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A new approach to integrals of discretizations by polarization

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Abstract

Recently, a family of unconventional integrators for ODEs with polynomial vector fields was proposed, based on the polarization of vector fields. The simplest instance is the by now famous Kahan discretization for quadratic vector fields. All these integrators seem to possess remarkable conservation properties. In particular, it has been proved that, when the underlying ODE is Hamiltonian, its polarization discretization possesses an integral of motion and an invariant volume form. In this note, we propose a new algebraic approach to derivation of the integrals of motion for polarization discretizations.

1 Introduction

The by now famous Kahan discretization [5] is a one-step numerical method designed specially for ODEs in $\mathbb{R}^d$,

$$\dot{x} = f(x), \tag{1}$$

with all components of the vector field f being polynomials of degree 2. The Kahan discretization with the stepsize ϵ is the following difference equation:

$$(x_{n+1} - x_n)/\epsilon = \mathrm{pol}_2 f(x_n, x_{n+1}). \tag{2}$$

Here, for any quadratic form $Q(x)$ on $\mathbb{R}^d$, its polarization is the corresponding symmetric bilinear form,

$$\mathrm{pol}_2 Q(x_1, x_2) = \frac{1}{2}\big(Q(x_1 + x_2) - Q(x_1) - Q(x_2)\big).$$

For a non-homogeneous polynomial $P(x)$ of degree 2, one extends it to a quadratic form in homogeneous coordinates, $\widetilde{P}(x,z)=z^2P(x/z)$, computes the bilinear symmetric form $\mathrm{pol}_2\widetilde{P}$ and then sets $\mathrm{pol}_2P=\mathrm{pol}_2\widetilde{P}|_{z_1=z_2=1}$. In particular, for a linear form $L(x)$ we obtain $\mathrm{pol}_2L(x_1,x_2)=(L(x_1)+L(x_2))/2$.

Equation (2) is linear with respect to x_{n+1}, thus can be solved to give a rational map

$$x_{n+1}=f_\epsilon(x_n). \tag{3}$$

Moreover, due to the symmetry of equation (2) with respect to $x_n\leftrightarrow x_{n+1}$ and $\epsilon\leftrightarrow-\epsilon$, we have $f_\epsilon^{-1}=f_{-\epsilon}$, in particular, f_ϵ is a birational map.

Kahan's discretization is known to inherit integrals and integral invariants much more frequently than could be anticipated, see [7, 8, 1, 2] and a more recent literature. In the present note, we will address the remarkable result of [1] which states that map f_ϵ always possesses an integral of motion, if $f(x)$ is a quadratic *Hamiltonian* vector field in the space of an even dimension d, that is, $f(x)=J\nabla H(x)$, where H is a polynomial of degree 3, and $J\in\mathrm{so}(d)$ is a non-degenerate skew-symmetric matrix. Our Theorem 1 in Section 2 gives a novel derivation and an algebraic interpretation of this result.

A wide generalization of the Kahan discretization for polynomial vector fields of higher degrees was proposed in [3]. The most interesting version of this approach deals with higher order differential equations, for which the discretization preserves the dimension of the phase space [4]. Consider a second order differential equation in $\mathbb{R}^d$,

$$\ddot{x}=g(x), \tag{4}$$

where all components of $g(x)$ are polynomials of degree 3. The polarization discretization of such an equation with the stepsize ϵ is the following second order difference equation:

$$(x_{n+1}-2x_n+x_{n-1})/\epsilon^2=\mathrm{pol}_3g(x_{n-1},x_n,x_{n+1}). \tag{5}$$

Here, the third order polarization pol_3 for a cubic form $C(x)$ is the corresponding symmetric trilinear form

$$\begin{aligned}\mathrm{pol}_3C(x_1,x_2,x_3) &= \frac{1}{6}\big(C(x_1+x_2+x_3)-C(x_1+x_2)-C(x_1+x_3)-C(x_2+x_3)\\ &\quad +C(x_1)+C(x_2)+C(x_3)\big).\end{aligned}$$

For a non-homogeneous polynomial $P(x)$ of degree 3, one first extends it to a cubic form in homogeneous coordinates, $\widetilde{P}(x,z)=z^3P(x/z)$, computes the trilinear symmetric form $\mathrm{pol}_3\widetilde{P}$, and then sets $\mathrm{pol}_3P=\mathrm{pol}_3\widetilde{P}|_{z_1=z_2=z_3=1}$. For a quadratic form $Q(x)$, we find:

$$\mathrm{pol}_3Q(x_1,x_2,x_3)=\frac{1}{3}\big(\mathrm{pol}_2Q(x_1,x_2)+\mathrm{pol}_2Q(x_1,x_3)+\mathrm{pol}_2Q(x_2,x_3)\big), \tag{6}$$

while for a linear form $L(x)$, we find:

$$\mathrm{pol}_3L(x_1,x_2,x_3)=\frac{1}{3}\big(L(x_1)+L(x_2)+L(x_3)\big). \tag{7}$$

Again, equation (5) is linear with respect to x_{n+1}, thus can be solved to give a birational map

$$(x_n,x_{n+1})=g_\epsilon(x_{n-1},x_n), \tag{8}$$

which enjoys the symmetry with respect to $x_{n-1} \leftrightarrow x_{n+1}$.

Let $g(x) = K\nabla W(x)$, where $K \in \mathrm{Symm}(d)$ is a non-degenerate symmetric matrix, and $W(x)$ is a polynomial of degree 4. Then equation (4) is equivalent to a canonical Hamiltonian system with the Hamilton function $H(x,p) = \frac{1}{2}\langle p, Kp\rangle + W(x)$. Indeed, equations of motion of the latter read $\dot{x} = Kp$, $\dot{p} = -\nabla W(x)$. A remarkable result of [4, 6] states that in this case map g_ϵ possesses an integral of motion. Our Theorem 2 in Section 3 gives a novel derivation and algebraic interpretation of this result.

2 Hamiltonian systems with a cubic integral

Consider a Hamiltonian system

$$\dot{x} = J\nabla H, \tag{9}$$

where $H : \mathbb{R}^d \to \mathbb{R}$ is a polynomial of degree 3, and $J \in \mathrm{so}(d)$ is a non-degenerate matrix (so that d is necessarily even). It is well known that $H(x)$ is an integral of motion for (9). We consider the Kahan discretization for (9), see equation (2).

Theorem 1. Separate H into homogeneous parts of degrees 3, 2, and 1:

$$H(x) = H_3(x) + H_2(x) + H_1(x). \tag{10}$$

Then the following quantity is a conserved quantity for the difference equation (2):

$$H_\epsilon(x_n, x_{n+1}) = \tfrac{1}{\epsilon}\langle x_n\,, J^{-1}x_{n+1}\rangle + \mathrm{pol}_2 H_2(x_n, x_{n+1}) + 2\,\mathrm{pol}_2 H_1(x_n, x_{n+1}). \tag{11}$$

Proof. We are dealing with the following difference equation:

$$J^{-1}(x_{n+1}-x_n)/\epsilon = \mathrm{pol}_2\nabla H_3(x_n, x_{n+1}) + \mathrm{pol}_2\nabla H_2(x_n, x_{n+1}) + \mathrm{pol}_2\nabla H_1(x_n, x_{n+1}). \tag{12}$$

Take the scalar product of equation (12) with x_{n-1}:

$$\begin{aligned} &\tfrac{1}{\epsilon}\langle x_{n-1}, J^{-1}x_{n+1}\rangle - \tfrac{1}{\epsilon}\langle x_{n-1}, J^{-1}x_n\rangle \\ &\quad = \; 3\,\mathrm{pol}_3 H_3(x_{n-1}, x_n, x_{n+1}) + \mathrm{pol}_2 H_2(x_{n-1}, x_n) + \mathrm{pol}_2 H_2(x_{n-1}, x_{n+1}) + H_1(x_{n-1}). \end{aligned} \tag{13}$$

Here we used Euler's theorem on homogeneous functions and have taken into account that for a quadratic form H_2 there holds $\mathrm{pol}_2\nabla H_2(x_n, x_{n+1}) = (\nabla H_2(x_n) + \nabla H_2(x_{n+1}))/2$, and for a linear form H_1 its gradient ∇H_1 is a constant vector. Similarly, take the scalar product of the downshifted (i.e., $n \to n-1$) equation (12) with x_{n+1}:

$$\begin{aligned} &\tfrac{1}{\epsilon}\langle x_{n+1}, J^{-1}x_n\rangle - \tfrac{1}{\epsilon}\langle x_{n+1}, J^{-1}x_{n-1}\rangle \\ &\quad = \; 3\,\mathrm{pol}_3 H_3(x_{n-1}, x_n, x_{n+1}) + \mathrm{pol}_2 H_2(x_n, x_{n+1}) + \mathrm{pol}_2 H_2(x_{n-1}, x_{n+1}) + H_1(x_{n+1}). \end{aligned} \tag{14}$$

Subtracting the latter two equations (taking into account the skew-symmetry of J^{-1}) leads to

$$\begin{aligned} &\tfrac{1}{\epsilon}\langle x_{n+1}, J^{-1}x_n\rangle - \tfrac{1}{\epsilon}\langle x_n, J^{-1}x_{n-1}\rangle \\ &\quad = \; \mathrm{pol}_2 H_2(x_n, x_{n+1}) - \mathrm{pol}_2 H_2(x_{n-1}, x_n) + H_1(x_{n+1}) - H_1(x_{n-1}). \end{aligned} \tag{15}$$

This is equivalent to (11) being a conserved quantity. ■

Discussion.

1) It is not very common to express conserved quantities of a first order difference equation in terms of more than one iterate. To avoid misconceptions, we stress that the statement that $H_\epsilon(x_n, x_{n+1})$ is a conserved quantity of the difference equation (12) means that

$$H_\epsilon(x, f_\epsilon(x)) = H_\epsilon(f_\epsilon(x), f_\epsilon^2(x)).$$

In other words, $H_\epsilon(x, f_\epsilon(x))$ is an integral of motion of the map f_ϵ. It is in this latter form that the integral has been found in [1]. Earlier examples of expressions of conserved quantities of Kahan discretizations in terms of more than one iterate have been found in [8, 10].

2) If $H(x)$ is homogeneous of degree 3, we get an especially simple conserved quantity $\epsilon H_\epsilon(x_n) = \langle x_n\,, J^{-1}x_{n+1}\rangle$. This particular result was found previously in [3] as a special case of a more general statement for discretization by polarization.

3) It is instructive to look at the continuous time counterpart of this result. We derive, by Euler's theorem on homogeneous functions:

$$\langle x, J^{-1}\dot{x}\rangle = \langle x, \nabla H(x)\rangle = 3H_3(x) + 2H_2(x) + H_1(x).$$

As a consequence, the quantity

$$\langle x, J^{-1}\dot{x}\rangle + H_2(x) + 2H_1(x)$$

is an integral of motion (equals $3H(x)$). In particular, if $H(x)$ is homogeneous of degree 3, we get a simple expression $\langle x, J^{-1}\dot{x}\rangle$ for the integral of motion.

Example. Take $d = 2$, $x = \begin{pmatrix} q \\ p \end{pmatrix}$, $J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$, so that $J^{-1} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, and set

$$\begin{aligned} H_3(q,p) &= a_{30}q^3 + a_{21}q^2p + a_{12}qp^2 + a_{03}p^3, &(16)\\ H_2(q,p) &= a_{20}q^2 + a_{11}qp + a_{02}p^2, &(17)\\ H_1(q,p) &= a_{10}q + a_{01}p. &(18) \end{aligned}$$

Thus, equations of motion (9) read

$$\begin{aligned} \dot{q} &= a_{21}q^2 + 2a_{12}qp + 3a_{03}p^2 + a_{11}q + 2a_{02}p + a_{01}, &(19)\\ \dot{p} &= -3a_{30}q^2 - 2a_{21}qp - a_{12}p^2 - 2a_{20}q - a_1p - a_{10}, &(20) \end{aligned}$$

while their Kahan discretization reads

$$\begin{aligned} (q_{n+1} - q_n)/\epsilon &= a_{21}q_nq_{n+1} + a_{12}(q_np_{n+1} + p_nq_{n+1}) + 3a_{03}p_np_{n+1} \\ &\quad + \tfrac{1}{2}a_{11}(q_n + q_{n+1}) + a_{02}(p_n + p_{n+1}) + a_{01}, &(21)\\ (p_{n+1} - p_n)/\epsilon &= -3a_{30}q_nq_{n+1} - a_{21}(q_np_{n+1} + p_nq_{n+1}) - a_{12}p_np_{n+1} \\ &\quad - a_{20}(q_n + q_{n+1}) - \tfrac{1}{2}a_{11}(p_n + p_{n+1}) - a_{10}. &(22) \end{aligned}$$

Conserved quantity (11) takes the form

$$\begin{aligned} H_\epsilon(q_n, p_n, q_{n+1}, p_{n+1}) &= \tfrac{1}{\epsilon}(p_nq_{n+1} - q_np_{n+1}) \\ &\quad + a_{20}q_nq_{n+1} + \tfrac{1}{2}a_{11}(p_nq_{n+1} + q_np_{n+1}) + a_{02}p_np_{n+1} \\ &\quad + a_{01}(p_n + p_{n+1}) + a_{10}(q_n + q_{n+1}). &(23) \end{aligned}$$

If $H(q,p)$ is homogeneous of degree 3, we get a quite simple conserved quantity $\epsilon H_\epsilon = p_n q_{n+1} - q_n p_{n+1}$. The continuous time limit of H_ϵ is the expression

$$p\dot{q} - q\dot{p} + H_2(q,p) + 2H_1(q,p),$$

which is an integral of motion (equals $3H(q,p)$). In particular, if $H(q,p)$ is homogeneous of degree 3, we get a simple "Wronskian" expression $p\dot{q} - q\dot{p}$ for the integral of motion.

3 Second order Hamiltonian systems with a quartic potential

Consider a Hamiltonian system

$$\ddot{x} = -K\nabla W, \tag{24}$$

where $W : \mathbb{R}^d \to \mathbb{R}$ is a polynomial of degree 4, and K is a symmetric $d \times d$ matrix. This system admits an integral of motion

$$H(x,\dot{x}) = \frac{1}{2}\langle \dot{x}, K^{-1}\dot{x}\rangle + W(x). \tag{25}$$

The right-hand side of equation (24) is of degree 3, and we consider the corresponding discretization by polarization, see (5).

Theorem 2. Separate the potential W into homogeneous parts of degrees 4, 3, 2, and 1:

$$W(x) = W_4(x) + W_3(x) + W_2(x) + W_1(x). \tag{26}$$

Then the following quantity is a conserved quantity of the difference equation (5):

$$\begin{aligned} H_\epsilon(x_{n-1},x_n,x_{n+1}) &= \tfrac{1}{\epsilon^2}\big(\langle x_{n-1}, K^{-1}x_n\rangle - 2\langle x_{n-1}, K^{-1}x_{n+1}\rangle + \langle x_n, K^{-1}x_{n+1}\rangle\big) \\ &\quad + \mathrm{pol}_3 W_3(x_{n-1},x_n,x_{n+1}) + 2\,\mathrm{pol}_3 W_2(x_{n-1},x_n,x_{n+1}) + 3\,\mathrm{pol}_3 W_1(x_{n-1},x_n,x_{n+1}). \end{aligned} \tag{27}$$

Proof. We are dealing with the following difference equation:

$$\begin{aligned} K^{-1}(x_{n+1} - 2x_n + x_{n-1})/\epsilon^2 \;=\; & -\mathrm{pol}_3\nabla W_4(x_{n-1},x_n,x_{n+1}) - \mathrm{pol}_3\nabla W_3(x_{n-1},x_n,x_{n+1}) \\ & -\mathrm{pol}_3\nabla W_2(x_{n-1},x_n,x_{n+1}) - \mathrm{pol}_3\nabla W_1(x_{n-1},x_n,x_{n+1}). \end{aligned} \tag{28}$$

Take the scalar product of this equation with x_{n+2}:

$$\begin{aligned} &\big(\langle x_{n+2}, K^{-1}x_{n+1}\rangle - 2\langle x_{n+2}, K^{-1}x_n\rangle + \langle x_{n+2}, K^{-1}x_{n-1}\rangle\big)/\epsilon^2 \\ &\quad = -4\,\mathrm{pol}_4 W_4(x_{n-1},x_n,x_{n+1},x_{n+2}) \\ &\qquad -\mathrm{pol}_3 W_3(x_{n-1},x_n,x_{n+2}) - \mathrm{pol}_3 W_3(x_{n-1},x_{n+1},x_{n+2}) - \mathrm{pol}_3 W_3(x_n,x_{n+1},x_{n+2}) \\ &\qquad -\frac{2}{3}\big(\mathrm{pol}_2 W_2(x_{n-1},x_{n+2}) + \mathrm{pol}_2 W_2(x_n,x_{n+2}) + \mathrm{pol}_2 W_2(x_{n+1},x_{n+2})\big) \\ &\qquad -W_1(x_{n+2}). \end{aligned} \tag{29}$$

Here we used Euler's theorem on homogeneous functions and have taken into account formulas (6) for the quadratic form ∇W_3 and (7) for the linear form ∇W_2, and that ∇W_1 is a constant vector. Similarly, take the scalar product of the shifted equation (28) (i.e., $n \to n+1$), by x_{n-1}:

$$\begin{aligned}
&\big(\langle x_{n-1}, K^{-1}x_{n+2}\rangle - 2\langle x_{n-1}, K^{-1}x_{n+1}\rangle + \langle x_{n-1}, K^{-1}x_n\rangle\big)/\epsilon^2\\
&\quad = \ -4\,\mathrm{pol}_4 W_4(x_{n-1}, x_n, x_{n+1}, x_{n+2})\\
&\qquad -\mathrm{pol}_3 W_3(x_{n-1}, x_n, x_{n+1}) - \mathrm{pol}_3 W_3(x_{n-1}, x_n, x_{n+2}) - \mathrm{pol}_3 W_3(x_{n-1}, x_{n+1}, x_{n+2})\\
&\qquad -\frac{2}{3}\big(\mathrm{pol}_2 W_2(x_{n-1}, x_n) + \mathrm{pol}_2 W_2(x_{n-1}, x_{n+1}) + \mathrm{pol}_2 W_2(x_{n-1}, x_{n+2})\big)\\
&\qquad -W_1(x_{n-1}).
\end{aligned} \tag{30}$$

Subtracting (30) from (29) leads to:

$$\begin{aligned}
&\big(\langle x_{n+2}, K^{-1}x_{n+1}\rangle - 2\langle x_{n+2}, K^{-1}x_n\rangle + 2\langle x_{n-1}, K^{-1}x_{n+1}\rangle - \langle x_{n-1}, K^{-1}x_n\rangle\big)/\epsilon^2\\
&\quad = \ -\mathrm{pol}_3 W_3(x_n, x_{n+1}, x_{n+2}) + \mathrm{pol}_3 W_3(x_{n-1}, x_n, x_{n+1})\\
&\qquad -\frac{2}{3}\big(\mathrm{pol}_2 W_2(x_n, x_{n+2}) + \mathrm{pol}_2 W_2(x_{n+1}, x_{n+2}) - \mathrm{pol}_2 W_2(x_{n-1}, x_{n+1}) - \mathrm{pol}_2 W_2(x_{n-1}, x_n)\big)\\
&\qquad -W_1(x_{n+2}) + W_1(x_{n-1}).
\end{aligned} \tag{31}$$

This is equivalent to the following expression being a conserved quantity:

$$\begin{aligned}
&\big(\langle x_{n-1}, K^{-1}x_n\rangle - 2\langle x_{n-1}, K^{-1}x_{n+1}\rangle + \langle x_n, K^{-1}x_{n+1}\rangle\big)/\epsilon^2\\
&\qquad +\mathrm{pol}_3 W_3(x_{n-1}, x_n, x_{n+1})\\
&\qquad +\frac{2}{3}\big(\mathrm{pol}_2 W_2(x_{n-1}, x_n) + \mathrm{pol}_2 W_2(x_{n-1}, x_{n+1}) + \mathrm{pol}_2 W_2(x_n, x_{n+1})\big)\\
&\qquad +W_1(x_{n-1}) + W_1(x_n) + W_1(x_{n+1}).
\end{aligned} \tag{32}$$

But this is the same as (27). ∎

Discussion.

1) Of course, in order to consider (27) as a function of (x_{n-1}, x_n), one has to substitute on the right-hand side the rational expression of x_{n+1} through (x_{n-1}, x_n), which follows from (28).

2) If $W(x)$ is homogeneous of degree 4, we get an especially simple conserved quantity:

$$\epsilon^2 H_\epsilon(x_{n-1}, x_n, x_{n+1}) = \langle x_{n-1}, K^{-1}x_n\rangle - 2\langle x_{n-1}, K^{-1}x_{n+1}\rangle + \langle x_n, K^{-1}x_{n+1}\rangle.$$

3) It is instructive to look at the continuous time counterpart of this result. The continuos limit of the expression on the right-hand side of (27) (performed according to $x_n = x$, $x_{n\pm1} = x \pm \epsilon\dot{x} + \frac{\epsilon^2}{2}\ddot{x} + O(\epsilon^3)$) equals

$$2\langle \dot{x}, K^{-1}\dot{x}\rangle - \langle x, K^{-1}\ddot{x}\rangle + W_3(x) + 2W_2(x) + 3W_1(x).$$

By virtue of equations of motion (24), this equals

$$2\langle \dot{x}, K^{-1}\dot{x}\rangle + \langle x, \nabla W(x)\rangle + W_3(x) + 2W_2(x) + 3W_1(x)$$

and, by Euler's theorem on homogeneous functions, we find:

$$
\begin{aligned}
&= 2\langle \dot{x}, K^{-1}\dot{x}\rangle + \big(4W_4(x)+3W_3(x)+2W_2(x)+W_1(x)\big) + W_3(x)+2W_2(x)+3W_1(x),\\
&= 2\langle \dot{x}, K^{-1}\dot{x}\rangle + 4W(x),
\end{aligned}
$$

which is an integral of motion $4H(x,\dot{x})$, see (25).

Example. We take $d=1$, $K=1$, and set

$$W(x) = \tfrac{1}{4}a_4x^4 + \tfrac{1}{3}a_3x^3 + \tfrac{1}{2}a_2x^2 + a_1x. \tag{33}$$

Thus, equations of motion (24) read

$$\ddot{x} = -a_4x^3 - a_3x^2 - a_2x - a_1, \tag{34}$$

while their polarization discretization reads

$$
\begin{aligned}
(x_{n+1}-2x_n+x_{n-1})/\epsilon^2 &= -a_4x_{n-1}x_nx_{n+1} - \tfrac{1}{3}a_3(x_{n-1}x_n + x_{n-1}x_{n+1} + x_nx_{n+1})\\
&\quad -\tfrac{1}{3}a_2(x_{n-1}+x_n+x_{n+1}) - a_1. \qquad (35)
\end{aligned}
$$

The following is a conserved quantity for the map $(x_{n-1},x_n)\mapsto(x_n,x_{n+1})$:

$$
\begin{aligned}
H_\epsilon(x_{n-1},x_n,x_{n+1}) &= \tfrac{1}{\epsilon^2}\big(x_{n-1}x_n - 2x_{n-1}x_{n+1} + x_nx_{n+1}\big)\\
&\quad + \tfrac{1}{3}a_3x_{n-1}x_nx_{n+1} + \tfrac{1}{3}a_2(x_{n-1}x_n + x_{n-1}x_{n+1} + x_nx_{n+1}) + a_1(x_{n-1}+x_n+x_{n+1}). \qquad (36)
\end{aligned}
$$

Upon expressing x_{n+1} through (x_{n-1},x_n) by virtue of equation (35), this coincides with the integral found in [4].

4 Conclusion

It is hoped that the algebraic approach to derivation of integrals of motion for the discrete time versions of Hamiltonian systems obtained by polarization will further stimulate the development of this fascinating area, towards an ultimate understanding of all the miraculous results discovered up to this day and yet to be discovered.

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