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A Collection of Test Problems for Ordinary Differential Equation Solvers Which Have Provisions for Rootfinding

S. Thompson

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Engineering Physics and Mathematics Division

Mathematical Sciences Section

A COLLECTION OF TEST PROBLEMS FOR ORDINARY DIFFERENTIAL EQUATION SOLVERS WHICH HAVE PROVISIONS FOR ROOTFINDING

S. Thompson

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ABSTRACT

Several popular ordinary differential equation (ode) solvers contain provisions for locating roots of functions which depend on the solution of the ode. A collection of problems for testing such solvers is described in this report. In addition to several well-known problems, the collection contains other interesting problems which have not previously appeared in the literature.

INTRODUCTION

Excellent collections of test problems are available for testing general ordinary differential equation (ode) solvers (for example, see [6, 7, 13, 19, 20]). This report presents a systematized collection of test problems for ordinary differential equation solvers and continuous simulation languages which have rootfinding capabilities. Such a solver is designed to integrate initial value problems of the form

$$\frac{dy}{dt} = f(t, y)$$
$$y(t_0) = y_0$$

while simultaneously locating roots of event functions

$$0 = g_i(t, y, \dot{y}), \quad i = 1, \cdots, m.$$

Such event functions sometimes correspond to derivative discontinuities, points at which the underlying initial value problem is changed, or simple rootfinding requirements such as locating the times at which a solution component attains a prescribed value. Prototype problems requiring rootfinding include the bouncing ball (Problem D-1) and stiction-friction (Problem B-3). The difficulties associated with rootfinding in the context of odes sometimes are not fully appreciated. (To emphasize this fact: the author is aware of no available ode solver with rootfinding which handles correctly all of the problems in this report, unless the user is extremely careful.) Excellent discussions of several of these difficulties are given in [11, 25].

Several good ode solvers are available which contain rootfinding capabilities of one type or another (for example, see [9, 11, 12, 13, 21, 22, 23, 24, 25]). Other such solvers will become available in the near future. In fact, it is anticipated that most new software for initial value problems in ordinary differential equations will contain provisions for rootfinding. It has been pointed out, for example, that the "next generation of Runge-Kutta code" will contain such provisions. The collection of problems described in this report should be useful in studying the performance of such solvers for problems requiring rootfinding.

The problems have been grouped roughly into several classes. Group A contains falling body problems with simple rootfinding (time-dependent event functions and functions of the form $y_i - \alpha$ where α is constant). Group B contains problems with switches in the derivative (multiple state-dependent branches which define the derivative). Group C contains problems for which it is desired to build tables of values. These problems involve the re-definition of the event function at roots. Group D contains problems in which the underlying initial value problem changes at each root of the event function. Each problem is equivalent to a sequence of initial value problems. The roots of the event functions also cluster at finite times. The problems in this section have the property that if any root of the event equation is ever missed, it will not be possible to correctly solve the problem thereafter. Group E contains problems with derivative singularities. These problems require that the derivative definition be extended in a suitable fashion at the singularity. Some of the problems in Group F involve more general event functions (for example, event functions which depend on more than one of the solution components). (Some ode solvers restrict the rootfinding to locating times when a solution component attains a prescribed value. Problems such as the ones in Group F can be handled by such solvers by adding solution components to the system.) Group G contains several interesting problems without simple solutions but for which the qualitative behavior of the solution is well-known. No test results are presented in this report. Extensive results for this collection of problems and several Runge-Kutta-Sarafyan integrators will be presented in a forthcoming report. In fact, one of the purposes of the present report is to serve as a basis for an evaluation of several such solvers.

A. FALLING BODY AND OTHER PROBLEMS WITH SIMPLE ROOTFINDING REQUIREMENTS

Problem A-1 is a simple mechanics problem. It describes the behavior of a body which falls from rest toward the earth from height H. The rootfinding of interest is to locate the time t at which the body strikes the earth, that is, for which $y_1(t) = H$ (where y_1 is the distance travelled from the initial resting position). Problem A-2 is similar to Problem A-1. The rootfinding of interest is to determine the time required for the moon to fall to earth under appropriate conditions. Due to the units used, it is necessary to integrate the problem for very large values of the independent variable. Problem A-3 describes the motion of a paratrooper whose parachute opens at time $t = t_1$. There is a strictly time-dependent discontinuity in the derivative at t_1. A second rootfinding requirement is to determine the time at which the paratrooper strikes the ground. Problems A-4 and A-5 are typical linear mechanics systems. If Problem A-4 is integrated for decreasing values of t, for say $4 \geqslant t \geqslant -1$, it is roughly linear at the beginning of the integration. The solution is damped and oscillatory for $t \leqslant 0$. Problem A-5 oscillates throughout the interval [0, 4] with considerably varying amplitude.

PROBLEM A-1 [17]

For $0 \leqslant t \leqslant H/2$,

$$\begin{aligned} \dot{y}_1 &= y_2 , & y_1(0) &= 0 \\ \dot{y}_2 &= (w - ky_2)/m, & y_2(0) &= 0 \\ g_1 &= y_1 - H \end{aligned}$$

where

$$m = 1/4$$
$$w = 8$$
$$k = 2$$
$$H = 10 \quad .$$

The exact solution is

$$y_1 = 4\left(t + \frac{1}{8}e^{-8t} - \frac{1}{8}\right)$$
$$y_2 = 4\left(1 - e^{-8t}\right) \quad .$$

PROBLEM A-2 [18]

$$\dot{y}_1 = -\sqrt{2gR^2}\ \sqrt{(H - y_1)/\ Hy_1}$$
$$y_1(0) = H$$
$$g_1 = y_1 - R$$

where

$$g = 32$$
$$R = 4000(5280)$$
$$H = 237000(5280) \quad .$$

The exact solution satisfies

$$t = \left(H^{3/2}\ /\ 8y_1\right)\left(\sqrt{y_1/\ H - (y_1/\ H)^2} + \frac{1}{2}\cos^{-1}(2y_1/\ H - 1)\right) \quad .$$

It is noted that $g_1 = 0$ for $t \approx 411152.54$.

PROBLEM A-3 [17]

For $0 \leqslant t \leqslant 20$,

$$\dot{y}_1 = y_2$$
$$\dot{y}_2 = \begin{cases} (w - k_1 y_2^2)/\ m & \text{if } t \leqslant t_1 \\ (w - k_2 y_2^2)/\ m & \text{if } t > t_1 \end{cases}$$
$$y_1(0) = 0$$
$$y_2(0) = 0$$
$$g_1 = t - t_1$$
$$g_2 = y_1 - H$$

where

$$w = 200$$
$$k_1 = 1/150$$
$$k_2 = 4/150$$
$$g = 32$$
$$m = w/g$$
$$t_1 = 5$$
$$H = 1000 \ .$$

The exact solution is given as follows:

For $0 \leqslant t \leqslant t_1$,

$$y_1 = \frac{1}{g}\frac{w}{k_1} \ln\left[\cosh\left(g\left(\frac{k_1}{w}\right)^{1/2} t\right)\right]$$
$$y_2 = \left(\frac{w}{k_1}\right)^{1/2} \tanh\left(g\left(\frac{k_1}{w}\right)^{1/2} t\right) \ .$$

For $t_1 < t$,

$$y_1 = \frac{1}{g}\frac{w}{k_2} \ln\left[\cosh\left(\frac{g}{\sqrt{w}}[\sqrt{k_2}(t - t_1) + \sqrt{k_1}t_1]\right)\right] + C$$
$$y_2 = \left(\frac{w}{k_2}\right)^{1/2} \tanh\left(\frac{g}{\sqrt{w}}\left[\sqrt{k_2}(t - t_1) + \sqrt{k_1}t_1\right]\right)$$

where

$$C = \frac{w}{g}\left(\frac{1}{k_1} - \frac{1}{k_2}\right)\ln\left[\cosh\left(g\left(\frac{k_1}{w}\right)^{1/2} t_1\right)\right] \ .$$

PROBLEM A-4 [8]

$$\dot{y}_1 = y_2$$
$$\dot{y}_2 = -(16\pi^2 e^{-2t} - 1/4)\, y_1$$
$$g_1 = y_1$$
$$g_2 = \dot{y}_1 \ .$$

The solution for which $y_1(0) = 1$ and $y_2(0) = 1/2$ is given by:

$$y_1(t) = e^{t/2}\cos(4\pi e^{-t})$$
$$y_2(t) = e^{t/2}\left(4\pi e^{-t}\sin(4\pi e^{-t}) + \frac{1}{2}\cos(4\pi e^{-t})\right) \ .$$

The roots of $g_1 = 0$ correspond to

$$t_k = \ln 8 - \ln(2k-1),\ k = 1, 2, \cdots .$$

Let $\theta = 4\pi e^{-t}$. For $k \geqslant 1$, the function $f(\theta) = \tan\theta + \frac{1}{2\theta}$ has exactly one root θ_k for which

$$(2k-1)\frac{\pi}{2} < \theta_k < (2k+1)\frac{\pi}{2} .$$

$t_k = \ln\left(\frac{\theta}{4\pi}\right)$ is the corresponding root of $g_2 = 0$.

PROBLEM A-5 [8]

$$\dot{y}_1 = y_2$$
$$\dot{y}_2 = -16\cos\left(\frac{\pi t}{2}\right)y_2 - \left(64\pi^2 + 64\cos^2\left(\frac{\pi t}{2}\right) - 4\pi\sin\left(\frac{\pi t}{2}\right)\right)y_1$$
$$g_1 = y_1 .$$

The solution for which $y_1(0) = 1$ and $y_2(0) = -8$ is given by:

$$y_1 = \exp\left(-\frac{16}{\pi}\sin\frac{\pi t}{2}\right)\cdot\cos(8\pi t)$$
$$y_2 = -8\exp\left(-\frac{16}{\pi}\sin\frac{\pi t}{2}\right) sixe\ 16\cdot\left(\pi\sin(8\pi t) + \cos\left(\frac{\pi}{2}t\right)\cos\left(8\pi t\right)\right) .$$

The roots of $g_1 = 0$ correspond to $t = (2k-1)/16,\ k = 1, 2, \cdots$.

B. PROBLEMS WITH DERIVATIVE SWITCHES

The problems in this section contain switches in the derivative definition. These switches introduce discontinuities in the derivative. Problem B-1 contains a simple switch. Any good adaptive integrator can handle the single discontinuity present in this problem. Problem B-2 is a well-known example which contains frequent discontinuities in the derivative. If rootfinding is not used and an integrator is not forced to hit exactly the times corresponding to these discontinuities, it is possible to obtain very inaccurate results for this problem. Problem B-3 is the well-known "stiction-friction" problem which describes the motion of an object sliding over a surface. A time-dependent force is applied to the body. The body tends to stick until the applied force overcomes friction and inertia. The derivative starts out on branch 3 of the ode. It switches to branch 1 at $t = 0.166$ and back to branch 3 near $t = 0.705$. At $t = 0.83$ it switches to branch 2. A final switch occurs near $t = 1.036$ when the derivative switches to branch 3. The performance of a solver is of interest for several cases:

Case (i)

ignore the points of discontinuity

Case (ii)

locate the points of discontinuity using rootfinding but allow the derivative to switch branches any time the conditions for a switch are satisfied

Case (iii)

locate the points of discontinuity but force the derivative calculation to be performed for the correct branch of the derivative at all values of time, that is, do not allow the derivative to switch branches until the next root is located.

Three of the event functions for this problem are strictly time-dependent. Three of the functions are also discontinuous step functions. In the latter cases, the rootfinder should be used to locate the break-points for the step functions. A rootfinder which does not reduce to bisection at points of discontinuity of the event function will have problems doing so. Problem B-4 is the ideal relay equation. The solution has jump discontinuities in its second derivative at multiples of $\pi/2$.

PROBLEM B-1 [21]

For $0 \leqslant t \leqslant 0.5$,

$$\dot{y}_1 = y_1 \ , \quad y_1(0) = 1$$

$$\dot{y}_2 = \begin{cases} -L & \text{if } E < -L/K \\ KE & \text{if } -L/K \leqslant E \leqslant L/K \\ L & \text{if } L/K < E \end{cases} \ , \quad y_2(0) = 1$$

where

$$E = y_1 - y_2$$

$$S = 17$$

$$K = 5/3$$

$$L = 1/4$$

$$g_1 = y_1 - y_2 + L/K$$

Denote by t_1 the positive root of

$$e^{-Kt} = e^t - L(K+1)/K \quad .$$

The exact solution is

$$y_1 = e^t$$

$$y_2 = \begin{cases} \dfrac{K}{K+1} e^t + \dfrac{1}{K+1} e^{-Kt} & \text{if } 0 \leqslant t \leqslant t_1 \\ L(t - t_1) + y_2(t_1) & \text{if } t_1 < t \leqslant 0.5 \end{cases} \quad .$$

It is noted that

$$t_1 \doteq 0.1569$$

and

$$y_2(t_1) \doteq 1.0199 \quad .$$

PROBLEM B-2 [4]

For $0 \leqslant t \leqslant 19$,

$$\dot{y}_1 = \begin{cases} y_1^2 & \text{if } y_2 > 0 \\ 0 & \text{if } y_2 \leqslant 0 \end{cases}$$

$$\dot{y}_2 = 4\pi \cos 4\pi t$$

$$y_1(0) = 0.1$$

$$y_2(0) = 0$$

$$g_1 = y_2 \quad .$$

The exact solution is given as follows:

For $i \geqslant 0$ define

$$S_i(t) = \frac{1}{10 + i/4 - t} \quad .$$

Then

$$y_1(t) = \begin{cases} S_i(t) & \text{if} \quad t \in \left[\frac{2i}{4}, \frac{2i+1}{4}\right] \\ S_i\left[\frac{2i+1}{4}\right] & \text{if} \quad t \in \left[\frac{2i+1}{4}, \frac{2i+2}{4}\right] \end{cases}$$

$$y_2(t) = \sin\ (4\pi t) \quad .$$

$g_1 = 0$ at integral multiples of 1/4.

PROBLEM B-3 [5]

For $0 \leqslant t \leqslant 1.5$,

$$\dot{y}_1 = y_2$$

$$\dot{y}_2 = \begin{cases} (F_a - F_1 - F_2 y_2)/\ m, & \text{if} \quad (y_2 = 0 \text{ and } F_a > F_s) \text{ or } y_2 > 0 \\ (F_a + F_1 - F_2 y_2)/\ m, & \text{if} \quad (y_2 = 0 \text{ and } F_a < -F_s) \text{ or } y_2 < 0 \\ 0 & \text{, if} \quad y_2 = 0 \text{ and } |F_a| \leqslant |F_s| \end{cases}$$

$$y_1(0) = 0$$
$$y_2(0) = 0$$

where

$$F_a = F_a(t) = \begin{cases} 0 & \text{if } 0 \leqslant t < 0.1 \ \ or \ \ 1.0 \leqslant t \\ 5t & \text{if } 0.1 \leqslant t < 0.5 \\ -t & \text{if } 0.5 \leqslant t < 1.0 \end{cases}$$

$$m = 0.64$$
$$F_s = 0.83$$
$$F_1 = 0.75$$
$$F_2 = 0.28$$

$$g_1 = \begin{cases} -1\,, & \text{if } (y_2 = 0 \text{ and } F_a > F_s) \text{ or } y_2 > 0 \\ +1\,, & \text{otherwise} \end{cases}$$

$$g_2 = \begin{cases} -1\,, & \text{if } (y_2 = 0 \text{ and } F_a < -F_s) \text{ or } y_2 < 0 \\ +1\,, & \text{otherwise} \end{cases}$$

$$g_3 = \begin{cases} -1\,, & \text{if } y_2 = 0 \text{ and } |F_a| \leqslant |F_s| \\ +1\,, & \text{otherwise} \end{cases}$$

$$g_4 = t - 0.1$$
$$g_5 = t - 0.5$$
$$g_6 = t - 1.0\ .$$

The exact solution for this problem is as follows:

i) for $0 \leqslant t < t_1 = 0.166$,

$$y_1 = y_{1,1} = 0$$
$$y_2 = y_{2,1} = 0$$

ii) for $t_1 < t \leqslant t_2 = 0.5$,

$$y_1 = y_{1,2} = -(C_2 m / F_2) \exp(-F_2 t / m) + 5\,t^2 / 2F_2 - 5mt / F_2^2 - F_1 t / F_2 + D_2$$

$$y_2 = y_{2,2} = C_2 \exp(-F_2 t / m) + 5t / F_2 - 5m / F_2^2 - F_1 / F_2$$

where

$$C_2 = -\exp(F_2 t_1 / m) \cdot \left\{ 5t_1 / F_2 - 5m / F_2^2 - F_1 / F_2 \right\}$$

$$D_2 = (C_2 m / F_2)\exp(-F_2 t_1 / m) - 5t_1^2 / 2F_2 + 5mt_1 / F_2^2 + F_1 t_1 / F_2$$

iii) for $t_2 < t \leqslant t_3 \approx 0.705$

$$y_1 = y_{1,3} = -(c_3 m / F_2) \exp(-F_2 t / m) - t^2 / 2F_2 + mt / F_2^2 - F_1 t / F_2 + D_3$$

$$y_2 = y_{2,3} = C_3 \exp(-F_2 t / m) - t / F_2 + m / F_2^2 - F_1 / F_2$$

where

$$C_3 = \exp(F_2 t_2 / m) \cdot \left\{ y_{2,2}(t_2) + t_2 / F_2 - m / F_2^2 + F_1 / F_2 \right\}$$

$$D_3 = y_{1,2}(t_2) + (C_3 m / F_2) \exp(-F_2 t_2 / m) + t_2^2 / 2F_2 - mt_2 / F_2^2 + F_1 t_2 / F_2$$

and t_3 satisfies

$$0 = C_3 \exp(-F_2 t_3 / m) - t_3 / F_2 + m / F_2^2 - F_1 / F_2$$

iv) for $t_3 < t \leqslant t_4 = 0.83$,

$$y_1 = y_{1,4} = y_{1,3}(t_3)$$
$$y_2 = y_{2,4} = 0$$

v) for $t_4 < t \leqslant t_5 = 1.0$,

$$y_1 = y_{1,5} = -(mC_5 / F_2) \exp(-F_2 t / m) - t^2 / 2F_2 + mt / F_2^2 + F_1 t / F_2 + D_5$$

$$y_2 = y_{2,5} = C_5 \exp(-F_2 t / m) - t / F_2 + m / F_2^2 + F_1 / F_2$$

where

$$C_5 = \exp(F_2 t_4 / m) \cdot \left\{ t_4 / F_2 - m / F_2^2 - F_1 / F_2 \right\}$$

$$D_5 = y_{1,3}(t_3) + (C_5 m / F_2) \exp(-F_2 t_4 / m) + t_4^2 / 2F_2 - mt_4 / F_2^2 - F_1 t_4 / F_2$$

vi) for $t_5 < t \leqslant t_6 \approx 1.036$,

$$y_1 = y_{1,6} = -(mC_6/F_2)\exp(-F_2 t/m) + F_1 t/F_2 + D_6$$

$$y_2 = y_{2,6} = C_6 \exp(-F_2 t/m) + F_1/F_2$$

where

$$C_6 = C_5 + \exp(F_2/m) \cdot \left\{ m/F_2^2 - 1/F_2 \right\}$$

$$D_6 = (m/F_2)(C_6 - C_5)\exp(-F_2/m) - 1/2F_2 + m/F_2^2 + D_5$$

and

$$t_6 = -(m/F_2)\ln(-F_1/C_6F_2)$$

vii) for $t_6 < t$,

$$y_1 = y_{1,7} = y_{1,6}(t_6)$$
$$y_2 = 0 .$$

PROBLEM B-4 [20, 25]

For $0 \leqslant t \leqslant 10$,

$$\dot{y}_1 = y_2 \qquad , \; y_1(0) = 0$$

$$\dot{y}_2 = -y_1 + sgn(y_1) - 3\sin 2t \; , \; y_2(0) = 3$$

where

$$sgn(y_1) = \begin{cases} +1 & \text{if } y_1 \geqslant 0 \\ -1 & \text{if } y_1 < 0 \end{cases}$$

$$g_1 = y_1 .$$

The exact solution is given by

$$y_1(t) = \begin{cases} -1 + \sqrt{2}\cos(\pi/4 - x) + \sin 2x & \text{for } 0 \leqslant x \leqslant \pi/2 \\ 1 + \sqrt{2}\cos(\pi/4 + x) + \sin 2x & \text{for } \pi/2 \leqslant x < \pi \end{cases}$$

where $x = t \; mod(\pi)$.

$g_1 = 0$ at multiples of $\pi/2$.

C. BUILDING TABLES OF VALUES

A common use of a rootfinding ode solver is to build a table of times at which the solution attains prescribed values. In Problem C-1, it is desired to locate the times at which the solution attains the values $k = 1, \cdots, 10$; these times correspond to $e^t = k$ or $t = \ln k$. This problem requires that the definition of the event function be changed at each root. (Initially $g_1 = y_1 - 1$, then $g_1 = y_1 - 2$, etc.) Problem C-2 is similar to C-1. For this problem, it is desired to calculate a table of definite integrals corresponding to specified values of the upper limit of integration.

PROBLEM C-1 [9]

For $0 \leqslant t \leqslant 3$,

$$\dot{y}_1 = y_1$$
$$y_1(0) = 1$$
$$g_1 = y_1 - k \ , \qquad k = 1, \cdots, 10 \ .$$

The exact solution is $y_1 = e^t$.

$g_1 = 0$ at $t = \ln k$, $k = 1, \cdots, 10$.

PROBLEM C-2 [16]

Evaluate integrals of the form

$$\int_{y_0}^{y_1} ds / \sqrt{f(s)}$$

for equally-spaced values of y_1 in some interval.

Assume f is smooth, nonnegative, and has a simple zero at some unknown point y^* in the interval. Denoting the integral by $t(y_1)$, leads to

$$\frac{d^2 y_1}{dt^2} = f'(y_1)/2$$
$$y_1(0) = 0$$
$$\frac{dy_1}{dt}(0) = \sqrt{f(y_0)} \ .$$

Denote the desired values of y_1 by $\bar{y}_1, \cdots, \bar{y}_m$ and use $g_1 = y_1 - \bar{y}_i$, $i = 1, \cdots, m$. Three cases are of interest:

<u>*Case (i)*</u>

$$f(s) = 1/\sqrt{s}$$

<u>*Cases (ii)*</u>

$$f(s) = 1/\sqrt{1-s^2}$$

Case (iii)

$f(s) = 1/\sqrt{1-s}$

In each case, $y_0 = 0$ and $\bar{y}_i = i/10, i = 1, \cdots, 10$.

D. PROBLEMS WITH DISCONTINUOUS SOLUTION COMPONENTS AND CLUSTERED ROOTS

These problems are variants of the "bouncing ball problem." The initial value problem is changed at each bounce, that is, at each point for which the height y_1 is zero. At each such point, the solution component y_2 is re-defined. In Problem D-1, y_2 is replaced by $-ky_2$ for a constant k between 0 and 1. In Problem D-2, y_2 is replaced by $k\,|y_2|^\alpha$ for constants k and α with $0 < k < 1$ and $0 < \alpha \leqslant 1$. For this problem, the maximum height between bounces decays exponentially. Problem D-3 simulates a bouncing ball on a 45° ramp. Observe that the ball does not necessarily reach the bottom of the ramp. For each of these problems, the bounce times cluster at a finite time. Near such cluster points, the ball bounces infinitely often. This provides an interesting test for rootfinding ode solvers. Problem D-4 provides another test for handling multiple or clustered roots. By picking appropriate values of k and α, it is possible to determine how well a solver performs in the presence of clustered roots.

PROBLEM D-1 [23]

$$\begin{aligned} \dot{y}_1 &= y_2, \quad y_1(0) = H_0 \\ \dot{y}_2 &= -g, \quad y_2(0) = 0 \\ g_1 &= y_1 \end{aligned}$$

where $g = 32.2$, $H_0 = 4$, and $0 < k < 1$. When $g_1 = 0$ replace y_2 by $-ky_2$.

Denote the bounce times (the times for which $y_1 = 0$) by $\{t_n\}_{n=1}^{\infty}$. Then $t_1 = \sqrt{2H_0/g}$ and for $n > 1$, $t_n = t_1(1 + 2k\sum_{m=0}^{n-2} k^m)$. The exact solution is given as follows:

For $0 \leqslant t < t_1$, the solution is given by

$$\begin{aligned} y_{1,0}(t) &= -\frac{g}{2}t^2 + 4 \\ y_{2,0}(t) &= -g\,t \quad . \end{aligned}$$

For $t_n \leqslant t < t_{n+1}$ and $n > 1$, the solution is given by

$$\begin{aligned} y_{1,n}(t) &= -\frac{g}{2}(t - t_n)(t - t_n - 2t_1k^n) \\ y_{2,n}(t) &= -g(t - t_n - t_1k^n) \quad . \end{aligned}$$

PROBLEM D-2

In Problem D-1 make the replacement $y_2 = k\,|y_2|^{\alpha}$ when $g_1 = 0$ $(0 < \alpha \leqslant 1)$.

In this case, $t_1 = \sqrt{2H_0/g}$ and for $n > 1$

$$t_n = t_1 + \frac{2}{g}\sum_{j=1}^{n-1} k^{(1-\alpha^j)/(1-\alpha)}(gt_1)^{\alpha^j} \quad .$$

For $0 \leqslant t < t_1$, the solution is given by

$$y_{1,0} = -\frac{g}{2}t^2 + H_0$$
$$y_{2,0} = -gt \quad .$$

For $t_n \leqslant t < t_{n+1}$ and $n > 1$, the solution is given by

$$y_{1,n}(t) = -\frac{g}{2}(t - t_n)^2 + A_n(t - t_n)$$
$$y_{2,n}(t) = -g(t - t_n) + A_n$$

where

$$A_n = k\,|\,y_{2,n-1}(t_n)\,|^{\alpha}$$
$$= k^{(1-\alpha^n)/(1-\alpha)}\,(gt_1)^{\alpha^n} \quad .$$

PROBLEM D-3

For $0 \leqslant y_1(t) \leqslant 1$ and $0 < y_3(t)$,

$$\begin{array}{lll} \dot{y}_1 = y_2 & , y_1(0) = x_0 & (0 \leqslant x_0 < 1) \\ \dot{y}_2 = 0 & , y_2(0) = 0 & \\ \dot{y}_3 = y_4 & , y_3(0) = y_0 & (y_0 > 1 - x_0) \\ \dot{y}_4 = g & , y_4(0) = 0 & \end{array}$$

where

$$g = -9.81$$
$$g_1 = y_1 + y_3 - 1$$
$$g_2 = y_1 - 1$$
$$g_3 = y_3 \quad .$$

When $g_1 = 0$ replace y_2 by $-ky_4$ and replace y_4 by $-ky_2$ where $0 < k < 1$. Terminate the integration when $g_2 = 0$ or $g_3 = 0$.

y_1 and y_3 correspond, respectively, to the horizontal and vertical components of the position of a ball bouncing on a ramp with vertices (0,0), (0,1), (1,0) in the (y_1, y_3) plane. The ball is initially at rest at the point (x_0, y_0) and is dropped from this position.

Denote the bounce times determined by g_1 by $\{t_n\}_{n=1}^{\infty}$ and let $t_0 = 0$. Then $t_1 = (\frac{2}{g}(1-x_0-y_0))^{1/2}$ and for $n \geqslant 1$

$$t_{n+1} = t_1(1 + 2k \sum_{m=0}^{n-1} k^m) \quad .$$

The exact solution is given as follows:

For $t_n \leqslant t < t_{n+1}$, the solution is given by

$$y_{1,n}(t) = A_n + B_n(t - t_n)$$
$$y_{2,n}(t) = B_n$$
$$y_{3,n}(t) = C_n + D_n(t - t_n) + \frac{g}{2}(t - t_n)^2$$
$$y_{4,n}(t) = D_n + g(t - t_n)$$

where

$$A_n = x_0 - 2gt_1^2k^2\left(\frac{1+(n-1)k^{2n} - nk^{2n-2}}{(1-k^2)^2}\right)$$
$$B_n = -ngt_1k^n$$
$$C_n = 1 - A_n \quad \text{for } n \geqslant 1 \ (C_0 = y_0)$$
$$D_n = (n-1)gt_1k^n \quad \text{for } n \geqslant 1 \ (D_0 = 0) \ .$$

Observe that $y_{1,n}(t_n) = A_n$ and $\{A_n\}$ converges to $x_0 - 2gt_1^2k^2 / (1-k^2)^2$. This value is less than one if and only if

$$y_0 < (1 - x_0)\left(\frac{1+k^2}{2k}\right)^2 \quad .$$

(In this case, the ball does not get to the bottom of the ramp.) Also observe that $\{t_n\}$ converges to

$$t^* = t_1\left(\frac{1+k}{1-k}\right) \quad .$$

PROBLEM D-4

In Problems D-1, D-2, and D-3, simulate the bouncing of more than one ball. Use slightly different values of k and the initial height for each ball. Dropping a shoebox of, say, twenty-five balls leads to interesting problems for rootfinding ode solvers. For example, it demonstrates the importance of locating the first root of any event function for a given integration step.

E. PROBLEMS WITH DERIVATIVE SINGULARITIES

This section contains problems which have singularities in the derivative. In each case it is necessary to extend the derivative definition in some manner at such singularities. In Problem E-1, the derivative is not defined beyond the final integration point. Problem E-2 involves $\ln y$ in the derivative calculation. Although the exact solution y is always positive, it is possible for a solver to request a derivative calculation for a negative value of y. The use of an event function such as the second one represents a common means of avoiding this type of difficulty, by locating the value of time for which the solution attains a cutoff value, and then terminating the integration. In Problems E-3 and E-4, the derivative is also not defined beyond the desired root of the event function.

PROBLEM E-1 [1]

For $20 \geqslant t \geqslant 5$,

$$\frac{dy_1}{dt} = -\frac{\sqrt{400-t^2}}{t}$$

$$y_1(20) = 0$$

$$g_1 = 22 - (y_1 + \sqrt{400-t^2}) \quad .$$

The exact solution is

$$y_1 = -\sqrt{400-t^2} + 20 \ln \frac{20+\sqrt{400-t^2}}{t} \quad .$$

$$g_1 = 0 \text{ at } t = 12 \text{ at which } y_1(12) = 6 \quad .$$

PROBLEM E-2 [12]

For $1 \leqslant t \leqslant 12$,

$$\dot{y}_1 = \left(\frac{2 \ln y_1 + 8}{t} - 5 \right) y_1$$

$$y_1(1) = 1$$

$$g_1 = \ln y_1 = 2.2491$$

$$g_2 = y_1 - \bar{\epsilon} \text{ where } \bar{\epsilon} = 10^{-8} \quad .$$

The exact solution is $y_1 = e^{-t^2+5t-4}$.

$g_1 = 0$ at $t = 2.47$, 2.53 .

$g_2 = 0$ at $t = (5 + (9 - 4 \ln \bar{\epsilon})^{1/2}) / 2$.

PROBLEM E-3

For $1 \geqslant t \geqslant 0$,

$$\dot{y}_1 = 1/\sqrt{y_1}$$
$$y_1(1) = 1$$
$$g_1 = y_1 \quad .$$

The exact solution is $y_1 = \left[\frac{3}{2}(t - 1/3)\right]^{2/3}$.

$g_1 = 0$ at $t = 1/3$.

PROBLEM E-4

For $0 \leqslant t \leqslant 5$,

$$\dot{y}_1 = \sqrt{1 - y_1}$$
$$y_1(0) = 0$$
$$g_1 = 1 - y_1 \quad .$$

The exact solution is $y_1 = t - t^2/4$.

$g_1 = 0$ at $t = 2$.

F. PROBLEMS WITH MORE GENERAL ROOTFINDING REQUIREMENTS

This section contains several miscellaneous problems which are of interest. Problems F-1 and F-2 are well-known ode test problems. Problem F-1 describes the integral surface of a torus. Problem F-2 involves orbit equations. Event functions involving both the solution and the derivative are included. If the ode solver provides an approximation for the derivative to the residual evaluation subroutine, the event functions which involve the derivative should be handled in each of two ways: using the derivative of the solver interpolant, and using the calculated exact derivative corresponding to the approximate solution. Problems F-3, F-4, and F-5 are standard demonstration problems for various rootfinding solvers. Problem F-6 has a boundary layer near the root of the event function.

PROBLEM F-1 [6,21]

For $0 \leqslant t \leqslant 2\pi$,

$$\dot{y}_1 = -y_2 - y_1 y_3/(y_1^2 + y_2^2)^{1/2} \quad , \quad y_1(0) = 3$$
$$\dot{y}_2 = y_1 - y_2 y_3/(y_1^2 + y_2^2)^{1/2} \quad , \quad y_2(0) = 0$$
$$\dot{y}_3 = y_1/(y_1^2 + y_2^2)^{1/2} \quad , \quad y_3(0) = 0$$

$$g_1 = y_1$$
$$g_2 = y_2 - y_1$$
$$g_3 = y_3 - .5$$
$$g_4 = \dot{y}_3 - .5 \quad .$$

The exact solution is

$$y_1 = \cos t \cdot (2 + \cos t)$$
$$y_2 = \sin t \cdot (2 + \cos t)$$
$$y_3 = \sin t \quad .$$

For $0 \leqslant t \leqslant 2\pi$, the event functions have roots at the following times:

$$g_1 = 0 \text{ at } \pi/2 \ , \ 3\pi/2$$
$$g_2 = 0 \text{ at } \pi/4 \ , \ 5\pi/4$$
$$g_3 = 0 \text{ at } \pi/6 \ , \ 5\pi/6$$
$$g_4 = 0 \text{ at } \pi/3 \ , \ 5\pi/3 \ .$$

PROBLEM F-2 [6,21]

For $0 \leqslant t \leqslant 2\pi$,

$$\begin{aligned}
\dot{y}_1 &= y_2 & , \ y_1(0) &= .4 \\
\dot{y}_2 &= -y_1/(y_1^2 + y_3^2)^{3/2} & , \ y_2(0) &= 0 \\
\dot{y}_3 &= y_4 & , \ y_3(0) &= 0 \\
\dot{y}_4 &= -y_3/(y_1^2 + y_3^2)^{3/2} & , \ y_4(0) &= 2
\end{aligned}$$

$$\begin{aligned}
g_1 &= y_3 \\
g_2 &= y_1 + .6 - y_3/.8 \\
g_3 &= y_3/.8 - .5 \\
g_4 &= \dot{y}_3/.8 - .5 \ .
\end{aligned}$$

The exact solution is

$$y_1 = \cos u - .6$$
$$y_2 = -\sin u/(1 - .6 \cos u)$$
$$y_3 = .8 \sin u$$
$$y_4 = .8 \cos u/(1 - .6 \cos u)$$

where u satisfies $u - .6 \sin u = t$.

For $0 \leqslant t \leqslant 2\pi$, the event functions have roots at the following times:

$$g_1 = 0 \text{ at } t = \pi, 2\pi$$
$$g_2 = 0 \text{ at } t = \pi/4 - .3\sqrt{2}, 5\pi/4 + .3\sqrt{2}$$
$$g_3 = 0 \text{ at } t = \pi/6 - .3, 5\pi/6 - .3$$
$$g_4 = 0 \text{ at } t = \cos^{-1}(5/13) - 7.2/13, \quad 2\pi - \cos^{-1}(5/13) + 7.2/13 \quad .$$

PROBLEM F-3 [9]

For $1 \leqslant t \leqslant 7$,

$$\dot{y}_1 = 2y_1/t + 5$$
$$y_1(1) = -4$$

$$g_1 = \dot{y}_1$$
$$g_2 = y_1 + 6.2491 \quad .$$

The exact solution is $y_1 = -5t + t^2$.

$g_1 = 0$ at $t = 2.5$.

$g_2 = 0$ at $t = 2.47, 2.53$.

PROBLEM F-4

For $0 \leqslant t \leqslant 4$,

$$\dot{y}_1 = -y_1 \qquad , y_1(0) = 1$$
$$\dot{y}_2 = -y_2^{3/2} \qquad , y_2(0) = 1$$
$$\dot{y}_3 = y_3 \cos t \qquad , y_3(0) = 1$$
$$\dot{y}_4 = y_4(1 - y_4/20)/4 \qquad , y_4(0) = 1$$
$$\dot{y}_5 = -y_5 + y_6 \qquad , y_5(0) = 2$$
$$\dot{y}_6 = y_5 - 2y_6 + y_7 \qquad , y_6(0) = 0$$
$$\dot{y}_7 = y_6 - y_7 \qquad , y_7(0) = 1$$

$$g_1 = y_6 + 2y_7 - 5/2 \quad .$$

The exact solution is

$$y_1 = e^{-t}$$
$$y_2 = 4/(t+2)^2$$
$$y_3 = e^{\sin t}$$
$$y_4 = 20/(1+19e^{-t/4})$$

$$y_5 = 1 + (e^{-t} + e^{-3t}) / 2$$
$$y_6 = 1 - e^{-3t}$$
$$y_7 = 1 - (e^{-t} - e^{-3t}) / 2 \quad .$$

$g_1 = 0$ at $t = \ln 2$.

PROBLEM F-5

For $-1 \leqslant t \leqslant 12$,

$$\begin{aligned}
\dot{y}_1 &= y_2 && , y_1(-1) = 1/2 \\
\dot{y}_2 &= 1 && , y_2(-1) = -1 \\
\dot{y}_3 &= y_1 + y_2 && , y_3(-1) = 1/3 \\
\dot{y}_4 &= y_3 && , y_4(-1) = -1/8 \\
\dot{y}_5 &= 3t^2 - 20t + 24 && , y_5(-1) = -35 \\
g_1 &= y_5 \\
g_2 &= \begin{cases} t - 9 & , \text{if } t < 1 \\ (3y_3 - 54y_2)/(y_1 + 6y_2) & , \text{if } t \geqslant 1 \end{cases} \\
g_3 &= y_2 - 9.9 \\
g_4 &= y_1 - y_2 - 1.5 \, .
\end{aligned}$$

The exact solution is

$$\begin{aligned}
y_1 &= t^2/2 \\
y_2 &= t \\
y_3 &= t^2(1 + t/3)/2 \\
y_4 &= t^3(1 + t/4)/6 \\
y_5 &= t(t-6)(t-4) \\
g_1 &= 0 \text{ at } t = 0, 4, 6 \\
g_2 &= 0 \text{ at } t = 9 \\
g_3 &= 0 \text{ at } t = 9.9 \\
g_4 &= 0 \text{ at } t = -1, 3 \quad .
\end{aligned}$$

PROBLEM F-6 [21]

For $-.1 \leqslant t \leqslant .1$,

$$\begin{aligned}
\dot{y}_1 &= y_2 \ , \ y_1(-.1) = -.1/(\epsilon + .01)^{1/2} \\
\dot{y}_2 &= \left[-3\epsilon / (\epsilon + t^2)^2\right] \cdot y_1 \ , \ y_2(-.1) = \epsilon/(\epsilon + .01)^{1/2} \\
g_1 &= y_1
\end{aligned}$$

where $\epsilon = 10^{-6}$.

The exact solution is

$$y_1 = t \,/\, (\epsilon + t^2)^{1/2}$$
$$y_2 = \epsilon \,/\, (\epsilon + t^2)^{3/2} \quad .$$

g_1 has a root at $t = 0$. Also, $y_1(\sqrt{\epsilon}) = \sqrt{2}/\,2$, $y_1(-\sqrt{\epsilon}) = -\sqrt{2}/\,2$ and $\dot{y}_1(0) = 1/\sqrt{\epsilon}$. The solution thus has a boundary layer of width $\sqrt{\epsilon}$ about $t = 0.0$.

PROBLEM F-7

For $0 \leqslant t \leqslant 0.2$,

$$\dot{y}_1 = y_1 - 2t \,/\, y_1 \quad , \; y_1(0) = 1$$
$$\dot{y}_2 = -\, y_2^2 \quad , \; y_2(0) = 1$$
$$\dot{y}_3 = -\, 1/\,(1+t)^2 \quad , \; y_3(0) = 1$$

$$g_1 = y_1 - y_2$$
$$g_2 = y_1 - \sqrt{779/343}\, y_2$$
$$g_3 = y_1 - \sqrt{779/343}\, y_3$$
$$g_4 = \dot{y}_1 - 1$$
$$g_5 = \dot{y}_1^2 + 1.01\dot{y}_2 \quad .$$

The exact solution is

$$y_1 = \sqrt{1 + 2t}$$
$$y_2 = 1/\,(1+t)$$
$$y_3 = 1/\,(1+t) \quad .$$

$$g_1 = 0 \text{ at } t = 0 \; .$$
$$g_2 = 0 \text{ at } t = 1/7 \; .$$
$$g_3 = 0 \text{ at } t = 1/7 \; .$$
$$g_4 = 0 \text{ at } t = 0 \; .$$
$$g_5 = 0 \text{ at } t = (0.02 + \sqrt{.0404})/2 \; .$$

G. SOME OTHER INTERESTING PROBLEMS WITHOUT SIMPLE SOLUTIONS

This section contains several interesting problems for which exact solutions are not readily available. In Problem G-1, it is desired to build a table of values corresponding to prescribed values of the solution. It is desired to do this for one complete swing of the corresponding pendulum. The accompanying table contains approximate values of the times of interest. In Problem G-2, it is desired to locate zeroes of van der Pol's equation for two cases. The roots of the event functions in Problem G-3 correspond to roots of Bessel functions of the first kind and orders 0 and 1. Four cases are of interest for the rootfinding. Two of the cases involve the derivative in the rootfinding. In Problem G-4, it

is desired to calculate orbits for the three-bodies problem, that is, to locate times at which the solution components return to their initial values. Since the event function also vanishes for other values of time, it is necessary to check whether a calculated root actually corresponds to an orbit.

PROBLEM G-1 [20]

$$\dot{y}_1 = y_2 \qquad , \; y_1(0) = 0$$
$$\dot{y}_2 = 2k^2 y_1^3 - (1+k^2)y_1 \quad , \; y_2(0) = 1$$

where $k = 1/2$.

$$g_1 = y_1 - i\,\Delta y\,,\; i = 1, \cdots, 8, 9, 8, \cdots, 1 \text{ where } \Delta y = 0.1.$$
$$g_2 = y_2$$

Denote the root of $g_2(t) = 0$ by $\bar{t}$. Then $y_1(\bar{t}) = 1$ and

$$\bar{t} = \int_0^1 \frac{ds}{[(1-s^2)(1-k^2s^2)]^{1/2}} \; .$$

For $0 \leqslant t^* \leqslant \bar{t}$ the value of t^* for which $y_1(t^*) = y^*$ is given by the elliptic integral of the first kind

$$t^* = \int_0^{y^*} \frac{ds}{[(1-s^2)(1-k^2s^2)]^{1/2}}$$

or

$$t^* = F(\phi \,|\, \alpha) = \int_0^{\phi} (1 - \sin^2\alpha \;\; \sin^2\theta)^{-1/2}\, d\theta$$

where

$$\alpha = \sin^{-1} k\,,\; \phi = \sin^{-1} y^* \quad .$$

For $\bar{t} \leqslant t^* \leqslant 2\bar{t}$, the value of t^* for which $y_1(t^*) = y^*$ is given by

$$t^* = 2\bar{t} - \int_0^{y^*} \frac{ds}{[(1-s^2)(1-k^2s^2)]^{1/2}} \quad .$$

The exact solution for y_1 may be computed to any desired degree of accuracy by using a rootfinder to invert the elliptic integral relationship.

PROBLEM G-2 [3,19]

$$\dot{y}_1 = y_2 \qquad , \; y_1(0) = 2$$
$$\dot{y}_2 = \eta(1-y_1^2)y_2 - y_1 \quad , \; y_2(0) = 0$$
$$g_1 = y_1 \quad .$$

Two cases are of interest:

Case (i)

$\eta = 3, \quad 0 \leqslant t \leqslant 20$

Case (ii)

$\eta = 100, \quad 0 \leqslant t \leqslant 400$.

The desired roots are approximately as follows.

Case (i)

3.60761267698567
8.03716042148430
12.4667081698911
16.8962559182921

Case (ii)

81.1723778705497
162.590913432667
244.009448787067
325.427984460614

[19] contains a discussion of values of η for which this problem behaves like a stiff problem.

PROBLEM G-3

For $0 \leqslant t \leqslant 20$,

$$\begin{aligned}
\dot{y}_1 &= y_2 & &, y_1(0) = 1 \\
\dot{y}_2 &= -y_2 / t - y_1 & &, y_2(0) = 0 \\
\dot{y}_3 &= y_4 & &, y_3(0) = 0 \\
\dot{y}_4 &= -y_4 / t - (1 - 1/ t^2) y_3 & &, y_4(0) = 1/ 2 \quad .
\end{aligned}$$

($\dot{y}_2(0) = -.5$ and $\dot{y}_4(0) = 0$.)

The exact solution is

$$\begin{aligned}
y_1 &= J_0(t) \\
y_2 &= J_0'(t) \\
y_3 &= J_1(t) \\
y_4 &= J_1'(t)
\end{aligned}$$

where J_0 and J_1 are the Bessel functions of the first kind and orders 0 and 1.

Four rootfinding cases are of interest:

Case (i)

$g_1 = \dot{y}_1$
$g_2 = y_1$

Case (ii)

$g_1 = y_3$
$g_2 = y_1$

Case (iii)

$g_1 = \dot{y}_1$
$g_2 = ty_4 + y_3$

Case (iv)

$g_1 = y_3$
$g_2 = ty_4 + y_3$.

In each case the roots of $g_1 = 0$ are the zeroes of $y_3 = J_1$ (recall that $J_0'(t) = -J_1(t)$); and the roots of $g_2 = 0$ are the zeroes of $y_1 = J_0$ (recall that $\frac{d}{dt}(tJ_1(t)) = tJ_0(t)$).

Within the interval of interest, the zeros of g_1 thus occur at approximately

$$t = 0.0,\ 3.8317,\ 7.0156,\ 10.1735,\ 13.3237,\ 16.4706;$$

and the zeros of g_2 occur at approximately

$$t = 2.4048,\ 5.5201,\ 8.6537,\ 11.7915,\ \text{and } 14.9309\ .$$

See [26] for an interesting discussion of using rootfinding ode solvers for other problems involving Bessel functions.

PROBLEM G-4 [15, 20]

For $0 \leqslant t \leqslant 10$,

$$\dot{y}_1 = y_3$$
$$\dot{y}_2 = y_4$$
$$\dot{y}_3 = y_1 + 2y_4 - v(y_1+u)/r_1 - u(y_1 - v)/r_2$$
$$\dot{y}_4 = y_2 - 2y_3 - vy_2/r_1 - uy_2/r_2$$
$$y_1(0) = 1.2$$
$$y_2(0) = 0$$
$$y_3(0) = 0$$
$$y_4(0) = K = -1.04935750983031990726$$

where

$$u = 1/\ 82.45$$
$$v = 1 - u$$
$$r_1 = \left[(y_1+u)^2 + y_2^2\right]^{3/2}$$
$$r_2 = \left[(y_1-v)^2 + y_2^2\right]^{3/2}$$
$$g_1 = (y_1 - y_1(0))\, y_3 + (y_2 - y_2(0))\, y_4 \quad .$$

The solution is periodic with period T where

$$T \doteq 6.19216933131963970674 \ .$$

The roots of g_1 which are of interest occur at integral multiples of T.

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