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SOLUTIONS SHEET 9

Exercise 24.

a. The source code can be found in listing 1. Remark: The code is based on the termination criterion given in [Kos89, p. 64] which states that for some user-specified tolerance $\varepsilon > 0$ the iteration will be stopped if for the $(k+1)$-th iterate $\|F(x^{k+1})\| \leqslant \varepsilon$ holds where $x^{(k+1)} := x^{(k)} - DF(x^{(k)})^{-1}F(x^{(k)})$ for $k = 0, 1, \ldots$.

```
function [ x ] = newton( F,invDF,x0,epsilon )
maxit = 1e+3;
s = invDF(x0) * F(x0);
x = x0 - s;
x0 = x;
it = 1;
while norm(F(x0)) > epsilon && it < maxit
    s = invDF(x0) * F(x0);
    x = x0 - s;
    x0 = x;
    it = it + 1;
end
end
```

LISTING 1. src/newton.m

b. The source code for the implicit midpoint rule can be found in listing 2 and the source code for the symplectic euler method can be found in 3.

```
function [ x,y ] = IM( f,Df,x0,xN,y0,N )
x = linspace(x0,xN,N+1);
h = (x0 - xN)/N;
y = zeros(length(y0),N+1);
y(:,1) = y0;
for k = 1:N
    F = @(eta) y(:,k) + h * f(1/2 * (y(:,k) + eta)) - eta;
    determinant = @(A) A(1,1) * A(2,2) - A(1,2) * A(2,1);
    inverse = @(A) 1/determinant(A) * [A(2,2),-A(1,2);-A(2,1),A(1,1)];
    invDF = @(eta) inverse(h/2 * Df(1/2 * (y0 + eta)) - eye(2));
    y(:,k+1) = newton( F,invDF,y(:,k),1e-6 );
end
end
```

LISTING 2. src/IM.m

First consider the *implicit midpoint rule* given by

```
function [ x,y ] = SEUL( a,b,aprime,x0,xN,y0,N )
x = linspace(x0,xN,N+1);
h = (x0 - xN)/N;
y = zeros(length(y0),N+1);
y(:,1) = y0;
for k = 1:N
    F = @(eta) y(1,k) + h * a(eta, y(2,k)) - eta;
    invDF = @(eta) 1/(h * aprime(eta, y(2,k)) - 1);
    y(1,k+1) = newton( F,invDF,y(1,k),1e-6 );
    y(2,k+1) = y(2,k) + h * b(y(1,k+1),y(2,k));
end
end
```

Listing 3. `src/SEUL.m`

$$y_{k+1} = y_k + hf\left(\frac{y_k + y_{k+1}}{2}\right) \qquad k = 0, 1, \ldots \tag{1}$$

Since we consider only systems of two ordinary differential equations we may write

$$\begin{bmatrix} y^1_{k+1} \\ y^2_{k+1} \end{bmatrix} = \begin{bmatrix} y^1_k \\ y^2_k \end{bmatrix} + h \begin{bmatrix} f^1\left(\frac{y_k+y_{k+1}}{2}\right) \\ f^2\left(\frac{y_k+y_{k+1}}{2}\right) \end{bmatrix} \qquad k = 0, 1, \ldots \tag{2}$$

the progressed discretization y_{k+1} occurs implicitely in equation (2) thus we may use the Newton method to solve it. We get that y_{k+1} is a root of the following function

$$F(\eta) := \begin{bmatrix} y^1_k \\ y^2_k \end{bmatrix} + h \begin{bmatrix} f^1\left(\frac{y_k+\eta}{2}\right) \\ f^2\left(\frac{y_k+\eta}{2}\right) \end{bmatrix} - \begin{bmatrix} \eta^1 \\ \eta^2 \end{bmatrix} \qquad k = 0, 1, \ldots \tag{3}$$

and further

$$\begin{aligned} DF(\eta) &= \begin{bmatrix} \frac{\partial F^1}{\partial \eta^1}(\eta) & \frac{\partial F^1}{\partial \eta^2}(\eta) \\ \frac{\partial F^2}{\partial \eta^1}(\eta) & \frac{\partial F^2}{\partial \eta^2}(\eta) \end{bmatrix} \\ &= \begin{bmatrix} hDf^1\left(\frac{y_k+\eta}{2}\right)\begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} - 1 & hDf^1\left(\frac{y_k+\eta}{2}\right)\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix} \\ hDf^2\left(\frac{y_k+\eta}{2}\right)\begin{bmatrix} \frac{1}{2} \\ 0 \end{bmatrix} & hDf^2\left(\frac{y_k+\eta}{2}\right)\begin{bmatrix} 0 \\ \frac{1}{2} \end{bmatrix} - 1 \end{bmatrix} \\ &= \frac{h}{2}\begin{bmatrix} \left(Df\left(\frac{y_k+\eta}{2}\right)\right)^1_1 & \left(Df\left(\frac{y_k+\eta}{2}\right)\right)^2_1 \\ \left(Df\left(\frac{y_k+\eta}{2}\right)\right)^1_2 & \left(Df\left(\frac{y_k+\eta}{2}\right)\right)^2_2 \end{bmatrix} - \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \end{aligned}$$

Hence

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$$(DF(\eta))^{-1} = \frac{2}{hd} \begin{bmatrix} \left(Df\left(\frac{y_k+\eta}{2}\right)\right)_2^2 & -\left(Df\left(\frac{y_k+\eta}{2}\right)\right)_1^2 \\ -\left(Df\left(\frac{y_k+\eta}{2}\right)\right)_2^1 & \left(Df\left(\frac{y_k+\eta}{2}\right)\right)_1^1 \end{bmatrix} \tag{4}$$

where

$$d := \left(\left(Df\left(\frac{y_k+\eta}{2}\right)\right)_1^1 - 1\right)\left(\left(Df\left(\frac{y_k+\eta}{2}\right)\right)_2^2 - 1\right) - \left(Df\left(\frac{y_k+\eta}{2}\right)\right)_2^1 \left(Df\left(\frac{y_k+\eta}{2}\right)\right)_1^2 \tag{5}$$

Now we consider the *symplectic Euler method* for a partitioned system

$$u' = a(u,v) \qquad v' = b(u,v) \tag{6}$$

given by

$$u_{k+1} = u_k + ha(u_{k+1}; v_k) \qquad v_{k+1} = v_k + hb(u_{k+1}; v_k) \qquad k = 0,1,\ldots \tag{7}$$

Thus we get u_{k+1} is a root of the function

$$F(\eta) := u_k + ha(\eta; v_k) - \eta \qquad k = 0,1,\ldots \tag{8}$$

And hence

$$(DF(\eta))^{-1} = (ha'(\eta; v_k) - 1)^{-1} \tag{9}$$

Exercise 25. Let us identify those two ODE systems as follows

$$\dagger \begin{cases} \dot{u} = (v-2)/v \\ \dot{v} = (1-u)/u \end{cases} \qquad \ddagger \begin{cases} \dot{u} = u^2 v(v-2) \\ \dot{v} = v^2 u(1-u) \end{cases} \tag{10}$$

As can be seen in figure 1 to 4 the numerical solution of the system † is periodical for the implicit midpoint rule as well as the symplectic Euler method for several initial values in a neighbourhood of $(u(0), v(0))^t = (1.5, 2.5)^t$. However the system ‡ behaves much more chaotic. In figures 1, 2 and 4 the numerical solution provided by the symplectic Euler method is obviously not periodical whereas the numerical solution generated by the implicit midpoint rule is (to a certain extent) periodical. In figure 3 we see that for the choosen initial value also the implicit midpoint rule is not periodical. In conclusion I say that both the implicit midpoint rule and the symplectic Euler are not suitable (this may be due to the low order of the methods) for solving the system ‡ numerically.

Exercise 26.

- The *implicit Euler method* is given by $y_1 = y_0 + hf(x_1, y_1)$. Hence we have obviously $s = 1$. Further we immediately see that $b_1 = 1$ and $k_1 = f(x_1, y_1)$. We have

$$k_1 = f(x_1, y_1) = f(x_0 + c_1 h, y_0 + ha_{11}k_1) \tag{11}$$

Thus we get $c_1 = 1$ and $a_{11} = 1$. Summarized in a *Butcher tableaux* the implicit Euler method is characterized by

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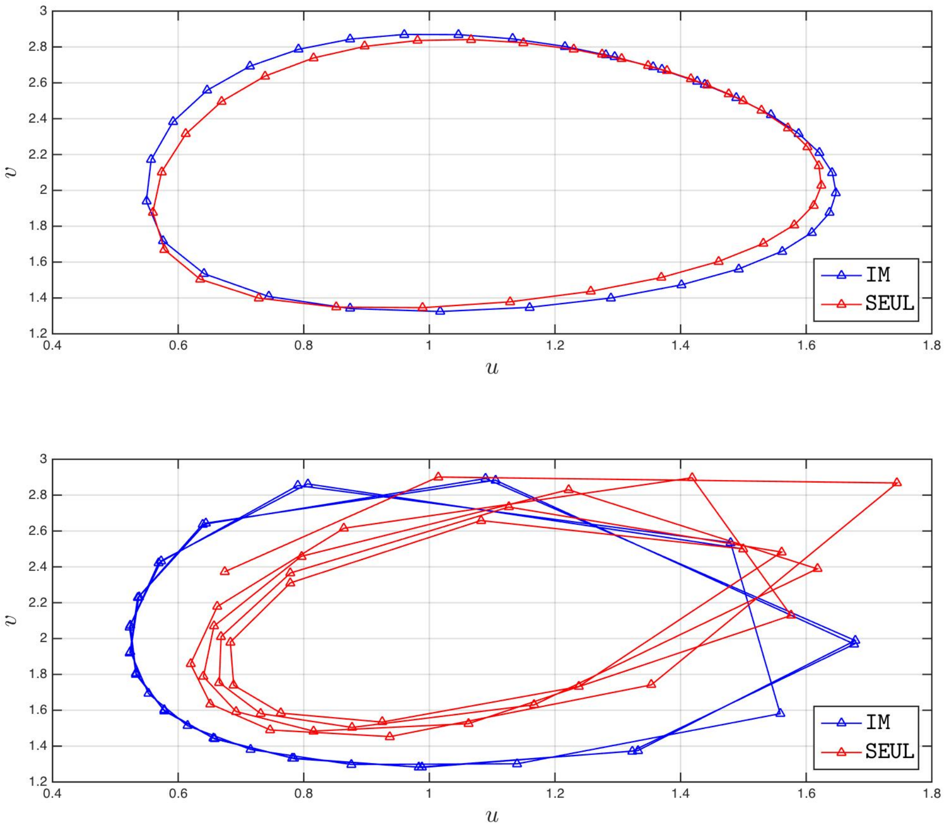

FIGURE 1. In the upper plot the discretized solution of the system † on the interval $[0, 10]$ with initial conditions $(u(0), v(0))^t = (1.5, 2.5)$ and $h = 10/35$ is shown. In the lower plot the discretized solution of ‡ with the same parameters is shown.

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

TABLE 1. Butcher tableaux of the implicit Euler method.

- The derivation of *Runge 2* follows standard text [HNW93, pp. 132–133]. Consider the IVP

$$y' = f(x) \qquad y(x_0) = y_0 \tag{12}$$

with exact solution $y(x) = y_0 + \int\limits_{x_0}^{x} f(\tau)d\tau$. By using the midpoint rule we get

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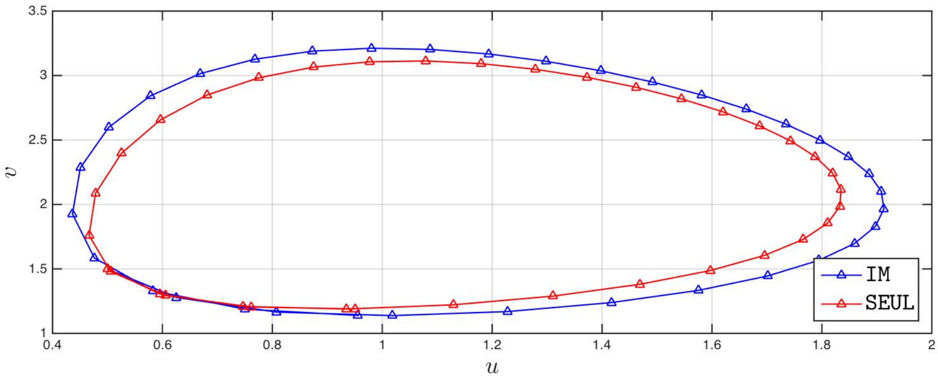

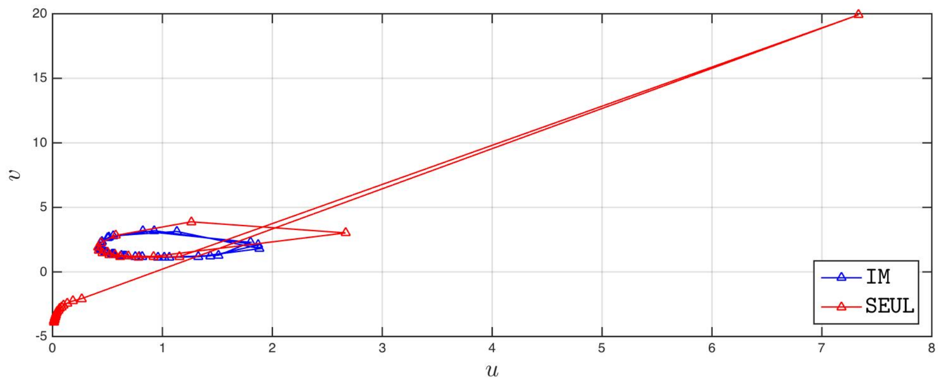

FIGURE 2. In the upper plot the discretized solution of the system † on the interval $[0, 10]$ with initial conditions $(u(0), v(0))^t = (0.5, 1.5)$ and $h = 10/35$ is shown. In the lower plot the discretized solution of ‡ with the same parameters is shown.

$$y(x_0 + h_0) \approx y_1 = y_0 + h_0 f\left(x_0 + \frac{h_0}{2}\right)$$
$$y(x_1 + h_1) \approx y_2 = y_1 + h_1 f\left(x_1 + \frac{h_1}{2}\right)$$
$$\vdots$$
$$y(x) \approx y_n = y_{n-1} + h_{n-1} f\left(x_{n-1} + \frac{h_{n-1}}{2}\right)$$

where $h_i = x_{i+1} - x_i$ and $x_0, x_1, \ldots, x_n = x$ is a subdivision of the interval $[x_0, x]$. If $f(x, y)$ is also dependent on the variable y, we can analogously consider for $x = x_0 + h$

$$y(x_0 + h) \approx y_1 := y_0 + hf\left(x_0 + \frac{h}{2}, y\left(x_0 + \frac{h}{2}\right)\right) \tag{13}$$

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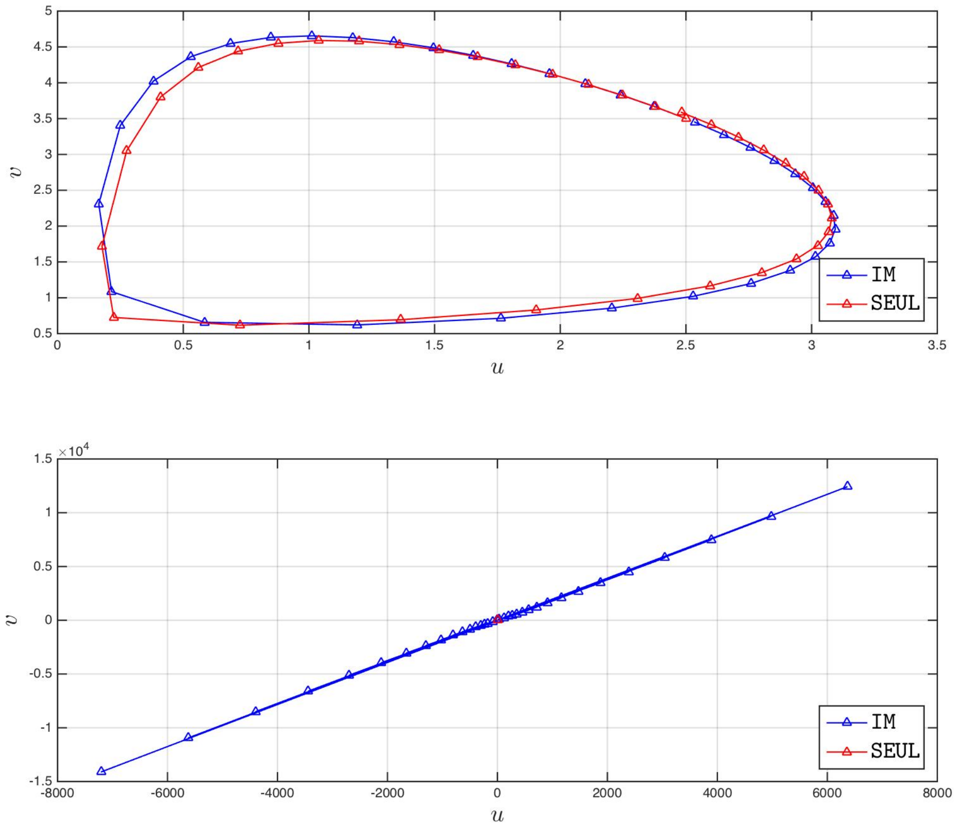


Figure 3. In the upper plot the discretized solution of the system † on the interval $[0, 10]$ with initial conditions $(u(0), v(0))^t = (2.5, 3.5)$ and $h = 10/35$ is shown. In the lower plot the discretized solution of ‡ with the same parameters is shown.

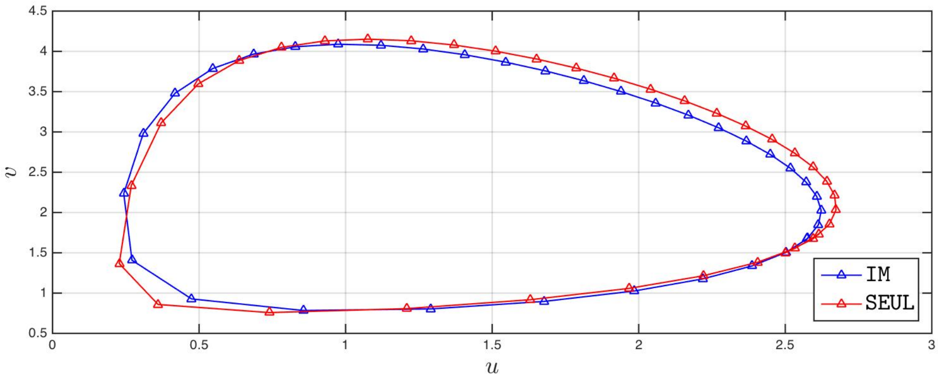
Since $y\left(x_0 + \frac{h}{2}\right)$ is unknown we may use explicit Euler for a further approximation. Thus we get $y\left(x_0 + \frac{h}{2}\right) \approx y_0 + \frac{h}{2} f(x_0, y_0)$. But now it is immediate that

$$\begin{aligned} k_1 &= f\left(x_0, y_0\right) \\ k_2 &= f\left(x_0 + \frac{h}{2}, y_0 + \frac{h}{2} k_1\right) \\ y_1 &= y_0 + h k_2 \end{aligned}$$

which is represented by the Butcher tableaux

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

Table 2. Butcher tableaux of Runge 2.



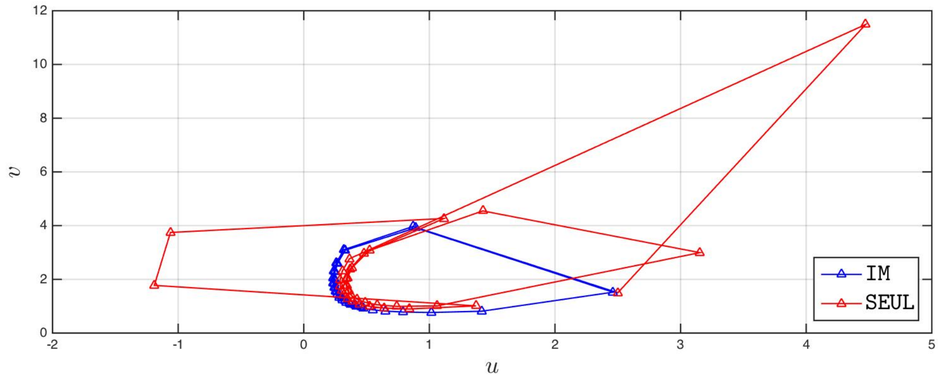


FIGURE 4. In the upper plot the discretized solution of the system † on the interval $[0, 10]$ with initial conditions $(u(0), v(0))^t = (2.5, 1.5)$ and $h = 10/35$ is shown. In the lower plot the discretized solution of ‡ with the same parameters is shown.

Exercise 27. By adding the equation $\dot{x} = 1$, we can assume without loss of generality that $f(x, y)$ does not depend on x *. Further we simplify notation by stipulating

$$k_i(h) = f\left(Y_i(h)\right), \qquad Y_i(h) := y_0 + h \sum_{j=1}^{s} a_{ij} k_j(h) \tag{15}$$

for $i = 1, \ldots, s$. Taylor expansion of the exact solution around $h = 0$ yields

* Assume we have a first order ODE system $y' = f(x, y)$, $f(x, y) \in C(I \times \mathbb{R}^n; \mathbb{R}^n)$ for some interval $I := [a, b]$. If we consider the first order system

$$\underbrace{\begin{bmatrix} y \\ x \end{bmatrix}'}_{=:\, z'} = \begin{bmatrix} y \\ y_{n+1} \end{bmatrix}' = \underbrace{\begin{bmatrix} f(y_{n+1}, y) \\ 1 \end{bmatrix}}_{=:\, \hat{f}(z)} \tag{14}$$

we get a new system $z' = \hat{f}(z)$ with $\hat{f} \in C(I \times \mathbb{R}^{n+1}; \mathbb{R}^{n+1})$ which is *autonomous*.

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$$\begin{aligned} y(x_0+h) =& y_0 + f(y_0)h + \frac{1}{2}f'(y_0)f(y_0)h^2 + \\ & \frac{1}{6}\left(f''(y_0)\left(f(y_0), f(y_0)\right) + \left(f'(y_0), f'(y_0)\right)f(y_0)\right)h^3 + O(h^4) \end{aligned}$$

Taylor expansion of the discretized solution provided by the s-stage Runge-Kutta method yields

$$\begin{aligned} y_1(h) =& y_0 + h\sum_{i=1}^{s} b_i k_i(h) \\ =& y_0 + \sum_{i=1}^{s} b_i k_i(0)h + \sum_{i=1}^{s} b_i \dot{k}_i(0)h^2 + \frac{1}{2}\sum_{i=1}^{s} b_i \ddot{k}_i(0) + O(h^4) \end{aligned}$$

Now we have

$$k_i(0) = f\left(Y_i(0)\right) = f(y_0) \tag{16}$$

Thus we get the condition $\boxed{\sum_{i=1}^{s} b_i = 1}$ for order one. Next

$$\dot{k}_i(h) = f'\left(Y_i(h)\right)\dot{Y}_i(h) \tag{17}$$

with $\dot{Y}_i(h) = \sum_{j=1}^{s} a_{ij}k_j(h) + h\sum_{j=1}^{s} a_{ij}\dot{k}_j(h)$. Thus we have $\dot{k}_i(0) = f'(y_0)\sum_{j=1}^{s} a_{ij}k_j(0) = f'(y_0)f(y_0)\sum_{j=1}^{s} a_{ij} = f'(y_0)f(y_0)c_i$ since by definition $c_i = \sum_{j=1}^{s} a_{ij}$ for $i = 1, \ldots, s$. Hence we have the order condition $\boxed{\sum_{i=1}^{s} b_i c_i = \frac{1}{2}}$ for order two. Finally we have

$$\ddot{k}_i = \frac{d}{dh}\dot{k}_i(h) = \frac{d}{dh}f'\left(Y_i(h)\right)\dot{Y}_i(h) = f''\left(Y_i(h)\right)\left(\dot{Y}_i(h), \dot{Y}_i(h)\right) + f'\left(Y_i(h)\right)\ddot{Y}_i(h) \tag{18}$$

with

$$\ddot{Y}_i(h) = \frac{d}{dh}\dot{Y}_i(h) = 2\sum_{j=1}^{s} a_{ij}\dot{k}_j(h) + h\sum_{j=1}^{s} a_{ij}\ddot{k}_j(h) \tag{19}$$

Thus we get

$$\ddot{k}_i(0) = f''(y_0)\left(\dot{Y}_i(0), \dot{Y}_i(0)\right) + f'(y_0)\ddot{Y}_i(0) \tag{20}$$

with

$$\ddot{Y}_i(0) = 2\sum_{j=1}^{s} a_{ij}\dot{k}_j(0) = 2f'(y_0)f(y_0)\sum_{j=1}^{s} a_{ij}c_j \tag{21}$$

and further

$$\ddot{k}_i(0) = f''(y_0)\left(f(y_0)c_i, f(y_0)c_i\right) + 2\left(f'(y_0), f'(y_0)\right)f(y_0)\sum_{j=1}^{s} a_{ij}c_j \tag{22}$$

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Hence we get the order conditions

$$\boxed{\sum_{i=1}^{s} b_i c_i^2 = \frac{1}{3} \qquad \sum_{i=1}^{s}\sum_{j=1}^{s} b_i a_{ij} c_j = \frac{1}{6}} \tag{23}$$

for order three. □

Remark: I have used the notation $(\cdot,\cdot)$ for $\cdot(\cdot,\cdot)$. Many thanks goes to Ernst Hairer[†] which sent me the essential proof steps on the 11^{th} of May, 2016 after electronic correspondence.

Exercise 28. The *implicit midpoint rule*[‡]is given by the Butcher tableaux

1/2	1/2
	1

TABLE 3. Butcher tableaux of the implicit midpoint rule.

Equivalently

$$y_1 = y_0 + hk_1 \qquad k_1 = f\left(x_0 + \frac{h}{2}, y_0 + \frac{h}{2}k_1\right) \tag{24}$$

Since the implicit midpoint method is a one-stage Runge Kutta method we have the ansatz $u(x) = y_0 + (x - x_0)k$ with $k = f(x_0 + c_1 h, y_0 + hc_1 k)$ for the collocation polynomial. Setting $c_1 = \frac{1}{2}$ we get the implicit midpoint rule since the numerical solution y_1 is given by $u(x_0 + h) = y_0 + hk$ (identical to the step provided by the implicit midpoint rule). Further we have

$$C(q): \qquad \sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{c_i^k}{k}, \qquad i = 1, \ldots, s, k = 1, \ldots, q$$

$$B(p): \qquad \sum_{i=1}^{s} b_i c_i^{k-1} = \frac{1}{k}, \qquad k = 1, \ldots, p$$

Consider $q = s = 1$. Then we have $C(1) = \sum_{j=1}^{s} a_{ij} c_j^{k-1} = \frac{1}{2} = c_i$ and

$$\sum_{i=1}^{s} b_i c_i^{k-1} = 1 = \frac{1}{k} \qquad \sum_{i=1}^{s} b_i c_i^{k-1} = \frac{1}{2} = \frac{1}{k} \tag{25}$$

for $k = 1$ and $k = 2$ respectively.

[†]http://www.unige.ch/~hairer/

[‡] Consider $y_1 = y_0 + hf\left(x_0 + \frac{h}{2}, \frac{y_0+y_1}{2}\right)$. Direct comparison with a one-stage Runge-Kutta scheme $y_1 = y_0 + hb_1 k_1$ yields $b_1 = 1$ and $k_1 = f\left(x_0 + \frac{h}{2}, \frac{y_0+y_1}{2}\right)$. Further comparison with $k_1 = f(x_0 + c_1 h, y_0 + ha_{11}k_1)$ yields $c_1 = \frac{1}{2}$. Now we have $\frac{y_0+y_1}{2} = \frac{1}{2}(y_0 + y_1 + y_0 - y_0) = y_0 + \frac{1}{2}(y_1 - y_0) = y_0 + \frac{h}{2h}(y_1 - y_0) = y_0 + \frac{1}{2}h\left(\frac{y_1 - y_0}{h}\right)$ and by using the definition of y_1 by the implicit midpoint rule we get $y_0 + \frac{1}{2}h\left(\frac{y_1-y_0}{h}\right) = y_0 + \frac{1}{2}hf\left(x_0 + \frac{h}{2}, \frac{y_0+y_1}{2}\right) = y_0 + \frac{1}{2}hk$. Thus $a_{11} = \frac{1}{2}$.

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[Kos89] Peter Kosmol. *Methoden zur numerischen Behandlung nichtlinearer Gleichungen und Optimierungsaufgaben*. B.G. Teubner Stuttgart, 1989.