Computational Physics

ODEs: Simple example, error and convergence

ODEs in physics

ODEs appear mainly in two type of problems:

Initial value problems:

- typical problem: time evolution of discrete system
  (e.g. point masses with strings)
- usually solved by numerical integration

Boundary value problems:

- typical problem: eigenstates of 1d continuous system
  (e.g. vibrating string)
- can be solved via self-constitent integration (e.g. shooting method)
  risk of poor condition
- can be solved via spatial discretization (e.g. finite elements)

Prototypical linear ODE

For the moment, we will study the first-order ODE with constant coefficient.

Scalar version:

$$y'(t) = \alpha(t)y(t)$$

Vectorial version:

$$\underbrace{\begin{pmatrix} y_1' \\ y_2' \\ \vdots \\ y_n' \end{pmatrix}}_{\mathbf{y}'(t)} = \underbrace{\begin{pmatrix} \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1n} \\ \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1n} \\ \vdots & \vdots & \ddots & \vdots \\ \alpha_{11} & \alpha_{12} & \cdots & \alpha_{1n} \end{pmatrix}}_{A(t)} \underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}}_{\mathbf{y}(t)}$$

Every arbitrary order system of linear ODEs can be brought to this form.

Initial value problems: numerical integration

Initial value problems are of the form

$$\begin{aligned} \mathbf{y}'(t) =& A(t)\mathbf{y}(t), \\ \mathbf{y}(0) =& \mathbf{y}_0, \end{aligned}$$

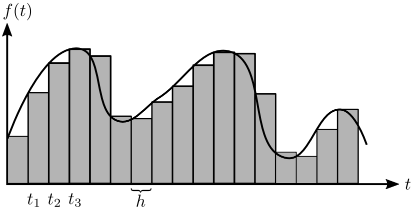
where $y(T)$ is sought for with $T > 0$.

Formal solution:

$$\mathbf{y}(T) = \int_0^T \mathrm{d}t\ \mathbf{y}'(t) = \int_0^T \mathrm{d}t\ A(t)\mathbf{y}(t).$$

Simplest ODE integration: Euler's method

Idea:



- Sample time at regular points $t_1, t_2, \ldots$, separated by time step h
- Approximate integral within each time step by integrand value on the left side.

Euler-integration for first order ODEs:

$$\begin{aligned} \mathbf{y}(t_0) =& \mathbf{y}_0, \\ \mathbf{y}(t_{n+1}) =& \mathbf{y}(t_n) + hA(t_n)\mathbf{y}(t_n). \end{aligned}$$

Examples

Exponential decay: Solve the linear initial value problem

$$
\begin{aligned}
y' =& \alpha y \qquad \text{with} \qquad y(0) = 1, \\
\alpha =& -1.
\end{aligned}
$$

using Euler's method and compare to the analytical solution:

$$y(x) = \exp(\alpha x)$$

Nonlinear decay: Do the same with the nonlinear problem

$$y' = -\sin^2 y, \qquad \text{with} \qquad y(0) = 1,$$

with the analytical solution:

$$y(x) = \operatorname{acot}(x + c), \qquad \text{with} \qquad c = \cot y(0).$$

Residual and error

Consider the initial value problem (IVP)

$$\mathbf{y}'(t) = A(t)\mathbf{y}(t) \qquad\qquad \mathbf{y}(0) = \mathbf{y}_0.$$

A numerical solver provides an approximate solution

$$\tilde{\mathbf{y}}(t) \approx \mathbf{y}(t).$$

The residual is the difference between true and numerical solution:

$$\mathbf{r}(t) = \mathbf{y}(t) - \tilde{\mathbf{y}}(t).$$

The norm of the residual is usually called the (absolute) error:

$$E = ||\mathbf{r}(t)|| = ||\mathbf{y}(t) - \tilde{\mathbf{y}}(t)||.$$

Convergence and consistency

Usually, numerical methods involve some parameter (e.g. time step size) that determines the accuracy and shall be labelled h.

- Assume there is a sequence $h_n = h_1, h_2, \ldots$ of such values.
- For each h, we find a different numerical solution $\tilde{\mathbf{y}}_h(t)$.
- If this sequence of numerical solutions converges, we say the numerical method converges; the limit is the converged result.

This does not imply that the converged numerical result is correct!

If the numerical solutions $\tilde{\mathbf{y}}_{h_n}(t)$ converge *to the true solution* $\mathbf{y}(t)$ (i.e. $E_n \to 0$), we call the method *consistent*.

**It is easy to show that calculation converges –
it is much harder to show that it is consistent!**

Consistency must be mathematically proven for each class of problem a method should be applied to. Using methods for "incompatible" problems can lead to inconsistent results.

Convergence rate and convergence order

Assuming consistency, convergence means that the (absolute) error at fixed time t decreases as we decrease h (or as we increase h depending on how it is defined).

Ideally, the solution is guaranteed to remain within an h-dependent region around the true solution:

$$E_{h_n}(t) \leq cf(h),$$

where the convergence rate function $f(h)$ contains the dependence on h and c is a problem-specific constant.

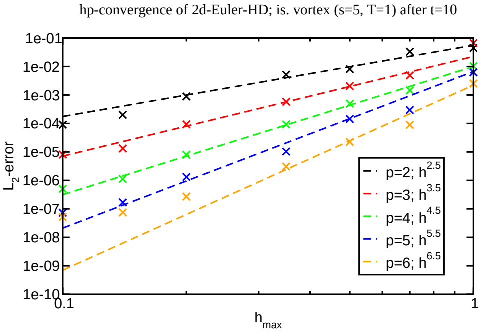
$f(h)$ is characteristic for a given method and usually a power law $f(h) = h^p$, where p is the convergence order.

The $f(h)$ describes how quickly the error decays as h is refined. It makes no statement about what h is required to obtain a certain error (c might be large for your problem).

Example: a "real-life" convergence plot

This is a convergence/consistency plot for a hydrodynamics method:

Error for an analytically solvable problem (rotating vortex in liquid). Comparison of simulation error (crosses) with expected behavior (lines) in a log-log plot.



If no analytical solution is available, one can make do with a trusted numerical high-accuracy solution.

Homework

Implement and test Euler's method for a harmonic oscillator and the Kepler problem (see problem sheet).