Numerical solution of ordinary differential equations

Trajectory

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

 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:

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

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

- 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.

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

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

$$y(t_{k+1}) - y(t_k) = \int_{t_k}^{t_{k+1}} f(t, y(t)) dt$$

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

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

This produces an ABM prediction

 $p(t_{k+1})$

Adams-Bashforth Moulton method

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

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

• and the point

$$(t_{k+1}, p(t_{k+1}))$$

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



Adams-Bashforth Moulton method

• The ABM formula's are:

$$p(t_{k+1}) = \hat{y}(t_k) + \frac{h}{24}(-9f_{k-3} + 37f_{k-2} - 59f_{k-1} + 55f_k)$$
$$\hat{y}(t_{k+1}) = \hat{y}(t_k) + \frac{h}{24}(9f_{k-2} - 5f_{k-1} + 19f_k + f_{k+1})$$

• 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 *h/2->y*₂): Δ = y₂ y₁
- RK4 has 5-th order error, so if the expected error is Δ_0 , then the optimal step is

$$h_0 = h \left| \frac{\Delta_0}{\Delta} \right|^{0.2}$$

Stability

• Take this simple example:

$$y' = -cy \quad c > 0$$

• Euler "explicit" solution:

$$y_{n+1} = y_n + hy'_n = (1 - ch)y_n$$

• If the step size is "too large" h > 2/c than the solution $|y_n|$ goes to infinity instead of the true solution, 0.

• Example 2 equations:

 $u' = 998u + 1998v \qquad v' = -999u - 1999v$

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

$$v = -y + z \qquad \qquad u = 2y - z$$

• the equations take the form:

$$v = -e^x + e^{-1000x} \qquad \qquad u = 2e^{-x} - e^{-1000x}$$

 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:

 $y_{n+1} = y_n + hy_{n+1}'$

- 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:

$$y' = -cy$$
 $c > 0$ $y_{n+1} = \frac{y_n}{1+ch}$

- 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

v = -y + z

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

 $u = 2y - z$

$$u' = 998u + 1998v$$

$$v' = -999u - 1999v$$

$$u(0) = 1, v(0) = 0$$

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