$

$\beta\gamma = 1/2,$

and $\beta\delta = 1/2$

→ Modified and improved Euler methods agree with Taylor series through terms of order h^2 and are said to be ***2nd-order RK methods***

Note: Such agreement requires that $\gamma=\delta$, but other parameters allow flexibility, e.g., h^3 is minimized when

$$\alpha = 1/3,\ \beta = 2/3,\ \text{and}\ \gamma=\delta=3/4$$

Runge-Kutta (RK)

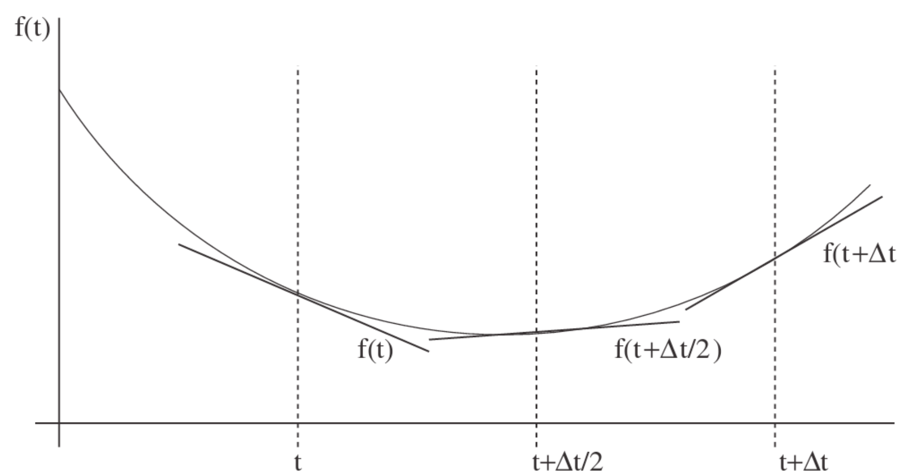
➢ 'Higher order' methods improve in a similar fashion to Riemann sums, for example:

- Euler → LEFT
- Modified Euler → MID
- Improved Euler → TRAP

➢ Most popular RK method is the 'fourth order' (RK4) and is equivalent to SIMP:

$$
\begin{aligned}
f_0 &= f(x_0, y_0),\\
f_1 &= f(x_0 + \frac{h}{2}, y_0 + \frac{h}{2} f_0),\\
f_2 &= f(x_0 + \frac{h}{2}, y_0 + \frac{h}{2} f_1),\\
f_3 &= f(x_0 + h, y_0 + h f_2).
\end{aligned}
$$

$$y(x_0 + h) = y(x_0) + \frac{h}{6}(f_0 + 2f_1 + 2f_2 + f_3)$$



Devries (1994)
Kutz (2013)

Adaptive step-size

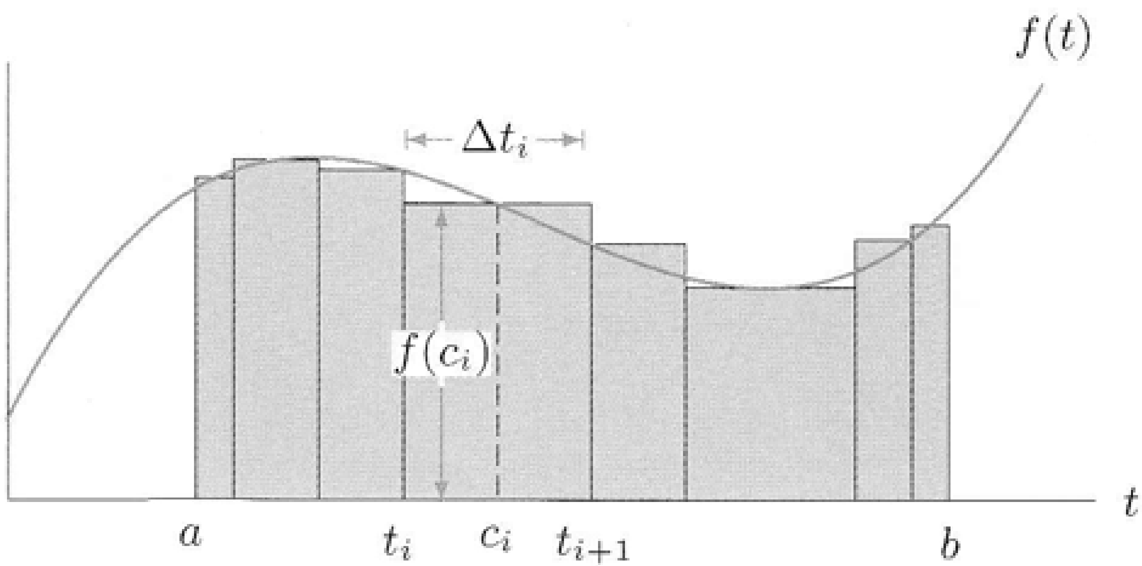
- How would you check the accuracy of your solver?

  <u>(Easy) Brute force way</u>: Calculate for two (or more) different step-sizes (e.g., Δt and $\Delta t/2$) and compare → if difference is small, then the error is assumed small

- Motivates the notion of some sort of *error tolerance*

- Further motivates that step-size need not be constant

→ Just like Riemann sums, Δt need not be constant



Hughes-Hallett et al. (2005)

(More advanced) RK methods

- Basic gist: 'adapt' the step size and see if *error* (ε) increases or decreases. Leads to the Runge-Kutta-Fehlberg method:

When the smoke clears....

$$f_0 = f(x_0, y_0),$$
$$f_1 = f(x_0 + \frac{h}{4}, y_0 + \frac{h}{4} f_0),$$
$$f_2 = f(x_0 + \frac{3h}{8}, y_0 + \frac{3h}{32} f_0 + \frac{9h}{32} f_1),$$
$$f_3 = f(x_0 + \frac{12h}{13}, y_0 + \frac{1932h}{2197} f_0 - \frac{7200h}{2197} f_1 + \frac{7296h}{2197} f_2),$$
$$f_4 = f(x_0 + h, y_0 + \frac{439h}{216} f_0 - 8h f_1 + \frac{3680h}{513} f_2 - \frac{845h}{4104} f_3),$$
$$f_5 = f(x_0 + \frac{h}{2}, y_0 - \frac{8h}{27} f_0 + 2h f_1 - \frac{3544h}{2565} f_2 + \frac{1859h}{4104} f_3 - \frac{11h}{40} f_4)$$

4th order
$$y = y_0 + h(\frac{25}{216} f_0 + \frac{1408}{2565} f_2 + \frac{2197}{4104} f_3 - \frac{1}{5} f_4)$$

5th order
$$\hat{y} = y_0 + h(\frac{16}{135} f_0 + \frac{6656}{12825} f_2 + \frac{28561}{56430} f_3 - \frac{9}{50} f_4 + \frac{2}{55} f_5)$$

→ At the most basic level, at least there is a clear numerical recipe one could cook up here!

- Can directly assess error (and set some sort of tolerance)

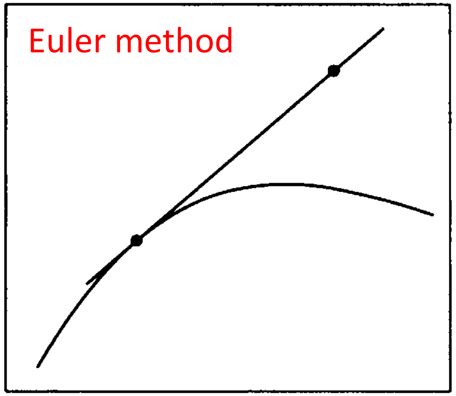
$$Err = \hat{y} - y = h\left(\frac{1}{360} f_0 - \frac{128}{4275} f_2 - \frac{2197}{75240} f_3 + \frac{1}{50} f_4 + \frac{2}{55} f_5\right)$$

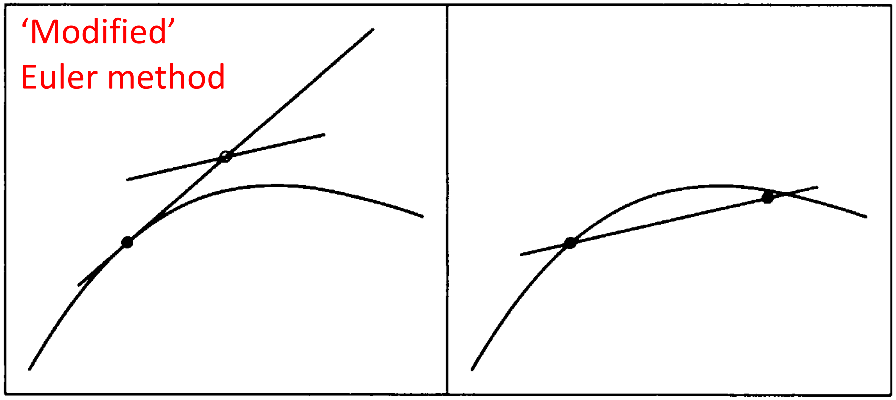
(conservative) estimate for step-size

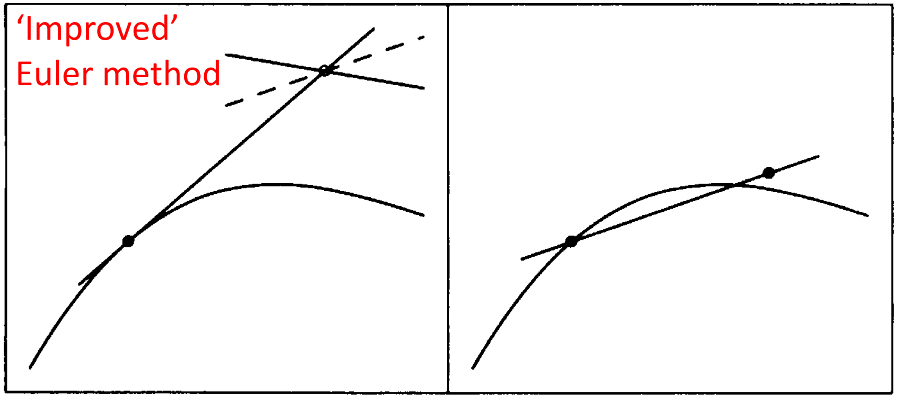
$$h_{new} = 0.9h \sqrt[4]{\frac{|h|\varepsilon}{|y(x_0+h) - \hat{y}(x_0+h)|}}.$$

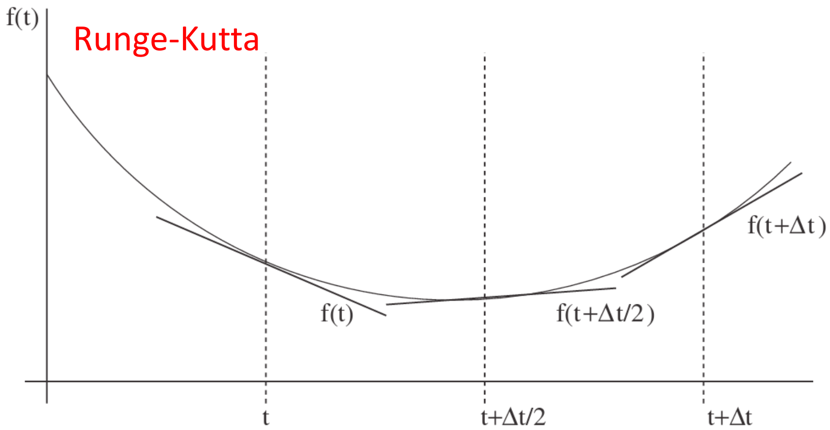
→ allows step-size to be adjusted on the fly!

Visual summary









Devries (1994)
Kutz (2013)

Post-class exercises

- Write your own code to use Euler's method to solve the logistic equation. How does it compare to dfield?

- Modify your code to (explicitly) solve via a RK4 method

- Looking ahead: Modify your code to use Matlab's ode45 (what do you need to do differently?)

- Looking ahead: Consider the equation for the simple harmonic oscillator

$$\frac{dv}{dt} = a = \frac{F}{m} = \frac{-kx}{m}$$

Is this a single 1st order ODE?

How might your strategy change to deal with this more complicated aspect?