Numerical Solution of Differential Equations I

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Lecture 11

Motivation

Example (MATLAB)

Compare the implicit midpoint rule with the explicit and implicit Euler methods for the following initial-value problem:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \qquad \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}(0) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

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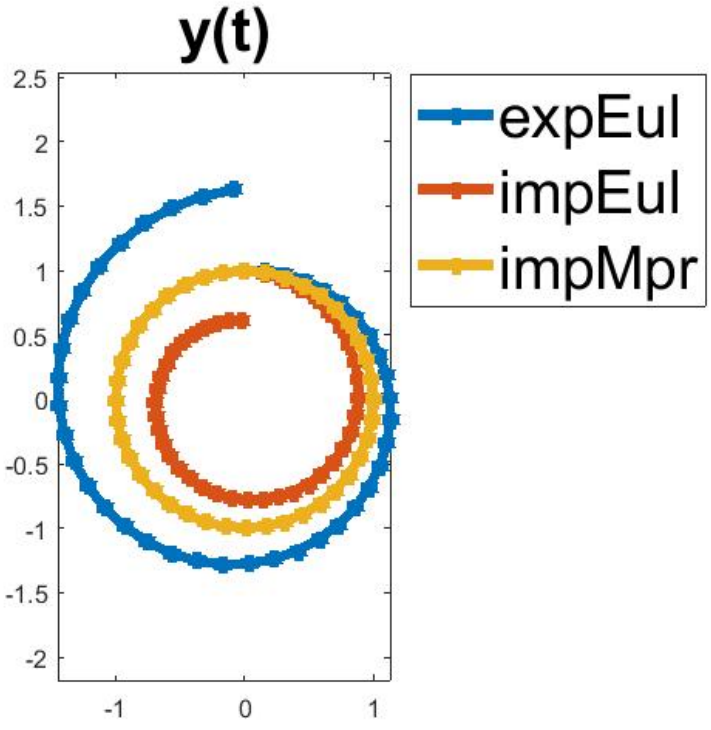
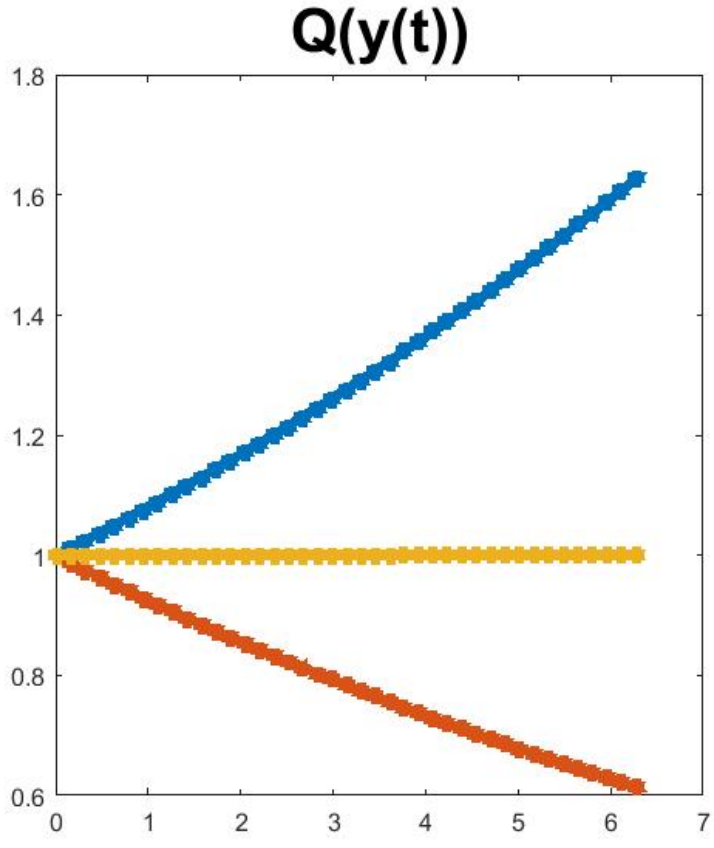
[Run the MATLAB code: testcase2a.m]


y(t)
2.5
2
1.5
1
0.5
0
-0.5
-1
-1.5
-2
-1
0
1
expEul
impEul
impMpr


Q(y(t))
1.8
1.6
1.4
1.2
1
0.8
0.6
0
1
2
3
4
5
6
7

The implicit midpoint rule for $\mathbf{y}'(t) = \mathbf{f}(\mathbf{y}(t))$, $\mathbf{y}(0) = \mathbf{x}$

$$\frac{\mathbf{y}_{n+1} - \mathbf{y}_n}{h} = \mathbf{f}\left(\frac{\mathbf{y}_{n+1} + \mathbf{y}_n}{2}\right), \quad n = 0, 1, \ldots,$$

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Exercise. Let $(\cdot, \cdot)$ be the inner product in $\mathbb{R}^d$ and let $\|\cdot\|$ be the associated Euclidean norm in $\mathbb{R}^d$. Suppose that $\mathbf{f} : D \subset \mathbb{R}^d \to \mathbb{R}^d$ and $(\mathbf{f}(\mathbf{z}), \mathbf{z}) = 0$ for all $\mathbf{z} \in D$. Show that if $\mathbf{y}' = \mathbf{f}(\mathbf{y})$, $\mathbf{y}(0) = \mathbf{x}$ and $\mathbf{y}_n$ is the implicit midpoint approximation of $\mathbf{y}$, then:

(a) $\|\mathbf{y}(t)\|^2 = \|\mathbf{x}\|^2$ for all $t \geq 0$;

(b) $\|\mathbf{y}_n\|^2 = \|\mathbf{x}\|^2$ for all $n \in \mathbb{N}_0 := \mathbb{N} \cup \{0\}$.

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Hint: Take the inner product of
(a) the ODE with $\mathbf{y}(t)$; and
(b) the implicit midpoint rule with $\frac{\mathbf{y}_{n+1}+\mathbf{y}_n}{2}$.

Structure-preserving integrators

In many time-dependent physical problems modelled by initial-value problems, certain relevant physical quantities (e.g. energy, mass, volume, etc.), are preserved during the course of evolution, i.e. they are constant in time.

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One needs to preserve some of these quantities at the discrete level.

For simplicity, we restrict ourselves to the autonomous ODE

$$\mathbf{y}' = \mathbf{f}(\mathbf{y}), \quad \text{where} \quad \mathbf{f} : D \to \mathbb{R}^d, \tag{1}$$

(where now $\mathbf{y}$ is considered to be a function of $t \in [0, \infty)$, and $\mathbf{y}' := \mathrm{d}\mathbf{y}/\mathrm{d}t$), subject to the initial condition

$$\mathbf{y}(0) = \mathbf{x},$$

where $\mathbf{x} \in D$, and D is a nonempty open subset of $\mathbb{R}^d$.

Definition

For $t \geq 0$, let $\mathbf{\Phi}^t : D \to \mathbb{R}^d$ denote the function that maps an initial datum $\mathbf{x} \in D$ into $\mathbf{y}(t) \in \mathbb{R}^d$, where $\mathbf{y}(t)$ is the solution at time t to $\mathbf{y}' = \mathbf{f}(\mathbf{y})$, $\mathbf{y}(0) = \mathbf{x}$ (tacitly assuming that the solution $t \in [0, \infty) \mapsto \mathbf{y}(t) \in \mathbb{R}^d$ to this initial-value problem, for each $\mathbf{x} \in D$, exists and that it is unique).

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The family $\{\mathbf{\Phi}^t\}_{t \geq 0}$ is called the *flow* of (1) (defined on $D \subset \mathbb{R}^d$).

Remark

The function $t \mapsto \mathbf{\Phi}^t \mathbf{x}$ *is the solution to* $\mathbf{y}' = \mathbf{f}(\mathbf{y})$, $\mathbf{y}(0) = \mathbf{x}$.

Using the concept of flow, we can clarify what is a “preserved quantity”.

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Definition

A *first integral* of (1) is a function $I : D \to \mathbb{R}$ that satisfies $I(\mathbf{\Phi}^t \mathbf{x}) = I(\mathbf{x})$ for every $\mathbf{x} \in D$ and every admissible $t \geq 0$.

Lemma

I is a first integral of (1) if, and only if, $\frac{\mathrm{d}}{\mathrm{d}t} I(\mathbf{\Phi}^t \mathbf{x}) = 0$ for every $\mathbf{x} \in D$ and every admissible $t \geq 0$. This is equivalent to:

$$\mathbf{D}I(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) = 0 \qquad \text{for every } \mathbf{x} \in D,$$

where $\mathbf{D}I(\mathbf{x}) := \mathbf{grad}\, I(\mathbf{x}) = (\frac{\partial I}{\partial x_1}, \ldots, \frac{\partial I}{\partial x_d})^{\mathrm{T}}$.

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where $\mathbf{y}$ is the solution of the initial-value problem $\mathbf{y}'(t) = \mathbf{f}(\mathbf{y}(t))$, $\mathbf{y}(0) = \mathbf{x} \in D$.

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where $\mathbf{y}$ is the solution of the initial-value problem $\mathbf{y}'(t) = \mathbf{f}(\mathbf{y}(t))$, $\mathbf{y}(0) = \mathbf{x} \in D$. Thus in particular $0 = \mathbf{D}I(\mathbf{y}(0)) \cdot \mathbf{f}(\mathbf{y}(0))$, and the assertion follows, because $\mathbf{y}(0) = \mathbf{x} \in D$. $\diamond$

For a systematic investigation, we consider first integrals that can be expressed as polynomials.

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Definition

We shall say that a first integral I of an autonomous system is a polynomial of degree $n \in \mathbb{N}$ if

$$I(\mathbf{x}) = \sum_{\boldsymbol{\alpha} \in \mathbb{N}_0^d,\, |\boldsymbol{\alpha}| \leq n} \beta_{\boldsymbol{\alpha}} \mathbf{x}^{\boldsymbol{\alpha}}, \tag{2}$$

where $\beta_{\boldsymbol{\alpha}} \in \mathbb{R}$, $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$, $|\boldsymbol{\alpha}| = \sum_{i=1}^d \alpha_i$, and $\mathbf{x}^{\boldsymbol{\alpha}} = x_1^{\alpha_1} \cdots x_d^{\alpha_d}$; in other words, I is a multivariate polynomial of degree n in $\mathbf{x} \in \mathbb{R}^d$.

Example

Linear first integrals are of the form $I(\mathbf{x}) = \mathbf{b}^{\mathrm{T}}\mathbf{x} + c$ (with $\mathbf{b} \in \mathbb{R}^d$, and $c \in \mathbb{R}$).

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Quadratic first integrals are of the form $I(\mathbf{x}) = \mathbf{x}^{\mathrm{T}}\mathbf{M}\mathbf{x} + \mathbf{b}^{\mathrm{T}}\mathbf{x} + c$ (with $\mathbf{M} = \mathbf{M}^{\mathrm{T}} \in \mathbb{R}^{d\times d}$, $\mathbf{b} \in \mathbb{R}^d$, and $c \in \mathbb{R}$).

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Consider the R-stage Runge–Kutta method

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h(c_1\mathbf{k}_1 + \cdots + c_R\mathbf{k}_R).$$

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Hence,

$$\begin{aligned} I(\mathbf{y}_{n+1}) - I(\mathbf{y}_n) &= \mathbf{b}^{\mathrm{T}}(\mathbf{y}_{n+1} - \mathbf{y}_n) \\ &= h\,\mathbf{b}^{\mathrm{T}}(c_1\mathbf{k}_1 + \cdots + c_R\mathbf{k}_R) = 0 + \cdots + 0 = 0. \end{aligned}$$

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Theorem

Gauss-collocation methods (i.e. Runge–Kutta methods based on function-evaluations at points of Gaussian quadrature rules) preserve quadratic first integrals.

Simple examples of Gauss-collocation methods are the Gauss–Legendre–Runge–Kutta methods, based on function-evaluations at points of Gauss–Legendre quadrature rules.

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Example

The Gauss–Legendre method of order two is the **implicit midpoint rule**,

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\,\mathbf{f}\left(t_n + \frac{1}{2}h, \frac{1}{2}\mathbf{y}_n + \frac{1}{2}\mathbf{y}_{n+1}\right)$$

which has Butcher tableau

$$\begin{array}{c|c} 1/2 & 1/2 \\ \hline & 1 \end{array} \quad .$$

Example

The Gauss–Legendre method of order four

$$\mathbf{y}_{n+1} = \mathbf{y}_n + h\left(\frac{1}{2}\mathbf{k}_1 + \frac{1}{2}\mathbf{k}_2\right), \qquad \text{where}$$

$$\mathbf{k}_1 = \mathbf{f}\left(t + \left(\frac{1}{2} - \frac{1}{6}\sqrt{3}\right)h, \mathbf{y}_n + \frac{1}{4}\mathbf{k}_1 + \left(\frac{1}{4} - \frac{1}{6}\sqrt{3}\right)\mathbf{k}_2\right),$$

$$\mathbf{k}_2 = \mathbf{f}\left(t + \left(\frac{1}{2} + \frac{1}{6}\sqrt{3}\right)h, \mathbf{y}_n + \left(\frac{1}{4} + \frac{1}{6}\sqrt{3}\right)\mathbf{k}_1 + \frac{1}{4}\mathbf{k}_2\right)$$

has Butcher tableau

$$\begin{array}{c|cc} \frac{1}{2} - \frac{1}{6}\sqrt{3} & \frac{1}{4} & \frac{1}{4} - \frac{1}{6}\sqrt{3} \\ \frac{1}{2} + \frac{1}{6}\sqrt{3} & \frac{1}{4} + \frac{1}{6}\sqrt{3} & \frac{1}{4} \\ \hline & \frac{1}{2} & \frac{1}{2} \end{array}.$$

Unfortunately, there is no consistent Runge–Kutta method that preserves polynomial first integrals of degree higher than 2; more precisely, the following negative result holds.

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Theorem

If $n \geq 3$, then there is no consistent Runge–Kutta method that preserves every polynomial first integral of degree n for every autonomous ODE.

We conclude with a few results concerning the conservation of a structure that is at the heart of classical mechanics: conservation of the symplectic product.

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Definition

A **Hamiltonian differential equation** is an ODE of the form

$$\mathbf{p}' = -\mathbf{D_q} H(\mathbf{p}, \mathbf{q}), \quad \mathbf{q}' = \mathbf{D_p} H(\mathbf{p}, \mathbf{q}), \tag{3}$$

where the function $H : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is called the *Hamiltonian*.

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Proof. This follows by applying the chain rule:

$$\frac{\mathrm{d}}{\mathrm{d}t} H(\mathbf{p}, \mathbf{q}) = \mathbf{D_p} H(\mathbf{p}, \mathbf{q}) \cdot \mathbf{p}' + \mathbf{D_q} H(\mathbf{p}, \mathbf{q}) \cdot \mathbf{q}' = 0. \qquad \diamond$$

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Lemma

The ODE (3) *is equivalent to*

$$\mathbf{y}' = \mathbf{J}^{-1} \mathbf{D} H(\mathbf{y}), \tag{4}$$

where $\mathbf{J} = \begin{pmatrix} \mathbf{0} & \mathbf{I} \\ -\mathbf{I} & \mathbf{0} \end{pmatrix} \in \mathbb{R}^{2d \times 2d}$ *and* $\mathbf{y} := \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix} \in \mathbb{R}^{2d}$.

The proof of this lemma is left as an exercise.

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Definition

The bilinear map

$$\omega : \mathbb{R}^{2d} \times \mathbb{R}^{2d} \to \mathbb{R}, \quad (\mathbf{a}, \mathbf{b}) \mapsto \omega(\mathbf{a}, \mathbf{b}) \coloneqq \mathbf{a}^{\mathrm{T}} \mathbf{J}\, \mathbf{b}$$

is called the *symplectic product* of $\mathbf{a}$ and $\mathbf{b}$.

Definition

A continuously differentiable map $\mathbf{\Phi} : D \subset \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is called *symplectic* if

$$\omega(\mathbf{D\Phi}(\mathbf{x})\mathbf{a}, \mathbf{D\Phi}(\mathbf{x})\mathbf{b}) = \omega(\mathbf{a}, \mathbf{b})$$

for every $\mathbf{x} \in D$ and every pair $(\mathbf{a}, \mathbf{b}) \in \mathbb{R}^{2d} \times \mathbb{R}^{2d}$.

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Remark

In other words, a map $\mathbf{\Phi}$ is symplectic if its Jacobian matrix $\mathbf{D\Phi}(\mathbf{x})$ (evaluated at a generic point $\mathbf{x}$) preserves the simplectic product.

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This concept is similar to the property of orthogonal matrices that they preserve the Euclidean inner product, i.e. if $\mathbf{O} \in \mathbb{R}^{d \times d}$ is an orthogonal matrix then $\langle \mathbf{Oa}, \mathbf{Ob} \rangle = \langle \mathbf{a}, \mathbf{b} \rangle$ for every pair $(\mathbf{a}, \mathbf{b})$ in $\mathbb{R}^d \times \mathbb{R}^d$, where $\langle \cdot, \cdot \rangle$ is the Euclidean inner product in $\mathbb{R}^d$.

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which explains why the concept of symplectic map is so relevant.

Theorem (Poincaré)

If H is a twice continuously differentiable Hamiltonian, then the flow $\mathbf{\Phi}^t$ of an Hamiltonian differential equation satisfies the following property: for each $\mathbf{x} \in D$ there exists a $\delta > 0$ such that

$$\omega(\mathbf{D\Phi}^t(\mathbf{x})\mathbf{a}, \mathbf{D\Phi}^t(\mathbf{x})\mathbf{b}) = \omega(\mathbf{a}, \mathbf{b})$$

for every $(\mathbf{a}, \mathbf{b}) \in \mathbb{R}^{2d} \times \mathbb{R}^{2d}$ and all $t \in [0, \delta)$.

Since Hamiltonian flows are symplectic, we are interested in symplectic one-step methods, in the following sense.

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Definition

Consider (4) subject to the initial condition $\mathbf{y}(0) = \mathbf{x}$, for $\mathbf{x} \in D$, and let $\mathbf{x} \mapsto \boldsymbol{\Psi}(0, \mathbf{x}; h)$ be a one-step method for (4), which maps the initial datum $\mathbf{x} \in D$ into a numerical approximation $\boldsymbol{\Psi}(0, \mathbf{x}; h) \in \mathbb{R}^d$ of $\mathbf{y}(h) \in \mathbb{R}^d$ over a single time step $h > 0$.

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The one-step method $\boldsymbol{\Phi}_h : \mathbf{x} \mapsto \boldsymbol{\Psi}(0, \mathbf{x}; h)$ is said to be *symplectic* if $\boldsymbol{\Phi}_h : \mathbf{x} \mapsto \boldsymbol{\Psi}(0, \mathbf{x}; h)$ defines a symplectic map on every compact subset $K \subset D$, whenever H is twice continuously differentiable and $h > 0$ is sufficiently small.

The following theorem provides a convenient sufficient condition for a Runge–Kutta being symplectic, although for an arbitrary one-step method one would still need to appeal to the previous definition to verify that the method in question is symplectic.

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Theorem

Every Runge–Kutta method that preserves quadratic first integrals is symplectic.