Numerical solution of SEIRD

```
library(comomodels)
library(deSolve)
library(ggplot2)
library(tidyverse)
#> -- Attaching packages --------------------------------------- tidyverse 1.3.1 --
#> v tibble  3.1.5     v dplyr   1.0.7
#> v tidyr   1.1.4     v stringr 1.4.0
#> v readr   2.0.2     v forcats 0.5.1
#> v purrr   0.3.4
#> -- Conflicts ------------------------------------------ tidyverse_conflicts() --
#> x dplyr::filter() masks stats::filter()
#> x dplyr::lag()    masks stats::lag()
library(glue)
#>
#> Attaching package: 'glue'
#> The following object is masked from 'package:dplyr':
#>
#>     collapse
```

Introduction

Compartmental epidemiological models (such as SEIRD and its variants) are *differential equation* models—that is, given particular values of the model parameters, the models do not directly specify a functional form over time, but rather they specify the instantaneous rate of change of the system, forming a system of differential equations whose solution is the model output over time. Like many differential equation models of interest in scientific applications, SEIRD differential equations do not admit analytical solutions. Instead, an approximation of the solution must be obtained using numerical methods.

Epidemiological differential equations can be solved easily using simple fixed time step solver such as the Euler method. In this notebook, we show that when such methods are employed without sufficient care in the selection of the time step, high error in the numerical solution may occur. We recommend more sophisticated adaptive step size solvers when solving SEIRD-type models, as implemented in the comomodels package.

This notebook begins with a review of a simple differential equation solver on a toy problem with a known solution. Then, it demonstrates the importance of accurate ODE solvers for comomodel's SEIRD model.

Numerical solution of a differential equation using forward Euler

One of the simplest numerical solvers for differential equations is the forward Euler method. This method assumes a first order differential equation

$$\frac{df}{dt} = g(t, f)$$

(note that f may be a vector-valued function), as well as an initial condition $f(t = t_0)$. Forward Euler forms an approximate solution $\{f_i\}_{i=0}^{N}$ on a set of time points $\{t_i = t_0 + i\Delta t\}_{i=0}^{N}$ which is given by:

$$f_0 = f(t = t_0);$$
$$f_{i+1} = f_i + g(t_i, f_i)\Delta t, \quad i = 1, \ldots, N-1.$$

Importance of the solver step size

Note that Δt—the time spacing between adjacent values in the approximate solution—is a critical parameter of the Euler method. While calculating the next function value f_{i+1}, the Euler method approximates the derivative $g(t, f)$ with the constant value $g(t_i, f_i)$ for the interval $(t_i, t_i + \Delta t)$. However, in actuality, $g(t, f)$ presumably varies over time—thus, as Δt is allowed to get larger, the approximation of $g(t, f)$ by a constant value on an interval of width Δt becomes more prone to error, which ultimately accumulates in the approximate solution and causes it to deviate from the true values.

However, obtaining a satisfactory solution to the differential equation is not as simple as setting Δt to some minuscule value, as decreasing the value of Δt will cause the runtime of the method to increase, and for very small values of Δt, the runtime may be prohibitive.

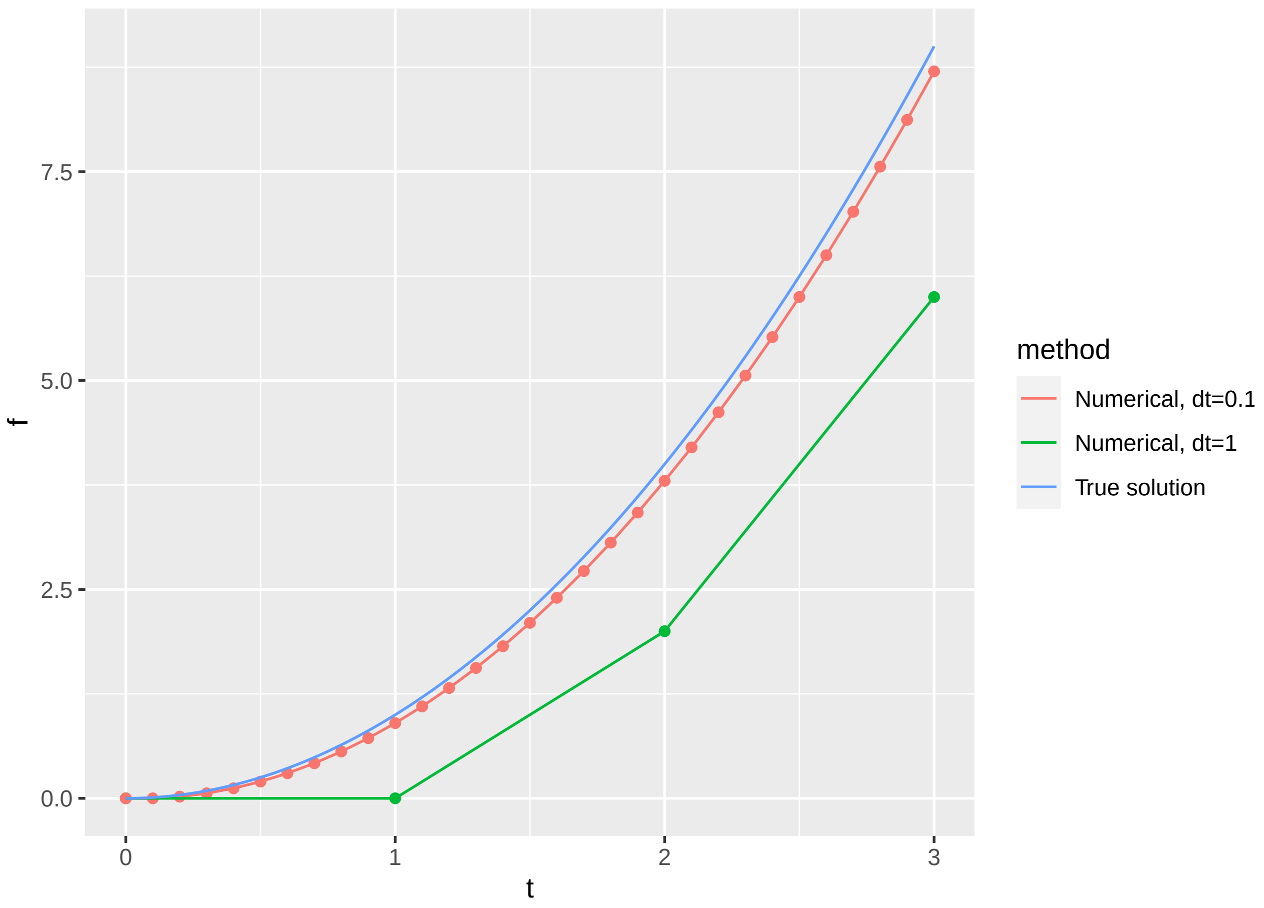
Effect of solver step size on solutions

Before looking at the epidemiological model, we examine the numerical error arising from the solver step size in a simple model for which we have an analytical solution. The differential equation is:

$$\frac{df}{dt} = 2t; \quad f(t = 0) = 0$$

We solve this differential equation on the interval from $t = 0$ to $t = 3$ with two different choices of the time step ($\Delta t = 1$ and $\Delta t = 0.1$). We compare the obtained approximate solutions with the known true solution.

```r
rhs <- function(t, state, params){
  list(2*t)
}

true_solution <- function(t){
  t ^ 2
}


sparse_times <- seq(0, 3, by=1)
dense_times <- seq(0, 3, by=0.1)


# Solve using "euler" from deSolve
# It uses the same times on which output is requested as the solver time points
numerical_solution_sparse = ode(
  y=0,
  times=sparse_times,
  parms=NULL,
  func=rhs,
  method="euler",
)

numerical_solution_dense = ode(
  y=0,
  times=dense_times,
  parms=NULL,
  func=rhs,
  method="euler",
)


# Save the results in data frames for plotting
results_sparse <- data.frame(
  t=numerical_solution_sparse[,1],
  f=numerical_solution_sparse[,2],
  method="Numerical, dt=1"
)

results_dense <- data.frame(
  t=numerical_solution_dense[,1],
  f=numerical_solution_dense[,2],
  method="Numerical, dt=0.1"
)

results_true <- data.frame(
  t=seq(0, 3, by=0.01),
  f=true_solution(seq(0, 3, by=0.01)),
  method="True solution"
)


ggplot() +
  geom_point(data=rbind(results_sparse, results_dense),
             aes(x=t, y=f, color=method),
             show.legend=F) +
  geom_line(data=rbind(results_sparse, results_dense, results_true),
            aes(x=t, y=f, color=method))
```



We observe that the large step size of $\Delta t = 1$ causes significant inaccuracy in the solution. In particular, because the derivative is increasing over time, the forward Euler method (which, between solver time steps, assumes that the derivative remains constant at an old value) produces an approximate solution that is too low. For the smaller time step $\Delta t = 0.1$, the approximate solution is more accurate, although a negative deviation is still apparent.

Effect of solver step size on the SEIRD model

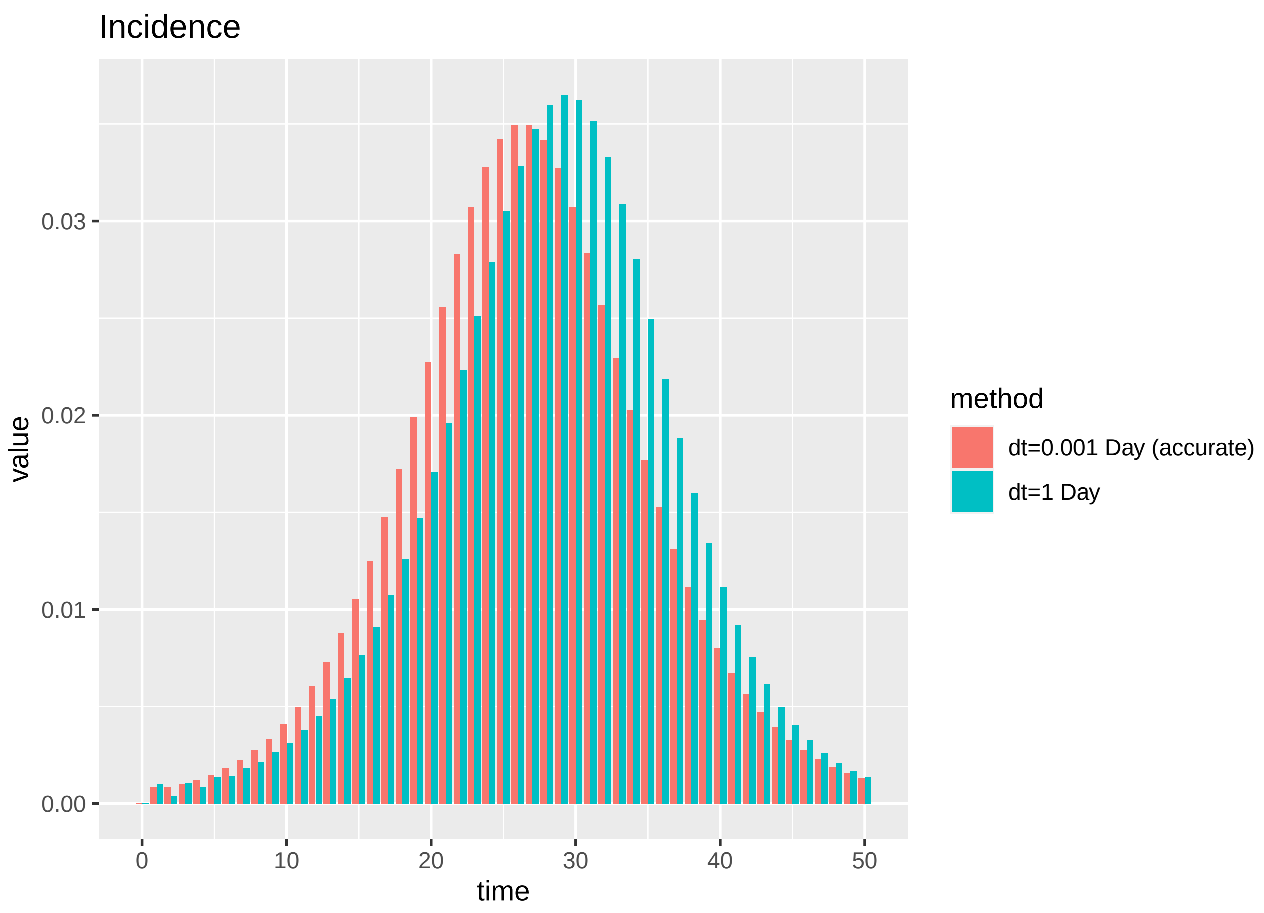
First, we load the SEIRD model from comomodels, and specify plausible parameter values and initial conditions.

```
model <- comomodels::SEIRD()
transmission_parameters(model) <- list(beta=1.0, kappa=0.9, gamma=0.5, mu=0.1)
initial_conditions(model) <- list(S0=0.999, E0=0, I0=0.001, R0=0)
```

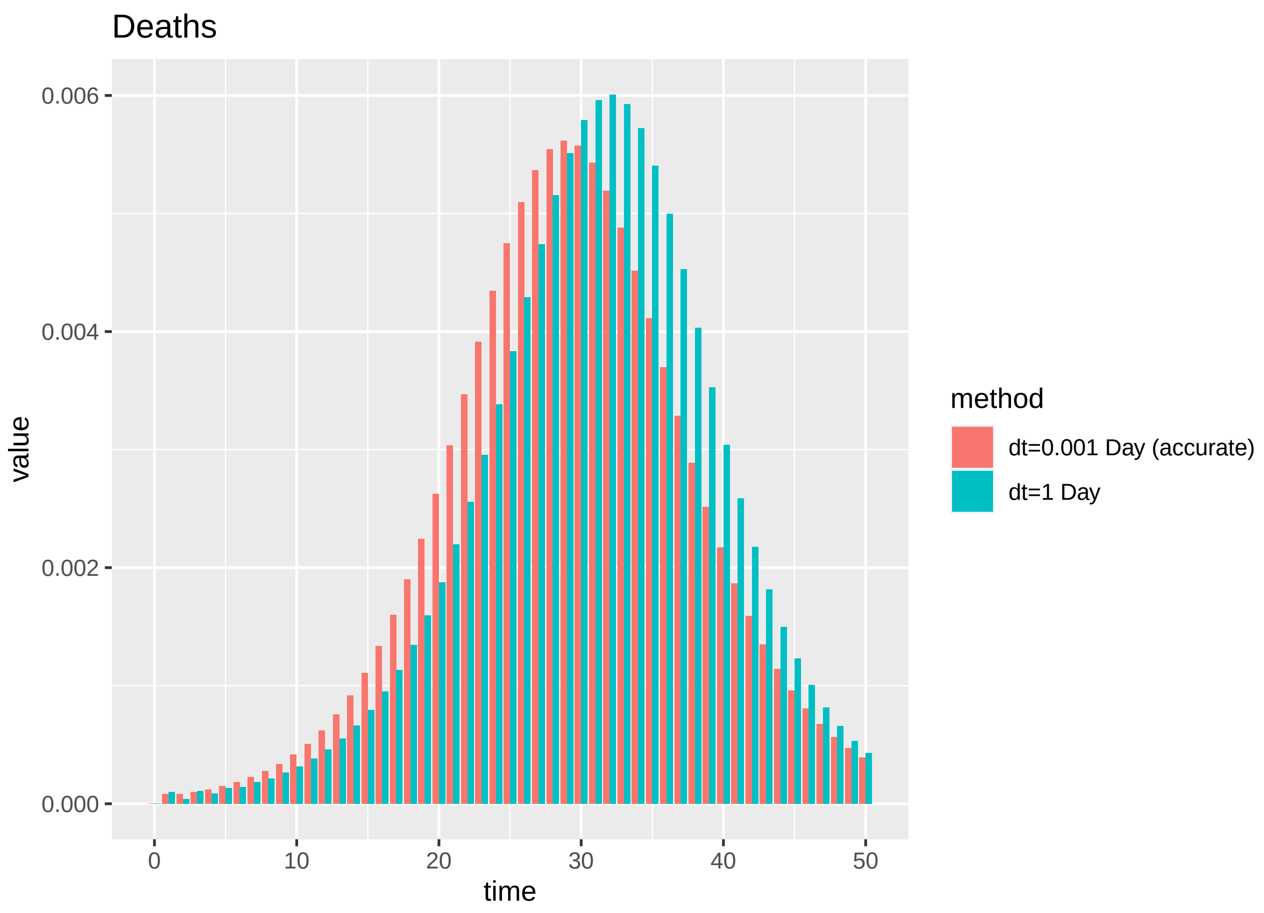
Next, we run the model using the forward Euler method. We investigate two different choices for the solver step size. The first is a daily time step, which naively might be considered an acceptable default choice, given that we are interested in simulating daily cases and deaths. We also consider a much smaller time step of 0.001 days, for which we know that the solution is sufficiently accurate (see the following section for further details on obtaining accurate numerical solutions).

```
times_daily <- seq(0, 50, by=1)
solution_daily <- run(model, times_daily, solve_method="euler")
changes_daily <- solution_daily$changes

times_dense <- seq(0, 50, by=0.001)
solution_dense <- run(model, times_dense, solve_method="euler")
```

```r
df <- solution_dense$changes
df <- as.data.frame(df)

# Sum the deaths and incidences from the dense output to obtain daily values
changes_dense <- data.frame(time=NULL, value=NULL, compartment=NULL)
for (t in times_daily) {
  cases <- subset(df, t-1<df[,1] & df[,1]<=t)
  incidence <- subset(cases, cases[,3]=="Incidence")
  death <- subset(cases, cases[,3]=="Deaths")
  changes_dense <- rbind(changes_dense,
                         data.frame(time=t,
                                    value=sum(incidence$value),
                                    compartment="Incidence",
                                    age_range="0-150"))
  changes_dense <- rbind(changes_dense,
                         data.frame(time=t,
                                    value=sum(death$value),
                                    compartment="Deaths",
                                    age_range="0-150"))
}

# Reorder the deaths and incidences
changes_dense <- changes_dense[order(changes_dense$compartment, changes_dense$time),]

# Save the labels and combine for plotting
changes_dense$method <- "dt=0.001 Day (accurate)"
changes_daily$method <- "dt=1 Day"
all_changes <- rbind(changes_dense, changes_daily)


ggplot(subset(all_changes, all_changes[,3]=="Incidence"),
       aes(x = time, y = value, fill = method)) +
  geom_bar(stat="identity", position = position_dodge()) +
  labs(title="Incidence")
```



```
ggplot(subset(all_changes, all_changes[,3]=="Deaths"),
       aes(x = time, y = value, fill = method)) +
  geom_bar(stat="identity", position = position_dodge()) +
  labs(title="Deaths")
```



These results indicate that for the SEIRD model with these parameters, a daily step size is much too large to obtain accurate results. The daily step size causes the date of the peak of the epidemic (for both incident cases and deaths) to be overestimated by several days.

Differential equations versus difference equations

The forward Euler recurrence relation defining the approximate solution to a *differential* equation,

$$f_{i+1} = f_i + \Delta t g(t_i, f_i),$$

is identical with a typical definition of a *difference* equation of the sort used in multiple fields of computational biology, including epidemiology.

Thus, what we have up till now treated as numerical error arising from the forward Euler method may alternatively be viewed as the discrepancy between an (accurately solved) differential equation model and a corresponding difference equation model. The results above show, for the parameter values considered, that this discrepancy is not negligible. While difference equations can be valid and tenable models for certain phenomena, we see that a daily SEIRD difference equation cannot be considered equivalent to the original SEIRD differential equation model, that is, the same parameter values can cause substantially different outputs from each model.

Adaptive step size methods

The chief advantage of numerical solvers such as forward Euler described above, which take a fixed grid of time points on which to calculate the approximate solution, is their ease of implementation. However, as seen above, these methods suffer because:

1. To obtain an accurate solution, the solver step size must be set to some small value, but it is often unknown how small this value must be.
2. When the solver step size is set to a small value, the method may be unpleasantly slow.

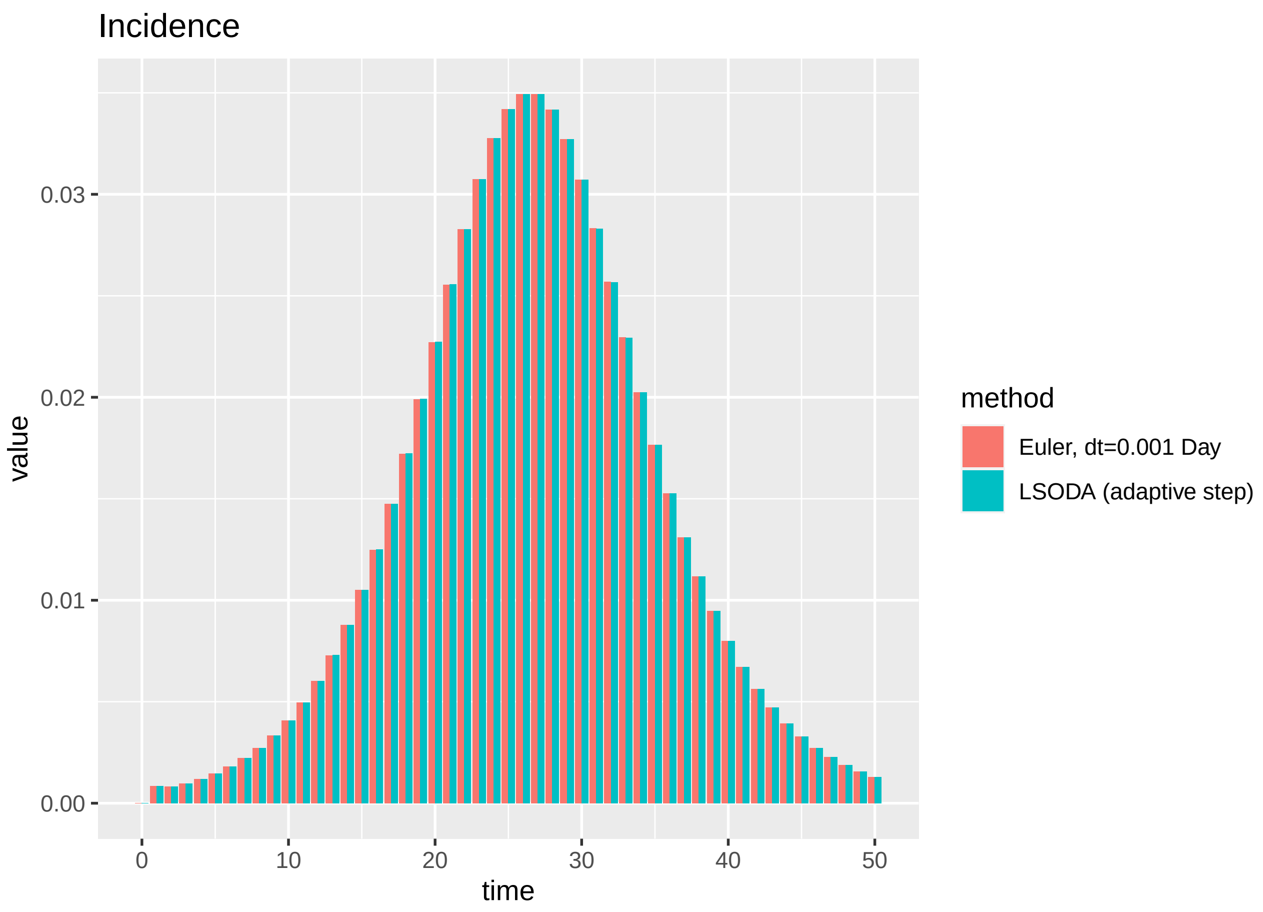
Both of these defects are addressed by adaptive step size methods. In these, the user specifies not a step size but a *tolerance*—some relative or absolute number which the local error in the approximate solution should not exceed. Then, the solver algorithm selects the appropriate step size in order for the solution to meet this tolerance. Adaptive solvers are able to vary the step size over the course of the solve, selecting very small values only in those regions of time where this is necessary, and otherwise increasing the step size to larger values. For this reason, they are much more efficient than fixed step solvers.

A wide variety of approaches to step size adaptation have been proposed. At each step, these methods typically use some heuristic to estimate the error introduced at that time step, and then select roughly the largest possible step such that the threshold imposed by the user-supplied tolerance is not exceeded.

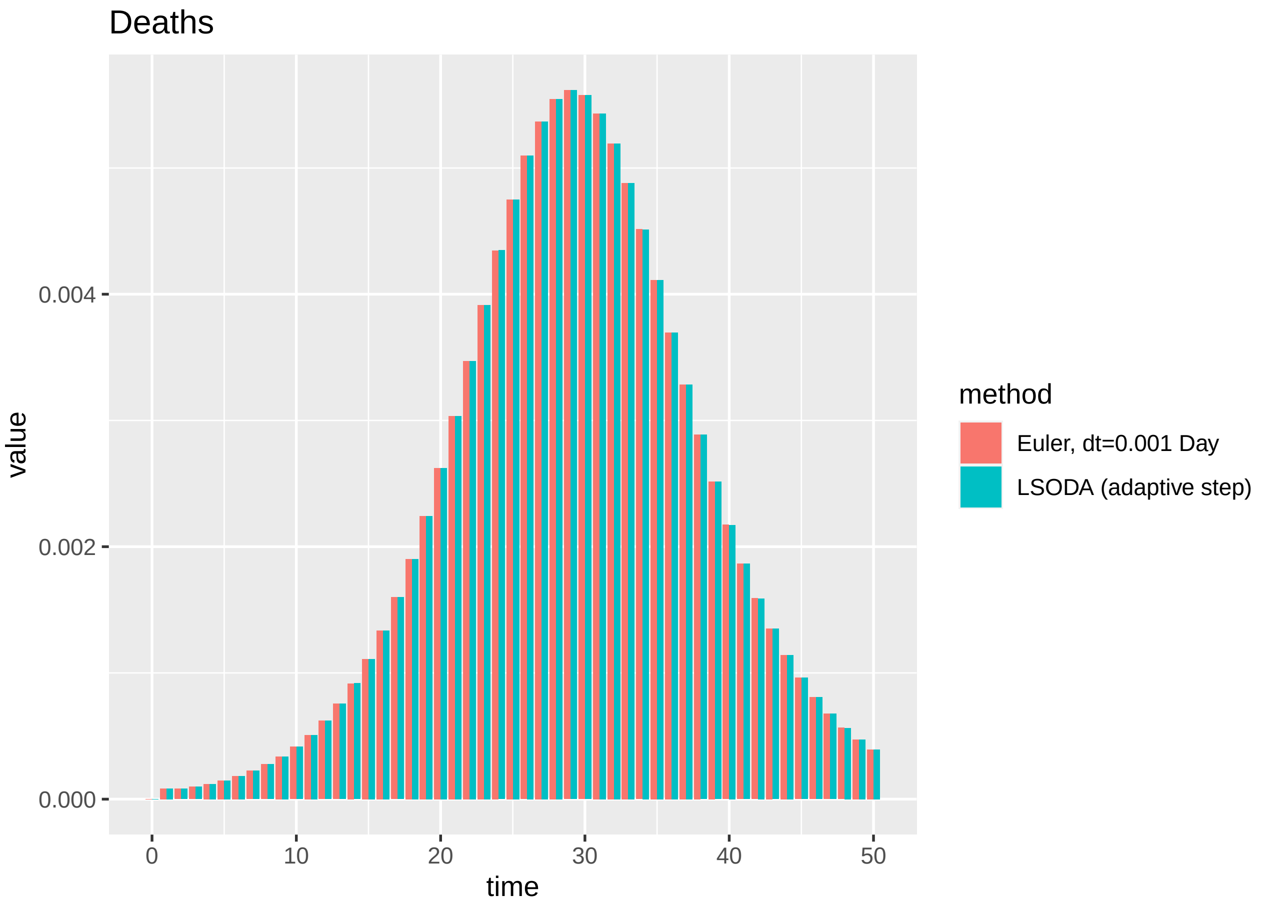
Although adaptive step size solvers are challenging to implement, it is often possible to rely on existing implementations. In R, a wide selection of adaptive step size solvers are provided by the deSolve package. The comomodels library uses deSolve to handle numerical solution of the systems of ODEs that arise in compartmental epidemiology models, giving users easy access to efficient adaptive step size solvers. In comomodels, default values of the local error tolerances are used, so these need not be specified manually. The default solver used in comomodels is LSODA (Hindmarsh and Petzold 2005). This method automatically switches between the Adams and backward differentiation formula (BDF) solvers (Gautschi 2012) based on the properties of the differential equation being solved.

In the following example, we compare the performance of the forward Euler solver with a fixed, small step size to that of the LSODA adaptive step size solver.

```r
times_dense <- seq(0, 50, by=0.001)
print("Timing for Euler (fixed step):")
#> [1] "Timing for Euler (fixed step):"
ptm <- proc.time()
solution_dense <- run(model, times_dense, solve_method='euler')
proc.time() - ptm
#>    user  system elapsed
#>   1.035   0.004   1.039

times_daily <- seq(0, 50, by=1)
print("Timing for LSODA (adaptive step):")
#> [1] "Timing for LSODA (adaptive step):"
ptm <- proc.time()
solution_adapt <- run(model, times_daily, solve_method='lsoda')
proc.time() - ptm
#>    user  system elapsed
#>   0.005   0.000   0.005

df <- solution_dense$changes
df <- as.data.frame(df)

# Sum the deaths and incidences from the dense output to obtain daily values
changes_dense <- data.frame(time=NULL, value=NULL, compartment=NULL)
for (t in times_daily) {
  cases = subset(df, t-1<df[,1] & df[,1]<=t)
  incidence = subset(cases, cases[,3]=="Incidence")
  death = subset(cases, cases[,3]=="Deaths")
  changes_dense = rbind(changes_dense,
                        data.frame(time=t,
                                 value=sum(incidence$value),
                                 compartment="Incidence",
                                 age_range="0-150"))
  changes_dense = rbind(changes_dense,
                      data.frame(time=t,
                                 value=sum(death$value),
                                 compartment="Deaths",
                                 age_range="0-150"))
}

# Save the labels and combine for plotting
changes_adapt <- solution_adapt$changes
changes_dense$method <- "Euler, dt=0.001 Day"
changes_adapt$method <- "LSODA (adaptive step)"
all_changes <- rbind(changes_dense, changes_adapt)


ggplot(subset(all_changes, all_changes[,3]=="Incidence"),
       aes(x = time, y = value, fill = method)) +
  geom_bar(stat="identity", position = position_dodge()) +
  labs(title="Incidence")
```



```
ggplot(subset(all_changes, all_changes[,3]=="Deaths"),
       aes(x = time, y = value, fill = method)) +
  geom_bar(stat="identity", position = position_dodge()) +
  labs(title="Deaths")
```



Both methods achieve the same accurate solution. However, for the LSODA solver, no fiddling with step sizes is necessary: we merely provide the time points at which we want to access the solution (daily), and the solver handles the selection of the step sizes. We also note the significant speed advantage of the LSODA solver, which may be more than 50 times faster (the actual runtimes will be system dependent).

Adaptive solvers are not infallible. On highly challenging differential equations, and when supplied with insufficient tolerances for the simulation or inference task at hand, they may be responsible for errors just as pernicious as those arising from fixed step solvers with too large step sizes. However, for the simulation of compartmental epidemiological models such as those covered by the comomodels package, we highly recommend the use of adaptive solvers such as LSODA (the default choice of solver in comomodels) for speed and accuracy.

Discontinuities in the RHS (interventions)

Differential equations of the form

$$\frac{df}{dt} = g(t, f)$$

where g is discontinuous present further challenges to both adaptive and fixed step size methods, whose error properties (and, for adaptive step size methods, the algorithms used to determine the time steps) typically assume differentiability of g.

In the epidemiological models of the sort described by comomodels, discontinuities of g in time are possible, most notably in the SEIRDV model where step function interventions may be used to specify the rate of vaccination.

Some of the numerical methods that can be used to increase efficiency and decrease error in the case of discontinuous g are:

1. Divide the time interval into sets where g is continuous, and solve the ODE on each set separately.
2. Replace the discontinuous g with a smooth approximation, and use a standard solver.

The second approach is adopted by the SEIRDV model, as a tanh approximation to the step function is used. Further details and a general treatment may be found in (Stewart 2011), Chapter 8.

References

Gautschi, Walter. 2012. *Numerical Analysis*. Springer Science & Business Media.

Hindmarsh, AC, and LR Petzold. 2005. "LSODA, Ordinary Differential Equation Solver for Stiff or Non-Stiff System."

Stewart, David E. 2011. *Dynamics with Inequalities: Impacts and Hard Constraints*. SIAM.