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SYMBOLIC INTEGRATION AND SUMMATION USING HOMOTOPY METHODS

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Abstract

The homotopy algorithm is a powerful method for indefinite integration of total derivatives, and for the indefinite summation of differences. By combining these ideas with straightforward Gaussian elimination, we construct an algorithm for the optimal symbolic integration or summation of expressions that contain terms that are not total derivatives or differences. The optimization consists of minimizing the number of terms that remain unintegrated or are not summed. Further, the algorithm imposes an ordering of terms so that the differential or difference order of these remaining terms is minimal.

1. *Introduction*

Homotopy methods are powerful tools originating in differential geometry and the calculus of variations for the integration and summation of exact expressions. In one continuous spatial dimension, this amounts to integrating total derivatives of expressions containing unknown functions and their derivatives. Such calculations occur frequently in applications. For instance, in soliton theory, the form of consecutive conserved densities and their fluxes are given by functional expressions of unknown functions and their derivatives. As shown in [**6**], the fluxes may be reconstructed by the indefinite integration of such expressions. A second application is the solution of an exact differential equation of arbitrary order [**10**].

The question addressed in this paper is the design of a *fully automated procedure* for the integration of expressions containing unknown functions and their derivatives, usable by a computer algebra system (CAS) such as Maple or Mathematica, especially if the input expressions are *not* exact. The current versions of both Maple (Release 10) and Mathematica (Release 5.1) are unable to integrate expressions that contain both derivative and nonderivative terms, even when the vast majority of the terms is exact. For example, suppose one wants to integrate the expression

$$E = u'(x)v(x) + v'(x)u(x) + u(x),$$

where $u(x)$ and $v(x)$ are unspecified functions of the independent variable x and $u'(x)$ denotes the derivative of u with respect to x. Immediately

$$\int E dx = u(x)v(x) + \int u(x)dx.$$

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Below we present an algorithm to obtain this answer systematically. The algorithm is especially suited for expressions containing many terms, not all of which are exact.

In addition to expressions depending on a continuous variable $x \in \mathbb{R}$, we also consider expressions with a discrete variable $n \in \mathbb{Z}$. Such expressions also occur frequently in applications (see [**8, 12**]). All of the above statements remain true, by replacing "integral" with "sum" and "derivative" with "shift". To illustrate this, consider the example of summing the expression

$$E_n = u_{n+1} - u_n + u_n^2.$$

Immediately

$$\sum_n E_n = u_{n+1} + \sum_n u_n^2,$$

where $\sum_n$ denotes indefinite summation with respect to n.

The current implementations of the symbolic integration and summation algorithms used by Maple 10 or Mathematica 5.1 do not perform these calculations, in part because of their refusal to make choices about which terms to integrate (sum) and which terms to leave unintegrated (unsummed). Indeed, this is a legitimate concern for more complicated expressions and one may argue about whether or not the answer our algorithm produces is optimal. Be that as it may, there should be no discussion on the resulting answer being an improvement over leaving the expressions untouched, which is the response of Maple 10 or Mathematica 5.1. This is demonstrated in examples. An implementation in Maple of the algorithm presented in this paper is available from [**3**]. It should be noted that the ideas in this paper are easily generalized to the multidimensional case, *i.e.*, the inversion of the divergence operator (or its discrete analog) [**7, 11**] . We state everything in one dimension because it is the most important and transparent case.

2. *Integrating exact expressions*

In this section we are concerned with expressions $E(x, \boldsymbol{u}, \boldsymbol{u}_x, \boldsymbol{u}_{2x}, \ldots, \boldsymbol{u}_{Nx})$ of an unknown (vector) function $\boldsymbol{u}$ and its derivatives with respect to x. Here N is the order of the highest derivative of any component of $\boldsymbol{u}$ with respect to x appearing in E . For ease of presentation, we assume that E is free of terms of the form $\hat{E}(x)$, *i.e.*, terms that are independent of the dependent variable. Such expressions are exact in a trivial sense. We also use the notation $\mathrm{D}_x F$ to denote the derivative of the expression F with respect to x.

We begin by introducing some mathematical tools from the calculus of variations and differential geometry, the Euler operators and the homotopy operator. These operators allow us to answer the following questions:

- **Question 1:** How does one check if an expression E is exact, *i.e.*, a total derivative, $E = \mathrm{D}_x F$ for some function F?
- **Question 2:** If an expression E is exact, how does one determine $F = \mathrm{D}_x^{-1}(E) = \int E dx$?

For clarity, we first introduce the more familiar zeroth-order Euler operator or the variational derivative, before introducing the higher-order versions. With the Euler operators in hand, we introduce the homotopy operator and demonstrate how it is used to integrate exact expressions. Most of the material presented in this section is not new. It may be found in a more abstract form in [**2, 11**], *e.g.*, or in a more concrete form in [**6, 7**], for instance.

2.1. *The continuous Euler operators*

DEFINITION 1. *The one-dimensional* **Euler operator of order zero** *(variational derivative), with independent variable x and dependent variable $\boldsymbol{u} = \big(u^{(1)}(x), \dots, u^{(M)}(x)\big)$, is defined as the operator $\mathcal{L}^{(0)}_{\boldsymbol{u}(x)}$ with M components*

$$\begin{aligned}\mathcal{L}^{(0)}_{\boldsymbol{u}(x)} &= \left(\mathcal{L}^{(0)}_{u^{(1)}(x)}, \dots, \mathcal{L}^{(0)}_{u^{(M)}(x)}\right) \\ &= \left(\sum_{k=0}^{\infty}(-\mathrm{D}_x)^k \frac{\partial}{\partial u^{(1)}_{kx}}, \dots, \sum_{k=0}^{\infty}(-\mathrm{D}_x)^k \frac{\partial}{\partial u^{(M)}_{kx}}\right).\end{aligned} \tag{1}$$

In particular, the explicit formula for the variational derivative with scalar component u and variable x is

$$\mathcal{L}^{(0)}_{u(x)} = \sum_{k=0}^{\infty}(-\mathrm{D}_x)^k \frac{\partial}{\partial u_{kx}} = \frac{\partial}{\partial u} - \mathrm{D}_x \frac{\partial}{\partial u_x} + \mathrm{D}_x^2 \frac{\partial}{\partial u_{2x}} - \mathrm{D}_x^3 \frac{\partial}{\partial u_{3x}} + \cdots . \tag{2}$$

The Euler operator of order zero allows us to answer Question 1 by the following theorem [**11**].

THEOREM 1. *A necessary and sufficient condition for an expression E to be exact is that $\mathcal{L}^{(0)}_{\boldsymbol{u}(x)}(E) \equiv 0$.*

Example. Consider

$$E = uv' + vu' = \mathrm{D}_x\,(uv)\,. \tag{3}$$

Then

$$\mathcal{L}^{(0)}_{u(x)}(E) = v' - D_x\,(v) = 0.$$

$$\mathcal{L}^{(0)}_{v(x)}(E) = u' - D_x\,(u) = 0.$$

To compute $F = \mathrm{D}_x^{-1}(E) = \int E dx$ we need the higher Euler operators.

DEFINITION 2. *The one-dimensional* **higher Euler operator** *of order i with variable x is given by*

$$\mathcal{L}^{(i)}_{\boldsymbol{u}(x)} = \sum_{k=i}^{\infty} \binom{k}{i} (-\mathrm{D}_x)^{k-i} \frac{\partial}{\partial \boldsymbol{u}_{kx}}, \tag{4}$$

where $\displaystyle\binom{k}{i} = \frac{k!}{i!(k-i)!}$.

In particular, the explicit formulas for the first four higher Euler operators (with component u and variable x) are

$$\mathcal{L}^{(0)}_{u(x)} = 1 \cdot \frac{\partial}{\partial u} - 1 \cdot \mathrm{D}_x \frac{\partial}{\partial u_x} + 1 \cdot \mathrm{D}_x^2 \frac{\partial}{\partial u_{2x}} - 1 \cdot \mathrm{D}_x^3 \frac{\partial}{\partial u_{3x}} + \cdots , \tag{5a}$$

$$\mathcal{L}^{(1)}_{u(x)} = 1 \cdot \frac{\partial}{\partial u_x} - 2 \cdot \mathrm{D}_x \frac{\partial}{\partial u_{2x}} + 3 \cdot \mathrm{D}_x^2 \frac{\partial}{\partial u_{3x}} - 4 \cdot \mathrm{D}_x^3 \frac{\partial}{\partial u_{4x}} + \cdots , \tag{5b}$$

$$\mathcal{L}^{(2)}_{u(x)} = 1 \cdot \frac{\partial}{\partial u_{2x}} - 3 \cdot \mathrm{D}_x \frac{\partial}{\partial u_{3x}} + 6 \cdot \mathrm{D}_x^2 \frac{\partial}{\partial u_{4x}} - 10 \cdot \mathrm{D}_x^3 \frac{\partial}{\partial u_{5x}} + \cdots , \tag{5c}$$

$$\mathcal{L}^{(3)}_{u(x)} = 1 \cdot \frac{\partial}{\partial u_{3x}} - 4 \cdot \mathrm{D}_x \frac{\partial}{\partial u_{4x}} + 10 \cdot \mathrm{D}_x^2 \frac{\partial}{\partial u_{5x}} - 20 \cdot \mathrm{D}_x^3 \frac{\partial}{\partial u_{6x}} + \cdots . \tag{5d}$$

Though not explicitly used in what follows, it is interesting to note that the higher-order analog of Question 1 is answered by the higher Euler operators (see [**9**]), $E = \mathrm{D}_x^m F$ for some F if and only if $\mathcal{L}^{(k)}_{\boldsymbol{u}(x)}(E) \equiv 0$ for $k = 0, \ldots, m-1$.

2.2. *The continuous homotopy operator*

We now define the homotopy operator, which reduces integration of an expression involving unknown functions to integration of a known function with respect to a single scalar variable.

DEFINITION 3. *The one-dimensional* **homotopy operator** *with variable x is given by*

$$\mathcal{H}_{\lambda_0}(E) = \int_{\lambda_0}^{1} \sum_{j=1}^{M} I_j(E)[\lambda \boldsymbol{u}] \, \frac{d\lambda}{\lambda}, \tag{6}$$

with

$$I_j(E) = \sum_{i=0}^{N-1} \mathrm{D}_x^i \left(u^{(j)} \, \mathcal{L}^{(i+1)}_{u^{(j)}(x)}(E) \right). \tag{7}$$

The integrand (7) involves the one-dimensional higher Euler operators and M is the number of components of $\boldsymbol{u}(x) = \left(u^{(1)}(x), \ldots, u^{(M)}(x)\right)$. The notation $I_j(E)[\lambda \boldsymbol{u}]$ implies that in $I_j(E)$ one replaces $\boldsymbol{u}(x)$ with $\lambda \boldsymbol{u}(x)$, $\boldsymbol{u}_x(x)$ with $\lambda \boldsymbol{u}_x(x)$, etc.

Remarks:

- This definition differs from that found in [**6, 11**] to avoid singularities as a consequence of the lower limit of integration, as discussed in [**1, 13**]. This is illustrated below.
- We have not included the part of the homotopy operator that deals with expressions whose only x-dependence is explicit (Sections 1.5 and 5.4 in [**11**]), as we have assumed that all such expressions are removed from E.
- The homotopy operator defined above is one of many homotopy operators introduced in [**11**] and elsewhere. For our purposes here, we simply refer to it as the homotopy operator.

The homotopy operator allows us to answer Question 2 by the following theorem (Section 5.4 in [**11**], with a more general lower bound used throughout).

THEOREM 2. *For an exact function $E = \mathrm{D}_x F$ one has*

$$\mathcal{H}_{\lambda_0}(E) = F[\boldsymbol{u}] - F[\lambda_0 \boldsymbol{u}]. \tag{8}$$

It is important to note that the kernel of the homotopy operator is non-trivial (see Appendix A). Because of this, different cases have to be considered: expressions which *vanish at zero or infinity* and expressions which do not. We can exclude mixed cases (containing both types of limit terms) since $\mathcal{H}_{\lambda_0}$ is a linear operator.

- **Expressions which vanish at zero or infinity:** If $\lim_{\lambda\to\lambda_0} E[\lambda\boldsymbol{u}] = 0$ for λ_0 equal to zero or infinity, then evaluating $\mathcal{H}_{\lambda_0}(E)$ gives $F[\boldsymbol{u}]$, up to an integration constant, according to (8). This can be seen by applying the chain rule: $\mathrm{D}_x F[\lambda_0\boldsymbol{u}] = E[\lambda_0\boldsymbol{u}] = 0$, from which $F[\lambda_0\boldsymbol{u}]$ is a constant independent of x.
- **Expressions which do not vanish at zero or infinity:** If $\lim_{\lambda\to\lambda_0} E[\lambda\boldsymbol{u}] = E_0[\boldsymbol{u}] \neq 0$ for both $\lambda_0 = 0$ and $\lambda_0 = \infty$, then: (i) $E_0[\boldsymbol{u}]$ is exact (since $E[\boldsymbol{u}]$ is exact) and (ii) $E_0[\boldsymbol{u}]$ is an expression of degree zero (see Appendix A). Therefore, $E_0[\boldsymbol{u}]$ is in the kernel of the homotopy operator (see Appendix A), and must be dealt with separately. One method of dealing with such terms is the introduction of a parameter, as demonstrated in the examples below. For an alternative approach, see [**1**]. Also, non-homotopy methods can be used (see [**10**], for instance).

Example. Returning to (3)

$$E = uv' + vu'.$$

In this case, $\boldsymbol{u} = (u, v)$ and

$$\lim_{\lambda\to\lambda_0} E[\lambda u, \lambda v] = \lim_{\lambda\to\lambda_0} \left((\lambda u)(\lambda v') + (\lambda v)(\lambda u')\right) = (uv' + vu') \lim_{\lambda\to\lambda_0} \lambda^2 = (uv' + vu')\lambda_0^2.$$

Thus we choose $\lambda_0 = 0$. Proceeding without this, we have

$$\mathcal{H}_{\lambda_0}(E) = \int_{\lambda_0}^{1} \left(I_u(E)[\lambda\boldsymbol{u}] + I_v(E)[\lambda\boldsymbol{u}]\right) \frac{d\lambda}{\lambda},$$

with

$$I_u(E) = \sum_{i=0}^{\infty} \mathrm{D}_x^i \left(u\, \mathcal{L}_{u(x)}^{(i+1)}(E)\right) \quad \text{and} \quad I_v(E) = \sum_{i=0}^{\infty} \mathrm{D}_x^i \left(v\, \mathcal{L}_{v(x)}^{(i+1)}(E)\right).$$

These formulas give

$$I_u(E) = u\mathcal{L}_{u(x)}^{(1)}(E) = u\frac{\partial E}{\partial u_x} = uv, \quad I_v(E) = v\mathcal{L}_{v(x)}^{(1)}(E) = v\frac{\partial E}{\partial v_x} = vu.$$

Thus, (6) gives

$$\mathcal{H}_{\lambda_0}(E) = \int_{\lambda_0}^{1} \left(\lambda^2 uv + \lambda^2 uv\right) \frac{d\lambda}{\lambda} = 2uv \int_{\lambda_0}^{1} \lambda d\lambda = uv - uv\lambda_0^2.$$

Using $\lambda_0 = 0$ results in

$$F = uv,$$

as desired.

Example. Consider

$$E = u'u^p. \tag{9}$$

Here

$$E[\lambda u] = \lambda^{(p+1)} u'u^p.$$

A similar calculation to that given above establishes that $\lambda_0 = 0$ for $p > -1$, whereas $\lambda_0 = \infty$ for $p < -1$. For $p \neq -1$, (7) gives

$$I_u(E) = u^{(p+1)}.$$

Therefore,

$$\mathcal{H}_{\lambda_0}(E) = \int_{\lambda_0}^{1} \lambda^p u^{(p+1)} d\lambda = \frac{1}{p+1} u^{(p+1)} - \frac{1}{p+1} u^{(p+1)} \lambda_0^{(p+1)}.$$

Evaluating at $\lambda_0 = \infty$ for $p < -1$ or $\lambda_0 = 0$ for $p > -1$ gives

$$\int E dx = \frac{u^{(p+1)}}{p+1}, \;\; p \neq -1. \tag{10}$$

Example. Suppose $p = -1$ in (9) from our previous example, then E is homogeneous of degree zero. In this case (7) gives

$$I_u(E) = 1,$$

resulting in

$$\mathcal{H}_{\lambda_0}(E) = \int_{\lambda_0}^{1} \frac{1}{\lambda} d\lambda = \ln\left(\frac{1}{\lambda_0}\right), \tag{11}$$

which is independent of $u(x)$. Nevertheless, this is correct since upon inspection one has

$$F[u] = \int E dx = \ln(u),$$

so that

$$F[u] - F[\lambda_0 u] = \ln(u) - \ln(\lambda_0 u) = \ln\left(\frac{u}{\lambda_0 u}\right) = \ln\left(\frac{1}{\lambda_0}\right),$$

in agreement with (8) and (11). Thus $F[u]$ cannot be recovered from the above expression.

In order to obtain the desired answer for the case $p = -1$, we can exploit the fact that the homotopy operator is defined up to a constant of integration. Using (10), we can remove the singularity at $p = -1$ by subtracting the constant of integration $1/(p+1)$ (this choice is unique among integration constants that cause an indefinite form as $p \to -1$):

$$\int \frac{u'}{u} dx = \lim_{p \to -1} \left(\frac{u^{(p+1)}}{p+1} - \frac{1}{p+1} \right) = \ln(u) .$$

Example. Only if a singularity is present in the obtained solution (depending on a parameter) is it necessary to subtract a suitable integration constant (depending on this parameter) to obtain the correct result, as in the previous example. Otherwise, a simple substitution of the desired parameter suffices. This second scenario is illustrated here. Let

$$E = \left(\frac{u^p}{u'^2} \right)' = \frac{pu^{p-1}}{u'} - \frac{2u^p u''}{u'^3},$$

which does not vanish at zero or infinity for $p = 2$. Proceeding for $p \neq 2$ gives

$$\mathcal{H}_{\lambda_0}(E) = \frac{u^p}{u'^2} - \lambda_0^{p-2} \left(\frac{u^p}{u'^2} \right).$$

Evaluating at $\lambda_0 = \infty$ for $p < 2$ or $\lambda_0 = 0$ for $p > 2$ gives

$$F = \frac{u^p}{u'^2},$$

which is correct. Note that this expression is well defined for $p = 2$. Taking the limit $p \to 2$ gives

$$\int \left(\frac{2u}{u'} - \frac{2u^2 u''}{u'^3} \right) dx = \frac{u^2}{u'^2},$$

as desired.

3. *Integrating non-exact expressions*

If an expression E is not exact, we aim to integrate as many total derivatives in E as possible, while optimizing the number and type of terms remaining in the integral. We use the following six-step method, which we refer to as *the homotopy method with optimization*.

Step 1. Integrate total derivatives in E. Calculate

$$F = \mathcal{H}_{\lambda_0}(E),$$

where λ_0 is equal to zero or infinity. Since E is not exact, $F \neq \int E dx$.

Step 2. Construct the set of all terms of F. Let p be the number of terms of $F = \sum_{i=1}^{p} c_i F^{(i)}$, such that no two $F^{(i)}$'s are constant multiples of each other and each c_i is a constant. Form the set $R = \{F^{(1)}, F^{(2)}, \ldots, F^{(p)}\}$ of all terms in F. Several choices may be possible for the set R. Preference should be given to the set with the largest p. To this end, expressions should be expanded when possible. It should be noted that working with a smaller set R will not result in a wrong answer, but merely in a less than optimal answer.

Step 3. Separate E into its derivative part and its non-derivative part. Using R,

$$\int E dx = \sum_{i=1}^{p} \alpha_i F^{(i)} + \int \left(E - \sum_{i=1}^{p} \alpha_i \mathrm{D}_x F^{(i)} \right) dx. \tag{12}$$

Note that choosing $\alpha_i = c_i$ for all i gives $\int E dx = F + \int (E - \mathrm{D}_x F) dx$, which is obviously true. Doing this is referred to as the *homotopy method without optimization*.

Step 4. Construct an ordered list of terms S occurring in $E - \sum_{i=1}^{p} \alpha_i \mathrm{D}_x F^{(i)}$. Reduce S to ensure no two elements are constant multiples of each other. The list starts with elements containing the highest derivatives, ending with those containing the lowest derivatives. Different choices for this ordering are possible, which may result in different but correct final results.

Step 5. Construct a linear algebraic system for $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_p)$. Construct a system of q linear equations such that the j-th equation is the coefficient of S_j in $\sum_{i=1}^{p} \alpha_i \mathrm{D}_x F^{(i)}$ equated to the coefficient of S_j in E. These equations are linear in the components of $\boldsymbol{\alpha}$, and the system of equations may be written as

$$\boldsymbol{C}\boldsymbol{\alpha} = \boldsymbol{b}, \tag{13}$$

where the matrix $\boldsymbol{C}$ is of dimension $q \times p$ and the vector $\boldsymbol{b}$ is of dimension q. Note that $q \geqslant p$, since S contains at least p elements obtained by taking a derivative of all elements of R. Thus, (13) is typically overdetermined.

Step 6. Solve for $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_p)$. Typically, the rank of $\boldsymbol{C}$ is p, and p of the equations in (13) can be satisfied. In any case, the goal is to solve as many as possible ($=$ rank $\boldsymbol{C}$) equations of (13) for the components of $\boldsymbol{\alpha}$. For every equation satisfied, a term disappears from the integrand of (12). It is preferable to solve the equations in the order they appear in (13), so as to minimize the order of differentiation of the remaining integrand of (12). This may be accomplished by Gaussian elimination, using a minimal number of row switching operations. Once this solution is obtained, (12) provides the final answer for $\int E dx$.

Example. Consider

$$E = 2uu'^3 + 3u^2u'u'' + 2uu',$$

which is easily checked not to be exact: $\mathcal{L}_u^{(0)}(E) \neq 0$.

Step 1. Applying the homotopy operator with $\lambda_0 = 0$ we get

$$F = \mathcal{H}_{\lambda_0}(E) = \frac{3}{4}u^2u'^2 + u^2.$$

Step 2. The above F gives,

$$R = \{u^2u'^2, u^2\},$$

thus $p=2$.

Step 3. Applying the homotopy method without optimization results in

$$\int E dx = \frac{3}{4}u^2u'^2 + u^2 + \frac{1}{2}\int \left(uu'^3 + 3u^2u'u''\right) dx, \tag{14}$$

which is correct, but not optimal. Instead, using (12) we get

$$\int E dx = \alpha_1 u^2u'^2 + \alpha_2 u^2 + \int \Big((2-2\alpha_1)\, uu'^3 + (3-2\alpha_1)\, u^2u'u'' + (2-2\alpha_2)\, uu'\Big) dx.$$

Step 4. Using this expression to construct the list S gives

$$S = \left[u^2u'u'', uu'^3, uu'\right],$$

so that $q=3$. Note that we have placed the term with the higher derivative first. The two terms of differential order 1 were ordered by degree of nonlinearity in their highest derivative.

Step 5. The resulting $q \times p = 3 \times 2$ linear system is

$$\begin{pmatrix} 2 & 0 \\ 2 & 0 \\ 0 & 2 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 3 \\ 2 \\ 2 \end{pmatrix}.$$

Step 6. As announced, this system is overdetermined. Performing Gaussian elimination with a minimal number of row switching operations gives the equivalent system

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 3/2 \\ 1 \\ -1 \end{pmatrix}.$$

Solving the first two of these equations results in $\alpha_1 = 3/2$ and $\alpha_2 = 1$, at which point no more equations can be solved. Therefore, our final answer is

$$\int E dx = \frac{3}{2}u^2u'^2 + u^2 - \int uu'^3 dx,$$

which is to be preferred over (14).

Example. Let

$$E = 3u'v^2 \sin u - u'^3 \sin u - 6vv' \cos u + 2u'u'' \cos u + 8v'v'' + v + uv^3 + e^u u'''.$$

Here we have two unknown functions and known functions of these. Using the homotopy method without optimization we obtain

$$\int E dx = -3\left(\frac{u'}{u}\right)^2 - 3\frac{u'^2 e^u}{u} + u'^2\cos u + e^u u'^2 + 3\frac{e^u u'^2}{u^2} + e^u u'' - 3v^2\cos u$$
$$+4v'^2 + \int\Big(v + uv^3 + 6\frac{u'u''}{u^2} - 6\Big(\frac{u'}{u}\Big)^3 - 6\frac{u'^3 e^u}{u^2} + 6\frac{u'u''e^u}{u^2}$$
$$+3\frac{u'^3e^u}{u} - e^u u'^3 - 3e^u u'u'' + 6e^u\Big(\frac{u'}{u}\Big)^3 - 6e^u\frac{u'u''}{u^2}\Big)dx,$$

not a desirable result. In this case, the homotopy method with optimization gives

$$\int E dx = u'^2\cos u - \frac{1}{2}e^u u'^2 + e^u u'' - 3v^2\cos u + 4v''^2 + \int\left(v + uv^3 + \frac{1}{2}e^u u'^3\right)dx,$$

which is a significant improvement over the non-optimized version.

Remarks:

- In essence, the homotopy operator is used as a guessing mechanism to generate a list of possible integrated terms, so that the size and the order of differentiation of the integrand in (12) can be reduced. However this does not always work as desired. Consider the example

  $$E = uu''.$$

  Then $\mathcal{L}_u^{(0)}(E) = 2uu'' \neq 0$, so that E is not exact. Next, $\mathcal{L}_u^{(1)}(E) = -2u'$ and $\mathcal{L}_u^{(2)}(E) = u$. The action of all remaining higher Euler operators results in zero. Then

  $$I(E) = \sum_{i=0}^{1} \mathrm{D}_x^i\left(u\mathcal{L}_u^{(i+1)}(E)\right) = u(-2u') + (u^2)' = 0 \quad\Rightarrow\quad \mathcal{H}_{\lambda_0}(E) = 0.$$

  Thus $E = uu''$ is in the kernel of the homotopy operator and this calculation gives no progress toward achieving

  $$\int E dx = uu' - \int u'^2 dx, \tag{15}$$

  which has a remaining integrand of lower differential order. This is a consequence of the cancellation occurring in (7). This problem may be avoided by introducing $J_{ji}(E) = \mathrm{D}_x^i\left(u^{(j)}\,\mathcal{L}_{u^{(j)}(x)}^{(i+1)}(E)\right)$, so that $I_j(E) = \sum_{i=0}^{N-1} J_{ji}(E)$. Now use (6) with $J_{ji}(E)$ instead of $I_j(E)$ for $i \in [0, N-1]$. This results in N homotopy-like constructions from which a set R may be constructed which will not suffer from cancellations internal to $I_j(E)$. For the above example $J_1(E) = -2uu' = -J_2(E)$. The resulting $R = \{uu'\}$. Using this R, our procedure gives the desired result.

- It should be noted that (12) is an identity for *all* choices of $\alpha_1, \ldots, \alpha_p$. Even without using the previous remark, the obtained answer,

  $$\int E dx = \int uu'' dx,$$

is correct, even though (15) may be more desirable. In summary, our procedure always gives a correct result, even though other guessing mechanisms may prove equally or more successful.

4. *Application: modulo derivatives*

In many applications [**4, 5, 11**], terms are considered equivalent if they are the same up to a total derivative. Applying the homotopy method with optimization may considerably simplify such computations.

Example. Consider

$$E_1 = 2uu'^3 + 3u^2u'u'',$$
$$E_2 = 3u'v^2 \sin u - u'^3 \sin u - 6vv' \cos u + 2u'u'' \cos u + 8v'v'' + v + uv^3.$$

Applying the homotopy method with optimization and only keeping terms which are left inside the resulting integral gives

$$E_1 \sim -uu'^3,$$

and

$$E_2 \sim v + uv^3,$$

where $E \sim \hat{E}$ means $E - \hat{E}$ is a total derivative.

Thus, the homotopy method with optimization allows one to efficiently reduce an expression to one of equal or lower differential order, equivalent to the original one up to a total derivative.

5. *Summing exact expressions*

We now turn our attention to the discrete case, where we are concerned with expressions of the form $E_n = E(n, \boldsymbol{u}_n, \boldsymbol{u}_{n+1}, \ldots, \boldsymbol{u}_{n+N})$ of an unknown (vector) function $\boldsymbol{u}_n$ and a finite number of its positive shifts, where N is the order of the highest shift of any component of $\boldsymbol{u}_n$ appearing in E_n. As in the continuous case, we assume that E_n contains no terms $\hat{E}(n)$ that are independent of the dependent variable. We will make use of the **shift operator** D, $\mathrm{D}E_n = E_{n+1}$. The identity operator is denoted by I, $\mathrm{I}E_n = E_n$, and $\Delta = \mathrm{D} - \mathrm{I}$, is the **forward difference operator**, $\Delta E_n = (\mathrm{D} - \mathrm{I})E_n = E_{n+1} - E_n$.

We begin by introducing the discrete analogs of the previously stated mathematical tools from the calculus of variations and differential geometry, the discrete Euler operators and the discrete homotopy operator. These operators will allow us to answer the following questions:

- **Question 1:** How does one check if an expression E_n is exact, i.e., a total difference, $E_n = \Delta F_n = F_{n+1} - F_n$ for some function F_n?
- **Question 2:** If an expression E_n is exact, how does one determine $F_{n+1} = \sum_n E_n$?

We first introduce the zeroth-order discrete Euler operator or the discrete variational derivative, before proceeding to introduce the higher-order versions. With the discrete Euler operators in hand, we introduce the discrete homotopy operator and demonstrate how it is used to sum exact expressions. Most of the material presented in this section is not new.

It may be found in a more abstract form in [**8**], or in a more concrete form in [**6, 7**], for instance.

5.1. *The discrete Euler operators*

DEFINITION 4. *The one-dimensional* **discrete Euler operator of order zero** *(discrete variational derivative), with the discrete independent variable n and dependent variable $\boldsymbol{u}_n = \left(u_n^{(1)}, \ldots, u_n^{(M)}\right)$, is defined as the operator $\mathcal{L}^{(0)}_{\boldsymbol{u}_n}$ with M components*

$$\mathcal{L}^{(0)}_{\boldsymbol{u}_n} = \left(\mathcal{L}^{(0)}_{u_n^{(1)}}, \ldots, \mathcal{L}^{(0)}_{u_n^{(M)}}\right) = \left(\sum_{k=0}^{N} \mathrm{D}^{-k} \frac{\partial}{\partial u^{(1)}_{n+k}}, \ldots, \sum_{k=0}^{N} \mathrm{D}^{-k} \frac{\partial}{\partial u^{(M)}_{n+k}}\right) \tag{16a}$$

$$= \left(\frac{\partial}{\partial u_n^{(1)}} \left(\sum_{k=0}^{N} \mathrm{D}^{-k}\right), \ldots, \frac{\partial}{\partial u_n^{(M)}} \left(\sum_{k=0}^{N} \mathrm{D}^{-k}\right)\right). \tag{16b}$$

Note the similarity of (16a) to the continuous Euler operator of order zero (1). In what follows, we use the second formulation (16b) because of its computational convenience.

The discrete variational derivative allows us to answer Question 1 by the following theorem [**8**].

THEOREM 3. *A necessary and sufficient condition for an expression E_n, with positive shifts, to be exact is that $\mathcal{L}^{(0)}_{\boldsymbol{u}_n}(E_n) \equiv 0$.*

Example. Consider

$$E_n = u_{n+3}v_{n+2}^2 + u_n^2 - v_n^5 - u_{n+1}v_n^2 + v_{n+1}^5 - u_{n+1}^2. \tag{17}$$

Note that $E_n = \Delta F_n$, $F_n = -u_n^2 + u_{n+1}v_n^2 + u_{n+2}v_{n+1}^2 + v_n^5$. Indeed,

$$\begin{aligned}\mathcal{L}^{(0)}_{u_n}(E_n) &= \frac{\partial}{\partial u_n}(u_{n+3}v_{n+2}^2 + v_{n+1}^5 - u_{n+1}^2 + u_{n+2}v_{n+1}^2 - u_{n-1}v_{n-2}^2 \\ &\quad + u_{n-3}^2 - v_{n-3}^5 - u_{n-2}v_{n-3}^2) \\ &= 0\end{aligned}$$

and

$$\begin{aligned}\mathcal{L}^{(0)}_{v_n}(E_n) &= \frac{\partial}{\partial v_n}(u_{n+3}v_{n+2}^2 + v_{n+1}^5 - u_{n+1}^2 + u_{n+2}v_{n+1}^2 - u_n v_{n-1}^2 + u_{n-2}^2 \\ &\quad - v_{n-2}^5 - u_{n-1}v_{n-2}^2) \\ &= 0.\end{aligned}$$

To compute $F_{n+1} = \sum_n E_n$, we need the discrete higher Euler operators.

DEFINITION 5. *The one-dimensional* **discrete higher Euler operator** *of order k with discrete independent variable n is given by*

$$\mathcal{L}^{(k)}_{\boldsymbol{u}_n} = \sum_{m=k}^{N} \binom{m}{k} \mathrm{D}^{-m} \frac{\partial}{\partial \boldsymbol{u}_{n+k}} = \frac{\partial}{\partial \boldsymbol{u}_n} \sum_{m=k}^{N} \binom{m}{k} \mathrm{D}^{-m}. \tag{18}$$

In particular, the first four higher Euler operators for component u_n are

$$\mathcal{L}^{(0)}_{u_n} = \frac{\partial}{\partial u_n}(1 \cdot \mathrm{I} + 1 \cdot \mathrm{D}^{-1} + 1 \cdot \mathrm{D}^{-2} + 1 \cdot \mathrm{D}^{-3} + \cdots), \tag{19a}$$

$$\mathcal{L}^{(1)}_{u_n} = \frac{\partial}{\partial u_n}\left(1 \cdot \mathrm{D}^{-1} + 2 \cdot \mathrm{D}^{-2} + 3 \cdot \mathrm{D}^{-3} + 4 \cdot \mathrm{D}^{-4} + \cdots\right), \tag{19b}$$

$$\mathcal{L}^{(2)}_{u_n} = \frac{\partial}{\partial u_n}\left(1 \cdot \mathrm{D}^{-2} + 3 \cdot \mathrm{D}^{-3} + 6 \cdot \mathrm{D}^{-4} + 10 \cdot \mathrm{D}^{-5} + \cdots\right), \tag{19c}$$

$$\mathcal{L}^{(3)}_{u_n} = \frac{\partial}{\partial u_n}\left(1 \cdot \mathrm{D}^{-3} + 4 \cdot \mathrm{D}^{-4} + 10 \cdot \mathrm{D}^{-5} + 20 \cdot \mathrm{D}^{-6} + \cdots\right). \tag{19d}$$

As in the continuous case, the higher-order analog of Question 1 is answered by the discrete higher Euler operators, $E_n = \Delta^m F_n$ for some F_n if and only if $\mathcal{L}^{(k)}_{\boldsymbol{u}_n}(E_n) \equiv 0$ for $k = 0, \ldots, m-1$ (the proof is analogous to the continuous version [**9**], using $\mathcal{L}^{(k)}_{\boldsymbol{u}_n}(\Delta E_n) = \mathcal{L}^{(k-1)}_{\boldsymbol{u}_n}(E_n)$).

5.2. *The discrete homotopy operator*

Next, we define the discrete homotopy operator, which reduces summation of an expression involving unknown functions to integration of a known function with respect to a single scalar variable.

DEFINITION 6. *The one-dimensional* **discrete homotopy operator** *with discrete independent variable n is*

$$\hat{\mathcal{H}}_{\lambda_0}(E_n) = \int_{\lambda_0}^{1} \sum_{j=1}^{M} I_j(E_n)[\lambda \boldsymbol{u}_n]\, \frac{d\lambda}{\lambda}, \tag{20}$$

with

$$I_j(E_n) = \sum_{i=0}^{N-1} \Delta^i \left(u_n^{(j)}\, \mathcal{L}^{(i+1)}_{u_n^{(j)}}(E_n) \right). \tag{21}$$

The integrand (21) involves the one-dimensional higher Euler operators and M is the number of components of $\boldsymbol{u}_n = \left(u_n^{(1)}, \ldots, u_n^{(M)}\right)$. The notation $I_j(E_n)[\lambda \boldsymbol{u}_n]$ implies that in $I_j(E_n)$ one replaces $\boldsymbol{u}_n$ with $\lambda \boldsymbol{u}_n$, $\boldsymbol{u}_{n+1}$ with $\lambda \boldsymbol{u}_{n+1}$, etc.

The discrete homotopy operator allows us to answer Question 2 by the following theorem [**8**].

THEOREM 4. *For an exact function $E_n = \Delta F_n$, one has*

$$\hat{\mathcal{H}}_{\lambda_0}(E_n) = F_n[\boldsymbol{u}_n] - F_n[\lambda_0 \boldsymbol{u}_n]. \tag{22}$$

As in the continuous case, the kernel of the discrete homotopy operator is non-trivial (see Appendix Appendix A). Thus, we consider two cases: expressions which *vanish at zero or infinity* and expressions which do not. Again, we can exclude mixed cases since $\hat{\mathcal{H}}_{\lambda_0}$ is a linear operator.

- **Expressions which vanish at zero or infinity:** If $\lim_{\lambda \to \lambda_0} E_n[\lambda \boldsymbol{u}_n] = 0$ for λ_0 equal to zero or infinity, then evaluating $\hat{\mathcal{H}}_{\lambda_0}(E_n)$ gives $F_n[\boldsymbol{u}_n]$, up to a summation constant, according to (22). This can be seen by noting that $\Delta F_n[\lambda_0 \boldsymbol{u}_n] =$

$E_n[\lambda_0 \boldsymbol{u}_n] = 0 \Rightarrow F_{n+1}[\lambda_0 \boldsymbol{u}_n] = F_n[\lambda_0 \boldsymbol{u}_n]$, thus $F_n[\lambda_0 \boldsymbol{u}_n]$ is a constant independent of n.

- **Expressions which do not vanish at zero or infinity:** If $\lim_{\lambda\to\lambda_0} E_n[\lambda \boldsymbol{u}_n] \neq 0$ for both $\lambda_0 = 0$ and $\lambda_0 = \infty$, then as in the continuous case, the limiting value is in the kernel of the discrete homotopy operator (see Appendix A), and must be dealt with separately. One method of dealing with such terms is the introduction of a parameter, as demonstrated in the examples below. A modified version of the homotopy operator may be used as well, as discussed in the remark at the end of the next section. Also, non-homotopy methods can be used (see Appendix B, for example).

Example. Returning to (17),

$$E_n = u_{n+3}v_{n+2}^2 + u_n^2 - v_n^5 - u_{n+1}v_n^2 + v_{n+1}^5 - u_{n+1}^2.$$

In this case, $\boldsymbol{u}_n = (u_n, v_n)$ and

$$\begin{aligned}
\lim_{\lambda\to\lambda_0} E_n[\lambda u_n, \lambda v_n] &= \lim_{\lambda\to\lambda_0} \Big(\lambda^3 u_{n+3}v_{n+2}^2 + \lambda^2 u_n^2 - \lambda^5 v_n^5 - \lambda^3 u_{n+1}v_n^2 \\
&\quad +\lambda^5 v_{n+1}^5 \lambda^2 u_{n+1}^2\Big) \\
&= \lambda_0^2\Big(\lambda_0 u_{n+3}v_{n+2}^2 + u_n^2 - \lambda_0^3 v_n^5 - \lambda_0 u_{n+1}v_n^2 + \lambda_0^3 v_{n+1}^5 \\
&\quad -u_{n+1}^2\Big).
\end{aligned}$$

Thus we choose $\lambda_0 = 0$. Proceeding without this, we have

$$\hat{\mathcal{H}}_{\lambda_0}(E_n) = \int_0^1 \left(I_{u_n}(f)[\lambda \mathbf{u}_n] + I_{v_n}(f)[\lambda \mathbf{u}_n]\right) \frac{d\lambda}{\lambda},$$

with

$$I_{u_n}(E_n) = \sum_{i=0}^{\infty} \Delta^i \left(u_n \mathcal{L}_{u_n}^{(i+1)}(E_n)\right) \quad \text{and} \quad I_{v_n}(E_n) = \sum_{i=0}^{\infty} \Delta^i \left(v_n \mathcal{L}_{v_n}^{(i+1)}(E_n)\right).$$

These formulas give

$$\begin{aligned}
I_{u_n}(E_n) &= u_n \mathcal{L}_{u_n}^{(1)}(E_n) + \Delta\left(u_n \mathcal{L}_{u_n}^{(2)}(E_n)\right) + \Delta^2\left(u_n \mathcal{L}_{u_n}^{(3)}(E_n)\right) \\
&= u_n \frac{\partial}{\partial u_n}\left(\mathrm{D}^{-1} + 2\mathrm{D}^{-2} + 3\mathrm{D}^{-3}\right)(E_n) + \Delta\left(u_n \frac{\partial}{\partial u_n}\left(\mathrm{D}^{-2} + 3\mathrm{D}^{-3}\right)(E_n)\right) \\
&\quad +\Delta^2\left(u_n \frac{\partial}{\partial u_n}\mathrm{D}^{-3}(E_n)\right) \\
&= -2u_n^2 + u_{n+1}v_n^2 + u_{n+2}v_{n+1}^2,
\end{aligned}$$

and

$$\begin{aligned}
I_{v_n}(E_n) &= v_n \mathcal{L}_{v_n}^{(1)}(E_n) + \Delta\left(v_n \mathcal{L}_{v_n}^{(2)}(E_n)\right) \\
&= v_n \frac{\partial}{\partial v_n}\left(\mathrm{D}^{-1} + 2\mathrm{D}^{-2}\right)(E_n) + \Delta\left(v_n \frac{\partial}{\partial v_n}\mathrm{D}^{-2}(E_n)\right) \\
&= 5v_n^5 + 2u_{n+1}v_n^2 + 2u_{n+2}v_{n+1}^2.
\end{aligned}$$

Thus, (20) gives

$$\begin{aligned}\hat{\mathcal{H}}_{\lambda_0}(E_n) &= \int_{\lambda_0}^{1} \left(I_{u_n}(E_n)[\lambda \mathbf{u}_n] + I_{v_n}(E_n)[\lambda \mathbf{u}_n]\right) \frac{d\lambda}{\lambda} \\ &= \int_{\lambda_0}^{1} \left(-2\lambda u_n^2 + 3\lambda^2 u_{n+1} v_n^2 + 3\lambda^2 u_{n+2} v_{n+1}^2 + 5\lambda^4 v_n^5\right) \, d\lambda \\ &= -u_n^2 + u_{n+1}v_n^2 + u_{n+2}v_{n+1}^2 + v_n^5 + \lambda_0^2 u_n^2 - \lambda_0^3 u_n^2 u_{n+1} v_n^2 \\ &\quad -\lambda_0^3 u_n^2 u_{n+2} v_{n+1}^2 - \lambda_0^5 u_n^2 v_n^5.\end{aligned}$$

Evaluating at $\lambda_0 = 0$ results in

$$F_n = -u_n^2 + u_{n+1}v_n^2 + u_{n+2}v_{n+1}^2 + v_n^5,$$

as desired.

Example. Consider

$$E_n = u_{n+2}u_{n+1}^p - u_{n+1}u_n^p. \tag{23}$$

Here we have

$$E_n[\lambda \boldsymbol{u}_n] = \lambda^{(p+1)} \left(u_{n+2}u_{n+1}^p - u_{n+1}u_n^p\right).$$

A similar calculation to that given above establishes that $\lambda_0 = 0$ for $p > -1$, whereas $\lambda_0 = \infty$ for $p < -1$. For $p \neq -1$, (21) gives

$$I_{u_n}(E_n) = (p+1)u_{n+1}u_n^p.$$

Therefore,

$$\hat{\mathcal{H}}_{\lambda_0}(E_n) = \int_{\lambda_0}^{1} \lambda^p (p+1) u_{n+1} u_n^p d\lambda = u_{n+1}u_n^p - \lambda_0^{(p+1)} u_{n+1} u_n^p.$$

Evaluating at $\lambda_0 = \infty$ for $p < -1$ or $\lambda_0 = 0$ for $p > -1$ gives

$$\sum_n E_n = u_{n+2}u_{n+1}^p, \;\; p \neq -1. \tag{24}$$

Example. Suppose $p = -1$ in (23) from our previous example, then E_n is homogeneous of degree zero. In this case (21) gives

$$I_u(E_n) = 0,$$

resulting in

$$\hat{\mathcal{H}}_{\lambda_0}(E_n) = \int_{\lambda_0}^{1} 0 \cdot \frac{1}{\lambda} d\lambda = 0. \tag{25}$$

This is correct: upon inspection one has

$$F_{n+1} = \sum_n E_n = \frac{u_{n+2}}{u_{n+1}},$$

giving

$$F_n[u_n] - F_n[\lambda_0 u_n] = \frac{u_{n+1}}{u_n} - \frac{\lambda_0 u_{n+1}}{\lambda_0 u_n} = 0,$$

in agreement with (22) and (25). However, $F_n[u_n]$ cannot be recovered from the above expression.

In order to obtain the desired answer for $p = -1$, we proceed as we did in the continuous case. Returning to our previous example, making note of the fact that there are no singularities with respect to the parameter p in (24), we make the substitution $p = -1$ giving

$$F_{n+1} = \sum_n E_n = \frac{u_{n+2}}{u_{n+1}},$$

as desired.

6. *Summing non-exact expressions*

If an expression E_n is not exact, we aim to sum as many differences in E_n as possible, while optimizing the number and type of terms remaining in the sum. We use the following six-step method, which we refer to as *the discrete homotopy method with optimization*.

Step 1. Sum total differences in E_n. Calculate

$$F_n = \hat{\mathcal{H}}_{\lambda_0}(E_n),$$

where λ_0 is equal to zero or infinity. Since E_n is not exact, $F_{n+1} \neq \sum_n E_n$.

Step 2. Construct the set of all terms of F_n. Let p be the number of terms of $F_n = \sum_{i=1}^{p} c_i F_n^{(i)}$, such that no two $F_n^{(i)}$'s are constant multiples of each other and each c_i is a constant. Form the set $R = \{F_n^{(1)}, F_n^{(2)}, \ldots, F_n^{(p)}\}$ of all terms in F_n. Several choices may be possible for the set R. Preference should be given to the set with the largest p. To this end, expressions should be expanded when possible. It should be noted that working with a smaller set R will not result in a wrong answer, but merely in a less than optimal answer.

Step 3. Separate E_n into its difference part and its non-difference part. Using R,

$$\sum_n E_n = \sum_{i=1}^{p} \alpha_i F_{n+1}^{(i)} + \sum_n \left(E_n - \sum_{i=1}^{p} \alpha_i \Delta F_n^{(i)} \right). \tag{26}$$

Note that choosing $\alpha_i = c_i$ for all i gives $\sum_n E_n = F_{n+1} + \sum_n (E_n - (F_{n+1} - F_n))$, which is obviously true. Doing this is referred to as the *discrete homotopy method without optimization*.

Step 4. Construct an ordered list of terms S occurring in $E_n - \sum_{i=1}^{p} \alpha_i \Delta F_n^{(i)}$. Reduce S to ensure no two elements are constant multiples of each other. The list starts with elements which contain the highest degree of non-locality (the difference between the highest shift and the lowest shift). Different choices for this ordering are possible, which may result in different but correct final results.

Step 5. Construct a linear algebraic system for $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_p)$. Construct a system of q linear equations such that the j-th equation is the coefficient of S_j in $\sum_{i=1}^{p} \alpha_i \Delta F_n^{(i)}$

equated to the coefficient of S_j in E_n. These equations are linear in the components of $\boldsymbol{\alpha}$, and the system of equations may be written as

$$\boldsymbol{C}\boldsymbol{\alpha} = \boldsymbol{b}, \tag{27}$$

where the matrix $\boldsymbol{C}$ is of dimension $q \times p$ and the vector $\boldsymbol{b}$ is of dimension q. Note that $q \geqslant p$, since S contains at least p elements obtained by applying D to all elements of R. Thus, (27) is typically overdetermined.

Step 6. Solve for $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_p)$. Typically, the rank of $\boldsymbol{C}$ is p, and p of the equations in (27) can be satisfied. In any case, the goal is to solve as many as possible ($=$ rank $\boldsymbol{C}$) equations of (27) for the components of $\boldsymbol{\alpha}$. For every equation satisfied, a term disappears from the summand of (26). It is preferable to solve the equations in the order they appear in (27), so as to minimize the degree of non-locality of the remaining summand of (26). Once this solution is obtained, (26) provides the final answer for $\sum_n E_n$.

Example. Consider

$$E_n = 2u_{n+3}^2 u_{n+2} - u_{n+1}^2 u_n + u_{n+2}, \tag{28}$$

which is easily checked not to be exact: $\mathcal{L}_{u_n}^{(0)} \neq 0$.

Step 1. Applying the discrete homotopy operator with $\lambda_0 = 0$ we get

$$\hat{\mathcal{H}}_{\lambda_0}(E_n) = \frac{2}{3} u_n^2 u_{n-1} + 2u_{n+1}^2 u_n + 2u_{n+2}^2 u_{n+1} + u_{n+1} + u_n.$$

Step 2. The above gives

$$R = \{u_{n+1}^2 u_n, u_{n+2}^2 u_{n+1}, u_n^2 u_{n-1}, u_{n+1}, u_n\},$$

thus $p = 5$.

Step 3. Applying the discrete homotopy method without optimization results in

$$\begin{aligned}\sum_n E_n &= \frac{2}{3} u_{n+1}^2 u_n + 2u_{n+2}^2 u_{n+1} + 2u_{n+3}^2 u_{n+2} + u_{n+2} + u_{n+1} \\ &\quad + \sum_n \left(\frac{1}{3} u_{n+1}^2 u_n + \frac{2}{3} {u_n}^2 u_{n-1} + u_n \right),\end{aligned} \tag{29}$$

which is correct, but not optimal. Instead, using (26) we get

$$\begin{aligned}\sum_n E_n &= \alpha_1 u_{n+2}^2 u_{n+1} + \alpha_2 u_{n+3}^2 u_{n+2} + \alpha_3 u_{n+1}^2 u_n + \alpha_4 u_{n+2} + \alpha_5 u_{n+1} \\ &\quad + \sum_n \Big((2-\alpha_2) u_{n+3}^2 u_{n+2} + (\alpha_2 - \alpha_1) u_{n+2}^2 u_{n+1} + (1-\alpha_4) u_{n+2} + \alpha_5 u_n \\ &\quad + (-1 + \alpha_1 - \alpha_3) u_{n+1}^2 u_n + \alpha_3 u_n^2 u_{n-1} + + (\alpha_4 - \alpha_5) u_{n+1} \Big).\end{aligned}$$

Step 4. Using this expression to construct the list S gives

$$S = \left[u_{n+3}^2 u_{n+2}, u_{n+2}^2 u_{n+1}, u_n^2 u_{n-1}, u_{n+1}^2 u_n, u_{n+2}, u_{n+1}, u_n \right],$$

so that $q = 7$. Note that in this case the first four terms have the same degree of non-locality, 1, while the last three terms have degree of non-locality 0. Terms with the same degree of non-locality have been ordered by the absolute value of their lowest shift, from highest to lowest (with negative shifts before positive shifts).

Step 5. The resulting $q \times p = 7 \times 5$ linear system is

$$\begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \alpha_5 \end{pmatrix} = \begin{pmatrix} 2 \\ 0 \\ 0 \\ 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}.$$

Step 6. As announced, this system is overdetermined. Performing Gaussian elimination with a minimal number of row switching operations gives the equivalent system

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \alpha_4 \\ \alpha_5 \end{pmatrix} = \begin{pmatrix} 2 \\ 2 \\ 0 \\ 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}.$$

Solving the first five of these equations results in $\alpha_1 = \alpha_2 = 2$, $\alpha_3 = 0$, and $\alpha_4 = \alpha_5 = 1$ at which point no more equations can be solved. Therefore, our final answer is

$$\sum_n E_n = 2u_{n+2}u_{n+3}^2 + 2u_{n+1}u_{n+2}^2 + u_{n+2} + u_{n+1} + \sum_n \left(u_{n+1}^2 u_n + u_n\right),$$

which is to be preferred over (29).

Example. Let

$$E_n = 7\,u_{n+3}^9 v_{n+2}^3 + u_{n+1}^2 v_n - e^{u_n} v_{n+1}^5 - u_{n+2}^9 v_{n+1}^3 + e^{u_{n+1}} v_{n+2}^5 - 3\,u_{n+2}^2 v_{n+1}.$$

Here we have two unknown functions and a known function of these. Using the discrete homotopy method without optimization gives

$$\begin{aligned} \sum_n E_n = {} & 7\,u_{n+3}^9 v_{n+2}^3 + 9/2\,u_{n+1}^9 v_n^3 + 6\,u_{n+2}^9 v_{n+1}^3 + e^{u_{n+1}} v_{n+2}^5 - 4/3\,u_{n+1}^2 v_n \\ & -3\,u_{n+2}^2 v_{n+1} + \sum_n \Big(-2/3\,u_{n+1}^2 v_n + 3/2\,u_{n+1}^9 v_n^3 + 9/2\,u_n^9 v_{n-1}^3 \\ & -4/3\,u_n^2 v_{n-1}\Big). \end{aligned}$$

In this case, the discrete homotopy method with optimization gives

$$
\begin{aligned}
\sum_n E_n = {} & 7\, u_{n+3}^9 v_{n+2}^3 + 6\, u_{n+2}^9 v_{n+1}^3 + e^{u_{n+1}} v_{n+2}^5 - 3\, u_{n+2}^2 v_{n+1} \\
& + \sum_n \left(6\, u_{n+1}^9 v_n^3 - 2\, u_{n+1}^2 v_n\right),
\end{aligned}
$$

which is an improvement over the non-optimized version.

Remark: The homotopy method with optimization also provides a way of summing exact expressions which do not vanish as the homotopy parameter λ approaches zero or infinity. As in the continuous case, we introduce

$$J_{ji}(E_n) = \Delta^i \left(u_n^{(j)}\, \mathcal{L}_{u_n^{(j)}}^{(i+1)}(E_n) \right),$$

so that $I_j(E_n) = \sum_{i=0}^{N-1} J_{ji}(E_n)$. Now use (20) with $J_{ji}(E_n)$ instead of $I_j(E_n)$ for $i \in [0, N-1]$. This results in N homotopy-like constructions from which a set R may be constructed which will not suffer from cancellations internal to $I_j(E_n)$. For example, returning to (23) with $p = -1$ we have

$$E_n = \frac{u_{n+2}}{u_{n+1}} - \frac{u_{n+1}}{u_n}.$$

This was shown to be in the kernel of the homotopy operator, thus, we were unable to recover F_n. Instead, using the above gives $J_1(E_n) = -u_{n+1}/u_n + u_n/u_{n-1} = -J_2(E_n)$. This results in $R = \{\frac{u_n}{u_{n-1}}, \frac{u_{n+1}}{u_n}\}$. Using this R, our procedure gives the desired result.

7. *Application: modulo differences*

In many applications [**6, 12**], terms are considered equivalent if they are identical up to differences. Applying the homotopy method with optimization may considerably simplify such computations.

Example. Consider

$$
\begin{aligned}
E_n^{(1)} &= n^2 u_{n+1} + 3\, n u_{n+1} + 2\, u_{n+1} - n^2 u_n - n u_n + u_n^7, \\
E_n^{(2)} &= -u_n u_{n+1} v_n - v_n^2 + u_{n+1} u_{n+2} v_{n+1} + v_{n+1}^2 + u_{n+3} v_{n+2} - u_{n+1} v_n + u_{n+1} \\
&\quad + v_n^{11} - u_n u_{n+1} v_{n+5}.
\end{aligned}
$$

Applying the homotopy method with optimization and retaining the remaining summand gives

$$E_n^{(1)} \sim u_n^7,$$

and

$$E_n^{(2)} \sim v_n^{11} + u_n - u_n u_{n+1} v_{n+5},$$

where $E_n \sim \hat{E}_n$ means $E_n - \hat{E}_n$ is a difference.

Thus, the homotopy method with optimization allows one to efficiently reduce an expression to a simpler (difference free) expression, equivalent to the original one up to a difference.

Appendix A. *The kernel of the homotopy operator*

Here we discuss the kernel of the continuous and discrete homotopy operators.

Definition. *An expression $E[\boldsymbol{u}]$ is* **equivalent to a term of degree zero** *if*

$$E[\lambda \boldsymbol{u}] = E[\boldsymbol{u}] + C_\lambda$$

where C_λ is a constant independent of $(\boldsymbol{u}, \boldsymbol{u}_x, \boldsymbol{u}_{2x}, \ldots)$. E is of **degree zero** *if $C_\lambda \equiv 0$.*

Theorem. *An exact expression $E = \mathrm{D}_x F$ is in the kernel of the homotopy operator if and only if E is of degree zero.*

Remark: The kernel is defined only up to a constant of integration. All constants of integration are considered equivalent to 0.

Lemma. *E is of degree zero if and only if F is equivalent to a term of degree zero.*

Proof of the lemma. First, suppose F is equivalent to a term of degree zero. Then

$$E[\lambda \boldsymbol{u}] = \mathrm{D}_x \left(F[\lambda \boldsymbol{u}] \right) = \mathrm{D}_x \left(F[\boldsymbol{u}] + C \right) = \mathrm{D}_x F[\boldsymbol{u}] = E[\boldsymbol{u}].$$

Therefore E is of degree zero.

Now, suppose E is of degree zero. Then

$$\mathrm{D}_\lambda \left(E[\lambda \boldsymbol{u}] \right) = \mathrm{D}_\lambda \left(E[\boldsymbol{u}] \right) = 0.$$

Thus,

$$0 = \mathrm{D}_\lambda \left(E[\lambda \boldsymbol{u}] \right) = \mathrm{D}_\lambda \left(\mathrm{D}_x F[\lambda \boldsymbol{u}] \right) = \mathrm{D}_x \left(\mathrm{D}_\lambda F[\lambda \boldsymbol{u}] \right).$$

This implies that $\mathrm{D}_\lambda F[\lambda \boldsymbol{u}]$ is some constant, $B(\lambda)$, independent of x. Integrating with respect to λ gives

$$\int_{\lambda_0}^{1} \mathrm{D}_\lambda F[\lambda \boldsymbol{u}] d\lambda = \int_{\lambda_0}^{1} B(\lambda) d\lambda \Rightarrow F[\boldsymbol{u}] - F[\lambda_0 \boldsymbol{u}] = \int_{\lambda_0}^{1} B(\lambda) d\lambda.$$

This implies,

$$F[\lambda_0 \boldsymbol{u}] = F[\boldsymbol{u}] - \int_{\lambda_0}^{1} B(\lambda) d\lambda.$$

Therefore, since λ_0 is arbitrary, F is equivalent to a term of degree zero. ■

Proof of the theorem. Now, suppose E is in the kernel of the homotopy operator. Then

$$\mathcal{H}_{\lambda_0}(E) = F[\boldsymbol{u}] - F[\lambda_0 \boldsymbol{u}] = A,$$

where A is some constant. This implies that

$$F[\lambda_0 \boldsymbol{u}] = F[\boldsymbol{u}] - A.$$

Thus, F is equivalent to a term of degree zero, which in turn implies E is of degree zero by the lemma.

Now, suppose E is of degree zero. This implies that F is equivalent to a term of degree zero by the lemma. Thus,

$$F[\lambda \boldsymbol{u}] = F[\boldsymbol{u}] + C_\lambda.$$

Therefore,

$$\mathcal{H}_{\lambda_0}(E) = F[\boldsymbol{u}] - F[\lambda_0 \boldsymbol{u}] = -C_{\lambda_0},$$

i.e., E is in the kernel of the homotopy operator. ■

We have the analogous result for the discrete case.

Theorem. *An exact expression $E_n = \Delta F_n$ is in the kernel of the discrete homotopy operator if and only if E_n is of degree zero.*

The proof closely resembles that of the continuous case, and it is omitted here.

Appendix B. *A non-homotopy summation algorithm*

Alternatively, we can use the following non-homotopy method to sum exact and non-exact expressions in one dimension. This method is devoid of the problem with the homotopy method when summing terms that do not vanish in the limit as λ goes to 0 or infinity. However, it is not easily generalized to the multi-dimensional setting unlike the homotopy method (see remark below).

Our goal is to reduce the summand to a *standard form*, which we define as an expression with every term having a lowest shift of zero. This will automatically eliminate differences from the summand since the standard form of a difference, $E_n = \Delta F_n = F_{n+1} - F_n$ (assuming, without loss of generality, that the lowest shift in F_n is 0), is $F_n - F_n = 0$. To accomplish this, we define the *minimum shift operator*, Z, such that $Z(E_n) = \mathrm{D}^{-m}(E_n)$, where m is the minimum shift occurring in E_n. In other words, Z returns an expression which has a minimum shift of zero. Applying Z to each term in the summand reduces it to standard form. Since we wish to apply Z to terms inside a sum, we need the *telescoping summand rule*, $\sum_n E_n = E_n + E_{n-1} + \cdots + E_{n-m+1} + \sum_n Z(E_n)$. This rule allows one to compensate for the action of Z on the summand. For $E_n = \Delta F_n$, this rule reduces to the more familiar identity $\sum_n \Delta F_n = \sum_n F_{n+1} - \sum_n F_n = F_{n+1} + \sum_n F_n - \sum_n F_n = F_{n+1}$.

Using the above remarks, the algorithm is as follows. Let p be the number of terms of $E_n = \sum_{i=1}^{p} E_n^{(i)}$, such that no two $E_n^{(i)}$'s are constant multiples of each other (see Step 2 of the discrete homotopy method). Then one has

$$\sum_n E_n = T_n + \sum_n G_n,$$

where

$$G_n = \sum_{i=1}^{p} Z(E_n^{(i)})$$

is in standard form, and is therefore difference free. Here T_n is found by use of the telescoping summand rule:

$$T_n = \sum_{i=1}^{p} T_n^{(i)},$$

where $T_n^{(i)} = E_n^{(i)} + E_{n-1}^{(i)} + \cdots + E_{n-m_i+1}^{(i)}$ and m_i is the lowest shift occurring in $E_n^{(i)}$.

For example, consider

$$E_n = \frac{u_{n+2}}{u_{n+1}} - \frac{u_{n+1}}{u_n} + 2u_{n+3}^2 u_{n+2} - u_{n+1}^2 u_n + u_{n+2},$$

a combination of our previous examples. We have

$$\begin{aligned}
&Z\left(u_{n+2}/u_{n+1}\right) = \mathrm{D}^{-1}\left(u_{n+2}/u_{n+1}\right) = u_{n+1}/u_n, \\
&Z\left(-u_{n+1}/u_n\right) = \mathrm{D}^{0}\left(-u_{n+1}/u_n\right) = -u_{n+1}/u_n, \\
&Z\left(2u_{n+3}^2 u_{n+2}\right) = \mathrm{D}^{-2}\left(2u_{n+3}^2 u_{n+2}\right) = 2u_{n+1}^2 u_n, \\
&Z\left(-u_{n+1}^2 u_n\right) = \mathrm{D}^{0}\left(-u_{n+1}^2 u_n\right) = -u_{n+1}^2 u_n, \\
&Z\left(u_{n+2}\right) = \mathrm{D}^{-2}\left(u_{n+2}\right) = u_n.
\end{aligned}$$

Thus,

$$G_n = \frac{u_{n+1}}{u_n} - \frac{u_{n+1}}{u_n} + 2u_{n+1}^2 u_n - u_{n+1}^2 u_n + u_n = u_{n+1}^2 u_n + u_n,$$

which is indeed difference free. Using the telescoping summand rule each time we apply Z to a term inside the sum gives

$$T_n = \frac{u_{n+2}}{u_{n+1}} + 2u_{n+3}^2 u_{n+2} + 2u_{n+2}^2 u_{n+1} + u_{n+2} + u_{n+1}.$$

Therefore, our final result is

$$\sum_n E_n = \frac{u_{n+2}}{u_{n+1}} + 2u_{n+3}^2 u_{n+2} + 2u_{n+2}^2 u_{n+1} + u_{n+2} + u_{n+1} + \sum_n \left(u_{n+1}^2 u_n + u_n\right),$$

in agreement with our results using homotopy methods.

Remark: This and other non-homotopy methods (see [**10**] for instance) rely on the fact that summation (integration) and the inversion of the discrete (continuous) divergence operator are equivalent in one-dimension. In the multi-dimensional setting, however, this equivalence no longer holds, *i.e.*, multiple summation (integration) is not the higher dimensional analog of the inversion of the discrete (continuous) divergence operator. As explicitly shown in [**7, 11**], the homotopy operator reduces this inversion in any dimension to a single integration. We see no clear extension of the algorithm presented in this appendix to higher dimensions, where as homotopy methods may still be used.

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