ÉCOLE POLYTECHNIQUE
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1 ► Order of implicit methods

For autonomous IVPs, find and prove the consistency order of the implicit midpoint rule given by the table $\begin{array}{c|c} 1/2 & 1/2 \\ \hline & 1 \end{array}$.

2 ► Implementation of implicit RK methods

(a) Write a function `z = newton(F,dF,z0,atol,maxiter)` which implements Newton's method

$$DF(\mathbf{z}^k)\Delta\mathbf{z}^k = -F(\mathbf{z}^k), \quad \mathbf{z}^{k+1} = \mathbf{z}^k + \Delta\mathbf{z}^k,$$

starting from $\mathbf{z}^0$, and terminating after `maxiter` steps, or when the criterion

$$\frac{\theta^k}{1-\theta^k}\|\Delta\mathbf{z}^k\| \le \texttt{atol}, \quad \theta^k = \|\Delta\mathbf{z}^k\|/\|\Delta\mathbf{z}^{k-1}\|$$

is satisfied (set $\theta_1 = 1$). If you find this boring you might download the method from the homepage.

(b) Implement the implicit trapezoidal rule $\begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}$ as a MATLAB function.
It could have the syntax `[t,y] = itrapez(f,tspan,y0,N,fjac,atol,maxiter)`.
Here `fjac(t,y)` should be the Jacobian of $\mathbf{y} \mapsto f(t,\mathbf{y})$.

For a general implicit RK method at iterate $\mathbf{y}_n$, let $G\colon \mathbb{R}^{ds} \to \mathbb{R}^{ds}$ be given by

$$G(\mathbf{z}) = \begin{pmatrix} \sum_{j=1}^s a_{1j} f(t+c_jh, \mathbf{y}_n + \mathbf{z}_j) \\ \vdots \\ \sum_{j=1}^s a_{sj} f(t+c_jh, \mathbf{y}_n + \mathbf{z}_j) \end{pmatrix} \in \mathbb{R}^{ds}, \quad \mathbf{z} = \begin{pmatrix} \mathbf{z}_1 \\ \vdots \\ \mathbf{z}_s \end{pmatrix} \in \mathbb{R}^{ds}.$$

The Newton method from (a) has to be called to solve for $F(\mathbf{z}) = \mathbf{z} - hG(\mathbf{y}_n, \mathbf{z}) = 0$ using $\mathbf{z}^0 = 0$ as a starting value.[1] The next step then is

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\sum_{j=1}^s b_j f(t + c_jh, \mathbf{y}_n + \mathbf{z}_j).$$

(c) Consider an interaction of three species modelled by

$$\mathbf{y}' = f(t,\mathbf{y}) = \begin{pmatrix} -0.04y_1 + 10^4 y_2y_3 \\ 0.04y_1 - 10^4y_2y_3 - 3\cdot 10^7 y_2^2 \\ 3\cdot 10^7 y_2^2 \end{pmatrix}, \quad \mathbf{y}(0) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}.$$

(i) Plot the solution component y_2 you obtain with `itrapez` on the time interval $[0, 0.3]$ using $N = 20, 50, 100, 200$ for $\texttt{atol} = 10^{-4}$ and 10^{-6} (use $\texttt{maxiter} = 10$). Compare to the explicit Runge-Kutta method for these values of N.

(ii) Now call the explicit `ode45` and the implicit `ode23s` from MATLAB, which both have a step size control. Try
`ode45(f,[0,0.3],[1 0 0]',odeset('Stats','on'))`,
`ode23s(f,[0,0.3],[1 0 0]',odeset('Stats','on'))`, and
`ode23s(f,[0,0.3],[1 0 0]',odeset('Stats','on','Jacobian',fjac))`
(where `fjac` should be the function handle of the Jacobian). Have a look on the number of steps sizes and number of rejected steps.

[1] In case of the implicit trapezoidal rule, if `tn` and `yn` are the current values, this amounts in, e.g., passing the following two function handles to the Newton method:

```
F = @(z) z - h*[zeros(d,1); f(tn,yn + z(1:d))/2 + f(tn + h,yn + z(d+1:2*d))/2];
dF = @(z) eye(2*d) - h*[zeros(d,2*d); fjac(tn,yn + z(1:d))/2, fjac(tn + h,yn + z(d+1:2*d))/2];
```

3 ► Stability of rational approximation

Assume the linear ODE

$$\mathbf{y}' = A\mathbf{y}$$

is stable. For a rational approximation S of the exponential function of consistency order p show the following: If the characteristic step size h_c is positive, then there exists $C > 0$ such that

$$\| \exp(nhA) - S(hA)^n \| \leq Ch^p \quad \text{for all } 0 < h < h_c.$$