Conservation of First Integrals and Projection Methods

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Outline

Conservation of First Integrals

Quadratic Invariants

Projection Methods

Numerical Examples of Projection Methods

Conclusion
Intuition

- ODEs often conserve certain quantities
- Numerical solutions also should
- How to design such a numerical method?
Definition of First Integrals

- Consider differential equation

\[ \dot{y} = f(y). \]
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A non-constant function \( I(y) \) is called a \textit{first integral} if
\[ I'(y)f(y) = 0 \quad \text{for all } y. \]
Consider differential equation
\[ \dot{y} = f(y). \]

A non-constant function \( I(y) \) is called a first integral if
\[ I'(y) f(y) = 0 \quad \text{for all } y. \]

This implies
\[ I(y(t)) = I(y_0) = \text{Const.} \]
for any solution \( y(t) \).
Example: Conservation of the Total Energy

- The Hamiltonian systems of the form

\[ \dot{p} = -H_q(p, q), \quad \dot{q} = H_p(p, q), \]

- \( H_q = \nabla_q H = \left( \frac{\partial H}{\partial q} \right)^T \) and \( H_p = \nabla_p H = \left( \frac{\partial H}{\partial p} \right)^T \)

- The Hamilton function \( H(p, q) \) is a first integral

\[ \frac{\partial H}{\partial p} \left( - \frac{\partial H}{\partial q} \right)^T + \frac{\partial H}{\partial q} \left( \frac{\partial H}{\partial p} \right)^T = 0. \]
Background: Explicit Runge-Kutta Methods

1. Given initial value problem \( y' = f(t, y), \ y(t_0) = y_0 \)
2. Given the current step \( y_n \) and \( t_n \)
3. Runge-Kutta methods are given by:

\[
\begin{align*}
    k_1 &= f(t_n, y_n), \\
    k_2 &= f(t_n + c_2 h, y_n + a_{21} h k_1), \\
    k_3 &= f(t_n + c_3 h, y_n + a_{31} h k_1 + a_{32} h k_2), \\
    \cdots \\
    \cdots \\
    k_s &= f(t_n + c_s h, y_n + a_{s1} h k_1 + a_{s2} h k_2 + \cdots + a_{s,s-1} h k_{s-1}), \\
    y_{n+1} &= y_n + h \sum_{i=1}^{s} b_i k_i,
\end{align*}
\]

4. \( y_{n+1} \) and \( t_{n+1} \) are the new step
Background: Runge-Kutta Method of Order 4

1. Given initial value problem $y' = f(t, y), y(t_0) = y_0$
2. Given the current step $y_n$ and $t_n$
3. Runge-Kutta method is given by:

   \[
   k_1 = f(t_n, y_n)
   \]

   \[
   k_2 = f(t_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_1)
   \]

   \[
   k_3 = f(t_n + \frac{1}{2}h, y_n + \frac{1}{2}hk_2)
   \]

   \[
   k_4 = f(t_n + h, y_n + hk_3)
   \]

   \[
   y_{n+1} = y_n + \frac{1}{6}h(k_1 + 2k_2 + 2k_3 + k_4)
   \]

4. $y_{n+1}$ and $t_{n+1}$ are the new step
Background: Runge-Kutta Method of Order 2

1. Given initial value problem \( y' = f(t, y) \), \( y(t_0) = y_0 \)
2. Given the last step \( y_n \) and \( t_n \)
3. Runge-Kutta method is given by:

\[
\begin{align*}
  k_1 &= f(t_n, y_n) \\
  k_2 &= f(t_n + h, y_n + hk_1) \\
  y_{n+1} &= y_n + \frac{1}{2}h(k_1 + k_2)
\end{align*}
\]

4. \( y_{n+1} \) and \( t_{n+1} \) are the new step
Theorem

All explicit and implicit Runge-Kutta methods conserve linear invariants.
A Quadratic Invariant

Theorem

Consider ODE of the form

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

if \(A(Y)\) is skew-symmetric for all \(Y\) (i.e., \(A^T = -A\)), then the quadratic function

\(I(Y) = Y^T Y\) is an invariant.
Consider ODE $\dot{y} = f(y)$ and quadratic functions

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

$Q(y)$ is an invariant if $y^T Cf(y) = 0$ for all $y$. 
If the coefficients of a Runge-Kutta method satisfy
\[ b_i a_{ij} + b_j a_{ji} = b_i b_j \quad \text{for all } i, j = 1, \ldots, s, \]
then it conserves quadratic invariants.
Suppose an \((n - m)\)-dimensional sub-manifold of \(\mathbb{R}^n\),

\[ M = \{ y; g(y) = 0 \} \quad (1) \]

\((g : \mathbb{R}^n \to \mathbb{R}^m)\),

And a differential equation \(\dot{y} = f(y)\) with the property that

\[ y_0 \in M \implies y(t) \in M \quad \text{for all } t. \]

It holds if \(g'(y)f(y) = 0\) for \(y \in M\).

We call \(g(y)\) a weak invariant.
Here the Standard Projection Methods are proposed as following:

**Algorithm**

Assume that $y_n \in \mathcal{M}$. One step $y_n \rightarrow y_{n+1}$ is defined as follows:

1. Compute $\tilde{y}_{n+1} = h(y_n)$, where $h$ is an arbitrary one-step method applied to $\dot{y} = f(y)$;
2. Project the value $\tilde{y}_{n+1}$ onto the manifold $\mathcal{M}$ to obtain $y_{n+1} \in \mathcal{M}$. 

Algorithm of Projection Methods

Here the Standard Projection Methods are proposed as following:

**Algorithm**

Assume that \( y_n \in M \). One step \( y_n \rightarrow y_{n+1} \) is defined as follows:

1. Compute \( \tilde{y}_{n+1} = \Phi_h(y_n) \), where \( \Phi_h \) is an arbitrary one-step method applied to \( \dot{y} = f(y) \);
Here the Standard Projection Methods are proposed as following:

**Algorithm**

*Assume that $y_n \in M$. One step $y_n \rightarrow y_{n+1}$ is defined as follows:*

1. *Compute $\tilde{y}_{n+1} = \Phi_h(y_n)$, where $\Phi_h$ is an arbitrary one-step method applied to $\dot{y} = f(y)$;*

2. *project the value $\tilde{y}_{n+1}$ onto the manifold $M$ to obtain $y_{n+1} \in M$.***
Given a function $f(x)$ and its derivative $f'(x)$

Want to solve an equation $f(x) = 0$

Repeat

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

until sufficiently accurate
In order to project $\tilde{y}_{n+1}$ onto $\mathcal{M}$ to obtain $y_{n+1}$, one needs to

- Solve the constrained minimization problem

\[
\| y_{n+1} - \tilde{y}_{n+1} \|_{L^2} \rightarrow \min \quad \text{subject to } g(y_{n+1}) = 0.
\]
A Minimization Problem

In order to project $\tilde{y}_{n+1}$ onto $\mathcal{M}$ to obtain $y_{n+1}$, one needs to

- Solve the constrained minimization problem

$$\|y_{n+1} - \tilde{y}_{n+1}\|_{L^2} \rightarrow \min \text{ subject to } g(y_{n+1}) = 0.$$ 

- Introduce Lagrange multipliers $\lambda = (\lambda_1, \ldots, \lambda_m)^T$, and the Langrange function

$$\mathcal{L}(y_{n+1}, \lambda) = \|y_{n+1} - \tilde{y}_{n+1}\|^2 / 2 - g(y_{n+1})^T \lambda.$$
The necessary condition leads to the system

\[ y_{n+1} = \tilde{y}_{n+1} + g'(\tilde{y}_{n+1})^T \lambda \]
\[ 0 = g(y_{n+1}). \]

Inserting the first equation into the second gives

\[ g(\tilde{y}_{n+1} + g'(\tilde{y}_{n+1})^T \lambda) = 0 \]

Solve the equation for \( \lambda \) with simplified Newton Method:

\[ \Delta \lambda_i = -\left(g'(\tilde{y}_{n+1})g'(\tilde{y}_{n+1})^T\right)^{-1}g(\tilde{y}_{n+1} + g'(\tilde{y}_{n+1})^T \lambda_i), \]

with \( \lambda_{i+1} = \lambda_i + \Delta \lambda_i \).
Consider the perturbed Kepler problem

\[ \dot{p} = -H_q(p, q), \quad \dot{q} = H_p(p, q), \]

with the Hamilton function

\[ H(p, q) = \frac{1}{2}(p_1^2 + p_2^2) - \frac{1}{\sqrt{q_1^2 + q_2^2}} - \frac{0.005}{2\sqrt{(q_1^2 + q_2^2)^3}} \]

Initial values: \( q_1(0) = 1 - e, q_2(0) = 0, p_2(0) = \sqrt{(1 + e)/(1 - e)} \), \( p_1(0) = 0 \) (\( e = 0.6 \) as the eccentricity)

Two known first integrals:
- the Hamilton function \( H(p, q) \)
- the angular momentum \( L(p, q) = q_1 p_2 - q_2 p_1 \)
Explicit Euler

(a) Without Projection

(b) With Projection onto $H$

(c) With Projection onto $H$ and $L$

Figure: Explicit euler, $h = 0.03$
Runge-Kutta of Order 2

(a) Without Projection

(b) With Projection onto $H$

(c) With Projection onto $H$ and $L$

Figure: RK2, $h = 0.03$
Runge-Kutta of Order 4

Figure: RK4, $h = 0.03$
Concluding Remarks

- A lot of ODEs have the property to conserve the *First Integrals*
- Certain numerical methods conserve the first integrals automatically
- If not, apply projection methods to conserve it manually
- Projection methods improve the numerical results
- Projections are especially effective for low order methods
Questions?
Thanks for your attention.