On the time-scale of B-series methods and symplectic integration

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We are concerned with the geometric numerical integration of

Hamiltonian systems

$$y' = J^{-1}\nabla H(y), \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}.$$

Example

Perturbed Kepler problem: We consider (for $0 < \epsilon << 1$)

$$H(p,q) = \frac{1}{2}||p||^2 + V(||q||), \quad \text{where} \quad V(r) = -\frac{1}{r} - \frac{\epsilon}{3r^3}.$$

Implicit midpoint: The approximations $y_n \approx y(t_n)$ for $t_n = nh$, are implicitly defined as

$$y_n = y_{n-1} + h\, f(\tfrac{1}{2}(y_{n-1} + y_n)), \quad f(y) = J^{-1}\nabla H(y).$$

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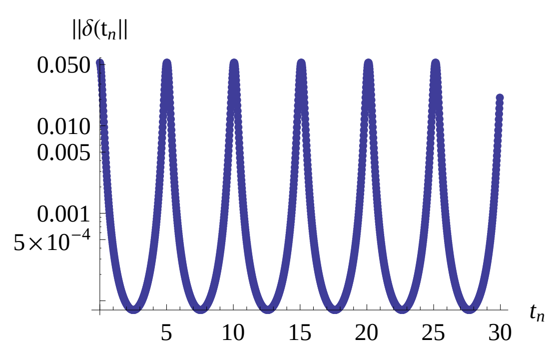
Example (Application to implicit midpoint to perturbed Kepler)

$y(0) = (1-e, 0, 0, \sqrt{\frac{1+e}{1-e}})$, $e = 0.6$, $\epsilon = 0.015$, $h = 0.02$.

Local error $\delta(t_n)$ (in logarithmic scale) versus time t_n:



$$\max_n ||\delta(t_n)|| = 0.052762, \quad \max_n ||y_n - y(t_n)|| = 0.92829.$$

Observed by Gladman, Duncan and Candy (1991), Calvo and Sanz-Serna (1992): Standard variable step-size implementation destroys the nice properties of symplectic integrators.

Time transformation

Consider a ficticious time variable τ such that $t = t(\tau)$ is defined as the solution of

$$\frac{d}{d\tau} t = s(y(t)), \quad t(0) = 0$$

for a suitably chosen function $s(y)$, and obtain $x(\tau) = y(t(\tau))$ by integrating

$$\frac{d}{d\tau} t = s(x), \quad \frac{d}{d\tau} x = s(y) f(x),$$

with $x(0) = y(0)$ and $t(0) = 0$.

- The function $s(y)$ needs to be chosen in advance.
- The new ODE system is not Hamiltonian.

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Adaptative symplectic integration (Hairer 1997, Reich 1999)

Consider a new Hamiltonian function

$$\mathcal{H}(y) = s(y)(H(y) - H_0), \quad H_0 = H(y(0)),$$

so that $t = t(\tau)$, $x(\tau) = y(t(\tau))$ is the solution of

$$\frac{d}{d\tau} t = s(x), \quad \frac{d}{d\tau} x = J^{-1} \nabla \mathcal{H}(x)$$

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We normalize s, when integrating for $t \in [0, t_f]$ in such a way that,

$$\int_0^{t_f} s(y(t(\tau)))\, d\tau = t_f.$$

Ideally: Find $s(y)$ such that, once normalized, minimize the discretization errors in some sense.

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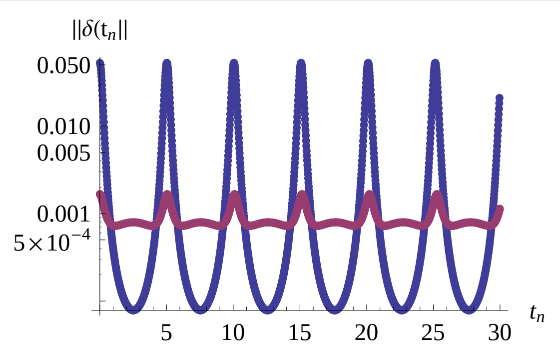
Example (Adaptative symplectic integration of perturbed Kepler)

We consider $s(p,q) = c\,||q||^{3/2}$ (Budd and Piggott 2003).
Local error $\delta(t_n)$ (in logarithmic scale) versus time t_n:



$$\max_n ||\delta(t_n)|| = 0.00166186, \quad \max_n ||y_n - y(t_n)|| = 0.00429137.$$

Backward error analysis for B-series methods

Modified equations of a one-step method of order N

$y_n = \bar{y}(t_n)$, where $\bar{y}(t)$ is the solution of a nearby problem

$$\frac{d}{dt}\bar{y} = f(\bar{y}) + h^N f_N(\bar{y}) + h^{N+1} f_{N+1}(\bar{y}) + \cdots, \quad \bar{y}(0) = y_0.$$

For a B-series method (RK, $\cdots$)

$$f_{j-1}(y) = \sum_{u \in \mathcal{T}_j} \frac{b(u)}{\sigma(u)} F(u)(y),$$

where $\mathcal{T}_j$ is the set of rooted trees with j vertices, and $\forall u \in \mathcal{T}_j$,

- $b(u) \in \mathbb{R}$ depends on the method,
- $F(u)(y)$ is the *elementary differential of u associated with f*,
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Rigorous backward error analysis for B-series methods

Rigorous backward error analysis: Benettin and Giorgilli (1994), Hairer and Lubich (1997), Reich (1999).

Estimates for real analytic ODE systems

There exists $\lambda : \cup \mathcal{T}_j \to \mathbb{R}$ such that, given a norm $||\cdot||$ on $\mathbb{R}^D$ and $f(y)$ real analytic, $\exists L(y), C(y) > 0$ such that $\forall u \in \mathcal{T}_j$,

$$\frac{1}{\sigma(u)} ||F(u)(y)|| \leq \lambda(u)\, C(y)\, L(y)^{j-1},$$

$$||h^j f_j(y)|| \leq d_j\, C(y)\, (hL(y))^{j-1},$$

, where $d_j = \sum_{u \in \mathcal{T}_j} \lambda(u)\, |b(u)|$.

If these estimates are tight enough, then $hL(y_n)$ somehow reflects the *time-scale* of $y_n = \bar{y}(t_n)$ at $t = t_n$.

Aim: Find a normalized $s(y)$ that minimizes $\max L(y_n)$.

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How to obtain $L(y)$? Let $||\cdot||$ be a norm in $\mathbb{C}^D$.

Preliminary estimates for real analytic $f(y)$

$$\tilde{L}(y) = \max_{||z-y||\leq 1} ||f(z)||,$$

where $f(z)$ is the complex analytic extension of $f(y)$. Then,

$$\frac{1}{\sigma(u)} ||F(u)(y)|| \leq \lambda(u)\, \tilde{L}(y)^j.$$

Observation: For invertible matrices $\mathcal{P} \in \mathbb{R}^{D\times D}$,

$$\begin{array}{ccccc} f(y) & \longrightarrow & \hat{f}(\hat{y}) & = \mathcal{P} f(\mathcal{P}^{-1}\hat{y}) \\ \downarrow & & \downarrow & \\ F(u)(y) & \longrightarrow & \hat{F}(u)(\hat{y}) & = \mathcal{P} F(u)(\mathcal{P}^{-1}\hat{y}) \end{array}$$

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Time-scale function $L(y)$

$$L(y) = \inf_{\mathcal{P}} \max_{||\mathcal{P}(z-y)||\leq 1} ||\mathcal{P}\,f(z)||.$$

If $\exists \mathcal{P} = \mathcal{P}(y)$ such that $L_{\mathcal{P}}(y) = L(y)$, then our estimates for the elementary differentials $||F(u)(y)||$ hold with $L(y)$ and

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Example (Perturbed Kepler problem)

If $H(p,q) < 0$, then there exist $\mu, \nu, c_1, c_2 > 0$ such that

$$L_{\mathcal{P}}(p,q) \;\leq\; \tilde{L}_{\mathcal{P}}(p,q) := c_1\,||q||^{-3/2} + \epsilon\, c_2\,||q||^{-7/2},$$

for

$$\mathcal{P} = \begin{pmatrix} \frac{\mu}{\sqrt{||q||}}\, I_2 & 0 \\ 0 & \nu\,||q||\, I_2 \end{pmatrix}.$$

It then seems reasonable to choose $s(p,q) \approx L_{\mathcal{P}}(p,q)^{-1}$, and $s(p,q) = c\,||q||^{3/2}$ when $\epsilon\,||q||^{-2} << 1$. Furthermore,

$$C_{\mathcal{P}}(p,q) \leq \tilde{C}_{\mathcal{P}}(p,q) := \max(\mu^{-1}||q||^{-1/2}, \nu^{-1}\,||q||^{-1}).$$

Consider $\hat{\delta}(t_n) = \delta(t_n)/(\tilde{C}_{\mathcal{P}}(y)\,\tilde{L}^2_{\mathcal{P}(y)})$, then compare

$$\frac{\max_n ||\hat{\delta}(t_n)||}{\min_n ||\hat{\delta}(t_n)||} = 1.29709, \quad \text{with} \quad \frac{\max_n ||\delta(t_n)||}{\min_n ||\delta(t_n)||} = 672.716.$$

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A simple rule of thumb for the case of a

Motion in a central field

Consider $H(p, q) = \frac{1}{2}||p||^2 + V(||q||)$, where

$$V(r) = \sum_{j=-l}^{l} c_j\, r^j,$$

then set

$$s(q) = \frac{||q||}{\sqrt{V^+(||q||)}}, \quad \text{where} \quad V^+(r) = \sum_{j=-l}^{l} |c_j|\, r^j.$$

When $V(r) = r^{\pm l}$, then it reduces to the recipe based on scaling invariance of Blanes and Budd (2004).
When one term $r^{\pm l}$ clearly dominates in $V(q)$, then both recipes give similar results.

A simple rule of thumb for the case of a

N-body problem

Consider $p_j, q_j \in \mathbb{R}^3$, $q = (q_1, \ldots, q_N)$, and $p = (p_1, \ldots, p_N)$, and

$$H(p, q) = \frac{1}{2}||p||^2 + \sum_{i<j} V(r_{ij}),$$

where $r_{ij} = ||q_i - q_j||$ and $V(r) = \sum_{j=-l}^{l} c_j\, r^j$. Then set

$$s(q) = \left(\sum_{i<j} V^+(r_{ij}) \right)^{-1/2} \left(\sum_{i<j} r_{ij}^{-2} \right)^{-1/2},$$

where $V^+(r) = \sum_{j=-l}^{l} |c_j|\, r^j$.

A variant of $L(y)$ for $||\cdot||_\infty$ and for

Real analytic Hamiltonian systems

For each $y \in \mathbb{R}^{2d}$, for each invertible matrix $\mathcal{P}$ consider

$$L_{\mathcal{P}}(y) \;=\; \max_{i,j} \left| \left(\mathcal{P} J^{-1} P^T \right)_{i,j} \right| \left(\max_{||\mathcal{P}(z-y)|| \le 1} |H(z)| \right),$$

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Example (Perturbed Kepler with $s(q) = ||q||^{3/2}$)

For the Hamiltonian system

$$\mathcal{H}(p,q) = ||q||^{3/2}(\frac{1}{2}||p||^2 + V(||q||) - H_0), \quad V(r) = \frac{1}{r} - \frac{\epsilon}{3r^3},$$

one can similarly obtain

$$\begin{aligned} L_{\mathcal{P}}(p,q) \;\leq\; & c_1\,||p||\,||q||^{1/2} + c_2\,||p||^{-1}\,||q||^{-1/2} \\ & + \epsilon\, c_3\,||p||^{-1}\,||q||^{-5/2} + \delta\, c_4\,||p||^{-1}\,||q||^{1/2}, \end{aligned}$$

where $|\frac{1}{2}||p||^2 + V(||q||) - H_0| \leq \delta$.

For $\epsilon = 0$ and $\delta = 0$ and $H_0 < 0$,

$$L_{\mathcal{P}}(p,q) \leq \sqrt{2}c_1 + c_2\,(2(1 + H_0||q||))^{-1/2}.$$

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Scaling invariance and adaptativity (Budd et al. 2003, ...)

If $\frac{d}{dt}y = f(y)$ is such that there exists a one-parameter family of invertible matrices Q_λ (for $\lambda \neq 0$) such that

$$\lambda f(Q_\lambda y) = Q_\lambda f(y),$$

then the time reparametrization function $s(y)$ should satisfy

$$s(Q_\lambda y) = \lambda s(y).$$

Actually, for the original system,

$$L(Q_\lambda y) = \lambda^{-1} L(y),$$

and thus cannot be bounded for all y. The criterium based on the scaling invariance guarantees that, for $\hat{f}(y) = s(y)f(y)$, it holds that $\hat{L}(Q_\lambda y) = \hat{L}(y)$.