FUNCTIONAL EQUIVARIANCE AND MODIFIED VECTOR FIELDS

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Abstract. This paper examines functional equivariance, recently introduced by McLachlan and Stern [Found. Comput. Math. (2022)], from the perspective of backward error analysis. We characterize the evolution of certain classes of observables (especially affine and quadratic) by structure-preserving numerical integrators in terms of their modified vector fields. Several results on invariant preservation and symplecticity of modified vector fields are thereby generalized to describe the numerical evolution of non-invariant observables.

1. Introduction

Functional equivariance, recently introduced by McLachlan and Stern [13], is a structure-preserving property of numerical integrators describing the evolution of certain observables. Given $\dot{y} = f(y)$, the chain rule implies that a C^1 observable $z = F(y)$ evolves according to $\dot{z} = F'(y)f(y)$. A numerical integrator is said to be *F-functionally equivariant* if, when the integrator is applied to $\dot{y} = f(y)$ for any f, the numerical evolution of $\bigl(y, F(y)\bigr)$ is identical to that obtained by numerically integrating the augmented system

$$\dot{y} = f(y), \qquad \dot{z} = F'(y)f(y).$$

If Φ is a one-step numerical integrator, Φ_f is its application to the vector field f, and Φ_g is its application to the augmented vector field $g(y,z) = \bigl(f(y), F'(y)f(y)\bigr)$, then this is the statement that the following diagram commutes:

$$\begin{array}{ccc} y_0 & \overset{\Phi_f}{\longmapsto} & y_1 \\ {\scriptstyle (\mathrm{id},F)}\big\downarrow & & \big\downarrow{\scriptstyle (\mathrm{id},F)} \\ (y_0, z_0) & \overset{\Phi_g}{\longmapsto} & (y_1, z_1) \end{array} .$$

A well-studied special case is when $F'(y)f(y) = 0$ and Φ preserves the invariance of $F(y)$ whenever F is, e.g., affine or quadratic; see Hairer, Lubich, and Wanner [9, Chapter IV] for a survey of such results. However, there are many important cases discussed in [13] where one may wish to preserve the evolution of *non-invariant* observables, e.g., local conservation laws in numerical PDEs.

In this paper, we examine functional equivariance from the perspective of *modified vector fields*, which form the foundation for backward error analysis of numerical integrators; cf. [9, Chapter IX] and references therein. From this point of view, a numerical trajectory of $\dot{y} = f(y)$ is formally viewed as a solution to a modified equation $\dot{\widetilde{y}} = \widetilde{f}(\widetilde{y})$, so the numerical evolution of the observable $\widetilde{z} = F(\widetilde{y})$ is given by $\dot{\widetilde{z}} = F'(\widetilde{y})\widetilde{f}(\widetilde{y})$. Therefore, F-functional equivariance corresponds to the condition

$$\widetilde{g}\bigl(\widetilde{y}, F(\widetilde{y})\bigr) = \bigl(\widetilde{f}(\widetilde{y}), F'(\widetilde{y})\widetilde{f}(\widetilde{y})\bigr), \tag{1}$$

where $\widetilde{g}$ is the modified vector field of the augmented vector field g given previously. As we will see, this approach generalizes several well-known results relating invariant-preserving integrators to modified vector fields, corresponding to the special case where $F'(y)f(y) = 0$ implies $F'(\widetilde{y})\widetilde{f}(\widetilde{y}) = 0$.

The paper is organized as follows:

- Section 2 develops a theory of functional equivariance for *integrator maps* $\phi\colon f \mapsto \widetilde{f}$, which take vector fields to modified vector fields, as in Munthe-Kaas and Verdier [14] and

McLachlan, Modin, Munthe-Kaas, and Verdier [11]. This section proves integrator-map versions of the key results in [13, Section 2].

- Section 3 considers modified vector fields of one-step integrators Φ. In this setting, $\widetilde{f}$ is a formal power series in the step size, and its finite truncations are integrator maps in the sense of the previous section. For F-functionally equivariant integrators, in the sense of [13], we show that the condition (1) holds term-by-term. Considering truncations therefore links the results in [13] to those in Section 2 of the present paper.
- Finally, Section 4 discusses the generalization of the results in the preceding sections to additive and partitioned integrator maps and integrators, including additive/partitioned Runge–Kutta methods and splitting/composition methods.

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2. Functional equivariance of integrator maps

2.1. **Integrator maps and affine equivariance.** Let $f \in \mathfrak{X}(Y)$ be a smooth vector field on a Banach space Y, and denote its time-h flow by $\exp hf \colon Y \to Y$. A one-step numerical integrator Φ approximates this flow by $\Phi_{hf} \colon Y \to Y$. In backward error analysis, one views this as the flow of a modified vector field $\widetilde{f}$, for which $\Phi_{hf} = \exp h\widetilde{f}$. However, $\widetilde{f}$ is typically a formal power series in h, which must be interpreted as a (possibly divergent) asymptotic expansion rather than a genuine vector field (Hairer, Lubich, and Wanner [9, Chapter IX]).

To sidestep these technicalities, at least until Section 3, we begin by following Munthe-Kaas and Verdier [14] and McLachlan, Modin, Munthe-Kaas, and Verdier [11] in first considering *integrator maps*, whose modified vector fields are genuine vector fields.

Definition 2.1. An *integrator map* ϕ is a collection of smooth maps $\phi_Y \colon \mathfrak{X}(Y) \to \mathfrak{X}(Y)$, for each Banach space Y. For $f \in \mathfrak{X}(Y)$, we will typically write $\phi(f)$ to mean the same thing as $\phi_Y(f)$, which we call the *modified vector field* of f with respect to ϕ. When ϕ is fixed, we will often denote the modified vector field simply by $\widetilde{f}$.

Remark 2.2. We allow for infinite-dimensional Banach spaces, which are used in some of the PDE applications discussed in McLachlan and Stern [13]. This is in contrast with [14, 11], who consider only vector fields on $\mathbb{R}^n$ for $n \in \mathbb{N}$. We are interested primarily in the *algebraic* properties of these methods, and we do not attempt to address the tricky *analytical* issues that may arise when considering backward error analysis of integrators on arbitrary Banach spaces.

Fox example, any ϕ defined by a finite B-series (e.g., a finite truncation of the B-series for the modified vector field of a Runge–Kutta method) gives an integrator map in the sense of the definition above. Note that infinite B-series may diverge for certain f, even on $\mathbb{R}^n$.

The integrator maps considered in this section will also be *affine equivariant* in the sense of [11]. By the main result of that paper, this means that they are B-series maps. However, we will usually not use the equivalent characterization of these maps in terms of trees and elementary differentials, instead relying primarily on the affine equivariance property in the results to follow.

Definition 2.3. Given a Gâteaux differentiable map $\chi \colon Y \to U$, a pair of vector fields $f \in \mathfrak{X}(Y)$ and $g \in \mathfrak{X}(U)$ is *χ-related* if $\chi'(y) f(y) = g\bigl(\chi(y)\bigr)$ for all $y \in Y$, and we write $f \sim_\chi g$. In particular, if $A \colon Y \to U$ is affine, then $f \sim_A g$ whenever $A' \circ f = g \circ A$. An integrator map ϕ is *affine equivariant* if $f \sim_A g$ implies $\phi(f) \sim_A \phi(g)$ for all affine maps A between Banach spaces.

2.2. **Functional equivariance.** We next define functional equivariance for integrator maps.

Definition 2.4. Given a Gâteaux differentiable map $F \colon Y \to Z$ and $f \in \mathfrak{X}(Y)$, define the *augmented vector field* $g \in \mathfrak{X}(Y \times Z)$ by $g(y, z) = \bigl(f(y), F'(y) f(y)\bigr)$. An integrator map ϕ is *F-functionally* *equivariant* if $\phi(f) \sim_{(\mathrm{id},F)} \phi(g)$ for all f, which is precisely the condition (1). Given a class of maps $\mathcal{F}$, we say that ϕ is *$\mathcal{F}$-functionally equivariant* if it is F-functionally equivariant for all $F \in \mathcal{F}(Y,Z)$ and all Banach spaces Y and Z.

Let us now restrict our attention to affine equivariant integrator maps. We first show that affine equivariance allows us to characterize $\widetilde{g}(\widetilde{y},\widetilde{z})$ for all $\widetilde{z} \in Z$, not just $\widetilde{z} = F(\widetilde{y})$. This gives a stronger notion of what it means for an affine equivariant integrator map to be F-functionally equivariant: *If g is the augmented vector field of f, then $\widetilde{g}$ is the augmented vector field of $\widetilde{f}$.*

Proposition 2.5. *If ϕ is affine equivariant, then $\widetilde{g}(\widetilde{y},\widetilde{z}) = \widetilde{g}\big(\widetilde{y},F(\widetilde{y})\big)$ for all $(\widetilde{y},\widetilde{z}) \in Y \times Z$. Consequently, the F-functional equivariance condition* (1) *holds if and only if $\widetilde{g}(\widetilde{y},\widetilde{z}) = \big(\widetilde{f}(\widetilde{y}), F'(\widetilde{y})\widetilde{f}(\widetilde{y})\big)$.*

Proof. Consider the affine map $A(y,z) = (y, z+c)$, where $c \in Z$ is a constant. Since g depends only on y, we have $g(y,z) = g(y,z+c)$, i.e., $g \sim_A g$. Affine equivariance therefore implies $\widetilde{g} \sim_A \widetilde{g}$, i.e., $\widetilde{g}(\widetilde{y},\widetilde{z}) = \widetilde{g}(\widetilde{y},\widetilde{z}+c)$. For any fixed $(\widetilde{y},\widetilde{z}) \in Y \times Z$, taking $c = F(\widetilde{y}) - \widetilde{z}$ completes the proof. □

We next consider the case where $\mathcal{F}(Y,Z)$ is the class of affine maps $Y \to Z$. Compare the following result with [13, Proposition 2.6].

Proposition 2.6. *Every affine equivariant integrator map is affine functionally equivariant.*

Proof. If $F\colon Y \to Z$ is affine, then so is $(\mathrm{id},F)\colon Y \to Y \times Z$. Since f and g in Definition 2.4 satisfy $f \sim_{(\mathrm{id},F)} g$, affine equivariance of ϕ implies $\phi(f) \sim_{(\mathrm{id},F)} \phi(g)$. □

We now characterize functional equivariance with respect to more general classes of maps $\mathcal{F}$, such as quadratic or higher-degree polynomial maps. Since the integrator maps under consideration are affine equivariant, we make the following natural set of assumptions on $\mathcal{F}$; cf. [13, Assumption 2.8].

Assumption 2.7. The class of maps $\mathcal{F}$ satisfies the following:
- $\mathcal{F}(Y,Y)$ contains the identity map for all Y;
- $\mathcal{F}(Y,Z)$ is a vector space for all Y and Z;
- $\mathcal{F}$ is invariant under composition with affine maps, in the following sense: If $A\colon Y \to U$ and $B\colon V \to Z$ are affine and $F \in \mathcal{F}(U,V)$, then $B \circ F \circ A \in \mathcal{F}(Y,Z)$.

The main result of this section will relate functional equivariance to the more well-studied notion of invariant preservation, which we now recall.

Definition 2.8. Given a Gâteaux differentiable map $F\colon Y \to Z$, an integrator map ϕ is *F-invariant preserving* if $F'f = 0$ implies $F'\phi(f) = 0$ for all f. We say that ϕ is *$\mathcal{F}$-invariant preserving*, for a class of maps $\mathcal{F}$, if ϕ is F-invariant preserving for all $F \in \mathcal{F}(Y,Z)$ and all Banach spaces Y and Z.

Although functional equivariance seems stronger than invariant preservation, since it accounts for both invariant and non-invariant observables F, the properties are in fact equivalent for affine equivariant integrator maps. Compare the following result with [13, Theorem 2.9].

Theorem 2.9. *Let $\mathcal{F}$ satisfy Assumption 2.7. An affine equivariant integrator map ϕ is $\mathcal{F}$-invariant preserving if and only if it is $\mathcal{F}$-functionally equivariant.*

Proof. ($\Rightarrow$) Suppose ϕ is $\mathcal{F}$-invariant preserving. If $F \in \mathcal{F}(Y,Z)$, Assumption 2.7 implies that $G(y,z) = F(y) - z$ is in $\mathcal{F}(Y \times Z, Z)$. Furthermore, G is an invariant of the augmented vector field g, since $G'(y,z)g(y,z) = F'(y)f(y) - F'(y)f(y) = 0$. Writing $\widetilde{g} = (\widetilde{g}_Y, \widetilde{g}_Z)$, the fact that ϕ is $\mathcal{F}$-invariant preserving implies

$$0 = G'(\widetilde{y},\widetilde{z})\widetilde{g}(\widetilde{y},\widetilde{z}) = F'(\widetilde{y})\widetilde{g}_Y(\widetilde{y},\widetilde{z}) - \widetilde{g}_Z(\widetilde{y},\widetilde{z}), \tag{2}$$

Now, letting $A(y,z) = y$ be linear projection onto the Y component, $g \sim_A f$ implies $\widetilde{g} \sim_A \widetilde{f}$ by affine equivariance. This says that $\widetilde{g}_Y(\widetilde{y},\widetilde{z}) = \widetilde{f}(\widetilde{y})$, so we conclude from (2) that $\widetilde{g}_Z(\widetilde{y},\widetilde{z}) = F'(\widetilde{y})\widetilde{f}(\widetilde{y})$. Hence, ϕ is $\mathcal{F}$-functionally equivariant.

($\Leftarrow$) Conversely, suppose ϕ is $\mathcal{F}$-functionally equivariant. If $F \in \mathcal{F}(Y,Z)$ is an invariant of $f \in \mathfrak{X}(Y)$, then the augmented vector field is $g(y,z) = \bigl(f(y), 0\bigr)$, and $\mathcal{F}$-functional equivariance implies $\widetilde{g}\bigl(\widetilde{y}, \widetilde{z}\bigr) = \bigl(\widetilde{f}(\widetilde{y}), F'(\widetilde{y})\widetilde{f}(\widetilde{y})\bigr)$ by Proposition 2.5. However, taking the linear projection $B(y,z) = z$ gives $g \sim_B 0$, so affine equivariance implies $\widetilde{g} \sim_B \widetilde{0} = 0$. (As in [11, Lemma 6.1], one proves $\widetilde{0} = 0$ by considering the affine map from the trivial Banach space to any point of Z.) Thus, $F'(\widetilde{y})\widetilde{f}(\widetilde{y}) = 0$, so ϕ is $\mathcal{F}$-invariant preserving. $\square$

Example 2.10. We illustrate functional equivariance for some simple B-series integrator maps, whose terms are elementary differentials corresponding to rooted trees.

(i) The integrator map $\bullet(f) = f$ is the identity, so it is trivially seen to be F-functionally equivariant with respect to all maps F.

(ii) Consider the integrator map $:(f) = f'f$. Applying this to the augmented vector field gives

$$\begin{aligned} :(g) &= \bigl(f'f, F'f'f + F''(f,f)\bigr) \\ &= \Bigl(:(f), F':(f) + F''\bigl(\bullet(f), \bullet(f)\bigr)\Bigr). \end{aligned}$$

If F is affine, then $F'' = 0$, so the last term vanishes and $:$ is F-functionally equivariant. However, if $F'' \neq 0$, then this generally does not hold. Thus, $:$ is affine functionally equivariant, as guaranteed by Proposition 2.6, but not quadratic functionally equivariant.

(iii) Consider the integrator map $\vdots(f) = f'f'f$, whose application to the augmented vector field is

$$\begin{aligned} \vdots(g) &= \bigl(f'f'f, F'f'f'f + F''(f'f, f)\bigr) \\ &= \Bigl(\vdots(f), F'\vdots(f) + F''\bigl(:(f), \bullet(f)\bigr)\Bigr). \end{aligned}$$

As in the previous example, $\vdots$ is affine functionally equivariant, since $F'' = 0$ for affine F, but not quadratic functionally equivariant.

(iv) Consider the integrator map $\vee(f) = f''(f,f)$, whose application to the augmented vector field is

$$\begin{aligned} \vee(g) &= \bigl(f''(f,f), F'f''(f,f) + 2F''(f'f,f) + F'''(f,f,f)\bigr) \\ &= \Bigl(\vee(f), F'\vee(f) + 2F''\bigl(:(f), \bullet(f)\bigr) + F'''\bigl(\bullet(f), \bullet(f), \bullet(f)\bigr)\Bigr) \end{aligned}$$

As in the last two examples, $\vee$ is affine functionally equivariant, since the F'' and F''' terms vanish, but not quadratic functionally equivariant.

(v) Finally, consider the integrator map $\phi(f) = f'f'f - \frac{1}{2}f''(f,f)$, i.e., $\phi = \vdots - \frac{1}{2}\vee$. Combining the calculations in the previous two examples, we get

$$\begin{aligned} \phi(g) &= \Bigl(f'f'f - \tfrac{1}{2}f''(f,f), F'\bigl(f'f'f - \tfrac{1}{2}f''(f,f)\bigr) - \tfrac{1}{2}F'''(f,f,f)\Bigr) \\ &= \Bigl(\phi(f), F'\phi(f) - \tfrac{1}{2}F'''\bigl(\bullet(f), \bullet(f), \bullet(f)\bigr)\Bigr), \end{aligned}$$

where subtraction causes the F'' terms to cancel. Thus, ϕ is quadratic functionally equivariant, since $F''' = 0$ for quadratic F, but not cubic functionally equivariant. Regarding the general impossibility of cubic functional equivariance for B-series methods (i.e., B-series other than the exact flow), see McLachlan and Stern [13, Corollary 2.10(c)], which uses results of Chartier and Murua [6] and Iserles, Quispel, and Tse [10] on cubic invariant preservation.

We remark that the modified vector field for the implicit midpoint method is given by a B-series

$$\bullet + \Bigl(\frac{1}{12}\vdots - \frac{1}{24}\vee\Bigr) + \cdots .$$

From (i) and (v), we see that the terms at each order are quadratic functionally equivariant integrator maps, corresponding to the fact that the implicit midpoint method is quadratic functionally equivariant. This is an example of a more general link between functional equivariance of integrators and their modified vector fields, which will be explored in Section 3.

2.3. **Closure under differentiation and observables involving variations.** We are often interested in the evolution of observables of the *variational equation*

$$\dot{y} = f(y), \qquad \dot{\eta} = f'(y)\eta, \tag{3}$$

where $\eta \in Y$ is called a *variation* of y. For example, the canonical symplectic two-form is a quadratic observable depending on two variations of y, and it is invariant whenever f is a canonical Hamiltonian vector field. In order to describe the numerical evolution of this and other observables depending on variations, we develop the notion of *closure under differentiation* for affine equivariant integrator maps. The idea of closure under differentiation and its connection with symplecticity, particularly for Runge–Kutta methods, was pioneered by Bochev and Scovel [3]. We adapt the approach of McLachlan and Stern [13, Section 2.3] for affine equivariant integrators.

Definition 2.11. Given $f \in \mathfrak{X}(Y)$, define $\delta f \in \mathfrak{X}(Y \times Y)$ by $\delta f(y,\eta) = \bigl(f(y), f'(y)\eta\bigr)$, corresponding to the variational system (3). An integrator map ϕ is *closed under differentiation* if $\phi(\delta f) = \delta\phi(f)$ for all f.

Remark 2.12. The vector field δf is called the *tangent lift* of f by Bochev and Scovel [3]; elsewhere, it is called the *complete lift* of f, cf. Yano and Kobayashi [15].

Compare the following result with [13, Theorem 2.12].

Theorem 2.13. *Affine equivariant integrator maps are closed under differentiation.*

Proof. Given $f \in \mathfrak{X}(Y)$, consider the system

$$\dot{x} = f(x), \qquad \dot{y} = f(y),$$

corresponding to the vector field $f \times f \in \mathfrak{X}(Y \times Y)$. Since $f \times f \sim_A f$, where A is either of the projections $(x,y) \mapsto x$ or $(x,y) \mapsto y$, affine equivariance of ϕ implies that $\phi(f \times f) \sim_A \phi(f)$ and thus $\phi(f \times f) = \phi(f) \times \phi(f)$. Now, taking $F(x,y) = (x-y)/\epsilon$ for $\epsilon > 0$ gives the augmented system

$$\dot{x} = f(x), \qquad \dot{y} = f(y), \qquad \dot{z} = \frac{f(x) - f(y)}{\epsilon}. \tag{4}$$

Since F is affine, Proposition 2.6 says that applying ϕ to this augmented system gives

$$\dot{\widetilde{x}} = \widetilde{f}(\widetilde{x}), \qquad \dot{\widetilde{y}} = \widetilde{f}(\widetilde{y}), \qquad \dot{\widetilde{z}} = \frac{\widetilde{f}(\widetilde{x}) - \widetilde{f}(\widetilde{y})}{\epsilon}, \tag{5}$$

which is the augmented system of $\phi(f \times f) = \phi(f) \times \phi(f)$. Now, letting $x = y + \epsilon\eta$ in (4) and taking $\epsilon \to 0$, the z-component converges to $f'(y)\eta$. Similarly, letting $\widetilde{x} = \widetilde{y} + \epsilon\widetilde{\eta}$ in (5) and taking $\epsilon \to 0$, the $\widetilde{z}$-component converges to $\widetilde{f}'(\widetilde{y})\widetilde{\eta}$. Since ϕ is smooth and maps (4) to (5) for all ϵ, we conclude that $\phi(\delta f) = \delta\phi(f)$, which completes the proof. □

We immediately obtain the following corollary for observables of the variational equation; compare [13, Corollary 2.13].

Corollary 2.14. *Let $f \in \mathfrak{X}(Y)$ and $F \colon Y \times Y \to Z$, and suppose ϕ is affine equivariant and F-functionally equivariant. If $g \in \mathfrak{X}(Y \times Y \times Z)$ is the augmented vector field of δf,*

$$g(y,\eta,z) = \Bigl(f(y), f'(y)\eta, F'(y,\eta)\bigl(f(y), f'(y)\eta\bigr)\Bigr),$$

then $\widetilde{g}$ is the augmented vector field of $\delta\widetilde{f}$,

$$\widetilde{g}(\widetilde{y},\widetilde{\eta},\widetilde{z}) = \Bigl(\widetilde{f}(\widetilde{y}), \widetilde{f}'(\widetilde{y})\widetilde{\eta}, F'(\widetilde{y},\widetilde{\eta})\bigl(\widetilde{f}(\widetilde{y}), \widetilde{f}'(\widetilde{y})\widetilde{\eta}\bigr)\Bigr).$$

That is, $\phi\big((\delta f, F'\delta f)\big) = \big(\delta\phi(f), F'\delta\phi(f)\big)$.

Proof. We have $\phi\big((\delta f, F'\delta f)\big) = \big(\phi(\delta f), F'\phi(\delta f)\big) = \big(\delta\phi(f), F'\delta\phi(f)\big)$, where the first equality holds by F-functional equivariance and the second equality holds by closure under differentiation. □

We can easily extend Corollary 2.14 to observables depending on two or more variations. For instance, if ξ and η are each variations of y, then $(y, \xi, \eta) \in Y \times Y \times Y$ satisfies

$$\dot{y} = f(y), \qquad \dot{\xi} = f'(y)\xi, \qquad \dot{\eta} = f'(y)\eta. \tag{6}$$

This is A-related to δf, where A is either of the projections $(y, \xi, \eta) \mapsto (y, \xi)$ or $(y, \xi, \eta) \mapsto (y, \eta)$, so affine equivariance of ϕ implies that we have

$$\dot{\widetilde{y}} = \widetilde{f}(\widetilde{y}), \qquad \dot{\widetilde{\xi}} = \widetilde{f}'(\widetilde{y})\widetilde{\xi}, \qquad \dot{\widetilde{\eta}} = \widetilde{f}'(\widetilde{y})\widetilde{\eta}. \tag{7}$$

If ϕ is F-functionally equivariant for some $F\colon Y \times Y \times Y \to Z$, we may then conclude that it maps the augmented vector field of (6) to that of (7).

A particularly important instance of this, which generalizes the result that quadratic invariant preserving B-series are symplectic, is worked out in the following example.

Example 2.15. If $F(y, \xi, \eta) = \omega(\xi, \eta)$, where $\omega\colon Y \times Y \to Z$ is a continuous bilinear map, then we augment (6) by the equation $\dot{z} = (L_f\omega)_y(\xi, \eta)$. Here, $(L_f\omega)_y$ is the Lie derivative of ω along f at y. Hence, the augmented vector field is

$$g(y, \xi, \eta, z) = \big(f(y), f'(y)\xi, f'(y)\eta, (L_f\omega)_y(\xi, \eta)\big).$$

If ϕ is quadratic functionally equivariant, then it follows that $\widetilde{g}$ is the augmented vector field of (7),

$$\widetilde{g}(\widetilde{y}, \widetilde{\xi}, \widetilde{\eta}, \widetilde{z}) = \big(\widetilde{f}(\widetilde{y}), \widetilde{f}'(\widetilde{y})\widetilde{\xi}, \widetilde{f}'(\widetilde{y})\widetilde{\eta}, (L_{\widetilde{f}}\omega)_{\widetilde{y}}(\widetilde{\xi}, \widetilde{\eta})\big).$$

In particular, if $L_f\omega = 0$, then Theorem 2.9 implies that $L_{\widetilde{f}}\omega = 0$ as well. As a special case, if (Y, ω) is a symplectic vector space and f is a symplectic vector field, then $\widetilde{f}$ is also symplectic.

2.4. **Quadratic functionally equivariant B-series.** McLachlan et al. [11] proved that affine equivariant integrator maps are precisely those that can be represented by a B-series. Let T denote the set of rooted trees. As in Example 2.10, we identify each $\tau \in T$ with the integrator map taking f to its corresponding elementary differential: $\bullet(f) = f$, $[\bullet](f) = f'f$, $[[\bullet]](f) = f'f'f$, $[\bullet,\bullet](f) = f''(f, f)$, etc. We can thus express any affine equivariant integrator map as a B-series

$$\phi = \sum_{\tau \in T} \frac{b(\tau)}{\sigma(\tau)} \tau,$$

where $\sigma(\tau)$ is the symmetry coefficient of τ. This section will assume that the reader is familiar with B-series, and we refer to Hairer et al. [9] and Butcher [4] for a comprehensive treatment.

Hairer et al. [9, Theorem IX.9.3] prove that the truncated modified vector field of a B-series integrator is symplectic, and thus also quadratic invariant preserving, if and only if

$$b(u \circ v) + b(v \circ u) = 0, \quad \forall u, v \in T, \tag{8}$$

where $\circ$ is the Butcher product on rooted trees. Example 2.10(v), which has $b([[\bullet]]) = 1$ and $b([\bullet,\bullet]) = -1$, can be seen to satisfy this condition condition, since $\bullet \circ [\bullet] = [[\bullet]]$ and $[\bullet] \circ \bullet = [\bullet,\bullet]$. The proof given in [9, Theorem IX.9.3] makes use of the symplecticity criterion of Calvo and Sanz-Serna [5] for B-series integrators in terms of their coefficients $a(\tau)$, along with a recursion formula relating these to the $b(\tau)$ coefficients of the modified vector field. We remark that preservation of quadratic invariants by Runge–Kutta methods was first characterized by Cooper [7].

Here, we give a new, direct proof of the criterion (8) for quadratic functional equivariance of integrator maps. Our task is simplified substantially by the fact that quadratic functional equivariance describes the evolution of observables for *arbitrary* vector fields f, not just Hamiltonian vector fields or those preserving a particular invariant.

Theorem 2.16. *A B-series integrator map is quadratic functionally equivariant if and only if its coefficients satisfy* $b(u \circ v) + b(v \circ u) = 0$ *for all* $u, v \in T$.

Proof. We write each rooted tree as $\tau = [\tau_1, \ldots, \tau_m]$, denoting that the root of τ has m children, which are the roots of subtrees $\tau_1, \ldots, \tau_m$. Let $F \colon Y \to Z$ be quadratic, meaning that $F''' = 0$. Applying τ to $g = (f, F'f)$ and using the Leibniz rule to differentiate the product $F'f$ gives

$$\tau(g) = \biggl(\tau(f), F'\tau(f) + \sum_{i=1}^{m} F''\bigl([\tau_1, \ldots, \widehat{\tau}_i, \ldots, \tau_m](f), \tau_i(f) \bigr) \biggr),$$

where $\widehat{\tau}_i$ denotes that the subtree τ_i is omitted. Letting $u = [\tau_1, \ldots, \widehat{\tau}_i, \ldots, \tau_m]$ and $v = \tau_i$, we see that each term in the sum above can be rewritten as $F''\bigl(u(f), v(f)\bigr)$ with $u \circ v = \tau$. However, this term can appear more than once if $v = \tau_i$ for multiple values of i. Recall that the symmetry coefficient $\sigma(\tau)$ is defined recursively by

$$\sigma(\tau) = \sigma(\tau_1) \cdots \sigma(\tau_m) \mu_1! \cdots \mu_k!,$$

where $\mu_1, \ldots, \mu_k$ count the number of occurrences of each unique tree in the list $\tau_1, \ldots, \tau_m$, $k \leq m$. If μ_j is the number of times τ_i appears in τ, then

$$\sigma(u) = \sigma(\tau_1) \cdots \widehat{\sigma(\tau_i)} \cdots \sigma(\tau_m) \mu_1! \cdots (\mu_j - 1)! \cdots \mu_k!,$$

and since $v = \tau_i$, it follows that

$$\mu_j = \frac{\sigma(u \circ v)}{\sigma(u)\sigma(v)}.$$

This is precisely the number of times $F''\bigl(u(f), v(f)\bigr)$ appears in the sum, which we now rewrite as

$$\sum_{i=1}^{m} F''\bigl([\tau_1, \ldots, \widehat{\tau}_i, \ldots, \tau_m](f), \tau_i(f) \bigr) = \sum_{u \circ v = \tau} \frac{\sigma(u \circ v)}{\sigma(u)\sigma(v)} F''\bigl(u(f), v(f)\bigr).$$

Thus, summing the terms of the B-series and rewriting $\sum_{\tau \in T} \sum_{u \circ v = \tau}$ as a sum over $u, v \in T$, we get

$$\phi(g) = \biggl(\phi(f), F'\phi(f) + \sum_{u, v \in T} \frac{b(u \circ v)}{\sigma(u)\sigma(v)} F''\bigl(u(f), v(f)\bigr) \biggr).$$

Now, ϕ is quadratic functionally equivariant if and only if the extra terms in this sum cancel for all f and F. We have $F''\bigl(u(f), v(f)\bigr) = F''\bigl(v(f), u(f)\bigr)$, by symmetry of the Hessian, but no other relations among the terms in general. (See below for further discussion of this claim.) Hence, these extra terms cancel generically if and only if $b(u \circ v) + b(v \circ u) = 0$ for all $u, v \in T$. □

The "only if" conclusion depends on the fact that, for all $u, v \in T$, one may construct f and F such that $F''\bigl(u(f), v(f)\bigr) = F''\bigl(v(f), u(f)\bigr)$ are the only nonvanishing Hessian terms at some point. When F corresponds to the canonical symplectic form, Calvo and Sanz-Serna [5, Lemma 5.1] construct a Hamiltonian vector field f that has this property. (See also Hairer et al. [9, Theorem VI.7.4], which gives a similar construction that works for both B-series and P-series.) We give a self-contained proof in Appendix A, where the construction of f and F is simplified by the fact that we are not constrained to the symplectic setting.

3. Modified vector fields of functionally equivariant integrators

3.1. **Modified vector fields and relatedness.** We now consider the case where we are given a numerical integrator Φ rather than an integrator map. As in Hairer et al. [9, Chapter IX], we suppose that Φ_{hf} may be expanded as a formal power series in h,

$$\Phi_{hf} = \mathrm{id} + hf + h^2 d_2 + h^3 d_3 + \cdots .$$

We then seek a modified vector field $\widetilde{f}$, also expressed as a formal power series,

$$\widetilde{f} = f + hf_2 + h^2 f_3 + \cdots ,$$

such that $\Phi_{hf} = \exp h\widetilde{f}$, in the sense that the power series match term-by-term. Matching these terms yields a recurrence for f_j in terms of the given d_j [9, Equation IX.1.4].

We begin by extending the notion of χ-relatedness to modified vector fields, then prove a general result linking this to properties of the integrator Φ. This result will be instrumental in characterizing the modified vector fields of affine equivariant and functionally equivariant integrators.

Definition 3.1. Let $\widetilde{f} = f + hf_2 + h^2 f_3 + \cdots$ and $\widetilde{g} = g + hg_2 + h^2 g_3 + \cdots$, where $f, f_2, f_3, \ldots \in \mathfrak{X}(Y)$ and $g, g_2, g_3, \ldots \in \mathfrak{X}(U)$. Given $\chi \colon Y \to U$, define $\widetilde{f} \sim_\chi \widetilde{g}$ to mean that $f \sim_\chi g$ and $f_j \sim_\chi g_j$ for all $j = 2, 3, \ldots$, i.e., $\widetilde{f}$ and $\widetilde{g}$ are term-by-term χ-related.

Theorem 3.2. *Given an integrator Φ, let $\widetilde{f}$ and $\widetilde{g}$ be the modified vector fields of f and g, respectively. If $\chi \circ \Phi_{hf} = \Phi_{hg} \circ \chi$ for all sufficiently small h, then $\widetilde{f} \sim_\chi \widetilde{g}$. Furthermore, if $\chi \circ \Phi_{hf}$ and $\Phi_{hg} \circ \chi$ are both real analytic in h at $h = 0$, then the converse holds.*

Proof. If $\widetilde{f}$ and $\widetilde{g}$ are actual vector fields, then $\chi \circ \exp h\widetilde{f} = \exp h\widetilde{g} \circ \chi$ for all h if and only if $\widetilde{f} \sim_\chi \widetilde{g}$. This is a standard result on vector fields and flows, cf. Abraham, Marsden, and Ratiu [1, Proposition 4.2.4]. To extend this to the case where $\widetilde{f}$ and $\widetilde{g}$ are formal power series in h, we use an induction argument on the truncations, which are actual vector fields.

First, observe that

$$\begin{aligned} \chi \circ \Phi_{hf}(y) &= \chi \circ \bigl[\mathrm{id} + hf + \mathcal{O}(h^2)\bigr](y) = \chi(y) + h\chi'(y)f(y) + \mathcal{O}(h^2),\\ \Phi_{hg} \circ \chi(y) &= \bigl[\mathrm{id} + hg + \mathcal{O}(h^2)\bigr] \circ \chi(y) = \chi(y) + hg\bigl(\chi(y)\bigr) + \mathcal{O}(h^2), \end{aligned}$$

where we have linearized χ about y on the first line. Matching terms implies $f \sim_\chi g$, which establishes the base case. For the induction step, suppose that $f \sim_\chi g, \ldots, f_{j-1} \sim_\chi g_{j-1}$. Then

$$\begin{aligned} \chi \circ \Phi_{hf}(y) &= \chi \circ \bigl[\exp(hf + \cdots + h^j f_j) + \mathcal{O}(h^{j+1})\bigr](y)\\ &= \chi \circ \bigl[\exp(hf + \cdots + h^{j-1} f_{j-1}) + h^j f_j + \mathcal{O}(h^{j+1})\bigr](y)\\ &= \chi \circ \exp(hf + \cdots + h^{j-1} f_{j-1})(y) + h^j \chi'(y) f_j(y) + \mathcal{O}(h^{j+1}). \end{aligned} \tag{9}$$

Here, the second line uses the fact that all higher-order exponential terms involving $h^j f_j$ are $\mathcal{O}(h^{j+1})$, and the third line linearizes χ about $\exp(hf + \cdots + h^{j-1} f_{j-1})(y)$. Similarly,

$$\begin{aligned} \Phi_{hg} \circ \chi(y) &= \bigl[\exp(hg + \cdots + h^j g_j) + \mathcal{O}(h^{j+1})\bigr] \circ \chi(y)\\ &= \bigl[\exp(hg + \cdots + h^{j-1} g_{j-1}) + h^j g_j + \mathcal{O}(h^{j+1})\bigr] \circ \chi(y)\\ &= \exp(hg + \cdots + h^{j-1} g_{j-1}) \circ \chi(y) + h^j g_j\bigl(\chi(y)\bigr) + \mathcal{O}(h^{j+1}). \end{aligned} \tag{10}$$

By the inductive assumption, $hf + \cdots + h^{j-1} f_{j-1} \sim_\chi hg + \cdots + h^{j-1} g_{j-1}$, i.e., the truncations are χ-related. Therefore, applying [1, Proposition 4.2.4], we have

$$\chi \circ \exp(hf + \cdots + h^{j-1} f_{j-1}) = \exp(hg + \cdots + h^{j-1} g_{j-1}) \circ \chi.$$

Hence, if (9) and (10) are equal, then we may cancel the first term of each to conclude $f_j \sim_\chi g_j$.

Conversely, the analyticity assumption allows us to conclude the equality of $\chi \circ \Phi_{hf}(y)$ and $\Phi_{hg} \circ \chi(y)$ for sufficiently small h from the equality of their power series. □

Remark 3.3. This can be seen as a generalization of Theorems IX.5.1 and IX.5.2 in Hairer et al. [9], which cover the case where χ is a parametrization of a manifold.

3.2. **Affine equivariant integrators.** The terms d_j and f_j in the power series for Φ_{hf} and $\widetilde{f}$, respectively, depend on f but not on h. Hence, they may be seen as arising from integrator maps $\delta_j(f) = d_j$ and $\phi_j(f) = f_j$. Moreover, each of these is homogeneous of degree j, meaning that $\delta_j(hf) = h^j d_j$ and $\phi_j(hf) = h^j f_j$.

We now discuss the relationship between affine equivariance of the integrator Φ and that of the integrator maps δ_j and ϕ_j.

Definition 3.4. An integrator Φ is *affine equivariant* if $f \sim_A g$ implies $A \circ \Phi_f = \Phi_g \circ A$ whenever A is an affine map.

Corollary 3.5. *If the integrator Φ is affine equivariant, then so are the integrator maps ϕ_j. The converse is true if Φ_{hf} is real analytic in h at $h = 0$ for all f.*

Proof. Apply Theorem 3.2, where $\chi = A$ is any affine map. □

An analogous result is true for the δ_j. One way to see this would be to apply the main result of McLachlan et al. [11] to conclude that $\widetilde{f}$ is a B-series in f, then use the fact that the exponential of a B-series is also a B-series. However, the following self-contained, tree-free proof uses only the basic properties of affine equivariance.

Proposition 3.6. *If the integrator Φ is affine equivariant, then so are the integrator maps δ_j. The converse is true if Φ_{hf} is real analytic in h at $h = 0$ for all f.*

Proof. Let $f \sim_A g$ for some affine map A. Since A is affine, we have $A \circ \Phi_{hf} - A = A' \circ (\Phi_{hf} - \mathrm{id})$, and therefore

$$A \circ \Phi_{hf} = A + h(A' \circ f) + h^2(A' \circ d_2) + h^3(A' \circ d_3) + \cdots .$$

Next, writing $\delta_j(g) = e_j$, we have

$$\Phi_{hg} \circ A = A + h(g \circ A) \ + h^2(e_2 \circ A) \ + h^3(e_3 \circ A) \ + \cdots .$$

Thus, if $A \circ \Phi_{hf} = \Phi_{hg} \circ A$, then the power series agree term-by-term, which means that $d_j \sim_A e_j$. Conversely, assuming analyticity, equality of the power series implies equality of the maps. □

Remark 3.7. The forward direction is essentially a version of the "transfer argument" in [11, Proposition 6.2]. Since Φ is an affine equivariant *integrator*, $\Phi - \mathrm{id}$ is an affine equivariant *integrator map*. Thus, the terms δ_j in the Taylor series of $\Phi - \mathrm{id}$ at 0 are also affine equivariant integrator maps.

3.3. **Functionally equivariant integrators.** We now consider the relationship between functional equivariance of integrators, in the sense of McLachlan and Stern [13], and that of the integrator maps ϕ_j constituting the terms of the modified vector field. We first recall the definition from [13] stated in the introduction.

Definition 3.8. Given a Gâteaux differentiable map $F\colon Y \to Z$, a numerical integrator Φ is *F-functionally equivariant* if $(\mathrm{id}, F) \circ \Phi_f = \Phi_g \circ (\mathrm{id}, F)$ for all $f \in \mathfrak{X}(Y)$, where $g \in \mathfrak{X}(Y \times Z)$ is the augmented vector field of f. Given a class of maps $\mathcal{F}$, the integrator is *$\mathcal{F}$-functionally equivariant* if this holds for all $F \in \mathcal{F}(Y, Z)$ and all Banach spaces Y and Z.

Corollary 3.9. *If the integrator Φ is F-functionally equivariant, then so are the integrator maps ϕ_j. The converse is true if F is real analytic and if Φ_{hf} is real analytic in h at $h = 0$ for all f.*

Proof. Apply Theorem 3.2, where $\chi = (\mathrm{id}, F)$. □

Remark 3.10. Unlike many of the results in Section 2, this corollary does not require the additional assumption of affine equivariance. However, if we *do* have affine equivariance, then combining Corollaries 3.5 and 3.9 links the results of Section 2 for affine equivariant integrator maps to the corresponding results of McLachlan and Stern [13] for affine equivariant integrators.

Remark 3.11. Except in the case where F is affine, we generally do *not* have a version of Proposition 3.6, in either direction, for F-functional equivariance of the integrator maps δ_j. For example, the implicit midpoint method $\Phi = \mathrm{id} + \bullet + \frac{1}{2}\overset{\bullet}{\bullet} + \cdots$ is a quadratic functionally equivariant integrator, but $\delta_2 = \frac{1}{2}\overset{\bullet}{\bullet}$ is not a quadratic functionally equivariant integrator map, as shown in Example 2.10(iii). On the other hand, Euler's method $\Phi = \mathrm{id} + \bullet$ has $\delta_j = 0$ for all $j = 2, 3, \ldots$, and trivially $0 \sim_{(\mathrm{id},F)} 0$ for any F whatsoever, but Euler's method is not quadratic functionally equivariant.

4. Generalization to additive and partitioned methods

The integrator maps and integrators discussed in the preceding sections include Runge–Kutta and B-series methods, but not additive methods (such as additive Runge–Kutta and NB-series methods [2] and splitting/composition methods [12]) or partitioned methods (such as partitioned Runge–Kutta methods and P-series methods [8]). In this section, we briefly discuss the extension of the foregoing theory to these two classes of methods. For each class, we modify the notion of integrator map and functional equivariance, similarly to how this was done for integrators in McLachlan and Stern [13, Section 5].

4.1. Additive methods.

An additive method is applied to a vector field $f \in \mathfrak{X}(Y)$ after it has been decomposed into a sum $f = f^{[1]} + \cdots + f^{[N]}$, and different decompositions of the same f may yield different numerical trajectories.

Definition 4.1. An *additive integrator map* is a collection of smooth maps

$$\phi_Y \colon \underbrace{\mathfrak{X}(Y) \times \cdots \times \mathfrak{X}(Y)}_{N} \to \mathfrak{X}(Y)$$

for each Banach space Y, where $N \in \mathbb{N}$ is the same for all Y. We denote the application of ϕ to $f = f^{[1]} + \cdots + f^{[N]} \in \mathfrak{X}(Y)$ by $\widetilde{f} = \phi(f^{[1]}, \ldots, f^{[N]})$, where it is understood that $\widetilde{f}$ depends on the decomposition and not just on f itself.

The following definitions extend the notions of affine equivariance and functional equivariance to additive integrator maps.

Definition 4.2. An additive integrator map ϕ is N*-affine equivariant* if, for all affine maps A, we have $\phi(f^{[1]}, \ldots, f^{[N]}) \sim_A \phi(g^{[1]}, \ldots, g^{[N]})$ whenever $f^{[\nu]} \sim_A g^{[\nu]}$ for all $\nu = 1, \ldots, N$.

Definition 4.3. Given a Gâteaux differentiable map $F \colon Y \to Z$ and $f^{[1]}, \ldots, f^{[N]} \in \mathfrak{X}(Y)$, let $g^{[\nu]}(y, z) = \bigl(f^{[\nu]}(y), F'(y) f^{[\nu]}(y)\bigr) \in \mathfrak{X}(Y \times Z)$ be the augmented vector field of $f^{[\nu]}$ for $\nu = 1, \ldots, N$. An additive integrator map ϕ is F*-functionally equivariant* if $\phi(f^{[1]}, \ldots, f^{[N]}) \sim_{(\mathrm{id},F)} \phi(g^{[1]}, \ldots, g^{[N]})$ for all $f^{[1]}, \ldots, f^{[N]} \in \mathfrak{X}(Y)$, and $\mathcal{F}$*-functionally equivariant* if this holds for all $F \in \mathcal{F}(Y, Z)$ and all Banach spaces Y and Z.

We next prove a version of Proposition 2.5, which strengthens the notion of functional equivariance for N-affine equivariant methods.

Proposition 4.4. *If ϕ is N-affine equivariant, then $\widetilde{g}(\widetilde{y}, \widetilde{z}) = \widetilde{g}\bigl(\widetilde{y}, F(\widetilde{y})\bigr)$ for all $(\widetilde{y}, \widetilde{z}) \in Y \times Z$. Consequently, the F-functional equivariance condition* (1) *holds if and only if $\widetilde{g}(\widetilde{y}, \widetilde{z}) = \bigl(\widetilde{f}(\widetilde{y}), F'(\widetilde{y})\widetilde{f}(\widetilde{y})\bigr)$.*

Proof. The proof is essentially the same as that of Proposition 2.5. Consider the affine map $A(y, z) = (y, z + c)$, where $c \in Z$ is a constant. Since each $g^{[\nu]}$ depends only on y, we have $g^{[\nu]} \sim_A g^{[\nu]}$ for $\nu = 1, \ldots, N$. Thus, N-affine equivariance implies $\widetilde{g} \sim_A \widetilde{g}$, i.e., $\widetilde{g}(\widetilde{y}, \widetilde{z}) = \widetilde{g}(\widetilde{y}, \widetilde{z} + c)$, so taking $c = F(\widetilde{y}) - \widetilde{z}$ completes the proof. □

Compare the following with [13, Proposition 5.3].

Proposition 4.5. *Every N-affine equivariant integrator map is affine functionally equivariant.*

Proof. As in the proof of Proposition 2.6, if F is affine, then so is (id, F). Since $f^{[\nu]} \sim_{(\mathrm{id},F)} g^{[\nu]}$ for $\nu = 1, \ldots, N$, if ϕ is N-affine equivariant, then $\phi(f^{[1]}, \ldots, f^{[N]}) \sim_{(\mathrm{id},F)} \phi(g^{[1]}, \ldots, g^{[N]})$. □

Before proving an additive version of Theorem 2.9, we note an important distinction between ordinary and additive integrator maps. Affine equivariant integrator maps preserve affine invariants, since $f \sim_A 0$ implies $\phi(f) \sim_A \phi(0) = 0$. In contrast, it is possible for an additive integrator map to be N-affine equivariant but *not* preserve affine invariants of f, since $f \sim_A 0$ does not necessarily imply $f^{[\nu]} \sim_A 0$ for all $\nu = 1, \ldots, N$, unless A is also an invariant of each individual $f^{[\nu]}$. This is illustrated in the following examples.

Example 4.6. We consider affine invariant preservation of some simple NB-series with $N = 2$. These can be represented in terms of trees with black and white vertices, cf. Araújo, Murua, and Sanz-Serna [2].

(i) The integrator maps $\bullet(f^{[1]}, f^{[2]}) = f^{[1]}$ and $\circ(f^{[1]}, f^{[2]}) = f^{[2]}$ do not necessarily preserve affine invariants of f, since we may have $A'f = 0$ but $A'f^{[\nu]} \neq 0$ for $\nu = 1, 2$. However, the integrator map $(\bullet + \circ)(f^{[1]}, f^{[2]}) = f$ clearly does preserve affine invariants of f.

(ii) Similarly, $\genfrac{}{}{0pt}{}{\bullet}{\bullet}(f^{[1]}, f^{[2]}) = f^{[1]\prime} f^{[1]}$ and $\genfrac{}{}{0pt}{}{\bullet}{\circ}(f^{[1]}, f^{[2]}) = f^{[2]\prime} f^{[1]}$ do not necessarily preserve affine invariants of f. However, $(\genfrac{}{}{0pt}{}{\bullet}{\bullet} + \genfrac{}{}{0pt}{}{\bullet}{\circ})(f^{[1]}, f^{[2]}) = f' f^{[1]}$ does, since $A'f = 0$ implies that $A' f' f^{[1]} = (A'f)' f^{[1]} = 0$.

In general, the condition for NB-series to preserve affine invariants of f, for arbitrary decompositions, is that trees must have the same coefficients if they differ only in the color of their roots. Indeed, if $[\tau_1, \ldots, \tau_m]^{[\nu]}$ denotes the N-colored tree whose root has the color ν, and whose children are the roots of the subtrees $\tau_1, \ldots, \tau_m$, then these having equal coefficients allows us to collect the terms

$$\begin{aligned} A' \sum_{\nu=1}^{N} [\tau_1, \ldots, \tau_m]^{[\nu]}(f^{[1]}, \ldots, f^{[N]}) &= A' \sum_{\nu=1}^{N} (f^{[\nu]})^{(m)} \Bigl(\tau_1(f^{[1]}, \ldots, f^{[N]}), \ldots, \tau_m(f^{[1]}, \ldots, f^{[N]}) \Bigr) \\ &= (A'f)^{(m)} \Bigl(\tau_1(f^{[1]}, \ldots, f^{[N]}), \ldots, \tau_m(f^{[1]}, \ldots, f^{[N]}) \Bigr), \end{aligned}$$

which vanishes if $A'f = 0$.

Thus, the ($\Leftarrow$) direction of Theorem 2.9 does not hold for N-affine equivariant integrators, even when $\mathcal{F}$ is the class of affine maps, but it does hold if we require the the additional condition of affine invariant preservation. Compare the following with [13, Theorem 5.7].

Theorem 4.7. *Let $\mathcal{F}$ satisfy Assumption 2.7. An N-affine equivariant integrator map ϕ is $\mathcal{F}$-invariant preserving if and only if it is $\mathcal{F}$-functionally equivariant and affine invariant preserving.*

Proof. ($\Rightarrow$) Suppose ϕ is $\mathcal{F}$-invariant preserving. The proof of $\mathcal{F}$-functional equivariance is essentially the same as in Theorem 2.9. The only notable modification is that, at the step where $A(y, z) = y$ is the linear projection onto Y, we use $g^{[\nu]} \sim_A f^{[\nu]}$ for $\nu = 1, \ldots, N$ to conclude that $\widetilde{g} \sim_A \widetilde{f}$ by N-affine equivariance. Furthermore, affine invariant preservation follows from $\mathcal{F}$-invariant preservation, since Assumption 2.7 implies that $\mathcal{F}$ includes all affine maps.

($\Leftarrow$) Conversely, suppose that ϕ is $\mathcal{F}$-functionally equivariant and affine invariant preserving. Just as in the proof of Theorem 2.9, if $F \in \mathcal{F}(Y, Z)$ is an invariant of $f \in \mathfrak{X}(Y)$, then $g(y, z) = \bigl(f(y), 0\bigr)$, and $\mathcal{F}$-functional equivariance implies $\widetilde{g}(\widetilde{y},\widetilde{z}) = \bigl(\widetilde{f}(\widetilde{y}), F'(\widetilde{y})\widetilde{f}(\widetilde{y})\bigr)$. Finally, the linear projection $B(y,z) = z$ is an affine invariant of g and thus of $\widetilde{g}$, so $F'(\widetilde{y})\widetilde{f}(\widetilde{y}) = 0$. □

We next give an integrator map version of [13, Corollary 5.9], which says that a consistent splitting method cannot preserve affine invariants unless it equals the exact flow. Modified vector fields of splitting methods contain only the terms $f^{[1]},\ldots,f^{[N]}$ and their iterated Jacobi–Lie brackets, as a consequence of the Baker–Campbell–Hausdorff formula [9, Section IX.4]. Since Jacobi–Lie brackets of χ-related vector fields are χ-related for *any* χ whatsoever [1, Proposition 4.2.25], it follows that modified vector fields of splitting methods are N-affine equivariant and F-functionally equivariant with respect to *all* maps F. To prove that any consistent integrator map with this property must agree with the exact flow, we first establish the following consequence of consistency.

Lemma 4.8. *Suppose an N-affine equivariant integrator map ϕ satisfies the consistency condition $\phi(hf^{[1]},\ldots,hf^{[N]}) = hf + o(h)$. If $f^{[\nu]}$ is constant for all $\nu = 1,\ldots,N$, then $\phi(f^{[1]},\ldots,f^{[N]}) = f$.*

Proof. Let $A(y) = y + c$ for some constant $c \in Y$. If each $f^{[\nu]}$ is constant, then $f^{[\nu]} \sim_A f^{[\nu]}$, so N-affine equivariance implies $\widetilde{f} \sim_A \widetilde{f}$, i.e., $\widetilde{f}$ is also constant. On the other hand, letting $B(y) = hy$, we have $f^{[\nu]} \sim_B hf^{[\nu]}$, so applying N-affine equivariance again, we have $\widetilde{f} \sim_B \widetilde{hf}$, i.e., $h\widetilde{f}(\widetilde{y}) = \widetilde{hf}(h\widetilde{y})$. Since both $h\widetilde{f}$ and $\widetilde{hf}$ are constant, we get $h\widetilde{f} = \widetilde{hf} = hf + o(h)$ by the consistency condition. Thus, $\widetilde{f} = f + o(1)$, but since this does not depend on h at all, we conclude that $\widetilde{f} = f$. □

Theorem 4.9. *Consider consistent, N-affine equivariant integrator maps that are F-functionally equivariant for all maps F (e.g., those arising from splitting methods). The unique such integrator map preserving affine invariants is $\phi(f^{[1]},\ldots,f^{[N]}) = f$, i.e., the exact flow.*

Proof. By Theorem 4.7, any such ϕ preserving affine invariants must preserve *all* invariants. Given $f \in \mathfrak{X}(Y)$, consider the vector field $(f,1) \in \mathfrak{X}(Y \times \mathbb{R})$. This augments $\dot{y} = f(y)$ by the equation $\dot{t} = 1$, where t may be seen as time. Thus, $F(y,t) = \exp(-tf)(y)$ is an invariant of $(f,1)$.

Now, suppose we split $(f,1)$ into $(f^{[\nu]}, c^{[\nu]})$, where $c^{[\nu]} \in \mathbb{R}$ are constants summing to 1. By Lemma 4.8 and N-affine equivariance with respect to $(y,t) \mapsto t$, we have $\widetilde{(f,1)} = (\widetilde{f},1)$. Since ϕ preserves the invariant F, we conclude that $\exp(-tf)(\widetilde{y})$ is an invariant of $(\widetilde{f},1)$, and thus $\widetilde{f} = f$. □

Remark 4.10. Without the consistency hypothesis, which allows us to use Lemma 4.8, $\dot{t} = 1$ does not necessarily imply $\dot{\widetilde{t}} = 1$. This allows for the possibility $\widetilde{f} = cf$ with $c \neq 1$, giving a time reparametrization of the exact flow.

Finally, we note that Theorem 3.2 holds virtually unchanged for the relationship of additive integrators to their modified vector fields, where we need only replace Φ_{hf} by $\Phi_{hf^{[1]},\ldots,hf^{[N]}}$ and Φ_{hg} by $\Phi_{hg^{[1]},\ldots,hg^{[N]}}$. Thus, we immediately get additive-integrator versions of Corollary 3.5 for N-affine equivariance and Corollary 3.9 for F-functional equivariance, in the sense of [13, Section 5.1].

4.2. **Partitioned methods.**

A partitioned method is based on a partitioning $Y = Y^{[1]} \oplus \cdots \oplus Y^{[N]}$. These are similar to additive methods, except the decomposition $f = f^{[1]} + \cdots + f^{[N]}$ is uniquely determined by the partitioning of Y.

Definition 4.11. A *partitioned integrator map* is a collection of smooth maps

$$\phi_{Y^{[1]}\oplus\cdots\oplus Y^{[N]}} \colon \mathfrak{X}(Y) \to \mathfrak{X}(Y),$$

for each partitioned Banach space $Y = \bigoplus_{\nu=1}^{N} Y^{[\nu]}$, where $N \in \mathbb{N}$ is fixed. For a given partitioning of Y, we simply write $\widetilde{f} = \phi(f)$ for $f \in \mathfrak{X}(Y)$.

For partitioned methods, rather than considering all affine maps between Banach spaces, we consider particular affine maps that respect the partitioning, cf. [13, Definition 5.10].

Definition 4.12. Given partitioned spaces $Y = \bigoplus_{\nu=1}^N Y^{[\nu]}$ and $U = \bigoplus_{\nu=1}^N U^{[\nu]}$, a map $A\colon Y \to U$ is *P-affine* if it decomposes as $A = \bigoplus_{\nu=1}^N A^{[\nu]}$, where each $A^{[\nu]}\colon Y^{[\nu]} \to U^{[\nu]}$ is affine. A partitioned integrator map ϕ is *P-affine equivariant* if $f \sim_A g$ implies $\phi(f) \sim_A \phi(g)$ for all P-affine maps A.

Remark 4.13. When A is P-affine, $f \sim_A g$ is equivalent to $f^{[\nu]} \sim_{A^{[\nu]}} g^{[\nu]}$ for all $\nu = 1, \ldots, N$.

In particular, let $A\colon Y \to \mathbb{R}$ be an affine functional, and partition $\mathbb{R}^{[\mu]} = \mathbb{R}$ and $\mathbb{R}^{[\nu]} = \{0\}$ for $\nu \neq \mu$. Then A is P-affine if and only if $A = A^{[\mu]}$, i.e., A depends only on $Y^{[\mu]}$ [13, Example 5.11].

The following integrator-map version of [13, Proposition 5.12] shows how N-affine equivariant integrator maps (e.g., NB-series) give rise to P-affine equivariant integrator maps (e.g., P-series).

Proposition 4.14. *If an additive integrator map ψ is N-affine equivariant, then the partitioned integrator map $\phi(f) = \psi(f^{[1]}, \ldots, f^{[N]})$ is P-affine equivariant.*

Proof. This follows immediately from the definitions, since P-affine maps are affine. □

The definition of F- and $\mathcal{F}$-functional equivariance is the same as in Definition 2.4, where given partitions $Y = \bigoplus_{\nu=1}^N Y^{[\nu]}$ and $Z = \bigoplus_{\nu=1}^N Z^{[\nu]}$, we apply ϕ to the augmented vector field by partitioning the product $Y \times Z = \bigoplus_{\nu=1}^N (Y^{[\nu]} \times Z^{[\nu]})$. To prove a partitioned version of Theorem 2.9, we must introduce a P-affine version of Assumption 2.7; cf. [13, Assumption 5.14]. Important examples of $\mathcal{F}$ satisfying these assumptions are P-affine maps, all affine maps, quadratic maps that are at most bilinear with respect to the partition, and all quadratic maps, cf. [13, Examples 5.16–5.19].

Assumption 4.15. Assume that:

- $\mathcal{F}(Y, Y)$ contains the identity map for all $Y = \bigoplus_{\nu=1}^N Y^{[\nu]}$;
- $\mathcal{F}(Y, Z)$ is a vector space for all $Y = \bigoplus_{\nu=1}^N Y^{[\nu]}$ and $Z = \bigoplus_{\nu=1}^N Z^{[\nu]}$;
- $\mathcal{F}$ is invariant under composition with P-affine maps, in the following sense: If $A\colon Y \to U$ and $B\colon V \to Z$ are P-affine and $F \in \mathcal{F}(U, V)$, then $B \circ F \circ A \in \mathcal{F}(Y, Z)$, for all $Y = \bigoplus_{\nu=1}^N Y^{[\nu]}$, $Z = \bigoplus_{\nu=1}^N Z^{[\nu]}$, $U = \bigoplus_{\nu=1}^N U^{[\nu]}$, and $V = \bigoplus_{\nu=1}^N V^{[\nu]}$.

Compare the following to [13, Theorem 5.15].

Theorem 4.16. *Let $\mathcal{F}$ satisfy Assumption 4.15. A P-affine equivariant integrator map ϕ is $\mathcal{F}$-invariant preserving if and only if it is $\mathcal{F}$-functionally equivariant.*

Proof. The proof is essentially identical to that of Theorem 2.9. For the ($\Rightarrow$) direction, we use the fact that the linear projection $A\colon Y \times Z \to Y$ is P-affine, since it decomposes into the projections $A^{[\nu]}\colon Y^{[\nu]} \times Z^{[\nu]} \to Y^{[\nu]}$. For the ($\Leftarrow$) direction, we similarly use the fact that $B\colon Y \times Z \to Z$ is P-affine, since it decomposes into $B^{[\nu]}\colon Y^{[\nu]} \times Z^{[\nu]} \to Z^{[\nu]}$. At the final step, we have $\widetilde{0} = 0$, since the affine map from the trivial Banach space (with trivial partitioning) to any point of Z is P-affine. □

Theorem 3.2 holds unchanged for the relationship of partitioned integrators to their modified vector fields. Thus, we immediately get partitioned-integrator versions of Corollary 3.5 for P-affine equivariance and Corollary 3.9 for F-functional equivariance, in the sense of [13, Section 5.2].

4.3. **Closure under differentiation and symplecticity.** Finally, we generalize Theorem 2.13 to N-affine and P-affine equivariant methods, allowing the functional equivariance results to be extended to observables depending on variations. Definition 2.11 of closure under differentiation is formally unchanged for partitioned integrator maps; for additive integrator maps, we modify it in the obvious way, as follows.

Definition 4.17. An additive integrator map ϕ is *closed under differentiation* if

$$\phi(\delta f^{[1]}, \ldots, \delta f^{[N]}) = \delta\phi(f^{[1]}, \ldots, f^{[N]}).$$

Compare the following to [13, Theorem 5.20].

Theorem 4.18. *N-affine and P-affine integrator maps are closed under differentiation.*

Proof. The proof is essentially the same as that of Theorem 2.13. The only modification needed is to specify the additive decomposition or partitioning of the augmented system (4) to which ϕ is applied in order to obtain (5). If ϕ is an additive integrator then we decompose (4) into

$$f(x) = \sum_{\nu=1}^{N} f^{[\nu]}(x), \qquad f(y) = \sum_{\nu=1}^{N} f^{[\nu]}(y), \qquad \frac{f(x) - f(y)}{\epsilon} = \sum_{\nu=1}^{N} \frac{f^{[\nu]}(x) - f^{[\nu]}(y)}{\epsilon}.$$

If ϕ is P-affine equivariant, we partition $Y \times Y \times Y = \bigoplus_{\nu=1}^{N} (Y^{[\nu]} \times Y^{[\nu]} \times Y^{[\nu]})$. □

When $\omega \colon Y \times Y \to Z$ is a continuous bilinear map on Y, it follows that Example 2.15 extends *mutatis mutandis* to N-affine and P-affine equivariant integrator maps—and in particular, those preserving quadratic invariants are symplectic.

For NB-series, a similar argument to Theorem 2.16 gives the quadratic functional equivariance condition $b(u \circ v) + b(v \circ u) = 0$ for all N-colored trees u and v. Together with the affine invariant preservation condition that $b(\tau)$ is independent of the color of the root (Example 4.6), we recover a modified-vector-field version of Araújo et al. [2, Theorem 3], which states that these maps must therefore correspond to ordinary symplectic B-series.

On the other hand, if ω is at most bilinear with respect to a partition $Y = \bigoplus_{\nu=1}^{N} Y^{[\nu]}$ (i.e., the $Y^{[\nu]} \times Y^{[\nu]}$ blocks are trivial), then $F''\bigl(u(f), v(f)\bigr) = 0$ when u and v have the same colored root. Hence, the condition $b(u \circ v) + b(v \circ u) = 0$ need only hold for trees with different-colored roots. In particular, when ω is the canonical symplectic form on $Y = E \oplus E^*$, applying this with $N = 2$ recovers Hairer et al. [9, Theorem IX.10.4] on modified vector fields of symplectic P-series.

Appendix A. Necessity proof for quadratic functionally equivariant B-series

In this appendix, we prove that for all $u, v \in T$, it is possible to construct a vector field f and quadratic F such that $F''\bigl(u(f), v(f)\bigr) = F''\bigl(v(f), u(f)\bigr)$ is the only nonvanishing Hessian term at some point (i.e., F'' vanishes on all other pairs of trees). This completes the proof of Theorem 2.16 by establishing the necessity of the condition $b(u \circ v) + b(v \circ u) = 0$ for quadratic functional equivariance of a B-series integrator map.

We begin with a vector field construction for an individual tree τ, which we subsequently apply to u and v to prove the claim above. Let $|\tau|$ denote the order of τ, i.e., its number of vertices.

Lemma A.1. *Given $\tau \in T$, there exists a vector field f on $\mathbb{R}^{|\tau|}$ such that*

$$\theta(f)_{|\tau|}(0) = \begin{cases} \sigma(\tau), & \text{if } \theta = \tau, \\ 0, & \text{otherwise.} \end{cases}$$

Proof. Label the vertices of τ by $1, \ldots, |\tau|$, where $i = |\tau|$ is the root. For each vertex i with children $j_1, \ldots, j_k$, define the ith component of f at $y = (y_1, \ldots, y_{|\tau|}) \in \mathbb{R}^{|\tau|}$ to be

$$f_i(y) = y_{j_1} \cdots y_{j_k}.$$

In the case $k = 0$ (i.e., vertex i is a leaf), we use the convention that the empty product is 1. We claim that this f has the desired property.

The proof of this claim is by induction on the height of τ. The base case $\tau = \bullet$ is trivial. For the induction step, write $\tau = [\tau_1, \ldots, \tau_m]$, and suppose without loss of generality that the children of the root are labeled $1, \ldots, m$ accordingly. By definition,

$$\tau(f) = f^{(m)}\bigl(\tau_1(f), \ldots, \tau_m(f)\bigr).$$

Using the inductive assumption, we have

$$\tau_j(f)_i(0) = \begin{cases} \sigma(\tau_j), & \text{if } \tau_i = \tau_j, \\ 0, & \text{otherwise,} \end{cases} \tag{11}$$

where i and j range over $1, \ldots, m$. Next, since $f_{|\tau|}(y) = y_1 \cdots y_m$, we have

$$f_{|\tau|}^{(m)}(0) = \sum_{\pi \in S_m} \mathrm{d}y_{\pi(1)} \otimes \cdots \otimes \mathrm{d}y_{\pi(m)}, \tag{12}$$

where S_m is the symmetric group on m elements, so that π is a permutation of $\{1, \ldots, m\}$. Applying this to (11), each nonvanishing term evaluates to $\sigma(\tau_1) \cdots \sigma(\tau_m)$, and the nonvanishing terms correspond to π that permute identical trees among $\tau_1, \ldots, \tau_m$. The number of such permutations is precisely $\mu_1! \cdots \mu_k!$, where the μ_j count the occurrences of each unique tree, as in the proof of Theorem 2.16. Therefore,

$$\tau(f)_{|\tau|}(0) = \sigma(\tau_1) \cdots \sigma(\tau_m) \mu_1! \cdots \mu_k! = \sigma(\tau).$$

Finally, suppose $\theta \neq \tau$, and write $\theta = [\theta_1, \ldots, \theta_n]$. If $n \neq m$, then we have $f_{|\tau|}^{(n)}(0) = 0$, so $\theta(f)_{|\tau|}(0) = 0$. Otherwise, $[\theta_1, \ldots, \theta_m]$ is not a permutation of $[\tau_1, \ldots, \tau_m]$, so for all $\pi \in S_m$, there exists some j such that $\theta_j \neq \tau_{\pi(j)}$. In this case, (11) implies $\theta_j(f)_{\pi(j)}(0) = 0$, so every term in (12) vanishes when evaluated on $\big(\theta_1(f)(0), \ldots, \theta_m(f)(0)\big)$, and again $\theta(f)_{|\tau|}(0) = 0$. □

Lemma A.2. *Given $u, v \in T$, there exists a vector field f and quadratic functional F on $Y = \mathbb{R}^{|u|+|v|}$ such that*

$$F''\big(\tau(f), \theta(f)\big)(0) \begin{cases} \neq 0, & \text{if } (\tau, \theta) = (u, v) \text{ or } (\tau, \theta) = (v, u), \\ = 0, & \text{otherwise.} \end{cases}$$

Proof. Similarly to Lemma A.1, label the vertices of u by $1, \ldots, |u|$, where $i = |u|$ is the root. For each vertex i with children $j_1, \ldots, j_k$, let

$$f_i(y) = y_{j_1} \cdots y_{j_k}.$$

Repeat this for v, labeling its vertices by $|u| + 1, \ldots, |u| + |v|$, where $i = |u| + |v|$ is the root. Now, define the quadratic functional

$$F(y) = y_{|u|} y_{|u|+|v|},$$

so that

$$F''\big(\tau(f), \theta(f)\big) = \tau(f)_{|u|} \theta(f)_{|u|+|v|} + \tau(f)_{|u|+|v|} \theta(f)_{|u|}.$$

If $\tau = u$ and $\theta = v$, or vice versa, then Lemma A.1 implies that evaluating this at $y = 0$ gives $2\sigma(u)\sigma(v)$ if $u = v$ and $\sigma(u)\sigma(v)$ if $u \neq v$. If τ and θ are not u and v, then Lemma A.1 implies that both terms vanish at $y = 0$. □

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