A new class of symplectic integration schemes based on generating functions

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Symplectic methods for general Hamiltonian systems

Although there are explicit symplectic methods for Hamiltonian systems with separable Hamiltonian function

$$H(p, q) = T(p) + V(q),$$

integration schemes that are symplectic for all Hamiltonian systems

$$y' = J^{-1}\nabla H(y)^T, \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$$

with arbitrary Hamiltonian function $H(y)$, need to be implicit.

Hamilton-Jacobi equation

If $S_t : \mathbb{R}^{2d} \to \mathbb{R}$ is a one-parameter family of functions (the generating functions) such that

$$\frac{\partial}{\partial t} S_t(y) = H\left(y + \frac{1}{2} J^{-1} \nabla S_t(y)\right)$$

then, for any solution $y(t)$ of $y' = J^{-1} \nabla H(y)^T$, it holds that

$$y(t+h) = y(t) + J^{-1} \nabla S_h \left(\frac{1}{2}(y(t) + y(t+h))\right).$$

Our aim is to explore symplectic methods based on some explicit approximation of $S_h(y)$.

Example: Implicit midpoint rule, $S_h(y) \approx hH(y)$.

The methods of Miesbach and Persch

One step $y^* = \psi_h(y)$ of the method is implicitly defined by

$$y^* = y + J^{-1}\nabla S_h(\tfrac{1}{2}(y + y^*)),$$

with the generating function $S_h(z)$ given as

$$S_h(z) = h\sum_{i=1}^{s} b_i H(Y_i),$$

where for $i = 1, \ldots, s$,

$$Y_i = z + hJ^{-1}\sum_{j=1}^{s} \alpha_{ij}\nabla H(Y_i)^T,$$

with appropriately chosen $b_i, \alpha_{ij} \in \mathbb{R}$.

Symplectic RK methods

One step $y^* = \psi_h(y)$ of the method can be written as

$$y^* = y + J^{-1}\nabla S_h(\tfrac{1}{2}(y + y^*)),$$

with the generating function $S_h(z)$ given as

$$S_h(z) = h\sum_{i=1}^{s} b_i H(Y_i) + \frac{h^2}{2}\sum_{i,j=1}^{s} b_i\alpha_{ij}\nabla H(Y_i)J^{-1}\nabla H(Y_j)^T,$$

where for $i = 1, \ldots, s$,

$$Y_i = z + hJ^{-1}\sum_{j=1}^{s}\alpha_{ij}\nabla H(Y_i)^T,$$

and $b_i\alpha_{ij} + b_j\alpha_{ji} = 0$ for all i, j $\;(a_{ij} = \alpha_{ij} + b_j/2)$.

The new family of symplectic integrators

One step $y^* = \psi_h(y)$ of the method is implicitly defined by

$$y^* = y + J^{-1}\nabla S_h(\tfrac{1}{2}(y + y^*)),$$

with the generating function $S_h(z)$ given as

$$S_h(z) = h\sum_{i=1}^{s} b_i H(Y_i) + \frac{h^2}{2}\sum_{i,j=1}^{s} \beta_{ij}\,\nabla H(Y_i)J^{-1}\nabla H(Y_j)^T,$$

where for $i = 1, \ldots, s$,

$$Y_i = z + hJ^{-1}\sum_{j=1}^{s}\alpha_{ij}\nabla H(Y_i)^T.$$

We assume without loss of generality that $\beta_{ij} = -\beta_{ji}$ for all i, j.

Methods of explicit type

If the matrix (α_{ij}) is lower triangular, then $S_h(z)$ is explicitly defined, and the definition of one step $y^* = \psi_h(y)$ of the method

$$y^* = y + J^{-1}\nabla S_h(\tfrac{1}{2}(y + y^*)), \tag{1}$$

is only implicit in y^*. The Jacobian of that system is

$$I - \frac{1}{2}J^{-1}\nabla^2 S_h(y) = I - \frac{h}{2}J^{-1}\nabla^2 H(y) + \mathcal{O}(h^3)$$

(if the method is at least of order 2), and its inverse

$$\left(I - \frac{1}{2}J^{-1}\nabla^2 S_h(y)\right)^{-1} = I + \frac{h}{2}J^{-1}\nabla^2 H(y) + \frac{h^2}{4}(J^{-1}\nabla^2 H(y))^2 + \mathcal{O}(h^3).$$

This allows to solve (**??**) very efficiently, provided that a good initial guess for y^* is available.

Efficient computation of the gradient of the generating function for methods of explicit type

$$\nabla S_h(z) = h \sum_{i=1}^{s} \left(b_i \nabla H(Y_i) - h \nabla^2 H(Y_i) v_i \right),$$

For $i = 1, \ldots, s$,

$$Y_i = z + hJ^{-1} \sum_{j<i} \alpha_{ij} \nabla H(Y_j),$$

For $i = s \ldots, 1$,

$$v_i = J^{-1} \sum_{j=1}^{s} \gamma_{ij} \nabla H(Y_j) - hJ^{-1} \sum_{j>i} \alpha_{ji} \nabla^2 H(Y_j) v_j,$$

where $\gamma_{ij} = \beta_{ij} + b_j \alpha_{ji}$ for all i, j.

It is required to compute

$$\nabla^2 H(y) \cdot v \text{ in addition to } \nabla H(y), \text{ for different } y, v \in \mathbb{R}^{2d}$$

Observation (from the theory of AD):

$$\mathrm{Cost}(\nabla H(y), \nabla^2 H(y) \cdot v) \approx k\,\mathrm{Cost}(\nabla H(y))$$

with small $k > 1$ (often $k = 1 + \varepsilon$ with small $\varepsilon > 0$).

Linear stability function

The method applied to the linear test equation $y' = \lambda y$ gives $y^* = R(h\lambda)y$, where $R(z)$ (the linear stability function) is

$$R(z) = \frac{2 + Q(z)}{2 - Q(z)},$$

where

$$Q(z) = z\left(b^T - ze^T(I + zA^T)^{-1}\Gamma\right)(I - zA)^{-1}e,$$

with $e^T = (1, \ldots, 1)$ and

$$b^T = (b_1, \ldots, b_s), \quad A = (\alpha_{ij}), \quad \Gamma = (\gamma_{ij}) = (\beta_{ij} + b_j\alpha_{ji})$$

Linear stability function for methods of explicit type

If the method is of order r, then

$$R(z) = \frac{2 + Q(z)}{2 - Q(z)} = e^z + \mathcal{O}(z^{r+1}) \quad \text{as } z \to 0,$$

or equivalently,

$$Q(z) = 2\tanh(z/2) + \mathcal{O}(z^{r+1}) \quad \text{as } z \to 0.$$

Order barriers for methods of explicit type:

- For methods of explicit type, $Q(z)$ is a polynomial of degree $d \leq 2s$. Whence the method has order $r \leq 2s$.
- For symmetric methods of explicit type, $Q(z)$ is an even polynomial of degree $d \leq (4s+2)/3$, and thus the method is of order $r \leq (4s+2)/3$.

Symmetric methods

A method is symmetric (or self-adjoint) if

$$\psi_h^{-1} = \psi_{-h}.$$

Symmetry is equivalent to

$$S_{-h}(z) \equiv -S_h(z).$$

If there exists a permutation π of the set of indices $\{1, \ldots, s\}$ such that $\pi^{-1} = \pi$, and

$$b_{\pi(i)} = b_i, \quad \alpha_{\pi(i),\pi(j)} = -\alpha_{i,j} \quad \beta_{\pi(i),\pi(j)} = -\beta_{i,j},$$

for all $i, j = 1, \ldots, s$, then the method is symmetric.

The order conditions

One order condition per non-superfluous free tree, linear in b_i, β_{ij}.
For order $r \geq 3$,

$$\sum_{i=1}^{s} b_i = 1, \quad \sum_{i=1}^{s} \left(b_i\, c_i^2 - 2c_i d_i\right) = \frac{1}{3},$$

where for each $i = 1, \ldots, s$,

$$c_i = \frac{1}{2} + \sum_{j=1}^{s} \alpha_{ij}, \quad d_i = \sum_{j=1}^{s} (\beta_{ij} + b_j \alpha_{ji}),$$

It is of order $r \geq 4$ if in addition

$$\sum_{i=1}^{s} \left(b_i\, c_i^3 - 3c_i^2 d_i\right) = \frac{1}{4}$$

(automatically fulfilled for symmetric methods of order $r \geq 3$).

The order conditions

The method is of order 5, if in addition,

$$\sum_{i=1}^{s} \left(b_i\, c_i^4 - 4c_i^3 d_i\right) = \frac{1}{5},$$

$$\sum_{i=1}^{s} \left(b_i\, c_i^2 e_i - c_i^2 f_i - 2c_i e_i d_i\right) = \frac{1}{10},$$

$$\sum_{i=1}^{s} \left(b_i\, e_i^2 - 2e_i f_i\right) = \frac{1}{20},$$

where for each $i = 1, \ldots, s$,

$$e_i = \frac{1}{4} + \sum_{j=1}^{s} \alpha_{ij}\, c_j, \quad f_i = \sum_{j=1}^{s} (\beta_{ij} + b_j \alpha_{ji}) c_j - \sum_{j=1}^{s} \alpha_{ji}\, d_j.$$

For symmetric methods, these conditions guarantee order $r \geq 6$.

A family of symmetric sixth order methods of explicit type

We have constructed a two-parameter family of symmetric methods of explicit type with $s = 4$, such that

- It is of order six,
- A initial guess $\widetilde{y}^*$ for $y^* = \psi_h(y)$ can be computed from the preceding step such that
$$\widetilde{y}^* - y^* = \mathcal{O}(h^5),$$
- A initial guess $\widetilde{y}^*$ for $y^* = \psi_h(y)$ can be computed from the preceding two steps such that
$$\widetilde{y}^* - y^* = \mathcal{O}(h^6).$$

Work in progress

- Fix some criteria to choose values for the two free parameters of our family of 6th order symmetric methods of explicit type, and find the optimal values.
- Construct other optimized 6th and 8th order symmetric methods of explicit type with higher number of stages ($s > 4$).
- Compare the efficiency of our schemes with respect to
  - Gauss methods,
  - Composition methods based on the implicit midpoint rule.