Continuous and Discrete Homotopy Operators with Applications in Integrability Testing

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Colloquium Talk Friday, October 31, 2003, 15:00

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Talk dedicated to Ryan Sayers

Research supported in part by NSF under Grant CCR-9901929

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

Future 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:

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

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)

$$8 v'v'' \longrightarrow 4 v'^{2}$$

$$2 u' u'' \cos(u) \longrightarrow u'^{2} \cos(u)$$

$$-u'^{3} \sin(u)$$

$$-6 v v' \cos(u) \longrightarrow -3 v^{2} \cos(u)$$

$$3 u' v^{2} \sin(u)$$

• Integral:

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

Remark: For simplicity we denote $f(\mathbf{u}, \mathbf{u}', \mathbf{u}'', \dots, \mathbf{u}^{(m)})$ 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 $f(\mathbf{u}) = D_x F(\mathbf{u})$ or equivalently $F(\mathbf{u}) = D_x^{-1} f(\mathbf{u}) = \int_x f(\mathbf{u}) dx$.

 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

$$\mathcal{L}_{\mathbf{u}}^{(0)} = \sum_{k=0}^{m_0} (-D_x)^k \frac{\partial}{\partial \mathbf{u}^{(k)}}$$

$$= \frac{\partial}{\partial u} - D_x \frac{\partial}{\partial \mathbf{u}'} + D_x^2 \frac{\partial}{\partial \mathbf{u}''} + \dots + (-1)^{m_0} D_x^{m_0} \frac{\partial}{\partial \mathbf{u}^{(m_0)}}$$

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):

$$\mathcal{L}_{u}^{(0)}(f) = \frac{\partial}{\partial u}(f) - D_{x}\frac{\partial}{\partial u'}(f) + D_{x}^{2}\frac{\partial}{\partial u''}(f)$$

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

$$-D_{x}[3v^{2} \sin(u) - 3u'^{2} \sin(u) + 2u'' \cos(u)] + D_{x}^{2}[2u' \cos(u)]$$

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

$$-[3u'v^{2} \cos(u) + 6v v' \sin(u) - 3u'^{3} \cos(u) - 6u u'' \sin(u)$$

$$-2u' u'' \sin(u) + 2u''' \cos(u)]$$

$$+[-2u''' \cos(u) - 6u' u'' \sin(u) + 2u''' \cos(u)]$$

$$\equiv 0$$

For component v (order 2):

$$\mathcal{L}_{v}^{(0)}(f) = \frac{\partial}{\partial v}(f) - D_{x}\frac{\partial}{\partial v'}(f) + D_{x}^{2}\frac{\partial}{\partial v''}(f)$$

$$= 6u'v\sin(u) - 6v'\cos(u) - D_{x}[-6v\cos(u) + 8v''] + D_{x}^{2}[8v']$$

$$= 6u'v\sin(u) - 6v'\cos(u) - [6u'v\sin(u) - 6v'\cos(u) + 8v'''] + 8v'''$$

$$\equiv 0$$

• Computation of the integral F

Definition (higher Euler operators):

The continuous higher Euler operators are defined by

$$\mathcal{L}_{\mathbf{u}}^{(i)} = \sum_{k=i}^{m_i} {k \choose i} (-D_x)^{k-i} \frac{\partial}{\partial \mathbf{u}^{(k)}}$$

These Euler operators all terminate at some maximal order m_i .

Examples (for component u):

$$\mathcal{L}_{u}^{(0)} = \frac{\partial}{\partial u} - D_{x} \frac{\partial}{\partial u'} + D_{x}^{2} \frac{\partial}{\partial u''} - D_{x}^{3} \frac{\partial}{\partial u'''} + \dots + (-1)^{m_{0}} D_{x}^{m_{0}} \frac{\partial}{\partial u^{(m_{0})}}$$

$$\mathcal{L}_{u}^{(1)} = \frac{\partial}{\partial u'} - 2D_{x} \frac{\partial}{\partial u'''} + 3D_{x}^{2} \frac{\partial}{\partial u''''} - 4D_{x}^{3} \frac{\partial}{\partial u^{(4)}} + \dots - (-1)^{m_{1}} m_{1} D_{x}^{m_{1} - 1} \frac{\partial}{\partial u^{(m_{1})}}$$

$$\mathcal{L}_{u}^{(2)} = \frac{\partial}{\partial u'''} - 3D_{x} \frac{\partial}{\partial u''''} + 6D_{x}^{2} \frac{\partial}{\partial u^{(4)}} - 10D_{x}^{3} \frac{\partial}{\partial u^{(5)}} + \dots + (-1)^{m_{2}} \binom{m_{2}}{2} D_{x}^{m_{2} - 2} \frac{\partial}{\partial u^{(m_{2})}}$$

$$\mathcal{L}_{u}^{(3)} = \frac{\partial}{\partial u''''} - 4D_{x} \frac{\partial}{\partial u^{(4)}} + 10D_{x}^{2} \frac{\partial}{\partial u^{(5)}} - 20D_{x}^{3} \frac{\partial}{\partial u^{(6)}} + \dots - (-1)^{m_{3}} \binom{m_{3}}{3} D_{x}^{m_{3} - 3} \frac{\partial}{\partial u^{(m_{3})}}$$

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

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

 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

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

and

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

Theorem (integration via homotopy operator):

Given an integrable function f

$$F = D_x^{-1} f = \int f \, dx = \mathcal{H}(\mathbf{u})(f)$$

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).

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

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

For component v (order 2):

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

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

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

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

$$= \int_0^1 [3\lambda^2 u v^2 \sin(\lambda u) - \lambda^2 u u'^2 \sin(\lambda u) + 2\lambda u'^2 \cos(\lambda u)$$

$$-6\lambda v^2 \cos(\lambda u) + 8\lambda v'^2] d\lambda$$

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

• Application: Conserved densities and fluxes for PDEs with transcendental nonlinearities

Definition (conservation law):

$$D_t \rho + D_x J = 0$$
 (on PDE)

conserved density ρ and flux J.

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

$$u_t = v$$

$$v_t = u_{xx} + \alpha \sin(u)$$

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:

$$w(D_x) = 1, \ w(D_t) = 1, \ w(u) = 0, \ w(v) = 1, \ w(\alpha) = 2$$

Conserved densities and fluxes

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

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

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

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

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

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

where $h_i(u)$ are unknown functions.

Step 2: Determine the functions h_i

Compute

$$E = D_t \rho = \frac{\partial \rho}{\partial t} + \rho'(\mathbf{u})[\mathbf{F}] \quad \text{(on PDE)}$$
$$= \frac{\partial \rho}{\partial t} + \sum_{k=0}^{m_1} \frac{\partial \rho}{\partial u_{kx}} D_x^k u_t + \sum_{k=0}^{m_2} \frac{\partial \rho}{\partial v_{kx}} D_x^k v_t$$

Since $E = D_t \rho = -D_x J$, 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):

$$h_{2}(u) - h_{3}(u) = 0$$

$$h_{2}'(u) = 0$$

$$h_{3}'(u) = 0$$

$$h_{4}'(u) = 0$$

$$h_{2}''(u) = 0$$

$$h_{4}''(u) = 0$$

$$2h_{2}''(u) - h_{3}'(u) = 0$$

$$2h_{2}''(u) - h_{3}''(u) = 0$$

$$h_{1}''(u) + 2\sin(u)h_{2}(u) = 0$$

$$h_{1}''(u) + 2\sin(u)h_{2}(u) = 0$$

Solution:

$$h_1(u) = 2c_1 \cos(u) + c_3$$

 $h_2(u) = h_3(u) = c_1$
 $h_4(u) = c_2$

(with arbitrary constants c_i).

Substitute in ρ

$$\rho = 2c_1\alpha\cos(u) + c_1v^2 + c_1u_x^2 + c_2u_xv + \alpha c_3$$

Step 3: Compute the flux J

First, compute

$$E = D_t \rho = c_1(-2\alpha u_t \sin u + 2vv_t + 2u_x u_{xt}) + c_2(u_{xt}v + u_x v_t)$$

$$= c_1(-2\alpha v \sin u + 2v(u_{2x} + \alpha \sin u) + 2u_x v_x)$$

$$+ c_2(v_x v + u_x(u_{2x} + \alpha \sin u))$$

$$= c_1(2u_{2x}v + 2u_x v_x) + c_2(vv_x + u_x u_{2x} + \alpha u_x \sin u)$$

Since $E = D_t \rho = -D_x J$, one must integrate.

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

For component u (order 2):

i	$\mathcal{L}_u^{(i+1)}(-E)$	$D_x^i \left(u \mathcal{L}_u^{(i+1)}(-E) \right)$
0	$2c_1v_x + c_2(u_{2x} - \alpha\sin u)$	$2c_1uv_x + c_2(uu_{2x} - \alpha u\sin u)$
1	$-2c_1v - c_2u_x$	$-2c_1(u_xv + uv_x) - c_2(u_x^2 + uu_{2x})$

Hence,
$$f_1(\mathbf{u})(f) = 2c_1u_xv - c_2(u_x^2 + \alpha u \sin u)$$

For component v (order 1):

$$\begin{array}{|c|c|c|c|}
\hline
i & \mathcal{L}_v^{(i+1)}(-E) & D_x^i \left(v \mathcal{L}_v^{(i+1)}(-E)\right) \\
\hline
0 & -2c_1u_x - c_2v & -2c_1u_xv - c_2v^2
\end{array}$$

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

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

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

$$= -\int_0^1 \left(4c_1 \lambda u_x v + c_2(\lambda u_x^2 + \alpha u \sin(\lambda u) + \lambda v^2) \right) d\lambda$$

$$= -2c_1 u_x v - c_2 \left(\frac{1}{2} v^2 + \frac{1}{2} u_x^2 - \alpha \cos u \right)$$

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

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

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

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:

$$u_t = v$$

$$v_t = u_{xx} + \alpha \sin(u)$$

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	$D_t \rho + D_x J = 0$	$\dot{\rho}_n + J_{n+1} - J_n = 0$
Symmetry	$D_t \mathbf{G} = \mathbf{F}'(\mathbf{u})[\mathbf{G}]$ $= \frac{\partial}{\partial \epsilon} \mathbf{F}(\mathbf{u} + \epsilon \mathbf{G}) _{\epsilon=0}$	$D_t \mathbf{G} = \mathbf{F}'(\mathbf{u}_n)[\mathbf{G}]$ $= \frac{\partial}{\partial \epsilon} \mathbf{F}(\mathbf{u}_n + \epsilon \mathbf{G}) _{\epsilon=0}$
Recursion Operator	$D_t \mathcal{R} + [\mathcal{R}, \mathbf{F}'(u)] = 0$	$D_t \mathcal{R} + [\mathcal{R}, \mathbf{F}'(\mathbf{u}_n)] = 0$

Table 1: Conservation Laws and Symmetries

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

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

$$DF_n = F_{n+1} = F_{n|_{n \to n+1}}$$

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

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

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

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

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

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

For k > 0, $D^k = D \circ D \circ \cdots \circ D$ (k times).

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

Problem to be solved:

Continuous case:

Given f. Find F so that $f = D_x F$ or $F = D_x^{-1} f = \int f dx$.

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)

$$-v_n^2 \longrightarrow v_n^2$$

$$v_{n+1}^2$$

$$-u_n u_{n+1} v_n \longrightarrow u_n u_{n+1} v_n$$

$$u_{n+1} u_{n+2} v_{n+1}$$

$$-u_{n+1} v_n \longrightarrow u_{n+1} v_n$$

$$+u_{n+2} v_{n+1}$$

$$-u_{n+2} v_{n+1}$$

$$-u_{n+2} v_{n+1}$$

$$u_{n+3} v_{n+2}$$

• 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 $\tilde{f}_n = D^2 f_n = u_n v_{n+2} v_{n+5}$.

• '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 $\mathcal{L}_{\mathbf{u}_n}^{(0)}(f_n) \equiv 0$, where $\mathcal{L}_{\mathbf{u}_n}^{(0)}$ is the discrete Euler operator (variational derivative) defined by

$$\mathcal{L}_{\mathbf{u}_{n}}^{(0)} = \sum_{k=0}^{m_{0}} D^{-k} \frac{\partial}{\partial \mathbf{u}_{n+k}}
= \frac{\partial}{\partial \mathbf{u}_{n}} + D^{-1} (\frac{\partial}{\partial \mathbf{u}_{n+1}}) + D^{-2} (\frac{\partial}{\partial \mathbf{u}_{n+2}}) + \dots + D^{-m_{0}} (\frac{\partial}{\partial \mathbf{u}_{n+m_{0}}})
= \frac{\partial}{\partial \mathbf{u}_{n}} (\sum_{k=0}^{m_{0}} D^{-k})
\mathcal{L}_{\mathbf{u}_{n}}^{(0)} = \frac{\partial}{\partial \mathbf{u}_{n}} (\mathbf{I} + \mathbf{D}^{-1} + \mathbf{D}^{-2} + \dots + \mathbf{D}^{-m_{0}})$$

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):

$$\mathcal{L}_{u_n}^{(0)}(f_n) = \frac{\partial}{\partial u_n} [I + D^{-1} + D^{-2} + D^{-3}](f_n)$$

$$= [-u_{n+1}v_n] + [-u_{n-1}v_{n-1} + u_{n+1}v_n - v_{n-1}] + [u_{n-1}v_{n-1}] + [v_{n-1}]$$

$$\equiv 0$$

For component v_n (highest shift 2):

$$\mathcal{L}_{v_n}^{(0)}(f_n) = \frac{\partial}{\partial v_n} [I + D^{-1} + D^{-2}](f_n)$$

$$= [-u_n u_{n+1} - 2v_n - u_{n+1}] + [u_n u_{n+1} + 2v_n] + [u_{n+1}]$$

$$\equiv 0$$

• Computation of F_n

Definition (higher Euler operators):

The discrete higher Euler operators are defined by

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

These Euler operators all terminate at some maximal shifts m_i .

Examples (for component u_n):

$$\mathcal{L}_{u_n}^{(0)} = \frac{\partial}{\partial u_n} (I + D^{-1} + D^{-2} + D^{-3} + \dots + D^{-m_0})$$

$$\mathcal{L}_{u_n}^{(1)} = \frac{\partial}{\partial u_n} (D^{-1} + 2D^{-2} + 3D^{-3} + 4D^{-4} + \dots + m_1 D^{-m_1})$$

$$\mathcal{L}_{u_n}^{(2)} = \frac{\partial}{\partial u_n} (D^{-2} + 3D^{-3} + 6D^{-4} + 10D^{-5} + \dots + \frac{1}{2} m_2 (m_2 - 1) D^{-m_2})$$

$$\mathcal{L}_{u_n}^{(3)} = \frac{\partial}{\partial u_n} (D^{-3} + 4D^{-4} + 10D^{-5} + 20D^{-6} + \dots + \binom{m_3}{3} D^{-m_3})$$

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

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

 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

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

and

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

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.

Higher Euler Operators Side by Side

Continuous Case (for component u)

$$\mathcal{L}_{u}^{(0)} = \frac{\partial}{\partial u} - D_{x} \frac{\partial}{\partial u_{x}} + D_{x}^{2} \frac{\partial}{\partial u_{2x}} - D_{x}^{3} \frac{\partial}{\partial u_{3x}} + \cdots$$

$$\mathcal{L}_{u}^{(1)} = \frac{\partial}{\partial u_{x}} - 2D_{x} \frac{\partial}{\partial u_{2x}} + 3D_{x}^{2} \frac{\partial}{\partial u_{3x}} - 4D_{x}^{3} \frac{\partial}{\partial u_{4x}} + \cdots$$

$$\mathcal{L}_{u}^{(2)} = \frac{\partial}{\partial u_{2x}} - 3D_{x} \frac{\partial}{\partial u_{3x}} + 6D_{x}^{2} \frac{\partial}{\partial u_{4x}} - 10D_{x}^{3} \frac{\partial}{\partial u_{5x}} + \cdots$$

$$\mathcal{L}_{u}^{(3)} = \frac{\partial}{\partial u_{3x}} - 4D_{x} \frac{\partial}{\partial u_{4x}} + 10D_{x}^{2} \frac{\partial}{\partial u_{5x}} - 20D_{x}^{3} \frac{\partial}{\partial u_{6x}} + \cdots$$

Discrete Case (for component u_n)

$$\mathcal{L}_{u_n}^{(0)} = \frac{\partial}{\partial u_n} (I + D^{-1} + D^{-2} + D^{-3} + \cdots)$$

$$\mathcal{L}_{u_n}^{(1)} = \frac{\partial}{\partial u_n} (D^{-1} + 2D^{-2} + 3D^{-3} + 4D^{-4} + \cdots)$$

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

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

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

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

and

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

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

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

and

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

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	$\mathcal{L}_{u_n}^{(i+1)}(f_n)$	$(D-I)^{i}[u_{n}\mathcal{L}_{u_{n}}^{(i+1)}(f_{n})]$
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_n u_{n+1} v_n + 3u_{n+1} v_n - u_{n-1} u_n v_{n-1} - 3u_n v_{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,
$$f_{1,n}(\mathbf{u}_n)(f_n) = 2u_n u_{n+1} v_n + u_{n+1} v_n + u_{n+2} v_{n+1}$$

For component v_n (highest shift 2):

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

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

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

$$F_{n}(\mathbf{u}_{n}) = \int_{0}^{1} \{f_{1,n}(\mathbf{u}_{n})(f_{n})[\lambda \mathbf{u}_{n}] + f_{2,n}(\mathbf{u}_{n})(f_{n})[\lambda \mathbf{u}_{n}]\} \frac{d\lambda}{\lambda}$$

$$= \int_{0}^{1} [2\lambda v_{n}^{2} + 3\lambda^{2}u_{n}u_{n+1}v_{n} + 2\lambda u_{n+1}v_{n} + 2\lambda u_{n+2}v_{n+1}] d\lambda$$

$$= v_{n}^{2} + u_{n}u_{n+1}v_{n} + u_{n+1}v_{n} + u_{n+2}v_{n+1}$$

Application: Conserved densities and fluxes for DDEs
 Definition (conservation law):

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

conserved density ρ_n and flux J_n .

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

$$\dot{u}_n = v_{n-1} - v_n$$

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

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

$$\rho_n^{(0)} = \ln(v_n) \qquad J_n^{(0)} = u_n
\rho_n^{(1)} = u_n \qquad J_n^{(1)} = v_{n-1}
\rho_n^{(2)} = \frac{1}{2}u_n^2 + v_n \qquad J_n^{(2)} = u_n v_{n-1}
\rho_n^{(3)} = \frac{1}{3}u_n^3 + u_n(v_{n-1} + v_n) \qquad J_n^{(3)} = u_{n-1}u_n v_{n-1} + v_{n-1}^2$$

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

$$E_{n} = D_{t}\rho_{n} = \frac{\partial \rho_{n}}{\partial t} + \rho'_{n}(\mathbf{u}_{n})[\mathbf{F}] \quad \text{(on DDE)}$$

$$= (3c_{1} - c_{2})u_{n}^{2}v_{n-1} + (c_{3} - 3c_{1})u_{n}^{2}v_{n} + (c_{3} - c_{2})v_{n-1}v_{n}$$

$$+c_{2}u_{n-1}u_{n}v_{n-1} + c_{2}v_{n-1}^{2} - c_{3}u_{n}u_{n+1}v_{n} - c_{3}v_{n}^{2}$$

Compute $\tilde{E}_n = DE_n$ 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

$$\mathcal{L}_{u_n}^{(0)}(\tilde{E}_n) = \frac{\partial}{\partial u_n} (I + D^{-1} + D^{-2})(\tilde{E}_n) = \frac{\partial}{\partial u_n} (D + I + D^{-1})(E_n)$$

$$= 2(3c_1 - c_2)u_n v_{n-1} + 2(c_3 - 3c_1)u_n v_n$$

$$+ (c_2 - c_3)u_{n-1}v_{n-1} + (c_2 - c_3)u_{n+1}v_n \equiv 0$$

and

$$\mathcal{L}_{v_n}^{(0)}(\tilde{E}_n) = \frac{\partial}{\partial v_n} (I + D^{-1})(\tilde{E}_n) = \frac{\partial}{\partial v_n} (D + I)(E_n)$$

$$= (3c_1 - c_2)u_{n+1}^2 + (c_3 - c_2)v_{n+1} + (c_2 - c_3)u_n u_{n+1}$$

$$+2(c_2 - c_3)v_n + (c_3 - 3c_1)u_n^2 + (c_3 - c_2)v_{n-1} \equiv 0.$$

Solve the linear system

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

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!

For component u_n (highest shift 2):

i	$\mathcal{L}_{u_n}^{(i+1)}(- ilde{E}_n)$	$\left (D-I)^{i} (u_{n} \mathcal{L}_{u_{n}}^{(i+1)} (-\tilde{E}_{n})) \right $
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	$u_{n-1}v_{n-1}$	$\left u_{n+1}u_nv_n-u_nu_{n-1}v_{n-1} \right $

Hence,
$$\tilde{j}_{1,n}(\mathbf{u}_n) = 2u_n u_{n+1} v_n$$

For component v_n (highest shift 1):

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

$$\tilde{J}_n = \int_0^1 (\tilde{j}_{1,n}(\mathbf{u}_n)[\lambda \mathbf{u}_n] + \tilde{j}_{2,n}(\mathbf{u}_n)[\lambda \mathbf{u}_n]) \frac{d\lambda}{\lambda}
= \int_0^1 (3\lambda^2 u_n u_{n+1} v_n + 2\lambda v_n^2) d\lambda
= u_n u_{n+1} v_n + v_n^2.$$

Final Result:

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

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:

$$\dot{u}_n = v_{n-1} - v_n$$

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

(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:

$$\dot{u}_n = u_{n+1} - 2u_n + u_{n-1} + u_n v_n (u_{n+1} + u_{n-1})$$

$$\dot{v}_n = -(v_{n+1} - 2v_n + v_{n-1}) - u_n v_n (v_{n+1} + v_{n-1}).$$

Future Research

- Generalize continuous homotopy operator in multi-dimensions (x, y, z, ...).
- Problem (in three dimensions):

Given
$$E = \nabla \cdot \mathbf{J} = J_x^{(1)} + J_y^{(2)} + J_z^{(3)}$$
.
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)

$$\mathcal{L}_{u}^{(0)} = \frac{\partial}{\partial u} - D_{x} \frac{\partial}{\partial u_{x}} + D_{x}^{2} \frac{\partial}{\partial u_{2x}} - D_{x}^{3} \frac{\partial}{\partial u_{3x}} + \cdots$$

$$\mathcal{L}_{u}^{(1)} = \frac{\partial}{\partial u_{x}} - 2D_{x} \frac{\partial}{\partial u_{2x}} + 3D_{x}^{2} \frac{\partial}{\partial u_{3x}} - 4D_{x}^{3} \frac{\partial}{\partial u_{4x}} + \cdots$$

$$\mathcal{L}_{u}^{(2)} = \frac{\partial}{\partial u_{2x}} - 3D_{x} \frac{\partial}{\partial u_{3x}} + 6D_{x}^{2} \frac{\partial}{\partial u_{4x}} - 10D_{x}^{3} \frac{\partial}{\partial u_{5x}} + \cdots$$

$$\mathcal{L}_{u}^{(3)} = \frac{\partial}{\partial u_{3x}} - 4D_{x} \frac{\partial}{\partial u_{4x}} + 10D_{x}^{2} \frac{\partial}{\partial u_{5x}} - 20D_{x}^{3} \frac{\partial}{\partial u_{6x}} + \cdots$$

Discrete Case (for component u_n)

$$\mathcal{L}_{u_n}^{(0)} = \frac{\partial}{\partial u_n} (I + D^{-1} + D^{-2} + D^{-3} + \cdots)$$

$$\mathcal{L}_{u_n}^{(1)} = \frac{\partial}{\partial u_n} (D^{-1} + 2D^{-2} + 3D^{-3} + 4D^{-4} + \cdots)$$

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

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

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

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

and

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

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

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

and

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