Volume Preservation by Runge-Kutta Methods

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- Consider an ODE of the form

$$\dot{x}(t) = f(x(t)), \quad x(0) = x_0 \in \mathbb{R}^n, \quad (f \in C^2)$$

  where $\mathrm{div}(f) = 0$.
- "Divergence free vector field".

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- "Divergence free vector field".
- These systems are **volume preserving**...

- The solution to an ODE $\dot{x} = f(x)$ is a **flow map**,

$$\varphi_t : \mathbb{R}^n \to \mathbb{R}^n,$$

for all times $t \geq 0$. It maps $x(0)$ to $x(t)$.

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- This is because

$$\int_{\varphi_t(A)} \mathrm{d}y = \int_A \det(\varphi_t'(x))\, \mathrm{d}x$$

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- A numerical method is volume preserving for $\dot{x} = f(x)$ if $\det(\phi_h'(x)) = 1$ for all x, h.

- An s-stage Runge-Kutta method is defined by

$$\begin{aligned}
\phi_h(x) &= x + h\sum_{i=1}^{s} b_i f(k_i) \\
k_1 &= x + h\sum_{j=1}^{s} a_{1j} f(k_j) \\
&\vdots \\
k_s &= x + h\sum_{j=1}^{s} a_{sj} f(k_j)
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- In what situations are Runge-Kutta methods volume preserving?

- Hamiltonian Systems are volume preserving ODEs. Why?

$$\dot{x} = J\nabla H(x), \quad J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix} \in \mathbb{R}^{2d\times 2d},$$

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- Compute determinants:

$$\det(\varphi_t'(x)^\top)\det(J)\det(\varphi_t'(x)) = \det(J).$$

Hence $\det(\varphi_t'(x))^2 = 1$. Note that $\det(\varphi_0'(x)) = 1$, so $\det(\varphi_t'(x)) = 1$.

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- There are **many more** divergence free vector fields!
- What about **non**-Hamiltonian systems, and in general?

Barriers for Volume Preserving Integrators

Theorem (Kang, Zai-Jiu 1995)

No **single** *analytic method (includes all RK methods) is volume preserving for* **all** *divergence free systems.*

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General volume preservation is **hard**!

- In their book on Geometric Numerical Integation, Hairer, Lubich and Wanner consider the following systems. $x \in \mathbb{R}^m$, $y \in \mathbb{R}^n$

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} u(y) \\ v(x) \end{pmatrix},$$

for functions $u : \mathbb{R}^n \to \mathbb{R}^m$, $v : \mathbb{R}^m \to \mathbb{R}^n$

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- These are many examples of **non**-Hamiltonian systems that have volume preserving Runge-Kutta integrators.

- Is there a large class of divergence free vector fields that have volume preserving Runge-Kutta methods?

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- Which Runge-Kutta methods are relevant?

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- **"The determinant condition"** is the necessary and sufficient condition for volume preservation for the implicit midpoint rule:

$$\det(I + \frac{h}{2} f'(x)) = \det(I - \frac{h}{2} f'(x)) \text{ for all } x \in \mathbb{R}^n, h > 0.$$

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- **Hairer-Lubich-Wanner separable** systems satisfy this condition.

Lemma (Generalises Hamiltonian systems)

Let $f : \mathbb{R}^n \to \mathbb{R}^n$ *be such that there exists* **an invertible matrix** $P \in \mathbb{R}^{n \times n}$ *with* $Pf'(x)P^{-1} = -f'(x)^\top$. *Then any Symplectic Runge-Kutta method is volume preserving.*

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If f is Hamiltonian: $f(x) = J^{-1}\nabla H(x)$, then $f'(x) = J^{-1}\nabla^2 H(x)$. Hence $Jf'(x)J^{-1} = \nabla^2 H(x)J^{-1} = -(J^{-1}\nabla^2 H(x))^\top = -f'(x)^\top$.

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Lemma (Generalises HLW separable systems)

Let $f : \mathbb{R}^n \to \mathbb{R}^n$ *be such that there exists* **an invertible matrix** $P \in \mathbb{R}^{n\times n}$ *with* $Pf'(x)P^{-1} = -f'(x)$*. Then any Symplectic Runge-Kutta method with 1 or 2 stages (and compositions) is volume preserving.*

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If f is a HLW system, $f(x, y) = (u(y), v(x))$, then

$$f'(x, y) = \begin{pmatrix} 0 & u'(y) \\ v'(x) & 0 \end{pmatrix}.$$

Hence $Pf'(x, y)P^{-1} = -f'(x, y)$, where $P = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$.

Further Examples

$$P = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad Pf'(x)P^{-1} = -f'(x)^\top, \quad Pf'(x)P^{-1} = -f'(x)$$

$$\begin{aligned} \dot{x} &= F(x-z) - 5y \\ \dot{y} &= 5z - 2x \\ \dot{z} &= F(x-z) + 2y \end{aligned} \qquad f'(x,y,z) = \begin{pmatrix} F'(x-z) & -5 & -F'(x-z) \\ -2 & 0 & 5 \\ F'(x-z) & 2 & -F'(x-z) \end{pmatrix}$$

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I don't know of any *real life examples* yet.

The Bigger Picture: Why are SRK methods symplectic?

- The system $\dot{x} = f(x)$ is Hamiltonian if and only if for every $x \in \mathbb{R}^{2d}$,

$$f'(x) \in \left\{\Omega \in \mathbb{R}^{2d \times 2d} : J\Omega + \Omega^\top J = 0\right\}$$

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- For each $x \in \mathbb{R}^{2d}$, this is a Lie group equation for $\varphi_t'(x)$. Hence

$$\varphi_t'(x) \in \mathrm{Sp}(2d) = \left\{ Q \in \mathbb{R}^{2d \times 2d} : Q^\top J Q = J \right\}$$

for all times t. The Symplectic Lie Group.

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Theorem (Cooper 1987, Sanz-Serna 1988, Bochev, Scovel 1994)

Symplectic Runge-Kutta methods preserve quadratic first integrals of both the solution $\varphi_t(x)$ **and** *the Jacobian* $\varphi_t'(x)$.

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- The constraint that $\varphi_t'(x) \in \mathrm{SP}(2d)$ (i.e. $\varphi_t'(x)^\top J \varphi_t'(x) = J$) is a set of $4d^2$ quadratic constraints of $\varphi_t'(x)$. One for each entry of the matrix.

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- Symplectic Runge-Kutta methods will preserve all of these first integrals, so "symplectic methods are symplectic".

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- The generated **quadratic Lie group** is

$$\mathcal{G}_P = \left\{Q \in \mathbb{R}^{n\times n} : Q^\top PQ = P\right\} \tag{1}$$

- Just like for Hamiltonian systems (but with P instead of J) SRK methods **preserve** the **quadratic Lie Group structure**:

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- The quadratic Lie algebraic structure **induces** the volume preservation in the ODE

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- Conjecture: 2-stage SRK methods preserve the appropriate structures.

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$$g(z) = Pf(P^{-1}z),$$

where P is a matrix and f is a basic foliation.

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Nice properties:

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- Runge-Kutta methods respect linear foliations.

We define the following families of volume preserving vector fields:

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\mathcal{H} &= \left\{ f \text{ such that there exists } P \text{ such that for all } x, Pf'(x)P^{-1} = -f'(x)^\top \right\}, \\
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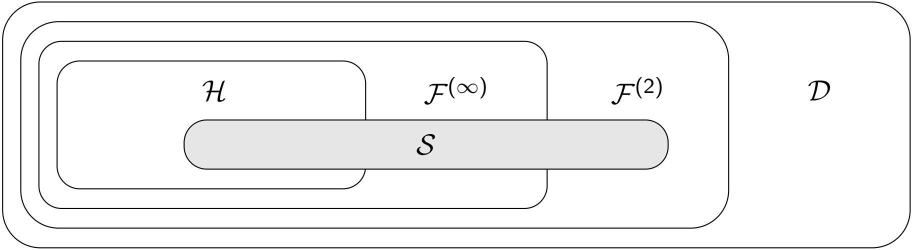
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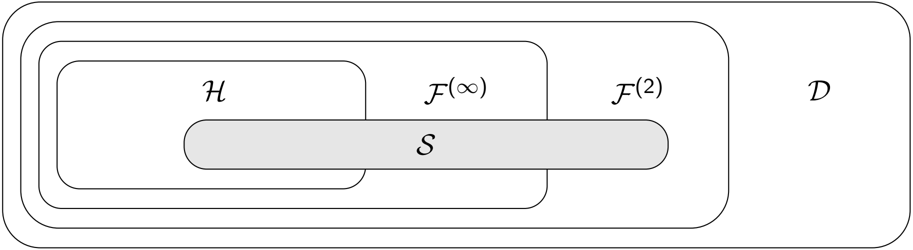

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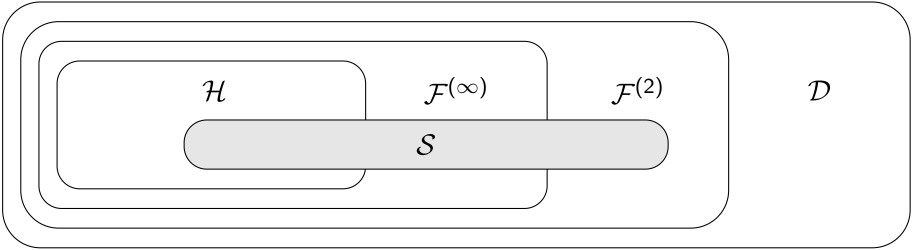
For vector fields in $\mathcal{F}^{(\infty)}$, all Symplectic Runge-Kutta methods are volume preserving.



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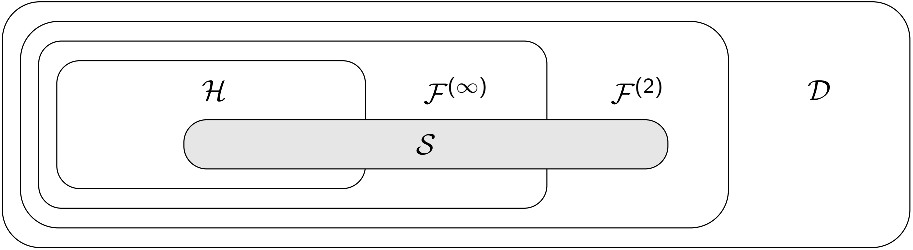

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For vector fields in $\mathcal{D}$ $(= \mathcal{F}^{(1)})$, the 1-stage implicit midpoint rule is volume preserving.

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- Thank you for listening.

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- Similarly, $\det((\phi \circ \cdots \circ \phi)'(x)) = \mu(x)/\mu((\phi \circ \cdots \circ \phi)(x))$

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- What is so good about this?

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- The **error** in volume preservation is committed by one operation at the beginning and one at the end, **no error from intermediate steps**.
- If the numerical solution stays in a region where $\mathrm{trace}(f'(\cdot)^2)$ is bounded, then we have a global $\mathcal{O}(h^2)$ error bound on our volume.

P. Bader, D.I. McLaren, R. Quispel, M. Webb *Volume Preservation by Runge-Kutta Methods* submitted, preprint available on arXiv and my website