Forward Time Integration of First-Order Initial-Value Problems

Euler's Method

given first-order initial-value differential equations of the form $\{\dot{y}\} = f(\{y\}, t)$

must know $\{y_i\}$ at time t_i for time step $h = t_{i+1} - t_i$

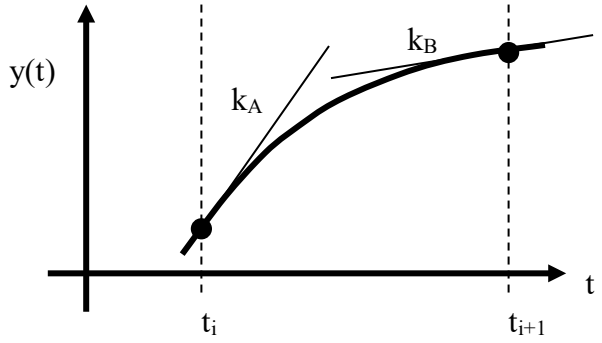
determine the slope at the beginning of the interval $k = f(y_i, t_i)$

$$y_{i+1} = y_i + k\,h$$

Second Order Runge-Kutta

given first-order initial-value differential equations of the form $\{\dot{y}\} = f(\{y\}, t)$

must know $\{y_i\}$ at time t_i for time step $h = t_{i+1} - t_i$



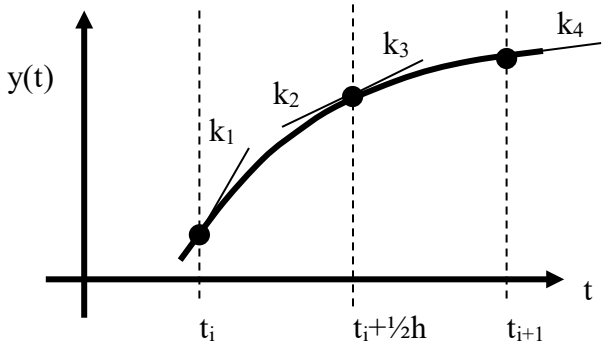
determine the slope at the beginning of the interval $k_A = f(y_i, t_i)$

estimate the slope at the end of the interval using Euler's method $k_B = f(y_i + k_A h,\, t_i + h)$

use the mean of these two slopes $k_M = \frac{1}{2}(k_A + k_B)$

$$y_{i+1} = y_i + k_M h$$

Fourth Order Runge-Kutta (RK4)



determine the slope at the beginning of the interval $k_1 = f(y_i, t_i)$

estimate the slope at the midpoint of the interval using Euler's method $k_2 = f\left(y_i + k_1 \frac{h}{2}, t_i + \frac{h}{2}\right)$

estimate the slope at the midpoint of the interval using the new value $k_3 = f\left(y_i + k_2 \frac{h}{2}, t_i + \frac{h}{2}\right)$

estimate the slope at the end of the interval using the newest value $k_4 = f(y_i + k_3 h, t_i + h)$

use a weighted mean of slopes $k_M = \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$

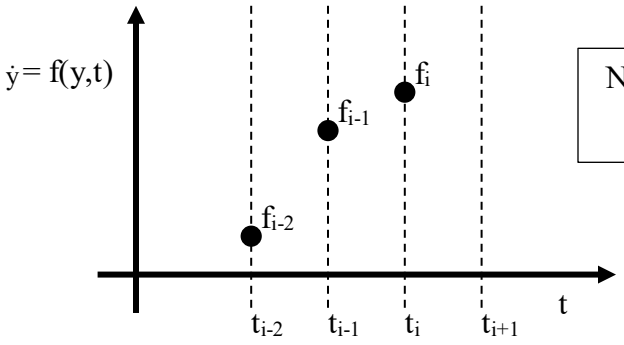
$$y_{i+1} = y_i + k_M h$$

Second-degree (Quadratic) Predictor and Third-degree (Cubic) Corrector

given first-order initial-value differential equations of the form $\{\dot{y}\} = f(\{y\}, t)$

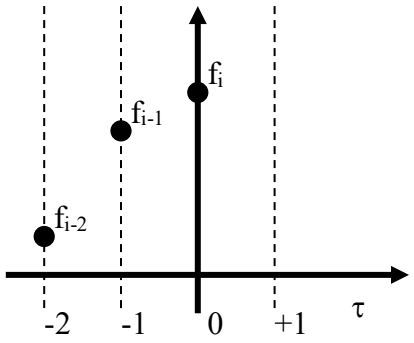
must know $\{y\}_i$, $\{y\}_{i-1}$, $\{y\}_{i-2}$ respectively at times t_i t_{i-1} and t_{i-2}

may determine $f_i = \{\dot{y}\}_i$ $f_{i-1} = \{\dot{y}\}_{i-1}$ $f_{i-2} = \{\dot{y}\}_{i-2}$



Note that the vertical axis is $\dot{y}$ NOT y

for fixed time step h $\tau = (t - t_i) / h$ $d\tau = dt / h$ $dt = h\, d\tau$



use second-degree polynomial predictor $f = a_0 + a_1 \tau + a_2 \tau^2 = \begin{bmatrix} 1 & \tau & \tau^2 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix}$

$$\begin{Bmatrix} f_i \\ f_{i-1} \\ f_{i-2} \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & -1 & 1 \\ 1 & -2 & 4 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} \qquad \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{bmatrix} 2 & 0 & 0 \\ 3 & -4 & 1 \\ 1 & -2 & 1 \end{bmatrix} \begin{Bmatrix} f_i \\ f_{i-1} \\ f_{i-2} \end{Bmatrix} / 2$$

know coefficients a_0, a_1 and a_2 for interpolant $f(\tau) = a_0 + a_1 \tau + a_2 \tau^2 = \dot{y}(\tau)$

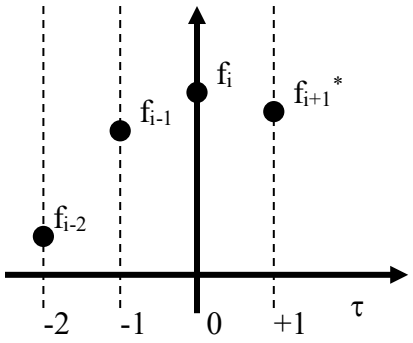
$$y_{i+1} = \int_{ti}^{ti+1} \dot{y}\, dt + y_i = h \int_0^1 f\, d\tau + y_i = h \left(a_0\tau + a_1\tau^2/2 + a_2\tau^3/3 \right)\Big|_0^1 + y_i$$

$$y_{i+1} = y_i + h \left(a_0 + a_1/2 + a_2/3 \right)$$

PREDICTOR (3-step Adams-Bashforth)

$$y_{i+1} = y_i + h\left(23\, f_i - 16\, f_{i-1} + 5\, f_{i-2}\right)/12$$

now use predicted value of y_{i+1} to compute $f(y_{i+1}) = f_{i+1}^*$



use third-degree polynomial <u>corrector</u> $f = b_0 + b_1 \tau + b_2 \tau^2 + b_3 \tau^3 = \begin{bmatrix} 1 & \tau & \tau^2 & \tau^3 \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix}$

$$\begin{Bmatrix} f_{i+1}^* \\ f_i \\ f_{i-1} \\ f_{i-2} \end{Bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 \\ 1 & -2 & 4 & -8 \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix} \qquad \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix} = \begin{bmatrix} 0 & 6 & 0 & 0 \\ 2 & 3 & -6 & 1 \\ 3 & -6 & 3 & 0 \\ 1 & -3 & 3 & -1 \end{bmatrix} \begin{Bmatrix} f_{i+1}^* \\ f_i \\ f_{i-1} \\ f_{i-2} \end{Bmatrix} / 6$$

know coefficients b_0, b_1, b_2 and b_3 for new interpolant $f(\tau) = b_0 + b_1 \tau + b_2 \tau^2 + b_3 \tau^3 = \dot{y}(\tau)$

$$y_{i+1} = \int_{ti}^{ti+1} \dot{y}\, dt + y_i = h \int_0^1 f\, d\tau + y_i = h \left(b_0\tau + b_1\tau^2/2 + b_2\tau^3/3 + b_3\tau^4/4 \right)\Big|_0^1 + y_i$$

$$y_{i+1} = y_i + h \left(b_0 + b_1/2 + b_2/3 + b_3/4 \right)$$

CORRECTOR (4-step Adams-Moulton)

$$y_{i+1} = y_i + h\left(9\, f_{i+1}^* + 19\, f_i - 5\, f_{i-1} + f_{i-2}\right)/24$$

variable time step second-degree polynomial <u>predictor</u> for f $\quad f = a_0 + a_1 (t-t_i) + a_2 (t-t_i)^2$

$$\begin{Bmatrix} f_i \\ f_{i-1} \\ f_{i-2} \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & (t_{i-1}-t_i) & (t_{i-1}-t_i)^2 \\ 1 & (t_{i-2}-t_i) & (t_{i-2}-t_i)^2 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = [A] \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} \qquad \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = [A]^{-1} \begin{Bmatrix} f_i \\ f_{i-1} \\ f_{i-2} \end{Bmatrix}$$

$$y_{i+1} = \int_{ti}^{ti+1} \dot{y}\, dt + y_i$$

PREDICTOR

$$y_{i+1} = y_i + a_0 (t_{i+1}-t_i) + a_1 (t_{i+1}-t_i)^2/2 + a_2 (t_{i+1}-t_i)^3/3$$

use predicted value of y_{i+1} to compute $f(y_{i+1},t) = f_{i+1}^*$

use third-degree polynomial <u>corrector</u> for f $\quad f = b_0 + b_1 (t-t_i) + b_2 (t-t_i)^2 + b_3 (t-t_i)^3$

$$\begin{Bmatrix} f_{i+1}^* \\ f_i \\ f_{i-1} \\ f_{i-2} \end{Bmatrix} = \begin{bmatrix} 1 & (t_{i+1}-t_i) & (t_{i+1}-t_i)^2 & (t_{i+1}-t_i)^3 \\ 1 & 0 & 0 & 0 \\ 1 & (t_{i-1}-t_i) & (t_{i-1}-t_i)^2 & (t_{i-1}-t_i)^3 \\ 1 & (t_{i-2}-t_i) & (t_{i-2}-t_i)^2 & (t_{i-2}-t_i)^3 \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix} = [B] \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix} \qquad \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix} = [B]^{-1} \begin{Bmatrix} f_{i+1}^* \\ f_i \\ f_{i-1} \\ f_{i-2} \end{Bmatrix}$$

CORRECTOR

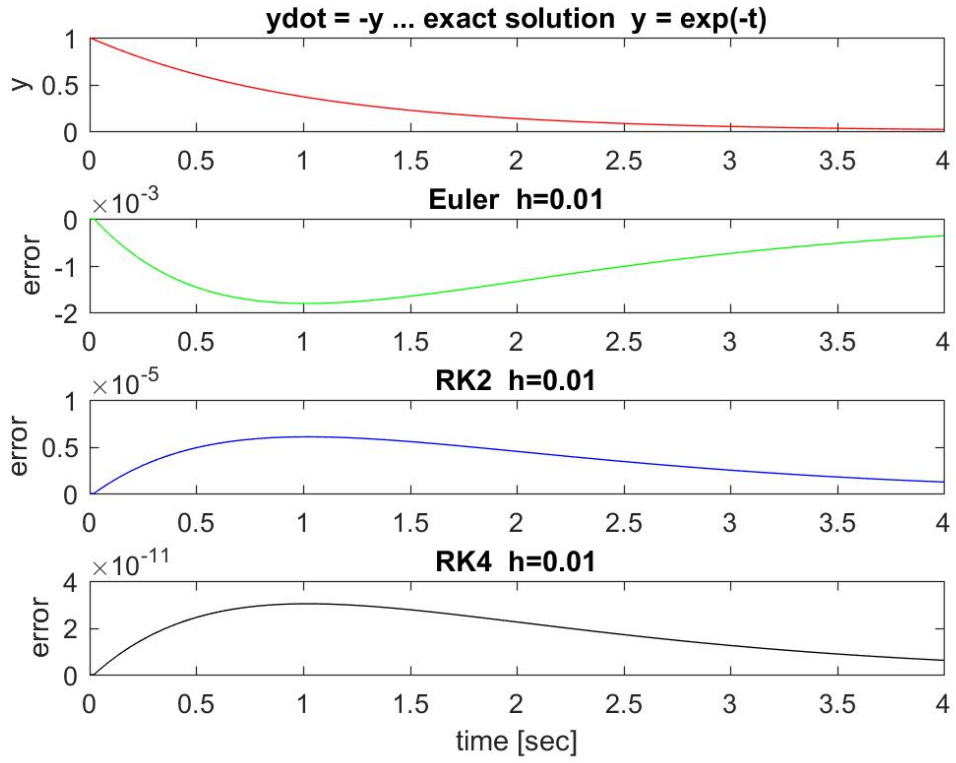
$$y_{i+1} = y_i + b_0 (t_{i+1}-t_i) + b_1 (t_{i+1}-t_i)^2/2 + b_2 (t_{i+1}-t_i)^3/3 + b_3 (t_{i+1}-t_i)^4/4$$

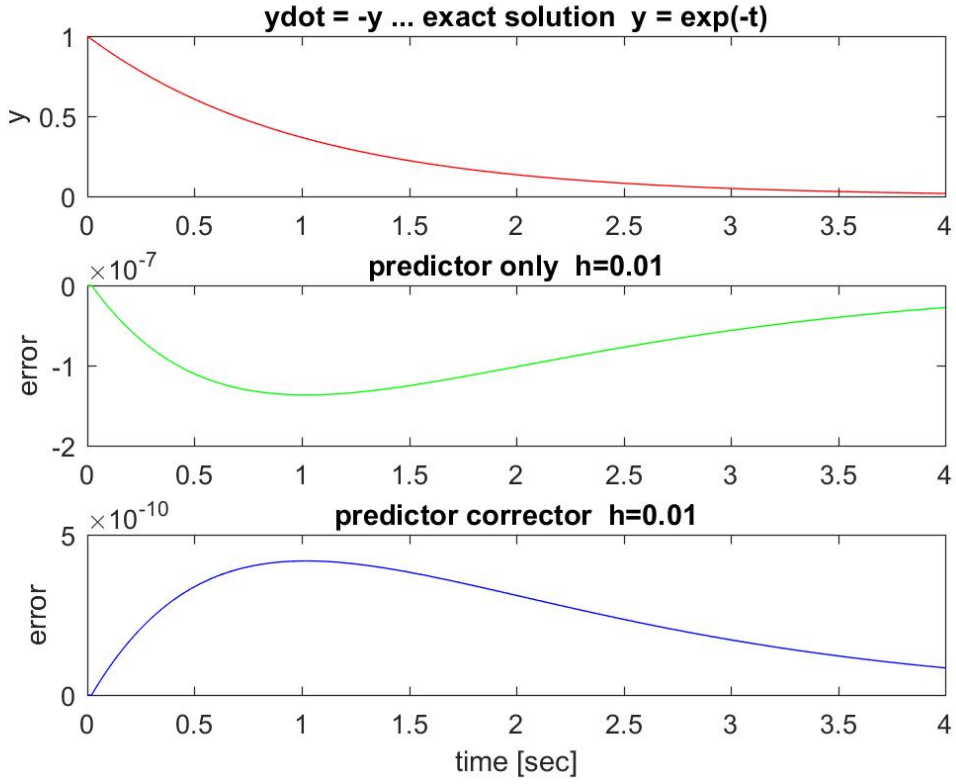
FIXED TIME STEP

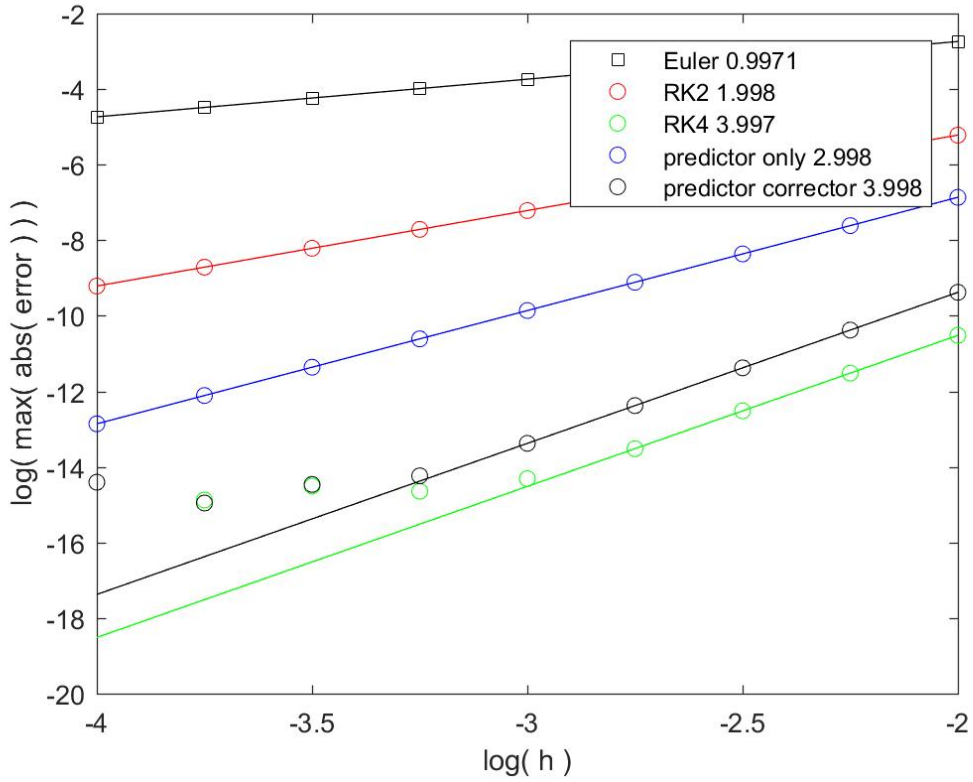
1) Predictor and corrector functions are constant coefficient, weighted sums of f_i.
2) Coefficients are the same for all functions $\{\dot{y}\} = f(\{y\}, t)$.

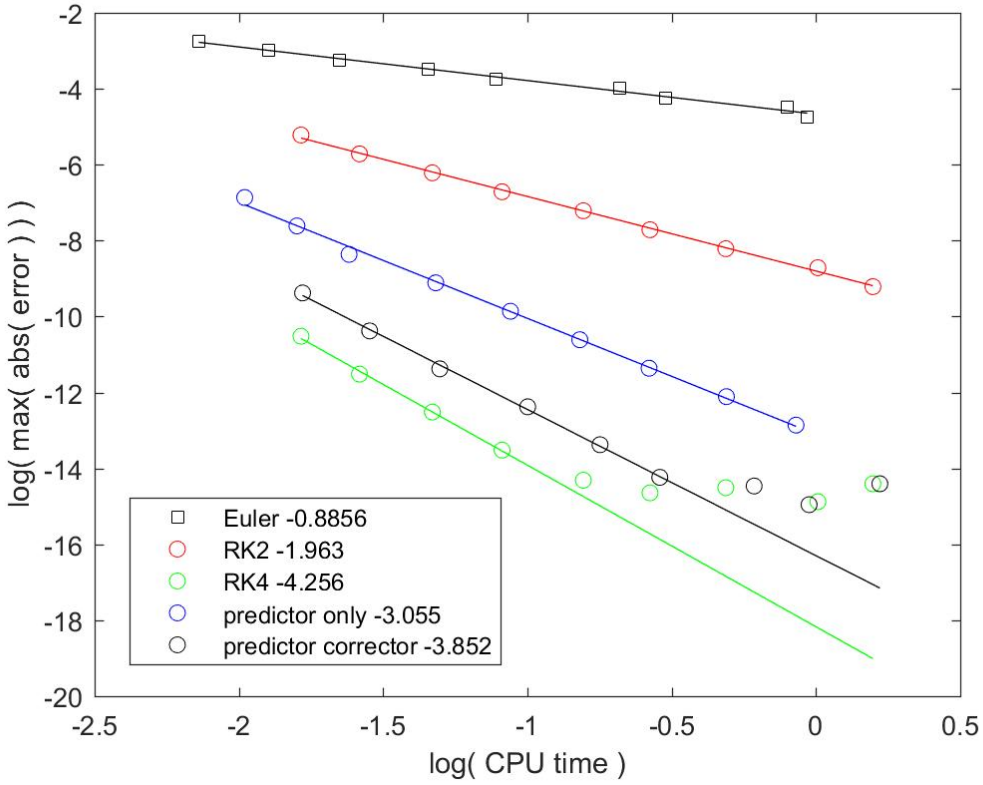
VARIABLE TIME STEP

1) Matrices [A] and [B] must be inverted at each time step.
2) Matrices [A] and [B] are the same for all functions $\{\dot{y}\} = f(\{y\}, t)$.


ydot = -y ... exact solution y = exp(-t)
y
Euler h=0.01
error
RK2 h=0.01
error
RK4 h=0.01
error
time [sec]


ydot = -y ... exact solution y = exp(-t)
y
predictor only h=0.01
error
predictor corrector h=0.01
error
time [sec]


Euler 0.9971
RK2 1.998
RK4 3.997
predictor only 2.998
predictor corrector 3.998
log(max(abs(error)))
log(h)
-2
-4
-6
-8
-10
-12
-14
-16
-18
-20
-4
-3.5
-3
-2.5
-2


Euler -0.8856
RK2 -1.963
RK4 -4.256
predictor only -3.055
predictor corrector -3.852
log(max(abs(error)))
log(CPU time)
-2
-4
-6
-8
-10
-12
-14
-16
-18
-20
-2.5
-2
-1.5
-1
-0.5
0
0.5

```
% comp_int.m - compare integrators
%   time integration using Euler, RK2, RK4, predictor, corrector
%   simulate ydot = -y     exact solution y = exp(-t)
% HJSIII, 21.03.12

clear

% predictor-corrector coefficients
pred_coeff = [ 23  -16   5    ] / 12;
corr_coeff = [  9   19  -5  1 ] / 24;

% time span [sec]
tend = 4;

% time step [sec]
keep_err = [];
keep_cpu = [];
for log10_h = -4 : 0.25 : -2,

% time values
  h = 10 ^ log10_h;
  n = floor( tend / h ) + 1;
  nm1 = n - 1;
  t = h * (0:nm1)';

% exact solution
  y_exact = exp( -t );

% allocate space for solutions
  y_euler     = zeros(n,1);
  y_rk2       = zeros(n,1);
  y_rk4       = zeros(n,1);
  y_pred_only = zeros(n,1);
  f_pred_only = zeros(n,1);
  y_pred_corr = zeros(n,1);
  f_pred_corr = zeros(n,1);

% use exact solution for first three samples to get started
  y_euler          =  y_exact(1:3);
  y_rk2            =  y_exact(1:3);
  y_rk4            =  y_exact(1:3);
  y_pred_only(1:3) =  y_exact(1:3);
  f_pred_only(1:3) = -y_pred_only(1:3);
  y_pred_corr(1:3) =  y_exact(1:3);
  f_pred_corr(1:3) = -y_pred_corr(1:3);

% integrate forward in time

% Euler
  tic;
  for i = 3 : nm1,
    k = -y_euler(i);
    q=inv( rand(18,18) );        % function evaluation
    y_euler(i+1) = y_euler(i) + k * h;
  end
  cpu_euler = toc;

% RK2
  tic;
  for i = 3 : nm1,
    kA = -y_rk2(i);
    q=inv( rand(18,18) );        % function evaluation
    yB = y_rk2(i) + kA * h;
    kB = -yB;
    q=inv( rand(18,18) );        % function evaluation
    kM = (kA + kB) / 2;
```

```
    y_rk2(i+1) = y_rk2(i) + kM * h;
  end
  cpu_rk2 = toc;

% RK4
  tic;
  for i = 3 : nm1,
    k1 = -y_rk4(i);
    q=inv( rand(18,18) );        % function evaluation
    y2 = y_rk4(i) + k1 * h/2;
    k2 = -y2;
    q=inv( rand(18,18) );        % function evaluation
    y3 = y_rk4(i) + k2 * h/2;
    k3 = -y3;
    q=inv( rand(18,18) );        % function evaluation
    y4 = y_rk4(i) + k3 * h;
    k4 = -y4;
    q=inv( rand(18,18) );        % function evaluation
    kM = (k1 + 2*k2 + 2*k3 + k4) / 6;
    y_rk4(i+1) = y_rk4(i) + kM * h;
  end
  cpu_rk4 = toc;

% predictor only
  tic;
  for i = 3 : nm1,
    y_pred_only(i+1) = y_pred_only(i) ...
        + h * pred_coeff * [ f_pred_only(i)  f_pred_only(i-1)  f_pred_only(i-2) ]';
    f_pred_only(i+1) = -y_pred_only(i+1);
    q=inv( rand(18,18) );        % function evaluation
  end
  cpu_pred_only = toc;

% predictor-corrector
  tic;
  for i = 3 : nm1,
    y_star = y_pred_corr(i) ...
        + h * pred_coeff * [ f_pred_corr(i)  f_pred_corr(i-1)  f_pred_corr(i-2) ]';
    f_star = -y_star;
    q=inv( rand(18,18) );        % function evaluation
    y_pred_corr(i+1) = y_pred_corr(i) ...
        + h * corr_coeff * [ f_star  f_pred_corr(i)  f_pred_corr(i-1)  f_pred_corr(i-2) ]';
    f_pred_corr(i+1) = -y_pred_corr(i+1);
    q=inv( rand(18,18) );        % function evaluation
  end
  cpu_pred_corr = toc;

% errors
  err_euler     = y_euler - y_exact;
  err_rk2       = y_rk2 - y_exact;
  err_rk4       = y_rk4 - y_exact;
  err_pred_only = y_pred_only - y_exact;
  err_pred_corr = y_pred_corr - y_exact;


% plot exact solution and errors
  figure( 1 )
    clf
    subplot( 4, 1, 1 )
      plot( t,y_exact,'r' )
      ylabel( 'y' )
      title( 'ydot = -y ... exact solution  y = exp(-t)' )
    subplot( 4, 1, 2 )
      plot( t,err_euler,'g')
      ylabel( 'error' )
      title( [ 'Euler  h=' num2str(h,4) ] )
    subplot( 4, 1, 3 )
      plot( t,err_rk2,'b')
      ylabel( 'error' )
      title( [ 'RK2  h=' num2str(h,4) ] )
    subplot( 4, 1, 4 )
```

```
      plot( t,err_rk4,'k')
      ylabel( 'error' )
      title( [ 'RK4  h=' num2str(h,4) ] )
      xlabel( 'time [sec]' )

  figure( 2 )
    clf
    subplot( 3, 1, 1 )
      plot( t,y_exact,'r' )
      ylabel( 'y' )
      title( 'ydot = -y ... exact solution  y = exp(-t)' )
    subplot( 3, 1, 2 )
      plot( t,err_pred_only,'g')
      ylabel( 'error' )
      title( [ 'predictor only  h=' num2str(h,4) ] )
    subplot( 3, 1, 3 )
      plot( t,err_pred_corr,'b' )
      xlabel( 'time [sec]' )
      ylabel( 'error' )
      title( [ 'predictor corrector  h=' num2str(h,4) ] )

  keep_err = [ keep_err ; [ log10_h  log10(max(abs(err_euler)))  ...
                                     log10(max(abs(err_rk2)))        log10(max(abs(err_rk4)))
...
                                     log10(max(abs(err_pred_only)))
log10(max(abs(err_pred_corr)))  ]  ];

  keep_cpu = [ keep_cpu ; [ log10_h  log10(cpu_euler)      log10(cpu_rk2)        log10(cpu_rk2)
...
                                     log10(cpu_pred_only)  log10(cpu_pred_corr)  ]  ];

end  % bottom - for log10_h

h =   keep_err(:,1);
eeu = keep_err(:,2);
er2 = keep_err(:,3);
er4 = keep_err(:,4);
epo = keep_err(:,5);
epc = keep_err(:,6);

ceu = keep_cpu(:,2);
cr2 = keep_cpu(:,3);
cr4 = keep_cpu(:,4);
cpo = keep_cpu(:,5);
cpc = keep_cpu(:,6);

% slopes for error
poly_eeu  = polyfit( h, eeu, 1 );
fit_eeu = polyval( poly_eeu, h );

poly_er2  = polyfit( h, er2, 1 );
fit_er2 = polyval( poly_er2, h );

poly_er4  = polyfit( h(6:end), er4(6:end), 1 );
fit_er4 = polyval( poly_er4, h );

poly_epo  = polyfit( h, epo, 1 );
fit_epo = polyval( poly_epo, h );

poly_epc = polyfit( h(6:end), epc(6:end), 1 );  % ignore noise floor
fit_epc = polyval( poly_epc, h );

% plot error
figure( 3 )
  clf
  plot( h,eeu,'ks',    h,er2,'ro',    h,er4,'go',    h,epo,'bo',    h,epc,'ko',  ...
        h,fit_eeu,'k', h,fit_er2,'r', h,fit_er4,'g', h,fit_epo,'b', h,fit_epc,'k' )
  xlabel( 'log( h )' )
  ylabel( 'log( max( abs( error ) ) )' )
  legend( [ 'Euler '               num2str(poly_eeu(1),4) ], ...
          [ 'RK2 '                 num2str(poly_er2(1),4) ], ...
```

```
          [ 'RK4 '                  num2str(poly_er4(1),4) ], ...
          [ 'predictor only '       num2str(poly_epo(1),4) ], ...
          [ 'predictor corrector '  num2str(poly_epc(1),4) ] )

% slopes for CPU time
poly_ceu  = polyfit( ceu, eeu, 1 );
fit_ceu = polyval( poly_ceu, ceu );

poly_cr2  = polyfit( cr2, er2, 1 );
fit_cr2 = polyval( poly_cr2, cr2 );

poly_cr4  = polyfit( cr4(6:end), er4(6:end), 1 );
fit_cr4 = polyval( poly_cr4, cr4 );

poly_cpo  = polyfit( cpo, epo, 1 );
fit_cpo = polyval( poly_cpo, cpo );

poly_cpc = polyfit( cpc(6:end), epc(6:end), 1 );  % ignore noise floor
fit_cpc = polyval( poly_cpc, cpc );

% plot CPU time
figure( 4 )
  clf
  plot( ceu,eeu,'ks',    cr2,er2,'ro',    cr4,er4,'go',    cpo,epo,'bo',    cpc,epc,'ko',  ...
        ceu,fit_ceu,'k', cr2,fit_cr2,'r', cr4,fit_cr4,'g', cpo,fit_cpo,'b', cpc,fit_cpc,'k' )
  xlabel( 'log( CPU time )' )
  ylabel( 'log( max( abs( error ) ) )' )
  legend( [ 'Euler '                  num2str(poly_ceu(1),4) ], ...
          [ 'RK2 '                    num2str(poly_cr2(1),4) ], ...
          [ 'RK4 '                    num2str(poly_cr4(1),4) ], ...
          [ 'predictor only '         num2str(poly_cpo(1),4) ], ...
          [ 'predictor corrector '    num2str(poly_cpc(1),4) ] )

% bottom of comp_int
```

Forward Time Integration in MATLAB

```
[T,Y] = solver(odefun,tspan,y0)
[T,Y] = solver(odefun,tspan,y0,options)
```

`odefun` A function handle that evaluates the right side of the differential equations. All solvers solve systems of equations in the form $y' = f(t,y)$ or problems that involve a mass matrix, $M(t,y)y' = f(t,y)$. The `ode23s` solver can solve only equations with constant mass matrices. `ode15s` and `ode23t` can solve problems with a mass matrix that is singular, i.e., differential-algebraic equations (DAEs).

`tspan` A vector specifying the interval of integration, `[t0,tf]`. The solver imposes the initial conditions at `tspan(1)`, and integrates from `tspan(1)` to `tspan(end)`. To obtain solutions at specific times (all increasing or all decreasing), use `tspan = [t0,t1,...,tf]`.

For `tspan` vectors with two elements `[t0 tf]`, the solver returns the solution evaluated at every integration step. For `tspan` vectors with more than two elements, the solver returns solutions evaluated at the given time points. The time values must be in order, either increasing or decreasing.

Specifying `tspan` with more than two elements does not affect the internal time steps that the solver uses to traverse the interval from `tspan(1)` to `tspan(end)`. All solvers in the ODE suite obtain output values by means of continuous extensions of the basic formulas. Although a solver does not necessarily step precisely to a time point specified in `tspan`, the solutions produced at the specified time points are of the same order of accuracy as the solutions computed at the internal time points.

Specifying `tspan` with more than two elements has little effect on the efficiency of computation, but for large systems, affects memory management.

`y0` A vector of initial conditions.

`options` Structure of optional parameters that change the default integration properties. This is the fourth input argument.

Solver	Problem Type	Order of Accuracy	When to Use
`ode45`	Nonstiff	Medium	Most of the time. This should be the first solver you try.
`ode23`	Nonstiff	Low	For problems with crude error tolerances or for solving moderately stiff problems.
`ode113`	Nonstiff	Low to high	For problems with stringent error tolerances or for solving computationally intensive problems.
`ode15s`	Stiff	Low to medium	If `ode45` is slow because the problem is stiff.
`ode23s`	Stiff	Low	If using crude error tolerances to solve stiff systems and the mass matrix is constant.
`ode23t`	Moderately Stiff	Low	For moderately stiff problems if you need a solution without numerical damping.
`ode23tb`	Stiff	Low	If using crude error tolerances to solve stiff systems.

MATLAB Algortihms

`ode45` is based on an explicit Runge-Kutta (4,5) formula, the Dormand-Prince pair. It is a *one-step* solver – in computing `y(tn)`, it needs only the solution at the immediately preceding time point, `y(tn-1)`. In general, `ode45` is the best function to apply as a *first try* for most problems. [3]

`ode23` is an implementation of an explicit Runge-Kutta (2,3) pair of Bogacki and Shampine. It may be more efficient than `ode45` at crude tolerances and in the presence of moderate stiffness. Like `ode45`, `ode23` is a one-step solver. [2]

`ode113` is a variable order Adams-Bashforth-Moulton PECE solver. It may be more efficient than `ode45` at stringent tolerances and when the ODE file function is particularly expensive to evaluate. `ode113` is a *multistep* solver — it normally needs the solutions at several preceding time points to compute the current solution. [7]

The above algorithms are intended to solve nonstiff systems. If they appear to be unduly slow, try using one of the stiff solvers below.

`ode15s` is a variable order solver based on the numerical differentiation formulas (NDFs). Optionally, it uses the backward differentiation formulas (BDFs, also known as Gear's method) that are usually less efficient. Like `ode113`, `ode15s` is a multistep solver. Try `ode15s` when `ode45` fails, or is very inefficient, and you suspect that the problem is stiff, or when solving a differential-algebraic problem. [9], [10]

`ode23s` is based on a modified Rosenbrock formula of order 2. Because it is a one-step solver, it may be more efficient than `ode15s` at crude tolerances. It can solve some kinds of stiff problems for which `ode15s` is not effective. [9]

`ode23t` is an implementation of the trapezoidal rule using a "free" interpolant. Use this solver if the problem is only moderately stiff and you need a solution without numerical damping. `ode23t` can solve DAEs. [10]

`ode23tb` is an implementation of TR-BDF2, an implicit Runge-Kutta formula with a first stage that is a trapezoidal rule step and a second stage that is a backward differentiation formula of order two. By construction, the same iteration matrix is used in evaluating both stages. Like `ode23s`, this solver may be more efficient than `ode15s` at crude tolerances. [8], [1]

References

[1] Bank, R. E., W. C. Coughran, Jr., W. Fichtner, E. Grosse, D. Rose, and R.Smith, "Transient Simulation of Silicon Devices and Circuits," *IEEE Trans. CAD*, 4 (1985), pp. 436–451.

[2] Bogacki, P. and L. F. Shampine, "A 3(2) pair of Runge-Kutta formulas," *Appl. Math. Letters*, Vol. 2, 1989, pp. 321–325.

[3] Dormand, J. R. and P. J. Prince, "A family of embedded Runge-Kutta formulae," *J. Comp. Appl. Math.*, Vol. 6, 1980, pp. 19–26.

[4] Forsythe, G. , M. Malcolm, and C. Moler, *Computer Methods for Mathematical Computations*, Prentice-Hall, New Jersey, 1977.

[5] Kahaner, D. , C. Moler, and S. Nash, *Numerical Methods and Software*, Prentice-Hall, New Jersey, 1989.

[6] Shampine, L. F. , *Numerical Solution of Ordinary Differential Equations*, Chapman & Hall, New York, 1994.

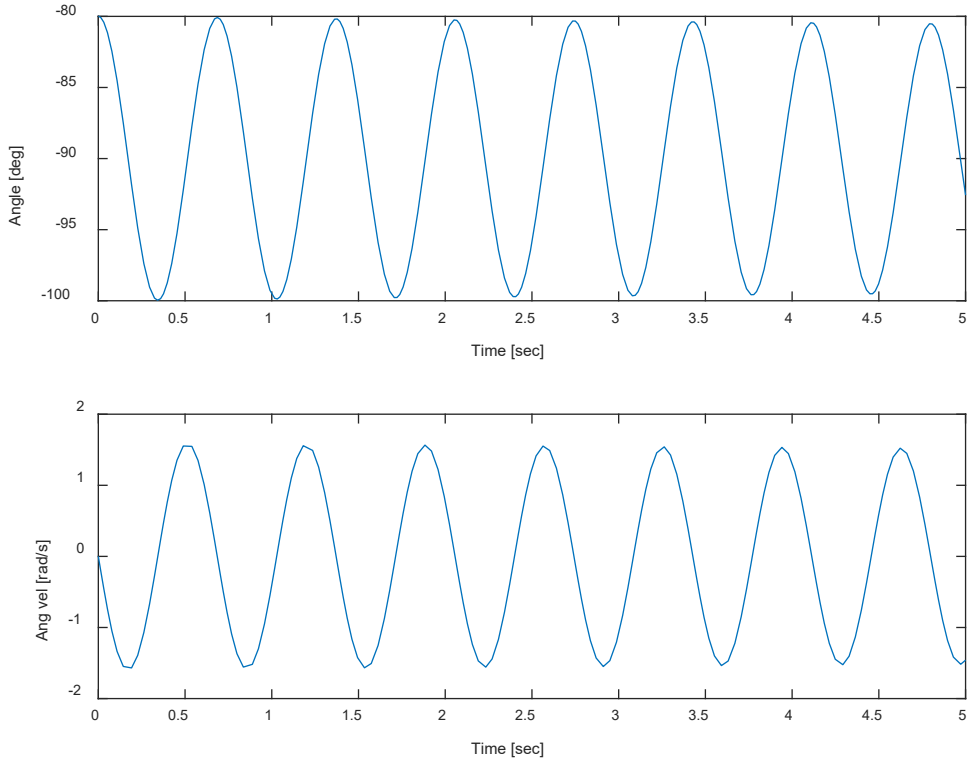
[7] Shampine, L. F. and M. K. Gordon, *Computer Solution of Ordinary Differential Equations: the Initial Value Problem*, W. H. Freeman, SanFrancisco, 1975.

[8] Shampine, L. F. and M. E. Hosea, "Analysis and Implementation of TR-BDF2," *Applied Numerical Mathematics 20*, 1996.

[9] Shampine, L. F. and M. W. Reichelt, "The MATLAB ODE Suite," *SIAM Journal on Scientific Computing,* Vol. 18, 1997, pp. 1–22.

[10] Shampine, L. F., M. W. Reichelt, and J.A. Kierzenka, "Solving Index-1 DAEs in MATLAB and Simulink," *SIAM Review*, Vol. 41, 1999, pp. 538–552.

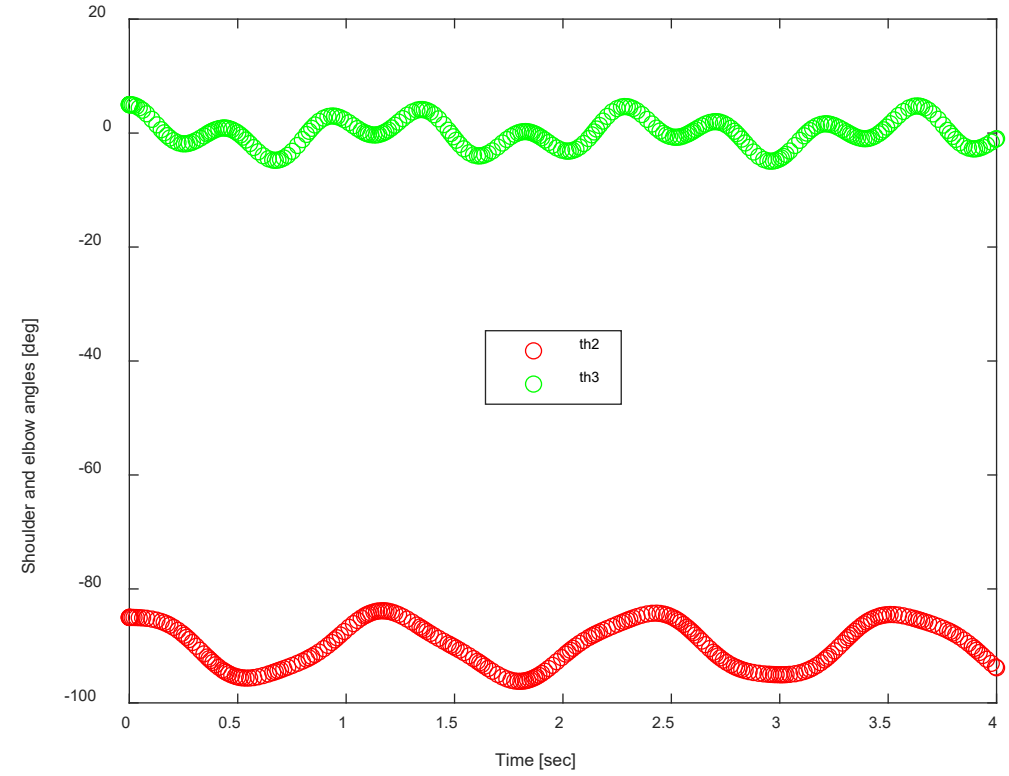
Simple pendulum from Notes_09_02

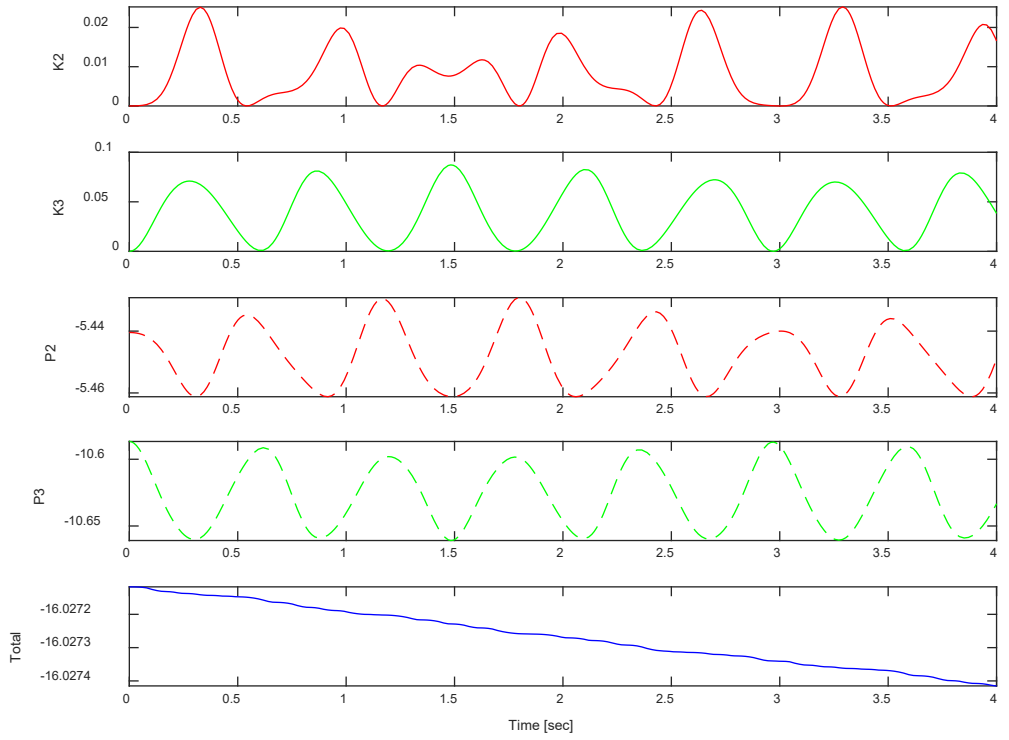



```
% ode_pendulum_main.m - main program for example use of ODE solver
%   simple pendulum Notes_09_02
% HJSIII, 20.04.09
%
% ODE coded in file ode_pendulum_yd.m  - (JG+m*a*a)*thdd = T - m*g*a*cos(th)
%
% {y} = { th  }          {yd} = { thd  }
%       { thd }                 { thdd }

clear

% global constants
global  m  JG  a  g

% constants
d2r = pi / 180;

% physical constants
% th [rad]
% thd [rad/sec]
% thdd [rad/sec^2]
m = 0.46;       % mass [lbm]
JG = 1.5;       % mass moment [lbm.in.in]
a = 3.7;        % centroid offset [in]
g = 386;        % acceleration of gravity [ipss]

% initial conditions
th0 = -80 * d2r;      % 10 degrees above vertical
y0 = [ th0  0  ]';    % free release

% time range
tspan = [ 0  5 ];
```

```
% ode23
[ t, y ] = ode23( 'ode_pendulum_yd', tspan, y0 );
th = y(:,1) / d2r;   % [deg]
thd = y(:,2);        % [rad/s]

% time domain results
figure( 1 )
  clf
  subplot( 2, 1, 1 )
    plot( t,th )
    xlabel( 'Time [sec]' )
    ylabel( 'Angle [deg]' )
%    axis( [ 0 5  -0.1 0.1 ] )

  subplot( 2, 1, 2 )
    plot( t,thd )
    xlabel( 'Time [sec]' )
    ylabel( 'Ang vel [rad/s]' )
%    axis( [ 0 5  -1.5 1.5 ] )

% bottom - ode_pendulum_main


************************************************************
function yd = ode_pendulum_yd( t, y )
% provides yd for integration
% simple pendulum Notes_09_02
%    (JG+m*a*a)*thdd = T - m*g*a*cos(th)
% HJSIII, 20.04.09

% global constants
global  m  JG  a  g

% free motion
T = 0;

% individual terms
th = y(1);
thd = y(2);

% free swing
thdd = ( T - m*g*a*cos(th) ) / (JG + m*a*a);

% simple Coulomb friction in revolute joint with bushing
mu = 0.1;              % coefficient of friction
radius = 0.25;         % [inch] radius for ID of bushing
W = m*g;               % [lbm.in/s/s] weight of pendulum
Tf = mu * radius * W;  % [lbf.in] frictional torque
%thdd = ( T -Tf*sign( thd ) -m*g*a*cos(th) ) / (JG + m*a*a);

yd(1,1) = thd;
yd(2,1) = thdd;

return
% bottom - ode_pendulum_yd
```

Double pendulum from Notes_09_02





```
% ode_dp_main.m - main program for example use of ODE solver
%   double pendulum Notes_09_02
% HJSIII, 20.04.09
%
% ODE coded in file ode_dp_yd.m
%
% {y} = { theta2     }      {ydot} = { theta2_dot     }
%       { theta3     }             = ( theta3_dot     }
%       { theta2_dot }             = ( theta2_dot_dot }
%       ( theta3_dot }             = ( theta3_dot_dot }

clear

% constants
d2r = pi /180;

% initial conditions - shoulder 5 deg above vertical, elbow 5 deg up
% th2=0 shoulder horizontal, th3=0 elbow straight
theta2_start = -85 * d2r;
theta3_start = 5 * d2r;

% free release
y0 = [  theta2_start   theta3_start   0   0  ]';

% time range
tspan = [ 0  4 ];

% time integration
[ t, y ] = ode23( 'ode_dp_yd', tspan, y0 );

% time domain results
th2 = y(:,1);
th3 = y(:,2);
th2d = y(:,3);
th3d = y(:,4);
figure( 1 )
  clf
  plot( t,th2/d2r,'ro',  t,th3/d2r,'go' )
  xlabel( 'Time [sec]' )
  ylabel( 'Shoulder and elbow angles [deg]' )
  legend( 'th2', 'th3' )

% check kinetic and potential energy

% units = m  kg  sec  m/sec  m/sec/sec  N  N.m
gravity = 9.81;  % [m/sec/sec]

% approximate human arm
d2 = 0.293;      % [m] upper arm
d3 = 0.225;      % [m] forearm

m2 = 3.80;       % [kg] upper arm
m3 = 2.68;       % [kg] forearm

J2 = 33300e-6;  % [kg.m.m] upper arm
J3 =  9900e-6;  % [kg.m.m] forearm

% symmetric links
a2 = d2 / 2;
a3 = d3 / 2;

% positions and velocities
x2 = a2*cos(th2);
y2 = a2*sin(th2);

x2d = -a2*th2d.*sin(th2);
y2d =  a2*th2d.*cos(th2);

x3 = d2*cos(th2) + a3*cos(th2+th3);
y3 = d2*sin(th2) + a3*sin(th2+th3);
```

```
x3d = -d2*th2d.*sin(th2) - a3*(th2d+th3d).*sin(th2+th3);
y3d =  d2*th2d.*cos(th2) + a3*(th2d+th3d).*cos(th2+th3);

% kinetic
K2 = m2*( x2d.*x2d + y2d.*y2d )/2 + J2*th2d.*th2d/2;
K3 = m3*( x3d.*x3d + y3d.*y3d )/2 + J3*(th2d+th3d).*(th2d+th3d)/2;

% potential
P2 = m2*y2*gravity;
P3 = m3*y3*gravity;

% show total energy
TE = K2 + K3 + P2 + P3;
figure( 2 )
  clf
  subplot( 5,1,1 )
  plot( t,K2,'r-' )
  ylabel( 'K2' )

  subplot( 5,1,2 )
  plot( t,K3,'g-' )
  ylabel( 'K3' )

  subplot( 5,1,3 )
  plot( t,P2,'r--' )
  ylabel( 'P2' )

  subplot( 5,1,4 )
  plot( t,P3,'g--' )
  ylabel( 'P3' )

  subplot( 5,1,5 )
  plot( t,TE,'b' )
  xlabel( 'Time [sec]' )
  ylabel( 'Total' )

% bottom - ode_dp_main

************************************************************
function ydot = ode_dp_yd( t, y )
% provides yd for integration
% double pendulum Notes_09_02
% HJSIII, 20.04.09

% units = m  kg  sec  m/sec  m/sec/sec  N  N.m
gravity = 9.81;  % [m/sec/sec]

% approximate human arm
d2 = 0.293;      % [m] upper arm
d3 = 0.225;      % [m] forearm

m2 = 3.80;       % [kg] upper arm
m3 = 2.68;       % [kg] forearm

J2 = 33300e-6;  % [kg.m.m] upper arm
J3 =  9900e-6;  % [kg.m.m] forearm

% symmetric links
a2 = d2 / 2;
a3 = d3 / 2;

% extract state variables
th2 =  y(1);
th3 =  y(2);
th2d = y(3);
th3d = y(4);

% coefficients
JB = m3*a3*a3 + J3;
JA = JB + m2*a2*a2 + m3*d2*d2 + J2 + 2*m3*d2*a3*cos(th3);
```

```
C = JB + m3*d2*a3*cos(th3);
D = m3*d2*a3*sin(th3);

G2 = (m2*a2+m3*d2) * gravity * cos(th2);
G3 = m3*a3 * gravity * cos(th2+th3);

% motor torques
T2 = 0;
T3 = 0;

% test
M = [ JA  C  ;
      C   JB ];
rhs = [ T2+D*th3d*th3d+2*D*th2d*th3d-G2-G3 ;
        T3-D*th2d*th2d-G3 ];
thdd = inv(M) * rhs;

% return derivatives of state derivatives
ydot =  [  th2d   th3d   thdd(1)   thdd(2)  ]';

return
% bottom - ode_dp_yd
```

Second-Order Initial-Value Problems

Taylor Series Using Second Derivatives

given second-order initial-value differential equations of the form
$\{\dot{y}\} = f(\{y\}, t)$ and $\{\ddot{y}\} = g(\{y\}, \{\dot{y}\}, t)$

must know y_i at time t_i

may determine $\dot{y}_i = f_i$ and $\ddot{y}_i = g_i$

for time step $h = t_{i+1} - t_i$

$$y_{i+1} = y_i + f_i\, h + \tfrac{1}{2} g_i h^2$$

Fourth Order Runge-Kutta-Nystrom Using Second Derivatives (Fehlberg)

given second-order initial-value differential equations of the form
$\{\dot{y}\} = f(\{y\}, t)$ and $\{\ddot{y}\} = g(\{y\}, \{\dot{y}\}, t)$

must know y_i at time t_i

may determine $\dot{y}_i = f_i$ and $\ddot{y}_i = g_i$

$$k_1 = g(y_i, t_i)$$

$$k_2 = g\left(y_i + \tfrac{1}{3} h f_i + \tfrac{1}{18} h^2 k_1, t_i + \tfrac{1}{3} h\right)$$

$$k_3 = g\left(y_i + \tfrac{2}{3} h f_i + \tfrac{2}{9} h^2 k_2, t_i + \tfrac{2}{3} h\right)$$

$$k_4 = g\left(y_i + h f_i + \tfrac{1}{6} h^2 (2k_1 + k_3), t_i + h\right)$$

$$y_{i+1} = y_i + h f_i + \tfrac{1}{120} h^2 \left(13 k_1 + 36 k_2 + 9 k_3 + 2 k_4\right)$$

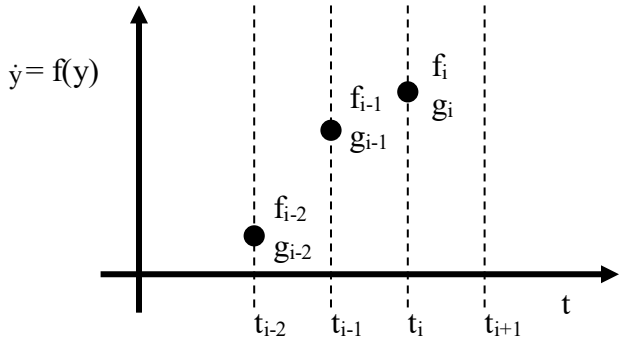
Fifth-degree (Quintic) Predictor and Seventh-degree (Heptic) Corrector with Second Derivatives

given second-order initial-value differential equations of the form

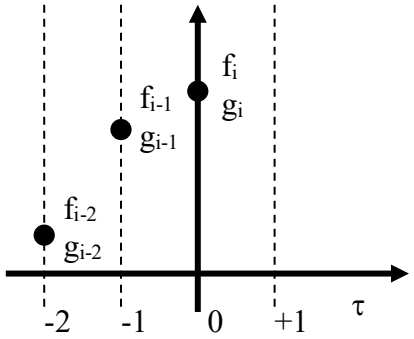
$$\{\dot{y}\} = f(\{y\}, t) \text{ and } \{\ddot{y}\} = g(\{y\}, \{\dot{y}\}, t)$$

must know $\{y\}_i, \{y\}_{i-1}, \{y\}_{i-2}$ respectively at times t_i, t_{i-1} and t_{i-2}

may determine $\{\dot{y}\}_i, \{\dot{y}\}_{i-1}, \{\dot{y}\}_{i-2}$ and $\{\ddot{y}\}_i, \{\ddot{y}\}_{i-1}, \{\ddot{y}\}_{i-2}$



fixed time step h $\quad \tau = (t - t_i) / h \quad d\tau = dt / h \quad dt = h\, d\tau \quad d\tau / dt = 1 / h$



use fifth degree polynomial <u>predictor</u> $\quad f = a_0 + a_1\tau + a_2\tau^2 + a_3\tau^3 + a_4\tau^4 + a_5\tau^5$

$$g = \frac{df}{dt} = \frac{\partial f}{\partial \tau}\frac{d\tau}{dt} \qquad g\,h = \frac{\partial f}{\partial \tau} \qquad g\,h = a_1 + 2a_2\tau + 3a_3\tau^2 + 4a_4\tau^3 + 5a_5\tau^4$$

$$\begin{Bmatrix} f \\ g\ h \end{Bmatrix} = \begin{bmatrix} 1 & \tau & \tau^2 & \tau^3 & \tau^4 & \tau^5 \\ 0 & 1 & 2\tau & 3\tau^2 & 4\tau^3 & 5\tau^4 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{Bmatrix}$$

$$\begin{Bmatrix} f_i \\ f_{i-1} \\ f_{i-2} \\ g_i\ h \\ g_{i-1}\ h \\ g_{i-2}\ h \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -2 & 4 & -8 & 16 & -32 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 3 & -4 & 5 \\ 0 & 1 & -4 & 12 & -32 & 80 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{Bmatrix}$$

$$\begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{Bmatrix} = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 & 0 \\ -23 & 16 & 7 & 12 & 16 & 2 \\ -33 & 16 & 17 & 13 & 32 & 5 \\ -17 & 4 & 13 & 6 & 20 & 4 \\ -3 & 0 & 3 & 1 & 4 & 1 \end{bmatrix} \begin{Bmatrix} f_i \\ f_{i-1} \\ f_{i-2} \\ g_i\ h \\ g_{i-1}\ h \\ g_{i-2}\ h \end{Bmatrix} / 4$$

know coefficients a_i for interpolant $\quad f(\tau) = a_0 + a_1\tau + a_2\tau^2 + a_3\tau^3 + a_4\tau^4 + a_5\tau^5 = \dot{y}(\tau)$

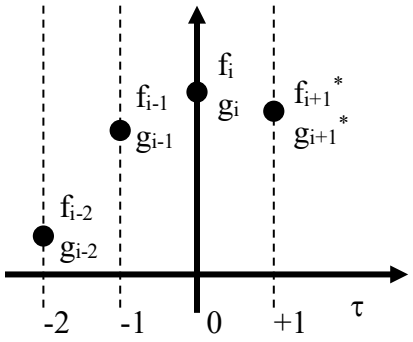
$$y_{i+1} = \int_{ti}^{ti+1} \dot{y}\, dt + y_i = h \int_0^1 f\, d\tau + y_i = y_i + h\left(a_0\tau + a_1\tau^2/2 + a_2\tau^3/3 + a_3\tau^4/4 + a_4\tau^5/5 + a_5\tau^6/6\right)\Big|_0^1$$

$$y_{i+1} = y_i + h\left(a_0 + a_1/2 + a_2/3 + a_3/4 + a_4/5 + a_5/6\right)$$

PREDICTOR (3-step Obreshkov)

$$y^*_{i+1} = y_i + h\left(-949\, f_i + 608\, f_{i-1} + 581\, f_{i-2} + h\left(637\, g_i + 1080\, g_{i-1} + 173\, g_{i-2}\right)\right)/240$$

now use predicted value of y^*_{i+1} to compute $f\left(y^*_{i+1}\right) = f^*_{i+1}$ and $g\left(y^*_{i+1}\right) = g^*_{i+1}$



use seventh degree polynomial corrector

$$f(\tau) = b_0 + b_1\tau + b_2\tau^2 + b_3\tau^3 + b_4\tau^4 + b_5\tau^5 + b_6\tau^6 + b_7\tau^7 = \dot{y}(\tau)$$

$$\begin{Bmatrix} f \\ g\ h \end{Bmatrix} = \begin{bmatrix} 1 & \tau & \tau^2 & \tau^3 & \tau^4 & \tau^5 & \tau^6 & \tau^7 \\ 0 & 1 & 2\tau & 3\tau^2 & 4\tau^3 & 5\tau^4 & 6\tau^5 & 7\tau^6 \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \\ b_7 \end{Bmatrix}$$

$$\begin{Bmatrix} f^*_{i+1} \\ f_i \\ f_{i-1} \\ f_{i-2} \\ g^*_{i+1} \\ g_i \\ g_{i-1} \\ g_{i-2} \end{Bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -2 & 4 & -8 & 16 & -32 & 64 & -128 \\ 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 3 & -4 & 5 & -6 & 7 \\ 0 & 1 & -4 & 12 & -32 & 80 & -192 & 448 \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \\ b_7 \end{Bmatrix}$$

$$\begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \\ b_7 \end{Bmatrix} = \begin{bmatrix} 0 & 108 & 0 & 0 & 0 & 0 & 0 & 01 \\ 0 & 0 & 0 & 0 & 0 & 108 & 0 & 0 \\ 56 & -297 & 216 & 25 & -12 & 108 & 108 & 6 \\ 124 & -27 & -108 & 11 & -24 & -189 & 0 & 3 \\ 50 & 270 & -270 & -50 & -3 & -216 & -189 & -12 \\ -59 & 54 & 27 & -22 & 21 & 54 & -27 & -6 \\ -52 & -81 & 108 & 25 & 15 & 108 & 81 & 6 \\ -11 & -27 & 27 & 11 & 3 & 27 & 27 & 3 \end{bmatrix} \begin{Bmatrix} f^*_{i+1} \\ f_i \\ f_{i-1} \\ f_{i-2} \\ g^*_{i+1} \\ g_i \\ g_{i-1} \\ g_{i-2} \end{Bmatrix} / 108$$

know coefficients b_i $\quad f(\tau) = b_0 + b_1\tau + b_2\tau^2 + b_3\tau^3 + b_4\tau^4 + b_5\tau^5 + b_6\tau^6 + b_7\tau^7 = \dot{y}(\tau)$

$$y_{i+1} = \int_{ti}^{ti+1} \dot{y}\, dt + y_i = h\int_0^1 f\, d\tau + y_i$$

$$= y_i + h\left(b_0\tau + b_1\tau^2/2 + b_2\tau^3/3 + b_3\tau^4/4 + b_4\tau^5/5 + b_5\tau^6/6 + b_6\tau^7/7 + b_7\tau^8/8\right)\Big|_0^1$$

$$y_{i+1} = y_i + h\left(b_0 + b_1/2 + b_2/3 + b_3/4 + b_4/5 + b_5/6 + b_6/7 + b_7/8\right)$$

CORRECTOR (4-step Obreshkov)

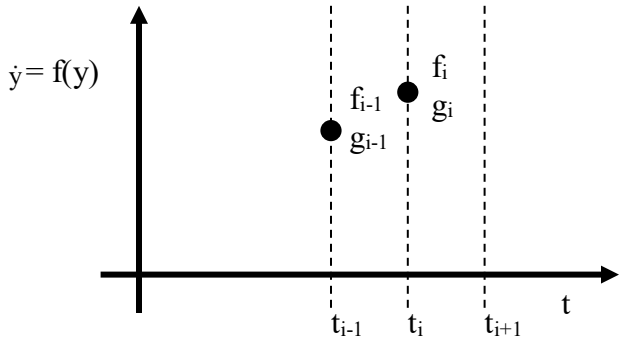
$$y_{i+1} = y_i + h\begin{pmatrix} 34465\, f^*_{i+1} + 42255\, f_i + 12015\, f_{i-1} + 1985\, f_{i-2} \\ + h\left(-3849\, g^*_{i+1} + 22977\, g_i + 7263\, g_{i-1} + 489\, g_{i-2}\right) \end{pmatrix} / 90720$$

Third-degree (Cubic) Predictor and Third-degree (Cubic) Corrector with Second Derivatives

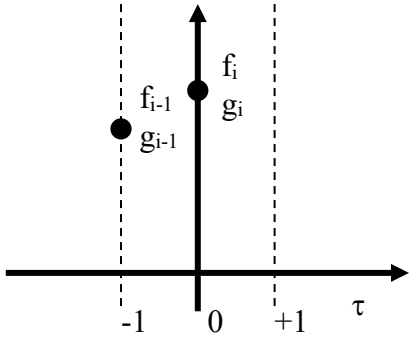
given second-order initial-value differential equations of the form
$\{\dot{y}\} = f(\{y\}, t)$ and $\{\ddot{y}\} = g(\{y\}, \{\dot{y}\}, t)$

must know $\{y\}_i$ and $\{y\}_{i-1}$ respectively at times t_i and t_{i-1}

may determine $\{\dot{y}\}_i$ $\{\dot{y}\}_{i-1}$ and $\{\ddot{y}\}_i$ $\{\ddot{y}\}_{i-}$



fixed time step h $\quad \tau = (t - t_i) / h \quad d\tau = dt / h \quad dt = h\, d\tau \quad d\tau / dt = 1 / h$



use third degree polynomial <u>predictor</u> $\quad f = a_0 + a_1\tau + a_2\tau^2 + a_3\tau^3$

$$g = \frac{df}{dt} = \frac{\partial f}{\partial \tau}\frac{d\tau}{dt} \qquad g\,h = \frac{\partial f}{\partial \tau} \qquad g\,h = a_1 + 2a_2\tau + 3a_3\tau^2$$

$$\begin{Bmatrix} f \\ g\,h \end{Bmatrix} = \begin{bmatrix} 1 & \tau & \tau^2 & \tau^3 \\ 0 & 1 & 2\tau & 3\tau^2 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{Bmatrix}$$

$$\begin{Bmatrix} f_i \\ f_{i-1} \\ g_i\ h \\ g_{i-1}\ h \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & -1 & 1 & -1 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & -2 & 3 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{Bmatrix}$$

$$\begin{Bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{Bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -3 & 3 & 2 & 1 \\ -2 & 2 & 1 & 1 \end{bmatrix} \begin{Bmatrix} f_i \\ f_{i-1} \\ g_i\ h \\ g_{i-1}\ h \end{Bmatrix}$$

know coefficients a_i for interpolant $f(\tau) = a_0 + a_1\tau + a_2\tau^2 + a_3\tau^3 = \dot{y}(\tau)$

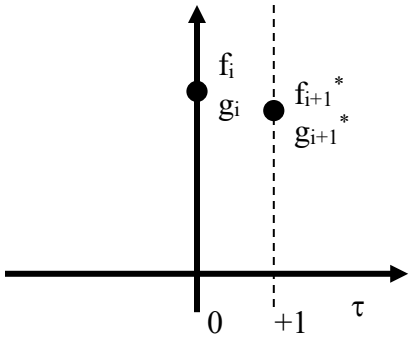
$$y_{i+1} = \int_{ti}^{ti+1} \dot{y}\, dt + y_i = h\int_0^1 f\, d\tau + y_i = y_i + h\left(a_0\tau + a_1\tau^2/2 + a_2\tau^3/3 + a_3\tau^4/4\right)\Big|_0^1$$

$$y_{i+1} = y_i + h\left(a_0 + a_1/2 + a_2/3 + a_3/4\right)$$

PREDICTOR (2-step Obreshkov per Sehnalova)

$$y^*_{i+1} = y_i + h\left(-6\,f_i + 18\,f_{i-1} + h\left(17\,g_i + 7g_{i-1}\right)\right)/12$$

now use predicted value of y^*_{i+1} to compute $f\left(y^*_{i+1}\right) = f^*_{i+1}$ and $g\left(y^*_{i+1}\right) = g^*_{i+1}$



use third degree polynomial <u>corrector</u> $f(\tau) = b_0 + b_1\tau + b_2\tau^2 + b_3\tau^3 = \dot{y}(\tau)$

$$\begin{Bmatrix} f \\ g\ h \end{Bmatrix} = \begin{bmatrix} 1 & \tau & \tau^2 & \tau^3 \\ 0 & 1 & 2\tau & 3\tau^2 \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix}$$

$$\begin{Bmatrix} f_{i+1} \\ f_i \\ g_{i+1}\ h \\ g_i\ h \end{Bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 2 & 3 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix}$$

$$\begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 3 & -3 & -1 & -2 \\ -2 & 2 & 1 & 1 \end{bmatrix} \begin{Bmatrix} f_{i+1} \\ f_i \\ g_{i+1}\ h \\ g_i\ h \end{Bmatrix}$$

know coefficients b_i $\quad f(\tau) = b_0 + b_1\tau + b_2\tau^2 + b_3\tau^3 = \dot{y}(\tau)$

$$y_{i+1} = \int_{ti}^{ti+1} \dot{y}\, dt + y_i = h \int_0^1 f\, d\tau + y_i$$
$$= y_i + h\left(b_0\tau + b_1\tau^2/2 + b_2\tau^3/3 + b_3\tau^4/4\right)\Big|_0^1$$

$$y_{i+1} = y_i + h\left(b_0 + b_1/2 + b_2/3 + b_3/4\right)$$

CORRECTOR (2-step Obreshkov per Sehnalova)

$$y^*_{i+1} = y_i + h\left(6 f_{i+1} + 6 f_i + h\left(-g_{i+1} + g_i\right)\right)/12$$

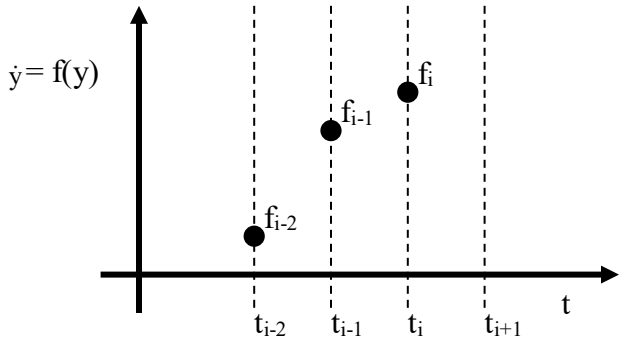
Least-Squares Quadratic Predictor and Cubic Corrector with Second Derivatives

given second-order initial-value differential equations of the form

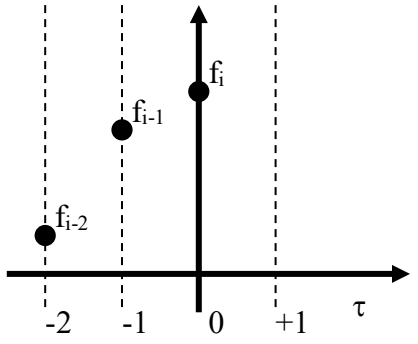
$\{\dot{y}\} = f(\{y\}, t)$ and $\{\ddot{y}\} = g(\{y\}, \{\dot{y}\}, t)$

must know $\{y\}_i, \{y\}_{i-1}, \{y\}_{i-2}$ respectively at times t_i, t_{i-1} and t_{i-2}

may determine $\{\dot{y}\}_i, \{\dot{y}\}_{i-1}, \{\dot{y}\}_{i-2}$ and $\{\ddot{y}\}_i, \{\ddot{y}\}_{i-1}, \{\ddot{y}\}_{i-2}$



fixed time step h $\quad \tau = (t - t_i) / h \quad d\tau = dt / h \quad dt = h\, d\tau \quad d\tau / dt = 1 / h$



use quadratic polynomial <u>predictor</u> $\quad f = a_0 + a_1 \tau + a_2 \tau^2$

$$g = \frac{df}{dt} = \frac{\partial f}{\partial \tau}\frac{d\tau}{dt} \qquad g = (a_1 + 2a_2\tau)/h \qquad g\,h = a_1 + 2a_2\tau$$

$$\begin{Bmatrix} f \\ g\,h \end{Bmatrix} = \begin{bmatrix} 1 & \tau & \tau^2 \\ 0 & 1 & 2\tau \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix}$$

$$\begin{Bmatrix} f_i \\ g_i\ h \\ f_{i-1} \\ g_{i-1}\ h \\ f_{i-2} \\ g_{i-2}\ h \end{Bmatrix} \approx \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & -2 \\ 1 & -2 & 4 \\ 0 & 1 & -4 \end{bmatrix} \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix}$$

$$\{Y\} \approx [X]\{\beta\} \qquad \{Y\} = \begin{Bmatrix} f_i \\ g_i\ h \\ f_{i-1} \\ g_{i-1}\ h \\ f_{i-2} \\ g_{i-2}\ h \end{Bmatrix} \qquad [X] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & -1 & 1 \\ 0 & 1 & -2 \\ 1 & -2 & 4 \\ 0 & 1 & -4 \end{bmatrix} \qquad \{\beta\} = \begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix}$$

$$\{\beta\} = \left([X]^T [X]\right)^{-1} [X]^T \{Y\} \qquad \text{least squares solution}$$

$$\begin{Bmatrix} a_0 \\ a_1 \\ a_2 \end{Bmatrix} = \begin{bmatrix} 71 & 36 & 40 & 26 & 19 & 16 \\ 36 & 86 & -20 & 26 & -16 & -34 \\ 5 & 30 & -10 & 0 & 5 & -30 \end{bmatrix} \begin{Bmatrix} f_i \\ g_i\ h \\ f_{i-1} \\ g_{i-1}\ h \\ f_{i-2} \\ g_{i-2}\ h \end{Bmatrix} / 130$$

know coefficients a_0, a_1 and a_2 for interpolant $f(\tau) = a_0 + a_1 \tau + a_2 \tau^2 = \dot{y}(\tau)$

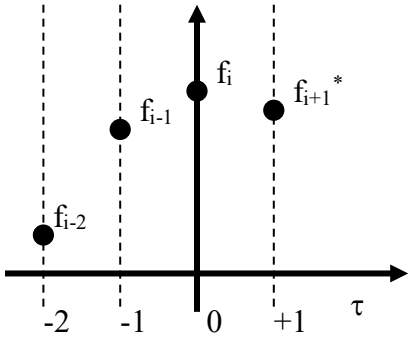
$$y_{i+1} = \int_{ti}^{ti+1} \dot{y}\, dt + y_i = h \int_0^1 f\, d\tau + y_i = h \left(a_0\tau + a_1\tau^2/2 + a_2\tau^3/3 \right)\Big|_0^1 + y_i$$

$$y_{i+1} = y_i + h \left(a_0 + a_1/2 + a_2/3 \right)$$

PREDICTOR (least-squares 3-step Adams-Bashforth)

$$y_{i+1} = y_i + h\left(272\, f_i + 80\, f_{i-1} + 38\, f_{i-2} + h\left(267\, g_i + 117\, g_{i-1} - 33\, g_{i-2}\right)\right)/390$$

now use predicted value of y_{i+1} to compute $f(y_{i+1}) = f_{i+1}^*$ and $g(y_{i+1}) = g_{i+1}^*$



use cubic polynomial <u>corrector</u> $f = b_0 + b_1 \tau + b_2 \tau^2 + b_3 \tau^3$

$$\begin{Bmatrix} f \\ g\ h \end{Bmatrix} = \begin{bmatrix} 1 & \tau & \tau^2 & \tau^3 \\ 0 & 1 & 2\tau & 3\tau^2 \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix}$$

$$\begin{Bmatrix} f_{i+1}^* \\ g_{i+1}^*\ h \\ f_i \\ g_i\ h \\ f_{i-1} \\ g_{i-1}\ h \\ f_{i-2} \\ g_{i-1}\ h \end{Bmatrix} \approx \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & -1 & 1 & -1 \\ 0 & 1 & -2 & 3 \\ 1 & -2 & 4 & -8 \\ 0 & 1 & -4 & 12 \end{bmatrix} \begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix}$$

$$\begin{Bmatrix} b_0 \\ b_1 \\ b_2 \\ b_3 \end{Bmatrix} = \begin{bmatrix} 754 & -438 & 851 & 175 & 542 & 374 & 241 & 159 \\ 590 & 126 & 175 & 593 & -374 & 394 & -391 & -471 \\ 32 & 618 & -203 & -67 & 4 & -266 & 167 & 21 \\ -45 & 213 & -69 & -111 & 69 & -111 & 45 & 213 \end{bmatrix} \begin{Bmatrix} f_{i+1}^* \\ g_{i+1}^*\ h \\ f_i \\ g_i\ h \\ f_{i-1} \\ g_{i-1}\ h \\ f_{i-2} \\ g_{i-1}\ h \end{Bmatrix} / 2388$$

know coefficients b_0, b_1, b_2 and b_3 for new interpolant $f(\tau) = b_0 + b_1 \tau + b_2 \tau^2 + b_3 \tau^3 = \dot{y}(\tau)$

$$y_{i+1} = \int_{ti}^{ti+1} \dot{y}\, dt + y_i = h \int_0^1 f\, d\tau + y_i = h\,(b_0\tau + b_1\tau^2/2 + b_2\tau^3/3 + b_3\tau^4/4)\Big|_0^1 + y_i$$

$$y_{i+1} = y_i + h\,(b_0 + b_1/2 + b_2/3 + b_3/4)$$

CORRECTOR (least-squares 4-step Adams-Moulton)

$$y_{i+1} = y_i + h \begin{pmatrix} 12581\, f^*_{i+1} + 10243\, f_i + 4483\, f_{i-1} + 1349\, f_{i-2} \\ + h\left(-1389\, g^*_{i+1} + 5057\, g_i + 5455\, g_{i-1} - 195\, g_{i-2}\right) \end{pmatrix} / 28656$$

does not work as well as Obreshkov