Package bvpSolve, solving boundary value problems in R

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Abstract

This document is about package **bvpSolve** (Soetaert 2009a), designed for the numerical solution of boundary value problems for (first-order) ordinary differential equations (ODE) in R .

Package **bvpSolve** contains:

- function `bvpshoot` which implements the shooting method. This method makes use of the initial value problem solvers from packages **deSolve** (Soetaert, Petzoldt, and Setzer 2009) and the root-finding solver from package **rootSolve** (Soetaert 2009b).

- function `bvptwp`, the mono-implicit Runge-Kutta (MIRK) method with deferred corrections, code TWPBVP (Cash and Wright 1991), for solving two-point boundary value problems

The R functions have an interface which is similar to the interface of the solvers in package **deSolve**

Keywords: ordinary differential equations, boundary value problems, shooting method, mono-implicit Runge-Kutta, R.

1. Introduction

bvpSolve numerically solves boundary value problems (BVP) of first-order ordinary differential equations (ODE), which for one ODE can be written as:

$$\frac{d^2y}{dx^2} = f(x, y, \frac{dy}{dx}) a \le x \le b$$
$$g_1(y)|_a = 0$$
$$g_2(y)|_b = 0$$

where `y` is the dependent, `x` the independent variable, function `f` is the differential equation, g_a and g_b the boundary conditions at the end points a and b.

The problem must be specified as a first-order system. Thus, higher-order ODEs need to be rewritten as a set of first-order systems. For instance:

$$\frac{d^2y}{dx^2} = f(x, y, \frac{dy}{dx})$$

can be rewritten as:

$$\frac{dy}{dx} = z$$
$$\frac{dz}{dx} = f(x, y, z)$$

Note that in the current implementation, the boundary conditions must be defined at the end of the interval over which the ODE is specified (i.e. at `a` and/or `b`).

More examples of boundary value problems can be found in the packages `examples` subdirector. They include a.o. all problems found in `http://www.ma.ic.ac.uk/~jcash/BVP_software`.

2. A simple BVP example

Here is a simple ODE (which is problem 7 from a test problem available from `http://www.ma.ic.ac.uk/~jcash/BVP_software/readme.php`):

$$
\begin{aligned}
\xi y'' + xy' - y &= -(1 + \xi \pi^2)\cos(\pi x) - \pi x \sin(\pi x) \\
y(-1) &= -1 \\
y(1) &= 1
\end{aligned}
$$

The second-order ODE is expanded as two first-order ODEs as:

$$
\begin{aligned}
y_1' &= y_2 \\
y_2' &= 1/\xi \cdot (-xy_2 + y_1 - (1 + \xi \pi^2)\cos(\pi x) - \pi x \sin(\pi x))
\end{aligned}
$$

with boundary conditions

$$
\begin{aligned}
y_1(-1) &= -1 \\
y_1(1) &= 1
\end{aligned}
$$

This is implemented as:

```
> fun<- function(x,y,pars)
+ {
+  list(c(y[2],
+    1/ks*(-x*y[2]+y[1]-(1+ks*pi*pi)*cos(pi*x)-pi*x*sin(pi*x)))
+      )
+ }
```

and solved, using the two methods, as:

```
> ks <- 0.1
> x  <- seq(-1,1,by=0.01)
> print(system.time(
+ sol1  <- bvpshoot(yini=c(-1,NA),yend=c(1,NA),x=x,func=fun,guess=0)
+ ))

   user  system elapsed
   0.04    0.00    0.16


> print(system.time(
+ sol2  <- bvptwp(yini=c(-1,NA),yend=c(1,NA),x=x,func=fun, guess=0)
+ ))

   user  system elapsed
   0.14    0.00    0.14
```
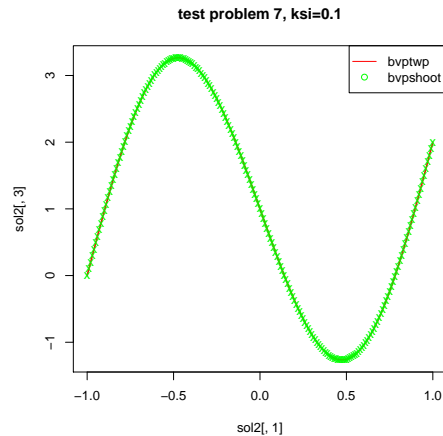
Figure 1: Solution of the simple BVP, for ksi=0.1 - see text for R -code

Note how the boundary conditions at the start (`yini`) and end `yend` of the integration interval are specified, where `NA` is used for boundary conditions that are not known.

A reasonable `guess` of the unknown initial condition is also inputted.

As is often the case, the shooting method is faster than the other method. However, there are particular problems where `bvpshoot` does not lead to a solution, whereas the MIRK method does (see below).

The plot shows that the two methods give the same solution:

```
> plot(sol2[,1],sol2[,3],type="l",main="test problem 7, ksi=0.1",
+      lwd=2,col="red")
> points(sol1[,1],sol1[,3],col="green",pch="x")
> legend("topright",c("bvptwp", "bvpshoot"),
+        lty=c(1,NA,NA), pch=c(NA,1,3),col=c("red", "green") )
```

When the parameter ξ is decreased, `bvpshoot` cannot solve the problem anymore, due to the presence of a zone of rapid change near x=0.

However, it can still easily be solved with the MIRK method:

```
> ks <-0.0001
> print(system.time(
+ sol2  <- bvptwp(yini=c(-1,NA),yend=c(1,NA),x=seq(-1,1,by=0.01),
+           func=fun, guess=0)
+ ))

   user   system elapsed
   1.78    0.00    1.78


> plot(sol2[,1],sol2[,3],type="l",main="test problem 7, ksi=0.0001",
+      lwd=2,col="red")
```
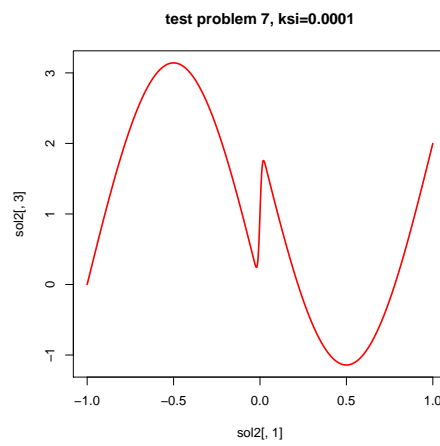
Figure 2: Solution of the simple BVP, for ksi=0.0001 - see text for R -code. Note that this problem cannot be solved with `bvpshoot`

3. A more complex BVP example

Here the test problem referred to as "swirling flow III" is solved (Ascher, Mattheij, and Russell 1995).

The original problem definition is:

$$
\begin{aligned}
g'' &= (gf' - fg')/\xi \\
f'''' &= (-ff''' - gg')/\xi
\end{aligned}
$$

on the interval [0,1] and subject to boundary conditions:

$$
\begin{aligned}
g(0) &= -1, f(0) = 0, f'(0) = 0 \\
g(1) &= 1, f(1) = 0, f'(1) = 0
\end{aligned}
$$

This is rewritten as a set of 1st order ODEs as follows:

$$
\begin{aligned}
y_1' &= y_2 \\
y_2' &= (y_1 * y_4 - y_3 * y_2)/\xi \\
y_3' &= y_4 \\
y_4' &= y_5 \\
y_5' &= y_6 \\
y_6' &= (-y_3 y_6 - y_1 y_2)/\xi
\end{aligned}
$$

Its implementation in R is:

```
> fsub <- function (t,Y,pars)
+ { return(list(c(f1 = Y[2],
+                 f2 = (Y[1]*Y[4] - Y[3]*Y[2])/eps,
+                    f3 = Y[4],
+                    f4 = Y[5],
+                    f5 = Y[6],
+                    f6 = (-Y[3]*Y[6] - Y[1]*Y[2])/eps)))
+ }
> eps <- 0.001
> x <- seq(0,1,len=100)
```

This model cannot be solved with the shooting method. However, it can be solved using bvptwp:

```
> print(system.time(
+ Soltwp <- bvptwp(x=x,func=fsub,guess= c(2,0,0),
+                   yini=c(-1,NA,0,0,NA,NA), yend=c(1,NA,0,0,NA,NA))
+ ))

   user  system elapsed
   1.83    0.00    1.83
```
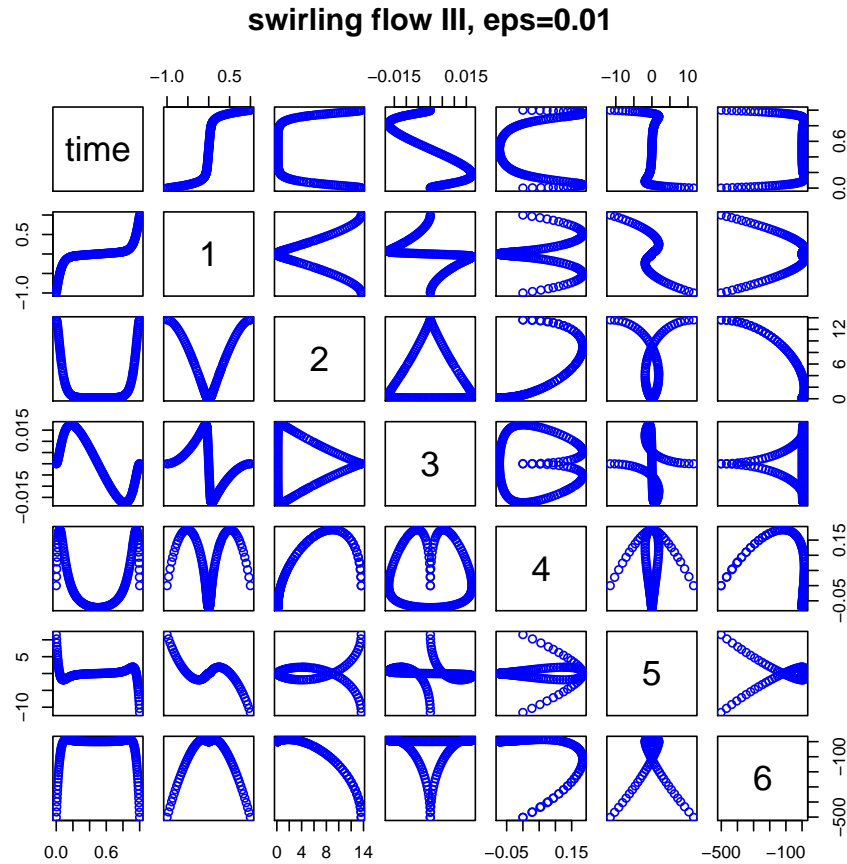
swirling flow III, eps=0.01

Figure 3: Solution of the swirling flow III problem - see text for R -code. Note that this problem cannot be solved with `bvpshoot`

where the reported system time is in seconds

The problem cannot be solved with too small values of eps:

```
> eps <- 1e-9
> Soltwp2 <- NA
> Soltwp2 <- try(bvptwp(x=x,func=fsub,guess= c(2,0,0),
+                 yini=c(-1,NA,0,0,NA,NA), yend=c(1,NA,0,0,NA,NA)),
+      silent = TRUE)
> cat(Soltwp2)

Error in bvptwp(x = x, func = fsub, guess = c(2, 0, 0), yini = c(-1, NA,  :
  The Expected No. Of Subintervals Exceeds Storage Specifications.

> pairs(Soltwp, main="swirling flow III, eps=0.01", col="blue")
```

The problem is more efficiently solved if an initial guess of the solution is given:

```
> eps <- 0.001
> xguess <- x
> yguess <- matrix(nr=6, nc=length(xguess), data=0.)
> slope  <- 0.375-0.9129
> yguess[1,] <- 2*xguess -1
> yguess[2,] <- 2
> print(system.time(Sol2 <- bvptwp(x=x,func=fsub,guess= c(2,0,0),
+   xguess=xguess,yguess=yguess,yini=c(-1,NA,0,0,NA,NA),
+   yend=c(1,NA,0,0,NA,NA))))

   user  system elapsed
   1.39    0.00    1.40
```

4. More complex initial or end conditions

Problem `musn` was described in (Ascher *et al.* 1995).

The problem is:

$$
\begin{aligned}
u' &= 0.5u(w-u)/v \\
v' &= -0.5(w-u) \\
w' &= (0.9 - 1000(w-y) - 0.5w(w-u))/z \\
z' &= 0.5(w-u) \\
y' &= -100(y-w)
\end{aligned}
$$

on the interval [0,1] and subject to boundary conditions:

$$
\begin{aligned}
u(0) = v(0) = w(0) &= 1 \\
z(0) &= -10 \\
w(1) &= y(1)
\end{aligned}
$$

Note the last boundary conditions which expresses `w` as a function of `y`.

Implementation of the ODE function is simple:

```
> musn <- function(x,Y,pars)
+ {
+   with (as.list(Y),
+   {
+     du=0.5*u*(w-u)/v
+     dv=-0.5*(w-u)
+     dw=(0.9-1000*(w-y)-0.5*w*(w-u))/z
+     dz=0.5*(w-u)
+     dy=-100*(y-w)
+     return(list(c(du,dv,dw,dz,dy)))
+   })
+ }
```

There are 4 boundary values specified at the start of the interval; a value for `y` is lacking:

```
> init <- c(u=1,v=1,w=1,z=-10,y=NA)
```

The boundary condition at the end of the integration interval (1) specifies the value of `w` as a function of `y`.

Because of that, `yend` cannot be simply inputted as a vector. It is rather implemented as a function that has as input the values at the end of the integration interval (`Y`), the values at the start (`yini`) and the parameters, and that returns the residual function (`w-y`):

```
> yend  <- function (Y,yini,pars)  with (as.list(Y), w-y)
```

This problem is most efficiently solved with `bvpshoot`: [1]

---

[1]Note that there are at least two solutions to this problem, the second solution can simply be found by setting `guess` equal to 0.9.
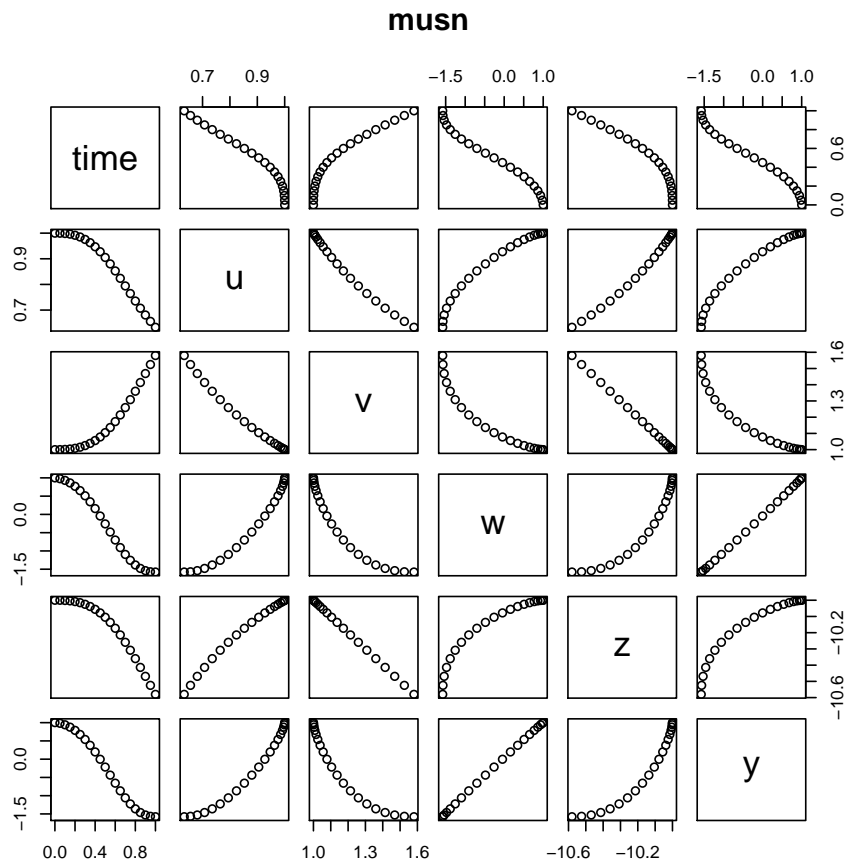
Figure 4: Solution of the musn model, using `bvpshoot` - see text for R -code.

```
> print(system.time(
+ sol    <-bvpshoot(yini= init, x=seq(0,1,by=0.05),func=musn,
+          yend=yend,guess=1,atol=1e-10,rtol=0)
+ ))

   user  system elapsed
   0.34    0.00    0.37

> pairs(sol,main="musn")
```

5. a BVP problem including an unknown parameter

In the next BVP problem, a parameter λ is to be found such that:

$$\frac{d^2y}{dt^2} + (\lambda - 10\cos(2t)) \cdot y = 0$$

on $[0,\pi]$ with boundary conditions $\frac{dy}{dt}(0) = 0$ and $\frac{dy}{dt}(\pi) = 0$ and $y(0) = 1$

Here all the initial values (at t=0) are prescribed. If λ would be known the problem would be overdetermined.

The 2nd order differential equation is first rewritten as two 1st-order equations:

$$\begin{aligned}
\frac{dy}{dt} &= y2 \\
\frac{dy2}{dt} &= -(\lambda - 10\cos(2t)) \cdot y
\end{aligned}$$

and the function that estimates these derivatives is written (`derivs`).

```
> mathieu <- function(x,y,lambda)
+     list(c(y[2],
+         -(lambda-10*cos(2*x))*y[1]))
```

which is easily solved using `bvpshoot`:

```
> init <- c(1,0)
> sol  <- bvpshoot(yini=init,yend=c(NA,0),x=seq(0,pi,by=0.01),
+         func=mathieu, guess=NULL, extra=15)
```

and plotted:

```
> plot(sol)
```

Note how the extra parameter to be fitted is passed (`extra`). The value of `lam` can be printed:

```
> attr(sol,"roots")  # root gives the value of "lam" (17.10684)

      root        f.root iter
2 17.10683 2.347269e-12    6
```
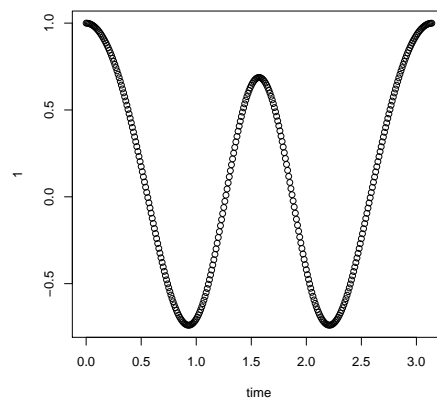
Figure 5: Solution of the BVP ODE problem including an unknown parameter, see text for R-code

References

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