Geometric Numerical Integration:
Examples of 1st Integrals, Quadratic Invariants

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Introduction

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- two examples of first integrals
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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

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

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

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

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

$$A:\quad \dot{y}_1 = -0.04y_1 + 10^4y_2y_3$$

$$B:\quad \dot{y}_2 = 0.04y_1 - 10^4y_2y_3 - 3 \cdot 10^7y_2^2$$

$$C:\quad \dot{y}_3 = 3 \cdot 10^7y_2^2$$

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 $I(Y) = Y^TY$ is an invariant. Particularly, if the initial value $Y_0$ consists of orthonormal columns ($Y_0^T Y_0 = I$), then the columns of the solution $Y(t)$ of $\dot{Y} = A(Y)Y$ remain orthonormal $\forall t$, i.e. $Y(t)^T Y(t) = \text{const.}$
Rigid Body

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

\[
\begin{align*}
\dot{y}_1 &= a_1 y_2 y_3 \\
\dot{y}_2 &= a_1 y_1 y_3 \\
\dot{y}_3 &= a_1 y_1 y_2
\end{align*}
\]

where

\[
\begin{align*}
a_1 &= \frac{I_2 - I_3}{I_2 I_3}, \quad a_2 = \frac{I_3 - I_1}{I_1 I_3}, \quad a_3 = \frac{I_1 - I_2}{I_1 I_2}.
\end{align*}
\]

\[y = (y_1, y_2, y_3)^T\] 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

\[ Q(y, z) = y^T Dz. \]
Theorem

If the coefficients of a partitioned Runge Kutta method satisfy

\[
\begin{align*}
\hat{b}_i \hat{b}_j &= b_i \hat{a}_{ij} + \hat{b}_j a_{ji} \quad i, j = 1, \ldots, s \\
\hat{b}_i &= \hat{b}_i \quad \forall \ i = 1, \ldots, s.
\end{align*}
\]

Then it conserves quadratic invariants of the form \(Q(y, z) = y^T Dz\). If the partitioned differential equation is of the special form

\[
\begin{align*}
\dot{y} &= f(z) \\
\dot{z} &= g(y),
\end{align*}
\]

then the first condition alone implies that invariants of the form \(Q(y, z) = y^T Dz\) are conserved.
Thank you.
Thank you.

Questions?
Thank you.
Questions?
The End.