Continuous and Discrete Homotopy Operators with Applications in Integrability Testing of Nonlinear PDEs and Lattices

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Purpose

- Design symbolic code (in *Mathematica*) to automate the computation of conservation laws (symmetries, recursion operators) of nonlinear systems of PDEs and DDEs.

- Systems of PDEs in $(1+1)$ and $(3+1)$ dimensions with polynomial as well as transcendental nonlinearities.

- Systems involving arbitrary parameters (classification problems).

- Extend the algorithms to differential-difference equations (DDEs, semi-discrete lattices), continuous in time and one discretized space variable.

Motivation

- Conservation laws describe the conservation of fundamental physical quantities (linear momentum, energy, etc.).

  Compare with constants of motion (linear momentum, energy) in mechanics.

- Conservation laws provide a method to study quantitative and qualitative properties of equations and their solutions,
  e.g. Hamiltonian structures.

- Conserved densities can be used to test numerical integrators.

- For PDEs and DDEs, the existence of a sufficiently large (in principal infinite) number of conservation laws or symmetries assures complete **integrability**.

- Conserved densities and symmetries aid in finding the recursion operator (which guarantees the existence of infinitely many symmetries).

Definitions:

- Conservation law in $(1+1)$ dimensions

$$\mathrm{D}_t\rho + \mathrm{D}_x J = 0 \qquad \text{(on PDE)}$$

conserved density ρ and flux J.

- Conservation law in $(3+1)$ dimensions

$$\mathrm{D}_t\rho + \nabla\cdot\mathbf{J} = \mathrm{D}_t\rho + \mathrm{D}_x J^{(1)} + \mathrm{D}_y J^{(2)} + \mathrm{D}_z J^{(3)} = 0 \qquad \text{(on PDE)}$$

conserved density ρ and flux $\mathbf{J} = (J^{(1)}, J^{(2)}, J^{(3)})$.

Typical examples:

- Korteweg-de Vries (KdV) equation

$$u_t + uu_x + u_{3x} = 0$$

First few conservation laws:

$$\rho_{(1)} = u, \qquad \mathrm{D}_t(u) + \mathrm{D}_x\left(\frac{u^2}{2} + u_{2x}\right) = 0.$$

$$\rho_{(2)} = u^2, \qquad \mathrm{D}_t(u^2) + \mathrm{D}_x\left(\frac{2u^3}{3} + 2uu_{2x} - {u_x}^2\right) = 0.$$

$$\rho_{(3)} = u^3 - 3{u_x}^2,$$

$$\mathrm{D}_t\left(u^3 - 3{u_x}^2\right) + \mathrm{D}_x\left(\frac{3}{4}u^4 - 6u{u_x}^2 + 3u^2u_{2x} + 3{u_{2x}}^2 - 6u_xu_{3x}\right) = 0.$$

$$\vdots$$

$$\begin{aligned}\rho_{(6)} &= u^6 - 60u^3{u_x}^2 - 30{u_x}^4 + 108u^2{u_{2x}}^2 \\ &\quad + \frac{720}{7}{u_{2x}}^3 - \frac{648}{7}u{u_{3x}}^2 + \frac{216}{7}{u_{4x}}^2.\end{aligned}$$

- Sine-Gordon equation

$$\begin{aligned} u_t &= v \\ v_t &= u_{xx} + \alpha \sin(u) \end{aligned}$$

First few density-flux pairs:

$$\begin{aligned} \rho_{(1)} &= 2\alpha \cos(u) + v^2 + {u_x}^2, \qquad J_{(1)} = -2u_x v \\ \rho_{(2)} &= 2u_x v, \qquad J_{(2)} = 2\alpha \cos(u) - v^2 - {u_x}^2 \\ \rho_{(3)} &= 12 \cos(u) v u_x + 2v^3 u_x + 2v{u_x}^3 - 16 v_x u_{2x} \\ \rho_{(4)} &= 2\cos^2(u) - 2\sin^2(u) + v^4 + 6v^2 {u_x}^2 + {u_x}^4 + 4\cos(u) v^2 \\ &+ \ 20 \cos(u) {u_x}^2 - 16 {v_x}^2 - 16 {u_{2x}}^2 \end{aligned}$$

$J_{(3)}$ and $J_{(4)}$ are not shown (too long).

- A class of fifth-order evolution equations

$$u_t + \alpha u^2 u_x + \beta u_x u_{2x} + \gamma u u_{3x} + u_{5x} = 0$$

where α, β, γ are nonzero parameters.

Special cases:

$\alpha = 30$	$\beta = 20$	$\gamma = 10$	Lax Equation
$\alpha = 5$	$\beta = 5$	$\gamma = 5$	Sawada – Kotera Equation
$\alpha = 20$	$\beta = 25$	$\gamma = 10$	Kaup–Kupershmidt Equation
$\alpha = 2$	$\beta = 6$	$\gamma = 3$	Ito Equation

Conditions for α, β and γ so that conserved densities exist?

- Shallow water wave equations with an inhomogeneous layer (Dellar)

$$
\begin{aligned}
&\mathbf{u}_t + (\mathbf{u}\cdot\nabla)\mathbf{u} + 2\,\mathbf{\Omega}\times\mathbf{u} + \nabla(\theta h) - \frac{1}{2}h\nabla\theta = \mathbf{0}\\
&h_t + \nabla\cdot(\mathbf{u}h) = 0\\
&\theta_t + \mathbf{u}\cdot(\nabla\theta) = 0
\end{aligned}
$$

$\mathbf{\Omega}$ is constant. In components, $\nabla = (\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, 0)$, $\mathbf{u} = (u, v, 0)$, $\mathbf{\Omega} = (0, 0, \Omega)$:

$$
\begin{aligned}
&u_t + uu_x + vu_y - 2\,\Omega v + \frac{1}{2}h\theta_x + \theta h_x = 0\\
&v_t + uv_x + vv_y + 2\,\Omega u + \frac{1}{2}h\theta_y + \theta h_y = 0\\
&h_t + hu_x + uh_x + hv_y + vh_y = 0\\
&\theta_t + u\theta_x + v\theta_y = 0
\end{aligned}
$$

First few conserved densities and fluxes:

$$
\rho_{(1)} = h, \qquad \mathbf{J}_{(1)} = \begin{pmatrix} uh \\ vh \\ 0 \end{pmatrix}, \qquad \rho_{(2)} = h\theta, \qquad \mathbf{J}_{(2)} = \begin{pmatrix} uh\theta \\ vh\theta \\ 0 \end{pmatrix}
$$

$$
\rho_{(3)} = h\theta^2, \qquad \mathbf{J}_{(3)} = \begin{pmatrix} uh\theta^2 \\ vh\theta^2 \\ 0 \end{pmatrix}
$$

$$
\rho_{(4)} = (u^2 + v^2)h + h^2\theta, \qquad \mathbf{J}_{(4)} = \begin{pmatrix} u^3h + uv^2h + 2uh^2\theta \\ v^3h + u^2vh + 2vh^2\theta \\ 0 \end{pmatrix}
$$

$$
\rho_{(5)} = v_x\theta - u_y\theta + 2\Omega\theta
$$

$$
\mathbf{J}_{(5)} = \frac{1}{6}\begin{pmatrix} 12\Omega u\theta - 4uu_y\theta + 6uv_x\theta + 2vv_y\theta + u^2\theta_y + v^2\theta_y - h\theta\theta_y + h_y\theta^2 \\ 12\Omega v\theta + 4vv_x\theta - 6vu_y\theta - 2uu_x\theta - u^2\theta_x - v^2\theta_x + h\theta\theta_x - h_x\theta^2 \\ 0 \end{pmatrix}
$$

Definition:

Conservation law for DDE:

$$\mathrm{D}_t\,\rho_n + \Delta J_n = \mathrm{D}_t\,\rho_n + J_{n+1} - J_n = 0 \qquad \text{on DDE}$$

conserved density ρ_n and associated flux J_n.

Typical Examples:

- Kac-van Moerbeke (Volterra) lattice

$$\dot{u}_n = u_n(u_{n+1} - u_{n-1})$$

$$\begin{aligned}
\rho_n^{(1)} &= u_n, \qquad\qquad \rho_n^{(2)} = \tfrac{1}{2}{u_n}^2 + u_n u_{n+1} \\
\rho_n^{(3)} &= \tfrac{1}{3}{u_n}^3 + u_n u_{n+1}(u_n + u_{n+1} + u_{n+2}) \\
\rho_n^{(4)} &= \tfrac{1}{4}{u_n}^4 + {u_n}^3 u_{n+1} + \tfrac{3}{2}{u_n}^2 {u_{n+1}}^2 + u_n {u_{n+1}}^2(u_{n+1} + u_{n+2}) \\
&\quad + u_n u_{n+1} u_{n+2}(u_n + u_{n+1} + u_{n+2} + u_{n+3})
\end{aligned}$$

- Combined KdV-mKdV lattice (Taha & Herbst)

$$\begin{aligned}
\dot{u}_n &= -(1 + \alpha h^2 u_n + \beta h^2 u_n^2)\,\Big\{\, \tfrac{1}{h^3}\,(\tfrac{1}{2}u_{n+2} - u_{n+1} + u_{n-1} - \tfrac{1}{2}u_{n-2}) \\
&\quad + \tfrac{\alpha}{2h}[u_{n+1}^2 - u_{n-1}^2 + u_n(u_{n+1} - u_{n-1}) + u_{n+1}u_{n+2} - u_{n-1}u_{n-2}] \\
&\quad + \tfrac{\beta}{2h}[u_{n+1}^2(u_{n+2} + u_n) - u_{n-1}^2(u_{n-2} + u_n)]\,\Big\}
\end{aligned}$$

discretizes the combined KdV-mKdV equation

$$u_t + 6\alpha u u_x + 6\beta u^2 u_x + u_{xxx} = 0$$

$$\begin{aligned}
\rho_n^{(1)} &= \alpha u_n + \beta u_n u_{n+1} \\
\rho_n^{(2)} &= \frac{\alpha^2}{2\beta}{u_n}^2 + \frac{\alpha^2}{\beta}u_n u_{n+1} - u_n u_{n+1} + \alpha {u_n}^2 u_{n+1} + \alpha u_n {u_{n+1}}^2 \\
&+ \frac{1}{2}\beta {u_n}^2 {u_{n+1}}^2 + u_n u_{n+2} + \alpha u_n u_{n+1} u_{n+2} + \beta u_n {u_{n+1}}^2 u_{n+2}.
\end{aligned}$$

- Toda lattice

$$
\begin{aligned}
\dot{u}_n &= v_{n-1} - v_n \\
\dot{v}_n &= v_n(u_n - u_{n+1})
\end{aligned}
$$

First few conserved densities (fluxes not shown):

$$
\begin{aligned}
\rho_n^{(1)} &= u_n, \qquad\qquad \rho_n^{(2)} = \tfrac{1}{2}{u_n}^2 + v_n \\
\rho_n^{(3)} &= \tfrac{1}{3}{u_n}^3 + u_n(v_{n-1} + v_n) \\
\rho_n^{(4)} &= \tfrac{1}{4}{u_n}^4 + {u_n}^2(v_{n-1} + v_n) + u_n u_{n+1} v_n + \tfrac{1}{2}{v_n}^2 + v_n v_{n+1} \\
\rho_n^{(5)} &= \tfrac{1}{5}{u_n}^5 + {u_n}^3(v_{n-1} + v_n) + u_n u_{n+1} v_n(u_n + u_{n+1}) \\
&\quad + u_n v_{n-1}(v_{n-2} + v_{n-1} + v_n) + u_n v_n(v_{n-1} + v_n + v_{n+1}).
\end{aligned}
$$

- Ablowitz-Ladik lattice

$$
i\,\dot{u}_n = u_{n+1} - 2u_n + u_{n-1} + \kappa u_n^* u_n(u_{n+1} + u_{n-1}),
$$

discretizes the nonlinear Schrödinger equation

$$
iu_t + u_{xx} + \kappa u^2 u^* = 0
$$

u_n^* is the complex conjugate of u_n. Treat u_n and $v_n = u_n^*$ as independent variables and add the complex conjugate equation.

Set $\kappa = 1$ (scaling), absorb i in scale on t, introduce auxiliary parameter α (with weight):

$$
\begin{aligned}
\dot{u}_n &= \alpha(u_{n+1} - 2u_n + u_{n-1}) + u_n v_n(u_{n+1} + u_{n-1}), \\
\dot{v}_n &= -\alpha(v_{n+1} - 2v_n + v_{n-1}) - u_n v_n(v_{n+1} + v_{n-1}).
\end{aligned}
$$

First few conserved densities ($\alpha = 1$, in original variables):

$$\rho_n^{(1)} = u_n u_{n-1}^*$$

$$\rho_n^{(2)} = u_n u_{n+1}^*$$

$$\rho_n^{(3)} = \tfrac{1}{2} u_n^2 u_{n-1}^{*2} + u_n u_{n+1} u_{n-1}^* v_n + u_n u_{n-2}^*$$

$$\rho_n^{(4)} = \tfrac{1}{2} u_n^2 u_{n+1}^{*2} + u_n u_{n+1} u_{n+1}^* u_{n+2}^* + u_n u_{n+2}^*$$

$$\begin{aligned}\rho_n^{(5)} = {} & \tfrac{1}{3} u_n^3 u_{n-1}^{*3} + u_n u_{n+1} u_{n-1}^* u_n^* (u_n u_{n-1}^* + u_{n+1} u_n^* + u_{n+2} u_{n+1}^*) \\ & + u_n u_{n-1}^* (u_n u_{n-2}^* + u_{n+1} u_{n-1}^*) + u_n u_n^* (u_{n+1} u_{n-2}^* + u_{n+2} u_{n-1}^*) + u_n u_{n-3}^*\end{aligned}$$

$$\begin{aligned}\rho_n^{(6)} = {} & \tfrac{1}{3} u_n^3 u_{n+1}^{*3} + u_n u_{n+1} u_{n+1}^* u_{n+2}^* (u_n u_{n+1}^* + u_{n+1} u_{n+2}^* + u_{n+2} u_{n+3}^*) \\ & + u_n u_{n+2}^* (u_n u_{n+1}^* + u_{n+1} u_{n+2}^*) + u_n u_{n+3}^* (u_{n+1} u_{n+1}^* + u_{n+2} u_{n+2}^*) + u_n u_{n+3}^*\end{aligned}$$

Density missed:

$$\rho_n^{(0)} = \ln(1 + u_n u_n^*).$$

We cannot find the Hamiltonian (constant of motion):

$$H = -i \sum [u_n^* (u_{n-1} + u_{n+1}) - 2 \ln(1 + u_n u_n^*)],$$

Key Observations

Conserved densities, generalized symmetries, and recursion operators are invariant under the dilation symmetry of the given PDE or DDE.

Overall Strategy

Exploit dilation symmetry as much as possible.

Keep the computations as simple as possible.

Use linear algebra

* solve linear systems
* construct basis vectors (building blocks)
* use linear independence
* work in finite dimensional spaces

Use calculus and differential equations

* derivatives
* integrals (as little as possible)
* solve systems of linear ODEs

Use tools from variational calculus

* variational derivative (Euler operator)
* Fréchet derivative
* Homotopy operator

Use analogy between continuous and semi-discrete cases

OUTLINE

Part I: Continuous Case

Integration by Parts on the Jet Space (by hand) + Mathematica Experiment

Exactness or Integrability Criterion: Continuous Euler Operator

Continuous Homotopy Operator

Application of Continuous Homotopy Operator

Demo of Mathematica software

Part II: Discrete Case

Inverting the Total Difference Operator (by hand)

Exactness or 'Total Difference' Criterion: Discrete Euler Operator

Discrete Homotopy Operator

Application of Discrete Homotopy Operator

Demo of Mathematica Software

Conclusions and Ongoing Research

Problem Statement

For continuous case:

Given, for example,

$$f = 3\,u'\,v^2\,\sin(u) - u'^3\,\sin(u) - 6\,v\,v'\,\cos(u) + 2\,u'\,u''\,\cos(u) + 8\,v'v''$$

Find F so that $f = D_x F$ or $F = \int f\,dx$.

Result:

$$F = 4\,v'^2 + u'^2\,\cos(u) - 3\,v^2\,\cos(u)$$

Can this be done without integration by parts?

Can the problem be reduced to a single integral in one variable?

For discrete case:

Given, for example,

$$f_n = -u_n\,u_{n+1}\,v_n - v_n^2 + u_{n+1}\,u_{n+2}\,v_{n+1} + v_{n+1}^2 + u_{n+3}\,v_{n+2} - u_{n+1}\,v_n$$

Find F_n so that $f_n = \Delta F_n = F_{n+1} - F_n$ or $F_n = \Delta^{-1} f_n$.

Result:

$$F_n = v_n^2 + u_n\,u_{n+1}\,v_n + u_{n+1}\,v_n + u_{n+2}\,v_{n+1}.$$

How can this be done algorithmically?

Can this be done in the same way as the continuous case?

Part I: Continuous Case

Integration by Parts on the Jet Space

- Given f involving $u(x)$ and $v(x)$ and their derivatives

  $f = 3\,u'\,v^2\,\sin(u) - u'^3\,\sin(u) - 6\,v\,v'\,\cos(u) + 2\,u'\,u''\,\cos(u) + 8\,v'v''$

- Find F so that $f = D_x F$ or $F = \int f\,dx$.

  Integrate by parts (compute F by hand)

f		F
$8\,v'v''$	$\longrightarrow$	$4\,v'^2$
$2\,u'\,u''\,\cos(u)$	$\longrightarrow$	$u'^2\,\cos(u)$
$-u'^3\,\sin(u)$		
$-6\,v\,v'\,\cos(u)$	$\longrightarrow$	$-3\,v^2\,\cos(u)$
$3\,u'\,v^2\,\sin(u)$		

- Integral:

$$F = 4\,v'^2 + u'^2\,\cos(u) - 3\,v^2\,\cos(u)$$

Remark: For simplicity we denote $f(\mathbf{u}, \mathbf{u}', \mathbf{u}'', \cdots, \mathbf{u}^{(m)})$ as $f(\mathbf{u})$.

- **Exactness Criterion:**

  Continuous Euler Operator (variational derivative)

  Definition (exactness):

  A function $f(\mathbf{u})$ is exact, i.e. can be integrated fully, if there exists a function $F(\mathbf{u})$, such that $f(\mathbf{u}) = \mathrm{D}_x\, F(\mathbf{u})$ or equivalently $F(\mathbf{u}) = \mathrm{D}_x^{-1} f(\mathbf{u}) = \int_x f(\mathbf{u})\, dx$.

  D_x is the (total) derivative with respect to x.

  Theorem (exactness or integrability test):

  A necessary and sufficient condition for a function f to be exact, i.e. the derivative of another function, is that $\mathcal{L}_{\mathbf{u}}^{(0)}(f) \equiv 0$ where $\mathcal{L}_{\mathbf{u}}^{(0)}$ is the continuous Euler operator (variational derivative) defined by

  $$\begin{aligned}\mathcal{L}_{\mathbf{u}}^{(0)} &= \sum_{k=0}^{m_0} (-\mathrm{D}_x)^k \frac{\partial}{\partial \mathbf{u}^{(k)}} \\ &= \frac{\partial}{\partial \mathbf{u}} - \mathrm{D}_x \frac{\partial}{\partial \mathbf{u}'} + \mathrm{D}_x^2 \frac{\partial}{\partial \mathbf{u}''} + \cdots + (-1)^{m_0} \mathrm{D}_x^{m_0} \frac{\partial}{\partial \mathbf{u}^{(m_0)}}\end{aligned}$$

  where m_0 is the order (of f).

  Proof:
  See calculus of variations (derivation of Euler-Lagrange equations — the forgotten case!).

Example: Apply the continuous Euler operator to

$$f(\mathbf{u}) = 3u'\,v^2\,\sin(u) - u'^3\,\sin(u) - 6v\,v'\,\cos(u) + 2u'\,u''\,\cos(u) + 8v'v''$$

Here $\mathbf{u} = (u, v)$.

For component u (order 2):

$$\begin{aligned}
\mathcal{L}_u^{(0)}(f) &= \frac{\partial}{\partial u}(f) - \mathrm{D}_x \frac{\partial}{\partial u'}(f) + \mathrm{D}_x^2 \frac{\partial}{\partial u''}(f) \\
&= 3u'\,v^2\,\cos(u) - u'^3\,\cos(u) + 6v\,v'\,\sin(u) - 2u'\,u''\,\sin(u) \\
&\quad -\mathrm{D}_x[3v^2\,\sin(u) - 3u'^2\,\sin(u) + 2u''\,\cos(u)] + \mathrm{D}_x^2[2u'\,\cos(u)] \\
&= 3u'\,v^2\,\cos(u) - u'^3\,\cos(u) + 6v\,v'\,\sin(u) - 2u'\,u''\,\sin(u) \\
&\quad -[3u'v^2\,\cos(u) + 6v\,v'\,\sin(u) - 3u'^3\,\cos(u) - 6u\,u''\,\sin(u) \\
&\quad -2u'\,u''\,\sin(u) + 2u'''\,\cos(u)] \\
&\quad +[-2u'''\cos(u) - 6u'\,u''\sin(u) + 2u'''\cos(u)] \\
&\equiv 0
\end{aligned}$$

For component v (order 2):

$$\begin{aligned}
\mathcal{L}_v^{(0)}(f) &= \frac{\partial}{\partial v}(f) - \mathrm{D}_x \frac{\partial}{\partial v'}(f) + \mathrm{D}_x^2 \frac{\partial}{\partial v''}(f) \\
&= 6u'\,v\,\sin(u) - 6v'\,\cos(u) - \mathrm{D}_x[-6v\,\cos(u) + 8v''] + \mathrm{D}_x^2[8v'] \\
&= 6u'v\sin(u) - 6v'\cos(u) - [6u'v\sin(u) - 6v'\cos(u) + 8v'''] + 8v''' \\
&\equiv 0
\end{aligned}$$

- **Computation of the integral F**

  Definition (higher Euler operators):

  The continuous higher Euler operators are defined by

$$\mathcal{L}_{\mathbf{u}}^{(i)} = \sum_{k=i}^{m_i} \binom{k}{i} (-\mathrm{D}_x)^{k-i} \frac{\partial}{\partial \mathbf{u}^{(k)}}$$

  These Euler operators all terminate at some maximal order m_i.

Examples (for component u) :

$$\mathcal{L}_u^{(0)} = \frac{\partial}{\partial u} - \mathrm{D}_x \frac{\partial}{\partial u'} + \mathrm{D}_x^2 \frac{\partial}{\partial u''} - \mathrm{D}_x^3 \frac{\partial}{\partial u'''} + \cdots + (-1)^{m_0} \mathrm{D}_x^{m_0} \frac{\partial}{\partial u^{(m_0)}}$$

$$\mathcal{L}_u^{(1)} = \frac{\partial}{\partial u'} - 2\mathrm{D}_x \frac{\partial}{\partial u''} + 3\mathrm{D}_x^2 \frac{\partial}{\partial u'''} - 4\mathrm{D}_x^3 \frac{\partial}{\partial u^{(4)}} + \cdots - (-1)^{m_1} m_1 \mathrm{D}_x^{m_1-1} \frac{\partial}{\partial u^{(m_1)}}$$

$$\mathcal{L}_u^{(2)} = \frac{\partial}{\partial u''} - 3\mathrm{D}_x \frac{\partial}{\partial u'''} + 6\mathrm{D}_x^2 \frac{\partial}{\partial u^{(4)}} - 10\mathrm{D}_x^3 \frac{\partial}{\partial u^{(5)}} + \cdots + (-1)^{m_2} \binom{m_2}{2} \mathrm{D}_x^{m_2-2} \frac{\partial}{\partial u^{(m_2)}}$$

$$\mathcal{L}_u^{(3)} = \frac{\partial}{\partial u'''} - 4\mathrm{D}_x \frac{\partial}{\partial u^{(4)}} + 10\mathrm{D}_x^2 \frac{\partial}{\partial u^{(5)}} - 20\mathrm{D}_x^3 \frac{\partial}{\partial u^{(6)}} + \cdots - (-1)^{m_3} \binom{m_3}{3} \mathrm{D}_x^{m_3-3} \frac{\partial}{\partial u^{(m_3)}}$$

Similar formulae for component $\mathcal{L}_v^{(i)}$

Definition (homotopy operator):

The continuous homotopy operator is defined by

$$\mathcal{H}_{\mathbf{u}} = \int_0^1 \sum_{r=1}^{N} f_r(\mathbf{u})[\lambda \mathbf{u}] \frac{d\lambda}{\lambda}$$

where

$$f_r(\mathbf{u}) = \sum_{i=0}^{p_r} \mathrm{D}_x^i [u_r \boldsymbol{\mathcal{L}}_{u_r}^{(i+1)}]$$

p_r is the maximum order of u_r in f

N is the number of dependent variables

$f_r(\mathbf{u})[\lambda \mathbf{u}]$ means that in $f_r(\mathbf{u})$ one replaces $\mathbf{u} \to \lambda \mathbf{u}$, $\mathbf{u}' \to \lambda \mathbf{u}'$, etc.

Example:

For a two-component system ($N = 2$) where $\mathbf{u} = (u, v)$:

$$\mathcal{H}_{\mathbf{u}} = \int_0^1 \{ f_1(\mathbf{u})[\lambda \mathbf{u}] + f_2(\mathbf{u})[\lambda \mathbf{u}] \} \frac{d\lambda}{\lambda}$$

with

$$f_1(\mathbf{u}) = \sum_{i=0}^{p_1} \mathrm{D}_x^i [u \boldsymbol{\mathcal{L}}_{u}^{(i+1)}]$$

and

$$f_2(\mathbf{u}) = \sum_{i=0}^{p_2} \mathrm{D}_x^i [v \boldsymbol{\mathcal{L}}_{v}^{(i+1)}]$$

Theorem (integration via homotopy operator):

Given an integrable function f

$$F = \mathrm{D}_x^{-1} f = \int f \, dx = \mathcal{H}_{\mathbf{u}}(f)$$

Proof: Olver's book 'Applications of Lie Groups to Differential Equations', p. 372. Proof is given in terms of differential forms.

Work of Henri Poincaré (1854-1912), George de Rham (1950), and Ian Anderson & Tom Duchamp (1980).

Proofs based on calculus: Deconinck and Hereman.

Example: Apply the continuous homotopy operator to integrate

$$f(\mathbf{u}) = 3u'v^2\sin(u) - u'^3\sin(u) - 6vv'\cos(u) + 2u'u''\cos(u) + 8v'v''$$

For component u (order 2):

i	$\mathcal{L}_u^{(i+1)}(f)$	$\mathrm{D}_x^i\left(u\mathcal{L}_u^{(i+1)}(f)\right)$
0	$\frac{\partial}{\partial u'}f - 2\mathrm{D}_x(\frac{\partial}{\partial u''}f)$ $=3v^2\sin u - 3u'^2\sin u + 2u''\cos u$ $-2\mathrm{D}_x(2u'\cos u)$ $=3v^2\sin u + u'^2\sin u - 2u''\cos u$	$3uv^2\sin u + uu'^2\sin u - 2uu''\cos u$
1	$\frac{\partial}{\partial u''}f = 2u'\cos u$	$\mathrm{D}_x[2uu'\cos u]$ $=2u'^2\cos u + 2uu''\cos u - 2uu'^2\sin u$

Hence, $f_1(\mathbf{u})(f) = 3uv^2\sin(u) - uu'^2\sin(u) + 2u'^2\cos(u)$

For component v (order 2):

i	$\mathcal{L}_v^{(i+1)}(f)$	$\mathrm{D}_x^i[v\mathcal{L}_v^{(i+1)}(f)]$
0	$-6v\cos(u) + 8v'' - 2\mathrm{D}_x[8v']$ $= -6v\cos(u) - 8v''$	$-6v^2\cos(u) - 8vv''$
1	$8v'$	$\mathrm{D}_x[8vv'] = 8v'^2 + 8vv''$

Hence, $f_2(\mathbf{u})(f) = -6v^2\cos(u) + 8v'^2$

The homotopy operator leads to an integral for (auxiliary) variable λ. (Use standard integration by parts to work the integral).

$$\begin{aligned} F(\mathbf{u}) &= \mathcal{H}_{\mathbf{u}}(f) = \int_0^1 \{f_1(\mathbf{u})(f)[\lambda\mathbf{u}] + f_2(\mathbf{u})(f)[\lambda\mathbf{u}]\}\,\frac{d\lambda}{\lambda} \\ &= \int_0^1 [3\lambda^2uv^2\sin(\lambda u) - \lambda^2uu'^2\sin(\lambda u) + 2\lambda u'^2\cos(\lambda u) \\ &\qquad -6\lambda v^2\cos(\lambda u) + 8\lambda v'^2]\,d\lambda \\ &= 4v'^2 + u'^2\cos(u) - 3v^2\cos(u) \end{aligned}$$

- **Application: Conserved densities and fluxes for PDEs with transcendental nonlinearities**

  Definition (conservation law):

$$\mathrm{D}_t \rho + \mathrm{D}_x J = 0 \qquad \text{(on PDE)}$$

conserved density ρ and flux J.

Example: Sine-Gordon system (type $\mathbf{u}_t = \mathbf{F}$)

$$\begin{aligned} u_t &= v \\ v_t &= u_{xx} + \alpha \sin(u) \end{aligned}$$

has scaling symmetry

$$(t, x, u, v, \alpha) \rightarrow (\lambda^{-1} t, \lambda^{-1} x, \lambda^0 u, \lambda v, \lambda^2 \alpha)$$

In terms of weights:

$$w(\mathrm{D}_x) = 1,\ w(\mathrm{D}_t) = 1,\ w(u) = 0,\ w(v) = 1,\ w(\alpha) = 2$$

Conserved densities and fluxes

$$\rho_{(1)} = 2\alpha \cos(u) + v^2 + {u_x}^2 \qquad J_{(1)} = -2 u_x v$$

$$\rho_{(2)} = u_x v \qquad J_{(2)} = -[\frac{1}{2} v^2 + \frac{1}{2} {u_x}^2 - \alpha \cos(u)]$$

$$\rho_{(3)} = 12 \cos(u) v u_x + 2 v^3 u_x + 2 v {u_x}^3 - 16 v_x u_{2x}$$

$$\begin{aligned} \rho_{(4)} = &\ 2 \cos^2(u) - 2 \sin^2(u) + v^4 + 6 v^2 {u_x}^2 + {u_x}^4 + 4 \cos(u) v^2 \\ &+ 20 \cos(u) {u_x}^2 - 16 {v_x}^2 - 16 {u_{2x}}^2. \end{aligned}$$

are all scaling invariant!

Remark: $J_{(3)}$ and $J_{(4)}$ are not shown (too long).

- **Algorithm for Conserved Densities and Fluxes**

Example: Density and flux of rank 2 for sine-Gordon system

Step 1: **Construct the form of the density**

$$\rho = \alpha h_1(u) + h_2(u)v^2 + h_3(u){u_x}^2 + h_4(u)u_x v$$

where $h_i(u)$ are unknown functions.

Step 2: **Determine the functions** h_i

Compute

$$\begin{aligned} E = \mathrm{D}_t \rho &= \frac{\partial \rho}{\partial t} + \rho'(\mathbf{u})[\mathbf{F}] \quad \text{(on PDE)} \\ &= \frac{\partial \rho}{\partial t} + \sum_{k=0}^{m_1} \frac{\partial \rho}{\partial u_{kx}} \mathrm{D}_x^k u_t + \sum_{k=0}^{m_2} \frac{\partial \rho}{\partial v_{kx}} \mathrm{D}_x^k v_t \end{aligned}$$

Since $E = \mathrm{D}_t \rho = -\mathrm{D}_x J$, the expression E must be integrable.

Require that $\mathcal{L}_u^{(0)}(E) \equiv 0$ and $\mathcal{L}_v^{(0)}(E) \equiv 0$.

Solve the system of linear mixed system (algebraic eqs. and ODEs):

$$\begin{aligned}
&h_2(u) - h_3(u) = 0 \\
&{h_2}'(u) = 0 \\
&{h_3}'(u) = 0 \\
&{h_4}'(u) = 0 \\
&{h_2}''(u) = 0 \\
&{h_4}''(u) = 0 \\
&2{h_2}'(u) - {h_3}'(u) = 0 \\
&2{h_2}''(u) - {h_3}''(u) = 0 \\
&{h_1}'(u) + 2\sin(u) h_2(u) = 0 \\
&{h_1}''(u) + 2\sin(u) {h_2}'(u) + 2\cos(u) h_2(u) = 0
\end{aligned}$$

Solution:

$$
\begin{aligned}
h_1(u) &= 2c_1\cos(u) + c_3 \\
h_2(u) &= h_3(u) = c_1 \\
h_4(u) &= c_2
\end{aligned}
$$

(with arbitrary constants c_i).

Substitute in ρ

$$\rho = c_1(2\alpha\cos(u) + v^2 + {u_x}^2) + c_2(u_x v) + c_3\alpha$$

Step 3: **Compute the flux** J

First, compute

$$
\begin{aligned}
E = \mathrm{D}_t\rho &= c_1(-2\alpha u_t \sin u + 2vv_t + 2u_x u_{xt}) + c_2(u_{xt}v + u_x v_t) \\
&= c_1(-2\alpha v\sin u + 2v\,(u_{2x} + \alpha\sin u) + 2u_x v_x) \\
&\quad + c_2(v_x v + u_x\,(u_{2x} + \alpha\sin u)) \\
&= c_1(2u_{2x}v + 2u_x v_x) + c_2(vv_x + u_x u_{2x} + \alpha u_x \sin u)
\end{aligned}
$$

Since $E = \mathrm{D}_t\rho = -\mathrm{D}_x J$, one must integrate $f = -E$.

Apply the homotopy operator for each component of $\mathbf{u} = (u, v)$.

For component u (order 2):

i	$\mathcal{L}_u^{(i+1)}(f)$	$\mathrm{D}_x^i\left(u\mathcal{L}_u^{(i+1)}(f)\right)$
0	$2c_1 v_x + c_2(u_{2x} - \alpha\sin u)$	$2c_1 uv_x + c_2(uu_{2x} - \alpha u\sin u)$
1	$-2c_1 v - c_2 u_x$	$-2c_1(u_x v + uv_x) - c_2(u_x^2 + uu_{2x})$

Hence, $f_1(\mathbf{u})(f) = -2c_1 u_x v - c_2(u_x^2 + \alpha u\sin u)$

For component v (order 1):

i	$\mathcal{L}_v^{(i+1)}(f)$	$\mathrm{D}_x^i\left(v\mathcal{L}_v^{(i+1)}(f)\right)$
0	$-2c_1u_x - c_2v$	$-2c_1u_xv - c_2v^2$

Hence, $f_2(\mathbf{u})(f) = -2c_1u_xv - c_2v^2$

The homotopy operator leads to an integral for (one) variable λ :

$$\begin{aligned} J(\mathbf{u}) &= \mathcal{H}_{\mathbf{u}}(f) = \int_0^1 \left(f_1(\mathbf{u})(f)[\lambda\mathbf{u}] + f_2(\mathbf{u})(f)[\lambda\mathbf{u}]\right)\,\frac{d\lambda}{\lambda} \\ &= -\int_0^1 \left(4c_1\lambda u_xv + c_2(\lambda u_x^2 + \alpha u\sin(\lambda u) + \lambda v^2)\right)\,d\lambda \\ &= -2c_1u_xv - c_2\left(\frac{1}{2}v^2 + \frac{1}{2}u_x^2 - \alpha\cos u\right) \end{aligned}$$

Split the density and flux in independent pieces (for c_1 and c_2):

$$\begin{aligned} \rho_{(1)} &= 2\alpha\cos u + v^2 + {u_x}^2 \qquad J_{(1)} = -2u_xv \\ \rho_{(2)} &= u_xv \qquad J_{(2)} = -\frac{1}{2}v^2 - \frac{1}{2}u_x^2 + \alpha\cos u \end{aligned}$$

Remark: Computation of $J_{(3)}$ and $J_{(4)}$ requires integration with the homotopy operator!

Computer Demos

(1) Use continuous homotopy operator to integrate

$$f = 3\,u'\,v^2\,\sin(u) - u'^3\,\sin(u) - 6\,v\,v'\,\cos(u) + 2\,u'\,u''\,\cos(u) + 8\,v'v''$$

(2) Compute densities of rank 8 and fluxes for 5th-order Korteweg-de Vries equation with three parameters:

$$u_t + \alpha u^2 u_x + \beta u_x u_{2x} + \gamma u u_{3x} + u_{5x} = 0$$

(α, β, γ are nonzero constant parameters).

(3) Compute density of rank 4 and flux for sine-Gordon system:

$$\begin{aligned} u_t &= v \\ v_t &= u_{xx} + \alpha \sin(u) \end{aligned}$$

Analogy PDEs and DDEs

	Continuous Case (PDEs)	Semi-discrete Case (DDEs)
System	$\mathbf{u}_t = \mathbf{F}(\mathbf{u}, \mathbf{u}_x, \mathbf{u}_{2x}, ...)$	$\dot{\mathbf{u}}_n = \mathbf{F}(..., \mathbf{u}_{n-1}, \mathbf{u}_n, \mathbf{u}_{n+1}, ...)$
Conservation Law	$\mathrm{D}_t \rho + \mathrm{D}_x J = 0$	$\dot{\rho}_n + J_{n+1} - J_n = 0$
Symmetry	$\mathrm{D}_t \mathbf{G} = \mathbf{F}'(\mathbf{u})[\mathbf{G}] = \frac{\partial}{\partial \epsilon} \mathbf{F}(\mathbf{u} + \epsilon \mathbf{G})\|_{\epsilon=0}$	$\mathrm{D}_t \mathbf{G} = \mathbf{F}'(\mathbf{u}_n)[\mathbf{G}] = \frac{\partial}{\partial \epsilon} \mathbf{F}(\mathbf{u}_n + \epsilon \mathbf{G})\|_{\epsilon=0}$
Recursion Operator	$\mathrm{D}_t \mathcal{R} + [\mathcal{R}, \mathbf{F}'(u)] = 0$	$\mathrm{D}_t \mathcal{R} + [\mathcal{R}, \mathbf{F}'(\mathbf{u}_n)] = 0$

Table 1: Conservation Laws and Symmetries

	KdV Equation	Volterra Lattice
Equation	$u_t = 6uu_x + u_{3x}$	$\dot{u}_n = u_n\,(u_{n+1} - u_{n-1})$
Densities	$\rho = u, \quad \rho = u^2$ $\rho = u^3 - \frac{1}{2}u_x^2$	$\rho_n = u_n, \quad \rho_n = u_n(\frac{1}{2}u_n + u_{n+1})$ $\rho_n = \frac{1}{3}u_n^3 + u_n u_{n+1}(u_n + u_{n+1} + u_{n+2})$
Symmetries	$G = u_x, \quad G = 6uu_x + u_{3x}$ $G = 30u^2 u_x + 20u_x u_{2x} + 10uu_{3x} + u_{5x}$	$G = u_n u_{n+1}\,(u_n + u_{n+1} + u_{n+2}) - u_{n-1}u_n(u_{n-2} + u_{n-1} + u_n)$
Recursion Operator	$\mathcal{R} = \mathrm{D}_x^2 + 4u + 2u_x \mathrm{D}_x^{-1}$	$\mathcal{R} = u_n(\mathrm{I} + \mathrm{D})(u_n \mathrm{D} - \mathrm{D}^{-1} u_n)(\mathrm{D} - \mathrm{I})^{-1} \frac{1}{u_n}$

Table 2: Prototypical Examples

Part II: Discrete Case

Definitions (shift and total difference operators):

D is the **up-shift** (forward or right-shift) operator if for F_n

$$\mathrm{D}F_n = F_{n+1} = F_{n|_{n\to n+1}}$$

D^{-1} the **down-shift** (backward or left-shift) operator if

$$\mathrm{D}^{-1}F_n = F_{n-1} = F_{n|_{n\to n-1}}$$

$\Delta = \mathrm{D} - \mathrm{I}$ is the total **difference operator**

$$\Delta F_n = (\mathrm{D} - \mathrm{I})F_n = F_{n+1} - F_n$$

D (up-shift operator) corresponds the differential operator D_x

$$\mathrm{D}_x F(x) \to \frac{F_{n+1} - F_n}{\Delta x} = \frac{\Delta F_n}{\Delta x} \quad (\text{set } \Delta x = 1)$$

For $k > 0$, $\mathrm{D}^k = \mathrm{D} \circ \mathrm{D} \circ \cdots \circ \mathrm{D} \quad (k \text{ times})$.

Similarly, $\mathrm{D}^{-k} = \mathrm{D}^{-1} \circ \mathrm{D}^{-1} \circ \cdots \circ \mathrm{D}^{-1}$.

Problem to be solved:

Continuous case:

Given f. Find F so that $f = \mathrm{D}_x F$ or $F = \mathrm{D}_x^{-1} f = \int f\, dx$.

Discrete case:

Given f_n. Find F_n so that $f_n = \Delta F_n = F_{n+1} - F_n$ or $F_n = \Delta^{-1} f_n$.

Inverting the Δ Operator

- Given f_n involving u_n and v_n and their shifts:

  $f_n = -u_n\, u_{n+1}\, v_n - v_n^2 + u_{n+1}\, u_{n+2}\, v_{n+1} + v_{n+1}^2 + u_{n+3}\, v_{n+2} - u_{n+1}\, v_n$

- Find F_n so that $f_n = \Delta F_n = F_{n+1} - F_n$ or $F_n = \Delta^{-1} f_n$.

  Invert the Δ operator (compute F_n by hand)

f_n		F_n
$-v_n^2$	$\longrightarrow$	v_n^2
v_{n+1}^2		
$-u_n\, u_{n+1}\, v_n$	$\longrightarrow$	$u_n\, u_{n+1}\, v_n$
$u_{n+1}\, u_{n+2}\, v_{n+1}$		
$-u_{n+1}\, v_n$	$\longrightarrow$	$u_{n+1}\, v_n$
$+u_{n+2}\, v_{n+1}$ $-u_{n+2}\, v_{n+1}$	$\longrightarrow$	$u_{n+2}\, v_{n+1}$
$u_{n+3}\, v_{n+2}$		

- Result:

$$F_n = v_n^2 + u_n\, u_{n+1}\, v_n + u_{n+1}\, v_n + u_{n+2}\, v_{n+1}.$$

Remarks: We denote $f(\mathbf{u}_n, \mathbf{u}_{n+1}, \mathbf{u}_{n+2}, \cdots, \mathbf{u}_{n+p})$ as $f(\mathbf{u}_n)$.

Assume that all negative shifts have been removed via up-shifting

Replace $f_n = u_{n-2}\, v_n\, v_{n+3}$ by $\tilde{f}_n = \mathrm{D}^2 f_n = u_n\, v_{n+2}\, v_{n+5}$.

- **'Total Difference' Criterion:**

  Discrete Euler Operator (variational derivative)

  Definition (exactness):

  A function $f_n(\mathbf{u}_n)$ is exact, i.e. a total difference, if there exists a function $F_n(\mathbf{u}_n)$, such that $f_n = \Delta\, F_n$ or equivalently $F_n = \Delta^{-1} f_n$.

  D is the up-shift operator.

  Theorem (exactness or total difference test):

  A necessary and sufficient condition for a function f_n to be exact, i.e. a total difference, is that $\mathcal{L}^{(0)}_{\mathbf{u}_n}(f_n) \equiv 0$, where $\mathcal{L}^{(0)}_{\mathbf{u}_n}$ is the discrete Euler operator (variational derivative) defined by

$$
\begin{aligned}
\mathcal{L}^{(0)}_{\mathbf{u}_n} &= \sum_{k=0}^{m_0} \mathrm{D}^{-k} \frac{\partial}{\partial \mathbf{u}_{n+k}} \\
&= \frac{\partial}{\partial \mathbf{u}_n} + \mathrm{D}^{-1}(\frac{\partial}{\partial \mathbf{u}_{n+1}}) + \mathrm{D}^{-2}(\frac{\partial}{\partial \mathbf{u}_{n+2}}) + \cdots + \mathrm{D}^{-m_0}(\frac{\partial}{\partial \mathbf{u}_{n+m_0}}) \\
&= \frac{\partial}{\partial \mathbf{u}_n}(\sum_{k=0}^{m_0} \mathrm{D}^{-k}) \\
\mathcal{L}^{(0)}_{\mathbf{u}_n} &= \frac{\partial}{\partial \mathbf{u}_n}(\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \cdots + \mathrm{D}^{-m_0})
\end{aligned}
$$

  where m_0 is the highest forward shift (in f_n).

Example: Apply the discrete Euler operator to

$$f_n(\mathbf{u}_n) = -u_n\, u_{n+1}\, v_n - v_n^2 + u_{n+1}\, u_{n+2}\, v_{n+1} + v_{n+1}^2 + u_{n+3}\, v_{n+2} - u_{n+1}\, v_n$$

Here $\mathbf{u}_n = (u_n, v_n)$.

For component u_n (highest shift 3):

$$\begin{aligned}
\mathcal{L}^{(0)}_{u_n}(f_n) &= \frac{\partial}{\partial u_n}[\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3}](f_n) \\
&= [-u_{n+1}v_n] + [-u_{n-1}v_{n-1} + u_{n+1}v_n - v_{n-1}] + [u_{n-1}v_{n-1}] + [v_{n-1}] \\
&\equiv 0
\end{aligned}$$

For component v_n (highest shift 2):

$$\begin{aligned}
\mathcal{L}^{(0)}_{v_n}(f_n) &= \frac{\partial}{\partial v_n}[\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2}](f_n) \\
&= [-u_n u_{n+1} - 2v_n - u_{n+1}] + [u_n u_{n+1} + 2v_n] + [u_{n+1}] \\
&\equiv 0
\end{aligned}$$

- **Computation of F_n**

  Definition (higher Euler operators):

  The discrete higher Euler operators are defined by

$$\mathcal{L}_{\mathbf{u}_n}^{(i)} = \frac{\partial}{\partial \mathbf{u}_n}\left(\sum_{k=i}^{m_i} \binom{k}{i} \mathrm{D}^{-k}\right)$$

  These Euler operators all terminate at some maximal shifts m_i.

  Examples (for component u_n):

$$\mathcal{L}_{u_n}^{(0)} = \frac{\partial}{\partial u_n}(\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3} + \cdots + \mathrm{D}^{-m_0})$$
$$\mathcal{L}_{u_n}^{(1)} = \frac{\partial}{\partial u_n}(\mathrm{D}^{-1} + 2\mathrm{D}^{-2} + 3\mathrm{D}^{-3} + 4\mathrm{D}^{-4} + \cdots + m_1\,\mathrm{D}^{-m_1})$$
$$\mathcal{L}_{u_n}^{(2)} = \frac{\partial}{\partial u_n}(\mathrm{D}^{-2} + 3\mathrm{D}^{-3} + 6\mathrm{D}^{-4} + 10\mathrm{D}^{-5} + \cdots + \frac{1}{2}m_2(m_2 - 1)\,\mathrm{D}^{-m_2})$$
$$\mathcal{L}_{u_n}^{(3)} = \frac{\partial}{\partial u_n}(\mathrm{D}^{-3} + 4\mathrm{D}^{-4} + 10\mathrm{D}^{-5} + 20\mathrm{D}^{-6} + \cdots + \binom{m_3}{3}\mathrm{D}^{-m_3})$$

  Similar formulae for $\mathcal{L}_{v_n}^{(i)}$.

- **Definition** (homotopy operator):

The discrete homotopy operator is defined by

$$\mathcal{H}_{\mathbf{u}_n} = \int_0^1 \sum_{r=1}^{N} f_{r,n}(\mathbf{u}_n)[\lambda \mathbf{u}_n] \frac{d\lambda}{\lambda}$$

where

$$f_{r,n}(\mathbf{u}_n) = \sum_{i=0}^{p_r} (\mathrm{D} - \mathrm{I})^i [u_{r,n} \mathcal{L}^{(i+1)}_{u_{r,n}}]$$

p_r is the maximum shift of $u_{r,n}$ in f_n
N is the number of dependent variables
$f_{r,n}(\mathbf{u}_n)[\lambda \mathbf{u}_n]$ means that in $f_{r,n}(\mathbf{u}_n)$ one replaces $\mathbf{u}_n \to \lambda \mathbf{u}_n$, $\mathbf{u}_{n+1} \to \lambda \mathbf{u}_{n+1}$, etc.

Example:
For a two-component system ($N = 2$) where $\mathbf{u}_n = (u_n, v_n)$:

$$\mathcal{H}_{\mathbf{u}_n} = \int_0^1 \{f_{1,n}(\mathbf{u}_n)[\lambda \mathbf{u}_n] + f_{2,n}(\mathbf{u}_n)[\lambda \mathbf{u}_n]\} \frac{d\lambda}{\lambda}$$

with

$$f_{1,n}(\mathbf{u}_n) = \sum_{i=0}^{p_1} (\mathrm{D} - \mathrm{I})^i [u_n \mathcal{L}^{(i+1)}_{u_n}]$$

and

$$f_{2,n}(\mathbf{u}_n) = \sum_{i=0}^{p_2} (\mathrm{D} - \mathrm{I})^i [v_n \mathcal{L}^{(i+1)}_{v_n}]$$

Theorem (total difference via homotopy operator):

Given a function f_n which is a total difference, then

$$F_n = \Delta^{-1} f_n = \mathcal{H}_{\mathbf{u}_n}(f_n)$$

Proof: Recent work by Mansfield and Hydon on discrete variational bi-complexes. Proof is given in terms of differential forms.
Proof based on calculus: Deconinck and Hereman.

Higher Euler Operators Side by Side

Continuous Case (for component u)

$$\mathcal{L}_u^{(0)} = \frac{\partial}{\partial u} - \mathrm{D}_x \frac{\partial}{\partial u_x} + \mathrm{D}_x^2 \frac{\partial}{\partial u_{2x}} - \mathrm{D}_x^3 \frac{\partial}{\partial u_{3x}} + \cdots$$
$$\mathcal{L}_u^{(1)} = \frac{\partial}{\partial u_x} - 2\mathrm{D}_x \frac{\partial}{\partial u_{2x}} + 3\mathrm{D}_x^2 \frac{\partial}{\partial u_{3x}} - 4\mathrm{D}_x^3 \frac{\partial}{\partial u_{4x}} + \cdots$$
$$\mathcal{L}_u^{(2)} = \frac{\partial}{\partial u_{2x}} - 3\mathrm{D}_x \frac{\partial}{\partial u_{3x}} + 6\mathrm{D}_x^2 \frac{\partial}{\partial u_{4x}} - 10\mathrm{D}_x^3 \frac{\partial}{\partial u_{5x}} + \cdots$$
$$\mathcal{L}_u^{(3)} = \frac{\partial}{\partial u_{3x}} - 4\mathrm{D}_x \frac{\partial}{\partial u_{4x}} + 10\mathrm{D}_x^2 \frac{\partial}{\partial u_{5x}} - 20\mathrm{D}_x^3 \frac{\partial}{\partial u_{6x}} + \cdots$$

Discrete Case (for component u_n)

$$\mathcal{L}_{u_n}^{(0)} = \frac{\partial}{\partial u_n}(\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3} + \cdots)$$
$$\mathcal{L}_{u_n}^{(1)} = \frac{\partial}{\partial u_n}(\mathrm{D}^{-1} + 2\mathrm{D}^{-2} + 3\mathrm{D}^{-3} + 4\mathrm{D}^{-4} + \cdots)$$
$$\mathcal{L}_{u_n}^{(2)} = \frac{\partial}{\partial u_n}(\mathrm{D}^{-2} + 3\mathrm{D}^{-3} + 6\mathrm{D}^{-4} + 10\mathrm{D}^{-5} + \cdots)$$
$$\mathcal{L}_{u_n}^{(3)} = \frac{\partial}{\partial u_n}(\mathrm{D}^{-3} + 4\mathrm{D}^{-4} + 10\mathrm{D}^{-5} + 20\mathrm{D}^{-6} + \cdots)$$

Homotopy Operators Side by Side

Continuous Case (for components u and v)

$$\mathcal{H}_{\mathbf{u}} = \int_0^1 \{ f_1(\mathbf{u})[\lambda \mathbf{u}] + f_2(\mathbf{u})[\lambda \mathbf{u}] \} \, \frac{d\lambda}{\lambda}$$

with

$$f_1(\mathbf{u}) = \sum_{i=0}^{p_1} \mathrm{D}_x^i [u \mathcal{L}_u^{(i+1)}]$$

and

$$f_2(\mathbf{u}) = \sum_{i=0}^{p_2} \mathrm{D}_x^i [v \mathcal{L}_v^{(i+1)}]$$

Discrete Case (for components u_n and v_n)

$$\mathcal{H}_{\mathbf{u}_n} = \int_0^1 \{ f_{1,n}(\mathbf{u}_n)[\lambda \mathbf{u}_n] + f_{2,n}(\mathbf{u}_n)[\lambda \mathbf{u}_n] \} \frac{d\lambda}{\lambda}$$

with

$$f_{1,n}(\mathbf{u}_n) = \sum_{i=0}^{p_1} (\mathrm{D} - \mathrm{I})^i [u_n \mathcal{L}_{u_n}^{(i+1)}]$$

and

$$f_{2,n}(\mathbf{u}_n) = \sum_{i=0}^{p_2} (\mathrm{D} - \mathrm{I})^i [v_n \mathcal{L}_{v_n}^{(i+1)}]$$

Example: Apply the discrete homotopy operator to

$$f_n(\mathbf{u}_n) = -u_n\, u_{n+1}\, v_n - v_n^2 + u_{n+1}\, u_{n+2}\, v_{n+1} + v_{n+1}^2 + u_{n+3}\, v_{n+2} - u_{n+1}\, v_n$$

For component u_n (highest shift 3):

i	$\mathcal{L}_{u_n}^{(i+1)}(f_n)$	$(\mathrm{D}-\mathrm{I})^i[u_n \mathcal{L}_{u_n}^{(i+1)}(f_n)]$
0	$u_{n-1}v_{n-1}+u_{n+1}v_n+2v_{n-1}$	$u_{n-1}u_nv_{n-1}+u_nu_{n+1}v_n+2u_nv_{n-1}$
1	$u_{n-1}v_{n-1}+3v_{n-1}$	$u_nu_{n+1}v_n+3u_{n+1}v_n-u_{n-1}u_nv_{n-1}-3u_nv_{n-1}$
2	v_{n-1}	$u_{n+2}v_{n+1}-u_{n+1}v_n-u_{n+1}v_n+u_nv_{n-1}$

Hence, $f_{1,n}(\mathbf{u}_n)(f_n) = 2u_nu_{n+1}v_n + u_{n+1}v_n + u_{n+2}v_{n+1}$

For component v_n (highest shift 2):

i	$\mathcal{L}_{v_n}^{(i+1)}(f_n)$	$(\mathrm{D}-\mathrm{I})^i[v_n \mathcal{L}_{v_n}^{(i+1)}(f_n)]$
0	$u_nu_{n+1}+2v_n+2u_{n+1}$	$u_nu_{n+1}v_n+2v_n^2+2u_{n+1}v_n$
1	u_{n+1}	$u_{n+2}v_{n+1}-u_{n+1}v_n$

Hence, $f_{2,n}(\mathbf{u}_n)(f_n) = u_nu_{n+1}v_n + 2v_n^2 + u_{n+1}v_n + u_{n+2}v_{n+1}$

The homotopy operator leads to an integral for variable λ. (Use standard integration by parts to work the integral).

$$\begin{aligned}
F_n(\mathbf{u}_n) &= \mathcal{H}_{\mathbf{u}_n}(f_n) = \int_0^1 \{f_{1,n}(\mathbf{u}_n)(f_n)[\lambda\mathbf{u}_n] + f_{2,n}(\mathbf{u}_n)(f_n)[\lambda\mathbf{u}_n]\} \frac{d\lambda}{\lambda} \\
&= \int_0^1 [2\lambda v_n^2 + 3\lambda^2 u_nu_{n+1}v_n + 2\lambda u_{n+1}v_n + 2\lambda u_{n+2}v_{n+1}]\, d\lambda \\
&= v_n^2 + u_nu_{n+1}v_n + u_{n+1}v_n + u_{n+2}v_{n+1}
\end{aligned}$$

- **Application: Conserved densities and fluxes for DDEs**

Definition (conservation law):

$$\mathrm{D}_t\rho_n + \Delta J_n = \mathrm{D}_t\rho_n + J_{n+1} - J_n = 0 \qquad \text{(on DDE)}$$

conserved density ρ_n and flux J_n.

Example The Toda lattice (type $\dot{\mathbf{u}}_n = \mathbf{F}$) :

$$\begin{aligned} \dot{u}_n &= v_{n-1} - v_n \\ \dot{v}_n &= v_n(u_n - u_{n+1}) \end{aligned}$$

has scaling symmetry

$$(t, u_n, v_n) \to (\lambda^{-1}t, \lambda u_n, \lambda^2 v_n).$$

In terms of weights:

$w(\frac{\mathrm{d}}{\mathrm{dt}}) = 1,\ w(u_n) = w(u_{n+1}) = 1,\ w(v_n) = w(v_{n-1}) = 2.$

Conserved densities and fluxes

$$\begin{aligned} \rho_n^{(0)} &= \ln(v_n) & J_n^{(0)} &= u_n \\ \rho_n^{(1)} &= u_n & J_n^{(1)} &= v_{n-1} \\ \rho_n^{(2)} &= \tfrac{1}{2}u_n^2 + v_n & J_n^{(2)} &= u_n v_{n-1} \\ \rho_n^{(3)} &= \tfrac{1}{3}u_n^3 + u_n(v_{n-1} + v_n) & J_n^{(3)} &= u_{n-1}u_n v_{n-1} + v_{n-1}^2 \end{aligned}$$

are all scaling invariant!

- **Algorithm for Conserved Densities and Fluxes**

Example: Density of rank 3 for Toda system

Step 1: **Construct the form of the density.**

$$\rho_n = c_1\, u_n^3 + c_2\, u_n v_{n-1} + c_3\, u_n v_n$$

where c_i are unknown constants.

Step 2: **Determine the constants c_i.**

Compute

$$\begin{aligned} E_n = \mathrm{D}_t \rho_n \;&=\; \frac{\partial \rho_n}{\partial t} + \rho_n'(\mathbf{u}_n)[\mathbf{F}] \quad \text{(on DDE)} \\ &=\; (3c_1 - c_2)u_n^2 v_{n-1} + (c_3 - 3c_1)u_n^2 v_n + (c_3 - c_2)v_{n-1}v_n \\ &\quad + c_2 u_{n-1}u_n v_{n-1} + c_2 v_{n-1}^2 - c_3 u_n u_{n+1} v_n - c_3 v_n^2 \end{aligned}$$

Compute $\tilde{E}_n = \mathrm{D}E_n$ to remove negative shift $n-1$.

Since $\tilde{E}_n = -\Delta \tilde{J}_n$, the expression $\tilde{E}_n$ must be a total difference.

Require

$$\begin{aligned} \mathcal{L}_{u_n}^{(0)}(\tilde{E}_n) &= \frac{\partial}{\partial u_n}(\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2})(\tilde{E}_n) = \frac{\partial}{\partial u_n}(\mathrm{D} + \mathrm{I} + \mathrm{D}^{-1})(E_n) \\ &= 2(3c_1 - c_2)u_n v_{n-1} + 2(c_3 - 3c_1)u_n v_n \\ &\quad + (c_2 - c_3)u_{n-1}v_{n-1} + (c_2 - c_3)u_{n+1}v_n \equiv 0 \end{aligned}$$

and

$$\begin{aligned} \mathcal{L}_{v_n}^{(0)}(\tilde{E}_n) &= \frac{\partial}{\partial v_n}(\mathrm{I} + \mathrm{D}^{-1})(\tilde{E}_n) = \frac{\partial}{\partial v_n}(\mathrm{D} + \mathrm{I})(E_n) \\ &= (3c_1 - c_2)u_{n+1}^2 + (c_3 - c_2)v_{n+1} + (c_2 - c_3)u_n u_{n+1} \\ &\quad + 2(c_2 - c_3)v_n + (c_3 - 3c_1)u_n^2 + (c_3 - c_2)v_{n-1} \equiv 0. \end{aligned}$$

Solve the linear system

$$\mathcal{S} = \{3c_1 - c_2 = 0, c_3 - 3c_1 = 0, c_2 - c_3 = 0\}.$$

Solution: $3c_1 = c_2 = c_3$ Choose $c_1 = \frac{1}{3}$, and $c_2 = c_3 = 1$.

Substitute in ρ_n

$$\rho_n = \frac{1}{3}\,u_n^3 + u_n(v_{n-1} + v_n)$$

Step 3: **Compute the flux** J_n**.**

Start from $-\tilde{E}_n = -u_n u_{n+1} v_n - v_n^2 + u_{n+1} u_{n+2} v_{n+1} + v_{n+1}^2$

Apply the discrete homotopy operator to $f_n = -\tilde{E}_n$.

For component u_n (highest shift 2):

i	$\mathcal{L}_{u_n}^{(i+1)}(f_n)$	$(\mathrm{D}-\mathrm{I})^i(u_n \mathcal{L}_{u_n}^{(i+1)}(-\tilde{E}_n))$
0	$u_{n-1}v_{n-1}+u_{n+1}v_n$	$u_n u_{n-1} v_{n-1}+u_n u_{n+1} v_n$
1	$u_{n-1}v_{n-1}$	$u_{n+1}u_n v_n - u_n u_{n-1} v_{n-1}$

Hence, $f_{1,n}(\mathbf{u}_n)(f_n) = 2u_n u_{n+1} v_n$

For component v_n (highest shift 1):

i	$\mathcal{L}_{v_n}^{(i+1)}(f_n)$	$(\mathrm{D}-\mathrm{I})^i(v_n \mathcal{L}_{v_n}^{(i+1)}(-\tilde{E}_n))$
0	$u_n u_{n+1}+2v_n$	$v_n u_n u_{n+1}+2v_n^2$

Hence, $f_{2,n}(\mathbf{u}_n)(f_n) = u_n u_{n+1} v_n + 2v_n^2$

$$\begin{aligned}
\tilde{J}_n &= \mathcal{H}_{\mathbf{u}_n}(f_n) = \int_0^1 (f_{1,n}(\mathbf{u}_n)(f_n)[\lambda \mathbf{u}_n] + f_{2,n}(f_n)(\mathbf{u}_n)[\lambda \mathbf{u}_n])\,\frac{d\lambda}{\lambda} \\
&= \int_0^1 (3\lambda^2 u_n u_{n+1} v_n + 2\lambda v_n^2)\, d\lambda \\
&= u_n u_{n+1} v_n + v_n^2.
\end{aligned}$$

Final Result:

$$J_n = \mathrm{D}^{-1}\tilde{J}_n = u_{n-1} u_n v_{n-1} + v_{n-1}^2$$

Computer Demos

(1) Use discrete homotopy operator to compute $F_n = \Delta^{-1} f_n$ for

$f_n = -u_n\, u_{n+1}\, v_n - v_n^2 + u_{n+1}\, u_{n+2}\, v_{n+1} + v_{n+1}^2 + u_{n+3}\, v_{n+2} - u_{n+1}\, v_n$

(2) Compute density of rank 4 and flux for Toda system:

$$\begin{aligned} \dot{u}_n &= v_{n-1} - v_n \\ \dot{v}_n &= v_n(u_n - u_{n+1}) \end{aligned}$$

(3) Compute density of rank 2 for Ablowitz-Ladik system:

$$i\,\dot{u}_n = u_{n+1} - 2u_n + u_{n-1} + \kappa u_n^* u_n (u_{n+1} + u_{n-1})$$

(u_n^* is the complex conjugate of u_n).

This is an integrable discretization of the NLS equation:

$$iu_t + u_{xx} + \kappa u^2 u^* = 0$$

Take equation and its complex conjugate.
Treat u_n and $v_n = u_n^*$ as dependent variables. Absorb i in t:

$$\begin{aligned} \dot{u}_n &= u_{n+1} - 2u_n + u_{n-1} + u_n v_n (u_{n+1} + u_{n-1}) \\ \dot{v}_n &= -(v_{n+1} - 2v_n + v_{n-1}) - u_n v_n (v_{n+1} + v_{n-1}). \end{aligned}$$

Conclusions and Ongoing Research

- Generalize continuous homotopy operator in multi-dimensions $(x, y, z, ...)$.

- Problem (in three dimensions):

  Given $E = \boldsymbol{\nabla}\cdot\mathbf{J} = \mathrm{D}_x J^{(1)} + \mathrm{D}_y J^{(2)} + \mathrm{D}_z J^{(3)}$

  Find $\mathbf{J} = (J^{(1)},\ J^{(2)},\ J^{(3)})$.

- Application:

  Compute densities and fluxes of multi-dimensional systems of PDEs (in t, x, y, z).

- Generalize discrete homotopy operator in multi-dimensions $(n, m, ...)$.

Higher Euler Operators Side by Side

Continuous Case (for component u)

$$\mathcal{L}_u^{(0)} = \frac{\partial}{\partial u} - \mathrm{D}_x \frac{\partial}{\partial u_x} + \mathrm{D}_x^2 \frac{\partial}{\partial u_{2x}} - \mathrm{D}_x^3 \frac{\partial}{\partial u_{3x}} + \cdots$$
$$\mathcal{L}_u^{(1)} = \frac{\partial}{\partial u_x} - 2\mathrm{D}_x \frac{\partial}{\partial u_{2x}} + 3\mathrm{D}_x^2 \frac{\partial}{\partial u_{3x}} - 4\mathrm{D}_x^3 \frac{\partial}{\partial u_{4x}} + \cdots$$
$$\mathcal{L}_u^{(2)} = \frac{\partial}{\partial u_{2x}} - 3\mathrm{D}_x \frac{\partial}{\partial u_{3x}} + 6\mathrm{D}_x^2 \frac{\partial}{\partial u_{4x}} - 10\mathrm{D}_x^3 \frac{\partial}{\partial u_{5x}} + \cdots$$
$$\mathcal{L}_u^{(3)} = \frac{\partial}{\partial u_{3x}} - 4\mathrm{D}_x \frac{\partial}{\partial u_{4x}} + 10\mathrm{D}_x^2 \frac{\partial}{\partial u_{5x}} - 20\mathrm{D}_x^3 \frac{\partial}{\partial u_{6x}} + \cdots$$

Discrete Case (for component u_n)

$$\mathcal{L}_{u_n}^{(0)} = \frac{\partial}{\partial u_n}(\mathrm{I} + \mathrm{D}^{-1} + \mathrm{D}^{-2} + \mathrm{D}^{-3} + \cdots)$$
$$\mathcal{L}_{u_n}^{(1)} = \frac{\partial}{\partial u_n}(\mathrm{D}^{-1} + 2\mathrm{D}^{-2} + 3\mathrm{D}^{-3} + 4\mathrm{D}^{-4} + \cdots)$$
$$\mathcal{L}_{u_n}^{(2)} = \frac{\partial}{\partial u_n}(\mathrm{D}^{-2} + 3\mathrm{D}^{-3} + 6\mathrm{D}^{-4} + 10\mathrm{D}^{-5} + \cdots)$$
$$\mathcal{L}_{u_n}^{(3)} = \frac{\partial}{\partial u_n}(\mathrm{D}^{-3} + 4\mathrm{D}^{-4} + 10\mathrm{D}^{-5} + 20\mathrm{D}^{-6} + \cdots)$$

Homotopy Operators Side by Side

Continuous Case (for components u and v)

$$\mathcal{H}_{\mathbf{u}} = \int_0^1 \{ f_1(\mathbf{u})[\lambda \mathbf{u}] + f_2(\mathbf{u})[\lambda \mathbf{u}] \} \, \frac{d\lambda}{\lambda}$$

with

$$f_1(\mathbf{u}) = \sum_{i=0}^{p_1} \mathrm{D}_x^i [u \mathcal{L}_u^{(i+1)}]$$

and

$$f_2(\mathbf{u}) = \sum_{i=0}^{p_2} \mathrm{D}_x^i [v \mathcal{L}_v^{(i+1)}]$$

Discrete Case (for components u_n and v_n)

$$\mathcal{H}_{\mathbf{u}_n} = \int_0^1 \{ f_{1,n}(\mathbf{u}_n)[\lambda \mathbf{u}_n] + f_{2,n}(\mathbf{u}_n)[\lambda \mathbf{u}_n] \} \frac{d\lambda}{\lambda}$$

with

$$f_{1,n}(\mathbf{u}_n) = \sum_{i=0}^{p_1} (\mathrm{D} - \mathrm{I})^i [u_n \mathcal{L}_{u_n}^{(i+1)}]$$

and

$$f_{2,n}(\mathbf{u}_n) = \sum_{i=0}^{p_2} (\mathrm{D} - \mathrm{I})^i [v_n \mathcal{L}_{v_n}^{(i+1)}]$$

Implementation in Mathematica – Software

* P.J. Adams and W. Hereman
  TransPDEDensityFlux.m: Symbolic computation of conserved densities and fluxes for systems of partial differential equations with transcendental nonlinearities (2002).

* D. Baldwin and W. Hereman, **PDERecursionOperator.m**: A Mathematica program for the symbolic computation of recursion operators for nonlinear partial differential equations (2004).

* H. Eklund and W. Hereman
  DDEDensityFlux.m: Symbolic computation of conserved densities and fluxes for nonlinear systems of differential-difference equations (2002).

* Ü. Göktaş and W. Hereman
  InvariantsSymmetries.m: A Mathematica integrability package for the computation of invariants and symmetries (1997).
  Available from MathSource
  (Item: 0208-932, Applications/Mathematics) via FTP:
  mathsource.wolfram.com or URL
  http://www.mathsource.com/cgi-bin/MathSource/Applications/

* Ü. Göktaş and W. Hereman
  CONDENS.M: A Mathematica program for the symbolic computation of conserved densities for systems of nonlinear evolution equations (1996).

* Ü. Göktaş and W. Hereman
  DIFFDENS.M: A Mathematica program for the symbolic computation of conserved densities for systems of nonlinear differential-difference equations (1997).

All codes are available via the Internet
URL: http://www.mines.edu/fs_home/whereman/
and via anonymous FTP from mines.edu in directory
pub/papers/math_cs_dept/software/

Publications

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6). Ü. Göktaş, W. Hereman, and G. Erdmann, Computation of conserved densities for systems of nonlinear differential-difference equations, Phys. Lett. A, 236 (1997) 30–38.

7). Ü. Göktaş and W. Hereman, Computation of conserved densities for nonlinear lattices, Physica D, 123 (1998) 425–436.

8). Ü. Göktaş and W. Hereman, Algorithmic computation of higher-order symmetries for nonlinear evolution and lattice equations, Advances in Computational Mathematics 11 (1999), 55-80.

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10). W. Hereman, Ü. Göktaş, M. Colagrosso, and A. Miller, Algorithmic integrability tests for nonlinear differential and lattice equations, Computer Physics Communications 115 (1998) 428–446.

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