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Directional Quaternion Step Differentiation and a Bicomplex Double-Step Calculus for Cancellation-Free First and Second Derivatives

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Abstract

Accurate derivative information is central to sensitivity analysis and optimization, yet standard finite differences can lose many digits when the step size is small because of subtractive cancellation. Complex-step differentiation largely resolves this issue for first derivatives, but robust second derivatives and mixed partials remain delicate: several practical complex-step variants for f'' still subtract nearly equal quantities, and quaternion-step rules are often presented as separate constructions. We develop a unified slice-based framework that extracts first and second derivatives from a single evaluation by projecting algebraic coefficients in commutative subalgebras of the complexified quaternions. First, we formulate a directional quaternion-step rule parameterized by an arbitrary unit pure quaternion u and provide an explicit projection operator that makes the underlying complex slice $\mathbb{C}_u \simeq \mathbb{C}$ transparent; the resulting first-derivative formula is rotation invariant and recovers classical j -step and planar (j, k) -step rules as special cases. Second, we construct a *bicomplex double-step* calculus in the commuting imaginary units i and u and show that one evaluation at $z + (i + u)h$ separates derivative information into distinct coefficients, with the iu -component equal to $h^2 f''(z) + \mathcal{O}(h^4)$, giving a subtraction-free $\mathcal{O}(h^2)$ approximation of f'' . For bivariate analytic functions we additionally derive one-shot identities for f_x , f_y , and f_{xy} from $f(x + uh, y + ih)$ and supply practical extraction identities, step-size guidance for h^2 -scaled coefficients, and branch-consistency diagnostics for non-entire functions. The “cancellation-free” property here refers to avoiding the subtraction of nearly equal *real* quantities at the level of the differentiation formula; in floating-point arithmetic, coefficient extraction and the $1/h^2$ scaling for second-order quantities still interact with roundoff, and we quantify the resulting stable regimes numerically.

Keywords: complex-step differentiation; quaternion step; bicomplex numbers; mixed partial derivatives; Hessian approximation; cancellation-free numerics; sensitivity analysis

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1. Introduction

Numerical differentiation underpins sensitivity analysis, inverse problems, optimal control, and many routines in scientific computing. In practice, however, straightforward finite differences can be limited by subtractive cancellation when the step size h is small, so that the observed accuracy may fall far short of the nominal truncation order. A widely used

alternative is the complex-step derivative approximation: if f is analytic and real-valued on the real axis, then

$$f'(x) \approx \frac{\operatorname{Im} f(x + ih)}{h}, \quad h \rightarrow 0, \quad (1)$$

which has truncation error $\mathcal{O}(h^2)$ while avoiding the subtraction of nearly equal real numbers [1,2]. This combination of accuracy and robustness has made the complex-step method a standard tool, including in black-box settings where only a function evaluator is available.

Second derivatives are more delicate. The classical stencil

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

has $\mathcal{O}(h^2)$ truncation error, yet its differencing structure can magnify roundoff dramatically as h decreases. Several complex-step extensions exist [3], but many practical formulas for f'' ultimately reintroduce subtraction (for instance through combinations such as $f(x) - \operatorname{Re} f(x + ih)$). Exact second derivatives can be obtained by hyper-dual numbers [4] or by multicomplex methods [5]; these approaches are powerful, but they typically require additional algebraic infrastructure beyond complex arithmetic.

Quaternion-step differentiation provides another route to cancellation-free differentiation by embedding an imaginary step into a commutative slice of a (complexified) quaternion algebra and recovering derivatives by projection [6]. The present work develops this idea in a direction-agnostic form and shows that, once one works systematically inside a commuting $\{i, u\}$ -slice, second derivatives and mixed partials can also be extracted from *one* evaluation without subtraction.

Main Results

We separate our contributions into (i) new constructions and (ii) a unifying viewpoint clarifying scope and limitations.

New constructions.

Directional quaternion-step calculus with explicit projection. For an arbitrary unit pure quaternion u we prove a u -step rule that computes $f'(z)$ from a single slice evaluation $f(z + uh) \in \mathbb{C}_u$ via an explicit projection onto the u -component. The construction makes the slice isomorphism $\mathbb{C}_u \simeq \mathbb{C}$ explicit and yields a clean rotation-invariance statement.

A bicomplex double-step for subtraction-free f'' . Working in the commutative bicomplex slice $\mathbb{B}_u = \operatorname{span}_{\mathbb{R}}\{1, i, u, iu\}$, we show that one evaluation at $z + (i + u)h$ separates derivative information into algebraic coefficients. Under a local analyticity assumption near the perturbed points, the iu -coefficient equals $h^2 f''(z) + \mathcal{O}(h^4)$, providing an $\mathcal{O}(h^2)$ approximation of f'' without subtracting nearly equal real numbers.

One-shot mixed partials with controlled higher-order coupling. For bivariate analytic $f(x, y)$ we derive identities that recover f_x , f_y , and f_{xy} simultaneously from a single evaluation at $(x + uh, y + ih)$. We record explicit Taylor expansions showing that the first f_{xy} -coupling terms enter at order h^4 (and hence produce an $\mathcal{O}(h^2)$ truncation after scaling by $1/h^2$), which informs step-size selection.

Unifying viewpoint and scope.

Unification of existing quaternion-step variants. Classical j -step and planar (j, k) -step formulas arise from particular choices of u and the same projection principle on $\mathbb{C}_u$.

What is (and is not) handled about noncommutativity. The methods do not “resolve” noncommutativity in full quaternionic algebras; rather, they exploit commutative slices where standard analytic expansions are valid and coefficient extraction is well defined.

Practical safeguards. For non-entire functions we discuss branch-aware direction choice and provide diagnostics for violations of the slice-evaluability assumption.

The paper is organized as follows. Section 2 reviews related differentiation paradigms. Section 3 summarizes quaternionic and bicomplex preliminaries and fixes notation. Section 4 presents the directional quaternion-step rule and its invariance properties. Section 5 discusses direction selection. Section 6 analyzes truncation and rounding errors. Section 7 develops the bicomplex double-step formula for f'' and provides coefficient identities. Section 8 derives one-shot mixed partial formulas and discusses Hessian assembly. Section 9 gives implementation notes. Section 10 reports numerical experiments and comparisons. Appendices A–E collect additional algebraic identities, an idempotent decomposition viewpoint, and reference pseudocode.

2. Related Work

2.1. Complex-Step and Finite-Difference Methods

The idea of differentiating analytic functions through complex perturbations goes back at least to [7]. The modern complex-step approximation (1) was popularized in [1] and systematized for algorithmic use in [2]; see also [8] for a concise discussion. For holomorphic f , the method can be interpreted through Taylor expansion and the absence of real subtraction. Finite-difference methods remain widely used due to minimal requirements on function evaluators, but their error is typically governed by a trade-off between truncation $\mathcal{O}(h^p)$ and rounding/cancellation $\mathcal{O}(\epsilon/h)$.

Second derivatives via complex perturbations have been investigated in, e.g., [3], but many formulas still involve subtraction of close real quantities and, thus, lose accuracy for very small h . Higher-order finite-difference stencils and Richardson extrapolation can reduce truncation but often worsen cancellation and increase evaluation cost.

2.2. Dual, Hyper-Dual, and Multicomplex Approaches

Dual numbers encode first derivatives exactly, and hyper-dual numbers encode second derivatives exactly via nilpotent elements and an extended arithmetic [4,9]. Multicomplex numbers generalize complex-step ideas to higher orders and mixed derivatives, providing a systematic coefficient-extraction framework [5]. These methods can achieve very high accuracy, at the expense of working in enlarged algebras and implementing elementary functions therein. Several software packages implement multicomplex or multidual variants (see, e.g., [10]).

2.3. Quaternionic and Bicomplex Function Theory

Quaternionic analysis offers multiple notions of analyticity, including slice regularity [11]. For numerical differentiation of real-valued functions, a common pragmatic approach is to embed a complex step into a commutative subalgebra of $\mathbb{H}$ (or its complexification), thereby retaining the cancellation-free property while allowing “directional” steps. Such quaternion-step rules can be implemented with a black-box interface by working inside a commutative slice and extracting the appropriate component by projection.

Bicomplex numbers provide a commutative algebra with two commuting square roots of -1 and a hyperbolic unit [12,13]. They offer a natural environment for extracting second-order information from a single evaluation, via a separation of coefficients that is not available in ordinary complex arithmetic.

3. Preliminaries

3.1. Quaternions and Pure Unit Directions

The quaternion algebra $\mathbb{H}$ is generated by $1, i, j, k$ with relations $i^2 = j^2 = k^2 = ijk = -1$. Every $q \in \mathbb{H}$ decomposes as $q = q_0 + \mathbf{q}$ with scalar part $q_0 \in \mathbb{R}$ and vector part $\mathbf{q} \in \mathbb{R}^3$. The quaternionic conjugate is $\bar{q} = q_0 - \mathbf{q}$ and $|q|^2 = q\bar{q} = \bar{q}q$.

A pure unit quaternion is any $u \in \mathbb{H}$ with $\text{Re}(u) = 0$ and $u^2 = -1$. Such u can be written as $u = bi + cj + dk$ with $b^2 + c^2 + d^2 = 1$. For a fixed u , the set $\mathbb{C}_u := \{x + uy : x, y \in \mathbb{R}\}$ is a commutative subalgebra isomorphic to $\mathbb{C}$. Concretely, the isomorphism $\phi_u : \mathbb{C} \rightarrow \mathbb{C}_u$ may be taken as

$$\phi_u(x + iy) = x + uy,$$

and different choices of u correspond to rotated slices: if s is a unit quaternion with $u = sjs^{-1}$, then $\phi_u(x + iy) = s(x + jy)s^{-1}$. In computations, writing an element of $\mathbb{C}_u$ as $\alpha + \beta u$ (with $\alpha, \beta \in \mathbb{R}$) is equivalent to extracting its 1- and u -coefficients via the projection operator introduced in Section 4.

3.2. Complexified Quaternions and Bicomplex Slices

For step calculus we work in the complexified quaternion algebra $\mathbb{H}_{\mathbb{C}} := \mathbb{H} \otimes_{\mathbb{R}} \mathbb{C}$, whose elements have the form

$$q = a + bi + cu + diu,$$

where the scalar imaginary unit i commutes with all quaternionic units and u is a chosen pure unit quaternion. The commutative subalgebra

$$\mathbb{B}_u := \{a + bi + cu + diu : a, b, c, d \in \mathbb{R}\} \quad (2)$$

is isomorphic to the bicomplex algebra $\mathbb{B} \cong \mathbb{C} \otimes_{\mathbb{R}} \mathbb{C}$ [12]. Note that $(iu)^2 = +1$, so iu plays the role of a hyperbolic unit.

We use the basis $(1, i, u, iu)$ and write, for $w \in \mathbb{B}_u$,

$$w = [w]_1 + [w]_i i + [w]_u u + [w]_{iu} iu.$$

3.3. Analytic Functions on Slices and an Evaluability Assumption

Our formulas require that the target function can be evaluated on complex and bicomplex perturbations. This can be formalized as follows.

Assumption 1 (Holomorphic slice evaluability). *Let $\Omega \subset \mathbb{C}$ be a domain containing a real interval of interest. A scalar function $f : \Omega \rightarrow \mathbb{C}$ is slice-evaluable if it admits a convergent power-series expansion on Ω (or an analytic continuation there), so that f can be evaluated on $\mathbb{C}_u$ and $\mathbb{B}_u$ by replacing i with u and using the same coefficients.*

Remark 1. *Assumption 1 is a local requirement: it asks only that the function admit an analytic continuation on a neighborhood of the base point and of the perturbed evaluation points. For entire elementary functions (e.g., polynomials, exp, sin, cos), this holds globally. For multi-valued functions with branch points (e.g., log and $\sqrt{\cdot}$), the assumption is “mild” provided the base point z lies in a simply connected region on which a single branch is fixed and the step size is chosen so that the evaluation path stays inside that region. Concretely, if z is not on a branch cut for the chosen branch, then there exists $r > 0$ such that the disk $D(z, r)$ avoids the cut; taking $|h| < r$ guarantees that $z + uh$ and $z + (i + u)h$ remain on the same branch and the slice evaluation is well defined. In Section 9 we describe practical safeguards (step-size selection and branch-consistency checks) and illustrate the effect of branch geometry in the logarithm experiment.*

4. Directional Quaternion Step Differentiation

4.1. A Projection-Based u -Step Rule

Let u be a pure unit quaternion and let f be slice-evaluable in the sense of Assumption 1. For $z \in \mathbb{C}$ and small $h \in \mathbb{R}$, consider the slice evaluation $f(z + uh) \in \mathbb{C}_u$. Write the Taylor expansion in $\mathbb{C}_u$:

$$f(z + uh) = f(z) + uh f'(z) - \frac{h^2}{2} f''(z) - u \frac{h^3}{6} f^{(3)}(z) + \mathcal{O}(h^4). \quad (3)$$

Because the perturbation $z + uh$ lies in the commutative slice $\mathbb{C}_u$, powers $(uh)^k$ are unambiguous and the usual Taylor expansion (with the same coefficient ordering as in $\mathbb{C}$) applies. Moreover, if f is holomorphic on a disk containing the segment between z and $z + uh$, the remainder admits the standard bound in terms of higher derivatives, so the truncation $\mathcal{O}(h^4)$ in (3) is justified exactly as in the complex case. The u -coefficient isolates the odd terms.

Theorem 1 (u -step first derivative). *Let f satisfy Assumption 1 on a neighborhood of $z \in \mathbb{C}$. Then, for any pure unit quaternion u and sufficiently small h ,*

$$f'(z) = \frac{[f(z + uh)]_u}{h} + \mathcal{O}(h^2). \quad (4)$$

Equivalently, writing $f(z + uh) = \alpha(h) + u \beta(h)$ with $\alpha, \beta \in \mathbb{C}$,

$$f'(z) = \frac{\beta(h)}{h} + \mathcal{O}(h^2).$$

Proof. From (3), we read off the u -coefficient: $[f(z + uh)]_u = h f'(z) - \frac{h^3}{6} f^{(3)}(z) + \mathcal{O}(h^5)$. Dividing by h gives (4). $\square$

Remark 2 (On the scope of the unification). *Theorem 1 unifies previously proposed quaternion-step formulas in the setting of slice evaluations: once an imaginary direction u is fixed, the perturbation $z + uh$ lives in the commutative copy $\mathbb{C}_u \subset \mathbb{H}_{\mathbb{C}}$, and the derivative is obtained by projecting onto the u -component. Classical j -step and (j, k) -step rules correspond to particular choices of u (and, for mixed information, to evaluating in a commuting slice) and hence are instances of the same projection principle. Outside this setting—for example, if one perturbs in genuinely noncommuting directions and attempts to interpret products without restricting to a commutative slice—the clean coefficient separation generally breaks down and additional commutator terms can appear. This is why our mixed-partial and double-step constructions are formulated explicitly in a commuting $\{i, u\}$ -slice.*

4.2. Recovering j -Step and Planar (j, k) -Step Rules

Setting $u = j$ specializes Theorem 1 to a j -step rule. More generally, any unit direction in the j - k plane,

$$u(\theta) = \cos \theta j + \sin \theta k,$$

produces an equivalent family of directional formulas. Theorem 1 shows that these variants are all instances of the same projection-based u -step method and differ only by a rotation of the chosen imaginary direction.

4.3. A Chain Rule and Jacobian Templates

The u -step derivative is compatible with composition for analytic maps.

Proposition 1 (Chain rule in a slice). *Let $g : \Omega \rightarrow \mathbb{C}$ and $f : g(\Omega) \rightarrow \mathbb{C}$ be slice-evaluable and analytic. Then for any pure unit u ,*

$$\frac{[f(g(z + uh))]_u}{h} = f'(g(z))g'(z) + \mathcal{O}(h^2).$$

Proof. Expand $g(z + uh) = g(z) + uhg'(z) + \mathcal{O}(h^2)$ in $\mathbb{C}_u$ and insert into the analytic expansion of f around $g(z)$. The u -coefficient is $hf'(g(z))g'(z) + \mathcal{O}(h^3)$. $\square$

For a vector-valued mapping $F : \mathbb{R}^n \rightarrow \mathbb{R}^m$ that is analytic in each component under complex perturbations, one may compute Jacobian columns by stepping one coordinate at a time:

$$\partial_{x_j} F(x) \approx \frac{1}{h} [F(x + uh e_j)]_u, \quad j = 1, \dots, n.$$

In Section 8, we discuss mixed partials and Hessian assembly.

5. Rotation Invariance and Direction Selection

A useful feature of quaternionic steps is the freedom to choose the direction u . This section formalizes the invariance of the u -step derivative under rotations and highlights practical consequences.

5.1. Conjugation Rotates Slices

Let $q \in \mathbb{H}$ be a unit quaternion, $|q| = 1$. Conjugation by q acts on pure unit quaternions by a 3D rotation:

$$u \mapsto u' := q u q^{-1}, \quad (u')^2 = -1.$$

Moreover,

$$q(z + uh)q^{-1} = z + (quq^{-1})h = z + u'h,$$

because the scalar complex variable $z \in \mathbb{C}$ commutes with q in $\mathbb{H}_{\mathbb{C}}$.

Lemma 1 (Equivariance of scalar-coefficient power series). *Let $p(w) = \sum_{k=0}^N a_k w^k$ be a polynomial with coefficients $a_k \in \mathbb{C}$ (hence commuting with $\mathbb{H}$). Then for all $w \in \mathbb{H}_{\mathbb{C}}$ and all unit quaternions q ,*

$$p(qwq^{-1}) = q p(w) q^{-1}.$$

The same identity holds for analytic functions defined by absolutely convergent power series.

Proof. For monomials w^k the identity follows by repeated insertion of $q^{-1}q = 1$: $(qwq^{-1})^k = qw^kq^{-1}$. Linearity gives the polynomial case; the analytic case follows by termwise convergence. $\square$

5.2. Invariance of the u -Step Derivative

Equivariance implies that the u -step derivative does not depend on the chosen unit direction.

Theorem 2 (Rotation invariance). *Let f satisfy Assumption 1 near $z \in \mathbb{C}$. Let u be a pure unit quaternion and let $u' = quq^{-1}$ for some unit quaternion q . Then, for sufficiently small h ,*

$$\frac{[f(z + uh)]_u}{h} = \frac{[f(z + u'h)]_{u'}}{h} + \mathcal{O}(h^2).$$

In particular, the limit $h \rightarrow 0$ (when it exists) is independent of u .

Proof. By Lemma 1, $f(z + u'h) = f(q(z + uh)q^{-1}) = qf(z + uh)q^{-1}$. Writing $f(z + uh) = \alpha(h) + u\beta(h)$ with $\alpha, \beta \in \mathbb{C}$, we obtain $f(z + u'h) = \alpha(h) + u'\beta(h)$ because conjugation rotates u to u' and fixes scalars. Thus, $[f(z + u'h)]_{u'} = [f(z + uh)]_u = \beta(h)$, and Theorem 1 yields the claim. $\square$

5.3. Practical Direction Choice

The freedom to choose u is helpful when the analytic continuation of f has restricted domains (e.g., branch cuts). Given a real evaluation point x , one may select u to avoid pushing $x + uh$ toward a cut in the complex plane of the chosen slice. For entire functions, direction choice is mostly irrelevant; for non-entire functions, this additional degree of freedom can improve robustness. Section 10 illustrates invariance numerically and provides a logarithm example where branch awareness matters.

6. Error and Stability Analysis

6.1. Truncation Order

Equation (4) shows that the u -step first derivative has truncation error $\mathcal{O}(h^2)$. This matches the complex-step method. One may raise the formal truncation order by Richardson extrapolation applied after coefficient extraction, e.g.,

$$f'(z) = \frac{4[f(z + uh/2)]_u - [f(z + uh)]_u}{h} + \mathcal{O}(h^4),$$

provided the function evaluation is stable on the slice. However, the linear combination involves subtraction of two close coefficient estimates; it does not reintroduce subtraction of nearly equal real function values, but it can still amplify roundoff when h is very small. Accordingly, we do not interpret Richardson extrapolation as preserving the cancellation-free behavior of the base u -step rule in floating-point arithmetic.

6.2. Rounding Error Model and Step-Size Guidance

Assume the computed value $\widehat{f(z + uh)}$ satisfies a relative error model $\widehat{f} = f(1 + \delta)$ with $|\delta| \lesssim \varepsilon$. For the first derivative, coefficient extraction is linear and does not involve subtracting close reals, so the rounding contribution to $[f(z + uh)]_u$ is typically of size $\mathcal{O}(\varepsilon|f|)$. Consequently, the total error behaves like

$$|\widehat{f'(z)} - f'(z)| \lesssim C_1 h^2 + C_2 \varepsilon,$$

which permits choosing h near machine precision (up to function evaluation limitations).

For second-order quantities (e.g., f'' or f_{xy}) the extracted coefficient is of size $\mathcal{O}(h^2)$ and the approximation divides it by h^2 . If the evaluation error in f is of size $\mathcal{O}(\varepsilon|f|)$, then after coefficient extraction and scaling one expects a roundoff contribution of order $\mathcal{O}(\varepsilon|f|/h^2)$. Combined with the $\mathcal{O}(h^2)$ truncation term, this yields the standard balance

$$\text{error} \approx C_{\text{tr}} h^2 + C_{\text{ro}} \frac{\varepsilon}{h^2}, \quad h \sim \varepsilon^{1/4}.$$

Coefficient extraction itself is a fixed linear projection (implemented by a few additions/-subtractions and scalar multiplications), so its conditioning is mild; the dominant sensitivity comes from the $1/h^2$ scaling inherent to any method that reads off a second derivative from an h^2 -small signal. The experiments in Section 10 illustrate the resulting optimal regime.

7. A Bicomplex Double-Step Calculus for Second Derivatives

7.1. *Key Algebra:* $(i + u)^2 = -2 + 2iu$

Inside $\mathbb{B}_u$ we have $i^2 = u^2 = -1$ and $iu = ui$, hence

$$(i + u)^2 = i^2 + 2iu + u^2 = -2 + 2iu. \quad (5)$$

The iu term is precisely what enables a clean separation of second-order information.

7.2. *Double-Step Expansion and a No-Subtraction Formula*

Consider the bicomplex perturbation $z + (i + u)h$ with $z \in \mathbb{C}$ and $h \in \mathbb{R}$. Since i and u commute inside $\mathbb{B}_u$, the Taylor series can be written unambiguously as

$$f(z + (i + u)h) = \sum_{k \geq 0} \frac{f^{(k)}(z)}{k!} (i + u)^k h^k. \quad (6)$$

The crucial observation is that *odd powers carry no iu component*. Indeed, letting $k := iu$ (so $k^2 = 1$) and using $(i + u)^2 = -2 + 2k$, we have

$$(i + u)^{2m+1} = (i + u)((i + u)^2)^m = (i + u)(-2 + 2k)^m,$$

and $(-2 + 2k)^m$ is a linear combination of 1 and k only; multiplying by $(i + u)$ produces terms in the span of $\{i, u\}$, but not iu . Consequently,

$$[(i + u)^{2m+1}]_{iu} = 0 \quad (m \geq 0). \quad (7)$$

Keeping the first two even orders gives a transparent truncation:

$$\begin{aligned} f(z + (i + u)h) &= f(z) + (i + u)h f'(z) + \frac{(i + u)^2 h^2}{2} f''(z) + \frac{(i + u)^4 h^4}{24} f^{(4)}(z) + \mathcal{O}(h^5) \\ &= f(z) + (i + u)h f'(z) + (-h^2 + iu h^2) f''(z) + \frac{1}{3}(1 - iu)h^4 f^{(4)}(z) + \mathcal{O}(h^5). \end{aligned} \quad (8)$$

Therefore, the iu -coefficient satisfies

$$[f(z + (i + u)h)]_{iu} = h^2 f''(z) - \frac{1}{3} h^4 f^{(4)}(z) + \mathcal{O}(h^6). \quad (9)$$

Theorem 3 (Bicomplex double-step for f''). *Let f be holomorphic on a neighborhood of the complex line segment joining z and $z + 2ih$ (for $|h|$ in a sufficiently small range), and assume f is slice-evaluable in the sense of Assumption 1. Then, for any pure unit quaternion u and sufficiently small real h ,*

$$f''(z) = \frac{[f(z + (i + u)h)]_{iu}}{h^2} + \mathcal{O}(h^2). \quad (10)$$

The leading term uses only coefficient extraction in the commutative algebra $\mathbb{B}_u$. The formula is subtraction-free at the level of real differencing, i.e., it avoids subtracting nearly equal real numbers as in classical second-difference stencils; in floating-point arithmetic, the $1/h^2$ scaling still imposes a practical lower bound on h (Section 6).

Proof. Equation (9) shows that the iu coefficient equals $h^2 f''(z) + \mathcal{O}(h^4)$. Dividing by h^2 yields (10) with $\mathcal{O}(h^2)$ truncation. The improved remainder order in (9) follows from the parity cancellation (7), which eliminates all odd Taylor contributions from the iu component. $\square$

Remark 3 (Comparison with a subtractive complex-step second derivative). A popular complex-step second derivative formula is

$$f''(x) \approx \frac{2(f(x) - \operatorname{Re} f(x + ih))}{h^2},$$

which involves the subtraction $f(x) - \operatorname{Re} f(x + ih)$ and, thus, loses accuracy when h is too small. By contrast, (10) isolates f'' as an algebraic coefficient in $\mathbb{B}_u$.

7.3. Coefficient Extraction via Involutions

Define three commuting involutions on $\mathbb{B}_u$:

$$\overline{(\cdot)}^{(i)} : i \mapsto -i, u \mapsto u, \quad \overline{(\cdot)}^{(u)} : i \mapsto i, u \mapsto -u, \quad \overline{(\cdot)}^{(iu)} : i \mapsto -i, u \mapsto -u.$$

These yield explicit coefficient formulas.

Lemma 2 (Extraction identities). For $w \in \mathbb{B}_u$,

$$\begin{aligned} [w]_1 &= \frac{w + \overline{w}^{(i)} + \overline{w}^{(u)} + \overline{w}^{(iu)}}{4}, \\ [w]_i &= \frac{w - \overline{w}^{(i)} + \overline{w}^{(u)} - \overline{w}^{(iu)}}{4i}, \\ [w]_u &= \frac{w + \overline{w}^{(i)} - \overline{w}^{(u)} - \overline{w}^{(iu)}}{4u}, \\ [w]_{iu} &= \frac{w - \overline{w}^{(i)} - \overline{w}^{(u)} + \overline{w}^{(iu)}}{4iu}. \end{aligned}$$

Remark 4 (Why Lemma 2 matters). Lemma 2 provides explicit coefficient-extraction identities on $\mathbb{B}_u$ using only involutions (conjugations) and elementary arithmetic. These formulas are the computational core of the proposed methods: they turn a single bicomplex evaluation such as $f(z + (i + u)h)$ into the scalar components $[\cdot]_i$, $[\cdot]_u$, and $[\cdot]_{iu}$ that encode $f'(z)$, $f''(z)$, and mixed information. Because the extraction uses additions and sign changes rather than subtracting two close function values, it preserves the cancellation-free character of the complex/quaternion-step idea and leads to straightforward implementations (see Section 9 and Appendix D).

Proof. Write $w = a + bi + cu + diu$ and apply the involutions; solving the resulting 4×4 linear system yields the identities. $\square$

8. Mixed Partial and Hessians from One Evaluation

8.1. One-Shot Extraction for f_x , f_y , and f_{xy}

Let $f : \mathbb{R}^2 \rightarrow \mathbb{R}$ be analytic and slice-evaluable in each variable. Consider the bivariate perturbation

$$(x, y) \mapsto (x + uh, y + ih),$$

which lives in the commutative slice $\mathbb{B}_u$. A Taylor expansion gives

$$\begin{aligned} f(x + uh, y + ih) &= f(x, y) + uh f_x + ih f_y + iu h^2 f_{xy} \\ &\quad - \frac{h^2}{2}(f_{xx} + f_{yy}) + \mathcal{O}(h^3), \end{aligned} \tag{11}$$

where all partial derivatives are evaluated at (x, y) .

In particular, the iu -coefficient has no contribution at total degree 3; the first coupling correction appears at degree 4:

$$[f(x + uh, y + ih)]_{iu} = h^2 f_{xy}(x, y) - \frac{h^4}{6} (f_{xxxy}(x, y) + f_{xyyy}(x, y)) + \mathcal{O}(h^6). \quad (12)$$

After dividing by h^2 , this yields an $\mathcal{O}(h^2)$ truncation error for f_{xy} and motivates the $h \sim \varepsilon^{1/4}$ guideline for mixed partials.

Derivation of (11). Let $\Delta x = uh$ and $\Delta y = ih$. The bivariate Taylor expansion gives

$$f(x + \Delta x, y + \Delta y) = f + \Delta x f_x + \Delta y f_y + \frac{1}{2} (\Delta x^2 f_{xx} + 2\Delta x \Delta y f_{xy} + \Delta y^2 f_{yy}) + \mathcal{O}(h^3).$$

Since i commutes with u in the slice $\mathbb{B}_u$, $\Delta x \Delta y = \Delta y \Delta x = iu h^2$. Moreover, $\Delta x^2 = u^2 h^2 = -h^2$ and $\Delta y^2 = i^2 h^2 = -h^2$. Substituting these identities yields (11).

Theorem 4 (One evaluation yields three derivatives). *Under the above assumptions,*

$$f_x(x, y) = \frac{[f(x + uh, y + ih)]_u}{h} + \mathcal{O}(h^2), \quad f_y(x, y) = \frac{[f(x + uh, y + ih)]_i}{h} + \mathcal{O}(h^2),$$

and

$$f_{xy}(x, y) = \frac{[f(x + uh, y + ih)]_{iu}}{h^2} + \mathcal{O}(h^2).$$

Proof. Expand f in two variables and collect the coefficients of u , i , and iu as in (11). $\square$

8.2. Hessian Assembly

For $f : \mathbb{R}^n \rightarrow \mathbb{R}$, the full Hessian requires access to $f_{x_i x_j}$. The double-step formula in Section 7 provides the diagonal entries $f_{x_i x_i}$ from a one-dimensional perturbation in each coordinate (one evaluation per diagonal entry). For mixed entries $f_{x_i x_j}$ one may use the two-variable perturbation of Theorem 4 by stepping coordinates i and j together; this requires one evaluation per unordered pair (i, j) . Thus, a direct Hessian assembly requires $1 + \frac{n(n+1)}{2}$ evaluations, comparable to hyper-dual methods but with simpler coefficient extraction in a commutative slice. When only Hessian-vector products are required, directional variants can reduce cost.

9. Algorithms and Implementation Notes

9.1. Elementary Functions on $\mathbb{B}_u$

For polynomials and power series, evaluation on $\mathbb{B}_u$ is immediate. For elementary transcendental functions, a reliable strategy is to use the *idempotent decomposition* of bicomplex numbers [12] (see Appendix B): any $w \in \mathbb{B}_u$ splits into two complex components, and functions can be applied componentwise. This reduces implementation to two complex evaluations, which are typically available in numerical libraries.

9.2. Branch Cuts and Domain Restrictions

For functions with branch cuts (e.g., $\log$ and $\sqrt{\cdot}$), one must ensure that the perturbed arguments remain in a domain where the chosen branch is analytic. In practice, this requires choosing h small enough and, when needed, selecting a direction u that does not cross a cut. Rotation invariance (Section 10) can be exploited to pick numerically safe directions.

9.3. Diagnostics for Slice Evaluability and Branch Consistency

Assumption 1 can fail in practice when f contains non-holomorphic operations (e.g., $|\cdot|$, $\text{Re}(\cdot)$, conditionals that depend on the sign of $\text{Im}(\cdot)$) or when a multi-valued analytic

function is evaluated on different branches after a complex/bicomplex perturbation. Since such failures may be silent in black-box codes, we recommend lightweight diagnostics:

Direction-consistency check. Compute the same derivative using two independent directions u_1, u_2 (e.g., orthogonal unit pure quaternions) with the *same* step size. For slice-evaluable functions, the results agree up to roundoff; a discrepancy well above a few hundred machine epsilons typically indicates a violation of the slice assumption or an unstable choice of h .

Step-halving stability. For a fixed direction u , compare the extracted coefficient at h and $h/2$. For second-order quantities where the leading truncation is $\mathcal{O}(h^2)$, the difference should decay by roughly a factor of 4 until roundoff dominates.

Branch consistency for multi-valued functions. When using $\log$ or $\sqrt{\cdot}$, verify that the perturbed points remain inside a simply connected region where the branch is fixed. A practical surrogate is to compare evaluations at $z + ih$ and $z - ih$; if f is real on the real axis and branch-consistent, then one expects $f(z - ih) \approx \overline{f(z + ih)}$ for small h .

These checks are inexpensive (one or two extra evaluations) and are useful to prevent overconfident claims of “cancellation-free” accuracy when the analytic continuation assumption is violated.

9.4. Step-Size Heuristics

For first derivatives, h may be taken as small as permitted by the function evaluator and overflow/underflow constraints (complex-/quaternion-step does not involve subtraction of close real values). For second-order quantities extracted from an h^2 -scaled coefficient (double-step f'' and one-shot f_{xy}), the relevant model is

$$\text{error} \approx C_{\text{tr}} h^2 + C_{\text{ro}} \frac{\varepsilon}{h^2},$$

so the balancing choice is

$$h \approx \varepsilon^{1/4} \max(1, |z|),$$

up to problem-dependent constants. This matches the empirically observed “sweet spot” in Sections 10 and 10.7.

9.5. Evaluation Cost Comparison

Table 1 summarizes the *evaluation counts* required by representative $\mathcal{O}(h^2)$ approximations, which is the right metric when function calls dominate (e.g., PDE solves, legacy simulators, or expensive objective functions). Two practical caveats are worth noting.

First, a “bicomplex evaluation” is not free: if bicomplex arithmetic is implemented via the standard idempotent decomposition, then one bicomplex call typically reduces to two complex calls (and thus, roughly, two real-valued runs for codes that already support complex arithmetic). Even with this overhead, the double-step can remain attractive when it replaces multi-point real stencils that suffer cancellation or require additional bookkeeping.

Second, in high dimensions the dominant scaling is combinatorial: assembling a full $n \times n$ Hessian from mixed partials requires $\mathcal{O}(n^2)$ evaluations for *any* black-box coefficient-extraction approach (finite differences, hyper-dual, or multicomplex variants). When only Hessian-vector products or selected entries are needed, directional variants (Section 8) reduce cost substantially and are often the right compromise in large-scale optimization.

Table 1. Function evaluation counts for representative derivative approximations (scalar functions). “Evaluations” counts calls to the underlying function evaluator in the indicated arithmetic. For methods that also require $f(x)$, we list the total calls assuming $f(x)$ is not already cached (in which case one call can be saved).

Quantity	Method	Evaluations	Cancellation Risk
$f'(x)$	Forward difference	2 ($x, x+h$)	High
$f'(x)$	Central difference	2 ($x-h, x+h$)	Medium
$f'(x)$	Complex-step/ u -step	1 ($x+ih$ or $x+uh$)	Low
$f'(x)$	Hyper-dual (if available)	1 (hyper-dual)	Low
$f''(x)$	Central second difference	3 ($x-h, x, x+h$)	High
$f''(x)$	Subtractive complex-step	2 ($x, x+ih$)	Medium–High
$f''(x)$	Bicomplex double-step	2 ($x, x+2ih$) ¹	Low (real differencing)
$f''(x)$	Hyper-dual (if available)	1 (hyper-dual)	Low
$f_{xy}(x, y)$	Central mixed stencil	4	High
$f_{xy}(x, y)$	One-shot bicomplex (u, i) step	1 (bicomplex)	Low (real differencing)
$f_{xy}(x, y)$	Hyper-dual (if available)	1 (hyper-dual)	Low

¹ Via idempotent decomposition, a bicomplex evaluation reduces to two complex evaluations at the conjugate points x and $x+2ih$ for scalar analytic functions; for general black-box codes the bicomplex extension may be implemented explicitly.

Remark 5 (comparison with hyper-dual approaches). *Hyper-dual numbers can return first and second derivatives “exactly” (up to floating-point roundoff) in a single evaluation provided the entire computation of f is implemented over the hyper-dual algebra (typically via operator overloading). This is powerful for source-available codes, but it is often unavailable for black-box solvers (e.g., legacy PDE codes) that only accept real/complex inputs. By contrast, the slice-based rules here require only the ability to evaluate f at complex/quaternionic perturbations and then apply a fixed projection to extract coefficients.*

10. Numerical Experiments

All computations were performed in IEEE double precision. The figures report relative errors versus step size h on logarithmic scales.

10.1. Compact Numeric Summary

To complement the log–log plots, Table 2 reports (for the representative points used in Figures 1–4) the smallest relative error observed over the step-size sweep and the corresponding minimizer h_{opt} . All values were computed in IEEE double precision by sweeping $h \in [10^{-1}, 10^{-40}]$ on a log grid.

Table 2. Compact numeric summary of the step-size sweeps: minimum observed relative error and the corresponding h_{opt} .

Test	Quantity	Method	Min Rel. Error	h_{opt}
e^x at $x=1$	$f'(1)$	complex-step/ u -step	1.63×10^{-16}	2.38×10^{-8}
e^x at $x=1$	$f''(1)$	central second difference	3.40×10^{-9}	2.00×10^{-4}
e^x at $x=1$	$f'''(1)$	subtractive complex-step	2.14×10^{-9}	3.68×10^{-5}
e^x at $x=1$	$f'''(1)$	bicomplex double-step	2.14×10^{-9}	3.68×10^{-5}
$\log(1+x)$ at $x=0.3$	$f'(0.3)$	complex-step/ u -step	1.44×10^{-16}	4.38×10^{-9}
$\log(1+x)$ at $x=0.3$	$f''(0.3)$	central second difference	9.80×10^{-9}	6.48×10^{-5}
$\log(1+x)$ at $x=0.3$	$f'''(0.3)$	subtractive complex-step	2.47×10^{-9}	1.14×10^{-4}
$\log(1+x)$ at $x=0.3$	$f'''(0.3)$	bicomplex double-step	1.38×10^{-9}	6.48×10^{-5}

10.2. First Derivative Accuracy and Comparison

Figure 1 compares forward differences, central differences, and complex-step/ u -step differentiation for $f(x) = e^x$ at $x=1$. As expected, complex-step achieves $\mathcal{O}(h^2)$ truncation

without cancellation and remains accurate for very small steps, while finite differences deteriorate once rounding dominates.

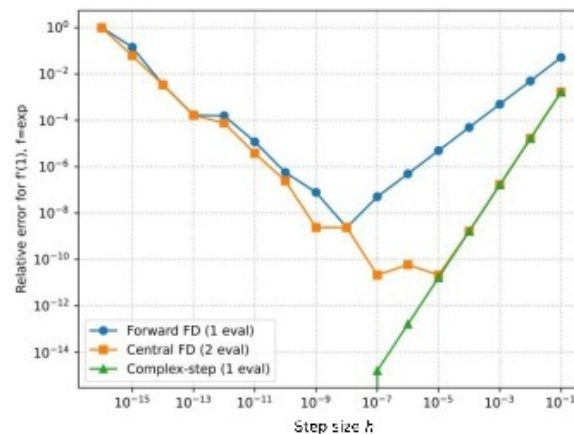


Figure 1. Relative error for $f'(1)$ with $f(x) = e^x$ using forward difference, central difference, and complex-step/ u -step.

10.3. Second Derivatives: Subtraction vs. Bicomplex Double-Step

Figure 2 compares three $\mathcal{O}(h^2)$ methods for $f''(1)$ with $f(x) = e^x$: central differences, a subtractive complex-step second derivative formula, and the bicomplex double-step (10). The subtractive complex-step method eventually loses accuracy as h decreases due to cancellation in $f(x) - \operatorname{Re} f(x + ih)$. In contrast, the bicomplex double-step follows the predicted error model from Section 6: truncation decreases like $\mathcal{O}(h^2)$ until the unavoidable amplification of floating-point noise by the $1/h^2$ scaling becomes visible, producing a characteristic “sweet spot” near $h \approx \varepsilon^{1/4}$.

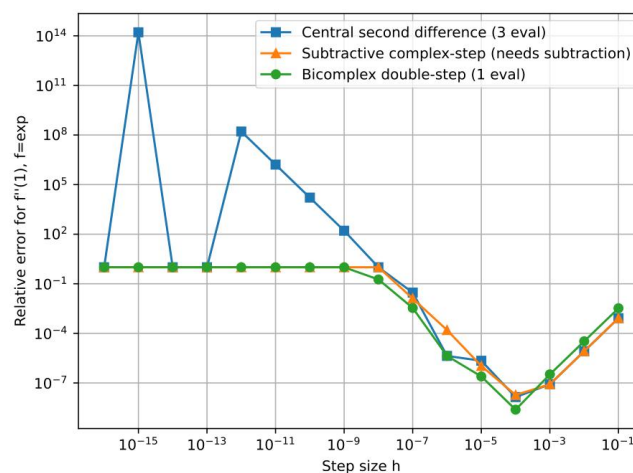


Figure 2. Relative error for $f''(1)$ with $f(x) = e^x$: central finite differences, subtractive complex-step second derivative, and bicomplex double-step.

10.4. Mixed Partial from One Evaluation

For $f(x, y) = e^{xy}$ at $(x, y) = (0.7, -0.2)$, Figure 3 reports errors for f_x , f_y , and f_{xy} extracted from one bicomplex evaluation as in Theorem 4. A standard central mixed-partial stencil (four evaluations) is included for comparison.

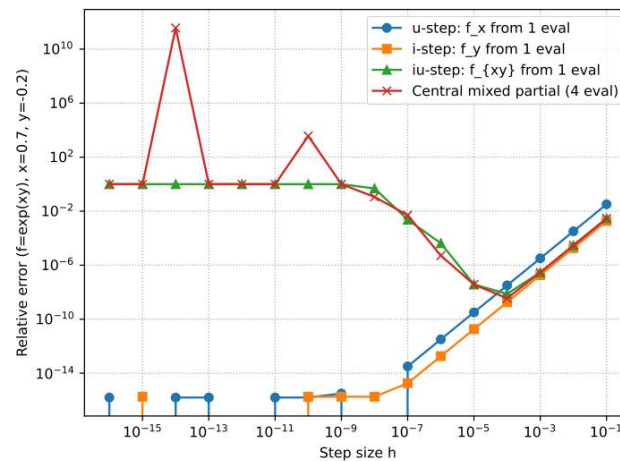


Figure 3. Relative errors for f_x , f_y , and f_{xy} of $f(x, y) = e^{xy}$ extracted from one evaluation at $(x + uh, y + ih)$. The central mixed-partial stencil requires four evaluations and exhibits cancellation for small h .

10.5. A Non-Entire Example: $f(x) = \log(1 + x)$

To illustrate behavior for a function with a branch cut, we test $f(x) = \log(1 + x)$ at $x = 0.3$ using the principal branch. Since $1 + x$ stays away from the negative real axis under small imaginary perturbations, the complex-step and bicomplex evaluations are well-defined. Figure 4 reports relative errors for $f'(x)$ and $f''(x)$ using representative methods. As in the exponential case, the subtractive complex-step second derivative loses accuracy for very small h , while the bicomplex double-step remains stable until the h^2 scaling reaches rounding limits.

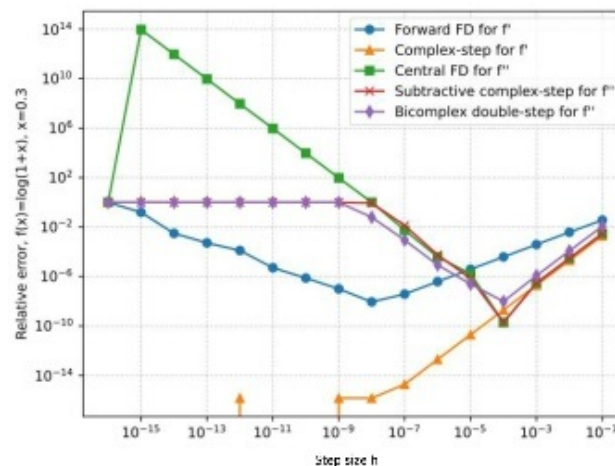


Figure 4. Relative errors for $f'(0.3)$ and $f''(0.3)$ with $f(x) = \log(1 + x)$: forward difference and complex-step for f' , and central differences, subtractive complex-step, and bicomplex double-step for f'' .

10.6. Direction Invariance in the j - k Plane

We verified numerically that the u -step derivative is independent of the chosen unit direction u up to rounding error. Figure 5 plots (i) the range across directions $u(\theta) = \cos \theta j + \sin \theta k$ of the computed derivative and (ii) the mean relative error. The range is at the level of 10^{-15} across the tested steps, confirming invariance to floating-point accuracy.

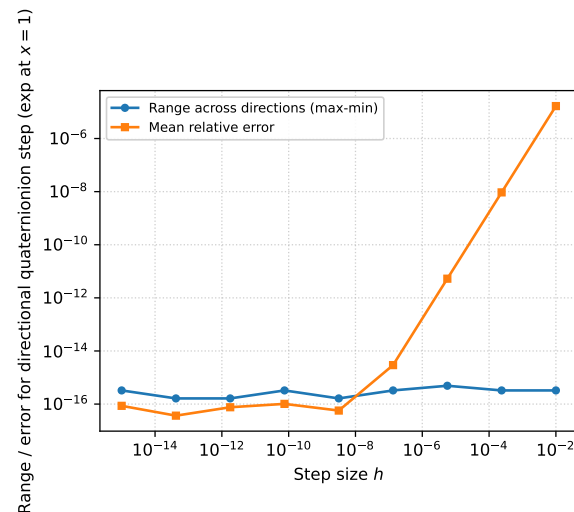


Figure 5. Directional invariance for $f'(1)$ with $f(x) = e^x$ using $u(\theta)$ in the j - k plane: range across directions (max-min) and mean relative error.

10.7. A PDE-Driven Sensitivity Example (Screened Poisson)

To demonstrate that the double-step remains effective when a single “function evaluation” involves a nontrivial solver, we consider a parameter-dependent elliptic model on $\Omega = (0, 1)^2$:

$$-\Delta u(x, y; p) + p u(x, y; p) = \sin(\pi x) \sin(\pi y), \quad u|_{\partial\Omega} = 0,$$

and take as quantity of interest the point value $J(p) := u(x_*, y_*; p)$ at the grid point closest to $(x_*, y_*) = (1/2, 1/2)$ after a standard five-point finite-difference discretization. For real p , the discrete solve returns a real $J(p)$; for complex (or bicomplex) p the same linear system is solved in complex arithmetic.

Figure 6 reports the relative error in $J''(p)$ at $p = 0.7$ computed by (i) a central second difference in p , (ii) the subtractive complex-step second derivative, and (iii) the bicomplex double-step (10). The reference $J''(p)$ is obtained by differentiating the shifted linear system $(A + pI)u = b$ analytically and solving two auxiliary linear systems. The experiment is consistent with the scalar tests: the bicomplex double-step exhibits an $\mathcal{O}(h^2)$ regime and delays the small-step breakdown compared with subtraction-based alternatives.

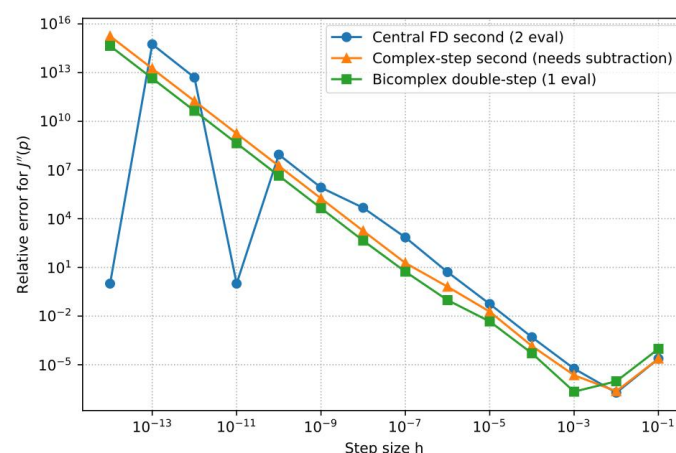


Figure 6. Relative error for the PDE sensitivity $J''(p)$ at $p = 0.7$ (screened Poisson discretization): central second differences, subtractive complex-step, and bicomplex double-step.

11. Conclusions

We have developed two complementary, cancellation-free differentiation tools:

Directional quaternion-step rule that computes $f'(z)$ from a single evaluation $f(z + uh)$ by an explicit projection onto the u -component and is rotation invariant with respect to the choice of unit pure quaternion u ; and bicomplex double-step calculus on the commuting slice generated by i and u , in which one evaluation at $z + (i + u)h$ separates derivative information into distinct coefficients and yields a subtraction-free $\mathcal{O}(h^2)$ approximation of $f''(z)$ from the iu -component.

For bivariate analytic functions, the same slice viewpoint leads to one-shot identities for mixed partials from $f(x + uh, y + ih)$, and Lemma 2 supplies practical coefficient-extraction formulas needed for robust implementations. The numerical experiments support the analysis, highlight stable step-size regimes for second-order quantities, and confirm direction-independence up to rounding.

Several extensions are natural. First, higher-order derivative extraction via multicomplex/hypercomplex embeddings can be developed in a way that preserves the projection-based invariance principle. Second, for non-entire functions with branch points, a more systematic treatment of branch-cut geometry on bicomplex slices would sharpen the practical safeguards discussed in Section 9. Finally, integrating these ideas with modern automatic differentiation pipelines may offer hybrid methods that retain cancellation-free behavior while scaling to very large parameter dimensions.

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Conflicts of Interest: The authors declare no conflict of interest.

Appendix A. Coefficient Extraction Identities

For completeness, we record identities useful in code. Lemma 2 gives closed forms based on involutions. In implementations it is often more efficient to work with an explicit representation

$$w = (a + bi) + (c + di)u, \quad a, b, c, d \in \mathbb{R},$$

and then read off $[w]_{iu} = d$.

Appendix B. Idempotent Decomposition of $\mathbb{B}_u$

Let $j := iu$ so that $j^2 = 1$. Define idempotents $e_{\pm} = (1 \pm j)/2$ satisfying $e_{\pm}^2 = e_{\pm}$ and $e_+e_- = 0$. Every $w \in \mathbb{B}_u$ can be written uniquely as

$$w = w_+e_+ + w_-e_-,$$

where $w_{\pm} \in \mathbb{C}(i)$ are complex numbers. If $w = x + yu$ with $x, y \in \mathbb{C}(i)$, then $w_{\pm} = x \mp iy$. For any holomorphic function f (defined by power series), one has

$$f(w) = f(w_+)e_+ + f(w_-)e_-,$$

reducing bicomplex evaluation to two complex evaluations. This provides a robust route to implement elementary functions on $\mathbb{B}_u$ [12].

Appendix C. Exactness for Low-Degree Polynomials and Scaling Limits

The coefficient-extraction viewpoint clarifies when the step formulas are exact.

Appendix C.1. Exactness Statements

If f is a polynomial of degree ≤ 1 , then $[f(z + uh)]_u/h$ equals $f'(z)$ exactly for all h . If f is a polynomial of degree ≤ 2 , then the bicomplex double-step coefficient $[f(z + (i + u)h)]_{iu}/h^2$ equals $f''(z)$ exactly for all h . More generally, for analytic f the truncation error is governed by the first omitted odd (respectively even) term in the Taylor expansion.

Appendix C.2. Why Second-Order Coefficients Cannot Use Arbitrarily Tiny Steps

For f'' and mixed partials, the informative coefficient is proportional to h^2 . In floating-point arithmetic, if the computed function value has relative error $\mathcal{O}(\varepsilon)$, then the smallest reliably representable h^2 -scaled coefficient is typically $\mathcal{O}(\varepsilon|f|)$. Hence the effective floor for the relative error of f'' is reached once $h^2|f''| \lesssim \varepsilon|f|$. This motivates the standard balance for second-order quantities $h \approx \varepsilon^{1/4} \max(1, |z|)$ (cf. Section 6).

Appendix D. Reference Pseudocode

The following pseudocode illustrates the minimal logic needed to compute f' and f'' from one evaluation.

Listing A1. Skeleton pseudocode for the u -step and bicomplex double-step methods.

```
# Input: analytic scalar function f, point z (real or complex), step h, unit direction u
# Output: approximations to f'(z) and f''(z)

# First derivative (u-step):
w1 = f(z + u*h)           # evaluation in the slice C_u
fprime = coeff_u(w1)/h     # extract u-coefficient

# Second derivative (double-step):
w2 = f(z + (i + u)*h)      # evaluation in bicomplex slice B_u
fsecond = coeff_iu(w2)/h**2 # extract i*u coefficient
```

Appendix E. Reference Wall-Clock Timings

To support the practical efficiency discussion, we report indicative wall-clock timings from a simple *Python* prototype (double precision). These timings are not meant as definitive performance claims (they depend strongly on language, compiler, BLAS/LAPACK backends, and implementation details), but they provide an order-of-magnitude reference.

Environment. Python 3.11.2 with NumPy 1.24.0 and SciPy 1.14.1 on Linux-4.4.0-x86_64-with-glibc2.36.

Scalar microbenchmark. We compute $f''(x)$ for $f(x) = e^x$ at $x = 1$ with $h = \varepsilon^{1/4}$ and report average time per call over 2×10^4 repetitions (after warm-up).

Table A1. Scalar microbenchmark (average time per f'' call).

Method	Time [μ s]
Central second difference (3 real evals)	0.40
Subtractive complex-step (1 real + 1 complex eval)	0.39
Double-step (1 real + 1 complex eval at $x + 2ih$)	0.41

PDE sensitivity microbenchmark. We solve $(-\Delta + p)u = 1$ on the unit square with Dirichlet boundary conditions using a standard 5-point finite difference discretization

($n = 35$ interior points per direction, $N = n^2$ unknowns) and a sparse direct solve. We set $J(p) := \text{mean}(u)$ and compute $J''(p)$ at $p = 1$ with $h = \varepsilon^{1/4}$. The central second difference requires three real solves; the complex-step variants require one real and one complex solve.

Table A2. PDE microbenchmark (average time per J'' call).

Method	Time [ms]
Central second difference (3 real solves)	10.0
Subtractive complex-step (1 real + 1 complex solve)	6.5
Double-step (1 real + 1 complex solve at $p + 2ih$)	6.2

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