ON QUADRATIC INVARIANTS AND SYMPLECTIC STRUCTURE

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Abstract.

We show that the theorems of Sanz-Serna and Eirola and Sanz-Serna concerning the symplecticity of Runge-Kutta and Linear Multistep methods, respectively, follow from the fact that these methods preserve quadratic integral invariants and are closed under differentiation and restriction to closed subsystems.

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1. Introduction.

Concerning the numerical solution of ordinary differential equations, Cooper [4] has shown that Runge-Kutta methods with vanishing stability matrix preserve the quadratic invariants of the system, and Sanz-Serna [11] and Lasagni [9] have shown them to be symplectic when applied to Hamiltonian systems. See the review articles of Scovel [13], Yoshida [14], Sanz-Serna [12], and section II.16 of Hairer et al. [8] for more details concerning the symplectic methods. Moreover, Eirola and Sanz-Serna [5] have shown that, for symmetric one-leg multistep methods (OLM), the quadratic invariants of the system can be extended to quadratic invariants of the multistep method by a tensor product of Λ, a matrix associated with the OLM, and the matrix associated with the quadratic invariant. They also show that the symmetric OLM is symplectic with respect to a tensor product of Λ and the symplectic matrix. See also Ge [7].

These results suggest that there is some relation between the preservation of quadratic invariants and symplectic structure. Indeed, since both the Runge-Kutta and the OLM's are equivariant under linear symmetry groups, being symplectic implies the preservation of quadratic invariants of Hamiltonian

systems by a result of Feng and Ge [6]. On the other hand, we observe that
the invariance of the symplectic structure determines an integral invariant for
the natural extension to the Whitney sum $TN \oplus TN$ (cf. [2]) where N is the
original phase space. If N is a linear symplectic space, then this Whitney sum
can be trivialized to a vector space $N \oplus N \oplus N$ such that this integral invariant
is *quadratic*.

Our main theorem is that if the method is closed under differentiation, closed
under restriction to closed subsystems (to be defined shortly), and preserves
quadratic invariants generated by those of the original system, then the method
is symplectic when applied to a Hamiltonian system. We then obtain Sanz-
Serna's [11] and Eirola and Sanz-Serna's [5] results concerning symplecticity,
as a consequence of quadratic invariant preservation, by verifying that those
methods are closed under differentiation and restriction to closed subsystems.
However, we remark that presently it is questionable if this result can be used
to prove the symplecticity of a method since the direct proof that a method
preserves quadratic invariants is not necessarily simpler than the direct proof
that it preserves the symplectic structure. Indeed, this result seems to indicate
that, for a large class of linear methods, the converse should be true.

2. Quadratic invariants and symplectic maps.

Let $N = R^d \times R^d$ be the standard symplectic vector space with symplectic
form

$$\omega = d\mathbf{q} \wedge d\mathbf{p} = \sum_{i=1}^{d} dq_i \wedge dp_i = J d\mathbf{y} \wedge d\mathbf{y}$$

where $\mathbf{y} = (\mathbf{q}, \mathbf{p})$ and

$$J = \begin{pmatrix} 0 & -I_d \\ I_d & 0 \end{pmatrix}.$$

See Abraham and Marsden [1] for a treatment of Hamiltonian mechanics. For
a Hamiltonian H, the Hamilton equations of motion are

(1) $\dot{\mathbf{y}} = J^{-1}\nabla H(\mathbf{y})$.

Since N is a vector space, we trivialize TN to $N \times N$, but will still refer to it
as TN.

Consider the tangent lift of these equations to TN obtained by differentiation:

(2) $\dot{\mathbf{y}} = J^{-1}\nabla H(\mathbf{y})$

$$\dot{\mathbf{z}} = J^{-1}d\nabla H(\mathbf{y})\mathbf{z}.$$

Now consider a numerical method for the solution of the Hamiltonian system
(1). We adopt the notation

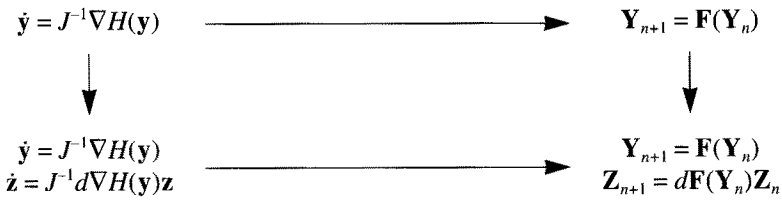(3) $\mathbf{Y}_{n+1} = \mathbf{F}(\mathbf{Y}_n)$

$$\dot{\mathbf{y}} = J^{-1}\nabla H(\mathbf{y}) \quad\longrightarrow\quad \mathbf{Y}_{n+1} = \mathbf{F}(\mathbf{Y}_n)$$

$$\begin{aligned}\dot{\mathbf{y}} &= J^{-1}\nabla H(\mathbf{y})\\ \dot{\mathbf{z}} &= J^{-1}d\nabla H(\mathbf{y})\mathbf{z}\end{aligned} \quad\longrightarrow\quad \begin{aligned}\mathbf{Y}_{n+1} &= \mathbf{F}(\mathbf{Y}_n)\\ \mathbf{Z}_{n+1} &= d\mathbf{F}(\mathbf{Y}_n)\mathbf{Z}_n\end{aligned}$$

Figure 1. Tangent lift of a system and a method.

for such a method where $\mathbf{Y}_n$ is a point in an appropriate numerical phase space M. For one-step methods $M = N$, and for k-step methods M can be identified with N^k. The tangent lift of the method (3) to one on TM is

(4) $$\mathbf{Y}_{n+1} = \mathbf{F}(\mathbf{Y}_n)$$

(5) $$\mathbf{Z}_{n+1} = d\mathbf{F}(\mathbf{Y}_n)\mathbf{Z}_n.$$

If the numerical method applied to the tangent lift system (2) gives the lift (4), (5) of the numerical method applied to the original system, we say that the method is closed under differentiation and that Figure 1 is commutative. The left hand side of the figure consists of differential equations and the right hand side along the horizontal arrows is the numerical method applied to those differential equations.

We say that the method is closed under restriction to closed subsystems if the method restricted to a closed subsystem is the same as the method applied to the full system and then evaluated on the variables of the subsystem. Namely, restriction commutes with the method. To be precise, consider the system $\dot{\mathbf{y}}$ = $\mathbf{f}(\mathbf{y})$ where $\mathbf{y} = (\mathbf{y}_1, \mathbf{y}_2)$ and $\mathbf{y}_1$ are the subsystem variables. If

$$\mathbf{f}(\mathbf{y}) = (\mathbf{f}_1(\mathbf{y}_1), \mathbf{f}_2(\mathbf{y})),$$

then the system $\dot{\mathbf{y}}_1 = \mathbf{f}_1(\mathbf{y}_1)$ is a closed subsystem. The method is closed under restriction to the $\mathbf{Y}_1$ variables if

$$F(\mathbf{Y}) = (F_1(\mathbf{Y}), F_2(\mathbf{Y})) = (F(\mathbf{Y}_1), F_2(\mathbf{Y})),$$

where $F(\mathbf{Y}_1)$ is the method applied to the subsystem alone. For example, the tangent lift of a method closed under differentiation is closed under restriction to the original $\mathbf{Y}$ variables since the top half of the method applied to the $(\mathbf{Y}, \mathbf{Z})$ variables in (4), (5) is the same as the method applied to the $\mathbf{Y}$ variables alone (eqn. 3).

We say that the method (3) has a quadratic invariant Q, generated by a quadratic invariant Q of the original system if $Q = Q$ for single-step methods and $Q = \Lambda \otimes Q$ for multistep methods, where Λ is a symmetric matrix which depends on the method but does not depend on the specific system being integrated. We require $\Lambda = 1$ for single-step methods so that the condition can simply be stated as $Q = \Lambda \otimes Q$. The single step $Q = Q$ corresponds to the result

of Cooper [4], and the multistep $Q = \Lambda \otimes Q$ corresponds to the result of Eirola and Sanz-Serna [5].

Consider the skew-symmetric bilinear function $\langle Jz, \mathbf{w} \rangle$. It corresponds to a quadratic function $\langle \check{J} \cdot, \cdot \rangle$ on the Whitney sum $N \oplus N \oplus N$ where the matrix $\check{J}$ is

(6)
$$\check{J} = \frac{1}{2} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -J \\ 0 & J & 0 \end{pmatrix}.$$

Similarly, the skew-symmetric bilinear function $\langle (\Lambda \otimes J)\mathbf{Z}, \mathbf{W} \rangle$, defined on the numerical phase space M gives a quadratic function

(7) $\langle (\Lambda \otimes \check{J})(\mathbf{Y}, \mathbf{Z}, \mathbf{W}), (\mathbf{Y}, \mathbf{Z}, \mathbf{W}) \rangle = \Lambda_{ij}\langle J\mathbf{Z}_i, \mathbf{W}_j \rangle = \langle (\Lambda \otimes J)\mathbf{Z}, \mathbf{W} \rangle$

on $M \oplus M \oplus M$ and we also refer to $\mathbb{J} = \Lambda \otimes J$ as being generated by J. Since J is a symplectic structure, $\Lambda \otimes J$ is skew symmetric, but its nondegeneracy must be established for it to be a symplectic structure. Eirola and Sanz-Serna [5] have shown it to be symplectic for the symmetric OLM's. However, we are not concerned with this issue here and will broadly refer to $\Lambda \otimes J$ as a symplectic structure.

THEOREM 1. *Suppose that the numerical method is both closed under differentiation and closed under restriction to closed subsystems. Suppose also that the method preserves the quadratic invariant Q generated by each quadratic invariant Q of the original system. Then the mapping $\mathbf{Y}_n \mapsto \mathbf{Y}_{n+1}$ is canonical with respect to the symplectic structure $\mathbb{J} = \Lambda \otimes J$ when applied to the Hamiltonian system (1).*

PROOF. Consider the system of ODE's extended to the Whitney sum $TN \oplus TN \approx N \oplus N \oplus N$

(8)
$$\dot{\mathbf{y}} = J^{-1}\nabla H(\mathbf{y})$$
$$\dot{\mathbf{z}} = J^{-1}d\nabla H(\mathbf{y})\mathbf{z}$$
$$\dot{\mathbf{w}} = J^{-1}d\nabla H(\mathbf{y})\mathbf{w}.$$

Since the subsystems

$$\dot{\mathbf{y}} = J^{-1}\nabla H(\mathbf{y})$$
$$\dot{\mathbf{z}} = J^{-1}d\nabla H(\mathbf{y})\mathbf{z}$$

and

$$\dot{\mathbf{y}} = J^{-1}\nabla H(\mathbf{y})$$
$$\dot{\mathbf{w}} = J^{-1}d\nabla H(\mathbf{y})\mathbf{w}$$

are both closed subsystems and tangent lifts of the original system, the numerical method applied to (8) must be of the form

$$\mathbf{Y}_{n+1} = \mathbf{F}(\mathbf{Y}_n)$$

$$\mathbf{Z}_{n+1} = d\mathbf{F}(\mathbf{Y}_n)\mathbf{Z}_n$$

$$\mathbf{W}_{n+1} = d\mathbf{F}(\mathbf{Y}_n)\mathbf{W}_n.$$

Now observe that the system (8) has a quadratic invariant generated by the symplectic structure of the original system. Namely,

$$\langle \hat{J}(\mathbf{y}, \mathbf{z}, \mathbf{w}), (\mathbf{y}, \mathbf{z}, \mathbf{w}) \rangle = \langle J\mathbf{z}, \mathbf{w} \rangle = const.$$

where J is defined in (6). This is proved by straightforward differentiation:

$$\langle J\mathbf{z}, \mathbf{w} \rangle = \langle J\dot{\mathbf{z}}, \mathbf{w} \rangle + \langle J\mathbf{z}, \dot{\mathbf{w}} \rangle = \langle JJ^{-1}B\mathbf{z}, \mathbf{w} \rangle + \langle J\mathbf{z}, J^{-1}B\mathbf{w} \rangle = 0,$$

where $B = d\nabla H(\mathbf{y})$ is symmetric and J is skew symmetric.

The hypothesis of the theorem is that there is some Λ such that $\hat{J} = \Lambda \otimes \hat{J}$ is preserved. By equation (7), preservation of the quadratic invariant determined by $\hat{J}$ is equivalent to the preservation of the bilinear function determined by $\mathcal{J} = \Lambda \otimes \mathcal{J}$. Thus

$$\langle \mathcal{J}\mathbf{Z}_{n+1}, \mathbf{W}_{n+1} \rangle = \langle \mathcal{J}\mathbf{Z}_n, \mathbf{W}_n \rangle.$$

Since

$$\mathbf{Z}_{n+1} = d\mathbf{F}(\mathbf{Y}_n)\mathbf{Z}_n$$

and

$$\mathbf{W}_{n+1} = d\mathbf{F}(\mathbf{Y}_n)\mathbf{W}_n$$

and the invariant is preserved for all $\mathbf{Z}_n$ and $\mathbf{W}_n$, we deduce that

$$d\mathbf{F}(\mathbf{Y}_n)^T \mathcal{J} d\mathbf{F}(\mathbf{Y}_n) = \mathcal{J}.$$

Namely, the method is symplectic with respect to $\mathcal{J}$. The proof is finished.

3. Applications.

In this section, we show that the Runge-Kutta methods, Linear Multistep methods, and more generally the General Linear Methods are closed under differentiation and restriction to closed subsystems. See Hairer et al. [8] for a more detailed discussion of these methods. Consequently, by Theorem 1, to demonstrate symplecticity, one only needs to know when they preserve quadratic invariants. We consider the methods applied to the general ODE

$$(9) \qquad\qquad \dot{\mathbf{y}} = \mathbf{f}(\mathbf{y}).$$

3.1. *Runge-Kutta methods.*

The s-stage Runge-Kutta for solving (9) is defined by the equations

$$(10) \qquad\qquad Y_i = \mathbf{y}_n + h \sum_{j=1}^{s} a_{ij}\mathbf{f}(Y_j)$$

$$(11) \qquad \mathbf{y}_{n+1} = \mathbf{y}_n + h \sum_{i=1}^{s} b_i \mathbf{f}(Y_i).$$

To show that the Runge-Kutta methods are closed under differentiation, we apply (10), (11) to the system

$$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$$

$$\dot{\mathbf{z}} = d\mathbf{f}(\mathbf{y})\mathbf{z}.$$

The new approximation to the vectors $\mathbf{y}$ and $\mathbf{z}$ is now computed according to the formulae

$$\begin{pmatrix} Y_i \\ Z_i \end{pmatrix} = \begin{pmatrix} \mathbf{y}_n \\ \mathbf{z}_n \end{pmatrix} + h \sum_{j=1}^{s} a_{ij} \begin{pmatrix} \mathbf{f}(Y_j) \\ d\mathbf{f}(Y_j)Z_j \end{pmatrix}$$

$$\begin{pmatrix} \mathbf{y}_{n+1} \\ \mathbf{z}_{n+1} \end{pmatrix} = \begin{pmatrix} \mathbf{y}_n \\ \mathbf{z}_n \end{pmatrix} + h \sum_{i=1}^{s} b_i \begin{pmatrix} \mathbf{f}(Y_i) \\ d\mathbf{f}(Y_i)Z_i \end{pmatrix}$$

Note that in the above equations the stages Y_i for the closed subsystem of variables $\mathbf{y}$ can be determined independently from the stages Z_i. Once the Y_i are found, then the stages Z_i can also be computed. Therefore, the equations for Y_i and $\mathbf{y}_{n+1}$ can be decoupled from the equations for Z_i and $\mathbf{z}_{n+1}$. Equations for the first pair are identical with the equations (10) and (11) for the system (9). For the second pair we have a similar situation with

$$Z_i = \mathbf{z}_n + h \sum_{j=1}^{s} a_{ij} d\mathbf{f}(Y_j)Z_j$$

$$\mathbf{z}_{n+1} = \mathbf{z}_n + h \sum_{i=1}^{s} b_i d\mathbf{f}(Y_i)Z_i$$

being equivalent to (10) and (11) applied to $\dot{\mathbf{z}} = d\mathbf{f}(\mathbf{y})\mathbf{z}$. On the other hand, differentiation of (10) and (11) results in equations identical to the above. Since h is small enough that the solutions are unique, we find that the tangent lift of the method (10) and (11) gives the same map as the method applied to the tangent lift of the system (9). Consequently, the Runge-Kutta methods are closed under differentiation.

The Runge-Kutta methods are homogeneous in the vector indices. Namely, the method treats all indices the same and does not mix components. Therefore, it is easy to see that if a subset of the indices corresponds to a closed subsystem, then the Runge-Kutta method applied to the full system but then evaluated on the subsystem is the same as the method applied directly to the subsystem. Consequently, the Runge-Kutta methods are also closed under restriction to closed subsystems.

Therefore, since Cooper has shown that Runge-Kutta methods with vanishing stability matrix ($BA + A^TB - bb^T = 0$ where B denotes the diagonal matrix

with entries b_i) preserve all quadratic invariants, Theorem 1 tells us that such methods are also symplectic when applied to a Hamiltonian system 1.

3.2 Multistep methods.

A general linear multistep method is defined by its two real characteristic polynomials

$$\rho(x) = \sum_{j=0}^{k} \alpha_j x^j; \quad \alpha_k \neq 0; \quad \sigma(x) = \sum_{j=1}^{k} \beta_j x^j; \quad \sigma(1) = 1.$$

The standard Linear Multistep Method (LMM) and the corresponding One-Leg Method (OLM) are then given by the equations

(12) $\rho(E)\mathbf{y}_n = h\sigma(E)\mathbf{f}(\mathbf{y}_n)$

(13) $\rho(E)\mathbf{y}_n = h\mathbf{f}(\sigma(E)\mathbf{y}_n),$

where E denotes the shift operator $E\mathbf{y}_n = \mathbf{y}_{n+1}$. The methods (12) and (13) are called symmetric if $\alpha_j = -\alpha_{k-j}$ and $\beta_j = \beta_{k-j}$. It is convenient to regard a multistep method as a one-step method defined on a suitable product space. For this let us solve (13) for $\mathbf{y}_{n+k}$:

$$\mathbf{y}_{n+k} = -\frac{\alpha_{k-1}}{\alpha_k}\mathbf{y}_{n+k-1} - \cdots - \frac{\alpha_0}{\alpha_k}\mathbf{y}_n - \frac{h}{\alpha_k}\mathbf{f}(\sigma(E)\mathbf{y}_n).$$

If we introduce the vectors

$$\mathbf{Y}_n = (\mathbf{y}_n^T, \cdots, \mathbf{y}_{n+k-1}^T)^T$$
$$b^T = (\beta_k, \cdots, \beta_0)$$

and the matrix

$$A = \begin{pmatrix} -\dfrac{\alpha_{k-1}}{\alpha_k} & -\dfrac{\alpha_{k-2}}{\alpha_k} & \cdots & -\dfrac{\alpha_1}{\alpha_k} & -\dfrac{\alpha_0}{\alpha_k} \\ 1 & 0 & \cdots & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & 1 & 0 \end{pmatrix}$$

then the OLM (13) can be written as a one-step method which maps $\mathbf{Y}_n$ to $\mathbf{Y}_{n+1}$ as follows:

(14) $\mathbf{Y}_{n+1} = (A \otimes I)\mathbf{Y}_n + (e_1 \otimes I)\dfrac{h}{\alpha_k}\mathbf{f}((b^T \otimes I)\mathbf{Y}_{n+1}),$

where we refer to Lancaster [10] for the basic definitions of tensor products.

To verify that the OLM (13) is closed under differentiation, we apply the one-step representation (14) to the tangent lift

$$\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y})$$

$$\dot{\mathbf{z}} = d\mathbf{f}(\mathbf{y})\mathbf{z}.$$

Let $\mathbf{X}_n = (\mathbf{Y}_n^T, \mathbf{Z}_n^T)^T$ where $\mathbf{Y}_n$ and $\mathbf{Z}_n$ denote the respective approximations for $\mathbf{y}$ and $\mathbf{z}$. It is easy to see that the formula for computation of $\mathbf{X}_{n+1}$ from $\mathbf{X}_n$ can be decoupled into two separate equations

$$\mathbf{Y}_{n+1} = (A \otimes I)\mathbf{Y}_n + (e_1 \otimes I)\frac{h}{\alpha_k}\mathbf{f}((b^T \otimes I)\mathbf{Y}_{n+1})$$

and

$$\mathbf{Z}_{n+1} = (A \otimes I)\mathbf{Z}_n + (e_1 \otimes I)\frac{h}{\alpha_k}d\mathbf{f}((b^T \otimes I)\mathbf{Y}_{n+1})(b^T \otimes I)\mathbf{Z}_{n+1}.$$

Differentiation of (14) produces exactly the same as the above with $\mathbf{Y}'_{n+1}$ instead of $\mathbf{Z}_{n+1}$. For h sufficiently small, it follows that $\mathbf{Y}'_{n+1}$ can be identified with $\mathbf{Z}_{n+1}$ which establishes that the method is closed under differentiation. It is straightforward to show that the one-step representation is closed under restriction to the direct product of closed subsystem variables in M. Similarly, the LMM's are also closed under both differentiation and restriction to closed subsystems.

Since Eirola and Sanz-Serna [5] have shown that for any quadratic invariant Q the symmetric OLM preserves the quadratic invariant $Q = \Lambda \otimes Q$, Theorem 1 now implies that the symmetric OLM is symplectic with respect to the symplectic matrix $\mathcal{J} = \Lambda \otimes J$ when applied to the Hamiltonian system 1. However, it is not known which of the LMM's preserve quadratic invariants.

3.3 *General linear methods.*

In this section we turn our attention to the so-called General Linear Methods (GLM) introduced in [3]. Indeed, being linear means that we solve a system which is linear in the state vectors and the vector field evaluated at the state vectors.

A GLM for the autonomous system (9) is defined by the equations

$$v_i^n = \sum_{j=1}^{k} \tilde{a}_{ij} y_j^n + h \sum_{j=1}^{s} \tilde{b}_{ij} \mathbf{f}(v_j^n); \quad i = 1, \ldots, k$$

$$y_i^{n+1} = \sum_{j=1}^{k} a_{ij} y_j^n + h \sum_{j=1}^{s} b_{ij} \mathbf{f}(v_j^n); \quad i = 1, \ldots, s.$$

Each $\mathbf{y}_i$ is an m-dimensional vector, where m is dimension of the system (9). These vectors are called external stages since they contain all information from the previous step necessary for the computation of the new approximation. The vectors v_i^n are the internal stages of the current step. By the linearity and homogeneity of the method with respect to vector indices, an elementary calculation similar to those given above shows that GLM's are closed under both

differentiation and restriction to closed subsystems. Consequently, to apply Theorem 1 and establish the symplecticity of any GLM method, we need only to find whether the method preserves invariants generated by the quadratic invariants of the original system. It might be possible to formulate a general condition in this sense similar to the condition on the Runge-Kutta methods, but at present we do not know whether such a condition actually exists. One of the difficulties here is that now we have to determine the form of the quadratic invariants to be preserved by the method simultaneously with the conditions on the coefficients of the GLM which will guarantee the preservation of these invariants. In contrast, in the Runge-Kutta case and in the symmetric OLM case these problems were not related. Indeed, since Runge-Kutta are one-step methods, we search only for the conditions on the coefficients which will preserve the canonical symplectic structure. In the case of the symmetric OLM we only had to identify the appropriate symplectic structure on the product space $M = N^k$ without searching for conditions on the coefficients. Consequently, we simultaneously seek conditions on the GLM and Λ such that the method is symplectic with respect to $\Lambda \otimes J$.

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