

Numerical ODE integrators in Stan/Torsten

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July 30, 2019

Nonlinear ODEs without analytical solution

```
functions {  
    real[] reaction(real t, real[] x, real[] p, real[] r, int[]  
i){  
    /*  $k_{1r} = k_{-1}$  */  
    real k1  = p[1];  
    real k1r = p[2];  
    real k2  = p[3];  
    real S   = x[1];  
    real E   = x[2];  
    real ES  = x[3];  
    real P   = x[4];  
    real dSdt = k1r * ES - k1 * S * E;  
    real dEdt = k1r * ES + k2 * ES - k1 * S * E;  
    real dESdt = k1 * S * E - k1r * ES - k2 * ES;  
    real dPdt  = k2 * ES;  
  
    return {dSdt, dEdt, dESdt, dPdt};  
}  
}
```

Numerical integrators

- ▶ Runge-Kutta 4th/5th (rk45)
 - ▶ non-stiff equations
 - ▶ Most popular, try this if you don't know the nature of the ODE, or what you're doing, or both.
- ▶ Backward differentiation formula (bdf)
 - ▶ stiff equations
 - ▶ More expensive to use
- ▶ Adams-Moulton
 - ▶ non-stiff equations
 - ▶ higher-order of accuracy(do you really need it?)
 - ▶ scales better with number of steps

Numerical integrators

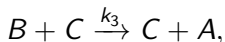
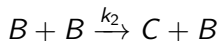
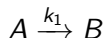
Integrators	Stan	Torsten
rk45	integrate_ode_rk45	pmx_integrate_ode_rk45
BDF	integrate_ode_bdf	pmx_integrate_ode_bdf
Adams	integrate_ode_adams	pmx_integrate_ode_adams

```
real[ , ] pmx_integrate_ode_rk45(ODE_RHS, real[] y0, real t0,  
  ↪ real[] ts, real[] theta, real[] x_r, int[] x_i, real rtol =  
  ↪ 1.e-6, real atol = 1.e-6, int max_step = 1e6);
```

- ▶ ODE_RHS: ODE right-hand-side f in $y' = f(y, t, \theta, x_r, x_i)$.
- ▶ y0: initial condition at time t0.
- ▶ t0: initial time.
- ▶ ts: times at which we require a solution.
- ▶ theta: parameters to be passed to f .
- ▶ x_r: real data to be passed to f .
- ▶ x_i: integer data to be passed to f .

Exercise

We consider the kinetics of an autocatalytic reaction [1]. The structure of the reactions is



where k_1 , k_2 , k_3 are the rate constants and A , B and C are the chemical species involved. The corresponding ODEs are

$$x_1' = -k_1 x_1 + k_3 x_2 x_3$$

$$x_2' = k_1 x_1 - k_2 y_2^2 - k_3 x_2 x_3$$

$$x_3' = k_2 y_2^2$$

Given $k_1 = 0.04$, $k_2 = 1.0e4$, $k_3 = 3.0e7$, we seek the initial condition for $x_1(t = 0)$.

Exercise

- ▶ Write the `functions` block for f .
- ▶ What's the initial conditions for x_2 and x_3 ?
- ▶ Which numerical integrator to use? Why? Did you try other options?

Exercise

How to build & run?

Edit/Add cmdstan/make/local

```
TORSTEN_MPI = 1  # flag on torsten's MPI solvers  
CXXFLAGS += -isystem /usr/local/include    # path to MPI  
↪      library's headers
```

Build in cmdstan

```
make ../example-models/ttpn2/ttpn2_group
```

Run

```
./chem sample adapt delta=0.95 random seed=1104508041 data  
↪   file=chem.data.R init=chem.init.R
```

Reference



H. H. Robertson.

Numerical analysis, an introduction, chapitre The solution of a set of reaction rate equations.

Academic Press, 1966.