

Diversi Problemi-Test

(Metodi numerici per le ODEs)

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METODI NUMERICI PER ODEs

Test cases: Initial Value Problems

1. Consider the initial value problem in \mathbb{R}^2 :

$$\dot{y} = Ay \quad t \in [0, T], \quad y \in \mathbb{R}^n ,$$

with $n = 2$, $T = 10$ and initial data $y(0) = [1, 1]^T$ where the matrix $A \in \mathbb{R}^{n \times n}$ is given by:

$$A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

2. Brusselator-ODEs

$$(0.1) \quad \begin{cases} \dot{y}_1 = 1 + y_1^2 y_2 - 4y_1 \\ \dot{y}_2 = 3y_1 - y_1^2 y_2 , \end{cases}$$

with initial data $y_1(0) = 1.01$, $y_2(0) = 3$, in the time intervall $[0, 20]$.

3. Van der Pol system:

$$(0.2) \quad \begin{cases} \dot{y}_1 = y_2(A - y_1) \\ \dot{y}_2 = \varepsilon ((1 - y_1^2)y_2 - y_1) (A - y_1) , \quad \varepsilon > 0 . \end{cases}$$

For different values of ε . Take also $\varepsilon = 1$. For such value, the system has a limit cycle with period $6 < T < 7$ that passes through $y = [A, 0]$, with

$$A = 1.00861986087484313650940188 .$$

Take as initial data $y_1(0) = 1$, $y_2(0) = 0$, and study how well the methods can approximate the limit cycle.

4. Full Brusselator (in the time interval $[0, 20]$):

$$(0.3) \quad \begin{cases} \dot{y}_1 = 1 + y_1^2 y_2 - (y_3 + 1)y_1 \\ \dot{y}_2 = y_1 y_3 - y_1^2 y_2, \\ \dot{y}_3 = -y_1 y_3 + \alpha, \end{cases}$$

with initial data $y_1(0) = 1.01$, $y_2(0) = 3$, $y_3(0) = 0$. In the above equations $\alpha \in \mathbb{R}^+$. Take different values of $\alpha \in [1, 1.5]$ and study how the approximation (qualitatively) depends on different values of α . What happens if $\alpha \mapsto \infty$ is taken arbitrary large??

5. Consider the problem(s) in \mathbb{R}^2 :

$$\dot{y} = Ay + g(t) \quad t \in [0, T], \quad y \in \mathbb{R}^n,$$

with $n = 2$, $T = 10$ and initial data $y(0) = [2, 3/2]^T$ where $A \in \mathbb{R}^{n \times n}$ and $g(t)$ are respectively, the matrix and functions given by:

- Case 1:

$$A = \begin{pmatrix} -2 & 1 \\ 1 & -2 \end{pmatrix} \quad g(t) = \begin{bmatrix} 2 \sin(t) \\ 2(\cos(t) - \sin(t)) \end{bmatrix}$$

- Case 2:

$$A = \begin{pmatrix} -2 & 1 \\ 998 & -999 \end{pmatrix} \quad g(t) = \begin{bmatrix} 2 \sin(t) \\ 999(\cos(t) - \sin(t)) \end{bmatrix}$$

6. Pendulum system in $[0, t_f]$

$$(0.4) \quad \begin{cases} \dot{z}_1 = y_1 \\ \dot{y}_1 = 0 \\ \dot{z}_2 = y_2, \\ \dot{y}_2 = -\omega^2 z_2, \end{cases}$$

with initial data $z_1(0) = 1$, $y_1(0) = 1$, $z_2(0) = \omega^{-1}$, $y_2(0) = 1$. The Hamiltonian is given by

$$H(z_1, y_1, z_2, y_2) = \frac{1}{2}(y_1^2 + y_2^2) + \frac{\omega^2}{2}(z_1^2 + z_2^2),$$

Besides the Hamiltonian (total energy), you can also measure the energy of each spring

$$I_1(z_1, y_1) = \frac{1}{2}(y_1^2 + \omega^2 z_1^2) \quad I_2(z_2, y_2) = \frac{1}{2}(y_2^2 + \omega^2 z_2^2)$$

To integrate effectively the system, one should use a method that is able to reproduce the qualitative features of the solution, and in particular methods able to conserve the Hamiltonian (total energy). Study the effect for large values of $\omega = 10, 50, 100, \dots$

7. Lotka-Volterra Model (used in bio-mathematics to model the grow of different species)

$$(0.5) \quad \begin{aligned} \dot{u} &= u(v - 2) \\ \dot{v} &= v(1 - u), \end{aligned}$$

and consider different values of initial data $[u(0), v(0)]^T = [4, 8]^T, [4, 2]^T, [6, 2]^T$. The solutions of the above system are periodic, and it would be desirable to verify which numerical methods can preserve this property. The system has the following Invariant :

$$(0.6) \quad I(u, v) = \log(u) - u + 2 \log(v) - v .$$

and as such it remains constant along a solution to (0.5). Which methods are able to preserve the invariant?

8. Consider the initial value problems:

$$(0.7) \quad (a) \quad \begin{cases} u' = \frac{(v-2)}{v} \\ v' = \frac{(1-u)}{u} \end{cases} \quad (b) \quad \begin{cases} u' = u^2 v(v-2) \\ v' = v^2 u(1-u) \end{cases}$$

Both systems have the same invariant (0.6) as the Lotka-Volterra system and therefore their solutions are also periodic. Which methods produce numerical solutions having this behaviour?

9. The (mathematical) Pendulum is a system with one degree of freedom and Hamiltonian (operator that *represents* total energy of the system)

$$H(p, q) = \frac{1}{2}(p^2 - \cos(q)) ,$$

where q denote the position coordinates and p the momenta. The equations of motion in $[0, 2\pi]$ are:

$$(0.8) \quad \begin{cases} \dot{p} = -\sin(q), \\ \dot{q} = p \end{cases}$$

Along the solution of the above system, the Hamiltonian (so the Energy) remains constant. To integrate effectively the system, one should use a method that is able to reproduce the qualitative features of the solution, and in particular verify the property of the Hamiltonian.

10. Two-Body problem (Kepler problem): models the motion of two bodies which attract to each other. The center of the coordinate system is located at one of the bodies, and the motion will stay in a plane. The position of the second body is given by $q = (q_1, q_2)$ and its motion is given by the system:

$$(0.9) \quad \begin{cases} \ddot{q}_1 = -\frac{q_1}{(q_1^2 + q_2^2)^{3/2}} \\ \ddot{q}_2 = -\frac{q_2}{(q_1^2 + q_2^2)^{3/2}} \end{cases}$$

It can be converted into a first order system introducing the momentum variable $p_1 = \dot{q}_1$, $p_2 = \dot{q}_2$. The Hamiltonian of the system (total energy) is

$$H(p_1, p_2, q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}}$$

The system has also the angular momentum as another invariant:

$$L(p_1, p_2, q_1, q_2) = q_1 p_2 - q_2 p_1 .$$

This is what you might know as *Kepler's second law* (a planet sweeps equal area at equal times).

Consider as initial data for the system:

$$(0.10) \quad q_1(0) = 1 - e, \quad q_2(0) = 0, \quad \dot{q}_1(0) = 0, \quad \dot{q}_2(0) = \sqrt{\frac{1+e}{1-e}}$$

where $e \in [0, 1)$ is the eccentricity of the ellipse. Study which numerical methods are able to reproduce the qualitative features of the solution and study which conserve the invariants of the system.

For the case $e = 0.6$ the values for the exact solution at time $t = 7.5$ are given by:

$$\begin{aligned} q_1 &= -0.828164402690770818204757585370 \\ q_2 &= 0.778898095658635447081654480796 \\ p_1 &= -0.856384715343395351524486215030 \\ p_2 &= -0.160552150799838435254419104102 \end{aligned}$$

HINT: If you do not want to type the above numbers, you can copy them from this PDF.

11. The following example is taken from: [Hairer, Nørsett, Wanner: Solving Ordinary Differential Equations I, Springer 1993]. It is an instance of the restricted three body problem, and one may think about a small particle flying in the plane under the influence of the

earth clamped at the origin and the moon surrounding it on the unit circle. The plane has to be imagined as a relative coordinate system of the earth which rotates slowly around the sun. The equations of motion for the position $\mathbf{x} = (x_1, x_2)^T$ of the particle are

$$(0.11) \quad \ddot{\mathbf{x}} = \begin{pmatrix} x_1 + 2\dot{x}_2 \\ x_1 - 2\dot{x}_2 \end{pmatrix} = \frac{\tilde{\nu}}{((x_1 + \nu)^2 + x_2^2)^{3/2}} \begin{pmatrix} x_1 + \nu \\ x_2 \end{pmatrix} - \frac{\nu}{((x_1 - \tilde{\nu})^2 + x_2^2)^{3/2}} \begin{pmatrix} x_1 - \tilde{\nu} \\ x_2 \end{pmatrix},$$

where $\nu = 0.012277471$ is the mass of the moon, while $\tilde{\nu} = 1 - \nu$ is the mass of the earth. For the following starting values the solution should be periodic:

$$\mathbf{x}(0) = \begin{pmatrix} 0.994 \\ 0 \end{pmatrix}, \quad \dot{\mathbf{x}}(0) = \begin{pmatrix} 0 \\ -2.00158510637908252240537862224 \end{pmatrix},$$

The period is $T = 17.0652165601579625588917206249$.

Solve the equation using these values on the time interval $[0, T]$ using explicit Euler, a 4-th order Runge-Kutta and implicit euler with different values of h . Compare the results with those obtained with a RK embedded.

In particular compare efficiency. Plot the curves (in phase space) of $(x_1, x_2, \dot{x}_1, \dot{x}_2)$ to get an idea of the suitability of the methods.

HINT: If you do not want to type the above numbers, you can copy them from this PDF.

12. **(Eigenvalues of the discrete Laplacian)** Consider the following $N \times N$ matrix, used for the discretization (with finite differences) of the Laplacian in space-dimension one (say, in the unit interval) with Dirichlet boundary conditions,

$$(0.12) \quad \tilde{A} = \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & \ddots & \ddots \\ & & \ddots & -2 \end{pmatrix}, \quad A = \frac{1}{h_x^2} \tilde{A} \in \mathbb{R}^{N \times N},$$

where $h_x = \frac{1}{N+1}$.

Show that the eigenvalues of \tilde{A} are:

$$(0.13) \quad \lambda_k = -2 + 2 \cos \left(\frac{k\pi}{N+1} \right), \quad k = 1, \dots, N.$$

with associated eigenvectors $v^k = (v_1^k, v_2^k, \dots, v_N^k)^T$ given by

$$(0.14) \quad v_j^k = C \sin \left(\frac{jk\pi}{N+1} \right), \quad 1 \leq j, k \leq N.$$

13. **(Application to PDEs)** Consider the Brusselator problem: find $u, v \in \mathcal{C}^0([0, T]; H^1([0, 1])) \cap \mathcal{C}^1((0, T); L^2([0, 1]))$ solution to the system of PDEs

$$(0.15) \quad \begin{aligned} \frac{\partial u}{\partial t} &= a + u^2 v - (b+1)u + \nu \frac{\partial^2 u}{\partial x^2}, & x \in (0, 1) \\ \frac{\partial v}{\partial t} &= bu - u^2 v + \nu \frac{\partial^2 v}{\partial x^2}, & x \in (0, 1) \end{aligned}$$

with the boundary conditions

$$(0.16) \quad u(0, t) = u(1, t) = 1, \quad v(0, t) = v(1, t) = 3,$$

and initial conditions

$$(0.17) \quad u(x, 0) = 1 + \sin(2\pi x), \quad v(x, 0) = 3.$$

We consider the parameters $a = 1, b = 3$ and $\nu = 0.02$. Give explicitly the system of ODEs obtained by discretizing the spatial variable of the above system applying the method of lines (discretize the space variable using finite differences; see below). Using previous test/exercise, perform a linear stability analysis of the resulting system of ODEs and give the time-step restriction for the methods you decide to use for the approximation. (Start with euler...)

PRELIMINARIES: SPACE DISCRETIZATION We consider the discretization of the space $[0, 1]$ into $N + 1$ subintervals of length $h_x = 1/(N + 1)$:

$$(0.18) \quad 0 = x_0 < x_1 < \dots < x_N < x_{N+1} = 1 \quad x_i = \frac{i}{N+1}, \quad i = 0, \dots, N+1,$$

The space discretization for $u(x, t)$ (and similarly for $v(x, t)$) is then

$$(0.19) \quad U_i(t) \approx u(x_i, t) \quad V_i(t) \approx v(x_i, t) \quad x_i = \frac{i}{N+1}, \quad i = 0, \dots, N+1,$$

Since $U_0(t)$ and $U_{N+1}(t)$ (resp. $V_0(t)$ and $V_{N+1}(t)$) are already known from the boundary conditions (0.16), the unknown functions become the vectors of size N : $\mathbf{U}(t) = [U_1(t), \dots, U_N(t)]^T$ and $\mathbf{V}(t) = [V_1(t), \dots, V_N(t)]^T$ which are solution of a (possibly large)

nonlinear system of ODEs.

Chemical reaction: one should create a separate function that computes the (nonlinear) terms corresponding to the chemical reaction in (0.15), (i.e., without the diffusion terms) that takes as input the two vectors when two $\mathbf{U} = [U_1, \dots, U_N]^T$, $\mathbf{V} = [V_1, \dots, V_N]^T$ and provides the output vectors with components:

$$\mathbf{f}\mathbf{u}_i = a + U_i^2 V_i - (b + 1)U_i, \quad \mathbf{f}\mathbf{v}_i = bU_i - U_i^2 V_i, \quad i = 1, \dots, N.$$

Diffusion terms: the second derivatives can be discretized with the second order divided differences (can you verify is second order?) which correspond to

$$\Delta \mathbf{U} \longrightarrow A \mathbf{U}$$

with $A \in \mathbb{R}^{N \times N}$ being the matrix in (0.12).

STABILITY OF EXPLICIT EULER: Take a reasonable space discretization (e.g., $N = 30, 40, \dots$) and compute the numerical solution of the Brusselator problem (0.15), with diffusion in the time interval $[0, 10]$ using different time steps. Study what happen taking a small ($\nu = 1e - 04$) or larger diffusion coefficient. Verify numerically (and deduce!) that the explicit Euler method is stable for

$$dt \leq \frac{h_x^2}{2\nu} \quad \text{Courant-Friedrichs-Lewy (CFL) condition}$$

This condition is the so-called **Courant-Friedrichs-Lewy (CFL) condition**.

STABILITY OF IMPLICIT EULER: this is a good example to study what happen with the different iterations for solving the nonlinear system at each time step in implicit Euler integration.