Continuous and Discrete Homotopy Operators: A Theoretical Approach made Concrete ⋆

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Abstract

Using standard calculus, explicit formulas for the one-dimensional continuous and discrete homotopy operators are derived. It is shown that these formulas are equivalent to those in terms of Euler operators obtained from the variational complex.

The continuous homotopy operator automates integration by parts on the jet space. Its discrete analogue can be used in applications where summation by parts is essential. Several example illustrate the use of the homotopy operators.

The calculus-based formulas for the homotopy operators are easy to implement in computer algebra systems such as *Mathematica* and *Maple*. The homotopy operators can be readily applied to the symbolic computation of conservation laws of nonlinear partial differential equations and differential-difference equations.

Key words: homotopy operator, exactness, conservation law, computer algebra
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1 Introduction

During the development of symbolic algorithms [4–6] for the computation of conservation laws of nonlinear partial differential equations (PDEs) and nonlinear differential-difference equations (DDEs) we encountered powerful tools from the calculus of variations and differential geometry that deserve

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attention in their own right. This paper focuses on one of these tools: the homotopy operator.

Inspired by work of Kruskal *et al.* [9], we give a straightforward derivation of formulas for the continuous homotopy operator and its discrete counterpart. We show that our formulas are equivalent to those in terms of Euler operators obtained from the variational complex [6]. For lack of space, we only cover the one-dimensional cases (1D) with independent variable x or lattice variable n. The generalization to multiple independent variables is cumbersome [5].

The continuous homotopy operator goes back to Volterra's work [13] on the inverse problem of the calculus of variations. The homotopy operator also appears in the proof of the converse of Poincaré's lemma [12], which states that exact differential forms are closed and vice versa (at least on a star-shaped domain in Euclidean space). Poincaré's lemma is a special case of the so-called *de Rham complex*, where one investigates the equivalence of closedness and exactness of differential $k-$forms in generality. The key to exactness proofs of various complexes (such as the de Rham complex) is the construction of suitable homotopy operators [12].

In basic terms, the 1D continuous homotopy operator reduces the problem of integration by parts on the jet space to a sequence of differentiations followed by a single definite integration with respect to an auxiliary variable. In 2D and 3D, the homotopy operator allows one to invert the total divergence operator [12]. Irrespective of the number of independent or dependent variables, the problem can be reduced to a single definite integral. Applications of the continuous homotopy operator in multi-dimensions can be found in [4,5,12].

Likewise, the discrete homotopy operator is a tool to invert the forward difference operator whatever the application is. It circumvents summation by parts by applying shifts and differentiations followed by a one-dimensional integration with respect to an auxiliary variable [6]. Applications of the discrete homotopy operator are given in [5,6].

As shown in [8,10], the parallelism between the continuous and discrete cases can be made rigorous as both can be formulated in terms of variational bicomplexes. We do not use the abstract framework in order to make this paper accessible to as wide an audience as possible. Aficionados of *de Rham* complexes should consult [2,3] and [8,10,11]. The latter set of papers covers the discrete variational bicomplex.

Several examples illustrate the inner workings of the homotopy operator at the calculus level, without "wedges and hooks" or differential forms. Avoiding sophisticated arguments from differential geometry, we can introduce the powerful concept of homotopy operators to a wider audience.

In [4–6] we apply homotopy operators to the symbolic computation of conservation laws of nonlinear PDEs and DDEs. Beyond DDEs, the discrete homotopy operator is useful in the study of difference equations [8,10,11].

Despite their universality and applicability, homotopy operators have not been implemented in major computer algebra systems (CAS) like *Mathematica* and *Maple*. CAS offer few reliable tools for integration (or summation) by parts of expressions involving *unknown* functions and their derivatives (or shifts). We hope that the calculus-based formulas for the homotopy operator presented in this paper will lead to more sophisticated integration algorithms within CAS.

In summary, our paper has the following objectives: (i) Give a straightforward derivation of the 1D continuous homotopy operator, (ii) Present the discrete homotopy operator by analogy with the continuous case, (iii) Illustrate the inner workings of the homotopy operators at the calculus level, (iv) Present alternate, readily applicable formulas for the homotopy operators which lead to efficient and fast symbolic codes for integration and summation by parts.

2 Derivation of the continuous homotopy operator in 1D

In [4,5], we presented the homotopy operator and referred to [12] for a proof, which involves working with differential forms. Inspired by [9], we give a calculus-based derivation of the homotopy operator $\mathcal{H}_{u(x)}$. For simplicity and clarity, we show the derivation for one dependent variable u and one independent variable x (henceforth referred to as the 1D case).

To do so, we first introduce a "degree" operator $\mathcal{M}$ and its inverse, the total derivative $\mathcal{D}_x$, and the Euler operator $\mathcal{L}^{(0)}_{u(x)}$. The latter is also called the variational derivative or Euler-Lagrange operator.

The calculations below are carried out in the *jet space* where one treats u, u_x, u_{2x}, etc., as independent. As usual, $u_x = \frac{\partial u}{\partial x}, u_{2x} = \frac{\partial^2 u}{\partial x^2}$, etc. The operators act on $f(u, u_x, u_{2x}, \ldots, u_{Mx})$. Such functions are called *differential functions* [12]. Throughout this paper we assume that the differential functions lack constant terms and that the upper bounds in the summations equal the order M of the differential function the operators are applied to.

Definition 1 *The degree operator $\mathcal{M}$ is defined by*

$$\mathcal{M}f = \sum_{i=0}^{M} u_{ix} \frac{\partial f}{\partial u_{ix}} = u\frac{\partial f}{\partial u} + u_x \frac{\partial f}{\partial u_x} + u_{2x}\frac{\partial f}{\partial u_{2x}} + \cdots + u_{Mx}\frac{\partial f}{\partial u_{Mx}}, \tag{1}$$

where f is a differential function of order M.

Example 2 *If $f = u^p u_x^q u_{3x}^r$, where p, q, and r are non-negative integers, then*

$$g = \mathcal{M}f = \sum_{i=0}^{3} u_{ix}\frac{\partial f}{\partial u_{ix}} = (p+q+r)\, u^p u_x^q u_{3x}^r. \tag{2}$$

Thus, application of $\mathcal{M}$ to a monomial results in multiplication of the monomial with its *degree*, i.e. the total number of factors in that monomial.

We use the homotopy concept to construct the inverse operator, $\mathcal{M}^{-1}$. Given a differential function $g(u)$, let $g[\lambda u]$ denote $g(u)$ where u is replaced by λu, u_x is replaced by λu_x, etc., where λ is an auxiliary parameter. We now show

$$\mathcal{M}^{-1} g(u) = \int_0^1 g[\lambda u] \, \frac{d\lambda}{\lambda}. \tag{3}$$

Indeed, if $g(u)$ has order M then so does $g[\lambda u]$, and

$$\frac{d}{d\lambda} g[\lambda u] = \sum_{i=0}^{M} \frac{\partial g[\lambda u]}{\partial \lambda u_{ix}} \frac{d\lambda u_{ix}}{d\lambda} = \frac{1}{\lambda} \sum_{i=0}^{M} u_{ix} \frac{\partial g[\lambda u]}{\partial u_{ix}} = \frac{1}{\lambda} \mathcal{M} g[\lambda u]. \tag{4}$$

Upon integration of both sides with respect to λ, we get

$$\int_0^1 \frac{d}{d\lambda} g[\lambda u] \, d\lambda = g[\lambda u]|_{\lambda=0}^{\lambda=1} = g(u) - g(0) = \int_0^1 \mathcal{M} g[\lambda u] \, \frac{d\lambda}{\lambda} = \mathcal{M} \int_0^1 g[\lambda u] \, \frac{d\lambda}{\lambda}. \tag{5}$$

Assuming $g(0) = 0$ and applying $\mathcal{M}^{-1}$ to both sides of (5), Eq. (3) readily follows. The assumption $g(0) = 0$ restricts the choice for f. We only consider differential functions involving monomials in u, u_x, etc., and on occasion multiplied by $\sin u$ or $\cos u$.

Example 3 *For g in (2), we have $g[\lambda u] = (p + q + r)\lambda^{p+q+r} \, u^p u_x^q u_{3x}^r$. Using (3),*

$$\mathcal{M}^{-1} g = \int_0^1 (p + q + r) \, \lambda^{p+q+r-1} \, u^p u_x^q u_{3x}^r \, d\lambda \tag{6}$$

$$= u^p u_x^q u_{3x}^r \; \lambda^{p+q+r} \Big|_{\lambda=0}^{\lambda=1} = u^p u_x^q u_{3x}^r. \tag{7}$$

Definition 4 *The total derivative operator $\mathcal{D}_x$ is defined by*

$$\mathcal{D}_x f = \sum_{i=0}^{M} u_{(i+1)x} \frac{\partial f}{\partial u_{ix}} = u_x \frac{\partial f}{\partial u} + u_{2x} \frac{\partial f}{\partial u_x} + \cdots + u_{(M+1)x} \frac{\partial f}{\partial u_{Mx}}. \tag{8}$$

Example 5 *If $f = u^p u_x^q u_{3x}^r$, then*

$$\mathcal{D}_x f = \sum_{i=0}^{3} u_{(i+1)x} \frac{\partial f}{\partial u_{ix}} = p u^{p-1} u_x^q u_{3x}^r + q u^p u_x^{q-1} u_{2x} u_{3x}^r + r u^p u_x^q u_{3x}^{r-1} u_{4x}. \tag{9}$$

Theorem 6 *The operators $\mathcal{M}$ and $\mathcal{D}_x$ commute as do $\mathcal{M}^{-1}$ and $\mathcal{D}_x$.*

Proof. The proof that $\mathcal{M}$ and $\mathcal{D}_x$ commute is straightforward: applying $\mathcal{M}$ to $\mathcal{D}_x f$ gives the same result as applying $\mathcal{D}_x$ to $\mathcal{M} f$, using standard calculus manipulations. Proving that $\mathcal{M}^{-1}$ commutes with $\mathcal{D}_x$ is then immediate. ■

Definition 7 *The continuous Euler operator of order zero (variational derivative) $\mathcal{L}^{(0)}_{u(x)}$ is defined [12] by*

$$\mathcal{L}^{(0)}_{u(x)} f = \sum_{k=0}^{M} (-\mathcal{D}_x)^k \frac{\partial f}{\partial u_{kx}}$$
$$= \frac{\partial f}{\partial u} - \mathcal{D}_x \frac{\partial f}{\partial u_x} + \mathcal{D}_x^2 \frac{\partial f}{\partial u_{2x}} - \mathcal{D}_x^3 \frac{\partial f}{\partial u_{3x}} + \cdots + (-1)^M \mathcal{D}_x^M \frac{\partial f}{\partial u_{Mx}}. \quad (10)$$

Definition 8 *A differential function f of order M is called exact if there exists a differential function F of order $M-1$ so that $f = \mathcal{D}_x F$.*

Theorem 9 *A necessary and sufficient condition for a differential function f to be exact is that $\mathcal{L}^{(0)}_{u(x)} f \equiv 0$.*

Proof. A proof is given in e.g. [9].

Example 10 *Let $f = 2u_x u_{2x} \cos u - u_x^3 \sin u$. Note that $f = \mathcal{D}_x F$ with $F = u_x^2 \cos u$.*

We show that f is indeed exact. Using (10), we readily verify that

$$\mathcal{L}^{(0)}_{u(x)} f = \frac{\partial f}{\partial u} - \mathcal{D}_x \frac{\partial f}{\partial u_x} + \mathcal{D}_x^2 \frac{\partial f}{\partial u_{2x}}$$
$$= -2u_x u_{2x} \sin u - u_x^3 \cos u - \mathcal{D}_x [2u_{2x} \cos u - 3u_x^2 \sin u] + \mathcal{D}_x^2 [2u_x \cos u]$$
$$= -2u_x u_{2x} \sin u - u_x^3 \cos u - [2u_{3x} \cos u - 8u_x u_{2x} \sin u - 3u_x^3 \cos u]$$
$$+ [2u_{3x} \cos u - 6u_x u_{2x} \sin u - 2u_x^3 \cos u] \equiv 0. \quad (11)$$

Definition 11 *The continuous homotopy operator with variable $u(x)$ is*

$$\mathcal{H}_{u(x)} f = \int_0^1 (I_u f)[\lambda u] \frac{d\lambda}{\lambda}, \quad (12)$$

where the integrand $I_u f$ is given by

$$I_u f = \sum_{i=0}^{M-1} u_{ix} \sum_{k=i+1}^{M} (-\mathcal{D}_x)^{k-(i+1)} \frac{\partial f}{\partial u_{kx}}. \quad (13)$$

Theorem 12 *Given an exact differential function f of order M one has $F = \mathcal{D}_x^{-1} f = \int f \, dx = \mathcal{H}_{u(x)} f$.*

Proof. We multiply $\mathcal{L}^{(0)}_{u(x)} f = \sum_{k=0}^{M} (-\mathcal{D}_x)^k \frac{\partial f}{\partial u_{kx}}$ by u to restore the degree. Next, we split off $u \frac{\partial f}{\partial u}$. Then, we integrate by parts and split off $u_x \frac{\partial f}{\partial u_x}$. We repeat this process until we split off $u_{Mx} \frac{\partial f}{\partial u_{Mx}}$. In detail,

$$u \mathcal{L}^{(0)}_{u(x)} f = u \sum_{k=0}^{M} (-\mathcal{D}_x)^k \frac{\partial f}{\partial u_{kx}}$$
$$= u \frac{\partial f}{\partial u} - \mathcal{D}_x \left(u \sum_{k=1}^{M} (-\mathcal{D}_x)^{k-1} \frac{\partial f}{\partial u_{kx}} \right) + u_x \sum_{k=1}^{M} (-\mathcal{D}_x)^{k-1} \frac{\partial f}{\partial u_{kx}}$$

$$
\begin{aligned}
&= u\frac{\partial f}{\partial u} + u_x\frac{\partial f}{\partial u_x} - \mathcal{D}_x\left(u\sum_{k=1}^{M}(-\mathcal{D}_x)^{k-1}\frac{\partial f}{\partial u_{kx}}\right.\\
&\quad \left.+u_x\sum_{k=2}^{M}(-\mathcal{D}_x)^{k-2}\frac{\partial f}{\partial u_{kx}}\right) + u_{2x}\sum_{k=2}^{M}(-\mathcal{D}_x)^{k-2}\frac{\partial f}{\partial u_{kx}}\\
&= \ldots\\
&= u\frac{\partial f}{\partial u} + u_x\frac{\partial f}{\partial u_x} + \ldots + u_{Mx}\frac{\partial f}{\partial u_{Mx}} - \mathcal{D}_x\left(u\sum_{k=1}^{M}(-\mathcal{D}_x)^{k-1}\frac{\partial f}{\partial u_{kx}}\right.\\
&\quad \left.+u_x\sum_{k=2}^{M}(-\mathcal{D}_x)^{k-2}\frac{\partial f}{\partial u_{kx}} + \ldots + u_{(M-1)x}\sum_{k=M}^{M}(-\mathcal{D}_x)^{k-M}\frac{\partial f}{\partial u_{kx}}\right)\\
&= \sum_{i=0}^{M} u_{ix}\frac{\partial f}{\partial u_{ix}} - \mathcal{D}_x\left(\sum_{i=0}^{M-1} u_{ix}\sum_{k=i+1}^{M}(-\mathcal{D}_x)^{k-(i+1)}\frac{\partial f}{\partial u_{kx}}\right)\\
&= \mathcal{M}f - \mathcal{D}_x\left(\sum_{i=0}^{M-1} u_{ix}\sum_{k=i+1}^{M}(-\mathcal{D}_x)^{k-(i+1)}\frac{\partial f}{\partial u_{kx}}\right). \qquad (14)
\end{aligned}
$$

Since f is exact we have $\mathcal{L}^{(0)}_{u(x)}f = 0$. Eq. (14) then implies

$$
\mathcal{M}f = \mathcal{D}_x\left(\sum_{i=0}^{M-1} u_{ix}\sum_{k=i+1}^{M}(-\mathcal{D}_x)^{k-(i+1)}\frac{\partial f}{\partial u_{kx}}\right). \qquad (15)
$$

Applying $\mathcal{M}^{-1}$ and using $\mathcal{M}^{-1}\mathcal{D}_x = \mathcal{D}_x\mathcal{M}^{-1}$ from Theorem 6, we obtain

$$
f = \mathcal{D}_x\left(\mathcal{M}^{-1}\sum_{i=0}^{M-1} u_{ix}\sum_{k=i+1}^{M}(-\mathcal{D}_x)^{k-(i+1)}\frac{\partial f}{\partial u_{kx}}\right). \qquad (16)
$$

Applying $\mathcal{D}_x^{-1}$ and using (3), we get

$$
F = \mathcal{D}_x^{-1}f = \int_0^1\left(\sum_{i=0}^{M-1} u_{ix}\sum_{k=i+1}^{M}(-\mathcal{D}_x)^{k-(i+1)}\frac{\partial f}{\partial u_{kx}}\right)[\lambda u]\,\frac{d\lambda}{\lambda} = \mathcal{H}_{u(x)}f \qquad (17)
$$

using (12) and (13). ■

Example 13 *Let $f = 2u_xu_{2x}\cos u - u_x^3\sin u$ which is exact as shown in Example 10. Using (13) with $M = 2$, we readily compute*

$$
\begin{aligned}
I_uf &= \sum_{i=0}^{1} u_{ix}\sum_{k=i+1}^{2}(-\mathcal{D}_x)^{k-i-1}\frac{\partial f}{\partial u_{kx}} = u\frac{\partial f}{\partial u_x} - u\mathcal{D}_x(\frac{\partial f}{\partial u_{2x}}) + u_x(\frac{\partial f}{\partial u_{2x}})\\
&= u(2u_{2x}\cos u - 3u_x^2\sin u) - u\mathcal{D}_x(2u_x\cos u) + u_x(2u_x\cos u)\\
&= -uu_x^2\sin u + 2u_x^2\cos u. \qquad (18)
\end{aligned}
$$

Using (12),

$$
\begin{aligned}
F &= \mathcal{H}_{u(x)}f = \int_0^1 (I_uf)\,[\lambda u]\,\frac{d\lambda}{\lambda} = \int_0^1\Big(-\lambda^2uu_x^2\sin(\lambda u) + 2\lambda u_x^2\cos(\lambda u)\Big)\,d\lambda\\
&= u_x^2\cos u. \qquad (19)
\end{aligned}
$$

Thus, application of (12) yields F without integration by parts with respect to x. Indeed, F can be computed via repeated differentiation followed by a one-dimensional integration with respect to an auxiliary variable λ.

3 Alternate form of the continuous homotopy operator in 1D

Formulas (12) and (13) are valid for one dependent variable u. In [5] we presented a calculus-based formula for the homotopy operator for N dependent variables in 1D based on work by Anderson and Olver in [12, p. 372]:

$$\mathcal{H}_{\mathbf{u}(x)} f = \int_0^1 \sum_{j=1}^{N} \left(I_{u^{(j)}} f\right)[\lambda \mathbf{u}] \frac{d\lambda}{\lambda}, \tag{20}$$

where $u^{(j)}$ is the jth component of $\mathbf{u} = (u^{(1)}, u^{(2)}, \cdots, u^{(j)}, \cdots, u^{(N)})$. The integrand,

$$I_{u^{(j)}} f = \sum_{i=0}^{M^{(j)}-1} \mathcal{D}_x^i \left(u^{(j)} \, \mathcal{L}_{u^{(j)}(x)}^{(i+1)} f \right), \tag{21}$$

where $M^{(j)}$ is the order of the variable $u^{(j)}$ in f, involves the continuous 1D higher Euler operators [9,12] defined as follows.

Definition 14 *The continuous higher Euler operators for component $u^{(j)}(x)$ are*

$$\mathcal{L}_{u^{(j)}(x)}^{(i)} f = \sum_{k=i}^{M^{(j)}} \binom{k}{i} (-\mathcal{D}_x)^{k-i} \frac{\partial f}{\partial {u^{(j)}}_{kx}}, \tag{22}$$

where $\binom{k}{i}$ is the binomial coefficient.

Note that the higher Euler operator for $i = 0$ and one dependent variable $u^{(1)}(x) = u(x)$ matches the variational derivative (10).

In the case of one dependent variable, u, we denote $M^{(1)}$ by M. After substitution of $\mathcal{L}_{u(x)}^{(i+1)} f$ into (21), we obtain

$$I_u f = \sum_{i=0}^{M-1} \mathcal{D}_x^i \left(u \sum_{k=i+1}^{M} \binom{k}{i+1} (-\mathcal{D}_x)^{k-(i+1)} \frac{\partial f}{\partial u_{kx}} \right). \tag{23}$$

Theorem 15 *The integrands (13) and (23) are equal.*

Proof. Starting from (23), we use Leibniz's rule to propagate $\mathcal{D}_x$ to the right

$$\begin{aligned} I_u f &= \sum_{i=0}^{M-1} \mathcal{D}_x^i \left(u \sum_{k=i+1}^{M} \binom{k}{i+1} (-\mathcal{D}_x)^{k-(i+1)} \frac{\partial f}{\partial u_{kx}} \right) \\ &= \sum_{i=0}^{M-1} \sum_{j=0}^{i} \binom{i}{j} u_{jx} \mathcal{D}_x^{i-j} \left(\sum_{k=i+1}^{M} \binom{k}{i+1} (-\mathcal{D}_x)^{k-(i+1)} \frac{\partial f}{\partial u_{kx}} \right) \\ &= \sum_{i=0}^{M-1} \sum_{j=0}^{i} \binom{i}{j} u_{jx} (-1)^{j-i} \sum_{k=i+1}^{M} \binom{k}{i+1} (-\mathcal{D}_x)^{k-(j+1)} \frac{\partial f}{\partial u_{kx}}. \end{aligned} \tag{24}$$

Next, we interchange the sums over i and j (to bring u_{jx} up front), followed by an interchange of the sums over i and k (to bring $\mathcal{D}_x$ and $\partial f/\partial u_{kx}$ outside the sum over i). So,

$$
\begin{aligned}
I_u f &= \sum_{j=0}^{M-1} u_{jx} \sum_{i=j}^{M-1} \binom{i}{j} (-1)^{j-i} \sum_{k=i+1}^{M} \binom{k}{i+1} (-\mathcal{D}_x)^{k-(j+1)} \frac{\partial f}{\partial u_{kx}} \\
&= \sum_{j=0}^{M-1} u_{jx} \sum_{k=j+1}^{M} (-\mathcal{D}_x)^{k-(j+1)} \frac{\partial f}{\partial u_{kx}} \sum_{i=j}^{k-1} (-1)^{i-j} \binom{i}{j} \binom{k}{i+1} \\
&= \sum_{j=0}^{M-1} u_{jx} \sum_{k=j+1}^{M} (-\mathcal{D}_x)^{k-(j+1)} \frac{\partial f}{\partial u_{kx}},
\end{aligned}
\tag{25}
$$

where we have used the identity

$$
\sum_{i=j}^{k-1} (-1)^{i-j} \binom{i}{j} \binom{k}{i+1} = 1 \quad \text{if } k \geq j+1,
\tag{26}
$$

which is straightforward to prove using mathematical induction. ■

Homotopy operator (20) can easily be implemented in CAS. In our experience, integrand (13) leads to a more efficient and faster algorithm for it requires substantially less differentiations then (23).

4 Discrete Euler and homotopy operators

We now turn to the discrete analogues of differential functions, Euler operators and homotopy operators. For simplicity we consider the case of one lattice variable n which results, for example, from a discretization of the variable x. We allow N dependent variables, i.e. $\mathbf{u}_n = (u_n^{(1)}, u_n^{(2)}, \cdots, u_n^{(j)}, \cdots, u_n^{(N)})$. For simplicity, in the examples we denote these components by u_n, v_n, etc.

By analogy with $\mathcal{D}_x$ and $\mathcal{D}_x^{-1}$, we define shift operators acting on $f_n(\mathbf{u}_n)$.

Definition 16 D *is the up-shift operator (also known as forward- or right-shift) such that* $\mathrm{D}\, f_n = f_{n+1}$. *Its inverse,* D^{-1}, *is the down-shift operator (or backward- or left-shift) such that* $\mathrm{D}^{-1} f_n = f_{n-1}$. *The identity operator is denoted by* I. *Lastly,* $\Delta = \mathrm{D} - \mathrm{I}$ *is the forward difference operator so that* $\Delta\, f_n = (\mathrm{D} - \mathrm{I})\, f_n = f_{n+1} - f_n$.

Given are functions f_n in discrete variables $u_n, v_n, \ldots$ and their up and down shifts. If $f_n(u_{n-p}, v_{n-r}, \cdots, u_n, v_n, \cdots, u_{n+q}, v_{n+s})$ with $p \geq r$ involves negative shifts, one must first remove these by replacing f_n by $\tilde{f}_n = \mathrm{D}^p f_n$. From this point we assume that all negative shifts have been removed.

Definition 17 f_n *is called exact if it is a total difference, i.e. there exists a* F_n *so that* $f_n = \Delta\, F_n$.

Example 18 *Let*

$$f_n = \sin(u_{n+3})\cos^2(v_{n+2}^2) - \sin(u_{n+1})\cos^2(v_n^2). \tag{27}$$

By hand, we readily verify that $f_n = \Delta F_n$ *with*

$$F_n = \sin(u_{n+2})\cos^2(v_{n+1}^2) + \sin(u_{n+1})\cos^2(v_n^2). \tag{28}$$

So, f_n *is exact.*

Below we address the following questions. (i) How can one test whether or not f_n is exact? Equivalently, how does one know that F_n exists in closed form? (ii) Can one compute $F_n = \Delta^{-1} f_n$ in a way analogous to the continuous case?

Definition 19 $\mathcal{L}^{(0)}_{u_n^{(j)}}$ *is the discrete Euler operator of order zero (discrete variational derivative) for component* $u_n^{(j)}$, *defined [1] by*

$$\begin{aligned}\mathcal{L}^{(0)}_{u_n^{(j)}} f_n &= \sum_{k=0}^{M^{(j)}} \mathrm{D}^{-k} \frac{\partial f_n}{\partial u_{n+k}^{(j)}} = \frac{\partial}{\partial u_n^{(j)}} \sum_{k=0}^{M^{(j)}} \mathrm{D}^{-k} f_n \\ &= \frac{\partial}{\partial u_n^{(j)}} \left(\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \cdots + \mathrm{D}^{-M^{(j)}} \right) f_n, \end{aligned} \tag{29}$$

where $M^{(j)}$ *is the highest shift of* $u_n^{(j)}$ *occurring in* f_n.

With respect to the existence of F_n, the following exactness criterion is well-known and frequently used [1].

Theorem 20 *A necessary and sufficient condition for a function* f_n *with positive shifts to be exact is that* $\mathcal{L}^{(0)}_{u_n^{(j)}} f_n \equiv 0, \ j = 1, 2, 3, \cdots, N$.

Proof. A proof is given in e.g. [7]. ■

Example 21 *To test that (27) is exact we apply (29) to* f_n *for each component of* $\mathbf{u}_n = (u_n^{(1)}, u_n^{(2)}) = (u_n, v_n)$ *separately. For component* u_n *with maximum shift* $M^{(1)} = 3$ *we readily verify that* $\mathcal{L}^{(0)}_{u_n} f_n = \frac{\partial}{\partial u_n} (\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3}) f_n \equiv 0$. *Similarly, for component* v_n *with maximum shift* $M^{(2)} = 2$ *we check that* $\mathcal{L}^{(0)}_{v_n} f_n = \frac{\partial}{\partial v_n} (\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2}) f_n \equiv 0$.

Next, we compute F_n so that $f_n = \Delta F_n = F_{n+1} - F_n$.

Definition 22 *The discrete homotopy operator for* $\mathbf{u}_n$ *is*

$$\mathcal{H}_{\mathbf{u}_n} f_n = \int_0^1 \sum_{j=1}^{N} \left(I_{u_n^{(j)}} f_n \right) [\lambda \mathbf{u}_n] \frac{d\lambda}{\lambda}, \tag{30}$$

where the integrand $I_{u_n^{(j)}} f_n$ *is given by*

$$I_{u_n^{(j)}} f_n = \sum_{i=0}^{M^{(j)}-1} u_{n+i}^{(j)} \frac{\partial}{\partial u_{n+i}^{(j)}} \sum_{k=i+1}^{M^{(j)}} \mathrm{D}^{-(k-i)} f_n. \tag{31}$$

As in the continuous case, $\left(I_{u_n^{(j)}} f_n\right)[\lambda \mathbf{u}_n]$ means that after $I_{u_n^{(j)}} f_n$ is computed one replaces $\mathbf{u}_n$ by $\lambda \mathbf{u}_n$, $\mathbf{u}_{n+1}$ by $\lambda \mathbf{u}_{n+1}$, etc.

One can use the following theorem [6,8,10] to compute F_n.

Theorem 23 *Given an exact function f_n one has $F_n = \Delta^{-1} f_n = \mathcal{H}_{\mathbf{u}_n} f_n$.*

Proof. The proof is similar to that of Theorem 12. For simplicity we show it for one dependent variable, $u_n^{(1)} = u_n$, and we denote $M^{(1)}$ by M. After multiplication of $\mathcal{L}_{u_n}^{(0)} f_n = \frac{\partial}{\partial u_n} \sum_{k=0}^{M} \mathrm{D}^{-k} f_n$ with u_n, we isolate $u_n \frac{\partial f_n}{\partial u_n}$ and apply Δ to the remaining term in order to sum by parts. Next, we isolate $u_{n+1} \frac{\partial f_n}{\partial u_{n+1}}$, followed by another summation by parts.
This process is repeated $M-1$ times, so that

$$u_n \mathcal{L}_{u_n}^{(0)} f_n = \sum_{i=0}^{M} u_{n+i} \frac{\partial f_n}{\partial u_{n+i}} - \Delta \left(\sum_{i=0}^{M-1} u_{n+i} \frac{\partial}{\partial u_{n+i}} \sum_{k=i+1}^{M} \mathrm{D}^{-(k-i)} f_n \right). \qquad (32)$$

The inverse of the discrete operator $\mathcal{M} f_n = \sum_{i=0}^{M} u_{n+i} \frac{\partial f_n}{\partial u_{n+i}}$ is computed as $\mathcal{M}^{-1} f_n = \int_0^1 f_n[\lambda u_n] \frac{d\lambda}{\lambda}$. Since f_n is exact and $\mathcal{M}^{-1}$ and Δ commute, we get

$$F_n = \Delta^{-1} f_n = \int_0^1 \left(\sum_{i=0}^{M-1} u_{n+i} \frac{\partial}{\partial u_{n+i}} \sum_{k=i+1}^{M} \mathrm{D}^{-(k-i)} f_n \right) [\lambda u_n] \frac{d\lambda}{\lambda} = \mathcal{H}_{u_n} f_n \qquad (33)$$

using (30) and (31). ■

Thus, the homotopy operator reduces summation by parts needed for the inversion of Δ to a set of shifts and differentiations followed by a single definite integral with respect to a scaling parameter λ.

Example 24 *We return to (27) where f_n involves u_n and v_n with maximal shifts $M^{(1)} = 3$ and $M^{(2)} = 2$. Using (31), we get*

$$\begin{aligned}
I_{u_n} f_n &= u_n \frac{\partial}{\partial u_n} (\mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3}) f_n + u_{n+1} \frac{\partial}{\partial u_{n+1}} (\mathrm{D}^{-1} + \mathrm{D}^{-2}) f_n + u_{n+2} \frac{\partial}{\partial u_{n+2}} \mathrm{D}^{-1} f_n \\
&= u_n \frac{\partial}{\partial u_n} \Big(\sin(u_{n+2}) \cos^2(v_{n+1}^2) + \sin(u_{n+1}) \cos^2(v_n^2) \\
&\quad - \sin(u_{n-1}) \cos^2(v_{n-2}^2) - \sin(u_{n-2}) \cos^2(v_{n-3}^2) \Big) \\
&\quad + u_{n+1} \frac{\partial}{\partial u_{n+1}} \Big(\sin(u_{n+2}) \cos^2(v_{n+1}^2) - \sin(u_n) \cos^2(v_{n-1}^2) \\
&\quad + \sin(u_{n+1}) \cos^2(v_n^2) - \sin(u_{n-1}) \cos^2(v_{n-2}^2) \Big) \\
&\quad + u_{n+2} \frac{\partial}{\partial u_{n+2}} \Big(\sin(u_{n+2}) \cos^2(v_{n+1}^2) - \sin(u_n) \cos^2(v_{n-1}^2) \Big). \\
&= u_{n+1} \cos(u_{n+1}) \cos^2(v_n^2) + u_{n+2} \cos(u_{n+2}) \cos^2(v_{n+1}^2). \qquad (34)
\end{aligned}$$

and, analogously,

$$I_{v_n} f_n = -4\left(v_n^2 \sin(u_{n+1}) \cos(v_n^2) \sin(v_n^2) + v_{n+1}^2 \sin(u_{n+2}) \cos(v_{n+1}^2) \sin(v_{n+1}^2)\right). \quad (35)$$

Based on (30), we compute

$$\begin{aligned}
F_n &= \int_0^1 \left(I_{u_n} f_n + I_{v_n} f_n\right)[\lambda \mathbf{u}_n] \frac{d\lambda}{\lambda} \\
&= \int_0^1 \Big(u_{n+1} \cos(\lambda u_{n+1}) \cos^2(\lambda^2 v_n^2) + u_{n+2} \cos(\lambda u_{n+2}) \cos^2(\lambda^2 v_{n+1}^2) \\
&\qquad - 4\,\lambda\, v_n^2 \,\sin(\lambda u_{n+1}) \cos(\lambda^2 v_n^2) \sin(\lambda^2 v_n^2) \\
&\qquad - 4\,\lambda\, v_{n+1}^2 \,\sin(\lambda u_{n+2}) \cos(\lambda^2 v_{n+1}^2) \sin(\lambda^2 v_{n+1}^2)\Big)\, d\lambda \\
&= \sin(u_{n+2}) \cos^2(v_{n+1}^2) + \sin(u_{n+1}) \cos^2(v_n^2), \qquad (36)
\end{aligned}$$

which agrees with (28) previously computed by hand in Example 18.

5 Alternate form of the discrete homotopy operator

In [5] we presented the following formula for the discrete homotopy operator with one lattice variable (n) and with N dependent variables $u_n^{(j)}$:

$$\mathcal{H}_{\mathbf{u}_n} f_n = \int_0^1 \sum_{j=1}^{N} \left(I_{u_n^{(j)}} f_n\right)[\lambda \mathbf{u}_n] \frac{d\lambda}{\lambda} \qquad (37)$$

with

$$I_{u_n^{(j)}} f_n = \sum_{i=0}^{M^{(j)}-1} \Delta^i \left(u_n^{(j)} \mathcal{L}_{u_n^{(j)}}^{(i+1)} f_n\right), \qquad (38)$$

where the discrete higher Euler operators are defined as follows.

Definition 25 *The discrete higher Euler operators for component $u_n^{(j)}$ are*

$$\mathcal{L}_{u_n^{(j)}}^{(i)} f_n = \sum_{k=i}^{M^{(j)}} \binom{k}{i} \mathrm{D}^{-k} \frac{\partial f_n}{\partial u_{n+k}^{(j)}} = \frac{\partial}{\partial u_n^{(j)}} \sum_{k=i}^{M^{(j)}} \binom{k}{i} \mathrm{D}^{-k} f_n. \qquad (39)$$

Theorem 26 *The integrands (31) and (38) are equal, i.e.*

$$\begin{aligned}
I_{u_n^{(j)}} f_n &= \sum_{i=0}^{M^{(j)}-1} \Delta^i \left(u_n^{(j)} \frac{\partial}{\partial u_n^{(j)}} \sum_{k=i+1}^{M^{(j)}} \binom{k}{i+1} \mathrm{D}^{-k} f_n\right) \\
&= \sum_{i=0}^{M^{(j)}-1} u_{n+i}^{(j)} \frac{\partial}{\partial u_{n+i}^{(j)}} \sum_{k=i+1}^{M^{(j)}} \mathrm{D}^{-(k-i)} f_n \qquad (40)
\end{aligned}$$

Proof. The proof is analogous to that of Theorem 15. ■

6 Conclusions

In this paper we derived formulas for the 1D continuous and discrete homotopy operators. We showed that our calculus-based formulas are equivalent to those obtained from the variational complexes. The simplified formulas no longer involve higher Euler operators which makes them easier to implement and faster to execute in major computer algebra systems. Simplified versions of the continuous homotopy operator in 2D and 3D will be presented elsewhere.

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