Ordinary Differential Equations

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Ordinary Differential Equations (refresher)

- Are equations with derivatives with respect to 1 variable, e.g.

$$\frac{dx}{dt} = f(x,t)$$

- There can be several coupled such equations, e.g.

$$\frac{dx^{(1)}}{dt} = f^{(1)}(x^{(1)}, x^{(2)}, t); \quad \frac{dx^{(2)}}{dt} = f^{(2)}(x^{(1)}, x^{(2)}, t)$$

- The derivative can be of higher order to, e.g. $\frac{d^2x}{dt^2} = f(x,t)$

  Many numerical techniques expect a first order equation.

  Not an issue: set $x^{(1)} = x$, $x^{(2)} = dx/dt$, to arrive at

$$\frac{dx^{(1)}}{dt} = x^{(2)}; \qquad \frac{dx^{(2)}}{dt} = f(x^{(1)}, t)$$

ODE Examples

Lotka–Volterra (predator/pray)

$$\frac{dx^{(1)}}{dt} = x^{(1)}(\alpha - \beta x^{(2)})$$
$$\frac{dx^{(2)}}{dt} = -x^{(2)}(\gamma - \delta x^{(1)})$$

Harmonic oscillator

$$\frac{dx^{(1)}}{dt} = x^{(2)}$$
$$\frac{dx^{(2)}}{dt} = -x^{(1)}$$

Rate equations (chemistry))

$$\begin{aligned}
\frac{dx^{(1)}}{dt} &= -2k_1[x^{(1)}]^2x^{(2)} + 2k_2[x^{(3)}]^2 \\
\frac{dx^{(2)}}{dt} &= -k_1[x^{(1)}]^2x^{(2)} + k_2[x^{(3)}]^2 \\
\frac{dx^{(3)}}{dt} &= 2k_1[x^{(1)}]^2x^{(2)} - 2k_2[x^{(3)}]^2
\end{aligned}$$

Lorenz system (weather)

$$\begin{aligned}
\frac{dx^{(1)}}{dt} &= \sigma(x^{(2)} - x^{(1)}) \\
\frac{dx^{(2)}}{dt} &= x^{(1)}(\rho - x^{(3)}) - x^{(2)} \\
\frac{dx^{(3)}}{dt} &= x^{(1)}x^{(2)} - \beta x^{(3)}
\end{aligned}$$

Numerical approaches

Start from the general form:

$$\frac{dx^{(i)}}{dt} = f(x^{(1)}, x^{(2)}, ..., t)$$

- Initial conditions: specify $x^{(i)}(t_0)$.
- Algorithms for numerically solving ODEs are called integrators.
- All integrators will evaluate f at discrete points t_0, t_1, ...
- The time step is typically denoted with h.
- Consecutive points may have a fixed step size $h = t_{k+1} - t_k$
- or the size of h may be adaptive, e.g. because some regions require a smaller step for a given accuracy.

Reasonable qualities for an integrator

- *Accuracy*
- *Efficiency*
- *Stability*
- Respect physical laws, e.g.

  Time reversal symmetry
  Conservation of energy
  Conservation of linear momentum
  Conservation of angular momentum
  Conservation of phase space volume

The most efficient algorithm is then the one that allows the largest possible time step for a given level of **accuracy**, while maintaining **stability** and preserving **conservation laws**.

This is a trade-off between accuracy and physicality.

ODE solvers: Forward Euler

To solve:

$$\frac{dx}{dt} = f(x,t)$$

We get a simple approximation of the solution:

$$x_{n+1} \approx x_n + hf(x_n, t_n) \qquad \text{"forward Euler"}$$

How? By truncating the Taylor series of $x_{n+1} = x(t+h)$ around $x_n = x(t)$:

$$x(t_n + h) = x(t_n) + h\frac{dx}{dt}(t_n) + \mathcal{O}(h^2)$$

So:

$$x(t_n + h) = x(t_n) + hf(x_n, t_n) + \mathcal{O}(h^2)$$

So when taking small time steps, this should be accurate.

Accuracy of the forward Euler method

$$x(t_n + h) = x(t_n) + hf(x_n, t_n) + \mathcal{O}(h^2)$$

- $\mathcal{O}(h^2)$ is the local error, i.e., the error in each time step.
- For given trajectory from $t = t_1$ to t_2, we need $n = (t_2 - t_1)/h$ steps.
- The global error, i.e., the error accumulated over the trajectory, is therefore: $n \times \mathcal{O}(h^2) = \mathcal{O}(h)$
- Not very accurate.

Stability of the forward Euler method

To solve harmonic oscillator:

$$\frac{dx^{(1)}}{dt} = x^{(2)}$$

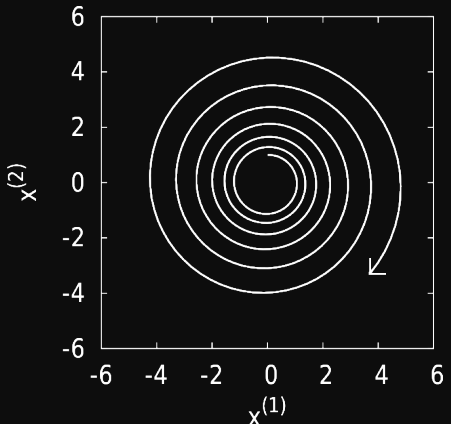
$$\frac{dx^{(2)}}{dt} = -x^{(1)}$$

with forward Euler gives:

$$\begin{pmatrix} x^{(1)}_{n+1} \\ x^{(2)}_{n+1} \end{pmatrix} = \begin{pmatrix} 1 & h \\ -h & 1 \end{pmatrix} \begin{pmatrix} x^{(1)}_{n} \\ x^{(2)}_{n} \end{pmatrix}$$

Stability governed by eigenvalues.

$\lambda_\pm = 1 \pm ih$ of that matrix.

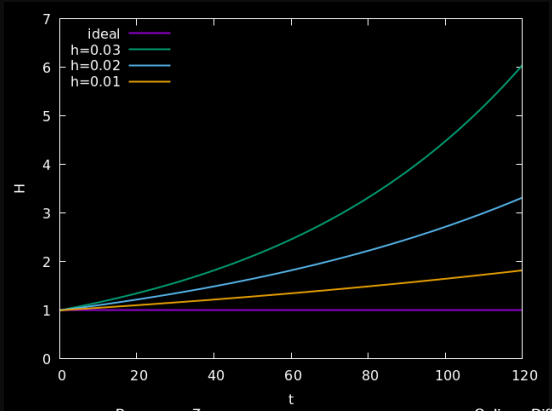


$$|\lambda_\pm| = \sqrt{1+h^2} > 1$$

Unstable for any h!

Monitoring Stability

- For the harmonic oscillator, we know the exact answer, so it's easy to see that the forward Euler integrator is unstable.
- For systems without an exact solution, one may still know that some quantities should be bounded.
- Many physical systems have conserved energy, so we can monitor the energy as a function of time.



Harmonic oscillator:

$$H = \frac{1}{2}[x^{(1)}]^2 + \frac{1}{2}[x^{(1)}]^2$$

So smaller h does help, but in the long run ($t \sim \mathcal{O}(1/h)$), unstable.

ODE solvers: implicit mid-point Euler

Equation to solve:

$$\frac{dx}{dt} = f(x,t)$$

Forward Euler explodes, backward Euler would implode $\Rightarrow$ Symmetric approximation:

$$x_{n+1} \approx x_n + hf((x_n + x_{n+1})/2, t_n) \qquad \textit{"mid-point Euler"}$$

This is an implicit formula, i.e., has to be solved for x_{n+1}.

Example: Harmonic oscillator

$$\begin{bmatrix} 1 & -\frac{h}{2} \\ \frac{h}{2} & 1 \end{bmatrix} \begin{bmatrix} x^{(1)}_{n+1} \\ x^{(2)}_{n+1} \end{bmatrix} = \begin{bmatrix} 1 & \frac{h}{2} \\ -\frac{h}{2} & 1 \end{bmatrix} \begin{bmatrix} x^{(1)}_{n} \\ x^{(2)}_{n} \end{bmatrix} \Rightarrow \begin{bmatrix} x^{(1)}_{n+1} \\ x^{(2)}_{n+1} \end{bmatrix} = M \begin{bmatrix} x^{(1)}_{n} \\ x^{(2)}_{n} \end{bmatrix}$$

Eigenvalues M are $\lambda_\pm = \frac{(1 \pm ih/2)^2}{1+h^2/4}$ so $|\lambda_\pm| = 1$

Stable for all h!

Implicit methods often more stable and allow larger step size h.

ODE solvers: implicit mid-point Euler

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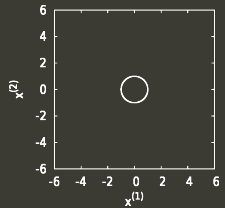


ODE solvers: Predictor-Corrector

- Computation of new point
- Correction using that new point
- Gear P.C.: keep previous values of x to do higher order Taylor series (predictor), then use f in last point to correct.

  Can suffer from catastrophic cancellation at very low h.
- Runge-Kutta: Refines by using mid-points. 4th order version:

$$
\begin{aligned}
k_1 &= hf(x,t) \\
k_2 &= hf(x+k_1/2, t+h/2) \\
k_3 &= hf(x+k_2/2, t+h/2) \\
k_4 &= hf(x+k_3, t+h) \\
x' &= y + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6}
\end{aligned}
$$

Adaptive Step-size Control

Rather than taking a fixed h, we can vary h such that the solution has a certain accuracy.

Methods that adjust the time step as the computation proceeds are known as adaptive methods.

Such an approach needs four components:

1. The basic algorithm for a single h time step,
2. An algorithm to determine the best h time step based on given absolute or relative precision,
3. A evolution algorithm combining these two to take the best possible single time step.
4. A driver routine to step forward in time, using the evolution, for the desired time points.

Don't code this yourself (except for the 'driver')!

Adaptive schemes are implemented in libraries such as the `gsl` and `boost::numeric::odeint`.

ODE example: Van der Pol equation

The Van der Pol oscilator satisfies the following equation:

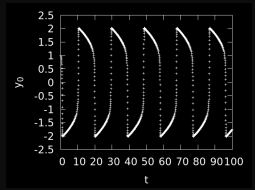
$$\frac{d^2y}{dt^2} - \mu(1-y^2)\frac{dy}{dt} + y = 0$$

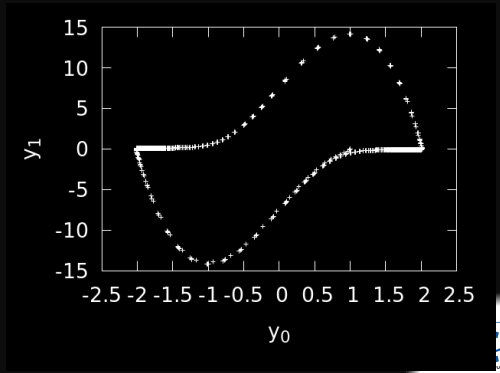
or, writing $y_0 = y =$, $y_1 = dy/dt$,

$$\frac{dy_0}{dt} = y_1$$

$$\frac{dy_1}{dt} = -y_0 - \mu(y_0^2 - 1)y_1$$

Solution for $t = 0..100$ starting from $(y_0, y_1) = (1, 0)$





GSL ODE example: Van der Pol equation

```
#include <print>
#include <memory>
#include <gsl/gsl_errno.h>
#include <gsl/gsl_odeiv2.h>
```

```
const unsigned vdpdim = 2;

int vdprhs(double t, const double y[],
           double f[], void *params)
{
 double mu = *reinterpret_cast<double*>(params);
 f[0] = y[1];
 f[1] = -y[0] - mu*y[1]*(y[0]*y[0] - 1);
 return GSL_SUCCESS;
}
```

```
int main() {
 const gsl_odeiv2_step_type*
   step_type = gsl_odeiv2_step_rk8pd;
 double abstol = 1.e-8;
 auto stepper = std::shared_ptr<gsl_odeiv2_step>
   (gsl_odeiv2_step_alloc(step_type, vdpdim),
    gsl_odeiv2_step_free);
```

```
auto control = std::shared_ptr<gsl_odeiv2_control>
  (gsl_odeiv2_control_y_new (abstol, 0.0),
   gsl_odeiv2_control_free);
auto evolver = std::shared_ptr<gsl_odeiv2_evolve>
  (gsl_odeiv2_evolve_alloc(vdpdim),
   gsl_odeiv2_evolve_free);
```

```
double mu = 10;
gsl_odeiv2_system sys = {vdprhs, 0, vdpdim, &mu};
```

```
double t = 0.0;
double maxt = 100.0;
double h = 1.e-6;
double y[vdpdim] = { 1.0, 0.0 };
```

```
while (t < maxt) {
 int status = gsl_odeiv2_evolve_apply
  (evolver.get(), control.get(), stepper.get(),
   &sys, &t, maxt, &h, y);
```

```
 if (status != GSL_SUCCESS) break;
 std::println("{:.5e} {:.5e} {:.5e}",
              t,     y[0],  y[1]);
}
```

Boost ODE example: Van der Pol equation

```
#include <iostream>
#include <array>
#include <boost/numeric/odeint.hpp>

const unsigned vdpdim = 2;
typedef std::array<double,vdpdim> State;

struct van_der_pol {
 double mu;
 van_der_pol(double mu) : mu(mu) {}
 void operator()(const State &y,
                 State &f, double t) const {
  f[0] = y[1];
  f[1] = -y[0] - mu*y[1]*(y[0]*y[0] - 1);
 }
};

void write_state(const State &y, double t) {
 std::cout<<std::scientific<<std::setprecision(5)
          <<t<<" "<<y[0]<<" "<<y[1]<<"\n";
}
```

```
int main(int argc, char* argv[])
{
 using namespace boost::numeric::odeint;

 double abstol = 1.e-8;
 auto control = make_controlled(abstol, 0.0,
                    runge_kutta_dopri5<State>());
 double mu = 10.0;
 auto system = van_der_pol(mu);

 double t = 0.0;
 double maxt = 100.0;
 double h = 1.e-6;
 State y = { 1.0, 0.0 };

 integrate_adaptive(control, system,
                    y, t, maxt, h,
                    write_state);
}
```

Compilation on Teach

GSL example:

```
$ module load gcc/14
$ # have gsl installed
$ g++ -Wall -I$HOME/gsl/include -g -O3 -march=native -c -o gslvdp.o gslvdp.cpp
$ g++ -g -O3 -L$HOME/gsl/lib -o gslvdp gslvdp.o -lgsl -lgslcblas
$ export LD_LIBRARY_PATH="$LD_LIBRARY_PATH:$HOME/gsl/lib"
$ ./gslvdp
```

Boost:

```
$ module load gcc/14 boost
$ g++ -Wall -g -O3 -march=native -c -o boostvdp.o boostvdp.cpp
$ g++ -g -o boostvdp.cpp boostvdp.o
$ ./boostvdp
```

(note that boost's ode implementation is header-only).

Remember the GSL installation from lecture 8

```
$ module load gcc/14
$ mkdir $HOME/buildgsl
$ cd $HOME/buildgsl
$ wget ftp://ftp.gnu.org/gnu/gsl/gsl-2.8.tar.gz
$ tar xzf gsl-2.8.tar.gz
$ cd gsl-2.8
$ ./configure CFLAGS="-O2 -march=native -ffp-contract=off" --prefix=$HOME/gsl
$ make -j4
$ make check
$ make install
```

then set

```
export CPATH="$CPATH:$HOME/gsl/include"
export LIBRARY_PATH="$LIBRARY_PATH:$HOME/gsl/lib"
export LD_LIBRARY_PATH="$LD_LIBRARY_PATH:$HOME/gsl/lib"
```