MATH 350: Introduction to Computational Mathematics

Chapter VII: Numerical Differentiation and Solution of Ordinary Differential Equations

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Outline

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Introduction

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However, first we think about how to deal with derivatives numerically since being able to do this accurately is often essential for a good ODE or PDE solver.

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Let $f(x) = mx + b$ so that $f'(x) = m$. Then

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This gives us a new symmetric difference method:

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Since we have an “exact” error estimate for these methods we can be more precise about the impact of Richardson extrapolation.

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$$f'(x) = \underbrace{\frac{f(x+h) - f(x-h)}{2h}}_{=\overline{D}_h f(x)} + k_2 h^2 + k_4 h^4 + \ldots,$$

where k_2, k_4, etc., are appropriate constants independent of h.

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So symmetric differences with Richardson extrapolation are $\mathcal{O}(h^4)$ accurate (see `Differentiation.mw`).

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This gives us

$$f''(x) \approx D_h^{(2)} f(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

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3. *The accuracy of such a method can be obtained via error estimates for the polynomial interpolant (which we didn't study).*
4. *The approach based on polynomial interpolation is very general and can be used for arbitrary degree (i.e., arbitrarily many points), arbitrarily spaced points (symmetric, non-symmetric, etc.), and arbitrary order derivatives.*

Example

- The linear interpolant of f at $(x-h, f(x-h))$ and $(x+h, f(x+h))$ has slope

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- Differentiation of the quadratic interpolant

$$p(x) = \frac{(x-x_2)(x-x_3)}{(x_1-x_2)(x_1-x_3)}f(x_1) + \frac{(x-x_1)(x-x_3)}{(x_2-x_1)(x_2-x_3)}f(x_2) + \frac{(x-x_1)(x-x_2)}{(x_3-x_1)(x_3-x_2)}f(x_3)$$

to f followed by evaluation at $x_1 = x-h$, $x_2 = x$ and $x_3 = x+h$ will provide the formula for $f''(x)$ from the previous slide (for details see HW).

Outline

First-order initial value problems

We will consider problems of the form

$$\begin{aligned}\frac{\mathrm{d}y(t)}{\mathrm{d}t} &= f(t, y(t)) \\ y(t_0) &= y_0.\end{aligned}$$

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Namely,

$$y(t) = \frac{1}{\mu(t)} \int_{t_0}^{t} \mu(\tau) b(\tau) \mathrm{d}\tau$$

with integrating factor

$$\mu(t) = \mathrm{e}^{-\int a(t)\mathrm{d}t}.$$

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Remark

In many cases f will not be as simple, and numerical methods are required.

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Theorem

Let $f = f(t, y)$ and $\frac{\partial f}{\partial y}$ be continuous near the initial point (t_0, y_0). Then there is a unique solution y defined on the interval $[t_0 - \alpha, t_0 + \alpha]$ for some α such that

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Remark

This theorem can be found in any introductory ODE book (such as [Zill]). For a proof see for example [Boyce and DiPrima].

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Example

The predator-prey model from Chapter 1 provides such a system:

$$\begin{aligned} \frac{\mathrm{d}H(t)}{\mathrm{d}t} &= aH(t) - bH(t)L(t) \\ \frac{\mathrm{d}L(t)}{\mathrm{d}t} &= -cL(t) + dH(t)L(t) \\ H(t_0) &= H_0, \quad L(t_0) = L_0, \end{aligned}$$

where t denotes time, H population of hares, L population of lynx, and a, b, c, d, H_0, L_0 are given constants.
This system is coupled and nonlinear and does not possess an analytical solution.

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Example

The angle θ that a pendulum with mass m and length ℓ makes with the vertical satisfies the following second-order IVP (which is based on Newton's second law of motion):

$$\begin{aligned} m\ell\frac{\mathrm{d}^2\theta(t)}{\mathrm{d}t^2} &= -mg\sin(\theta(t)) \\ \theta(t_0) &= \theta_0 \\ \theta'(t_0) &= v_0. \end{aligned}$$

Here g is the gravitational constant, θ_0 is the initial angle, and v_0 the initial angular velocity.

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This problem can be converted to a system of two first-order equations.

Example (cont.)

We introduce a vector $\boldsymbol{y}(t) = [y_1(t), y_2(t)]^T$ of new variables such that $[y_1(t), y_2(t)]^T = [\theta(t), \frac{\mathrm{d}\theta(t)}{\mathrm{d}t}]^T$.

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Therefore, all we need to numerically solve any ODE initial value problem is a vectorized first-order solver.

The simplest such solver is given by `Euler.m` used in Chapter 1 (see details below).

Example

Rewrite the coupled system of second-order initial-value problems

$$[x''(t)]^2 + te^{y(t)} + y'(t) = x'(t) - x(t)$$
$$y'(t)y''(t) - \cos(x(t)y(t)) + \sin(tx'(t)y(t)) = x(t)$$
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as a first-order system.

Solution

Since there are two second-order equations we will need four new variables leading to four first-order equations.
Therefore we take $\boldsymbol{y}(t) = [y_1(t), y_2(t), y_3(t), y_4(t)]^T$ with

$$[y_1(t), y_2(t), y_3(t), y_4(t)]^T = [x(t), x'(t), y(t), y'(t)]^T.$$

Solution (cont.)

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Outline

From IVPs to Integral Equations

As before, we consider the IVP

$$\begin{aligned} y'(t) &= f(t, y(t)) \\ y(t_0) &= y_0 \end{aligned}$$

and integrate both sides of the differential equation from t to $t + h$ to obtain

$$y(t+h) - y(t) = \int_t^{t+h} f(\tau, y(\tau)) \mathrm{d}\tau. \tag{3}$$

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Remark

For simplicity we limit our discussion to single ODEs of one variable. However, everything goes through analogously for the first-order systems discussed on the previous slides.

Example

Apply the left endpoint rule $\int_a^b f(x)\mathrm{d}x \approx \sum_{i=1}^{n} \underbrace{h}_{=\frac{b-a}{n}} f(x_{i-1})$ on a single interval, i.e., with $n = 1$, and $a = t$, $b = t + h$ to the RHS of (3).

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Solution

In this case the left endpoint rule is

$$L_1(f) = \sum_{i=1}^{1} \frac{b-a}{1} f(x_{i-1})$$

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Thus, solving (3) with the left endpoint rule is equivalent to Euler's method (see also Chapter 6).

Euler's Method

In order to advance the solution of the IVP in time we introduce a sequence of points $t_n = t_0 + nh$, $n = 0, 1, \ldots, N$ that divide a time interval $[t_0, t_N]$ into N equal subintervals (i.e., $h = \frac{t_N - t_0}{N}$).

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With this notation the approximate solution of the integral equation (3)

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Algorithm (see also `Euler.m`)

- Input t_0, y_0, f, h, N
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Euler's method is illustrated in the MATLAB script `EulerDemo350.m`.

Graphical interpretation of Euler's method

Graphically, Euler's method comes down to taking straight line approximations of the unknown solution y over small time intervals from t_n to $t_{n+1} = t_n + h$.

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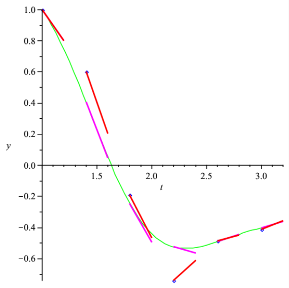

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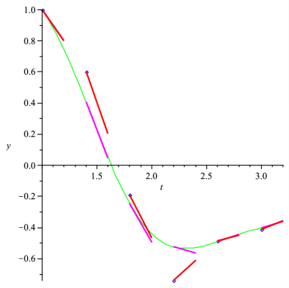

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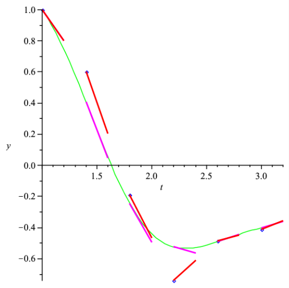

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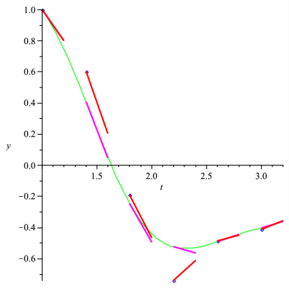

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See the Maple worksheet `EulerDemo.mw`.

Example

Apply the basic trapezoidal rule $\int_a^b f(x)\mathrm{d}x \approx \frac{b-a}{2}[f(a)+f(b)]$ with $a = t$ and $b = t+h$ to the RHS of (3).

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This gives us

$$\int_t^{t+h} f(\tau, y(\tau))\mathrm{d}\tau \approx \frac{h}{2}\left[f(t, y(t)) + f(t+h, y(t+h))\right].$$

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Note that we have a y_{n+1} term on both sides of the equation (and cannot explicitly solve for it). This means that we have an implicit method. This method is also called trapezoidal rule (for IVPs).

How to deal with an implicit IVP solver?

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Remark

We will not focus on implicit methods. They are more difficult to implement, but have better stability properties (see MATH 478). In MATLAB *we find them as stiff solvers.*

In order to make the trapezoidal rule

$$y_{n+1} = y_n + \frac{h}{2} f(t_n, y_n) + \frac{h}{2} f(t_{n+1}, y_{n+1}).$$

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$$y_{n+1} = y_n + h\frac{s_1 + s_2}{2}$$

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For an example see the MATLAB files `RK2.m` and `RK2Demo.m`.

Graphical Interpretation of Classical 2nd-Order RK

Since the 2nd-order RK method is given by

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  so that we obtain an approximate slope s_2 at $t_n + h$.
- The actual Euler step then uses the average of the slopes s_1 at t_n and s_2 at $t_n + h$ to obtain

  $$y_{n+1} = y_n + h\frac{s_1 + s_2}{2}.$$

Example

Apply the basic midpoint rule $\int_a^b f(x)\mathrm{d}x \approx (b-a)f\left(\frac{a+b}{2}\right)$ with $a = t$, $b = t + h$ to the RHS of (3).

Example

Apply the basic midpoint rule $\int_a^b f(x)dx \approx (b-a)f\left(\frac{a+b}{2}\right)$ with $a = t$, $b = t + h$ to the RHS of (3).

Solution

This gives us $\int_t^{t+h} f(\tau, y(\tau))d\tau \approx hf(t + \frac{h}{2}, y(t + \frac{h}{2}))$.

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$$y_{n+1} = y_n + hf(t_n + \frac{h}{2}, y_n + \frac{h}{2}f(t_n, y_n)).$$

This is known as the modified Euler method or midpoint rule (for IVPs).

If we write the modified Euler method (midpoint rule)

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then this is also a second-order Runge Kutta method.

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Remark

Runge-Kutta methods are characterized by having several stages ($s_1, s_2, \ldots$) for each time step.

Graphical Interpretation of Modified Euler

Based on the Runge-Kutta formulation of the modified Euler method/midpoint rule we can see that it corresponds to

- taking an Euler step with only half the step length, $\frac{h}{2}$, resulting in

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- followed by an Euler step with full step length h using the slope at the half-way point $(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}})$ so that

$$y_{n+1} = y_n + hf(t_{n+\frac{1}{2}}, y_{n+\frac{1}{2}}).$$

Here $t_{n+\frac{1}{2}}$ is used symbolically to denote the time $t_n + \frac{h}{2}$.

Example

Apply the basic midpoint rule $\int_a^b f(x)\mathrm{d}x \approx (b-a)f\left(\frac{a+b}{2}\right)$ with $a = t$, $b = t + 2h$ to the RHS of (3).

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This gives us

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This is an explicit 2-step method (and *not* a Runge-Kutta method). In the context of PDEs this method appears as the leapfrog method.

Example

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- Simpson's rule yields the classical fourth-order Runge-Kutta method (see below) in case there is no dependence of f on y.
- Gauss quadrature leads to so-called Gauss-Runge-Kutta or Gauss-Legendre methods. One such method is the implicit midpoint rule

$$y_{n+1} = y_n + hf(t_n + \tfrac{h}{2}, \tfrac{1}{2}(y_n + y_{n+1})).$$

Outline

Methods for which the value y_{n+1} depends only on the previous time level t_n are called single step methods. All methods mentioned so far (except for the explicit midpoint rule) fall into this category.

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We now take a closer look at the family of Runge-Kutta methods named after the late 19th/early 20th century German mathematicians Carl Runge and Martin Kutta.

Second-order Runge-Kutta Methods

We already met the classical second-order Runge-Kutta (improved Euler) method

$$y_{n+1} = y_n + h\frac{s_1 + s_2}{2}$$

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One can imagine many other possibilities to complete these two stages.

A general explicit two-stage Runge-Kutta method is of the form

$$y_{n+1} = y_n + h\left[\gamma_1 s_1 + \gamma_2 s_2\right]$$

where

$$\begin{aligned} s_1 &= f(t_n, y_n) \\ s_2 &= f(t_n + \alpha_2 h, y_n + h\beta_{21} s_1), \end{aligned}$$

with $\alpha_2 = \beta_{21}$ (which ensures that the method is consistent[1] or first-order).

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Remark

The somewhat arbitrary notation comes from a more general discussion that includes implicit as well as higher-order methods.

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Butcher Tableaux

It is customary to arrange the coefficients α_i, β_{ij}, and γ_i in a so-called Runge-Kutta or Butcher tableaux.

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An explicit two-stage RK method will always look like

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with $\alpha_2 = \beta_{21}$.
Using Taylor series expansions one can show (see MATH 478) that for the method to be second-order it needs to also satisfy

$$\gamma_1 + \gamma_2 = 1$$
$$\beta_{21}\gamma_2 = \frac{1}{2}$$

— a system of two nonlinear equations in three unknowns. It is not difficult to generate solutions of this system.

Remark

The choice $\gamma_1 = 1$, $\gamma_2 = 0$ leads to Euler's method. However, since now we can't have $\beta_{21}\gamma_2 = \frac{1}{2}$ Euler's method is only a first-order method.

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The Butcher tableaux for the classical RK2 method is

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}.$$

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The Butcher tableaux for the modified Euler method is

$$\begin{array}{c|cc} 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \hline & 0 & 1. \end{array}$$

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Another interesting second-order Runge-Kutta method has the tableaux

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We will see later how it can be embedded into a third-order method that uses the same slopes as the second-order method (plus one additional one) resulting in an adaptive method.

Fourth-order Runge-Kutta Methods

Probably the most famous Runge-Kutta method is the four-stage classical fourth-order method:

$$y_{n+1} = y_n + \frac{h}{6}\left[s_1 + 2s_2 + 2s_3 + s_4\right]$$

with

$$\begin{aligned} s_1 &= f(t_n, y_n) \\ s_2 &= f\left(t_n + \tfrac{h}{2}, y_n + \tfrac{h}{2}s_1\right) \\ s_3 &= f\left(t_n + \tfrac{h}{2}, y_n + \tfrac{h}{2}s_2\right) \\ s_4 &= f\left(t_n + h, y_n + hs_3\right) \end{aligned}$$

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For an example see the MATLAB files `RK4.m` and `RK4Demo.m`.

Convergence Experiments

In the MATLAB script `EulerRKConvergenceDemo.m` we compare the orders (convergence rates) of three single step methods:

- Euler's method (first-order),
- classical second-order Runge-Kutta (or improved Euler) method (second-order),
- classical fourth-order Runge-Kutta method (fourth-order).

Outline

In order to be able to implement an adaptive step size control as we did for numerical integration in `quadtx` we need to have two IVP solvers of different orders that can be paired together efficiently.

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- using so-called predictor-corrector methods (also based on multistep methods such as Adams methods),
- using two totally different methods (such as `ode23t` and `ode23tb` which both couple the trapezoidal rule with something else).

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For more general Runge-Kutta methods the situation is as follows:

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However, certain higher-order methods are still useful if we want to construct adaptive embedded Runge-Kutta methods.

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Earlier we mentioned the second-order Runge-Kutta method

$$y_{n+1} = y_n + \frac{h}{4}\left[s_1 + 3s_2\right]$$

with

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The combination uses only three function evaluations per time step.

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while the related four-stage third-order method is

$$\tilde{y}_{n+1} = y_n + \frac{h}{24}(7s_1 + 6s_2 + 8s_3 + 3s_4)$$

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while the related four-stage third-order method is

$$\tilde{y}_{n+1} = y_n + \frac{h}{24}(7s_1 + 6s_2 + 8s_3 + 3s_4)$$

with s_1, s_2 and s_3 as above, and

$$s_4 = f(t_{n+1}, y_{n+1})$$

using the second-order approximation y_{n+1}.

Adaptive step size control

Using a technique similar to Richardson extrapolation we can obtain an error estimate which we can use to adaptively control the stepsize:

$$e_{n+1} = \frac{h}{72}(-5s_1 + 6s_2 + 8s_3 - 9s_4).$$

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  Note that the fourth stage is not wasted since it is used as the first stage for the next time step. Thus, only three function evaluations are required per time step.
- If the error is too large, then we forget the y_{n+1} calculation and try again with a smaller value of h.

Slightly simplified main ingredients of `ode23tx.m`

Function header:

```
function [tout,yout] = ode23tx(F,tspan,y0,arg4,varargin)
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Initialize a few variables:

```
rtol = 1.e-3,  atol = 1.e-6;
t0 = tspan(1);
tfinal = tspan(2);
tdir = sign(tfinal - t0);      % "forward" or "backward"
threshold = atol / rtol;
hmax = abs(0.1*(tfinal-t0));
t = t0,  y = y0(:);
```

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hmax = abs(0.1*(tfinal-t0));
t = t0,  y = y0(:);
```

Set initial time step size depending on scale of the problem:

```
s1 = F(t, y, varargin{:});
r = norm(s1./max(abs(y),threshold),inf) + realmin;
h = tdir*0.8*rtol^(1/3)/r;
```

The cube root appears because we have a third-order method.

Main loop

```
while t ~= tfinal
    hmin = 16*eps*abs(t);
    if abs(h) > hmax, h = tdir*hmax; end
    if abs(h) < hmin, h = tdir*hmin; end
    % Stretch the step if t is close to tfinal.
    if 1.1*abs(h) >= abs(tfinal - t)
        h = tfinal - t;
    end
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The Runge-Kutta step

```
    s2 = F(t+h/2, y+h/2*s1, varargin{:});
    s3 = F(t+3*h/4, y+3*h/4*s2, varargin{:});
    tnew = t + h;
    ynew = y + h*(2*s1 + 3*s2 + 4*s3)/9;
    s4 = F(tnew, ynew, varargin{:});
```

Error estimate scaled to match the tolerances (realmin prevents err from being exactly zero):

```
e = h*(-5*s1 + 6*s2 + 8*s3 - 9*s4)/72;
err = norm(e./max(max(abs(y),abs(ynew)),threshold),
        ... inf) + realmin;
```

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        ... inf) + realmin;
```

See if we advance or repeat

```
if err <= rtol
    t = tnew;
    y = ynew;
    tout(end+1,1) = t;
    yout(end+1,:) = y.';
    s1 = s4; % Reuse final function value in new step
% else forget the latest calculation
end
```

Compute new step size:

```
    h = h*min(5,0.8*(rtol/err)^(1/3));
end   % of function ode23tx
```

Here

$$\texttt{rtol/err} \begin{cases} > 1 & \text{if advance} \\ < 1 & \text{otherwise,} \end{cases}$$

and the factors 0.8 and 5 prevent excessive changes in step size.

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has solution $y(t) = 1$.
In MATLAB we can use `ode23tx` to solve this problem by running this MATLAB code:

```
f = @(t,y) 0;
ode23tx(f,[0 10],1);
```

Example

The harmonic oscillator (see Pendulum example)

$$\begin{aligned} \frac{d^2}{dt^2} y(t) &= -y(t), \quad 0 \le t \le 2\pi \\ y(0) &= 1 \quad y'(0) = 0 \end{aligned}$$

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We can then use `ode23tx` and ‣ run this MATLAB code:

```
f = @(t,y) [y(2); -y(1)];
ode23tx(f,[0 2*pi],[1; 0]);
```

Example (cont.)

In order to get a phase plane plot, i.e., a plot of the y_2 component (velocity) vs. the y_1 component (position) parametrized by time, we use

Run this MATLAB code

```
f = @(t,y) [y(2); -y(1)];
[t,y] = ode23tx(f,[0 2*pi],[1; 0]);
plot(y(:,1),y(:,2),'-o')
axis([-1.2 1.2 -1.2 1.2])
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A few other ways to achieve this (such as by defining your own plotting function) are described in [NCM].

Example

In the two-body problem we model the orbit of a small body (such as a spaceship) as it moves under the gravitational attraction of a much heavier body (a planet).
A model for the path of the small body (specified by the Cartesian coordinates of its position at time t relative to the large body) is

$$
\begin{aligned}
x''(t) &= -\frac{x(t)}{r(t)^3} \\
y''(t) &= -\frac{y(t)}{r(t)^3}
\end{aligned}
$$

where

$$r(t) = \sqrt{x(t)^2 + y(t)^2}.$$

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This is illustrated in `twobody.m` and `TwobodyDemo.m`.

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A mathematical model for this is given by the nonlinear first-order equation

$$\begin{aligned} y'(t) &= y^2(t) - y^3(t), \quad 0 \le t \le \frac{2}{\delta} \\ y(0) &= \delta, \end{aligned}$$

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$$\begin{aligned} y'(t) &= y^2(t) - y^3(t), \quad 0 \le t \le \tfrac{2}{\delta} \\ y(0) &= \delta, \end{aligned}$$

- $y(t)$: radius of the ball of flame at time t,
- y^2: comes from surface area,
- y^3: comes from volume,
- δ: initial radius (assumed to be “small”, transition to critical size occurs at $\frac{1}{\delta}$).

Example (cont.)

The exact solution is given by

$$y(t) = \frac{1}{W(ae^{a-t}) + 1}, \quad a = \frac{1}{\delta} - 1,$$

where W is the Lambert W function (the solution of the equation $W(z)e^{W(z)} = z$, see also the Maple worksheet `MatchDemo.mw`).

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This problem is initially well-behaved, but becomes stiff as the solution approaches the steady state of 1. See an illustration of the stiffness in `MatchDemo.mw`.

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The stiff solver `ode23s` used to solve this problem much more efficiently is an embedded second-third order implicit Runge-Kutta (or Rosenbrock) method.

Using `odeset` to add special options to MATLAB's IVP solvers

Example

In the match problem we used the `odeset` function to reduce the default relative tolerance from 10^{-3} to 10^{-4} via

```
tol = 1e-4;
opts = odeset('RelTol',tol);
ode23tx(f,[t0 tmax],y0,opts);
```

Example

Let's consider again the skydive model of Chapters 1 and 4:

$$\frac{\mathrm{d}v}{\mathrm{d}t}(t) = \frac{F_g + F_d}{m} = g - \frac{c}{m}v^2(t), \quad v(0) = v_0 = 0.$$

Here we used the second model according to which the drag force due to air resistance is proportional to the square of the velocity.

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Here we used the second model according to which the drag force due to air resistance is proportional to the square of the velocity.
In addition, let's assume that the gravitational "constant" g depends on the altitude x according to Newton's inverse square law of gravitational attraction

$$g(x) = g(0)\frac{R^2}{(R + x(t))^2}$$

with

- $R \approx 6.37 \times 10^6 (m)$: earth's radius,
- $g(0) = 9.81 (m/s^2)$: value of the gravitational constant at the earth's surface.

Example (cont.)

Combining the above information we get

$$\frac{\mathrm{d}v}{\mathrm{d}t}(t) = g(0)\frac{R^2}{(R + x(t))^2} - \frac{c}{m}v^2(t), \quad v(0) = v_0 = 0.$$

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$$\begin{aligned}
\frac{\mathrm{d}x}{\mathrm{d}t}(t) &= -v(t) \\
\frac{\mathrm{d}v}{\mathrm{d}t}(t) &= g(0)\frac{R^2}{(R+x(t))^2} - \frac{c}{m}v^2(t) \\
x(0) &= x_0 \\
v(0) &= 0.
\end{aligned}$$

A standard jumping altitude is about $x_0 = 4000(m)$.

Example (cont.)

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This is quite complicated, and luckily MATLAB offers a simpler approach based on event handling.

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This is quite complicated, and luckily MATLAB offers a simpler approach based on event handling.

The MATLAB programs `Skydive3Demo.m`, `Skydive3.m`, and `Skydive3Event.m` illustrate how this works.

Example (cont.)

Event handling for the skydive problem works as follows:
In the main program we call `ode23`

```
opts = odeset('events',@Skydive3Event);
[t,y,te,ye] = ode23(@Skydive3,[t0 tend],y0,opts,g,c,m,R);
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where `t0,tend,y0,g,c,m,R` are specified values.

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where `t0,tend,y0,g,c,m,R` are specified values.
The event handler `Skydive3Event.m` consists of

```
function [stopval,isterm,dir] = Skydive3Event(t,y,g,c,m,R)
stopval = y(1); % the value we want to make 0
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- `y(1)` contains the altitude, so the solver stops when this value becomes zero.
- `isterm` specifies whether we stop when the stop event occurs, or continue to `tend` (`isterm = 0`).

Example

As a small challenge you should try to modify the previous skydive example to cover the model of Problem 3 of Homework Assignment 1 and Problem 1 of Computer Assignment 1 in which the skydiver was allowed to use a parachute.

Outline

What is Stiffness?

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Other similar descriptions from the literature are:

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- A problem is stiff if it contains widely varying time scales, i.e., some components of the solution decay much more rapidly than others.
- A problem is stiff if the stepsize is dictated by stability requirements rather than by accuracy requirements.
- A problem is stiff if explicit methods don't work, or work only extremely slowly.

Stiff ODEs arise in many applications; e.g.,

- when modeling chemical reactions,
- in control theory,
- in network analysis and simulation problems,
- in electrical circuits.

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This results in a second-order nonlinear IVP

$$y''(t) - \mu \left(1 - y^2(t)\right) y'(t) + y(t) = 0,$$

$$y(0) = y_0, \; y'(0) = yp_0,$$

where μ is a parameter that indicates the amount of damping.

For positive values of μ the solution describes deterministic chaos and ends up in a limit cycle.

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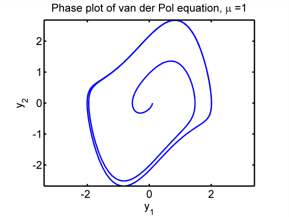

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For positive values of μ the solution describes deterministic chaos and ends up in a limit cycle.

For large values of μ the equation becomes stiff.

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$$
\begin{aligned}
y_1'(t) &= y_2(t) \\
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y_1(0) &= y_0 \\
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Solution of this system is illustrated in the MATLAB script `VanderPolDemo.m`.

Example (cont.)

Written as a first-order system we have

$$
\begin{aligned}
y_1'(t) &= y_2(t) \\
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\end{aligned}
$$

Solution of this system is illustrated in the MATLAB script `VanderPolDemo.m`.
Additional plots are provided in `VanderPolPlots.m`.

Remark

While our explicit solvers `ode23` *and* `ode45` *use adaptive stepsizes, there are stability constraints we have not discussed which prevent them from taking very large time steps — even if the problem would seem to allow this.*

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This is why explicit solvers don't work for stiff problems.

Implicit solvers have much better stability properties, and therefore adaptive implicit solvers (such as `ode23s` *and* `ode15s`*) can be used much more efficiently to deal with stiff problems.*

Outline

A single-step numerical method uses only the most recent history, y_n, to obtain the next value y_{n+1}.

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With an s-step method, on the other hand, more of the history of the solution will affect the next value, i.e., y_{n+s} depends on s previous values, $y_{n+s-1}, y_{n+s-2}, \ldots, y_{n+1}, y_n$.

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In its most general form an s-step method looks like

$$\sum_{m=0}^{s} a_m y_{n+m} = h \sum_{m=0}^{s} b_m f(t_{n+m}, y_{n+m}), \qquad n = 0, 1, \ldots,$$

where the coefficients a_m and b_m, $m = 0, 1, \ldots, s$, are independent of h, n, and the underlying ODE.

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Different choices of the a_m and b_m yield different numerical methods.

We have a true s-step formula if either a_0 or b_0 is different from zero.

General s-step method:

$$\sum_{m=0}^{s} a_m y_{n+m} = h \sum_{m=0}^{s} b_m f(t_{n+m}, y_{n+m}), \qquad n = 0, 1, \ldots,$$

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Adam-Bashforth methods are optimal order explicit methods.
Adam-Moulton methods with odd s are optimal order implicit methods.

Multistep methods require additional startup values. These are frequently obtained using one step of a higher-order single-step method (such as a Runge-Kutta method).

Explicit methods

Example

- First-order Adams-Bashforth method (Euler):

$$y_{n+1} = y_n + hf(t_n, y_n)$$

- Second-order Adams-Bashforth method:

$$y_{n+2} = y_{n+1} + \frac{h}{2}\left[3f(t_{n+1}, y_{n+1}) - f(t_n, y_n)\right]$$

- Third-order Adams-Bashforth method:

$$y_{n+3} = y_{n+2} + \frac{h}{12}\left[23f(t_{n+2}, y_{n+2}) - 16f(t_{n+1}, y_{n+1}) + 5f(t_n, y_n)\right]$$

Implicit methods

Example

- First-order Adams-Moulton method (backward Euler):

$$y_{n+1} = y_n + hf(t_{n+1}, y_{n+1})$$

- Second-order Adams-Moulton method (trapezoidal method, note only 1-step):

$$y_{n+2} = y_{n+1} + \frac{h}{2}\left[f(t_{n+2}, y_{n+2}) + f(t_{n+1}, y_{n+1})\right]$$

- Third-order Adams-Moulton method:

$$y_{n+3} = y_{n+2} + \frac{h}{12}\left[5f(t_{n+3}, y_{n+3}) + 8f(t_{n+2}, y_{n+2}) - f(t_{n+1}, y_{n+1})\right]$$

Usually one combines an implicit Adams-Moulton method with an explicit Adams-Bashforth method as a predictor-corrector pair. See, e.g., MATLAB's `ode113`, or

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Remark

Multistep methods tend to be more efficient than single-step methods for problems with smooth solutions and high accuracy requirements. For example, the orbits of planets and deep space probes are computed with multistep methods.

BDF multistep methods are implemented in MATLAB as `ode15s`. Many more details on multistep methods are provided in MATH 478.

Outline

Things to remember about this chapter

- The derivative estimates are important in and of themselves, but also play a fundamental role in finite difference solvers for BVPs and PDEs (see below).
- The ODE solvers we looked at are limited to initital value problems.
- Always convert your problem to a (system of) first-order ODEs before applying one of the standard solvers.
- Choose your method according to the guidelines on the next slide (from MATLAB's Help documentation).

MATLAB ODE Solvers

- `ode45`: Nonstiff problems, medium accuracy. Use most of the time. This should be the first solver you try.
- `ode23`: Nonstiff problems, low accuracy. Use for large error tolerances or moderately stiff problems.
- `ode113`: Nonstiff problems, low to high accuracy. Use for stringent error tolerances or computationally intensive ordinary differential equation functions.
- `ode15s` Stiff problems, low to medium accuracy. Use if ode45 is slow (stiff systems) or there is a mass matrix.
- `ode23s` Stiff problems, low accuracy. Use for large error tolerances with stiff systems or with a constant mass matrix.
- `ode23t` Moderately stiff problems, low accuracy. Use for moderately stiff problems where you need a solution without numerical damping.
- `ode23tb` Stiff problems, low accuracy. Use for large error tolerances with stiff systems or if there is a mass matrix.

Other things we did not discuss

- Accuracy issues, such as local vs. global truncation errors. See MATH 478 for details (or Section 7.13 in [NCM]).

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- Boundary value problems in one variable, such as

$$\begin{aligned} \frac{d^2}{dt^2} y(t) &= -y(t), \quad 0 \le t \le 2\pi \\ y(0) &= 1, \quad y(2\pi) = 0 \end{aligned}$$

MATLAB provides the finite difference solver `bvp4c` for such problems. Other popular methods are shooting methods, or collocation methods such as spectral methods. See MATH 478 for more on this.

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  MATLAB provides the finite difference solver `bvp4c` for such problems. Other popular methods are shooting methods, or collocation methods such as spectral methods. See MATH 478 for more on this.
- Partial differential equations, such as vibration of a string

$$\begin{aligned} \frac{\partial^2}{\partial t^2} u(x,t) &= c^2 \frac{\partial^2}{\partial x^2} u(x,t), \quad 0 \le x \le L,\ 0 \le t \le T \\ u(0,t) &= 0, \quad u(L,t) = 0, \quad 0 \le t \le T \\ u(x,0) &= f(x), \quad \frac{\partial}{\partial t} u(x,0) = g(x), \quad 0 \le x \le L. \end{aligned}$$

  A bit more is discussed in MATH 478 (and then MATH 589). See also Chapter 11 of [NCM].

References I

W. E. Boyce and R. C. DiPrima.
Elementary Differential Equations and Boundary Value Problems.
Wiley, 7th ed., 2001.

C. Moler.
Numerical Computing with MATLAB.
SIAM, Philadelphia, 2004.
Also http://www.mathworks.com/moler/.

D. G. Zill.
A First Course in Differential Equations with Modeling Applications.
Brooks/Cole, 8th ed., 2005.