IVPs for ODEs

THM: Suppose that $D = \{(t,y) \mid a \le t \le b \text{ and } -\infty < y < \infty\}$

and that $f(t,y)$ is continuous on D.

If f satisfies a Lipschitz condition on D (in the var y)

then the IVP $\begin{cases} y'(t) = f(t,y) & a \le t \le b \\ y(a) = \alpha \end{cases}$

has a unique solution $y(t)$ for $a \le t \le b$.

Comment: $f(t,y)$ is Lipschitz in y if $\exists L > 0$ s.t.

$|f(t,y_1) - f(t,y_2)| \le L|y_1 - y_2|$. L = Lipschitz constant.

Comment: If $f(t,y)$ is defined on a convex set $D \subset \mathbb{R}^2$

and $\exists L > 0$ s.t. $\left|\frac{\partial f}{\partial y}(t,y)\right| \le L \quad \forall (t,y) \in D$,

then f is Lipschitz on D in the variable y

with Lip constant L.

Example: $\begin{cases} y' = 1 + t\sin(ty) & 0 \le t \le 2 \\ y(0) = 0 \end{cases}$

$$\left|\frac{\partial f}{\partial y}\right| = \left|t^2 \cos(ty)\right| \le 4$$

So f is Lip with Lip-const. 4.

$\Rightarrow$ According to the THM, this IVP has a unique solution.

Well-posed problems

Def: The IVP $\begin{cases} \frac{dy}{dt} = f(t,y) & a \le t \le b \\ y(a) = \alpha \end{cases}$ (*)

is well-posed if

1) The exists a solution $y(t)$.

2) It is unique.

3) $\exists\ \varepsilon_0 > 0,\ k > 0$ s.t. $\forall \varepsilon$ with $\varepsilon_0 > \varepsilon > 0$ whenever $\delta(t)$ is continuous with $|\delta(t)| < \varepsilon$, and $|\delta_0| < \varepsilon$, the perturbed IVP:

$$\begin{cases} \frac{dz}{dt} = f(t,z) + \delta(t) \\ z(a) = \alpha + \delta_0 \end{cases}$$

has a unique solution that satisfies

$$|z(t) - y(t)| < k\varepsilon \quad \forall t \in [a,b].$$

why is this important? Numerical methods will always deal with perturbed problems due to round-off error.

THM: If f is Lip. in y & continuous, then (*) is well-posed.

Euler's Method

$$(\circledast)\quad \begin{cases} \dfrac{dy}{dt} = f(t,y), & a \le t \le b. \\ y(a) = \alpha \end{cases}$$

Mesh points: $t_i = a + ih \qquad i = 0, 1, \dots, N.$

$$h = \frac{b-a}{N} = t_{i+1} - t_i \qquad \underline{\text{step size}}$$

We generate an approximation to the solution at the grid points.

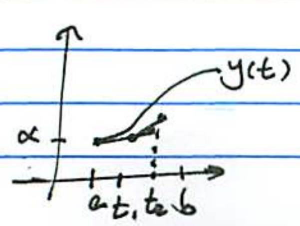
Assume that $y(t)$, the unique solution of $\circledast$ has two continuous derivatives on $[a,b]$. Then $\forall\, i = 0, \dots, N-1$

$$y(t_{i+1}) = y(t_i) + (t_{i+1} - t_i)\, y'(t_i) + \frac{(t_{i+1} - t_i)^2}{2} y''(\xi_i)$$
$$\big(\xi_i \in (t_i, t_{i+1})\big).$$

$$\Rightarrow\ y(t_{i+1}) = y(t_i) + h\, y'(t_i) + \frac{h^2}{2} y''(\xi_i)$$
$$y(t_{i+1}) = y(t_i) + h f(t_i, y(t_i)) + \frac{h^2}{2} y''(\xi_i)$$

Euler's method: Approximation $w_i \approx y(t_i)$:

$$\begin{cases} w_0 = \alpha \\ w_{i+1} = w_i + h f(t_i, w_i) & i = 0, \dots, N-1. \end{cases}$$



<u>Example:</u>

$$\begin{cases} y' = y - t^2 + 1 & 0 \le t \le 2 \\ y(0) = 0.5 \end{cases}$$

Set $h = 0.5$. $\quad f(t,y) = y - t^2 + 1$.

$w_0 = y(0) = 0.5$

$w_1 = w_0 + 0.5\left(w_0 - (0.0)^2 + 1\right) = 0.5 + 0.5 \cdot 1.5 = 1.25$.

$w_2 = w_1 + 0.5\left(w_1 - (0.5)^2 + 1\right) = 1.25 + 0.5 \cdot 2.0 = 2.25$.

$w_3 = w_2 + 0.5\left(w_2 - (1.0)^2 + 1\right) = 2.25 + 0.5 \cdot 2.25 = 3.375$.

$y(2) \approx w_4 = w_3 + 0.5\left(w_3 - (1.5)^2 + 1\right) = 3.375 + 0.5 \cdot 2.125$
$= 4.4375$.

The exact solution is $y(t) = (t+1)^2 - 0.5e^t$.

<u>ERROR</u>

<u>THM:</u> Suppose f is continuous & satisfies a Lip-condition on $D = \{(t,y) \mid a \le t \le b, \ -\infty < y < \infty\}$.

Suppose that $|y''(t)| \le M \ \ \forall t \in [a,b]$, where $y(t)$ is the unique solution of the IVP $\begin{cases} y' = f(t,y) & a \le t \le b \\ y(a) = \alpha \end{cases}$

Let $w_0, \dots, w_N$ be the approximations generated by Euler's method.

Then $\forall i = 0, \dots, N \quad |y(t_i) - w_i| \le \dfrac{hM}{2L}\left[e^{L(t_i - a)} - 1\right]$.

Another approach to deriving RK methods

Start with
$$\begin{cases} \frac{dy}{dt} = f(t, y(t)) \\ y(t_0) = y_0 \end{cases}$$

Integrate: $y(t+h) = y(t) + \int_t^{t+h} f(s, y(s))\, ds.$

Replace the integral by a quadrature:

1) Rectangular

$$y(t+h) = y(t) + h f(t, y(t)) \implies \text{Euler}$$

2) Midpoint

$$y(t+h) = y(t) + h f\left(t + \frac{h}{2}, y\left(t + \frac{h}{2}\right)\right)$$

Predict $y(t+\frac{h}{2})$ using an Euler step:

$$y\left(t+\frac{h}{2}\right) = y(t) + \frac{h}{2} f(t, y(t)).$$

This method can be summarized as:

$$k_1 = f(t, y(t))$$
$$k_2 = f\left(t+\frac{h}{2}, y(t) + \frac{h}{2} k_1\right)$$
$$y(t+h) = y(t) + h k_2. \implies \text{Modified Euler or Runge Method}$$

3) Trapezoid

$$y(t+h) = y(t) + \frac{h}{2}\left[f(t, y(t)) + f(t+h, y(t+h))\right]$$

The implicit trapezoidal rule

Predict the unknown on the RHS using an Euler step:

$$k_1 = f(t, y(t))$$

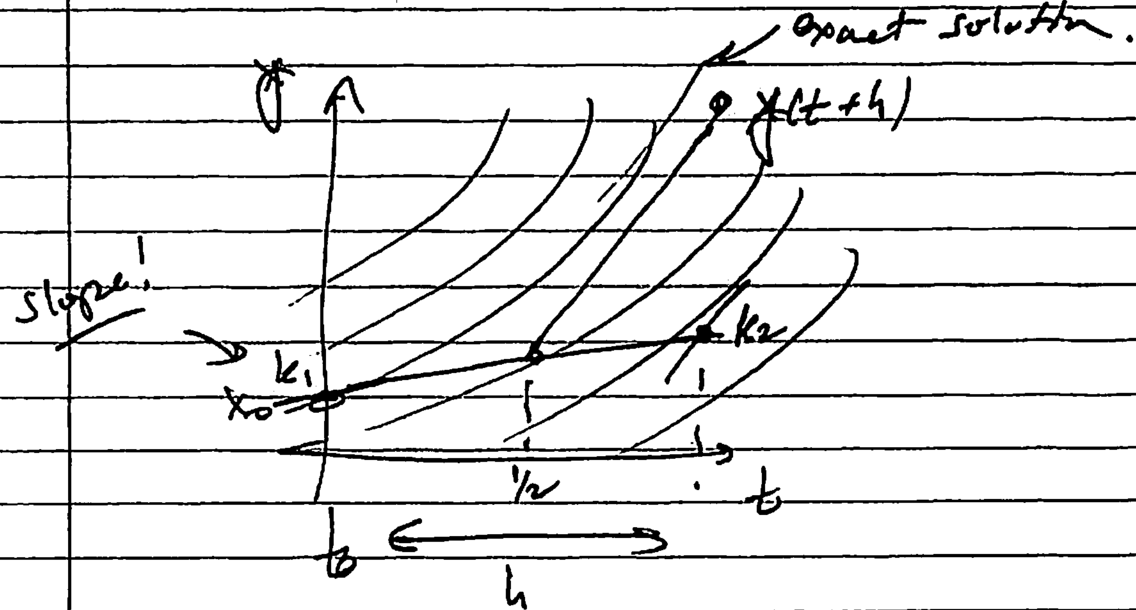
Euler: $x(t+h) = x(t) + hf(t,x)$

$$k_2 = f(t+h, y+hk_1)$$

$$y(t+h) = y(t) + \frac{h}{2}(k_1 + k_2)$$

This is Heun method

Geometrical interpretation:



Higher-order Taylor methods

Local truncation error at a step measures the amount by which the exact solution to the differential equation fails to satisfy the difference equation used for the approximation.

[Strange - it would have been better to measure how the approximations generated by the method satisfy the differential equation, but this is not accessible].

Def: (IVP) $\begin{cases} y' = f(t,y) & a \le t \le b \\ y(a) = \alpha \end{cases}$

The Difference method $\begin{cases} w_0 = \alpha \\ w_{i+1} = w_i + h\phi(t_i, w_i) \end{cases}$ $i = 0, \dots, N-1$

has local truncation error:

$$\tau_{i+1}(h) = \frac{y_{i+1} - (y_i + h\phi(t_i, y_i))}{h} = \frac{y_{i+1} - y_i}{h} - \phi(t_i, y_i).$$

(*) Local : measures the accuracy of a method at a specific step assuming it was exact on the previous step.

Example: Euler's method

$$\tau_{i+1}(h) = \frac{y_{i+1} - y_i}{h} - f(t_i, y_i)$$

We know that $y_{i+1} = y_i + h f(t_i, y_i) + \frac{h^2}{2} y''(\xi_i)$

$$\Rightarrow \quad \tau_{i+1}(h) = \frac{h}{2} y''(\xi_i) \qquad \xi_i \in (t_i, t_{i+1}).$$

If $|y''(t)| \le M$ on $[a,b]$, then $|\tau_{i+1}(h)| \le \frac{hM}{2}$.

$\Rightarrow$ local truncation error is $O(h)$.

Higher-order methods (Taylor methods)

$$y(t_{i+1}) = y(t_i) + h y'(t_i) + \frac{h^2}{2} y''(t_i) + \dots + \frac{h^n}{n!} y^{(n)}(t_i) + \frac{h^{n+1}}{(n+1)!} y^{(n+1)}(\xi_i)$$

$$y'(t) = f(t, y(t))$$
$$y''(t) = f'(t, y(t))$$
$$\vdots$$
$$y^{(k)}(t) = f^{(k-1)}(t, y(t)).$$

$$y(t_{i+1}) = y(t_i) + h f(t_i, y(t_i)) + \frac{h^2}{2} f'(t_i, y(t_i)) + \dots + \frac{h^n}{n!} f^{(n-1)}(t_i, y(t_i))$$
$$+ \frac{h^{n+1}}{(n+1)!} f^{(n)}(\xi_i, y(\xi_i)).$$

And a method is obtained by removing the remainder term:

$$w_0 = \alpha$$
$$w_{i+1} = w_i + h T^{(n)}(t_i, w_i)$$
with $T^{(n)}(t_i, w_i) = f(t_i, w_i) + \frac{h}{2} f'(t_i, w_i) + \dots + \frac{h^{n-1}}{n!} f^{(n-1)}(t_i, w_i)$.

RK2

In Taylor methods:

$$y(t_{i+1}) = y(t_i) + hy'(t_i) + \frac{h^2}{2}y''(t_i) + \dots$$

Which led to

We want to get rid of this term.

$$y(t_{i+1}) = y(t_i) + hf(t_i, y(t_i)) + \frac{h^2}{2}f'(t_i, y(t_i)) + \dots$$

The idea: evaluate f at other points.

We want to approximate $T^{(2)}(t,y) = f(t,y) + \frac{h}{2}f'(t,y)$

with error no greater than $O(h^2)$.

$$f'(t,y) = \frac{df}{dt}f(t,y) = \frac{\partial f}{\partial t}(t,y) + \frac{\partial f}{\partial y}(t,y)\overbrace{y'(t)}^{f(t,y)}$$

$$\Rightarrow T^{(2)}(t,y) = f(t,y) + \frac{h}{2}\frac{\partial f}{\partial t}(t,y) + \frac{h}{2}\frac{\partial f}{\partial y}(t,y) \cdot f(t,y).$$

We will approximate this with $f(t+\alpha_1, y+\beta_1)$

$$f(t+\alpha_1, y+\beta_1) = f(t,y) + \alpha_1\frac{\partial f}{\partial t}(t,y) + \beta_1\frac{\partial f}{\partial y}(t,y) + R_1(t+\alpha_1, y+\beta_1)$$

$$\Rightarrow \alpha_1 = \frac{h}{2}, \quad \beta_1 = \frac{h}{2}f(t,y) \qquad (\text{and } R_1 = O(h^2)).$$

$$\Longrightarrow \quad T^{(2)}(t,y) = f\left(t + \frac{h}{2}, y + \frac{h}{2}f(t,y)\right) + R_1$$

The resulting method:
$$\begin{cases} w_0 = \alpha \\ w_{i+1} = w_i + hf\left(t_i + \frac{h}{2}, w_i + \frac{h}{2}f(t_i, w_i)\right) \end{cases}$$

The midpoint Method. / Modified Euler

Runge Kutta methods

Taylor methods : high-order local truncation error.

Downside - requires computing & evaluating the derivatives of $f(t,y)$.

RK methods avoid that.

We need Taylor's THM in 2 variables:

THM: Suppose $f(t,y)$ & its partial derivatives of order $\leq n+1$ are conts on $D=\{(t,y) \mid a \leq t \leq b,\ c \leq y \leq d\}$.
Let $(t_0,y_0) \in D$.
Then $\forall (t,y) \in D$ $\exists$ $\underset{\min(t,t_0)\text{ etc...}}{t<\xi<t_0}$, $y<\mu<y_0$ with

$$f(t,y) = P_n(t,y) + R_n(t,y)$$

The n^{th} degree Taylor polynomial in 2 variables

$$P_n(t,y) = f(t_0,y_0) + \left[(t-t_0)\frac{\partial f}{\partial t}(t_0,y_0) + (y-y_0)\frac{\partial f}{\partial y}(t_0,y_0)\right]$$
$$+ \left[\frac{(t-t_0)^2}{2}\frac{\partial^2 f}{\partial t^2}(t_0,y_0) + (t-t_0)(y-y_0)\frac{\partial^2 f}{\partial t \partial y}(t_0,y_0)\right.$$
$$\left. + \frac{(y-y_0)^2}{2}\frac{\partial^2 f}{\partial y^2}(t_0,y_0)\right] + \cdots$$
$$+ \left[\frac{1}{n!}\sum_{j=0}^{n}\binom{n}{j}(t-t_0)^{n-j}(y-y_0)^j \frac{\partial^n f}{\partial t^{n-j}\partial y^j}(t_0,y_0)\right]$$

$$R_n(t,y) = \frac{1}{(n+1)!}\sum_{j=0}^{n+1}\binom{n+1}{j}(t-t_0)^{n+1-j}(y-y_0)^j \frac{\partial^{n+1} f}{\partial t^{n+1-j}\partial y^j}(\xi,\mu).$$

Explicit Runge-Kutta methods

s-stage explicit RK

$\downarrow$

$$\begin{cases} k_i = f\left(t_i + c_i h,\ \underset{w_i}{\cancel{x}} + h\displaystyle\sum_{j=1}^{i-1} a_{ij}k_j\right) & i=1,\dots,s \\ \underset{w_{i+1}}{\cancel{x(t+h)}} = \underset{w_i}{\cancel{x(t)}} + h\displaystyle\sum_{i=1}^{s} b_i k_i \end{cases}$$

k_i = the i^{th} stage of the method.

The coefficients of the method:

$$b = \begin{pmatrix} b_1 \\ \vdots \\ b_s \end{pmatrix}, \quad c = \begin{pmatrix} c_1 \\ \vdots \\ c_s \end{pmatrix}, \quad A = \begin{pmatrix} 0 & & \\ a_{21} & \ddots & \\ \vdots & & 0 \\ a_{s1} & \cdots & a_{s,s-1} \end{pmatrix}$$

<u>Butcher array</u> : $\begin{array}{c|c} c & A \\ \hline & b^t \end{array}$.

<u>Examples:</u>

(1) <u>Explicit Euler.</u>

$$\begin{array}{c|c} 0 & 0 \\ \hline & 1 \end{array}$$

$s=1.$

$k_1 = f(t,x) \Rightarrow c_1 = 0,\ A = 0.$

$\cancel{x(t+h) = x(t) + hk_1}$. $\Rightarrow b_1 = 1.$

$w_{i+1} = w_i + hk_1$

(2) <u>Modified Euler</u>

$\underset{y}{\cancel{x}}(t+h) = \underset{y}{\cancel{x}}(t) + h f\left(t + \frac{h}{2}, \underset{y}{\cancel{x}} + \frac{h}{2} f(t,y)\right)$

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

$k_1 = f(t,x) \Rightarrow c_1 = 0.$

$k_2 = f\left(t_i + \frac{h}{2}, x_i + h\frac{1}{2}k_1\right) \Rightarrow c_2 = a_{21} = \frac{1}{2}.$

Also $b_1 = 0$ and $b_2 = 1$

(3) Heun's method

$$y(t+h) = y(t) + \frac{1}{2}h\left[f(t,y) + f(t+h,\, y + h\, f(t,y))\right]$$

$$k_1 = f(t_i, x_i) \implies c_1 = 0.$$

$$k_2 = f(t_i + h,\, x_i + h k_1) \implies c_2 = a_{21} = 1.$$

$$\cancel{x(t+h) = x(t) + \tfrac{1}{2}k_1 + \tfrac{1}{2}k_2} \implies b^t = \left(\tfrac{1}{2}\ \tfrac{1}{2}\right).$$

$$w_{i+1} = w_i + \frac{1}{2}(k_1 + k_2)$$

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

(4) Classical RK-4

$$\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2} & & & \\
\frac{1}{2} & 0 & \frac{1}{2} & & \\
1 & 0 & 0 & 1 & \\
\hline
 & \frac{1}{6} & \frac{1}{3} & \frac{1}{3} & \frac{1}{6}
\end{array}$$

Many other versions of RK-4 are possible.

Higher-order RK methods

RK4: $w_0 = \alpha$

$$k_1 = hf(t_i, w_i)$$

$$k_2 = hf\left(t_i + \frac{h}{2}, w_i + \frac{k_1}{2}\right)$$

$$k_3 = hf\left(t_i + \frac{h}{2}, w_i + \frac{k_2}{2}\right)$$

$$k_4 = hf(t_{i+1}, w_i + k_3)$$

$$w_{i+1} = w_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4).$$

Multistep Methods

Starting point: ODE + IV : $\begin{cases} y'(t) = f(t, y(t)) \\ y(a) = \alpha \end{cases}$

Assume that we have $r \geq 2$ given approximate values of

$$\eta_k \approx y(t_k) \quad \text{for } k = j, \ldots, j+r-1.$$

We also assume that these approximations are given at equidistant points

$$t_k = a + kh.$$

From these values we want to compute η_{j+r}.

Step I: Initialization.

We need the first r values.

These can be obtained, e.g., from one-step methods.

Another option: using multistep methods with an increasing # of steps.

Step II: Assuming that we have the first r values, we integrate the ODE,

$$y(t_{p+k}) = y(t_{p-j}) + \int_{t_{p-j}}^{t_{p+k}} f(t, y(t))\, dt.$$

We now replace the integrand with a polynomial $P_q(t)$ that satisfies

(i) $\deg P_q(t) \le q$.

(ii) $P_q(t_i) = f(t_i, x(t_i))$ $\quad i = p, p-1, \dots, p-q$

Assuming a uniform mesh $h = t_{i+1} - t_i$, we write the Lagrange interpolant

$$P_q(t) = \sum_{i=0}^{q} f(t_{p-i}, x_{p-i})\, L_i(t)$$

with

$$L_i(t) = \prod_{\substack{l=0 \\ l \neq i}}^{q} \frac{t - t_{p-l}}{t_{p-i} - t_{p-l}}$$

Hence

$$\eta_{p+k} - \eta_{p-j} \approx \sum_{i=0}^{q} f(t_{p-i}, \eta_{p-i}) \int_{t_{p-j}}^{t_{p+k}} L_i(t)\,dt$$

$$= h \sum_{i=0}^{q} \beta_{qi}\, f(t_{p-i}, \eta_{p-i})$$

with (for $i = 0, \dots, q$):

$$\beta_{qi} = \frac{1}{h}\int_{t_{p-j}}^{t_{p+k}} L_i(t)\,dt = \frac{1}{h}\int_{t_{p-j}}^{t_{p+k}} \prod_{\substack{l=0\\ l\neq i}}^{q} \frac{t - t_{p-l}}{t_{p-i} - t_{p-l}}\,dt$$

$$= \frac{1}{h}\int_{-jh}^{kh} \prod_{\substack{l=0\\ l\neq i}}^{q} \frac{t + t_p - t_{p-l}}{t_{p-i} - t_{p-l}}\,dt$$

$$= \frac{1}{h}\int_{-jh}^{kh} \prod_{\substack{l=0\\ l\neq i}}^{q} \frac{t + hp - h(p-l)}{h(p-i) - h(p-l)}\,dt = \frac{1}{h}\int_{-jh}^{kh} \prod_{\substack{l=0\\ l\neq i}}^{q} \frac{t + hl}{h(-i+l)}\,dt$$

$$= \frac{1}{h}\int_{-j}^{k} \prod_{\substack{l=0\\ l\neq i}}^{q} \frac{s+l}{-i+l}\,ds .$$

$\Rightarrow$ The approximate method is

$$\eta_{p+k} = \eta_{p-j} + h\sum_{i=0}^{q} \beta_{qi} f_{p-i}$$

For different choices of k, j, q, we get different multistep methods.

Examples:

(1) Adams - Bashforth methods

$k=1$, $j=0$, $q=0,1,2,\ldots$

In this case

$$\eta_{p+1} = \eta_p + h\left[\beta_{q0} f_p + \beta_{q1} f_{p-1} + \ldots + \beta_{qq} f_{p-q}\right]$$

with $\beta_{qi} = \int_0^1 \prod_{\substack{l=0\\ l\neq i}}^{q} \frac{s+l}{-i+l}\, ds \qquad i=0,\ldots,q.$

Coefficients for AB:

i	0	1	2	3	4
β_{0i}	1				
$2\beta_{1i}$	3	-1			
$12\beta_{2i}$	23	-16	5		
$24\beta_{3i}$	55	-59	37	-9	
$720\beta_{4i}$	1901	-2774	2616	-1274	251

(2) <u>Adams - Moulton</u>

$k=0,\ j=1,\ q=0,1,\dots$

$$\eta_p = \eta_{p-1} + h\left[\beta_{q0} f_p + \dots + \beta_{qq} f_{p-q}\right]$$

Rewrite as $(p \to p+1)$

$$\eta_{p+1} = \eta_p + h\left[\beta_{q0} f_{p+1} + \dots + \beta_{qq} f_{p+1-q}\right]$$

$$\beta_{qi} = \int_{-1}^{0} \prod_{\substack{l=0 \\ l \neq i}}^{q} \frac{s+l}{-i+l}\, ds.$$

- Implicit method.

i	0	1	2	3	4
β_{0i}	1				
$2\beta_{1i}$	1	1			
$12\beta_{2i}$	5	8	-1		
$24\beta_{3i}$	9	19	-5	1	
$720\beta_{4i}$	251	646	-264	106	-19

- Can be solved using iterations:

$$\eta_{p+1}^{(i+1)} = \eta_p + h\left[\beta_{q0} f(t_{p+1}, \eta_{p+1}^{(i)}) + \beta_{q1} f_{q_1} + \dots + \beta_{qq} f_{p+1-q}\right]$$

For sufficiently small h, this is a contraction.

- A good initial iterate, e.g., using [AB].

(3) <u>Nyström</u>

$k=1, j=1$

$$\eta_{p+1} = \eta_{p-1} + h\left[\beta_{q0} f_p + \dots + \beta_{pq} f_{p-q}\right].$$

with $$\beta_{qi} = \int_{-1}^{1} \prod_{\substack{l=0\\ l\neq i}}^{q} \frac{s+l}{-i+l}\, ds \qquad i=0,\dots,q.$$

- Special case: $q=0 \Rightarrow \eta_{p+1} = \eta_{p-1} + 2h f_p$

The midpoint rule.

(4) <u>Milne</u>

$k=0, j=2. \quad p \to p+1$

$$\Rightarrow \eta_{p+1} = \eta_{p-1} + h\left[\beta_{q0} f_{p+1} + \dots + \beta_{qq} f_{p+1-q}\right]$$

with

$$\beta_{qi} = \int_{-2}^{0} \prod_{\substack{l=0\\ l\neq i}}^{q} \frac{s+l}{-i+l}\, ds \qquad i=0,\dots,q.$$

<u>Comment:</u>

More general form of multistep methods:

$$\eta_{j+r} + a_{r-1}\eta_{j+r-1} + \dots + a_0\eta_j = hF(t_j; \eta_{j+r}, \dots, \eta_j; h, f).$$