Geometric Numerical Integration
Exercises

Adrien Laurent

August 15, 2024

The exercises are not mandatory. They aim at helping you practice the main concepts of the course for the exam. A correction or some hints can be provided upon request. A solution is also generally provided in the associated references.

1 The flow and its properties

Exercise 1: Consider the following differential equation on $U = \mathbb{R}^2 \backslash \{(0,0)\}$.

$$\dot{p} = \frac{p}{p^2+q^2}, \qquad \dot{q} = \frac{q}{p^2+q^2}.$$

1. Show that the flow is symplectic on U.
2. Show that the system is locally Hamiltonian on U.
3. Show that the system is not globally Hamiltonian on U.

Hint: $H(p,q) = -\Im(\log(p+iq)) + const,$ $\qquad \log(z) = \log|z| + i\arg(z),$
Principal definition of logarithm: $\log(z) = \log|z| + 2i \arctan\left(\frac{\Im z}{\Re z + |z|}\right)$ $(z \in \mathbb{C} \backslash \mathbb{R}_-)$.

Exercise 2: Consider a differential equation of the form $y' = f(z)$, $z' = g(y)$. Compute the first terms of the Taylor expansion of the flow. Present an algebraic structure that allows to represent conveniently the expansion of the flow. What is the condition for symplecticity? for preservation of an invariant $I(y,z)$? for volume preservation?

2 Splitting and composition methods

Exercise 1: Compute the conditions of order up to 4 of a splitting method. Check that the Takahashi-Imada splitting is of order 4.

Exercise 2: Let Φ_h be a symmetric numerical method of order 2. Construct a composition method of the form

$$\Psi_h = \Phi_{\gamma_5 h} \circ \Phi_{\gamma_4 h} \circ \Phi_{\gamma_3 h} \circ \Phi_{\gamma_2 h} \circ \Phi_{\gamma_1 h}$$

such that $\gamma_1 = \gamma_2$ and which is of order 4.

Exercise 3: ([2]) Let a splitting method with coefficients a_i, b_i:

$$\psi_h = \varphi^B_{b_s h} \circ \varphi^A_{a_s h} \circ \dots \circ \varphi^B_{b_1 h} \circ \varphi^A_{a_1 h}.$$

Denote $\chi_t = \varphi^B_t \circ \varphi^A_t$.

1. Let $X_h = hX_1 + h^2 X_2 + \dots$ such that $\chi_h = \exp(X_h)$. Compute the X_i, $i \geqslant 3$. What is the adjoint method χ^*_h? Show that $\chi^*_h = \exp(-X_{-h})$.

2. Give conditions on the γ_i such that

$$\psi_h = \chi_{\gamma_{2s-1} h} \circ \chi^*_{\gamma_{2s-2} h} \circ \dots \circ \chi^*_{\gamma_2 h} \circ \chi_{\gamma_1 h}.$$

   You can use $\gamma_0 = \gamma_{2s} = 0$ for simplicity. Deduce that ψ_h is of order 1 if and only if

$$\sum_{i=1}^{s} a_i = \sum_{i=1}^{s} b_i = \sum_{i=1}^{2s-1} \gamma_i = 1.$$

   We observe that the splitting method ψ_h is of order p iff the composition method ψ_h is of order p.

3. Find f_1, f_2, $f_{3,1}$, $f_{3,2}$ in terms of the γ_i such that

$$\psi_h = \exp(hf_1 X_1 + h^2 f_2 X_2 + h^3(f_{3,1} X_3 + f_{3,2}[X_1, X_2]) + \mathcal{O}(h^4)).$$

   Deduce the conditions on the γ_i to have order 3 at least.

4. Assume the method has at least order 3. Using that $\text{sign}(x^3 + y^3) = \text{sign}(x + y)$, show that at least one a_i and one b_i are (strictly) negative.

3 Runge-Kutta methods

Exercise 1: Show that the Störmer-Verlet method, given by the following pair of Butcher tableaux, is symplectic for a Hamiltonian system:

$$
\begin{array}{c|cc}
0 & 0 & 0 \\
1 & 1/2 & 1/2 \\
\hline
 & 1/2 & 1/2
\end{array}
\qquad
\begin{array}{c|cc}
1/2 & 1/2 & 0 \\
1/2 & 1/2 & 0 \\
\hline
 & 1/2 & 1/2
\end{array}
$$

Show that the method is actually explicit for a partitioned problem of the form $\dot{y} = f(z), \dot{z} = g(y)$.

Exercise 2:

1. We consider a Runge-Kutta method $y_{n+1} = \Phi_h(y_n)$ with coefficients a_{ij}, b_i $(i = 1, \ldots, s)$. Show that the inverse of the numerical flow Φ_h^{-1} can still be expressed as a Runge-Kutta method for any sufficiently small step size h, and provide the corresponding coefficients.

2. If Φ_h is the numerical flow, we define the adjoint of this flow as $\Phi_h^* = \Phi_{-h}^{-1}$. What is the adjoint method to the explicit Euler method?

4 Runge-Kutta methods and geometry

Exercise 1: This exercise aims to prove the following result.

Theorem ([10])**.** *There is no Runge-Kutta method that exactly preserves the energy of polynomial Hamiltonian systems. However, for a fixed polynomial Hamiltonian, such a Runge-Kutta method exists.*

For a Hamiltonian system $\dot{y} = f(y) = J^{-1}\nabla H(y)$ with the Hamiltonian $H(y)$ assumed to be regular, consider the AVF (Average Vector Field) numerical method defined by

$$y_{n+1} = y_n + h \int_0^1 f(\theta y_n + (1-\theta)y_{n+1}) d\theta.$$

1. Show that this method is well-defined for sufficiently small h.
2. Show that for any sufficiently small h, we have

$$\int_0^1 \frac{y_{n+1} - y_n}{h} \cdot \nabla H(\theta y_n + (1-\theta)y_{n+1}) d\theta = 0,$$

   with the notation $u \cdot v = u^T v$.
3. Deduce that the numerical method exactly conserves energy, i.e., given y_n and considering y_{n+1} well-defined for sufficiently small h, we have:

$$H(y_{n+1}) = H(y_n).$$

4. Show that this integration method is not a Runge-Kutta method.
   Hint: Consider quadrature problems $\dot{y}(t) = f(t)$.
5. Show that a consistent Runge-Kutta method cannot preserve the Hamiltonian for all polynomial Hamiltonian systems.
   Hint: In dimension $d = 1$, set $H(p, q) = p - \int_0^q g(t)dt$ where $g(t)$ is an arbitrary polynomial.
6. In the case of a fixed polynomial Hamiltonian, show that a Runge-Kutta method can be constructed that exactly preserves the energy.
   Hint: Introduce a quadrature formula.

Exercise 2: Let $R(z)$ be an analytic function around $z = 0$ such that $R(0) = R'(0) = 1$. Recall that $R(z) = \sum_k a_k z^k$ induces an application on matrices close to 0 by $R(A) = \sum_k a_k A^k$.

1. Show that if $R(z) = \exp(z)$, then for any $A \in \mathbb{R}^{d\times d}$ such that $\mathrm{Tr}(A) = 0$, we have $\det(R(A)) = 1$.
2. Show that if for every $A \in \mathbb{R}^{d\times d}$ such that $\mathrm{Tr}(A) = 0$, we have $\det(R(A)) = 1$, then $R(z)$ satisfies $R(\mu + \nu) = R(\mu)R(\nu)$ for μ, ν close to 0.
   Hint: Consider matrices of the form $A = \mathrm{diag}(\mu, \nu, -\mu - \nu, 0, \dots, 0)$.

3. Deduce that $R(z) = \exp(z)$ if and only if for every $A \in \mathbb{R}^{d\times d}$ such that $\mathrm{Tr}(A) = 0$, we have $\det(R(A)) = 1$.

4. Show that a Runge-Kutta method for the problem $y' = \lambda y$, where $\lambda \in \mathbb{C}$, writes as $y_{n+1} = R(h\lambda)y_n$ for a specific R. Show that such a method is symmetric for the problem $y' = \lambda y$ if and only if R satisfies $R(-z)^{-1} = R(z)$. Provide an example of such a method.

Exercise 3: We are interested in matrix ODEs of the form $Y' = AY$, $Y(0) = I_d$ with $Y(t) \in \mathbb{R}^{d\times d}$ where $A \in \mathbb{R}^{d\times d}$ is constant and satisfies $\mathrm{Tr}(A) = 0$.

1. Explicitly state the solution of this ODE and show that $\det(Y)$ is a first integral. Deduce that the volume is preserved for the problem on $\mathbb{R}^d$, $y' = Ay$, $y(0) = y_0$.

2. Given a consistent Runge-Kutta method (of order at least 1) and denoting $R(z)$ its stability function (see previous exercise), we assume it preserves the determinant $\det(Y)$. Using the previous exercise, show that the stability function must satisfy $R(z) = \exp(z)$.

3. Deduce that a Runge-Kutta method cannot preserve the determinant.

4. Prove the following theorem.

   Theorem. *In dimension $d \geqslant 3$, there is no Runge-Kutta method that preserves* ***all*** *polynomial invariants of degree d.*

   Hint: The determinant is a polynomial of degree d.

5 Butcher series and algebraic structures

Exercise 1: Provide the list of trees $\tau \in \mathcal{T}$ with a number of nodes $|\tau| \leqslant 5$ in the set $\mathcal{T}$ of trees. For each of them, calculate the coefficients $\gamma(\tau)$ and $\sigma(\tau)$ as defined in the course. Show that the RK4 method is generally of exact order 4. Show it by simply using Taylor expansions and no trees.

Exercise 2:

1. Suppose $f : \mathbb{R}^d \to \mathbb{R}^d$ is linear. Show that the elementary differential $F(\tau)$ is zero for any tree $\tau \in \mathcal{T}$, unless τ is a "bamboo."
2. What does the B-series expansion of the exact solution become in the case where $f(y) = \lambda y$ and $\lambda \in \mathbb{C}$? Verify that the expected development is obtained by comparing it with the solution of $y' = f(y)$.
3. Deduce the value of the coefficients $a(\tau)$ for each bamboo-type tree τ in the B-series associated with the midpoint method.

Exercise 3:

1. For each $\hat{\tau} \in \mathcal{T}$, show that there exists y_0 and a vector field $f : \mathbb{R}^q \to \mathbb{R}^q$ with $q = |\hat{\tau}|$ such that $F(\hat{\tau})(y_0) \neq 0$ and $F(\tau)(y_0) = 0$ for all $\tau \in \mathcal{T}$ with $\tau \neq \hat{\tau}$ and $|\tau| = |\hat{\tau}|$.
   Hint: For a tree $\hat{\tau}$ with $q = |\hat{\tau}|$, number its nodes as $1, 2, \ldots, q$ (each node has a different index). Then, for each node of the tree with index i and indices of roots $i_1, \ldots, i_k$, where k is the number of branches, set

   $$f_i(y) = \prod_{j=1}^{k} y_{i_j}, \qquad (\textit{with } f_i(y) = 1 \textit{ if } k = 0).$$

   You may look at examples of trees with few nodes.

2. Deduce that the order conditions of Runge-Kutta methods indexed by Butcher trees are necessary and sufficient.

Exercise 4: Compute the first terms of the composition of two Runge-Kutta methods by first using Taylor expansions and then by using the Butcher-Connes-Kreimer Hopf algebra structure.

6 Backward error analysis

Exercise 1: Calculate the terms f_2, f_3, f_4 in the modified equation for the backward error analysis

$$\dot{\widetilde{y}} = f(\widetilde{y}) + hf_2(\widetilde{y}) + h^2 f_3(\widetilde{y}) + h^3 f_4(\widetilde{y}) + \dots$$

for the explicit Euler method applied to the following ODEs:

1. $\dot{y} = y$,
2. $\dot{y} = y^2$,
3. $\dot{y} = f(t)$,
4. $\dot{y} = f(y)$.

Use the method of your choice (Taylor expansions or Butcher series).

Exercise 2: For the ODE system $\dot{y} = f(y)$, consider a numerical method $y_{n+1} = \Phi_h(y_n)$ with a modified equation for the backward error analysis

$$\dot{\widetilde{y}} = f_h(\widetilde{y}) = f(\widetilde{y}) + hf_2(\widetilde{y}) + h^2 f_3(\widetilde{y}) + h^3 f_4(\widetilde{y}) + \dots$$

Show that the adjoint method $y_{n+1} = \Phi_h^*(y_n)$ has the modified equation

$$\dot{\widetilde{y}} = f_{-h}(\widetilde{y}) = f(\widetilde{y}) - hf_2(\widetilde{y}) + h^2 f_3(\widetilde{y}) - h^3 f_4(\widetilde{y}) + \dots$$

Verify this result for the first terms of the explicit and implicit Euler methods. Deduce that if the method is symmetric, its modified equation has a development in even powers of h.

Exercise 3: Compute the first terms of the modified Hamiltonian for the midpoint method applied to a general Hamiltonian problem. Use the method of your choice (Taylor expansions or Butcher series).

7 Going further

The exercises in this section will not appear at the exam in any way. They are here if you want a challenge or want to go further. There are a variety of different fields of mathematics represented in geometric numerical integration, that we aim to showcase here. If you find some (even partial) solutions to the open questions or if you want more details, feel free to ask me.

Exercise 1: This exercise studies some topological properties of Butcher series (see [18, 8, 24]). Consider the topology of formal series: a sequence of Butcher series $B_h^f(a_n)$ converges to $B_h^f(a)$ if for all $\tau \in \mathcal{T}$, $a_n(\tau) \to a(\tau)$. Show that Runge-Kutta methods are dense in the space of B-series.

Exercise 2: This exercise aims at observing properties of aromatic forests from different points of view (see [13, 19, 24, 25, 3, 22, 21, 5]).

1. Combinatorics: Let $t(z) = \sum_{n=1}^{\infty} t_n z^n$ with t_n the number of trees with n nodes and $a(z) = \sum_{n=0}^{\infty} a_n z^n$ with a_n the number of multiaromas with n nodes ($a_0 = 1$ by convention).
   (a) Compute the first values.
   (b) Show that t_n corresponds to the number of functions $\{1, \dots, n-1\} \to \{0, \dots, n-1\}$ modulo the symmetric group S_{n-1} and that t satisfies
   $$t(z) = z \exp\left(\sum_{k=1}^{\infty} \frac{1}{k} t(z^k)\right).$$
   (c) Show that a_n corresponds to the number of functions $\{1, \dots, n\} \to \{1, \dots, n\}$ modulo the symmetric group S_n and that a satisfies
   $$a(z) = \prod_{k=1}^{\infty} \left(1 - t(z^k)\right)^{-1}.$$
   (d) Deduce the generating series of the number of aromatic trees.
2. Geometric integration:
   (a) Open question: Create an aromatic B-series method that preserves volume. One could start from the method defined in [26]. Starting from Runge-Kutta methods and adding aromas here or there will not work.
   (b) Extend the Liouville theorem to the study of volume preservation on a Lie group, using the frozen flow methods described in the homework.
   (c) Open questions: how do aromatic series extend on homogeneous manifolds? Does the characterisation using backward error analysis extend?
3. Algebra: Show on examples that the composition of aromatic S-series indexed by (unordered) aromatic forests can be described by a BCK Hopf algebra. The substitution law cannot be described straightforwardly by Hopf algebra techniques and relies on a lift to the tensor symmetric algebra over aromatic trees (called clumped forests).

4. Variational calculus: We give details on the aromatic De Rham complex seen in the course.
   (a) Prove that $d^2 = 0$.
   (b) There exists a homotopy operator $h\colon \Omega_n \to \Omega_{n+1}$ such that $hd+dh = id$ (difficult, see [1, 22]). Show that the aromatic complex is exact, that is, $\mathrm{Ker}(d) = \mathrm{Im}(d)$.
   (c) Define the Euler operator on multiaromas $\gamma \in \Omega_0$:

$$\mathcal{E}\gamma = \sum_{v\in V} (-1)^{|\Pi(v)|} D^{\Pi(v)}\gamma_v,$$

   where $\Pi(v)$ contains the predecessors of v, and $D^{\Pi(v)}\gamma_v$ detaches all the predecessors of v and sum all the possible ways (with multiplicity) to plug them back on any node of γ **different from** v. Show that $\mathcal{E}d = 0$ on Ω_1. This newly obtained complex can be further extended into the Euler-Lagrange variational complex, which is an adimensional subcomplex of the standard Euler-Lagrange complex, where the Noether theorems are formulated.
   (d) Open questions: how does the Euler-Lagrange complex extends on manifolds? Is it still exact?

Exercise 3: The course only gives partial details on the proofs of the Hopf algebra structure over rooted forests. Show that the algebraic structures indeed are Hopf algebras and that the expressions of the antipodes are valid (see [7, 14, 6, 11, 18, 12, 9, 8, 17]).

Exercise 4: In this exercise, we extend some results of the course to stochastic numerical integration (see [29, 27, 28, 15, 16, 23, 4, 5]). We consider a stochastic differential equation of the form

$$dX = f(X)dt + dW,$$

where f is smooth, Lipschitz, and W is a d-dimensional Brownian motion defined on a probability space satisfying the usual assumptions. We approximate the law $u(t,x) = \mathbb{E}[\phi(X(t))]$. It satisfies the following PDE

$$\partial_t u = \mathcal{L}u, \quad \mathcal{L}\phi = \phi' f + \frac{1}{2}\Delta.$$

A stochastic Runge-Kutta method takes the form

$$H_i = Y_n + h\sum_{j=1}^{s} a_{ij} f(H_j) + \sqrt{h} d_i \xi_n,$$
$$Y_{n+1} = Y_n + h\sum_{i=1}^{s} b_i f(H_i) + \sqrt{h}\xi_n,$$

where the ξ_n are independent standard Gaussian vectors. Let us create a method of (weak) order two.

1. Give the first terms of the Taylor expansion of u.

2. We introduce decorated nodes to the Butcher forests. They are numbered by integers, only appear as leaves, and always come in pairs (the numbers do not matter and just serve as a way to identify the pairs). In particular, $F(①①)[\phi] = \Delta\phi = \sum_i \phi''(e_i, e_i)$, with e_i the canonical basis of $\mathbb{R}^d$. Propose a formalism of forests (called exotic) that allows to represent the Taylor expansion of u.

3. Following the idea of the Grossman-Larson Hopf algebra, write $u(h,x) = \exp(h\mathcal{L})[\phi]$ explicitly in terms of exotic forests (give the coefficient map). *Hint: the symmetry coefficient is the number of automorphisms of the forest.*

4. Give the expression in exotic forests of $\mathbb{E}[\phi(Y_1)]$ for the first orders. For the expression at any order, use [20].

5. Create a stochastic Runge-Kutta method of weak order two.

6. Observe that order conditions are indexed by forests and not trees. Identify the primitive elements and give the minimal number of order conditions.

References

[1] I. M. Anderson. The variational bicomplex. Unpublished, 1989.

[2] S. Blanes and F. Casas. On the necessity of negative coefficients for operator splitting schemes of order higher than two. *Appl. Numer. Math.*, 54(1):23–37, 2005.

[3] G. Bogfjellmo. Algebraic structure of aromatic B-series. *J. Comput. Dyn.*, 6(2):199–222, 2019.

[4] E. Bronasco. Exotic B-series and S-series: algebraic structures and order conditions for invariant measure sampling. *Found. Comput. Math.*, pages 1–31, 2024.

[5] E. Bronasco and A. Laurent. Hopf algebra structures for the backward error analysis of ergodic stochastic differential equations. *Submitted*, 2024.

[6] C. Brouder. Runge–Kutta methods and renormalization. *Eur. Phys. J. C*, 12(3):521–534, 2000.

[7] J. C. Butcher. An algebraic theory of integration methods. *Math. Comp.*, 26:79–106, 1972.

[8] J. C. Butcher. *Numerical methods for ordinary differential equations.* John Wiley & Sons, Ltd., Chichester, third edition, 2016.

[9] D. Calaque, K. Ebrahimi-Fard, and D. Manchon. Two interacting Hopf algebras of trees: a Hopf-algebraic approach to composition and substitution of B-series. *Adv. in Appl. Math.*, 47(2):282–308, 2011.

[10] E. Celledoni, V. Grimm, R. I. McLachlan, D. I. McLaren, D. O'Neale, B. Owren, and G. Quispel. Preserving energy resp. dissipation in numerical pdes using the "average vector field" method. *Journal of Computational Physics*, 231(20):6770–6789, 2012.

[11] P. Chartier, E. Hairer, and G. Vilmart. A substitution law for B-series vector fields. Research Report RR-5498, INRIA, 2005.

[12] P. Chartier, E. Hairer, and G. Vilmart. Algebraic structures of B-series. *Found. Comput. Math.*, 10(4):407–427, 2010.

[13] P. Chartier and A. Murua. Preserving first integrals and volume forms of additively split systems. *IMA J. Numer. Anal.*, 27(2):381–405, 2007.

[14] A. Connes and D. Kreimer. Hopf algebras, renormalization and noncommutative geometry. *Comm. Math. Phys.*, 199(1):203–242, 1998.

[15] K. Debrabant and A. Kværnø. Composition of stochastic B-series with applications to implicit Taylor methods. *Appl. Numer. Math.*, 61(4):501–511, 2011.

[16] L. C. Evans. *An introduction to stochastic differential equations.* American Mathematical Society, Providence, RI, 2013.

[17] L. Foissy. Introduction to hopf algebra of rooted trees. *Preprint.*

[18] E. Hairer, C. Lubich, and G. Wanner. *Geometric numerical integration*, volume 31 of *Springer Series in Computational Mathematics*. Springer-Verlag, Berlin, second edition, 2006. Structure-preserving algorithms for ordinary differential equations.

[19] A. Iserles, G. R. W. Quispel, and P. S. P. Tse. B-series methods cannot be volume-preserving. *BIT Numer. Math.*, 47(2):351–378, 2007.

[20] L. Isserlis. On a formula for the product-moment coefficient of any order of a normal frequency distribution in any number of variables. *Biometrika*, 12, 11 1918.

[21] A. Laurent. The Lie derivative and Noether's theorem on the aromatic bicomplex for the study of volume-preserving numerical integrators. *J. Comput. Dyn.*, 11(1):10–22, 2024.

[22] A. Laurent, R. I. McLachlan, H. Z. Munthe-Kaas, and O. Verdier. The aromatic bicomplex for the description of divergence-free aromatic forms and volume-preserving integrators. *Forum Math. Sigma*, 11:Paper No. e69, 2023.

[23] A. Laurent and G. Vilmart. Exotic aromatic B-series for the study of long time integrators for a class of ergodic SDEs. *Math. Comp.*, 89(321):169–202, 2020.

[24] R. I. McLachlan, K. Modin, H. Munthe-Kaas, and O. Verdier. B-series methods are exactly the affine equivariant methods. *Numer. Math.*, 133(3):599–622, 2016.

[25] H. Munthe-Kaas and O. Verdier. Aromatic Butcher series. *Found. Comput. Math.*, 16(1):183–215, 2016.

[26] G. R. W. Quispel. Volume-preserving integrators. *Phys. Lett. A*, 206(1-2):26–30, 1995.

[27] A. Rößler. Runge-Kutta methods for Stratonovich stochastic differential equation systems with commutative noise. In *Proceedings of the 10th International Congress on Computational and Applied Mathematics (ICCAM-2002)*, volume 164/165, pages 613–627, 2004.

[28] A. Rößler. Runge-Kutta methods for Itô stochastic differential equations with scalar noise. *BIT Numer. Math.*, 46(1):97–110, 2006.

[29] D. Talay and L. Tubaro. Expansion of the global error for numerical schemes solving stochastic differential equations. *Stochastic Anal. Appl.*, 8(4):483–509 (1991), 1990.