Geometric Numerical Integration:

Examples of 1st Integrals, Quadratic Invariants

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Introduction

- define a first integral

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- two examples of first integrals

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- RK methods and linear invariants

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Definition of first integral

Definition

Consider the differential equation $\dot{y} = f(y)$, where y is a vector or possibly a matrix. A non constant function $I(y)$ is called **first integral** of $\dot{y} = f(y)$, if:

$$I'(y)f(y) = 0 \quad \forall\, y.$$

Conservation of the total linear and angular momentum of N-body systems

Consider system of N particles interacting pairwise with potential forces, which depend on the distance of the particles. The Hamiltonian System is described as:

$$H(p,q) = \frac{1}{2}\sum_{i=1}^{N}\frac{1}{m_i}p_i^T p_i + \sum_{i=2}^{N}\sum_{j=1}^{i-1}V_{ij}(||q_i - q_j||)$$

where $q_i \in \mathbb{R}^3$ describes the position, $p_i \in \mathbb{R}^3$ the momentum, m_i the mass of particle i. V_{ij} describes the interaction potential between the i^{th} and j^{th} particle.

Conservation of mass in chemical reactions

Suppose we have three substances A, B, C undergoing chemical reactions

$$A \xrightarrow{0.04} B \qquad \text{(slow)}$$

$$B + B \xrightarrow{3\cdot 10^7} C + B \qquad \text{(very fast)}$$

$$B + C \xrightarrow{10^4} A + C \qquad \text{(fast)}$$

Let y_1, y_2, y_3 denote the masses of the substances. By the mass action law

$$\begin{aligned} A: \quad \dot{y}_1 &= -0.04 y_1 + 10^4 y_2 y_3 \\ B: \quad \dot{y}_2 &= 0.04 y_1 - 10^4 y_2 y_3 - 3\cdot 10^7 y_2^2 \\ C: \quad \dot{y}_3 &= 3\cdot 10^7 y_2^2 \end{aligned}$$

we see that $\dot{y}_1 + \dot{y}_2 + \dot{y}_3 = 0$, and therefore $I(y) = y_1 + y_2 + y_3$ is an invariant of the system.

Conservation of linear invariants

Theorem

All explicit and implicit Runge Kutta methods conserve linear invariants. Partitioned Runge Kutta methods conserve linear invariants if $b_i = \hat{b}_i$, $\forall\ i$.

Step towards quadratic invariants

Theorem

Consider differential equations of the form

$$\dot{Y} = A(Y)Y,$$

where Y *is a vector or a matrix. If* $A(Y)$ *is skew symmetric* $(A(Y)^T = -A(Y))$*, then* $I(Y) = Y^T Y$ *is an invariant. Particularly, if the initial value* Y_0 *consists of orthonormal columns* $(Y_0^T Y_0 = \mathbb{I})$*, then the columns of the solution* $Y(t)$ *of* $\dot{Y} = A(Y)Y$ *remain orthonormal* $\forall\ t$*, i.e.* $Y(t)^T Y(t) = const.$

Rigid Body

The motion of a rigid body, whose entire mass is at the origin is described by the Euler equations:

$$\begin{aligned} \dot{y}_1 &= a_1 y_2 y_3 \\ \dot{y}_2 &= a_1 y_1 y_3 \\ \dot{y}_3 &= a_1 y_1 y_2 \end{aligned}$$

where

$$a_1 = \frac{I_2 - I_3}{I_2 I_3}, \quad a_2 = \frac{I_3 - I_1}{I_1 I_3}, \quad a_3 = \frac{I_1 - I_2}{I_1 I_2}.$$

$y = (y_1, y_2, y_3)^T$ describes the angular momentum in the body frame and I_1, I_2, I_3 are the principal moments of inertia.

Rigid Body

The problem can be rewritten in the form of a skew-symmetric matrix:

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{pmatrix} = \begin{pmatrix} 0 & \frac{y_3}{I_3} & -\frac{y_2}{I_2} \\ -\frac{y_3}{I_3} & 0 & \frac{y_1}{I_1} \\ \frac{y_2}{I_2} & -\frac{y_1}{I_1} & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}.$$

Therefore, using the last Theorem, we find, that $y^T y = y_1^2 + y_2^2 + y_3^2$ is an invariant.

$$H(y_1, y_2, y_3) = \frac{1}{2}\left(\frac{y_1^2}{I_1} + \frac{y_2^2}{I_2} + \frac{y_3^2}{I_3}\right)$$

is also a quadratic invariant representing the kinetic energy.

Motivation

Quadratic invariants appear often in applications. We consider differential equations of the form

$$\dot{y} = f(y)$$

and quadratic functions

$$Q(y) = y^T C y,$$

where C is a symmetric square matrix. By definition $Q(y)$ is an invariant if $Q'(y)f(y) = 0$. Therefore it is an invariant if

$$y^T C f(y) = 0 \quad \forall\ y,$$

since $\frac{d}{dt}Q(y) = 2y^T C f(y)$.

Conservation of quadratic invariants

Theorem

The Gauss methods conserve quadratic invariants.

Cooper's Theorem

Theorem (Cooper, 1987)

If the coefficients of a Runge Kutta method satisfy

$$b_i a_{ij} + b_j a_{ji} = b_i b_j \quad \forall\ i, j = 1, \ldots, s,$$

then it conserves quadratic invariants.

Lobatto methods

Theorem

The Lobatto IIIA and IIIB pair conserves all quadratic invariants of the form

$$Q(y,z) = y^T Dz.$$

partitioned Runge Kutta methods

Theorem

If the coefficients of a partitioned Runge Kutta method satisfy

$$\begin{aligned} b_i \hat{b}_j &= b_i \hat{a}_{ij} + \hat{b}_j a_{ji} \quad i,j = 1,\dots,s \\ b_i &= \hat{b}_i \quad \forall\ i = 1,\dots,s. \end{aligned}$$

Then it conserves quadratic invariants of the form $Q(y,z) = y^T D z$. *If the partioned differential equation is of the special form*

$$\dot{y} = f(z) \quad \dot{z} = g(y),$$

then the first condition alone implies that invariants of the form $Q(y,z) = y^T D z$ *are conserved.*

- Thank you.

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- Questions?

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- The End.