Package bypSolve, solving testproblems

Karline Soetaert

The Netherlands

Jeff Cash

Francesca Mazzia

CEME

Department of mathematics Netherlands Institute of Ecology Imperial College London U.K.

Dipartimento di Matematica Universita' di Bari Italy

Abstract

This document implements several testproblems that can be found on http://www.ma. ic.ac.uk/~jcash/BVP_software/PROBLEMS.PDF, using solvers from package bvpSolve (Soetaert, Cash, and Mazzia 2009a).

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

1. introduction

bvpSolve numerically solves boundary value problems (BVP) of first-order ordinary differential equations (ODE), which for one (second-order) 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, $g_1(y)|_a$ and $g_2(y)|_b$ 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:

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

In this document, all boundary value problems that can be found on http://www.ma.ic.ac. uk/~jcash/BVP_software, are implemented and solved using solvers from package bvpSolve

For each solver, the default settings are used, i.e. without providing "initial guesses" of the solution.

With these settings, some methods cannot solve certain problems. This does not mean that other settings cannot be found that do solve the problem.

If available, then the analytical solution of the problem is plotted (as dots).

Note that another package **deSolve** (Soetaert, Petzoldt, and Setzer 2009b) is designed for solving initial value problems, i.e. where the boundary conditions are provided at the initial boundary point only.

Package **ReacTran** (Soetaert and Meysman 2010) provides numerical differences of first- and second- order derivatives and, using solvers form package **rootSolve** (Soetaert 2009), can solve certain boundary value problems. This is usually more efficient (but less precise) than the boundary value solvers from **bvpSolve**, but many problems cannot be solved this way.

2. Linear problems

2.1. problem 1

This problem is:

$$\xi y'' - y = 0$$
$$y_{(x=0)} = 1, y_{(x=1)} = 0$$

which is rewritten as:

$$y_1' = y2$$
$$y_2' = y_1/\xi$$

and implemented as:

```
> Prob1 <- function(t, y, pars) {
    list(c( y[2] , y[1]/xi ))
}</pre>
```

which is solved for different values of ξ

```
user system elapsed
        0.00
                   0.05
   0.03
> print(system.time(
    col \leftarrow bvpcol(yini = c(1, NA), yend=c(0, NA), x = seq(0, 1, by = 0.01),
              func = Prob1)))
   user system elapsed
         0.00
   0.02
                  0.02
for smaller \xi
> xi <-0.01
> shoot2 <- bvpshoot(yini=c(1,NA),yend=c(0,NA),x=seq(0,1,by=0.01),
              func=Prob1, guess=0)
and for a very small value
> xi <-0.001
> shoot3 < -bvpshoot(yini=c(1,NA),yend=c(0,NA),x=seq(0,1,by=0.01),
             func=Prob1, guess=0)
and the output plotted
> plot(shoot[,1],shoot[,2],type="1",main="test problem 1",col="blue",
    xlab="x",ylab="y")
> lines(shoot2[,1],shoot2[,2],col="red")
> lines(shoot3[,1],shoot3[,2],col="green")
> # exact solution
> curve(exp(-x/sqrt(xi))-exp((x-2)/sqrt(xi)))/(1-exp(-2/sqrt(xi))),
        0,1,add=TRUE,type="p")
```

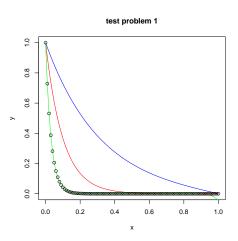


Figure 1: Solution of the BVP ODE problem 1, see text for R-code $\,$

2.2. problem 2

This problem is:

$$\xi y'' - y' = 0$$
$$y_{(x=0)} = 1, y_{(x=1)} = 0$$

which is rewritten as:

$$y_1' = y2$$
$$y_2' = y_2/\xi$$

For lower values of ξ (<0.1) this problem cannot be solved by the shooting method, but it is solvable by mono-implicit Runge-Kutta and collocation

The solution can be compared with the analytical solution:

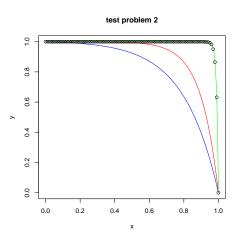


Figure 2: Solution of the BVP ODE problem 2, see text for R-code $\,$

2.3. problem 3

```
\xi y'' + (2 + \cos(\pi x))y' - y = -(1 + \xi \pi^2)\cos(\pi x) - (2 + \cos(\pi x))\pi\sin(\pi x)
                                                    y_{(x=-1)} = y_{(x=1)} = -1
> Prob3 <- function(x, y, pars) {
    list(c(y[2],
           1/xi * (-(2+cos(pi*x)) * y[2] + y[1]-
             (1 + xi*pi*pi) * cos(pi*x)-
             (2 + cos(pi*x))* pi * sin(pi*x))
        ))
  }
> xi <-0.1
> shoot <- bvpshoot(yini = c(-1, NA), yend = c(-1, NA),
                      x = seq(-1, 1, by=0.01), func = Prob3, guess = 0)
> xi <-0.01
         <- bvptwp(yini = c(-1, NA), yend = c(-1, NA),
                    x = seq(-1, 1, by=0.01), func = Prob3)
> xi <-0.001
> col1 <- bvpcol(yini = c(-1, NA), yend = c(-1, NA),
                    x = seq(-1, 1, by=0.01), func = Prob3)
> plot(shoot[,1], shoot[,2], type = "l", main = "test problem 3",
       col = "blue", xlab = "x", ylab = "y")
> lines(twp[,1], twp[,2], col = "red")
> curve(cos(pi*x),-1,1,type="p",add=TRUE)
```

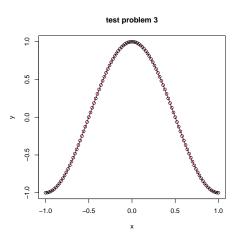


Figure 3: Solution of the BVP ODE problem 3, see text for R-code $\,$

2.4. problem 4

```
\xi y'' + y' - (1 + \xi)y = 0
                               y_{(x=-1)} = 1 + exp(-2)
                         y_{(x=1)} = 1 + exp(-2(1+\xi)/\xi)
> Prob4 <- function(t, y, pars) {</pre>
    list(c(y[2], (-y[2] + (1+xi)*y[1])/xi))
> yini <- c(1 + exp(-2), NA)
> xi <- 0.5
> yend <- c(1 + \exp(-2*(1+xi)/xi), NA)
> shoot <- bvpshoot(yini = yini, yend = yend, x = seq(-1, 1, by = 0.01),
                      func = Prob4, guess = 0)
> xi <- 0.1
> yend <- c(1 + \exp(-2*(1+xi)/xi), NA)
> twp \leftarrow bvptwp(yini = yini,yend = yend,x = seq(-1, 1, by = 0.01),
                   func = Prob4)
> xi <- 0.01
> yend <- c(1 + \exp(-2*(1+xi)/xi), NA)
         <- bvptwp(yini = yini, yend = yend, x = seq(-1, 1, by = 0.01),
                     func = Prob4)
> plot(shoot[,1], shoot[,2], type = "l", main = "test problem 4",
    ylim = c(0, 1.2), col = "blue", xlab = "x", ylab="y")
> lines(twp[,1], twp[,2],col = "red")
> lines(twp2[,1], twp2[,2],col = "green")
> curve(exp(x-1) + exp(-(1+xi)*(1+x)/xi), -1, 1, type = "p", add = TRUE)
```

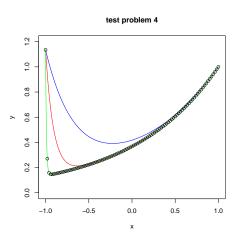


Figure 4: Solution of the BVP ODE problem 4, see text for R-code $\,$

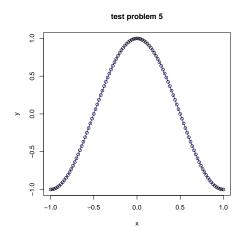


Figure 5: Solution of the BVP ODE problem 5, see text for R-code

2.5. problem 5

2.6. problem 6

$$\xi y'' + xy' = -\xi \pi^2 \cos(\pi x) - \pi x \sin(\pi x)$$
$$y_{(x=-1)} = -2$$
$$y_{(x=1)} = 0$$

This problem cannot be solved by the shooting method, except for the largest value of xi

```
> Prob6 <- function(t, y, pars) {</pre>
   list(c(y[2],
           1/xi * (-t*y[2] - xi*pi*pi*cos(pi*t) - pi*t*sin(pi*t)))
 }
> xi
      <- 0.1
> shoot <- bvpshoot(yini = c(-2, NA), yend = c(0, NA),
                    x = seg(-1, 1, by = 0.01), func = Prob6, guess = 0)
> xi
       <- 0.01
       <- bvptwp(yini = c(-2, NA), yend = c(0, NA),
                 x = seq(-1, 1, by = 0.01), func = Prob6)
> xi
       <- 0.001
> twp2 <- bvptwp(yini = c(-2, NA), yend = c(0, NA),
                 x = seq(-1, 1, by = 0.01), func = Prob6)
> plot(shoot[,1], shoot[,2], type = "l", main = "test problem 6",
       ylim = c(-2, 2), col = "blue", xlab = "x", ylab = "y")
> lines(twp[,1], twp[,2], col = "red")
> lines(twp2[,1], twp2[,2], col = "green")
> erf <- function(x) 2 * pnorm(x * sqrt(2)) - 1
> curve(cos(pi*x) + erf(x/sqrt(2*xi))/erf(1/sqrt(2*xi)), -1, 1,
        type = "p", add = TRUE)
```

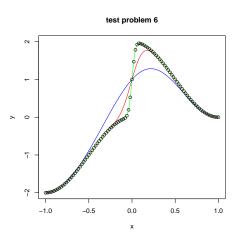


Figure 6: Solution of the BVP ODE problem 6, see text for R-code $\,$

2.7. problem 7

> par(mfrow = c(1,1))

$$\xi y'' + xy' - y = -(1 + \xi \pi^2) \cos(\pi x) - \pi x \sin(\pi x)$$

y(-1) = -1
y(1) = 1

This problem cannot be solved with the shooting method for small xi.

```
> prob7 <- function(x, y, pars) {</pre>
    list(c(y[2],
           1/xi * (-x*y[2]+y[1] - (1+xi*pi*pi)*cos(pi*x)-pi*x*sin(pi*x)))
  }
> x < - seq(-1, 1, by = 0.01)
> xi <- 0.01
> twp <- bvptwp(yini = c(-1, NA), yend = c(1, NA), x = x, func = prob7)
> xi <- 0.001
> twp2 < -bvptwp(yini = c(-1, NA), yend = c(1, NA), x = x, func = prob7)
For even smaller \xi, we need to provide good initial guesses:
> xi <- 0.0005
> twp3 <- bvptwp(yini = c(-1, NA), yend = c(1, NA), x = x, func = prob7,
    xguess = twp2[,1], yguess = t(twp2[,-1]))
> par(mfrow = c(1,2))
> plot(twp[,1], twp[,2], type = "l", main = "test problem 7",
    col = "blue", xlab = "x", ylab = "y")
> erf \leftarrow function(x) 2 * pnorm(x * sqrt(2)) - 1
> curve(cos(pi*x) + x + (x*erf(x/sqrt(2*xi))+sqrt(2*xi/pi)*exp(-x^2/2/xi))/
           (erf(1/(2*xi))+sqrt(2*xi/pi)*exp(-1/2/xi)),
           -1, 1, type = "p", add = TRUE)
> plot(twp[,1], twp[,3], type = "l", main = "test problem 7",
    col = "blue", xlab = "x", ylab = "y'")
> lines(twp2[,1], twp2[,3], col = "red")
> lines(twp3[,1], twp3[,3], col = "green")
```

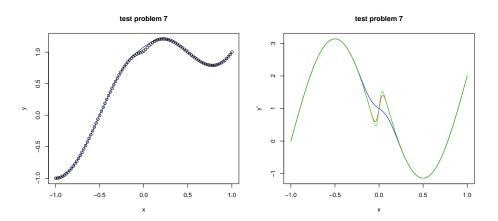


Figure 7: Solution of the BVP ODE problem 7, y and y' versus x- see text for R-code

2.8. problem 8

2.9. problem 9

$$(\xi + x^2)y'' + 4xy' + 2y = 0$$
$$y_{(x=-1)} = y_{(x=1)} = 1/(1+\xi)$$

This problem cannot be solved by the shooting method

```
> Prob9 <- function(x, y, pars) {
    list(c( y[2], -1/(xi+x^2)*(4*x*y[2]+2*y[1]) ))
}</pre>
```

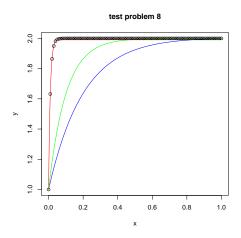


Figure 8: Solution of the BVP ODE problem 8, see text for R-code

```
<-0.05
> xi
       <- bvptwp(yini = c(1/(1+xi), NA), yend = c(1/(1+xi), NA),
                 x = seq(-1, 1, by = 0.01), func = Prob9)
> xi
       <-0.02
> twp2 <- bvptwp(yini = c(1/(1+xi), NA), yend = c(1/(1+xi), NA),
                 x = seq(-1, 1, by = 0.01), func = Prob9)
> xi
       <-0.01
> twp3 <- bvptwp(yini = c(1/(1+xi), NA), yend = c(1/(1+xi), NA),
                 x = seq(-1, 1, by = 0.01), func = Prob9)
> plot(twp[,1], twp[,2], type = "l", main = "test problem 9",
       ylim = c(0, 100), col = "blue", xlab = "x", ylab="y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp3[,1], twp3[,2], col = "green")
> # exact
> curve(1/(xi+x^2), -1, 1, type = "p", add = TRUE)
```

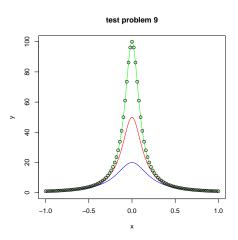


Figure 9: Solution of the BVP ODE problem 9, see text for R-code

2.10. problem 10

```
\xi y'' + xy' = 0
                                  y_{(x=-1)} = 0
                                   y_{(x=1)} = 2
> Prob10 <- function(x, y, pars) {</pre>
    list(c(y[2], -1/xi*x*y[2]))
> xi
       <-0.1
> shoot <- bvpshoot(yini = c(0, NA), yend = c(2, NA),
                    x = seq(-1, 1, by = 0.01), func=Prob10, guess = 0)
> xi
       <- 0.05
> twp <- bvptwp(yini = c(0, NA), yend = c(2, NA),
                 x = seq(-1, 1, by = 0.01), func=Prob10)
> xi <- 0.01
> twp2 \leftarrow bvptwp(yini = c(0, NA), yend = c(2, NA),
                 x = seq(-1, 1, by = 0.01), func=Prob10)
> plot(shoot[,1], shoot[,2], type = "l", main = "test problem 10",
       col = "blue", xlab = "x", ylab = "y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp[,1], twp[,2], col = "green")
> erf <- function(x) 2 * pnorm(x * sqrt(2)) - 1
> curve(1+erf(x/sqrt(2*xi))/erf(1/sqrt(2*xi)),
        -1, 1, type = "p", add = TRUE)
```

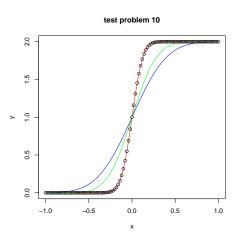


Figure 10: Solution of the BVP ODE problem 10, see text for R-code $\,$

2.11. problem 11

> curve(cos(pi*x), -1, 1, type = "p", add = TRUE)

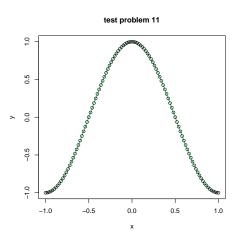


Figure 11: Solution of the BVP ODE problem 11, see text for R-code $\,$

2.12. problem 12

The same as problem 11, but with different boundary values:

$$\xi y'' = y = -(\xi \pi^2 + 1) cos(\pi x)$$

$$y_{(x=-1)} = -1$$

$$y_{(x=1)} = 0$$

```
> Prob12 <- function(x, y, pars) {</pre>
    list(c(y[2], 1/xi * (y[1]-(xi*pi*pi+1)*cos(pi*x))))
> xi <- 0.01
> shoot <- bvpshoot(yini = c(-1, NA), yend = c(0, NA),
                    x = seq(-1, 1, by = 0.01), func = Prob12, guess = 0)
> xi
       <- 0.0025
> twp <- bvptwp(yini = c(-1, NA), yend = c(0, NA),
                 x = seq(-1, 1, by = 0.01), func = Prob12)
       <- 0.0001
> xi
> twp2 \leftarrow bvptwp(yini = c(-1, NA), yend = c(0, NA),
                 x = seq(-1, 1, by = 0.01), func = Prob12)
> plot(shoot[,1], shoot[,2], type = "l", main="test problem 12",
       col = "blue", xlab = "x", ylab = "y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp[,1], twp[,2], col = "green")
> curve(cos(pi*x)+exp((x-1)/sqrt(xi)),
        -1, 1, type = "p", add = TRUE)
```

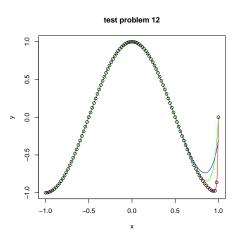


Figure 12: Solution of the BVP ODE problem 12, see text for R-code $\,$

2.13. problem 13

The same as problem 11, but with different boundary values:

-1, 1, type = "p", add = TRUE)

```
\xi y'' = y = -(\xi \pi^2 + 1)cos(\pi x)
                            y_{(x=-1)} = 0y_{(x=1)} = -1
> Prob13 <- function(x, y, pars) {</pre>
    list(c( y[2], 1/xi*(y[1]-(xi*pi*pi+1)*cos(pi*x)) ))
> xi <- 0.01
> shoot <- bvpshoot(yini = c(0, NA), yend = c(-1, NA),
                    x = seq(-1, 1, by=0.01), func = Prob13, guess = 0)
> xi
       <- 0.0025
> twp <- bvptwp(yini = c(0, NA), yend = c(-1, NA),
                 x = seq(-1, 1, by=0.01), func = Prob13)
        <- 0.0001
> xi
> twp2 <- bvptwp(yini = c(0, NA), yend = c(-1, NA),
                  x = seq(-1, 1, by=0.01), func = Prob13)
> plot(shoot[,1], shoot[,2], type = "l", main = "test problem 13",
       col = "blue", xlab = "x", ylab = "y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp[,1], twp[,2], col = "green")
> curve(cos(pi*x)+exp(-(x+1)/sqrt(xi)),
```

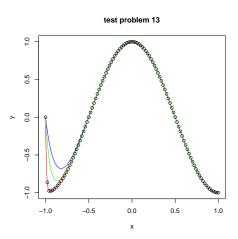


Figure 13: Solution of the BVP ODE problem 13, see text for R-code $\,$

2.14. problem 14

The same as problem 11, but with different boundary values:

$$\xi y'' = y = -(\xi \pi^2 + 1) cos(\pi x)$$

$$y_{(x=-1)} = 0$$

$$y_{(x=1)} = 0$$
 > Prob14 <- function(x, y, pars) { list(c(y[2], 1/xi*(y[1]-(xi*pi*pi+1)*cos(pi*xi*pi+1)

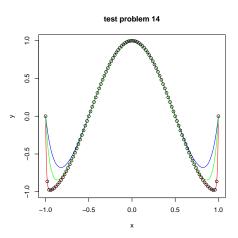


Figure 14: Solution of the BVP ODE problem 14, see text for R-code $\,$

2.15. problem 15

```
\xi y'' - xy = 0
                             y_{(x=-1)} = y_{(x=1)} = 1
> Prob15 <- function(x, y, pars) {</pre>
   list(c( y[2], 1/xi*x*y[1] ))
 }
> xi <-0.003
> print(system.time(
 shoot <- bvpshoot(yini = c(1, NA), yend = c(1, NA),
                     x = seq(-1, 1, by = 0.01), func = Prob15, guess = 0)
 ))
  user system elapsed
   0.09
           0.00
                   0.11
> xi <- 0.005
> print(system.time(
 twp \leftarrow bvptwp(yini = c(1, NA), yend = c(1, NA),
                 x = seq(-1, 1, by = 0.01), func = Prob15)
 ))
  user system elapsed
   0.10
         0.00
                  0.12
> xi <- 0.005
> print(system.time(
 col <- bvpcol(yini = c(1, NA), yend = c(1, NA),
                 x = seq(-1, 1, by = 0.01), func = Prob15)
 ))
  user system elapsed
                  0.23
  0.24
        0.00
> xi <- 0.01
> print(system.time(
  twp2 \leftarrow bvptwp(yini = c(1, NA), yend = c(1, NA),
              x = seq(-1, 1, by = 0.01), func = Prob15)
 ))
  user system elapsed
  0.13
        0.00
                   0.12
```

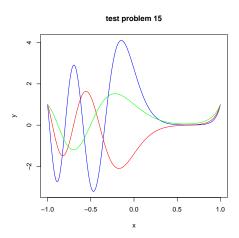


Figure 15: Solution of the BVP ODE problem 15, see text for R-code

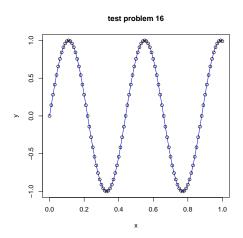


Figure 16: Solution of the BVP ODE problem 16, see text for R-code

2.16. problem 16

```
\xi^2 y'' + \pi^2 y / 4 = 0
                                       y_{(x=0)} = 0
                              y_{(x=1)} = \sin(\pi/(2\xi))
> Prob16 <- function(x, y, pars) {</pre>
    list(c(y[2], -1/xi^2*pi^2*y[1]/4))
  }
> xi <-0.11
> print(system.time(
  shoot <- bvpshoot(yini = c(0,NA), yend = c(\sin(pi/2/xi), NA),
                      x = seq(0, 1, by=0.01), func = Prob16, guess = 0,
                      atol = 1e-10)
  ))
         system elapsed
   user
           0.00
   0.11
                    0.11
> plot(shoot[,1], shoot[,2], type = "l", main = "test problem 16",
       col = "blue", xlab = "x", ylab = "y")
> curve(sin(pi*x/2/xi), 0, 1, type = "p", add = TRUE)
```

2.17. problem 17

$$y'' = -3\xi y/(\xi + x^2)^2$$
$$y_{(x=0.1)} = -y(-0.1) = \frac{0.1}{\sqrt{(\xi + 0.01)}}$$

only byptwp works.

```
> Prob17 <- function(x, y, pars) {</pre>
   list(c(y[2], -3*xi*y[1]/(xi+x^2)^2))
> xseq <- seq(-0.1, 0.1, by = 0.001)
> xi
       <- 0.01
> twp1 <- bvptwp(yini = c(-0.1/sqrt(xi+0.01), NA),
                  yend = c(0.1/sqrt(xi+0.01), NA), x = xseq,
                  func = Prob17, atol = 1e-10)
> xi <- 0.001
> twp2 < -bvptwp(yini = c(-0.1/sqrt(xi+0.01), NA),
                 yend = c(0.1/sqrt(xi+0.01), NA), x = xseq,
                  func = Prob17, atol = 1e-8)
> xi <- 0.0001
> twp3 < -bvptwp(yini = c(-0.1/sqrt(xi+0.01), NA),
                 yend = c(0.1/sqrt(xi+0.01), NA), x = xseq,
                 func = Prob17, atol = 1e-8)
> plot(twp1[,1], twp1[,2], type = "1", main = "test problem 17",
       ylim = c(-1, 1), col = "blue", xlab = "x", ylab = "y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp3[,1], twp3[,2], col = "red")
> curve(x/sqrt(xi+x^2), -0.1, 0.1, type = "p", add = TRUE)
```

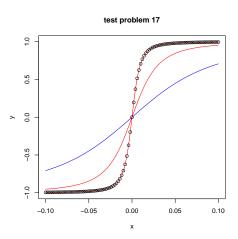


Figure 17: Solution of the BVP ODE problem 17, see text for R-code $\,$

2.18. problem 18

```
\xi y'' = -y'
                                     y_{(x=0)} = 1
                             y_{(x=1)} = exp(-1/\xi)
> Prob18 <- function(x, y, pars) {</pre>
   list(c(y[2], -1/xi*y[2]))
> xseq<-seq(0,1,by=0.01)
> xi <-0.2
> shoot <- bvpshoot(yini = c(1, NA), yend = c(exp(-1/xi), NA), x = xseq,
                     func = Prob18, guess = 0, atol = 1e-10)
> xi <- 0.1
> twp <- bvptwp(yini = c(1, NA), yend = c(exp(-1/xi), NA), x = xseq,
                 func = Prob18, atol = 1e-10)
> xi <- 0.01
> twp2 <- bvptwp(yini = c(1, NA), yend = c(exp(-1/xi), NA), x = xseq,
                 func = Prob18, atol = 1e-10)
> plot(shoot[,1], shoot[,2], type = "l", main = "test problem 18",
       ylim = c(0, 1), col = "blue", xlab = "x", ylab = "y")
> lines(twp[,1], twp[,2], col = "red")
> lines(twp2[,1], twp2[,2], col = "green")
> curve(exp(-x/xi), 0, 1, type = "p", add = TRUE)
```

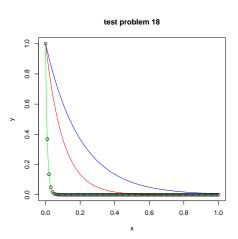


Figure 18: Solution of the BVP ODE problem 18, see text for R-code $\,$

3. nonlinear problems

For the nonlinear problems, the analytical solution is often not known.

3.1. problem 19

```
\xi y'' + exp(y)y' - \frac{\pi}{2}sin(\pi x/2)exp(2y) = 0
                                        y_{(x=0)} = y_{(x=1)} = 0
> Prob19 <- function(t, y, pars, ksi) {
    pit = pi*t
    list(c(y[2],(pi/2*sin(pit/2)*exp(2*y[1])-exp(y[1])*y[2])/ksi))
> xi
        <- 0.05
> shoot <- bvpshoot(yini = c(0, NA), yend = c(0, NA),
           x = seq(0, 1, by = 0.01), func = Prob19, guess = 0, ksi = xi)
> xi <- 0.03
> twp <- bvptwp(yini = c(0, NA), yend = c(0, NA),
                 x = seq(0, 1, by = 0.01), func = Prob19, ksi = xi,
                 atol = 1e-15)
> xi <- 0.005
> print(system.time(
  twp2 \leftarrow bvptwp(yini = c(0, NA), yend = c(0, NA),
                   x = seq(0, 1, by = 0.01), func = Prob19, ksi = xi,
                   atol = 1e-10)
  ))
   user system elapsed
   0.62
         0.00
                   0.54
> plot(shoot[,1], shoot[,2], type = "l", main = "test problem 19",
       ylim = c(-0.7, 0), col = "blue", xlab = "x", ylab = "y")
> lines(twp[,1], twp[,2], col = "red")
> lines(twp2[,1], twp2[,2], col = "green")
```

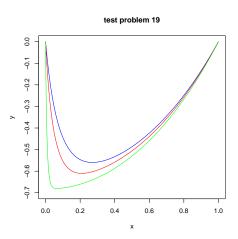


Figure 19: Solution of the BVP ODE problem 19, see text for R-code $\,$

3.2. problem 20

```
\xi y'' + y'^2 = 1
                         y_{x=0} = 1 + \xi ln(cosh(0.745/\xi))
                         y_{x=1} = 1 + \xi ln(cosh(0.255/\xi))
> Prob20 <- function(x, y, pars) {</pre>
    list(c(y[2], 1/xi *(1-y[2]^2)))
> xi <- 0.5
> ini <- c(1+xi * log(cosh(0.745/xi)), NA)</pre>
> end < c(1+xi * log(cosh(0.255/xi)), NA)
> twp1 < -bvptwp(yini = ini, yend = end, x = seq(0, 1, by=0.01),
                  func = Prob20)
> xi <- 0.3
> ini <- c(1+xi * log(cosh(0.745/xi)), NA)
> end < c(1+xi * log(cosh(0.255/xi)), NA)
> twp2 <- bvptwp(yini = ini, yend = end, x = <math>seq(0, 1, by=0.01),
                  func = Prob20)
> xi <- 0.01
> ini <- c(1+xi * log(cosh(0.745/xi)), NA)
> end <- c(1+xi * log(cosh(0.255/xi)), NA)
> twp3 <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by=0.01),
                   func = Prob20)
> plot(twp1[,1], twp1[,2], type = "1", main = "test problem 20",
       ylim = c(1, 1.8), col = "blue", xlab = "x", ylab = "y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp3[,1], twp3[,2], col = "green")
> curve(1+xi * log(cosh((x-0.745)/xi)),
        0, 1, add = TRUE, type = "p")
```

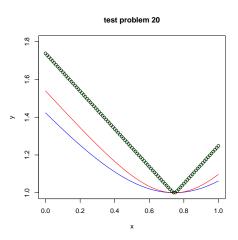


Figure 20: Solution of the BVP ODE problem 20, see text for R-code $\,$

3.3. problem 21

```
\xi y'' = y + y^2 - \exp(-2x/\sqrt{(\xi)})
                               y_{x=0} = 1
y_{x=1} = \exp(-1/\sqrt{(\xi)})
> Prob21 <- function(x, y, pars, xi) {</pre>
    list(c(y[2], 1/xi *(y[1]+y[1]^2-exp(-2*x/sqrt(xi)))))
> ini <- c(1, NA)
> xi <- 0.2
> end <- c(exp(-1/sqrt(xi)), NA)
> shoot <- bvpshoot(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                      func = Prob21, guess = 0, xi = xi)
> xi <- 0.1
> end <- c(exp(-1/sqrt(xi)), NA)
> twp <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob21, xi = xi)
> xi <- 0.01
> end <- c(exp(-1/sqrt(xi)), NA)
> twp2 <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                  func = Prob21, xi = xi)
> plot(shoot[,1], shoot[,2], type = "1", main = "test problem 21",
       ylim = c(0, 1), col = "blue", xlab = "x", ylab = "y")
> lines(twp[,1], twp[,2], col = "red")
> lines(twp2[,1], twp2[,2], col = "green")
> curve(exp(-x/sqrt(xi)), 0, 1, add = TRUE, type = "p")
```

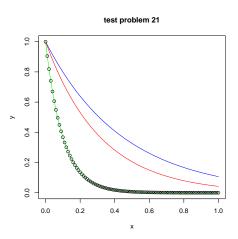


Figure 21: Solution of the BVP ODE problem 21, see text for R-code $\,$

3.4. problem 22

```
\xi y'' + y' + y^2 = 0
                                     y_{x=0} = 0
                                    y_{x=1} = 1/2
> Prob22 <- function(t, y, pars, xi) {</pre>
    list(c(y[2], -1/xi *(y[2]+y[1]^2)))
> ini <- c(0, NA)
> end <- c(1/2, NA)
> xi <-0.1
> shoot <- bvpshoot(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                      func = Prob22, guess = 0, xi = xi)
> xi <-0.05
> twp \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob22, xi = xi)
> xi <- 0.01
> twp2 <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                  func = Prob22, xi = xi)
> plot(shoot[,1], shoot[,2], type = "l", main = "test problem 22",
       ylim = c(0, 1), col = "blue", xlab = "x", ylab = "y")
> lines(twp[,1], twp[,2], col = "red")
> lines(twp2[,1], twp2[,2], col = "green")
```

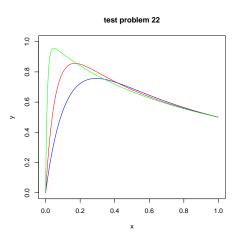


Figure 22: Solution of the BVP ODE problem 22, see text for R-code $\,$

3.5. problem 23

This is a difficult problem that cannot be solved with bypshoot

> lines(twp2[,1], twp2[,2], col = "green")

$$y'' = \mu sinh(\mu y)$$

$$y_{(x=0)} = y_{(x=1)} = 1$$
> $Prob23 \leftarrow function(t, y, pars, xi)$ {
$$list(c(y[2], sinh(y[1]/xi)/xi))$$
}
> $ini \leftarrow c(0, NA)$
> $end \leftarrow c(1, NA)$
> $xi \leftarrow 1/5$
> $twp1 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01), func = Prob23, xi = xi)$
> $xi \leftarrow 1/7$
> $twp \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01), func = Prob23, xi = xi)$
> $xi \leftarrow 1/9$
> $twp2 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01), func = Prob23, xi = xi)$
> $plot(twp1[,1], twp1[,2], type = "l", main = "test problem 23", col = "blue", xlab = "x", ylab = "y")$
> $lines(twp[,1], twp[,2], col = "red")$

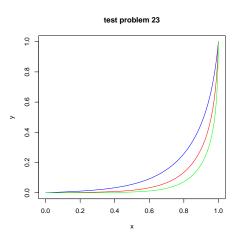


Figure 23: Solution of the BVP ODE problem 23, see text for R-code $\,$

3.6. problem 24

This is a particularly difficult problem to solve

$$\xi A(x)yy'' - (\frac{1+1.4}{2} - \xi A'(x))yy' + \frac{y'}{y} + \frac{A'(x)}{A(x)}(1 - \frac{1.4-1}{2}y^2) = 0$$

$$A(x) = 1 + x^2$$

$$y_{(x=0)} = 0.9129$$

$$y_{(x=1)} = 0.375$$
 > Prob24 <- function(t, y, pars, xi) {
$$A <- 1 + t * t$$

```
A \leftarrow 1+t*t
   AA <- 2*t
   ga <- 1.4
   list(c(y[2],
         (((1+ga)/2 -xi*AA)*y[1]*y[2]-y[2]/y[1]-
         (AA/A)*(1-(ga-1)*y[1]^2/2))/(xi*A*y[1]) ))
  }
> ini <- c(0.9129, NA)
> end <- c(0.375, NA)
> xi
       <-0.05
> mod1 <- bvpshoot(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                   func = Prob24, guess = 0.9, xi = xi)
> xi <-0.025
> mod2 < -bvpshoot(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                    func = Prob24, guess = 0.9, xi = xi)
> xi <-0.02
> mod3 <- bvpshoot(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                    func = Prob24, guess = 0.9, xi = xi)
> attributes(mod3)$roots
                                 # has FAILED: f.root too large!
       root
                f.root iter
1 0.8359306 -0.4355728
```

Function bypshoot cannot solve this problem for small ξ

Function byptwp can solve it for small ξ if initiated with good initial guesses:

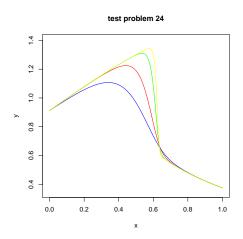


Figure 24: Solution of the BVP ODE problem 24, see text for R-code

3.7. problem 25

Now come a series of similar problems (problem 25-30), that differ only by their boundary conditions:

The differential equation is:

$$\xi y'' + yy' - y = 0$$

For problem 25, the boundary conditions are:

$$y_{x=0} = -1/3 y_{x=1} = 1/3$$

These problems are most easily solved with bvptwp

```
> Prob25 <- function(t, y, pars, xi) {
    list(c(y[2], -1/xi *(y[1]*y[2]-y[1])))
> ini <- c(-1/3 ,NA)
> end <- c(1/3, NA)
> xi <- 0.1
> twp1 <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob25, xi = xi)
> xi <- 0.01
> twp2 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob25, xi = xi)
> xi <- 0.001
> twp3 <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob25, xi = xi)
> plot(twp1[,1], twp1[,2], type = "l", main = "test problem 25",
       col = "blue", xlab = "x", ylab = "y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp3[,1], twp3[,2], col = "green")
```

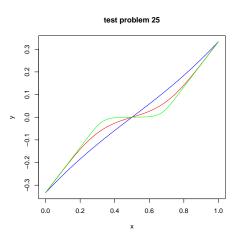


Figure 25: Solution of the BVP ODE problem 25, see text for R-code $\,$

3.8. problem 26

This problem equals previous problem, but with different boundary conditions:

$$y_{x=0} = 1$$
$$y_{x=1} = -1/3$$

```
> Prob26 <- function(t, y, pars, xi) {
    list(c(y[2], -1/xi *(y[1]*y[2]-y[1])))
  }
> ini <- c(1, NA)
> end <- c(-1/3, NA)
> xi
       <- 0.1
> twp1 <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob26, xi = xi)
> xi <- 0.02
> twp2 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob26, xi = xi)
       <- 0.005
> xi
> twp3 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob26, xi = xi)
> plot(twp1[,1], twp1[,2], type = "l", main = "test problem 26",
       col = "blue", xlab = "x", ylab = "y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp3[,1], twp3[,2], col = "green")
```

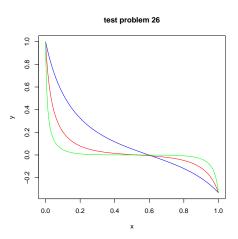


Figure 26: Solution of the BVP ODE problem 26, see text for R-code $\,$

3.9. problem 27

This problem equals previous problem, but with different boundary conditions:

$$y_{x=0} = 1$$
$$y_{x=1} = 1/3$$

```
> Prob27 <- function(t, y, pars, xi) {</pre>
    list(c(y[2], -1/xi *(y[1]*y[2]-y[1])))
  }
> ini <- c(1, NA)
> end <- c(1/3, NA)
> xi
       <- 0.1
> twp1 <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob27, xi = xi)
> xi
      <- 0.02
> twp2 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob27, xi = xi)
       <- 0.005
> twp3 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob27, xi = xi)
> plot(twp1[,1], twp1[,2], type = "l", main = "test problem 27",
       ylim = c(0, 1), col = "blue", xlab = "x", ylab = "y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp3[,1], twp3[,2], col = "green")
```

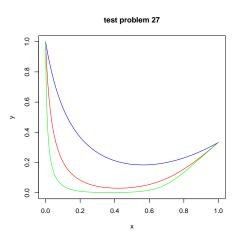


Figure 27: Solution of the BVP ODE problem 27, see text for R-code $\,$

3.10. problem 28

This problem equals previous problem, but with different boudnary conditions:

```
y_{x=0} = 1
                                 y_{x=1} = 3/2
> Prob28 <- function(t, y, pars, xi) {
    list(c(y[2], -1/xi *(y[1]*y[2]-y[1])))
  }
> ini <- c(1, NA)
> end <- c(3/2, NA)
> xi
       <- 0.1
> twp1 <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob28, xi = xi)
> xi
       <-0.02
> twp2 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob28, xi = xi)
> xi <-0.005
> twp3 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob28, xi = xi)
> plot(twp1[,1], twp1[,2], type = "l", main = "test problem 28",
       ylim = c(0.4, 1.5), col = "blue", xlab = "x", ylab = "y")
```

> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp3[,1], twp3[,2], col = "green")

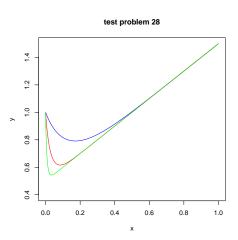


Figure 28: Solution of the BVP ODE problem 28, see text for R-code $\,$

3.11. problem 29

This problem equals previous problem, but with different boundary conditions:

$$y_{x=0} = 0$$
$$y_{x=1} = 3/2$$

```
> Prob29 <- function(t, y, pars, xi) {
    list(c(y[2], -1/xi *(y[1]*y[2]-y[1])))
  }
> ini <- c(0,NA)
> end <- c(3/2,NA)
> xi
       <- 0.1
> twp1 <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob29, xi = xi)
> xi <- 0.02
> twp2 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob29, xi = xi)
       <- 0.005
> twp3 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob29, xi = xi)
> plot(twp1[,1], twp1[,2], type = "l", main = "test problem 29",
       col = "blue", xlab = "x", ylab = "y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp3[,1], twp3[,2], col = "green")
```

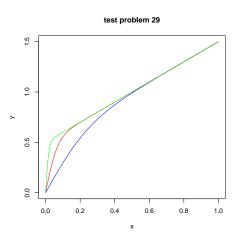


Figure 29: Solution of the BVP ODE problem 29, see text for R-code $\,$

3.12. problem 30

Similar to previous problems, with different boundary conditions:

$$y_{x=0} = -7/6$$

$$y_{x=1} = 3/2$$

```
> Prob30 <- function(t, y, pars, xi) {
    list(c(y[2], -1/xi *(y[1]*y[2]-y[1])))
  }
> ini <- c(-7/6, NA)
> end <- c(3/2, NA)
> xi
       <- 0.1
> twp1 <- bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob30, xi = xi)
> xi <- 0.02
> twp2 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob30, xi = xi)
       <- 0.01
> xi
> twp3 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01),
                 func = Prob30, xi = xi)
> plot(twp1[,1], twp1[,2], type = "l", main = "test problem 30",
       col = "blue", xlab = "x", ylab = "y")
> lines(twp2[,1], twp2[,2], col = "red")
> lines(twp3[,1], twp3[,2], col = "green")
```

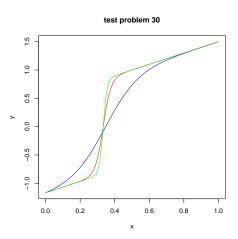


Figure 30: Solution of the BVP ODE problem 30, see text for R-code $\,$

3.13. problem 31

$$y' = \sin(\theta)$$

$$\theta' = M$$

$$\xi M' = -Q$$

$$\xi Q' = (y-1)\cos(\theta) - MT$$

$$T = \sec(\theta) + \xi Q \tan(\theta)$$

where

$$y_{x=0} = y_{x=1} = M_{x=0} = M_{x=1} = 0$$

```
> Prob31 <- function(t, Y, pars) {
    with (as.list(Y), {
        dy <- sin(Tet)
        dTet <- M
        dM <- -Q/xi
        T <- 1/cos (Tet) +xi*Q*tan(Tet)
        dQ <- 1/xi*((y-1)*cos(Tet)-M*T)
        list(c(dy, dTet, dM, dQ))
    })
    }
> ini <- c(y = 0, Tet = NA, M = 0, Q = NA)
> end <- c(y = 0, Tet = NA, M = 0, Q = NA)</pre>
```

Shooting does not work...

But the mono-implicit Runge-Kutta method does...

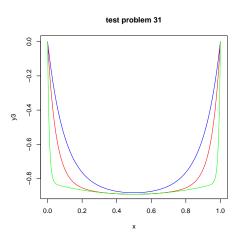


Figure 31: Solution of the BVP ODE problem 31, see text for R-code $\,$

3.14. problem 32

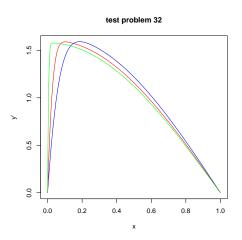


Figure 32: Solution of the BVP ODE problem 32, see text for R-code $\,$

3.15. problem 33

$$\xi z'''' = -z \cdot z''' - y \cdot y'$$

$$\xi y'' = y \cdot z' - z \cdot y'$$
where
$$y_{x=0} = -1y_{x=1} = 1z_{x=0} = z'_{x=0} = z_{x=1} = z'_{x=1} = 0$$
> $Prob33 \leftarrow function(t, z, pars, xi)$ {
 $list(c(z[2], z[3], z[4], 1/xi*(z[1]*z[4]-z[5]*z[6]), z[6], 1/xi*(z[5]*z[2]-z[1]*z[6]))$
}
> $ini \leftarrow c(0, 0, NA, NA, -1, NA)$
> $end \leftarrow c(0, 0, NA, NA, 1, NA)$
> $xi \leftarrow 0.1$
> $twp \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01), func = Prob33, xi = xi)$
> $xi \leftarrow 0.01$
> $twp2 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01), func = Prob33, xi = xi)$
> $xi \leftarrow 0.001$
> $twp3 \leftarrow bvptwp(yini = ini, yend = end, x = seq(0, 1, by = 0.01), func = Prob33, xi = xi)$
> $plot(twp[1], twp[2], type = 11, main = 1 test problem 33, col = 10 tup = 10 tup$

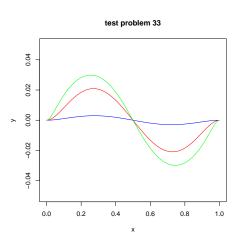


Figure 33: Solution of the BVP ODE problem 33, see text for R-code $\,$

3.16. problem 34

$$y'' = -\xi \cdot exp(y)$$
 where
$$y_{x=0} = y_{x=1} = 0$$
 > $Prob34 < -function(t, y, pars, xi)$ { $list(c(y[2], -xi*exp(y[1])))$ } } ini $< -c(0, NA)$ > $end < -c(0, NA)$

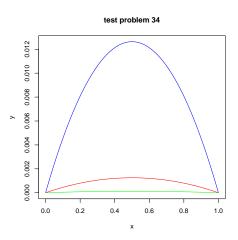


Figure 34: Solution of the BVP ODE problem 34, see text for R-code $\,$

3.17. problem 35

$$\xi y'' \ = \ xy' - y$$
 where
$$y_{x=-1} = 1; y_{x=1} = 2$$
 > $\operatorname{Prob35} < -\operatorname{function}(x, y, \operatorname{pars}, xi) \ \{ \ \operatorname{list}(c(y[2], 1/xi*(x*y[2]-y[1]))) \ \}$ > $\operatorname{ini} < -\operatorname{c}(1, \operatorname{NA})$ > $\operatorname{end} < -\operatorname{c}(2, \operatorname{NA})$ > $\operatorname{xi} < -1$ > $\operatorname{twp} < -\operatorname{bvptwp}(\operatorname{yini} = \operatorname{ini}, \operatorname{yend} = \operatorname{end}, \operatorname{x} = \operatorname{seq}(-1, 1, \operatorname{by} = 0.05), \ \operatorname{func} = \operatorname{Prob35}, \operatorname{xi} = \operatorname{xi})$ > $\operatorname{xi} < -0.1$ > $\operatorname{twp2} < -\operatorname{bvptwp}(\operatorname{yini} = \operatorname{ini}, \operatorname{yend} = \operatorname{end}, \operatorname{x} = \operatorname{seq}(-1, 1, \operatorname{by} = 0.05), \ \operatorname{func} = \operatorname{Prob35}, \operatorname{xi} = \operatorname{xi})$ > $\operatorname{xi} < -0.01$ > $\operatorname{twp3} < -\operatorname{bvptwp}(\operatorname{yini} = \operatorname{ini}, \operatorname{yend} = \operatorname{end}, \operatorname{x} = \operatorname{seq}(-1, 1, \operatorname{by} = 0.05), \ \operatorname{func} = \operatorname{Prob35}, \operatorname{xi} = \operatorname{xi})$ > $\operatorname{plot}(\operatorname{twp}[1], \operatorname{twp}[2], \operatorname{type} = "1", \operatorname{main} = "\operatorname{test} \operatorname{problem} 35", \ \operatorname{col} = "\operatorname{blue}", \operatorname{xlab} = "x", \operatorname{ylab} = "y", \operatorname{ylim} = \operatorname{c}(-1, 4))$ > $\operatorname{lines}(\operatorname{twp2}[1], \operatorname{twp2}[2], \operatorname{col} = "\operatorname{red}")$ > $\operatorname{lines}(\operatorname{twp3}[1], \operatorname{twp3}[2], \operatorname{col} = "\operatorname{green}")$

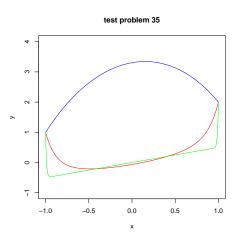


Figure 35: Solution of the BVP ODE problem 35, see text for R-code $\,$

References

Soetaert K (2009). rootSolve: Nonlinear root finding, equilibrium and steady-state analysis of ordinary differential equations. R package version 1.4.

Soetaert K, Cash J, Mazzia F (2009a). bvpSolve: solvers for boundary value problems of ordinary differential equations. R package version 1.1.

Soetaert K, Meysman F (2010). ReacTran: Reactive transport modelling in 1D, 2D and 3D. R package version 1.2.

Soetaert K, Petzoldt T, Setzer RW (2009b). deSolve: General solvers for initial value problems of ordinary differential equations (ODE), partial differential equations (PDE) and differential algebraic equations (DAE). R package version 1.3.

Affiliation:

Karline Soetaert

Centre for Estuarine and Marine Ecology (CEME)

Netherlands Institute of Ecology (NIOO)

4401 NT Yerseke, Netherlands

E-mail: k.soetaert@nioo.knaw.nl

URL: http://www.nioo.knaw.nl/users/ksoetaert

Jeff Cash

Imperial College London

South Kensington Campus

London SW7 2AZ, U.K.

E-mail: j.cash@imperial.ac.uk

URL: http://www.ma.ic.ac.uk/~jcash

Francesca Mazzia

Dipartimento di Matematica

Universita' di Bari

Via Orabona 4,

70125 Bari

Italy E-mail: mazzia@dm.uniba.it

URL: http://pitagora.dm.uniba.it/~mazzia