Numerical solution of ordinary differential equations

## Trajectory

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

- One of the task for ODE solvers is to find the trajectory starting from initial conditions



## True trajectory

- There are infinitely many possible trajectories
- The derivatives "show the correct path"


Note: some images, slides from RN Shorten, D. Leith: https://slideplayer.com/slide/4594068/)

## True trajectory



- We can calculate derivatives at all $(t, y)$ points
- It depends on $y$, too, not only on $t$ !


## Euler's method

- Using derivatives at the actual points to estimate solution
- Errors accumulate



## Discrete solution: sampling the true trajectory




## Smaller stepsize: closer to true solution



Multi-step concept

- Euler, RK4, ... all have the form:

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

$$
\hat{y}_{k+1}=K \hat{y}_{k}+g\left(t, \hat{y}_{k}\right)
$$

- Prediction depends only on previous value
- Multi-step methods attempt to gain efficiency by keeping and using the information from previous steps rather than discarding it. Consequently, multistep methods refer to several previous points and derivative values.


## Adams-Bashforth Moulton method

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

- The ABM predictor-corrector method is a multi-step method. It is obtained by approximating the integral in the formula

$$
y\left(t_{k+1}\right)-y\left(t_{k}\right)=\int_{t_{k}}^{t_{k}} f(t, y(t)) d t
$$

by an interpolation polynomial of third degree. This polynomial is chosen so that is passes through the points

$$
\left(t_{k-n}, f_{k-n}\right), \ldots, n=0,1,2
$$

This produces an ABM prediction

$$
p\left(t_{k+1}\right)
$$

## Adams-Bashforth Moulton method

- Having obtained the prediction, a second polynomial is constructed to fit the points

$$
\left(t_{k-n}, f_{k-n}\right), \ldots, n=0,1,2
$$

- and the point

$$
\left(t_{k+1}, p\left(t_{k+1}\right)\right)
$$

- This polynomial is then integrated to obtain the final prediction at time index $k+1$.

(a) The four nodes for the Adams-Bashforth predictor (extrapolation is used)

(a) The four nodes for the Adams-Moulton corrector (interpolation is used)


## Adams-Bashforth Moulton method

- The ABM formula's are:

$$
\begin{gathered}
p\left(t_{k+1}\right)=\hat{y}\left(t_{k}\right)+\frac{h}{24}\left(-9 f_{k-3}+37 f_{k-2}-59 f_{k-1}+55 f_{k}\right) \\
\hat{y}\left(t_{k+1}\right)=\hat{y}\left(t_{k}\right)+\frac{h}{24}\left(9 f_{k-2}-5 f_{k-1}+19 f_{k}+f_{k+1}\right)
\end{gathered}
$$

- The advantage of this technique is that the difference between the predictor and corrector gives an estimate of the truncation error.


## ABM: more precise



## ABM: but can be instable

- There is a range for step size where the method is instable



## Optimal step size

- Runge-Kutta: step size error can be calculated (make one step with $h->y_{1}$ and one with $\left.h / 2->y_{2}\right): \Delta=y_{2}-y_{1}$
- RK4 has 5 -th order error, so if the expected error is $\Delta_{0}$, then the optimal step is

$$
h_{0}=h\left|\frac{\Delta_{0}}{\Delta}\right|^{0.2}
$$

## Stability

- Take this simple example:

$$
y^{\prime}=-c y \quad c>0
$$

- Euler "explicit" solution:

$$
y_{n+1}=y_{n}+h y_{n}^{\prime}=(1-c h) y_{n}
$$

- If the step size is "too large" $h>2 / c$ than the solution $\left|y_{n}\right|$ goes to infinity instead of the true solution, 0 .
- Example 2 equations:

$$
u^{\prime}=998 u+1998 v \quad v^{\prime}=-999 u-1999 v
$$

- With boundary condition: $\quad u(0)=1, v(0)=0$
- With this variable transformation:

$$
v=-y+z
$$

$$
u=2 y-z
$$

- the equations take the form:

$$
v=-e^{x}+e^{-1000 x}
$$

$$
u=2 e^{-x}-e^{-1000 x}
$$

- Because of the second terms, stability ( $h<2 / c$ ) would require $h<2 / 1000$. But they are negligibly small, so because of the instability of equations very small steps are required.

Implicit Euler method

- Backwards Euler step:

$$
y_{n+1}=y_{n}+h y_{n+1}^{\prime}
$$

- This is an "implicit equation since $y_{n+1}$ appears on the right hand side, too.
- For our first example the equation can be reordered:

$$
y^{\prime}=-c y \quad c>0 \quad y_{n+1}=\frac{y_{n}}{1+c h}
$$

- This is always stable without any restriction on $h$.
- The price to be paid for stability: solution of set of (linear) equations in each step.


## Instability can be hidden

$$
\begin{gathered}
v=-e^{x}+e^{-1000 x} \\
v=-y+z \\
u^{\prime}=998 u+1998 v \\
v^{\prime}=-999 u-1999 v \\
u(0)=1, v(0)=0 \\
u=2 e^{-x}-e^{-1000 x}
\end{gathered}
$$

