Solving Differential Equations

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Outline

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1. Initial Value Problem
   - Euler's Method
   - Runge-Kutta Methods
   - Multistep Methods
   - Implicit Methods
   - Hybrid Method
2. Software Packages

Problem setting

Initial Value Problem (first order)

find $y(t)$ such that

$$y' = f(y,t)$$

initial value $y(t_0)$, usually assume $t_0 = 0$

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Generalization 1: system of first order ODEs: y is a vector and f a vector function.

Example

$$\begin{cases} y_1' = f_1(y_1, y_2, t) \\ y_2' = f_2(y_1, y_2, t) \end{cases}$$

or in vector notations:

$$\mathbf{y}' = \mathbf{f}(\mathbf{y}, t)$$

Problem setting (cont.)

Generalization 2: high order equation

$$u'' = g(u, u', t).$$

Let

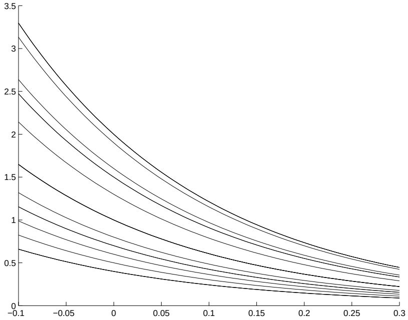
$$\begin{aligned} y_1 &= u \\ y_2 &= u' \end{aligned}$$

and transform the above into the following system of first order ODEs:

$$\begin{cases} y_1' = y_2 \\ y_2' = g(y_1, y_2, t) \end{cases}$$

Solution family

A differential equation has a family of solutions, each corresponds to an initial value.



$y' = -y$, solution family $y = Ce^{-t}$.

Euler's method

We consider the initial value problem:

$$y' = f(y,t), \qquad y(t_0) = y_0$$

Numerical solution: find approximations

$$y_n \approx y(t_n), \qquad \text{for} \quad n = 1, 2, \ldots$$

Note: $y_0 = y(t_0)$ (initial value)

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Note: $y_0 = y(t_0)$ (initial value)

A k-step method: Compute y_{n+1} using $y_n, y_{n-1}, \ldots, y_{n-k+1}$.

Euler's method (cont.)

A single-step method: Euler's method.

$$f(y_0, t_0) = y'(t_0) \approx \frac{y(t_1) - y(t_0)}{h_0},$$

where $h_0 = t_1 - t_0$. The first step:

$$y_1 = y_0 + h_0 f(y_0, t_0)$$

Euler's method (cont.)

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$$y_1 = y_0 + h_0 f(y_0, t_0)$$

Euler's method

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

Produces: $y_0 = y(t_0)$, $y_1 \approx y(t_1)$, $y_2 \approx y(t_2)$, ...

Example

$y' = -y$, $y(0) = 1.0$. (Solution $y = e^{-t}$)

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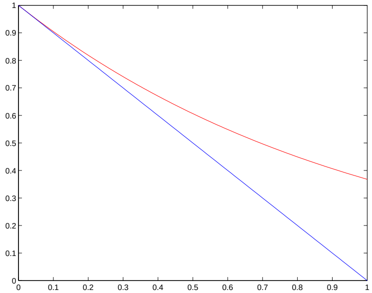
$h = 0.4$

Step 1:

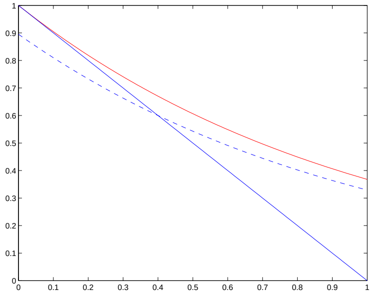
$y_1 = y_0 - hy_0 = 1.0 - 0.4 \times 1.0 = 0.6$
$(\approx y(0.4) = e^{-0.4} \approx 0.6703)$



Example

$u_1(t) = 0.6e^{-t+0.4} \approx 0.8951e^{-t}$ in the solution family.

$u_1' = -u_1$, $u_1(0) \approx 0.8951$ ($u_1(0.4) = 0.6$)



Example

Step 2:

$$y_2 = y_1 - hy_1 = 0.6 - 0.4 \times 0.6 = 0.36$$

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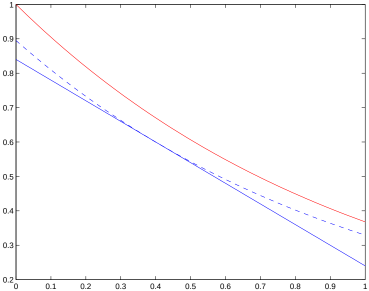
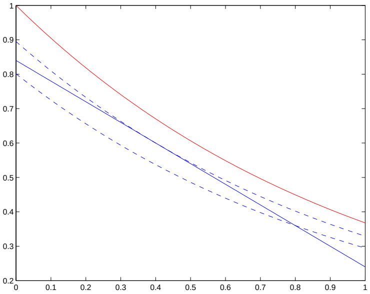


Example

$u_2(t) = 0.36e^{-t+0.8} \approx 0.8012e^{-t}$ in the solution family.

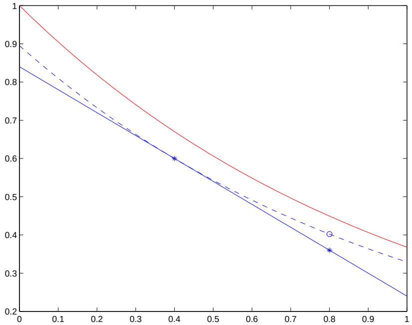
$u_2' = -u_2$, $u_2(0) \approx 0.8012$ ($u_2(0.8) = 0.36$)



Euler's method

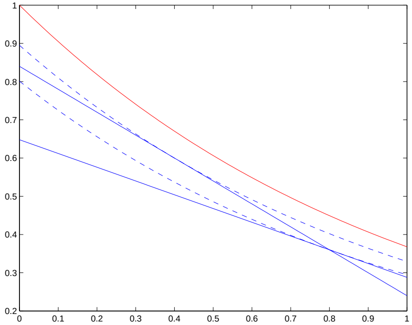
In general

$u_n'(t) = f(u_n(t), t)$, in the solution family
$u_n(t_n) = y_n$, passing (t_n, y_n)
$u_n(t_{n+1}) \approx u_n(t_n) + h_n u_n'(t_n) = y_n + h_n f(u_n(t_n), t_n) =$
$y_n + h_n f(y_n, t_n) = y_{n+1}$



Euler's method

Starting with t_0 and $y_0 = y(t_0)$, as we proceed, we jump from one solution in the family to another.



Errors

Two sources of errors: discretization error and roundoff error.

- *Discretization error*: caused by the method used, independent of the computer used and the program implementing the method.

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- *Discretization error*: caused by the method used, independent of the computer used and the program implementing the method.
- Two types of discretization error:
  - Global error: $e_n = y_n - y(t_n)$
  - Local error: the error in one step

Local error

Consider t_n as the starting point and the approximation y_n at t_n as the initial value , if $u_n(t)$ is the solution of

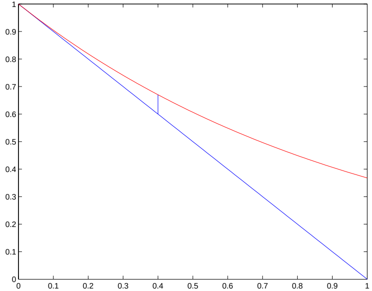
$$u_n' = f(u_n, t), \quad u_n(t_n) = y_n$$

then the local error is

$$d_n = y_{n+1} - u_n(t_{n+1})$$

Example

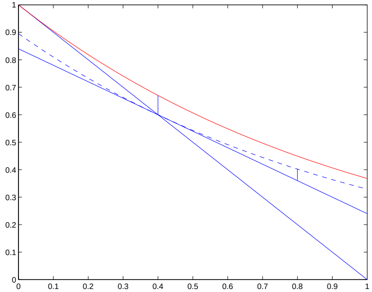
Step 1



Local error $d_0 = y_1 - y(t_1) = 0.6 - e^{-0.4} \approx -0.0703$.
Global error e_1 same as d_0.

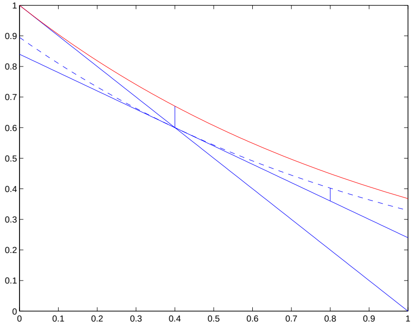
Example

Step 2



Local error $d_1 = y_2 - u_1(t_2) = 0.36 - u_1(0.8) \approx -0.0422.$
Global error $e_2 = y_2 - y(t_2) = 0.36 - e^{-0.8} \approx -0.0893.$

Example



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$$e_2 = y_2 - y(t_2) = 0.36 - e^{-0.8} \approx -0.0893$$

Stability

Relation between global error e_n and local error d_n
If the differential equation is unstable,

$$|e_N| > \sum_{n=0}^{N-1} |d_n|$$

If the differential equation is stable,

$$|e_N| \leq \sum_{n=0}^{N-1} |d_n|$$

In this case, $\sum_{n=0}^{N-1} |d_n|$ is an upper bound for the global error $|e_N|$.

Example

In the previous example:

Local errors $|d_0| = 0.0703$ and $|d_1| = 0.0422$

Global error $|e_2| = 0.0893$

$|e_2| < |d_0| + |d_1|$

Example

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$|e_2| < |d_0| + |d_1|$

More generally,
$y' = \alpha y$, solution family $y = Ce^{\alpha t}$.
Stable when $\alpha < 0$.

Accuracy

A measurement for the accuracy of a method

An order p method:

$$|d_n| \leq C h_n^{p+1} \qquad \text{(or } O(h_n^{p+1})\text{)}$$

C: independent of n and h_n.

Example: Euler's method $y_{n+1} = y_n + h_n f(y_n, t_n)$

Local solution $u_n(t)$

$$u_n'(t) = f(u_n(t), t), \quad u_n(t_n) = y_n$$

Taylor expansion at t_n:

$$u_n(t) = u_n(t_n) + (t - t_n)u'(t_n) + O((t - t_n)^2)$$

Since $y_n = u_n(t_n)$ and $u'(t_n) = f(y_n, t_n)$, we get

$$u_n(t_{n+1}) = y_n + h_n f(y_n, t_n) + O(h_n^2)$$

Local error

$$d_n = y_{n+1} - u_n(t_{n+1}) = O(h_n^2)$$

Euler's method is a first order method ($p = 1$)

Accuracy (cont.)

Consider the interval $[t_0, t_N]$ and partition $t_0, t_1, ..., t_N$. Roughly, the global error

$$|e_N| \approx \sum_{n=0}^{N-1} |d_n| \approx N \cdot O(h^{p+1}) \approx (t_N - t_0) \cdot O(h^p)$$

at the final point t_N is roughly $O(h^p)$ for a method of order p.

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For a pth order method, if the subintervals h_n are cut in half, then the average local error is reduced by a factor of 2^{p+1}, the global error is reduced by a factor of 2^p. (But double the number of steps, i.e., more work.)

Roundoff Error

Each step of the Euler's method

$$y_{n+1} = y_n + h_n f(y_n, t_n) + \epsilon \quad |\epsilon| = O(u).$$

Total rounding error: $N\epsilon = b\,\epsilon/h$ ($b = t_N - t_0$, fixed step size h)

$$\text{total error} \approx b\left(Ch + \frac{\epsilon}{h}\right)$$

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Remarks

- If h is too small, the roundoff error is large
- If h is too large, the discretization error is large

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The total error is minimized by

$$h_{\text{opt}} \approx \sqrt{\frac{u}{C}}$$

recalling that u is the unit of roundoff.

Runge-Kutta methods

Idea: Sample f at several spots to achieve high order.
Cost: More function evaluations

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Example. A second-order Runge-Kutta method
Suppose

$$y_{n+1} = y_n + \gamma_1 k_0 + \gamma_2 k_1$$

where γ_1 and γ_2 to be determined and
$k_0 = h_n f(y_n, t_n)$
$k_1 = h_n f(y_n + \beta k_0, t_n + \alpha h_n)$
α and β to be determined.

Runge-Kutta methods (cont.)

Taylor series (two variables):

$$k_1 = h_n(f_n + \beta k_0 f_y'(y_n, t_n) f_n + \alpha h_n f_t'(y_n, t_n) + \cdots)$$

Thus

$$\begin{aligned} y_{n+1} &= y_n + (\gamma_1 + \gamma_2) h_n f_n + \gamma_2 \beta h_n^2 f_n f_y'(y_n, t_n) \\ &\quad + \gamma_2 \alpha h_n^2 f_t'(y_n, t_n) + \ldots \end{aligned}$$

The Taylor expansion of the true local solution:

$$\begin{aligned} u_n(t_{n+1}) &= u_n(t_n) + h_n u_n'(t_n) + \frac{h_n^2}{2} u_n''(t_n) + \ldots \\ &= y_n + h_n f_n + \frac{h_n^2}{2}(f_y'(y_n, t_n) f_n + f_t'(y_n, t_n)) + \ldots \end{aligned}$$

Second order RK method

Comparing the two expressions, we set

$$\begin{cases} \gamma_1 + \gamma_2 = 1 \\ \gamma_2 \beta = 1/2 \\ \gamma_2 \alpha = 1/2 \end{cases}$$

Then the local error

$$d_n = y_{n+1} - u_n(t_{n+1}) = O(h_n^3)$$

The global error $O(h^2)$

Second order RK method

Let

$$\gamma_1 = 1 - \frac{1}{2\alpha}, \quad \gamma_2 = \frac{1}{2\alpha}, \quad \beta = \alpha$$

Second-order RK method

$$y_{n+1} = y_n + \left(1 - \frac{1}{2\alpha}\right) k_0 + \frac{1}{2\alpha} k_1$$

where

$k_0 = h_n f(y_n, t_n)$

$k_1 = h_n f(y_n + \alpha k_0, t_n + \alpha h_n)$

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where

$k_0 = h_n f(y_n, t_n)$

$k_1 = h_n f(y_n + \alpha k_0, t_n + \alpha h_n)$

When $\alpha = 1/2$, related to the rectangle rule

When $\alpha = 1$, related to the trapezoid rule

Classical fourth-order Runge-Kutta method

$$y_{n+1} = y_n + \frac{1}{6}(k_0 + 2k_1 + 2k_2 + k_3)$$

where

$$k_0 = hf(y_n, t_n)$$
$$k_1 = hf\left(y_n + \tfrac{1}{2}k_0, t_n + \tfrac{h}{2}\right)$$
$$k_2 = hf\left(y_n + \tfrac{1}{2}k_1, t_n + \tfrac{h}{2}\right)$$
$$k_3 = hf(y_n + k_2, t_n + h)$$

Multistep Methods

Compute y_{n+1} using $y_n, y_{n-1}, \ldots$ and $f_n, f_{n-1}, \ldots$ possibly f_{n+1} ($f_i = f(y_i, t_i)$).
General linear k-step method:

$$y_{n+1} = \sum_{i=1}^{k} \alpha_i y_{n-i+1} + h \sum_{i=0}^{k} \beta_i f_{n-i+1}$$

- $\beta_0 = 0$ (no f_{n+1}), explicit method
- $\beta_0 \neq 0$, implicit method

Examples

Adams-Bashforth methods.

$$y_{n+1} = y_n + \int_{t_n}^{t_{n+1}} p_{k-1}(t)dt$$

where $p_{k-1}(t)$ is a polynomial of degree $k-1$ which interpolates $f(y,t)$ at (y_{n-j}, t_{n-j}), $j = 0, ..., k-1$.

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For example.
$p_0(t) = f_n$, Euler's method
$p_1(t) = f_{n-1} + \frac{f_n - f_{n-1}}{h_{n-1}}(t - t_{n-1})$

Adams-Bashforth family

$y_{n+1} = y_n + hf_n$
local error $\frac{h^2}{2} y^{(2)}(\eta)$, order 1
$y_{n+1} = y_n + \frac{h}{2}(3f_n - f_{n-1})$
local error $\frac{5h^3}{12} y^{(3)}(\eta)$, order 2
$y_{n+1} = y_n + \frac{h}{12}(23f_n - 16f_{n-1} + 5f_{n-2})$
local error $\frac{3h^4}{8} y^{(4)}(\eta)$, order 3
$y_{n+1} = y_n + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3})$
local error $\frac{251h^5}{720} y^{(5)}(\eta)$, order 4

Multistep methods (cont.)

The “start-up” issue in multistep methods:

How to get the $k-1$ start values $f_j = f(y_j, t_j)$, $j = 1, \ldots, k-1$?

Multistep methods (cont.)

The “start-up” issue in multistep methods:

How to get the $k-1$ start values $f_j = f(y_j, t_j)$, $j = 1, ..., k-1$?

Use a single step method to get start values, then switch to multistep method.

Multistep methods (cont.)

The “start-up” issue in multistep methods:

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Use a single step method to get start values, then switch to multistep method.

Note. Careful about accuracy consistency.

Exmaple

The motion of two bodies under mutual gravitational attraction.

A coordination system:

origin: position of one body
$x(t)$, $y(t)$: position of the other body

Differential equations derived from Newton's laws of motion:

$$\begin{aligned} x''(t) &= \frac{-\alpha^2 x(t)}{r(t)} \\ y''(t) &= \frac{-\alpha^2 y(t)}{r(t)} \end{aligned}$$

where $r(t) = [x(t)^2 + y(t)^2]^{3/2}$ and α is a constant involving the gravitational constant, the masses of the two bodies, and the units of measurement.

Example

If the initial conditions are chosen as

$$\begin{aligned} x(0) &= 1 - e, & x'(0) &= 0, \\ y(0) &= 0, & y'(0) &= \alpha \left(\frac{1+e}{1-e}\right)^{1/2} \end{aligned}$$

for some e with $0 \leq e < 1$, then the solution is periodic with period $2\pi/\alpha$. The orbit is an ellipse with eccentricity e and with one focus at the origin.

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To write the two second-order differential equations as four first-order differential equations, we introduce

$$y_1 = x, \quad y_2 = y, \quad y_3 = x', \quad y_4 = y'$$

Exmaple

We have a system of first-order euquations

$$s = \frac{(y_1^2 + y_2^2)^{3/2}}{\alpha^2},$$

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}' = \begin{bmatrix} y_3 \\ y_4 \\ -\frac{y_1}{s} \\ -\frac{y_2}{s} \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -1/s & 0 & 0 & 0 \\ 0 & -1/s & 0 & 0 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

with the initial condition

$$\begin{bmatrix} y_1(0) \\ y_2(0) \\ y_3(0) \\ y_4(0) \end{bmatrix} = \begin{bmatrix} 1 - e \\ 0 \\ 0 \\ \alpha \left(\frac{1+e}{1-e} \right)^{1/2} \end{bmatrix}$$

Example

The function defining the system of equations;

```
function yp = orbit(y, t)

global a
global e

yp = zeros(size(y));
r = y(1)*y(1) + y(2)*y(2);
r = r*sqrt(r)/(a*a);
yp(1) = y(3);
yp(2) = y(4);
yp(3) = -y(1)/r;
yp(4) = -y(2)/r;

endfunction
```

Example

A script file `TwoBody.m` (Octave)

```
global a
global e

a = input('a = ');
e = input('e = ');

# initial value
x0 = [1-e; 0.0; 0.0; a*sqrt((1+e)/(1-e))];
# time span
t = [0.0:0.1:(2*pi/a)]';

# solve ode
[x, state, msg] = lsode('orbit', x0, t);
```

Matlab

```
[t, x] = ode45('orbit', [0.0 2*pi/a], x0);
```

Example

Output x: matrix of four columns

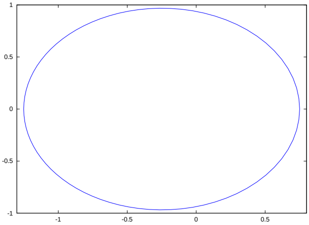
`x(:,1)`: $x(t)$

`x(:,2)`: $y(t)$

`x(:,3)`: $x'(t)$

`x(:,4)`: $y'(t)$

```
plot(x(:,1), x(:,2))
```



$e = 1/4$, $\alpha = \pi/4$

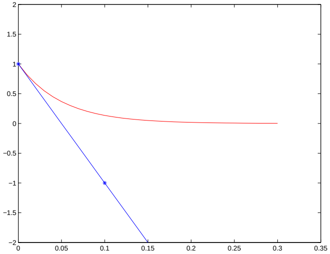
Implicit methods

Example

$y' = -20y$, $y(0) = 1$ (Solution e^{-20t})

Euler's method, $h = 0.1$

$$y_{n+1} = y_n - 20 \times 0.1 y_n = y_n - 2y_n$$



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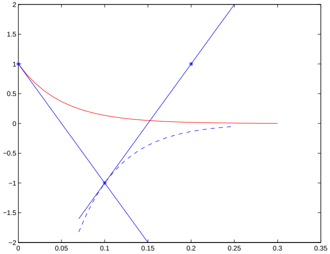


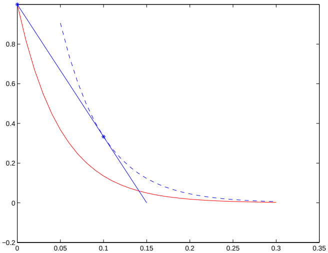
Backward Euler's method

Example

$y' = -20y$, $y(0) = 1$ (Solution y^{-20t})

Backward Euler's method, $h = 0.1$

$$y_{n+1} = y_n - 20 \times 0.1 y_{n+1} = y_n - 2y_{n+1}$$



Backward Euler's method

Taylor expansion of the solution $y(t)$ about $t = t_{n+1}$ (instead of $t = t_n$)

$$\begin{aligned} y(t_{n+1} + h) &\approx y(t_{n+1}) + y'(t_{n+1})h \\ &= y(t_{n+1}) + f(y(t_{n+1}), t_{n+1})h \end{aligned}$$

and set $h = -h_n = (t_n - t_{n+1})$, then we get

$$y(t_n) \approx y(t_{n+1}) - h_n f(y(t_{n+1}), t_{n+1})$$

Backward Euler's method (cont.)

$$y(t_n) \approx y(t_{n+1}) - h_n f(y(t_{n+1}), t_{n+1})$$

Substituting y_n for $y(t_n)$ and y_{n+1} for $y(t_{n+1})$, we have

Backward Euler's method

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

Backward Euler's method (cont.)

$$y(t_n) \approx y(t_{n+1}) - h_n f(y(t_{n+1}), t_{n+1})$$

Substituting y_n for $y(t_n)$ and y_{n+1} for $y(t_{n+1})$, we have

Backward Euler's method

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

Implicit methods tend to be more stable than their explicit counterparts. But there is a price, y_{n+1} is a zero of a usually nonlinear function.

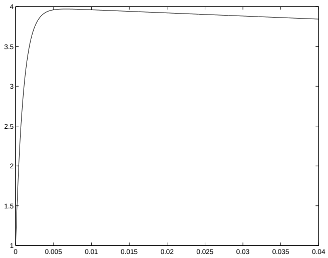
Example

A system of two differential equations.

$$\begin{cases} u' = 998u + 1998v \\ v' = -999u - 1999v \end{cases}$$

If the initial values $u(0) = v(0) = 1$, then the exact solution is

$$\begin{cases} u = 4e^{-t} - 3e^{-1000t} \\ v = -2e^{-t} + 3e^{-1000t} \end{cases}$$



Example (cont.)

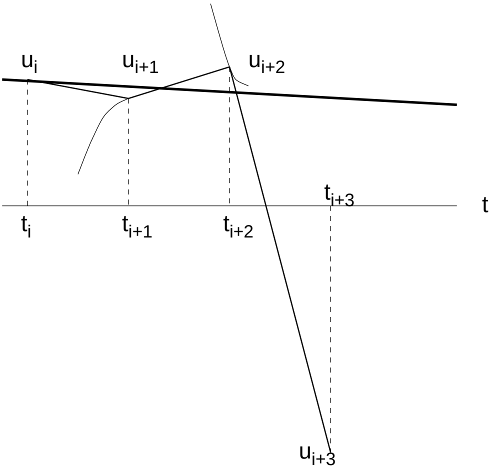
Suppose we use (forward) Euler's method

$$u_{n+1} = u_n + h(998u_n + 1998v_n)$$
$$v_{n+1} = v_n + h(-999u_n - 1999v_n)$$

with $u_0 = v_0 = 1.0$, then we get

```
        h = 0.01         h = 0.001
--------------------------------
  u0       1.0              1.0
  u1     30.96            3.996
  u2    -239.1            3.992
  u3     -9785           -7.988
  u4     52420           -31.92
```

Example (cont.)



Example (cont.)

If we use the backward Euler method

$$u_{n+1} = u_n + h(998u_{n+1} + 1998v_{n+1})$$
$$v_{n+1} = v_n + h(-999u_{n+1} - 1999v_{n+1})$$

Example (cont.)

If we use the backward Euler method

$$\begin{aligned} u_{n+1} &= u_n + h(998u_{n+1} + 1998v_{n+1}) \\ v_{n+1} &= v_n + h(-999u_{n+1} - 1999v_{n+1}) \end{aligned}$$

Solving the linear system

$$\begin{bmatrix} 1-998h & -1998h \\ 999h & 1+1999h \end{bmatrix} \begin{bmatrix} u_{n+1} \\ v_{n+1} \end{bmatrix} = \begin{bmatrix} u_n \\ v_n \end{bmatrix}$$

Example (cont.)

With initial values $u_0 = v_0 = 1.0$,

```
        h = 0.01       h = 0.001
-------------------------------
  u0      1.0             1.0
  u1    3.688           2.496
  u2    3.896           3.242
  u3    3.880           3.613
  u4    3.844           3.797
```

Example (cont.)

For comparison, the solution values

```
       h = 0.01      h = 0.001
-------------------------------
 u(0)     1.0          1.0
 u(1)   3.960        2.892
 u(2)   3.921        3.586
 u(3)   3.882        3.839
 u(4)   3.843        3.929
```

Hybrid methods

One of the difficulties in implicit methods is that they involve solving usually nonlinear systems.

Hybrid methods

One of the difficulties in implicit methods is that they involve solving usually nonlinear systems.
Combining both explicit and implicit:
Use an explicit method for predictor and an implicit method for corrector
Example. Fourth-order Adam's method
Predictor (fourth-order, explicit):

$$y_{n+1} = y_n + \frac{h}{24}(55f_n - 59f_{n-1} + 37f_{n-2} - 9f_{n-3})$$

Corrector (fourth-order, implicit):

$$y_{n+1} = y_n + \frac{h}{24}(9f_{n+1} + 19f_n - 5f_{n-1} + f_{n-2})$$

PECE methods

Algorithm:

1. Prediction: use the predictor to calculate $y_{n+1}^{(0)}$
2. Evaluation: $f_{n+1}^{(0)} = f(y_{n+1}^{(0)}, t_{n+1})$
3. Correction: use the corrector to calculate $y_{n+1}^{(1)}$

Steps 2 and 3 are repeated until $|y_{n+1}^{(i+1)} - y_{n+1}^{(i)}| \leq tol$. Then set $y_{n+1} = y_{n+1}^{(i+1)}$.

PECE methods

Algorithm:

1. Prediction: use the predictor to calculate $y_{n+1}^{(0)}$
2. Evaluation: $f_{n+1}^{(0)} = f(y_{n+1}^{(0)}, t_{n+1})$
3. Correction: use the corrector to calculate $y_{n+1}^{(1)}$

Steps 2 and 3 are repeated until $|y_{n+1}^{(i+1)} - y_{n+1}^{(i)}| \leq tol$. Then set $y_{n+1} = y_{n+1}^{(i+1)}$.

Usually, PECE, one iteration and a final evaluation for the next step.

Outline

Software packages

IMSL	ivprk (RK), ivpag (AB)
MATLAB	ode23, ode45 (RK), ode113 (AB), ode15s, ode23s (stiff), bvp4c (BVP)
NAG	d02baf (RK), d02caf (AB), d02eaf (stiff)
Netlib	dverk (RK), ode (AB), vode, vodpk (sfiff)
Octave	lsode

Summary

- Family of solutions of a differential equation, initial value problem
- Transform a high order ODE into a system of first order ODEs
- Errors: Discretization errors (global, local), stability of a differential equation (mathematical stability), roundoff error, total error
- Accuracy: Order of a method

Summary (cont.)

- Euler's method: Explicit, single step, first order
- Runge-Kutta methods: Explicit, single step
- Multistep methods: Adams-Bashforth family
- Implicit methods: Backward Euler's method
- Prediction-Correction scheme: Combination of explicit and implicit methods

References

[1] George E. Forsyth and Michael A. Malcolm and Cleve B. Moler. Computer Methods for Mathematical Computations. Prentice-Hall, Inc., 1977.
Ch 6.