Numerical ODE integrators in Stan/Torsten

Yi Zhang, Charles Margossian

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Outline

Nonlinear ODEs without analytical solution

```
functions {
  real[] reaction(real t, real[] x, real[] p, real[] r, int[]
i){
    /* k1r = 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

$$A \xrightarrow{k_1} B$$
$$B + B \xrightarrow{k_2} C + B$$
$$B + C \xrightarrow{k_3} C + A,$$

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.