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Birational maps from polarization and the preservation of measure and integrals

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Abstract

The main result of this paper is the discretization of second-order Hamiltonian systems of the form $\ddot{x} = -K\nabla W(x)$, where K is a constant symmetric matrix and $W: \mathbb{R}^n \rightarrow \mathbb{R}$ is a polynomial of degree $d \leq 4$ in any number of variables n . The discretization uses the method of polarization and preserves both the energy and the invariant measure of the differential equation, as well as the dimension of the phase space. This generalizes earlier work for discretizations of first order systems with $d = 3$, and of second order systems with $d = 4$ and $n = 1$.

Keywords: birational maps, Kahan mapping, geometric numerical integration

1. Introduction

1.1. Preamble

To any physicist, invariance and covariance are important properties. The significance of symmetries, integrals, symplectic structure, measure preservation, etc can hardly be overstated. For example, the above all play a role in Hamilton's equations. A fact of life is that, in most instances, Hamilton's equations cannot be solved in closed form, and one must rely on numerical computation.

A problem then arises. Most traditional numerical integration methods do not preserve symmetries, integrals, symplectic structure, etc. This has led to the development of a new area of computational physics, entitled geometric numerical integration, in which methods are

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developed to preserve each of the aforementioned properties (and more). For surveys of this area see [27, 32].

What has turned out to be more difficult is to preserve several properties at the same time. In particular, preserving the Hamiltonian and phase space volume simultaneously has proved to be hard in general. This situation improved when it was discovered that Kahan's method does preserve an integral as well as a volume form (albeit that it exactly preserves a nearby integral and a nearby measure) [6, 21, 30, 34]. This has led to a flurry of research extending and generalizing these results [4–7, 29–31]. The present paper follows in this tradition.

1.2. Darboux polynomials and birational integrators

The Cremona group of birational maps of a vector space—rational maps with a rational inverse—is studied both for its properties as an infinite group (for example, its generators and subgroups) and in terms of the dynamics of its elements [1, 8, 11]. (The Hénon map $(x, y) \mapsto (y + x^2 + c, ax)$ is an example.) Like the Cremona group, Darboux polynomials were also introduced in the nineteenth century, as a tool for the analysis of ordinary differential equations [9]. Yet only in recent years has it become apparent that there is a connection between these two objects. Gasull and Mañosa [12] constructed first integrals for some planar maps using Darboux polynomials. Celledoni *et al* [2, 3] gave an effective method for the construction of Darboux polynomials of birational maps, which in turn gave a method for the detection and determination of first integrals and invariant measures of birational maps.

In a parallel development, interesting new examples of birational maps have been discovered based on specific discretizations of ordinary differential equations [4–7, 10, 15–18, 20–24, 29–31, 33, 34, 36, 38, 39]. The Kahan (or Kahan–Hirota–Kimura) [21, 22] map is an example. In some cases these maps have been found to preserve first integrals, invariant measures, and/or integrability, which is a decidedly exceptional feature of a numerical discretization. Typically, the preserved structures are perturbations in the time step of the original ones.

An example is the Kahan map applied to a canonical Hamiltonian system with a cubic Hamiltonian [6]. Regardless of the dimension, the Kahan map has an invariant measure and first integral, which are perturbations of those of the continuous system. So in dimension 2, it generates integrable maps; in dimension 4 and greater, it provides examples of maps with nonlinear integrals and conserved measures unrelated (in general) to integrability or to obvious symmetries, a novel feature.

Darboux polynomials provide a route to discover new classes of such maps. In this paper we study maps associated with Hamiltonian systems of the form

$$\ddot{x} = -K\nabla W(x), \quad x \in \mathbb{R}^n, \quad (1)$$

where K is a constant symmetric matrix and $W: \mathbb{R}^n \rightarrow \mathbb{R}$ is a polynomial of degree ≤ 4 . These are canonical Hamiltonian systems with Hamiltonian

$$H(x, p) = \frac{1}{2} p^\top K p + W(x), \quad (2)$$

written in second-order form. The maps themselves take the form

$$\frac{x_{k+1} - 2x_k + x_{k-1}}{h^2} = f(x_{k-1}, x_k, x_{k+1}) \quad (3)$$

where f is linear in each argument, thus forming a family of birational maps parametrised by h with the same phase space as the associated continuous system. The function f is constructed from W by ‘polarization’, a standard technique in algebraic geometry that has been used to construct birational mappings from differential equations [5] and which provides a new viewpoint on the Kahan mapping. Its use in the form (3) was introduced by Hone and Quispel [18].

Our method is the following:

- (i) Find Darboux polynomials for specific instances or specific parametric families of maps (3).
- (ii) For cases such that the Darboux polynomials provide invariant integrals or measures of the maps, conjecture the general form of these integrals and measures.
- (iii) Prove the invariance of these integrals and measures directly.

Sections 2 and 3 review Darboux polynomials, the Kahan mapping, and polarization. In section 4 we establish the existence of an invariant measure for the polar map on $\mathbb{R}^{2n}$ associated with (1) when the potential $W(x)$ is a homogeneous quartic in n variables, while section 5 gives a first integral for this case. In section 6 these results are extended to the nonhomogeneous case and (for the invariant measure only) to non-conservative vector fields. Section 7 extends the results to polar maps associated with higher-order systems $\dot{x}^{(m)} = f(x)$, generalizing in addition a known result for the Kahan mapping in the case $m = 1$. Two results in section 8 point towards possible further generalizations: a polar map with a two integrals, and a polar map associated with a 4-parameter family of 4th order systems that has an integral.

It is not known which birational maps have invariants like the ones we find here, or how the specific functional form of the integral is related to the construction of the map. (We have no analogue of Noether’s theorem, for example.) We hope that our results here will lead in the direction of greater understanding of these questions.

2. Darboux polynomials for differential equations and maps

A *continuous Darboux polynomial* for an ODE $\dot{x} = f(x)$, $x \in \mathbb{R}^n$, is a polynomial $P: \mathbb{R}^n \rightarrow \mathbb{R}$ such that there exists a polynomial $C: \mathbb{R}^n \rightarrow \mathbb{R}$, called the *cofactor* of P , such that $\dot{P} = CP$ where $\dot{P} := (\nabla P)^\top f$. The level set $P^{-1}(0)$ is then invariant. Darboux polynomials have also been called ‘second integrals’ and ‘weak integrals’ of f . If P_1 and P_2 are Darboux polynomials with the same cofactor C , then P_1/P_2 is a first integral of f .

In addition, if $\dot{P}_i = C_i P_i$, then $\frac{d}{dt}(P_1 P_2) = (C_1 + C_2) P_1 P_2$, i.e. the product $P_1 P_2$ of two Darboux polynomials is a Darboux polynomial with cofactor equal to the *sum* $C_1 + C_2$. Moreover, if P is a Darboux polynomial for the polynomial vector field f , then all irreducible factors of P are Darboux polynomials [13].

However, even if P_1 , P_2 , and C are known to be polynomials of a given degree, determining their coefficients such that $\dot{P}_1 = CP_1$ and $\dot{P}_2 = CP_2$ is a nonlinear problem. This has tended to limit the discovery of Darboux polynomials to cases where either P or C is particularly simple (e.g. linear), or where an invariant set which may be identified as $P^{-1}(0)$ can be found by other means.

A *discrete Darboux polynomial* for a map $x \mapsto x' := \phi(x)$, $x \in \mathbb{R}^n$, is a polynomial $P: \mathbb{R}^n \rightarrow \mathbb{R}$ such that there exists a rational function $C: \mathbb{R}^n \rightarrow \mathbb{R}$ (again called the cofactor of P) such that $P' = CP$ where $P' := P \circ \phi$. As in the continuous case, the level set $P^{-1}(0)$ is then invariant,

and if P_1 and P_2 are Darboux polynomials with the same cofactor C , then P_1/P_2 is a first integral of ϕ .

The key difference between the discrete and the continuous cases is that in the discrete case if $P'_i = C_i P_i$ then $P'_1 P'_2 = (C_1 C_2)(P_1 P_2)$, i.e. the product $P_1 P_2$ of two Darboux polynomials is a Darboux polynomial with cofactor equal to the product $C_1 C_2$.

The maps ϕ in which we are interested are birational and not polynomial [28, 37]. In this case, an excellent ansatz is available for cofactors of birational maps, namely, that their factors are factors of the Jacobian determinant of the map. Therefore, the unique factorization of the Jacobian determinant of the map yields a finite number of choices of cofactor up to some chosen degree, which is not possible in the continuous case. For each such choice, the determination of the Darboux polynomials associated with that cofactor is a linear problem.

In addition, we have:

- (i) If P is a Darboux polynomial with cofactor $1/\det D\phi$, then $\frac{1}{P}dx_1 \wedge \cdots \wedge dx_n$ is an invariant measure of ϕ .
- (ii) If $P_1, \dots, P_k$ are Darboux polynomials with cofactors $C_1, \dots, C_k$, respectively, and $\prod_{i=1}^k C_i^{\alpha_i} = \det D\phi$, then $(\prod_{i=1}^k P_i^{\alpha_i})dx_1 \wedge \cdots \wedge dx_n$ is an invariant measure of ϕ .
- (iii) If $P_1, \dots, P_k$ are Darboux polynomials with cofactors $C_1, \dots, C_k$, respectively, and $\prod_{i=1}^k C_i^{\alpha_i} = 1$, then $\prod_{i=1}^k P_i^{\alpha_i}$ is a first integral of ϕ .
- (iv) If $P_1, \dots, P_k$ are Darboux polynomials with the same cofactor C , then $a_1 P_1 + \cdots + a_k P_k$ is a Darboux polynomial with cofactor C for any constants $a_1, \dots, a_k$. That is, the Darboux polynomials for a given cofactor form a vector space.

3. Kahan's method and polarization

Kahan's method [21, 22] for the quadratic ODE

$$\dot{x} = f(x) := Q(x, x) + Bx + c, \quad x \in \mathbb{R}^n \quad (4)$$

(where Q is an $\mathbb{R}^n$ -valued symmetric bilinear form, $B \in \mathbb{R}^{n \times n}$, and $c \in \mathbb{R}^n$) is the map $x \mapsto x'$ with step size h given by

$$\frac{x' - x}{h} = Q(x, x') + \frac{1}{2}B(x + x') + c. \quad (5)$$

Because the right-hand side of equation (5) is linear in x' , it can be solved explicitly to get the rational map

$$x' = x + h \left(I - \frac{h}{2} f'(x) \right)^{-1} f(x).$$

Its inverse is also rational,

$$x = x' - h \left(I + \frac{h}{2} f'(x') \right)^{-1} f(x'),$$

so the Kahan map is birational.

Moreover, a homogeneous quadratic vector field $f(x)$ can be expressed in terms of a bilinear form $Q(x, x)$, as in equation (4), using the technique of polarization:

$$Q(x_1, x_2) = \frac{1}{2}(f(x_1 + x_2) - f(x_1) - f(x_2)).$$

So the Kahan method can be obtained by polarizing the quadratic terms of the ODE, evaluating them at (x, x') and by replacing the linear and constant terms by the midpoint approximation.

Polarization is a map from a homogeneous polynomial to a symmetric multilinear form in more variables. For example, the polarization of the cubic $f(x)$ is the trilinear form

$$F(x_1, x_2, x_3) = \frac{1}{6} \frac{\partial}{\partial \lambda_1} \frac{\partial}{\partial \lambda_2} \frac{\partial}{\partial \lambda_3} f(\lambda_1 x_1 + \lambda_2 x_2 + \lambda_3 x_3) \Big|_{\lambda=0},$$

where $x, x_1, x_2, x_3 \in \mathbb{R}^n$. This is equal to $\frac{1}{6}$ of the coefficient of $\lambda_1 \lambda_2 \lambda_3$ in $f(\lambda_1 x_1 + \lambda_2 x_2 + \lambda_3 x_3)$. It satisfies $F(x, x, x) = f(x)$.

For example, consider $x = (y, z, w) \in \mathbb{R}^3$. The polarization of $3y^2z$ is $y_1 y_2 z_3 + y_2 y_3 z_1 + y_3 y_1 z_2$ and the polarization of $6yzw$ is $y_1 z_2 w_3 + y_2 z_3 w_1 + y_3 z_1 w_2 + y_1 z_3 w_2 + y_3 z_2 w_1 + y_2 z_1 w_3$.

Polarization of a homogeneous vector field of degree $k+1$ determines a multilinear form in $k+1$ variables. We call these variables $x_0, \dots, x_k$, where $x_k \in \mathbb{R}^n$.

Celledoni *et al* [5] considered the discretization of the first-order homogeneous ODE

$$\dot{x} = F(x, x, \dots, x), \quad x \in \mathbb{R}^n$$

of degree $k+1$ by the birational ‘polar map’ $(x_0, \dots, x_{k-1}) \rightarrow (x_1, \dots, x_k)$, where

$$\frac{x_k - x_0}{h} = F(x_0, \dots, x_k),$$

regarded as a k -step method. When the ODE is canonical Hamiltonian (or Poisson with a constant Poisson structure), this polar map has an invariant measure and its k th iterate has k independent integrals. For $k=1$ it coincides with Kahan’s method, but when $k>1$ its phase space $\mathbb{R}^{nk}$ is different from that of the ODE.

4. Polarization of homogeneous second order ODEs: invariant measure

In this paper, we consider the canonical Hamiltonian systems with phase space $\mathbb{R}^{2n}$, Hamiltonian (2), and Hamilton’s equations

$$\begin{aligned} \dot{x} &= Kp, \\ \dot{p} &= -\nabla W(x). \end{aligned}$$

Eliminating p gives the second-order ODE (1). When $W(x)$ is a homogeneous polynomial of degree 4, let $\frac{1}{4}V(x_0, x_1, x_2, x_3)$ be the polarization of W so that $W(x) = \frac{1}{4}V(x, x, x, x)$ and V is linear in each argument. Note that we then have

$$\begin{aligned} \nabla W(x) &= V(x, x, x, \cdot), \\ \text{Hess } W(x) &= 3V(x, x, \cdot, \cdot). \end{aligned} \tag{6}$$

Here $\text{Hess}W(x)$ is the Hessian of W , i.e. the matrix of second partial derivatives of W .

We consider the second-order map $(x_0, x_1) \mapsto (x_1, x_2)$ defined by

$$\frac{x_2 - 2x_1 + x_0}{h^2} = -KV(x_0, x_1, x_2, \cdot). \tag{7}$$

It is known from the work of Hone and Quispel [18] that the map (7) has an integral and a preserved measure for $n=1$. We now outline the strategy that we have used to discover analogous invariants in any dimension n .

We first consider specific examples of (7) for $n=2$. In these examples, we find that the Jacobian determinant factors as N/D^3 where N and D are polynomials. The cofactor

ansatz described above then leads to the determination of two linearly independent Darboux polynomials, P_4 of degree 4 and P_6 of degree 6, with cofactors both equal to the Jacobian determinant. As they have the same cofactor, any linear combination of P_4 and P_6 is again a Darboux polynomial. Thus, we look for a convenient basis. As the degree 4 polynomial has nonzero constant term, the constant term in P_6 can be eliminated. In this basis, the terms in P_6 of degree 2, 4, and 6 can be expressed as invariant functions of K and V . Using this approach, it was possible to discover general expressions for two independent Darboux polynomials for any n , and hence our two key results: the invariant measure of the map (proposition 1) and a first integral (theorem 1).

Proposition 1. *The map (7) on $\mathbb{R}^{2n}$ has invariant measure $(\det M_{01})^{-1} \prod dx$, where $\prod dx = dx_{0,1} \wedge \cdots \wedge dx_{0,n} \wedge dx_{1,1} \wedge \cdots \wedge dx_{1,n}$ is the standard Euclidean measure on $\mathbb{R}^{2n}$ and*

$$M_{01} := I + h^2 KV_{01}, \quad V_{01} := V(x_0, x_1, \cdot, \cdot).$$

Proof. Because $V(x_0, x_1, x_2, \cdot) = V_{01}x_2$, the equation (7) for x_2 can be written in the form

$$M_{01}x_2 = 2x_1 - x_0. \quad (8)$$

The map in first order form

$$\begin{pmatrix} x_1 \\ x_0 \end{pmatrix} \mapsto \begin{pmatrix} x_2 \\ x_1 \end{pmatrix}$$

has Jacobian derivative

$$\begin{pmatrix} D_{x_1}x_2 & D_{x_0}x_2 \\ I & 0 \end{pmatrix}$$

with determinant

$$\det(-D_{x_0}x_2). \quad (9)$$

Taking Jacobian derivatives of both sides of (8) with respect to x_0 and using the product rule on the left gives

$$M_{01}D_{x_0}x_2 + h^2KV_{12} = -I$$

or

$$I + h^2KV_{12} = M_{12} = -M_{01}D_{x_0}x_2.$$

Taking determinants gives

$$\det M_{12} = \det(-D_{x_0}x_2) \det M_{01}$$

which, together with (9), establishes the result. $\square$

5. Polarization of homogeneous second order ODEs: first integral

The following theorem establishes that the map (7) has a first integral for all nonsingular matrices K and for all homogeneous quartic potentials V , in any dimension. In the expression (10) for the integral, under the approximation $x_1 - x_0 \approx h\dot{x}$, the first term approximates

$h^2 \dot{x}^\top K^{-1} \dot{x}$, i.e. $2h^2$ times the kinetic energy, and the second term approximates $2h^2 W(x)$, i.e. $2h^2$ times the potential energy. That is, the integral is a perturbation of the Hamiltonian of (2).

Theorem 1. *Let K be a symmetric nonsingular $n \times n$ matrix. The map (7) has the rational first integral*

$$F(x_0, x_1) := \Delta x_0^\top K^{-1} M_{01}^{-1} \Delta x_0 - \frac{1}{2} x_0^\top K^{-1} (M_{01}^{-1} - I) x_1 \quad (10)$$

where Δ is the forward difference operator, i.e. $\Delta x_0 = x_1 - x_0$.

Proof. We need to show that $F(x_1, x_2) = F(x_0, x_1)$, that is, that $\Delta F(x_0, x_1) = 0$. We recall the product formula for forward differences,

$$\Delta(a_0 b_0 c_0) = a_0 b_0 (\Delta c_0) + a_0 (\Delta b_0) c_1 + (\Delta a_0) b_1 c_1.$$

From equation (7), we have

$$\begin{aligned} \Delta^2 x_0 &= -KV_{01} x_2 \\ &= (I - M_{01}) x_2 \\ &= (I - M_{12}) x_0, \end{aligned}$$

$$M_{01}^{-1} (2x_1 - x_0) = x_2,$$

and

$$M_{12}^{-1} (2x_1 - x_2) = x_0.$$

Note that both $M_{01}K$ (which is equal to $(I + h^2 KV_{01})K$) and its inverse $K^{-1}M_{01}^{-1}$ are symmetric matrices.

The forward difference of the first term in the integral F is

$$\begin{aligned} \Delta(\Delta x_0^\top M_{01}^{-1} \Delta x_0) &= \Delta x_0^\top K^{-1} M_{01}^{-1} \Delta^2 x_0 + \Delta x_0^\top K^{-1} \Delta M_{01}^{-1} \Delta x_1 + \Delta^2 x_0^\top K^{-1} M_{12}^{-1} \Delta x_1 \\ &= (x_1 - x_0)^\top K^{-1} (M_{01}^{-1} - I) x_2 + (x_1 - x_0)^\top K^{-1} (M_{12}^{-1} - M_{01}^{-1}) (x_2 - x_1) \\ &\quad - x_0^\top K^{-1} (I - M_{12}^{-1}) (x_2 - x_1). \end{aligned}$$

The forward difference of the second term in the integral is

$$\begin{aligned} & -\frac{1}{2} \Delta(x_0^\top K^{-1} (M_{01}^{-1} - I) x_1) \\ &= -\frac{1}{2} (x_0^\top K^{-1} (M_{01}^{-1} - I) \Delta x_1 + x_0^\top K^{-1} \Delta (M_{01}^{-1} - I) x_2 + (\Delta x_0)^\top K^{-1} (M_{01}^{-1} - I) x_2) \\ &= -\frac{1}{2} (x_0^\top K^{-1} (M_{01}^{-1} - I) (x_2 - x_1) + x_0^\top K^{-1} (M_{12}^{-1} - M_{01}^{-1}) x_2 \\ &\quad + (x_1 - x_0)^\top K^{-1} (M_{12}^{-1} - I) x_2). \end{aligned}$$

Each term is a quadratic form with coefficient matrix one of the symmetric matrices K^{-1} , $K^{-1}M_{01}^{-1}$, or $K^{-1}M_{12}^{-1}$.

The terms with coefficient matrix $K^{-1}M_{12}^{-1}$ are applied to the pairs of vectors

$$\begin{aligned} & (x_1, x_2) - (x_1, x_1) - (x_0, x_2) + (x_0, x_1) + (x_0, x_2) - (x_0, x_1) - \frac{1}{2} ((x_0, x_2) + (x_1, x_2) - (x_0, x_2)) \\ &= -\frac{1}{2} (x_1, 2x_1 - x_2), \end{aligned}$$

giving the value

$$-\frac{1}{2}x_1^\top K^{-1}M_{12}^{-1}(2x_1 - x_2) = -\frac{1}{2}x_1^\top K^{-1}x_0. \quad (11)$$

The terms with coefficient matrix K^{-1} are applied to the pairs of vectors

$$\begin{aligned} & -(x_1, x_2) + (x_0, x_2) - (x_0, x_2) + (x_0, x_1) + \frac{1}{2}((x_0, x_2) - (x_0, x_1) + (x_1, x_2) - (x_0, x_2)) \\ &= \frac{1}{2}(-(x_1, x_2) + (x_1, x_0)), \end{aligned}$$

giving the value

$$-\frac{1}{2}x_1^\top K^{-1}(x_2 - x_0). \quad (12)$$

The terms with coefficient matrix $K^{-1}M_{01}^{-1}$ are applied to the pairs of vectors

$$\begin{aligned} & (x_1, x_2) - (x_0, x_2) - (x_1, x_2) + (x_1, x_1) + (x_0, x_2) - (x_0, x_1) - \frac{1}{2}((x_0, x_2) - (x_0, x_1) - (x_0, x_2)) \\ &= \frac{1}{2}(x_1, 2x_1 - x_0) \end{aligned}$$

giving the value

$$\frac{1}{2}x_1^\top K^{-1}M_{01}^{-1}(2x_1 - x_0) = \frac{1}{2}x_1^\top K^{-1}x_2. \quad (13)$$

The forward difference $\Delta F(x_0, x_1)$ of the integral is the sum of the three terms (11)–(13), namely zero. $\square$

Remark. The denominator of the invariant measure (proposition 1) is equal to the denominator of the first integral (theorem 1). Therefore, both the numerator and the denominator of the first integral are Darboux polynomials with cofactor equal to the reciprocal of the Jacobian determinant of the map. Exactly the same structure holds for the Kahan map equation (5) in the Hamiltonian case [6].

6. Polarization of nonhomogeneous second order ODEs

A nonhomogeneous function $f: \mathbb{R}^n \rightarrow \mathbb{R}$ of degree $\leq d$ is associated with the homogeneous function $\tilde{f}: \mathbb{R}^{n+1} \rightarrow \mathbb{R}$ of degree d given by $\tilde{f}(x, z) := z^d f(x/z)$, where $z \in \mathbb{R}$. Therefore, nonhomogeneous potentials W can be handled by polarization by (i) homogenizing ∇W ; (ii) extending K to $\tilde{K} = \begin{bmatrix} K & 0 \\ 0 & 0 \end{bmatrix}$; discretizing the extended homogeneous system by polarization; and (iv) restricting to $z = 1$, noting that the level set $z = 1$ is invariant under both the extended differential equation and the polarized map.

Proposition 2 below shows, however, that the method resulting from steps (i)–(iv) above and the original method (7) for homogeneous potentials are both equivalent to the same Runge–Kutta–Nyström method.

For any (possibly nonhomogeneous) function or vector field $f(x)$ of degree $\leq d$, let

$$\text{pol}_d f(x_0, \dots, x_{d-1})$$

Table 1. Examples of degree- d polarization of polynomials of degree $\leq d$, for $d = 2$ and $d = 3$, illustrating how the Runge–Kutta-like formula (15), applied to nonhomogeneous polynomials, gives the same result as homogenization.

$\text{pol}_2 f = 2f\left(\frac{x_0+x_1}{2}\right) - \frac{1}{2}f(x_0) - \frac{1}{2}f(x_1)$
$\text{pol}_2 x^2 = 2\left(\frac{x_0+x_1}{2}\right)^2 - \frac{1}{2}x_0^2 - \frac{1}{2}x_1^2 = x_0x_1$
$\text{pol}_2 x = 2\frac{x_0+x_1}{2} - \frac{1}{2}x_0 - \frac{1}{2}x_1 = \frac{1}{2}(x_0 + x_1)$
$\text{pol}_2 1 = 2 - \frac{1}{2} - \frac{1}{2} = 1$
$\text{pol}_3 f = \frac{27}{6}f\left(\frac{x_0+x_1+x_2}{3}\right) - \frac{8}{6}f\left(\frac{x_0+x_1}{2}\right) - \frac{8}{6}f\left(\frac{x_0+x_2}{2}\right) - \frac{8}{6}f\left(\frac{x_1+x_2}{2}\right)$
$\quad + \frac{1}{6}f(x_0) + \frac{1}{6}f(x_1) + \frac{1}{6}f(x_2)$
$\text{pol}_3 x^3 = x_0x_1x_2$
$\text{pol}_3 x^2 = \frac{1}{3}(x_0x_1 + x_1x_2 + x_2x_0)$
$\text{pol}_3 x = \frac{1}{3}(x_0 + x_1 + x_2)$
$\text{pol}_3 1 = 1$

be the restriction to $z = 1$ of the polarization of the homogenization $\tilde{f}(x, z)$ of $f(x)$. (see the examples in table 1). The polar map of $\ddot{x} = f(x)$, $\deg(f) \leq 3$, is then defined by

$$x_2 - 2x_1 + x_0 = h^2 \text{pol}_3 f(x_0, x_1, x_2). \quad (14)$$

Proposition 2 ([18]). *The map (14) is equivalent to a specific 7-stage Runge–Kutta–Nyström method.*

Proof. We first establish an identity for arbitrary d that provides a Runge–Kutta-like expression for the polarization of nonhomogeneous functions.

For homogeneous f of degree d , a standard identity in algebraic polarization [14, p 110] recovers its polarization as a linear combination of its values:

$$\text{pol}_d f(x_0, \dots, x_{d-1}) = \frac{1}{d!} \sum_{\substack{1 \leq m \leq d \\ 0 \leq i_1 < \dots < i_m < d}} (-1)^{k-m} f(x_{i_1} + \dots + x_{i_m}),$$

where the sum is over all nonempty subsets of $\{0, \dots, d-1\}$. Using homogeneity of f , we get

$$\text{pol}_d f(x_0, \dots, x_{d-1}) = \frac{1}{d!} \sum_{\substack{1 \leq m \leq d \\ 0 \leq i_1 < \dots < i_m < d}} (-1)^{k-m} m^d f\left(\frac{x_{i_1} + \dots + x_{i_m}}{m}\right). \quad (15)$$

This is a linear combination of the values of f at $2^d - 1$ points, each of which is a convex combination of the x_j .

For $d = 3$ and the method (14), these points may be taken to be the seven stage values in x of a Runge–Kutta–Nyström method.

If, now, f is nonhomogeneous of degree $\leq d$, then $\tilde{f}([x, 1]) = f(x)$ and (on the right hand side of (15) in the last argument of $\tilde{f}$) $(1 + \dots + 1)/m = 1$, giving

$$\text{pol}_d \tilde{f}([x_0, 1], \dots, [x_{d-1}, 1]) = \text{pol}_d f(x_0, \dots, x_{d-1}),$$

while the final zero row of $\tilde{K}$ gives the discretization of the z component of the extended system as

$$z_2 - 2z_1 + z_0 = 0$$

which is satisfied by $z_k = 1$ for all k . $\square$

The invariant measure for the nonhomogeneous case can be determined by applying proposition 1 to the homogenized system. It can also be expressed directly in terms of the nonhomogeneous vector field, as follows.

Proposition 3. *Let $f = -K\nabla W$ be a nonhomogeneous vector field of degree ≤ 3 . The first-order map associated with (14) has invariant measure*

$$\frac{\prod dx}{\det\left(I - \frac{h^2}{3}\text{pol}_2 Df\right)}. \quad (16)$$

Proof. First, if f is homogeneous then from (6) we have

$$\begin{aligned} -KV(x_0, x_1, x_2, \cdot) &= -K\text{pol}_3 \nabla W(x_0, x_1, x_2) \\ &= \text{pol}_3 f(x_0, x_1, x_2) \end{aligned}$$

and

$$\begin{aligned} -KV(x_0, x_1, \cdot, \cdot) &= -K\frac{1}{3}\text{pol}_2 \text{Hess} W(x_0, x_1) \\ &= \frac{1}{3}\text{pol}_2 Df(x_0, x_1), \end{aligned}$$

establishing (16) for the homogeneous case.

If f is nonhomogeneous, we apply (16) to the homogenized system and restrict the invariant measure to the invariant set $z = 1$. The last row and column of $\tilde{K}$ are zero, and the top left $n \times n$ block of $D\tilde{f}$, evaluated at $z = 1$, is equal to Df . This gives the result. $\square$

The integral of the polar map for nonhomogeneous f cannot be obtained directly, as the extended matrix $\tilde{K}$ is noninvertible. Instead, we introduce a perturbation parameter ε and let $\tilde{K} = \begin{bmatrix} K & 0 \\ 0 & \varepsilon \end{bmatrix}$. Then the polar map of the perturbed homogenized system has the form

$$\begin{aligned} x_2 - 2x_1 + x_0 &= -h^2 K \nabla_x \tilde{V}(x, z) \\ z_2 - 2z_1 + z_0 &= -h^2 \varepsilon \nabla_z \tilde{V}(x, z). \end{aligned}$$

Its first integral from (10) has the form

$$F([x_0, z_0], [x_1, z_1]) = \frac{1}{\varepsilon}(z_1 - z_0)^2 + F_0([x_0, z_0], [x_1, z_1]) + \mathcal{O}(\varepsilon).$$

Restricting to $z_0 = z_1 = 1$, i.e. passing to the polar map (14) of the nonhomogeneous system, and then taking the limit $\varepsilon \rightarrow 0$, determines $F_0([x_0, 1], [x_1, 1])$ as a first integral of (14).

7. Higher order systems

The following proposition generalizes proposition 3 to m th order systems featuring degree $m + 1$ polynomials. The $m = 2$ case generalizes proposition 3 to arbitrary nonconservative vector fields f . The odd m case contains a restriction on f which is satisfied, for example, by Hamiltonian vector fields when $m = 1$.

Proposition 4. *The polar map*

$$x_m + \left(\sum_{i=1}^{m-1} c_i x_i \right) + (-1)^m x_0 = h^m \text{pol}_{m+1} f(x_0, \dots, x_m) \quad (17)$$

associated with the m th-order polynomial differential equation

$$x^{(m)} = f(x), \quad x \in \mathbb{R}^n, \quad \deg(f) \leq m + 1$$

preserves the measure

$$\frac{\prod dx}{\det(I - \frac{h^m}{m+1} \text{pol}_m Df)}$$

- (i) for all f when m is even; and
- (ii) for all f that satisfy $\det(I + Df) = \det(I - Df)$ when m is odd.

Proof. First consider the case that f is homogeneous, in which case the map (17) can be written in the form

$$x_m + \left(\sum_{i=1}^{m-1} c_i x_i \right) + (-1)^m x_0 = \frac{1}{m+1} h^m \text{pol}_m Df(x_0, \dots, x_{m-1}) x_m$$

or

$$\left(I - h^m \frac{1}{m+1} \text{pol}_m Df(x_0, \dots, x_{m-1}) \right) x_m = - \left(\sum_{i=1}^{m-1} c_i x_i \right) - (-1)^m x_0. \quad (18)$$

The map in first order form

$$\begin{pmatrix} x_{m-1} \\ \vdots \\ x_0 \end{pmatrix} \mapsto \begin{pmatrix} x_m \\ \vdots \\ x_1 \end{pmatrix}$$

has Jacobian derivative

$$\begin{pmatrix} D_{x_{m-1}} x_m & D_{x_{m-2}} x_m & \dots & D_{x_0} x_m \\ I & 0 & \dots & 0 \\ 0 & I & \dots & 0 \\ \dots & & & \end{pmatrix}$$

with determinant

$$\det((-1)^{m+1} D_{x_0} x_m). \quad (19)$$

Taking Jacobian derivatives of both sides of (18) with respect to x_0 and using the product rule on the left gives

$$\begin{aligned} & \left(I - h^m \frac{1}{m+1} \text{pol}_m \text{D}f(x_0, \dots, x_{m-1}) \right) D_{x_0} x_m - h^m \frac{1}{m+1} \text{pol}_m \text{D}f(x_1, \dots, x_m) \\ & = (-1)^{m+1} I \end{aligned}$$

or

$$\begin{aligned} & \left(I - h^m \frac{1}{m+1} \text{pol}_m \text{D}f(x_0, \dots, x_{m-1}) \right) ((-1)^{m+1} D_{x_0} x_m) \\ & = I + (-1)^{m+1} h^m \frac{1}{m+1} \text{pol}_m \text{D}f(x_1, \dots, x_m). \end{aligned}$$

Taking determinants gives

$$\begin{aligned} & \det \left(I - h^m \frac{1}{m+1} \text{pol}_m \text{D}f(x_0, \dots, x_{m-1}) \right) \det ((-1)^{m+1} D_{x_0} x_m) \\ & = \det \left(I + (-1)^{m+1} h^m \frac{1}{m+1} \text{pol}_m \text{D}f(x_1, \dots, x_m) \right). \end{aligned}$$

Together with equation (19), and $\det(I + \text{D}f) = \det(I - \text{D}f)$ when m is odd, this establishes the result. The nonhomogeneous case follows as in proposition 3. $\square$

Note that if $f = J^\top \nabla W$ for some $W: \mathbb{R}^n \rightarrow \mathbb{R}$ and some antisymmetric matrix J , then Sylvester's criterion gives $\det(I + \text{D}f) = \det(I + J \text{Hess} W) = \det(I + (\text{Hess} W)J) = \det(I + J^\top (\text{Hess} W)^\top) = \det(I - \text{D}f)$. However, other vector fields (such as $v(x) \frac{\partial}{\partial y} + w(y) \frac{\partial}{\partial x}$) also satisfy this condition.

8. A system with a linear symmetry

As we have seen, the discretization considered in this paper is equivalent to a Runge–Kutta–Nyström method. Therefore, it is equivariant with respect to (partitioned) linear maps [26]. That is, given any linear maps $A: X \rightarrow Y$, and any two A -related differential equations $\ddot{x} = f(x)$ ($x \in X$) and $\ddot{y} = g(y)$ ($y \in Y$) obeying $g \circ A = A \circ f$, the polar maps associated with the differential equations are themselves A -related. If A is invertible and $g = f$, then A is a symmetry of f and of its polar map. (Similar remarks hold for affine maps).

This suggests that polar maps of differential equations with linear symmetries may have further special properties. In this section we consider the special case of the system with $n = 2$ and rotationally-invariant Hamiltonian

$$H(x, p) = \frac{1}{2} \|p\|^2 + \alpha \|x\|^2 + \beta \|x\|^4. \quad (20)$$

The symmetry $x \mapsto Rx$, $R \in O(2)$, of Hamilton's equations extends to a symmetry $(x_0, x_1) \mapsto (Rx_0, Rx_1)$ of the polar map. The invariant measure of this map is rotationally invariant. Computing this measure using proposition 1 gives its explicit expression

$$\left((1 + \frac{2}{3} h^2 (\alpha + 4\beta(x_0 \cdot x_1)))^2 - \frac{16}{9} h^4 \beta^2 \|x_0\|^2 \|x_1\|^2 \right)^{-1} dx_{0,1} \wedge dx_{0,2} \wedge dx_{1,1} \wedge dx_{1,2}$$

in terms of the three fundamental invariants $x_0 \cdot x_1$, $\|x_0\|^2$, and $\|x_1\|^2$ of the group action. (Here $x_0 = (x_{0,1}, x_{0,2}) \in \mathbb{R}^2$.)

The Jacobian determinant of the polar map factors as $N_2 N_6 / D_4^3$, where the subscripts denote the degree of the polynomials. This provides more candidates for cofactors.

Indeed, we find immediately that the cofactor N_2 / D_4 has two rotationally-invariant Darboux polynomials P_1 and P_2 :

$$\begin{aligned} P_1 &= x_{1,1}x_{0,2} - x_{0,1}x_{1,2} \\ P_2 &= 3 + h^2(2\alpha + 4\beta(x_0 \cdot x_1)). \end{aligned}$$

These provide the integral P_1/P_2 , that approximates $\frac{1}{3}h$ times the integral of Hamilton's equations that is associated with the rotational symmetry, namely $x_2\dot{x}_1 - x_1\dot{x}_2$.

Trying other cofactors and Darboux polynomials up to degree 6 yields no further information other than those known for general systems and those generated by them.

The symmetry, integrals, and invariant measure are enough to ensure that the map is superintegrable in the sense of van der Kamp *et al* [35], i.e. it is a measure-preserving n -dimensional map with $n - 1$ functionally independent constants of motion.

Proposition 5. *The polar map associated with (20) is superintegrable.*

Proof. The map is four-dimensional with a one-dimensional measure-preserving symmetry group, and thus descends to a measure-preserving map on the three-dimensional quotient [19]. The two integrals are also invariant under the symmetry and hence descend to the quotient. This yields a three-dimensional measure-preserving map with two functionally independent integrals, thus superintegrable. $\square$

A different integrable discretization of this system is given in McLachlan [25].

Data availability statement

No new data were created or analysed in this study.

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