Geometric numerical integration of differential equations, THREAD Network-wide training event 6

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1 Symplectic integration with Runge-Kutta methods

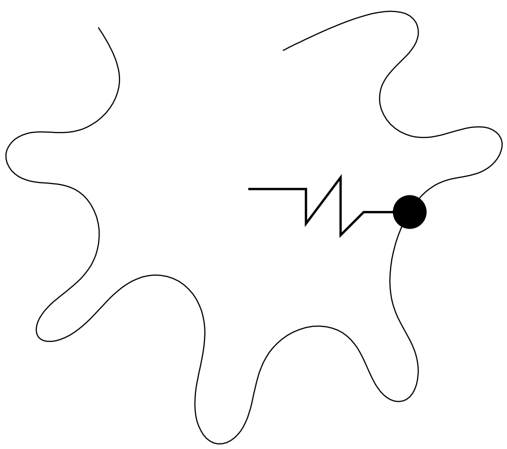

Figure 1: Spring pendulum

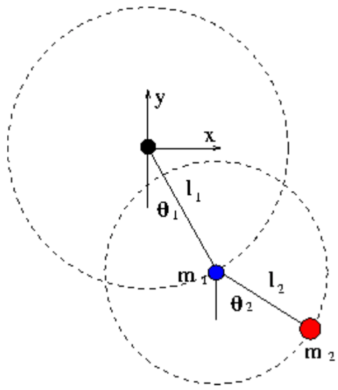

Figure 2: Double pendulum

1.1 Lagrangian mechanics, variational calculus.

We here denote by Q a n-dimensional configuration space (a vector space or a manifold) of generalized positions, and its tangent bundle TQ represents the velocity phase space, ($TQ = Q \times Q^*$ in the case of vector spaces). We introduce coordinates on Q, $(q_1, \ldots, q_n)$ which induce coordinates $(q_1, \ldots, q_n, v_1, \ldots, v_n)$ on TQ. The Lagrangian L is a function on TQ which we may express in coordinates

$$L : TQ \to \mathbb{R}, \qquad L(q_1, \ldots, q_n, v_1, \ldots, v_n).$$

For any differentiable curve $q(t) \in Q$ and real numbers $t_1 < t_2$ we define the *action integral*

$$S[q] = \int_{t_1}^{t_2} L(q(t), \dot{q}(t))\,\mathrm{d}t. \tag{1}$$

Hamilton's principle states that, among all curves with fixed end points, the path chosen by a dynamical system is a stationary path for the action integral (1).

Consider the curve $q_\varepsilon(t)$ on $[t_2, t_2]$ such that

$$q_\varepsilon(t)|_{\varepsilon=0} = q(t), \qquad \left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} q_\varepsilon(t) = \delta q(t) \in T_{q(t)}Q.$$

Then for all possible variations $\delta q(t)$ with $\delta(t_1) = \delta(t_2) = 0$, $q(t)$ satisfies the equations

$$\delta S[q] = 0, \qquad \delta S[q] = \left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} \int_{t_1}^{t_2} L(q_\varepsilon(t), \dot{q}_\varepsilon(t))\,\mathrm{d}t.$$

Now, assuming we can take the derivative inside the integral, we get

$$\delta S[q] = \int_{t_1}^{t_2} \left(\langle \frac{\partial L}{\partial q}(q, \dot{q}), \delta q \rangle + \langle \frac{\partial L}{\partial \dot{q}}(q, \dot{q}), \delta \dot{q} \rangle \right) \mathrm{d}t.$$

Integrating by parts on the second term in the integral, we obtain

$$\delta S[q] = \int_{t_1}^{t_2} \left\langle \frac{\partial L}{\partial q}(q, \dot{q}) - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \right), \delta q \right\rangle \mathrm{d}t + \left[\frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \delta q \right]_{t_1}^{t_2}$$

Using the boundary conditions on δq, and assuming that L is continuously differentiable with respect to both arguments, we conclude that $\delta S = 0$ for all δq requires

$$\frac{\partial L}{\partial q}(q, \dot{q}) - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}}(q, \dot{q}) \right) = 0$$

These are the *Euler-Lagrange equations.*

Exercise 1.1. *In the last step before arriving at the Euler-Lagrange equations, we made use of the following result. If $f(t)$ is a continuous function on $[a, b]$, then $\int_a^b f(t)h(t)\,\mathrm{d}t = 0$ for all continuous $h(t)$ requires $f(t) \equiv 0$ on $[a, b]$ (in fact it is even enough to assume that the integral vanishes for all $h \in C^\infty[a, b]$). Prove this result.*

Example 1.2. *Naturally, the Lagrangian L is the difference between the kinetic and potential energy of the system. We consider the dynamics of d particles*

$$L(q,\dot{q}) = \frac{1}{2}\sum_i m_i|\dot{q}_i|^2 - U(q)$$

Here, $q_i \in \mathbb{R}^3$ is the position coordinates of the ith particle, and its velocity is $\dot{q}_i$. So $q = (q_1,\ldots,q_d) \in \mathbb{R}^{3d}$. The potential energy $U(q)$ is assumed to only depend on the positions q. We compute

$$\frac{\partial L}{\partial q_i} = -\frac{\partial U}{\partial q_i}, \qquad \frac{\partial L}{\partial \dot{q}_i} = m_i\dot{q}_i$$

so that the Euler–Lagrange equations are

$$\frac{\mathrm{d}}{\mathrm{d}t}(m_i\dot{q}_i) = -\frac{\partial U}{\partial q_i}$$

This is nothing else than Newton's second law, mass times acceleration on the left, and a conservative force field on the right.

1.2 The Legendre transformation and Hamilton's equations.

The partial derivatives of L both with respect to q and $\dot{q}$ are dual vectors, i.e. elements of T_q^*Q. Let

$$p = \frac{\partial L}{\partial \dot{q}}(q,\dot{q}), \tag{2}$$

this is called the *Legendre transformation*, the map $(q,\dot{q}) \mapsto (q,p)$ maps TQ to T^*Q. The Legendre transform is invertible if its hessian matrix

$$\frac{\partial^2 L}{\partial \dot{q}^2}(q,\dot{q})$$

is non-singular. The Hamiltonian function $H(q,p)$ is obtained as

$$H(q,p) = \langle p,\dot{q}\rangle - L(q,\dot{q}) \tag{3}$$

where it is understood that (2) is solved for $\dot{q}$ in terms of (q,p) and inserted into (3). Now the differential equations for q and p can be found from

$$\dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial q} \tag{4}$$

Exercise 1.3. *For the Lagrangian in Example 1.2, determine the Legendre transformation and the resulting Hamiltonian function in terms of q and p.*

1.3 Hamiltonian systems and their properties

We consider a Hamiltonian system in the form

$$\dot{y} = J\,\nabla H(y) \tag{5}$$

$$y(0) = y_0 \tag{6}$$

where $y \in \mathbf{R}^{2n}$, $H : \mathbf{R}^{2n} \mapsto \mathbf{R}$, $H = H(q, p)$ is the Hamiltonian function, and

$$J := \begin{bmatrix} O & I \\ -I & O \end{bmatrix}$$

and I denotes the $n \times n$ identity matrix.

The ODE system (5) has the following properties.

1. The Hamiltonian function (typically representing an energy function) is preserved along solutions of (5). In fact we have that

$$\frac{d}{dt} H(y(t)) = \nabla H(y)^T \dot{y} = \nabla H(y)^T J \nabla H(y) = 0$$

   where the last equality follows because of the skew-symmetry of the matrix J. So the Hamiltonian function must be constant along solutions of the Hamiltonian system.

2. We will prove below that the flow of (5) is a symplectic map.

Definition 1.4. Symplectic transformation
A linear transformation $\Psi : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ is called a symplectic transformation if and only if it satisfies

$$\Psi^T J \Psi = J.$$

Definition 1.5. Symplectic map *A differentiable map $\gamma : U \subset \mathbb{R}^{2n} \to \mathbb{R}^{2n}$ (U open) is called symplectic if the Jacobian of γ is everywhere a symplectic transformation.*

Definition 1.6. Symplectic two-form *The symplectic two-form $\omega : \mathbb{R}^{2n} \times \mathbb{R}^{2n} \to \mathbb{R}$ is the map*

$$\omega(x, y) = x^T J y.$$

The space $(\mathbb{R}^{2n}, \omega)$ is called symplectic vector space. It is easily seen that ω is a bilinear form that satisfies the following three properties:

1. $\omega(x, y) = -\omega(y, x)$, skew-symmetry;
2. $\omega(x, x) = 0$;
3. $\omega(x, y) = 0$ for all $y \in \mathbb{R}^{2n}$ implies $x = 0$, non degenerate.

Denote with φ_t the flow map of (5). Recall that the flow map is the map $\varphi_t : \mathbf{R}^{2n} \to \mathbf{R}^{2n}$ such that

$$\varphi_t(y_0) = y(t),$$

and with $\Psi := \frac{\partial \varphi(y_0)}{\partial y_0}$ the derivative of the flow with respect to y_0.

The variational equation is the differential equation satisfied by Ψ and is obtained as follows. Differentiating Ψ with respect to t we have

$$\frac{d}{dt}\Psi = \frac{d}{dt}\frac{\partial \varphi_t(y_0)}{\partial y_0} = \frac{d}{dt}\frac{\partial y(t)}{\partial y_0} = \frac{\partial \dot{y}(t)}{\partial y_0} = \frac{\partial}{\partial y_0} J \nabla H(\varphi_t(y_0)) = J H''(y(t)) \frac{\partial \varphi_t(y_0)}{\partial y_0} = J H''(y(t)) \Psi$$

with the initial condition $\Psi(0) = I$. Since the vector field $JH''(y(t))\Psi$ depends on y, this equation is coupled to (5). All together the *variational equation*[1] for (5) reads:

$$\dot{y} = J\,\nabla H(y) \tag{7}$$
$$y(0) = y_0 \tag{8}$$
$$\dot{\Psi} = JH''(y)\Psi \tag{9}$$
$$\Psi(0) = I. \tag{10}$$

Theorem 1.7. *The flow of* (5) *is a symplectic map.*

Proof. The map φ_t is symplectic if the $\Psi = \frac{\partial \varphi(y_0)}{\partial y_0}$ is a symplectic transformation, i.e. we need to prove that

$$\Psi^T J \Psi = J.$$

To see that this is the case we differentiate $\Psi^T J \Psi$ with respect to t and get

$$\frac{d}{dt}\left(\Psi^T J \Psi\right) = \dot{\Psi}^T J \Psi + \Psi^T J \dot{\Psi}, \tag{11}$$
$$\tag{12}$$

using the variational equation i.e. $\dot{\Psi} = JH''(y)\Psi$ we get

$$\frac{d}{dt}\left(\Psi^T J \Psi\right) = \Psi^T H''(y) J^T J \Psi + \Psi^T J J H''(y)\Psi, \tag{13}$$

which since $J^T J = I$ and $J^2 = -I$, gives

$$\frac{d}{dt}\left(\Psi^T J \Psi\right) = O. \tag{14}$$

So $\Psi^T J \Psi$ is constant with respect to t and so

$$\Psi^T J \Psi = \Psi(0)^T J \Psi(0) = J.$$

Which shows that the condition for symplecticity of the flow of (5) is fulfilled. ■

1.4 Preservation of linear and quadratic invariants with Runge-Kutta methods

In this section we will discuss briefly the preservation of invariants for a general ordinary differential equation (ODE), as this will be used in the next sections. Consider the autonomous ODE

$$\dot{y} = f(y), \tag{15}$$

with $y(t) \in \mathbf{R}^m$ for all t.

[1]For a generic autonomous ODE $\dot{y} = f(y)$, $y(0) = y_0$, if $\Psi := \frac{\partial y(t)}{\partial y_0}$ the variational equations takes the form

$$\dot{y} = f(y),$$
$$y(0) = y_0,$$
$$\dot{\Psi} = f'(y)\Psi,$$
$$\Psi(0) = I.$$

Definition 1.8. *A function $\mathcal{I} : \mathbf{R}^m \to \mathbf{R}$ is a first integral (or invariant) of the ODE if and only if*

$$\nabla\mathcal{I}(y)^T f(y) = 0, \quad \forall y. \tag{16}$$

This implies that $\mathcal{I}(y(t)) = \mathcal{I}(y_0)$ is constant along solutions of the ODE, in fact $\frac{d\mathcal{I}(y(t))}{dt} = \nabla\mathcal{I}(y(t))^T f(y(t)) = 0$.

Linear invariants

Linear invariants have the form

$$\mathcal{I}(y) := d^T y,$$

where $d \in \mathbf{R}^m$ is a fixed vector not depending on t. These are homogeneous linear polynomials in the components of y.

Theorem 1.9. *All RK-methods preserve linear invariants.*

Proof. We want to prove that for a general Runge-Kutta method s.t. $y_{n+1} = \Phi_h(y_n)$, and a general linear invariant $\mathcal{I}(y) := d^T y$, we have that $d^T y_{n+1} = d^T y_n$. To see that this holds we consider the Runge-Kutta formulae and multiply from the left with d^T we obtain

$$d^T y_{n+1} = d^T y_n + h\sum_{i=1}^{s} b_i d^T K_i, \quad K_i = f(y_n + h\sum_{j=1}^{s} a_{i,j}K_j),\ i = 1,\dots,s,$$

but since $\nabla\mathcal{I}(y)^T = d^T$, and $\mathcal{I}$ is an invariant of (15), using the definition of invariant we have that

$$d^T f(y) = 0, \quad \forall y \in \mathbf{R}^m$$

and so also $d^T K_i = 0$ which concludes the proof. ∎

Quadratic invariants

Quadratic invariants have the form

$$Q(y) = y^T C y, \tag{17}$$

where $y \in \mathbf{R}^m$ and C is a symmetric $m \times m$ matrix. These are homogeneous quadratic polynomials in the components of y.

Theorem 1.10. *A Runge-Kutta method with coefficients $\{c_i\}_{i=1,\dots,s}$, $\{b_i\}_{i=1,\dots,s}$, $\{A_{i,j}\}_{i,j=1,\dots,s}$ satisfying the algebraic relation*

$$b_i a_{i,j} + b_j a_{j,i} = b_i b_j, \quad \forall i,j = 1,\dots,s, \tag{18}$$

preserves all quadratic invariants.

Proof. For a Runge-Kutta method we have

$$\begin{aligned} y_{n+1}^T C y_{n+1} &= (y_n + h\sum_{j=1}^{s} b_j K_j)^T (C y_n + h\sum_{i=1}^{s} b_i C K_i) \\ &= y_n^T C y_n + h\sum_{i=1}^{s} y_n^T C K_i + h\sum_{j=1}^{s} K_j^T C y_n + h^2 \sum_{i,j=1}^{s} b_i b_j K_j^T C K_i. \end{aligned}$$

Using the identity $y_n = y_n + h\sum_j a_{i,j}K_j - h\sum_j a_{i,j}K_j$ valid for $i = 1, \dots, s$, and the fact that

$$(y_n + h\sum_j a_{i,j}K_j)^T Cf(y_n + h\sum_j a_{i,j}K_j) = 0$$

(satisfied because $\forall y\ 0 = \nabla Q(y)^T f(y) = y^T Cf(y)$), we further obtain

$$\begin{aligned} y_{n+1}^T Cy_{n+1} &= y_n^T Cy_n - h^2\sum_{i,j=1}^s b_i a_{i,j} K_j^T CK_i - h^2\sum_{j,i=1}^s b_j a_{j,i} K_j^T CK_i + h^2\sum_{i,j=1}^s b_i b_j K_j^T CK_i, \\ &= y_n^T Cy_n + h^2\left(\sum_{i,j=1}^s \big(-b_i a_{i,j} - b_j a_{j,i} + b_i b_j\big) K_j^T CK_i\right), \end{aligned}$$

and from this last expression we see that if (18) is satisfied then $y_{n+1}^T Cy_{n+1} = y_n^T Cy_n$ for a generic C and so the Runge-Kutta method preserves all quadratic invariants. ∎

Exercise 1.11. *The midpoint rule satisfies* (18)*.*

Exercise 1.12. *The function* $\mathcal{I}_{i,j} : \mathbf{R}^{2n\times 2n} \to \mathbf{R}$*, defined by*

$$\mathcal{I}_{i,j}(\Psi) := (\Psi^T J\Psi)_{i,j} \tag{19}$$

is a quadratic invariant of the variational equation, (7)-(9)*.*

Proof. To see this we will write (19) in the form (17). Assume $m = 2n$ and consider the vector of length m^2 obtained by

$$\mathrm{vec}(\Psi)^T = [\Psi_1^T, \dots, \Psi_m^T]$$

where $\Psi_j = \Psi \cdot e_j$ is the j-th column of Ψ and e_j denotes the j-th canonical vector of $\mathbf{R}^m$. We have

$$\mathcal{I}_{i,j}(\Psi) = \mathrm{vec}(\Psi)^T C \mathrm{vec}(\Psi)^T$$

where C is the $m^2 \times m^2$ symmetric block matrix

$$C = \frac{1}{2}(e_i e_j^T + e_j e_i^T) \otimes J,$$

with $\otimes$ denoting the Kronecker tensor product of matrices. ∎

Cubic invariants

One can prove that there are no Runge-Kutta methods preserving all polynomial invariants of degree 3 or higher. We will prove this later with a counter example.

1.5 Symplecticity of Runge-Kutta methods

Definition 1.13. *A one-step method* $y_{n+1} = \Phi_h(y_n)$ *is symplectic if and only if*

$$\Psi_h := \frac{\partial \Phi_h(y_n)}{\partial y_n}, \quad \text{satisfies} \quad \Psi_h^T J\Psi_h = J,$$

i.e. the numerical flow is a symplectic map.

In the following lemma we consider an autonomous ODE together with its variational equation:

$$\begin{array}{rcl} \dot{y} & = & f(y) \\ y(0) & = & y_0, \\ \dot{\Psi} & = & f'(y)\Psi \\ \Psi(0) & = & I. \end{array} \tag{20}$$

Lemma 1.14. *For Runge-Kutta methods the following diagram commutes:*

$$\begin{array}{ccc} \begin{array}{rcl} \dot{y} & = & f(y) \\ y(0) & = & y_0 \end{array} & \xrightarrow{\text{differentiaiton w.r.t. } y_0} & \begin{array}{rcl} \dot{y} & = & f(y) \\ y(0) & = & y_0, \\ \dot{\Psi} & = & f'(y)\Psi \\ \Psi(0) & = & I \end{array} \\ \Big\downarrow \Phi_h & & \Big\downarrow \Phi_h \\ y_1 = \Phi_h(y_0, f) & \xrightarrow{\text{differentiaiton w.r.t. } y_0} & \begin{array}{rcl} y_1 & = & \Phi_h(y_0, f) \\ \Psi_1 & = & \Phi_h(\Psi_0, f'(y_1)) \end{array} \end{array}$$

where Φ_h *denotes the Runge-Kutta method.*

Proof. We first perform one step of a generic Runge-Kutta method on the ODE system $\dot{y} = f(y)$ and obtain

$$y_1 = y_0 + h\sum_{i=1}^{s} b_i K_i, \tag{21}$$

$$K_i = f(y_0 + h\sum_{j=1}^{s} a_{i,j}K_j). \tag{22}$$

We then differentiate with respect to y_0 and get

$$\frac{\partial y_1}{\partial y_0} = I + h\sum_{i=1}^{s} b_i \frac{\partial K_i}{\partial y_0}, \tag{23}$$

$$\frac{\partial K_i}{\partial y_0} = f'(y_0 + h\sum_{j=1}^{s} a_{i,j}K_j)\left(I + h\sum_{j=1}^{s} a_{i,j}\frac{\partial K_j}{\partial y_0}\right), \quad i = 1, \dots, s. \tag{24}$$

So this is the result of first applying Φ_h and then differentiating with respect to y_0. We want to show that if we first differente with respect to y_0 and then apply Φ_h we obtain the same result.

So by first differentiating the equation with respect to y_0 we obtain the variational equation (top right of the diagram), we next apply the same Runge-Kutta method as before to this set of equations. The result is equations (21), (22) and in addition

$$\Psi_1 = I + h\sum_{i=1}^{s} b_i \tilde{K}_i, \tag{25}$$

$$\tilde{K}_i = f'(y_0 + h\sum_{j=1}^{s} a_{i,j}K_j)\left(I + h\sum_{j=1}^{s} a_{i,j}\tilde{K}_j\right), \quad i = 1, \dots, s. \tag{26}$$

We conclude the proof observing that (24) is a system of linear equations in the unknowns $\frac{\partial K_i}{\partial y_0}$, $i = 1, \dots, s$, and (26) is the same system but in the unkonwns $\tilde{K}_i$, $i = 1, \dots, s$. It is easily seen that this system has an unique solution for sufficiently small h, so it must be $\frac{\partial K_i}{\partial y_0} = \tilde{K}_i$, $i = 1, \ldots, s$. From this it follows that $\Psi_1 = \frac{\partial y_1}{\partial y_0}$, and therefore the diagram commutes. ■

Theorem 1.15. *If the coefficients of a Runge-Kutta method satisfy* (18) *then the Runge-Kutta method is symplectic.*

Proof. Consider the Hamiltonian system and its variational equation

$$\begin{aligned} \dot{y} &= J\nabla H(y) \\ y(0) &= y_0, \\ \dot{\Psi} &= JH''(y)\Psi \\ \Psi(0) &= I, \end{aligned}$$

and apply a Runge-Kutta method satisfying (18) to it, to obtain the approximations y_1 and Ψ_1 after one step. Since $\Psi^T J\Psi - J$ is an invariant of the variational equation, it is exactly preserved by Runge-Kutta methods satisfying (18) so $\Psi_1^T J\Psi_1 = J$. But invoking Lemma 1.14 we have $\Psi_1 = \frac{\partial y_1}{\partial y_0}$ and so $\frac{\partial y_1}{\partial y_0}^T J \frac{\partial y_1}{\partial y_0} = J$ which means that the Runge-Kutta method restricted to the equations $\dot{y} = J\nabla H(y)$, $y(0) = y_0$, preserves symplecticity. ■

Exercise 1.16. *Prove directly, without invoking Theorem 1.15 and Theorem 1.10, that the midpoint rule is symplectic.*

Theorem 1.17. *An* **irreducible**[2] *Runge-Kutta method is symplectic if and only if* (18) *holds.*

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