CONSERVATION LAWS: FROM DIFFERENTIAL TO DIFFERENCE

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My research this past summer aimed at characterizing conservation laws of difference equations arising from differential equations, and their relationship to smooth conservation laws. Ultimately, the goal of such a characterization was to better understand admissible discretizations of differential equations that yield consistent and conservative numerical methods, which naturally have many desirable qualities [1–3]. This process began with reviewing the analogous theory for differential equations, which relies heavily on differential-geometric formalism [4, 5]. The translation of this theory to the discrete world and difference equations was the main "novel" portion of my work, and began largely by consolidating similar attempts [6–10].

1. *Conservation Laws of Differential Equations*

A **conservation law** of a (ordinary or partial) differential equation $F[\boldsymbol{x}, \boldsymbol{u}] \coloneqq F(x^1, ..., x^p; u^1, ..., u^q; u^\alpha_{x^i}; \cdots) = 0$ in p independent and q dependent variables is a function $\varphi[\boldsymbol{x}, \boldsymbol{u}]$ that is identically constant on solutions to F; in other words

$$(\text{Div } \varphi)|_{F=0} = 0. \tag{1}$$

Classical examples include conservation of mass, energy, momentum, and other physical quantities arising in physical systems. For instance, the classical Hamiltonian system in generalized coordinates with energy $H = H(p, q)$,

$$F(p, q, \dot{p}, \dot{q}) = \begin{pmatrix} \dot{p} \\ \dot{q} \end{pmatrix} - \begin{pmatrix} -\frac{\partial H}{\partial q} \\ \frac{\partial H}{\partial p} \end{pmatrix}, \tag{2}$$

has H as a conserved quantity

$$\text{Div } H \,|_{F=0} = \left[\dot{p} \cdot \partial_p H + \dot{q} \cdot \partial_q H\right]|_{F=0} = -\partial_q H \cdot \partial_p H + \partial_q H \cdot \partial_p H = 0. \tag{3}$$

The study of conservation laws is frequently used to study various properties of differential equations.

Under appropriate assumptions of nondegeneracy of F, domain, etc., every conservation law can be written in **characteristic form**

$$\text{Div } \varphi = \Lambda \cdot F, \tag{4}$$

where $\Lambda[\boldsymbol{x}, \boldsymbol{u}]$ is the **characteristic** or **multiplier** of φ [4]; for instance, the conservation law multiplier for H of Equation 2 is given by $\Lambda = \begin{pmatrix} H_q & H_p \end{pmatrix}$. Hence, finding conservation laws for F amounts to finding functions Λ such that $\Lambda \cdot F$ is a divergence term.

To this end, we introduce the **Euler operator** for the dependent variable u^α

$$\mathcal{E}_\alpha \coloneqq \sum_I (-D)_I \frac{\partial}{\partial u^\alpha_I}, \tag{5}$$

where the summation is over all multiindices $I = (i_1, ..., i_k)$ with $0 \leq i_j \leq p, k \geq 0$; we define $\mathcal{E} = \left(\mathcal{E}_1, ..., \mathcal{E}_q\right)$. Those familiar with the calculus of variations will recognize this operator as yielding determining (necessary, not sufficient) equations for extremals of variational problems. For our purposes, the real interest in this operator is in the characterization of its kernel (see [4]),

$$\ker\,\mathcal{E} = \{L : L = \text{Div}\ P\}, \tag{6}$$

that is, the kernel of $\mathcal{E}$ is composed precisely of divergence terms. Hence, taking $\mathcal{E}$ of both sides of Equation 4, we have that

$$\mathcal{E}(\Lambda \cdot F) = 0, \tag{7}$$

and thus finding conservation law multipliers for F amounts to solving the differential equation arising from the Euler-Langrange equations for $\Lambda \cdot F$ for Λ (see for instance [11] for examples); to study conservation laws, we study the Euler operator.

The Euler operator arises intrinsically as one of the operators (more precisely, as the composition of a quotient map and a "vertical" exterior derivative) in the **variational bicomplex**, a framework from differential geometry used to study variational calculus on abstract spaces [5]. While the rest of the complex is worth studying in its own right, the most notable (for our purposes) is the component known as the **Euler-Lagrange complex** (or "variational complex" in [4])

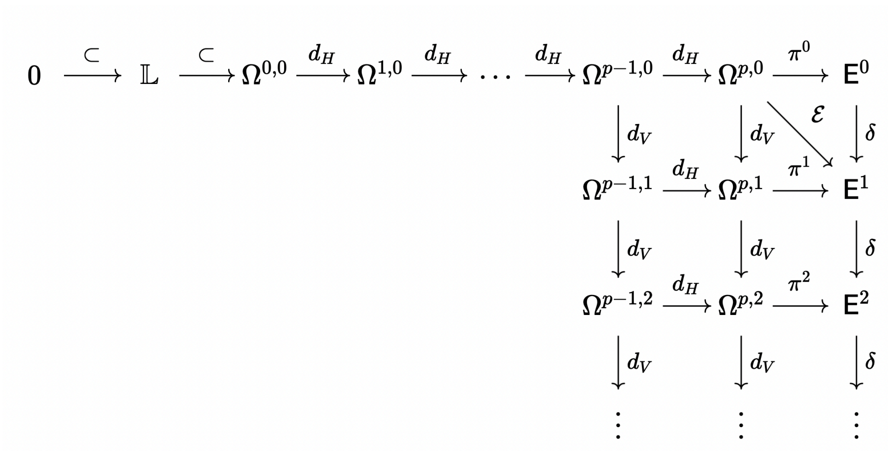

Figure 1. The Euler-Lagrange Complex

where $E^s := \Omega^{p,s}/\ \text{im}\{\mathrm{d}_H : \Omega^{p-1,s} \to \Omega^{p,s}\}$ are the relevant cohomology vector spaces. Without getting too into the details, this structure is analogous to the de Rham complex for functions on a manifold, but for differential equations viewed as smooth functions on the infinite jet bundle of a fibered manifold (which we typically take to be a trivial fiber $\pi : \mathbb{R}^p \times \mathbb{R}^q \to \mathbb{R}^p$ for simplicity); the vertical derivative d_V corresponds to partial differentiation with respect to the dependent variables $\boldsymbol{u}$, and the horizontal derivative d_H corresponds to total differentiation with respect to the independent variables $\boldsymbol{x}$. This results in a vertically unbounded and horizontally bounded (by the dimension of the independent variables) bicomplex; we denote in brief $\{\Omega^{i,\alpha}; \mathrm{d}_V, \mathrm{d}_H\}$.

A complex is **exact** if $\mathrm{d}\omega = 0$ if any only if $\omega = \mathrm{d}\eta$ for some appropriate form η. Exactness at the $\Omega^{p-1,0} \overset{\mathrm{d}_H}{\to} \Omega^{p,0} \overset{\mathcal{E}}{\to} E^1$ (where $\mathcal{E} = \pi^1 \circ \mathrm{d}_V$) is equivalent, in this framework, to the characterization of the kernel of the Euler operator given by Equation 6. In short, studying this complex, its exactness, and its overall structure is vital to understanding conservation laws of differential equations. We seek to create a similar complex in the discrete case of difference equations to study discrete conservation laws.

2. *Conservation Laws of Difference Equations*

A **difference equation** is an equation involving independent **lattice** variables $\boldsymbol{n} = (n^1, ..., n^p) \in \mathbb{L}^p$, unknown dependent variables $\boldsymbol{u_n} = (u^1_{\boldsymbol{n}}, ..., u^q_{\boldsymbol{n}})$, and finitely many **shifts** $\boldsymbol{u_{n+m}}$:

$$F[\boldsymbol{n}, \boldsymbol{u_n}] := F(\boldsymbol{n}; \boldsymbol{u_n}, ..., \boldsymbol{u_{n+m}}) = 0. \tag{8}$$

Solving a difference equations then amounts to finding a $\mathbb{L}$-indexed real-valued sequence $\{u^\alpha_{\boldsymbol{n}}\}_{\boldsymbol{n}\in\mathbb{L}}$ for each $\alpha = 1, ..., q$. These arise naturally in finite difference discretizations of difference equations, though we take the lead of [8, 6] of omitting explicit reference to any continuum limit until necessary (also allowing for consideration of more general difference equations).

A conservation law of a difference equation is a function $\varphi[\boldsymbol{n}, \boldsymbol{u_n}]$ that is constant on solutions to F, or equivalently,

$$(\boldsymbol{\Delta}\varphi)|_{F=0} = \sum_{i=1}^{p} \Delta_i \varphi|_{F=0} = \sum_{i=1}^{p} (S^1_i - \mathrm{id})\varphi|_{F=0} = 0, \tag{9}$$

where S^j_i denotes the **shift** operator by a shift j in the coordinate i; ie

$$S^j_i : \mathbb{L} \to \mathbb{L}, \quad (n^1, ..., n^i, ..., n^p) \mapsto (n^1, ..., n^i + j, ..., n^p). \tag{10}$$

We can again speak of characteristics of conservation laws here,

$$\boldsymbol{\Delta}\varphi = \Lambda \cdot F, \tag{11}$$

and we additionally have a discrete Euler operator

$$\hat{\mathcal{E}}_\alpha = \sum_{|I|=p} S^{-I} \frac{\partial}{\partial u^\alpha_I}, \tag{12}$$

where $S^{-I} = S^{-(i_1,...,i_p)} = S_1^{-i_1} \cdots S_p^{-i_p}$, with the characterization of its kernel (see [12] for a direct proof, or [8] for an "intrinsic" proof)

$$\ker \hat{\mathcal{E}} = \{L : L = \boldsymbol{\Delta}P\}; \tag{13}$$

one can find conservation laws by solving the "discrete Euler equations" for $\Lambda \cdot F$ [13, 14].

Both [6] and [8] construct discrete analogs to the variational bicomplex (with the former only considering the outer Euler-Lagrange complex) with the discrete Euler operator serving the same role; in this case vertical differentiation corresponds to partial differentiation in the independent variables u^α_i, and horizontal differentiation corresponds to the finite difference operators Δ_i. We denote the discrete variational bicomplex $\left\{\hat{\Omega}^{i,\alpha}; \hat{\mathrm{d}}_V, \hat{\mathrm{d}}_H\right\}$ to distinguish from the smooth.

3. *Novel Work and Future Directions*

The constructions of [6] and [8] are quite different in their approaches and a lot of time was spent consolidating them. In short, while the general complexes are compatible, the underlying algebra of functions in the former is far larger (in my opinion, too large to be practically useful), containing as a subalgebra the functions considered in the latter. Moreover, the notation, while not a major issue, varied widely. For instance, Hydon considers difference equations as in Equation 8, namely, the reliance on the dependent variables is explicitly tied to the dependence on the independent variable $\boldsymbol{n}$; upon changing $\boldsymbol{n}$, the specific $u_{\boldsymbol{n}}$ considered in the function also changes. On the other hand, Zhanirov allows the dependence on the two "types" of inputs to vary independently. The two, however, are identical under the change of variables $(\boldsymbol{n}, \boldsymbol{u}) \mapsto (\boldsymbol{n}, S^{\boldsymbol{n}}\boldsymbol{u})$. It is often easier to work in the variables of Zhanirov for the sake of technical proofs, but in that of Hydon for practical applications.

Another notable difference between the two complexes is in the proof of exactness. While the complex of Hydon is more practical, exactness is claimed, not proven. I have independently proven it, using techniques as outlined in [8], [4], but the proof would be too long (and not too interesting; it is largely computational) for inclusion here.

Exactness of the inner rows of the complex is yet to be resolved and is subject to further investigation. Proofs of exactness of complexes (say, $\{\Omega^\bullet, \mathrm{d}^\bullet\}$) tend to involve finding **homotopy operators**, linear maps

$$h^k : \Omega^k \to \Omega^{k-1} \tag{14}$$

such that for any $\omega \in \Omega^k$,

$$\omega = h^{k+1}\big(\mathrm{d}^k\omega\big) + \mathrm{d}^{k-1}\big(h^k\omega\big); \tag{15}$$

if $\mathrm{d}^k\omega = 0$, then by linearity of h^k, $\omega = \mathrm{d}^{k-1}\big(h^k\omega\big)$ and $h^k(\omega)$ gives the preimage of ω, hence proving exactness. The relevant homotopy operators in the proof of exactness of the inner rows of the smooth variational bicomplex as presented in [5] require the notion of contact forms, which (as [8] notes as well) is not a clear task in this context. Hence, it is not currently clear how to proceed in proving exactness of the inner rows of the complex.

With the general framework in place, there are several questions that I am still working to answer.

The first involves discussing convergence of the discrete variational bicomplex. I would like to be able to say that the discrete converges, in some sensible notion of convergence, to the true variational bicomplex. While this seems reasonable, it has still yet to be rigorously resolved. The issue in this sense lies mainly in properly defining what we mean by convergence. Namely, the underlying spaces in the smooth, discrete complexes are intrinsically different and hence the relevant function spaces are as well. One idea for consolidation is to identify the discrete functions in $\widehat{\Omega}^{i,\alpha}$ with piecewise polynomials in $\Omega^{i,\alpha}$. This clearly embeds the relevant function spaces, but doesn't clearly resolve the relationship between the differentiation operators $\widehat{\mathrm{d}}_V, \widehat{\mathrm{d}}_H$ and $\mathrm{d}_V, \mathrm{d}_H$. Notably, the discrete complex is *not* a subcomplex of the smooth complex; mapping a discrete function to a polynomial and differentiating is not equivalent, in general, to differentiating first and then mapping to a polynomial. This is the major difference between this approach and similar approaches to discretizing complexes in [15–17] where the complex built is by construction a subcomplex of the smooth.

A second question, also involving convergence, relates to discrete conservation laws of difference equations arising as discretizations of differential equations; namely, I'd like to be able to describe admissible discretizations for differential equations such that their discrete conservation laws are consistent with their smooth counterparts. This, too, has yet to be resolved; indeed many authors ignore the continuum case in general. We can summarize our ambitions pictorially

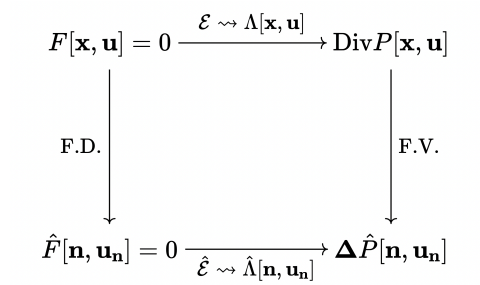

Figure 2. Our "goal": making this diagram commute

While the top (smooth) and bottom (discrete) rows of this diagram are well-understood, the "F.D." (finite difference) and "F.V." (finite volume) connecting arrows are our current areas of interest.

One current approach I have been taking is to try to develop more general discrete Euler operators for arbitrary finite difference schemes. Namely, if

$$\Delta = \sum_{i \in \mathbb{Z}} c_i \cdot S_i \tag{16}$$

is an arbitrary finite difference operator where only finitely many constants c_i are non-zero, I would like to construct a corresponding Euler-type operator $\mathcal{E}_\Delta$ with kernel $\{L : L = \Delta P\}$ and (this is a less clear task) who's image converges to that of the regular Euler operator. The main idea used here is to mirror the "natural derivation" of the Euler operator; the smooth Euler operator naturally arises after repeated integration by parts and modding out by divergence terms, while the discrete Euler arises from repeated summation by parts and modding out by forward differences $S^1 - \mathrm{id}$. Similarly, when working with a more general Δ, we can sum by parts and reduce the typical image of the operator $\pi^1 \circ \mathrm{d}_V$ to a form in E^1 that involves a constant, fixed number of basis forms. Explicit formulae for the resulting Euler-type operators are then directly computable. The question of convergence of these operators has not been resolved and requires deeper investigation, but their derivation is novel.

Overall, this research project has so far yielded a deeper understanding of discrete conservation laws. While my main goals have not yet been resolved, the constructions made and proofs established have made the path forward far clearer than before.

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