Dynamics of Multistep Methods

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Multistep Methods for First Order Problems

We define a linear multistep method as the following:

Definition (Linear Multistep Method)

For the first order system of differential equations we $\dot{y} = f(y)$, *linear multistep methods are defined by the formula:*

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f(y_{n+1}) \quad (0.1)$$

where α_j *and* β_j *are real variables* $a_j \neq 0$ *and* $|\alpha_0| + |\beta_0| > 0$. *To apply it we first need the initial conditions, then we also need approximations for the first* k, y_j.

Multistep Methods for First Order Problems

We also define the generating polynomials:

Definition (Generating Polynomials)

After Dahlquist († 2005) we write the characteristic polynomials of the coefficients by:

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j, \quad \sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j \tag{0.2}$$

Note that $\zeta \in \mathbb{C}$

Properties

Theorem (Order of Consistency)

A multistep method has order p if and only if when applied to with exact starting values to the problem:

$$\dot{y} = t^q, \quad (0 \leq q \leq p) \tag{0.3}$$

it integrates the problem without error. Written in terms of characteristic functions this is equivalent to the requirement that:

$$\rho(e^h) - h\sigma(e^h) = \mathcal{O}(h^{r+1}), \quad h \to 0 \tag{0.4}$$

Theorem (Stability)

The method is stable if and only if it yields for all $y_0, \ldots, y_{k-1}$ a bounded numerical solution. This is equivalent to that all roots of $\rho(\zeta)$ satisfy $|\zeta| \leq 1$, those on the unit circle are simple roots. Further it is called strictly stable if we have strict inequality with the exception of $\zeta = 1$.

Properties

Theorem (Convergence)

If a multistep method is stable and of order $r \leq 1$, it is convergent of order r for all sufficiently smooth problems. This means that, assuming starting approximations with an error bounded by $\mathcal{O}(h^r)$, the global error satisfies:

$$y_n - y(t_0 + nh) = \mathcal{O}(h^r) \tag{0.5}$$

on compact intervals $nh \leq T$

Theorem (Symmetri)

The method is symmetric if and only if:

$$\alpha_{k-j} = -\alpha_j, \quad \beta_{k-j} = \beta_j, \quad \forall j \tag{0.6}$$

For characteristic functions this is equivalent to that for every zero of $\rho(\zeta)$ then $\rho(\frac{1}{\zeta})$ is also a zero. Hence for stable methods, all zeros are simple and lie on the unit circle.

Multistep Methods for Second Order Problems

The above definitions can be extended to account for second order problems, of the form:

$$\ddot{y} = f(y) \tag{0.7}$$

Definition

For the secon order problems we obtain the following multistep method:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j f(y_{n+1}) \tag{0.8}$$

Properties

Theorem (Order of Consistency)

A multistep method applied to a second order problem has order r if and only if its generating polynomials satisfy:

$$\rho(e^h) - h^2\sigma(e^h) = \mathcal{O}(h^{r+2}), \quad h \to 0 \qquad (0.9)$$

Theorem (Stability)

The method is stable if and only if all the zeros of ρ satisfy $|\zeta| \leq 1$, and those on the unit circle are at most double zeros. The method is strictly stable if all zeros are inside the unit circle, with the exception $\zeta = 1$.
Note that all methods originating the first order problem, makes all zeros to doubles.

Properties

Theorem (Convergence)

If a multistep method is stable, of order $r \geq 1$ and if the starting values are accurate enough, then the global error satisfies:

$$y_n - y(t_0 + nh) = \mathcal{O}(h^r) \tag{0.10}$$

on compact intervals $nh \leq T$

Theorem (Symmetri)

A method if symmetric if and only if:

$$\alpha_{k-j} = \alpha_j, \quad \beta_{k-j} = \beta_j, \quad \forall j \tag{0.11}$$

Again for every zero of $\rho(\zeta)$ then $\rho(\frac{1}{\zeta})$ is also a zero. Hence symmetric and stable methods have all their zeros on the unit circle and they are at most of multiplicity 2.

The Underlying One-Step Method

As we know a lot of one step methods, one obvious way to investigate multistep methods is to rewrite them into their corresponding one step methods.

Theorem (Kirchgraber 1986)

Consider a strictly stable linear multistep method applied to $\dot{y} = f(y)$ *with sufficiently small step size* h*. Then there exists a one step method* Φ_h *such that for starting approximations computed by the same one step method.*
Then the approximations using the multistep method is identical to the ones using the one step method.

Recall that symmetric method cannot be strictly stable, hence this theorem is of no practical use.

The Underlying One-Step Method

Theorem (Feng 1995)

Consider a multistep method applied to $\dot{y} = f(y)$, and assume that $\zeta = 1$ is a single root of ρ. Then there exists a unique formal expansion:

$$\Phi_h(y) = y + hd_1(y) + h^2 d_2(y) + \dots \tag{1.1}$$

such that

$$\sum_{j=0}^{k} \alpha_j \Phi_h^j(y) = h \sum_{j=0}^{k} \beta_j f(\Phi_h^j(y)) \tag{1.2}$$

where identity is understood in the sense of formal power series in h.
If the multistep method is of order r, so is the one step method.

We call this "The underlying one step method".

Issue

The power series expansion:

$$\Phi_h(y) = y + hd_1(y) + h^2 d_2(y) + \dots \qquad (1.3)$$

does *not* converge in general, hence we have to truncate it at some point.

Backward Error Analysis

As we now have the underlying one step method, we can investigate the long time behaviour by applying backward analysis to this one step method. However care should be taken as:

- We have to truncate the power expansion of the one step method, one have to make sure that this does not alter the properties.
- One have to carefully calculate the initial approximations.

Modified Hamiltonian of Multistep Methods

Theorem

For a symmetric, consistent linear multistep method of order r applied to $\dot{y} = J^{-1}\nabla H(y)$, there exists a series of the form

$$\tilde{H}(y) = H(y) + h^r H_{r+1}(y) + h^{r+2} H_{r+3}(y) + \dots \qquad (2.1)$$

which is a formal first integral of the modified equation without truncation.

Theorem

For a symmetric, consistent linear multistep method of order r applied to $\ddot{y} = -\nabla U(y)$, there exists a series of the form

$$\tilde{H}(y) = \frac{1}{2}\dot{y}^T \dot{y} + U(y) + h^r H_{r+1}(y, \dot{y}) + h^{r+2} H_{r+3}(y, \dot{y}) + \dots \qquad (2.2)$$

which is a formal first integral of the modified equation without truncation.

Modified Hamiltonian of Multistep Methods

Theorem

Let $Q(y) = y^T Cy$ be a first integral of $\dot{y} = f(y)$. For a symmetric, consistent linear multistep method of order r, there then exists a series of the form:

$$\tilde{Q}(y) = y^T Cy + h^r Q_{r+1}(y) + h^{r+2} Q_{r+3}(y) \qquad (2.3)$$

which is a formal invariant of the modified equation without truncation.

Theorem

Suppose that $\ddot{y} = f(y)$ has $L(y, \dot{y}) = y^T E\dot{y}$ as first integral. For a symmetric, consistent linear multistep method of order r, there then exists a series of the form:

$$\tilde{L}(y, \dot{y}) = y^T E\dot{y} + h^r L_{r+1}(y, \dot{y}) + h^{r+2} L_{r+3}(y, \dot{y}) + \dots \qquad (2.4)$$

which is a formal invariant of the modified equation without truncation

Can Multistep Method be Symplectic?

As in the Backward error analysis, the obvious way to investigate symplecticity is say that a multistep method is symplectic if the underlying one step method is. However:

Theorem (Tang 1993)

The underlying one step method of a consistent linear multistep method cannot be symplectic.

However we can do a tiny bit better if we allow for partitioning:

Theorem

If the underlying one step method of a consistent, partitioned linear multistep method is symplectic for all separable Hamiltonians, then its order is ≤ 1

Note: Such a method is the symplectic Euler, it is in other words the best we can do in this setting.

Can Multistep Method be Symplectic?

If we however restrict ourself to a quadratic kinetic energy, we can do a bit better again:

Theorem

If the underlying one step method of a consistent, partitioned linear multistep method is symplectic for all Hamiltonian systems with Hamiltonians with at most quadratic kinetic energy term, then its order is ≤ 2

Long Time Behaviour

The following builds on theory made by Hairer and Lubich in 2004, where we consider the s-stable multistep method:

$$\sum_{j=0}^{k} \alpha_j y_{n+j} = -h^2 \sum_{j=0}^{k} \beta_j \nabla U(q_{n+j}) \tag{4.1}$$

for Hamiltonian systems:

$$\ddot{q} = -\nabla U(q) \tag{4.2}$$

Conservation of Energy

Theorem (Total Energy)

For a problem $\ddot{q} = -\nabla U(q)$ with a total energy $H(p, q) = \frac{1}{2}p^T p + U(q)$, the numerical solution of an s-stable symmetric multistep method of order r satisfies:

$$H(q_n, p_n) = H(q_0, p_0) + \mathcal{O}(h^r), \quad nh \leq h^{-r-2} \qquad (4.3)$$

If no root of $\rho(\zeta)$ other than 1 is a product of product of two other roots, the statement holds on intervals of length $\mathcal{O}(h^{-2r-3})$.

Conservation of Angular Momentum

Theorem (Angular Momentum)

Let $L(q,\dot q) = \dot q^T Aq$ be an invariant of $\ddot q = -\nabla U(q)$. The numerical solution of an s-stable symmetric multistep method of order r then satisfies:

$$L(q_n, p_n) = L(q_0, p_0) + \mathcal{O}(h^r), \quad nh \leq h^{-r-2} \qquad (4.4)$$

If no roots of $\rho(\zeta)$ other than 1 is a product of product of two other roots, the statement holds on intervals of length $\mathcal{O}(h^{-2r-3})$

Conservation of General Invariants

Theorem

Consider applying the s-stable symmetric multistep method of order r to an integrable reversible system $\ddot{q} = -\nabla U(q)$ with differentiable U. Suppose that $\omega^* \in \mathbb{R}^d$ satisfies the diophantine condition. Then there exists positive constants C, c and h_0 such that the following holds for all step sizes $h \leq h_0$: every numerical solution $(q_n, \dot{q})$ starting with frequencies $\omega_0 = \omega(I(q_0, \dot{q}_0))$ such that $\|\omega_0 - \omega^*\| \leq c|log(h)|^{-\nu-1}$ satisfies:

$$\begin{aligned} \|(q_n, \dot{q}_n) - (q(t), \dot{q}(t))\| &\leq Cth^r \\ \|I(q_n, \dot{q}_n) - I(q_0, \dot{q}_0)\| &\leq Ch^r, \quad 0 \leq t = nh \leq h^{-r} \end{aligned}$$

More Information

For more studies on the topic of multistep methods, I refer to:

- E. Hairer, S.P. Nørsett, G. Wanner, Solving Ordinary Differential Equations I, Non-Stiff Problems
- E. Hairer, G. Wanner, Solving Ordinary Differential Equations II, Stiff and Algebraic Problems

Where multistep methods is introduced in the first and highly used in the second to solve stiff problems