Generating Functions

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Idea: A certain function S moves a PDE problem and S is itself a solution of a partial differential equation (Hamilton-Jacobi PDE).

Such a function S is directly connected to any simplectic map.

The function S is called the Generating Function.

1. Existence of Generating Functions
2. Generating Function for Symplectic Runge-Kutta Methods
3. The Hamilton-Jacobi PDE
4. Methods Based on Generating Functions

Initial values: $p_1, \ldots, p_d$

$q_1, \ldots, q_d$

Final values: $P_1, \ldots, P_d$

$Q_1, \ldots, Q_d$

Theorem 1: A mapping $\varphi : (p, q) \mapsto (P, Q)$ is symplectic if and only if there exists locally a function $S(p, q)$ such that

$$P^T dQ - p^T dq = dS$$

This means that $P^T dQ - p^T dq$ is a total differential.

Change of Coordinates:

$$(p, q) \longrightarrow (q, Q)$$

$$S(p, q) \longrightarrow S(q, Q)$$

Reconstruction of the transformation from $S(q, Q)$

$$P = \frac{\partial S}{\partial Q}(q, Q) \qquad p = -\frac{\partial S}{\partial q}(q, Q)$$

Any sufficiently smooth and nondegenerate function S generates a symplectic mapping.

Lemma 1: Let $(p, q) \mapsto (P, Q)$ be a smooth transformation, close to identity. It is symplectic if and only if one of the following conditions hold locally:

1. $Q^T dP + p^T dq = d(P^T q + S^1)\,;\ S^1(P, q)$
2. $P^T dQ + q^T dp = d(p^T Q - S^2);\ S^2(p, Q)$
3. $(Q - q)^T d(P + p) - (P - p)^T d(Q + q) = 2S^3\,;$

$$S^3((P + p)/2, (Q + q)/2)$$

$S^1 \longrightarrow$ Symplectic Euler Method

$S^2 \longrightarrow$ Adjoint of the Symplectic Euler Method

$S^3 \longrightarrow$ Implicit Midpoint Rule

$$S^1 \longrightarrow p = P + \frac{\partial S^1}{\partial q}(P, q) \qquad Q = q + \frac{\partial S^1}{\partial P}(P, q)$$

$$S^3 \longrightarrow \begin{aligned} P &= p - \partial_2 S^3((P+p)/2, (Q+q)/2) \\ Q &= q + \partial_1 S^3((P+p)/2, (Q+q)/2) \end{aligned}$$

Theorem 2: Suppose, we have a Runge-Kutta method which satisfies

$$b_i a_{ij} + b_j a_{ji} = b_i b_j$$

i.e. it is symplectic. Then the method

$$P = p - h\sum_{i=1}^{s} b_i H_q(P_i, Q_i) \qquad P_i = p - h\sum_{j=1}^{s} a_{ij} H_q(P_j, Q_j)$$

$$Q = q + h\sum_{i=1}^{s} b_i H_p(P_i, Q_i) \qquad Q_i = q + h\sum_{j=1}^{s} a_{ij} H_p(P_j, Q_j)$$

can be written as

$$S^1(P, q, h) = h\sum_{j=1}^{s} b_i H(P_i, Q_i) - h^2 \sum_{i,j=1}^{s} b_i a_{ij} H_q(P_i, Q_i)^T H_p(P_j, Q_j)$$

Theorem 2 gives the explicit formula for the generating function.

Lemma 1 guarantees the local existence of a generating function where the explicit formula shows that the generating function is globally defined in the sense that it is well-defined in the region where $H(p, q)$ is defined.

We wish to construct a smooth generating function $S(q, Q, t)$ for a symplectic transformation but the final points shall move in the flow of the Hamiltonian system

$$P \longrightarrow P(t) \qquad\qquad Q \longrightarrow Q(t)$$

$S(q, Q, t)$ has to satisfy:

$$P_i(t) = \frac{\partial S}{\partial Q_i}(q, Q(t), t) \qquad p_i(t) = -\frac{\partial S}{\partial q_i}(q, Q(t), t) \quad \star$$

$$\Rightarrow 0 = \frac{\partial^2 S}{\partial q_i \partial t}(q, Q(t), t) + \sum_{j=1}^{d} \frac{\partial^2 S}{\partial q_i \partial Q_j}(q, Q(t), t) \cdot \frac{H}{P_j}(P(t), Q(t))$$

Using the chain rule:

$$\frac{\partial}{\partial q_i}\left(\frac{\partial S}{\partial t} + H\left(\frac{\partial S}{\partial Q_1}, \ldots, \frac{\partial S}{\partial Q_d}, Q_1, \ldots, Q_d\right)\right) = 0$$

Theorem 3: If $S(q, Q, t)$ is a smooth solution of

$$\frac{\partial S}{\partial t} + H\left(\frac{\partial S}{\partial Q_1}, \ldots, \frac{\partial S}{\partial Q_d}, Q_1, \ldots, Q_d\right) = 0$$

and if the matrix $\left(\frac{\partial^2 S}{\partial q_i \partial Q_j}\right)$ is invertible, there is a map defined by $\star$ which is the flow $\varphi_t(p, q)$ of the Hamiltonian system.

We write the Hamilton-Jacobi PDE in the coordinates used in Lemma 1:

$$S^1(P,q,t) = P^T(Q-q) - S(q,Q,t)$$

$$\longrightarrow \frac{\partial S^1}{\partial t}(P,q,t) = P^T\frac{\partial Q}{\partial t} - \frac{\partial S}{\partial Q}(q,Q,t)\frac{\partial Q}{\partial t} - \frac{\partial S}{\partial t}(q,Q,t) = -\frac{\partial S}{\partial t}(q,Q,t)$$

$$\longrightarrow \frac{\partial S^1}{\partial P}(P,q,t) = Q - q + P^T\frac{\partial Q}{\partial P} - \frac{\partial S}{\partial Q}(q,Q,t)\frac{\partial Q}{\partial P} = Q - q$$

Theorem 4: If $S^1(P,q,t)$ is a solution of the partial differential equation

$$\frac{\partial S^1}{\partial t}(P,q,t) = H(P, q + \frac{\partial S^1}{\partial P}(P,q,t)), S^1(P,q,t_0) = 0$$

then the mapping $(p,q) \mapsto (P(t), Q(t))$ is the exact flow of the Hamilton system.

Approximate solution of the Hamilton-Jacobi equation using the ansatz:

$$S^1(P,q,t) = tG_1(P,q) + t^2G_2(P,q) + t^3G_3(P,q) + \ldots$$

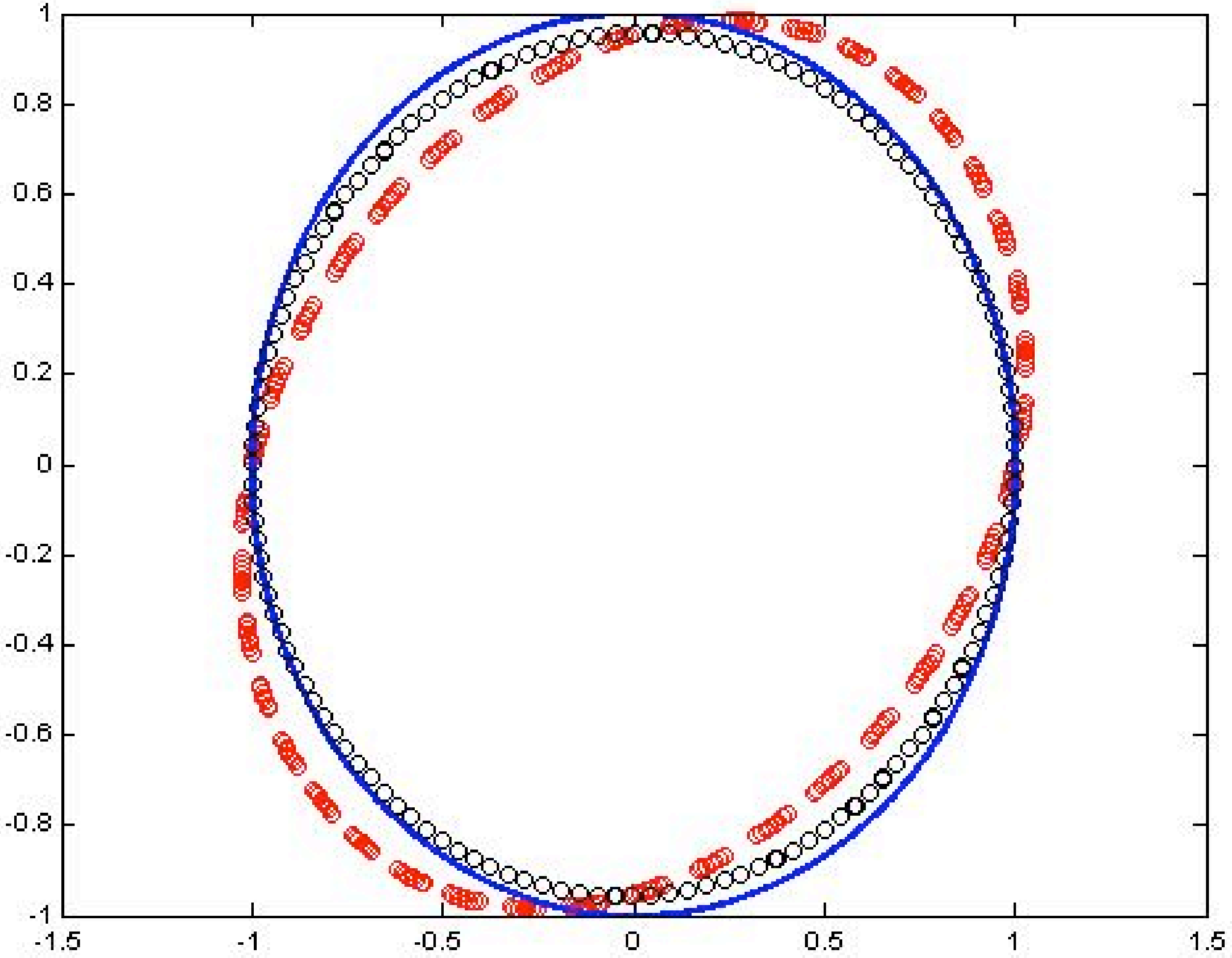
$$\longrightarrow \quad \begin{aligned} G_1(P,q) &= H(P,q) \\ G_2(P,q) &= \frac{1}{2}\left(\frac{\partial H}{\partial P}\frac{\partial H}{\partial q}\right)(P,q) \end{aligned}$$

Problem: Higher order derivatives!

Try to avoid higher order derivatives (Miesbach & Pesch). We use generating functions of the following form:

$$S^3(w,h) = h\sum_{i=1}^{s} b_i H(w + hc_i J^{-1}\nabla H(w))$$

We only have to determine the coefficients according to the solution of the Hamilton-Jacobi equation.
But: We still need second order derivatives.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