Automated parameters for troubled-cell indicators using outlier detection

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Recent Developments in the Numerics of Nonlinear Hyperbolic Conservation Laws
Oberwolfach workshop, September 15, 2015

Outline

1. Building blocks: DG and multiwavelets
2. Multiwavelet troubled-cell indicator (with parameter)
3. Outlier detection for parameter choice
4. Results

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Discontinuous Galerkin method

$$\begin{cases} u_t + f(u)_x = 0, & x \in [-1,1], \quad t > 0, \\ u(x,0) = u_0(x), & x \in [-1,1]. \end{cases}$$

- Discretize $[-1,1]$ into 2^n elements
- Approximation space V_h^k: kth-degree piecewise polynomials
- Approximate u by $u_h \in V_h^k$

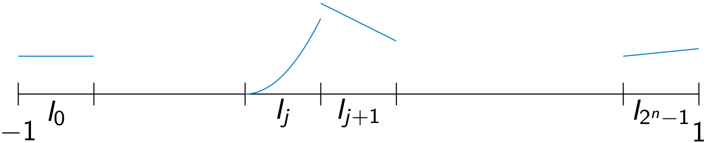
- Multiply PDE by $v_h \in V_h^k$, integrate over I_j
- Integrate by parts

TUDelft

DG approximations and multiwavelets

Global DG approximation, 2^n elements on $[-1,1]$:

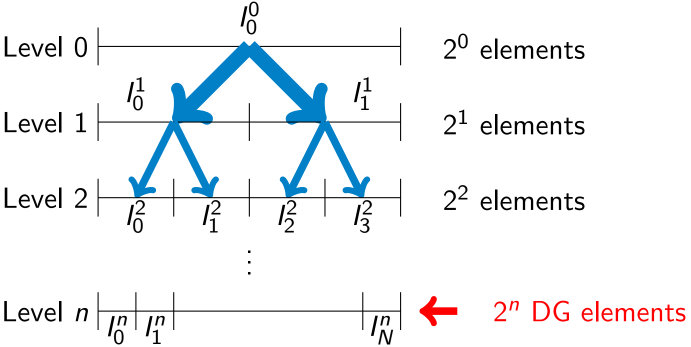
$$u_h(x) = \sum_{j=0}^{2^n-1} \sum_{\ell=0}^{k} u_j^{(\ell)} \phi_\ell(\xi_j)$$



Corresponding multiwavelet expansion:

$$u_h(x) = \underbrace{\sum_{\ell=0}^{k} s_{\ell 0}^{0} \phi_\ell(x)}_{\text{global average}} + \underbrace{\sum_{m=0}^{n-1} \sum_{j=0}^{2^m-1} \sum_{\ell=0}^{k} d_{\ell j}^{m} \psi_{\ell j}^{m}(x)}_{\text{finer details}}$$

Multiresolution idea



$$V_n^k = \{f : f \in \mathbb{P}^k(I_j^n), j = 0, \ldots, 2^n - 1\}$$

$$V_0^k \subset V_1^k \subset \cdots \subset V_n^k \subset \cdots$$

(Alpert, SIAM J. Math. Anal. 1993)

Scaling functions and DG basis

DG basis functions:

- Orthonormal Legendre polynomials
- Basis for V_0^k : scaling function basis
- Basis functions for V_n^k: dilation and translation

$$\phi_{\ell j}^n(x) = 2^{n/2}\phi_\ell(2^n(x+1) - 2j - 1),$$

$$\ell = 0, \ldots, k,\ j = 0, \ldots, 2^n - 1,\ x \in I_j^n$$

(Archibald et al., Appl. Num. Math. 2011)

Multiwavelets

Multiwavelet space W_m^k:

- Orthogonal complement of V_m^k in V_{m+1}^k:

$$V_m^k \oplus W_m^k = V_{m+1}^k, \quad W_m^k \perp V_m^k, \quad W_m^k \subset V_{m+1}^k$$

- V_n^k can be split into $n+1$ orthogonal subspaces:

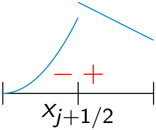
$$V_n^k = V_0^k \oplus W_0^k \oplus W_1^k \oplus \cdots \oplus W_{n-1}^k$$

Split up $f \in V_n^k$ into different levels:

$$u_h(x) = \sum_{\ell=0}^{k} s_{\ell 0}^0 \phi_\ell(x) + \sum_{m=0}^{n-1} \sum_{j=0}^{2^m-1} \sum_{\ell=0}^{k} d_{\ell j}^m \psi_{\ell j}^m(x)$$

Jumps in DG approximations

$$u_h(x) = \sum_{\ell=0}^{k} s_{\ell 0}^{0} \phi_\ell(x) + \sum_{m=0}^{n-1} \sum_{j=0}^{2^m-1} \sum_{\ell=0}^{k} d_{\ell j}^{m} \psi_{\ell j}^{m}(x)$$



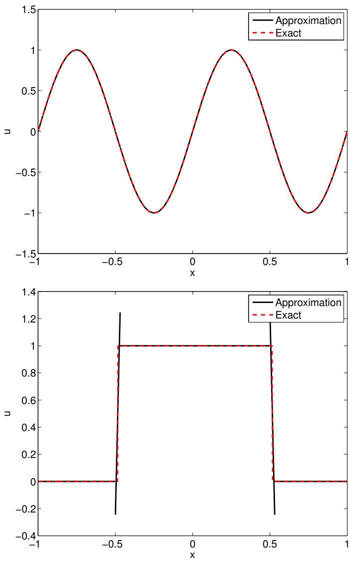
Coefficient $d_{\ell j}^{n-1}$: measures jump in (derivatives) approximation

$$d_{\ell j}^{n-1} = \sum_{m=0}^{k} c_{m\ell}^{n} \left(u_h^{(m)}(x_{j+1/2}^{+}) - u_h^{(m)}(x_{j+1/2}^{-}) \right),$$

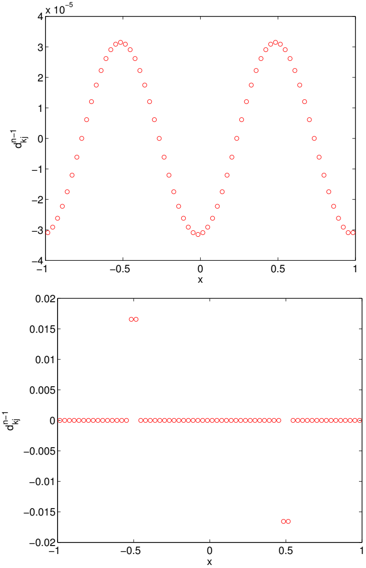
where

$$c_{m\ell}^{n} = \frac{2^{(-n+1)m}}{m!} \cdot \int_0^1 x^m \psi_\ell(x)\, dx.$$

(Vuik and Ryan, Proc. ICOSAHOM 2014)



Approximation



d_{kj}^{n-1}

Highest level

This means that $\mathbf{d}^{n-1}$:

- Measures element-boundary jumps in approximation (derivatives);
- Can be used for discontinuity detection.

(Vuik and Ryan, JCP 2014)

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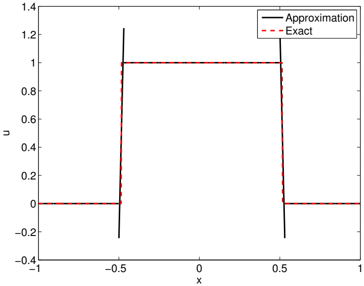
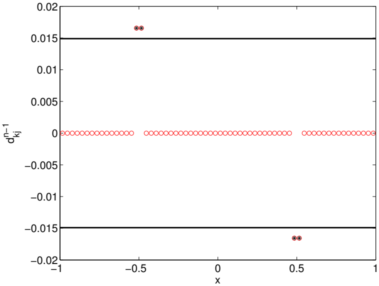
Original approach

Detect elements I_j and I_{j+1} if

$$|d_{kj}^{n-1}| > C \cdot \max_j |d_{kj}^{n-1}|, C \in [0, 1].$$



Approximation



Detected, $C = 0.9$

64 elements, $k = 1$

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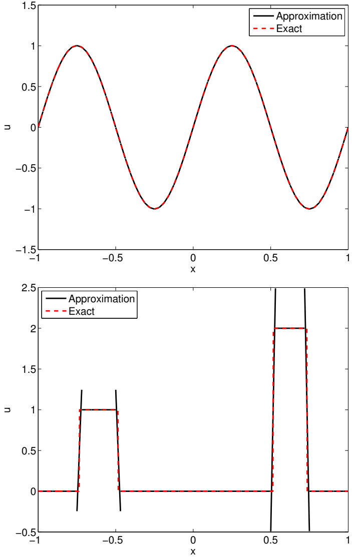
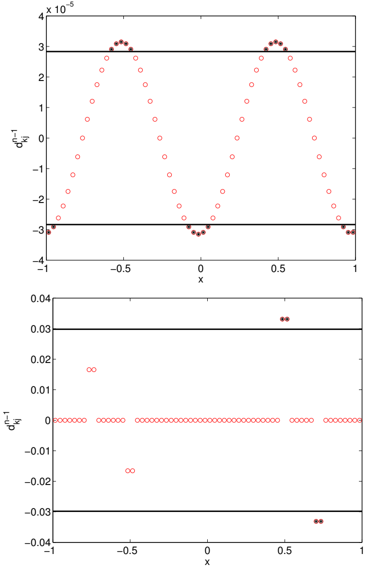


Approximation



Detected, $C = 0.9$

How to choose C?

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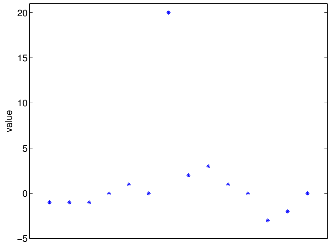
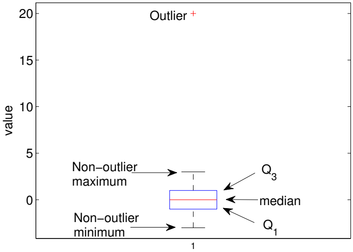
Outlier detection for parameter choice

d_{kj}^{n-1}:

- vector containing jumps over element boundaries
- coefficient big compared to neighbors: detect

$\Rightarrow$ Boxplot approach





(Tukey, 1977)

Outlier detection for parameter choice

Detect values in $\mathbf{D} = (d_0, \ldots, d_N)^\top$ which suddenly change:

1. Sort $\mathbf{D}$:

$$\mathbf{D}^s = (d_0^s, d_1^s, \ldots, d_N^s), \quad d_0^s \le d_1^s \le \ldots \le d_N^s$$

2. Compute quartiles $Q_1,\ Q_2,\ Q_3$ of $\mathbf{D}$
3. Construct outer fences
4. Determine outliers

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Quartile computation

- Median Q_2:

$$Q_2 = \begin{cases} d^s_{N/2}, & \text{if } N \text{ is even,} \\ \frac{1}{2}\left(d^s_{(N-1)/2} + d^s_{(N+1)/2}\right), & \text{if } N \text{ is odd.} \end{cases}$$

  Separates higher half from lower half.

- Q_1: value below which 25% data falls.
- Q_3: value below which 75% data falls.

Constructing fences

Outer fence: $[Q_1 - 3(Q_3 - Q_1),\ Q_3 + 3(Q_3 - Q_1)]$

Outside this region: extreme outlier

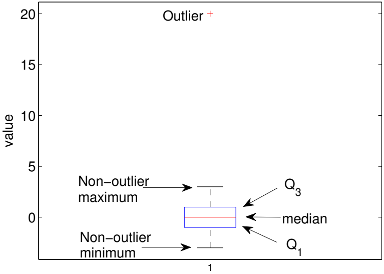
- Coverage of 99.9998%
- Normally distributed: 0.0002% detected asymptotically
- Few false positives if data well behaved
- Continuous function: no elements are detected!

(Hoaglin et al., J. Amer. Statist. Assoc. (1986))

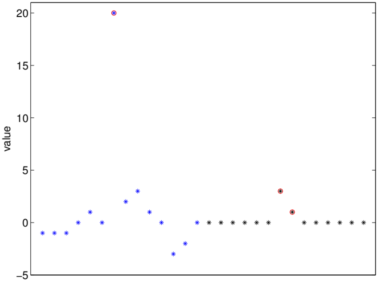
Boxplot

$$\mathbf{d} = \begin{pmatrix} -1 \\ -1 \\ -1 \\ 0 \\ 1 \\ 0 \\ 20 \\ 2 \\ 3 \\ 1 \\ 0 \\ -3 \\ -2 \\ 0 \end{pmatrix}, \quad \mathbf{d}^s = \begin{pmatrix} -3 \\ -2 \\ -1 \\ -1 \\ -1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \\ 1 \\ 2 \\ 3 \\ 20 \end{pmatrix}$$

- 25th and 75th percentiles:
  $Q_1 = -1, \quad Q_3 = 1$
- Lower bound:
  $Q_1 - 3(Q_3 - Q_1) = -7$
- Upper bound:
  $Q_3 + 3(Q_3 - Q_1) = 7$



Local information



- Divide global vector in local vectors
- Apply boxplot approach for each local vector
- Ignore 'outliers' near split boundaries

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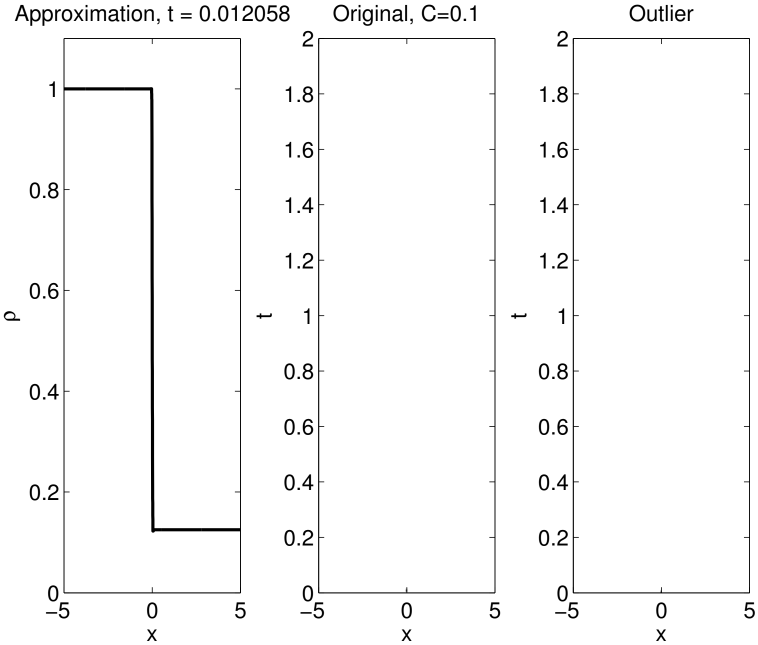
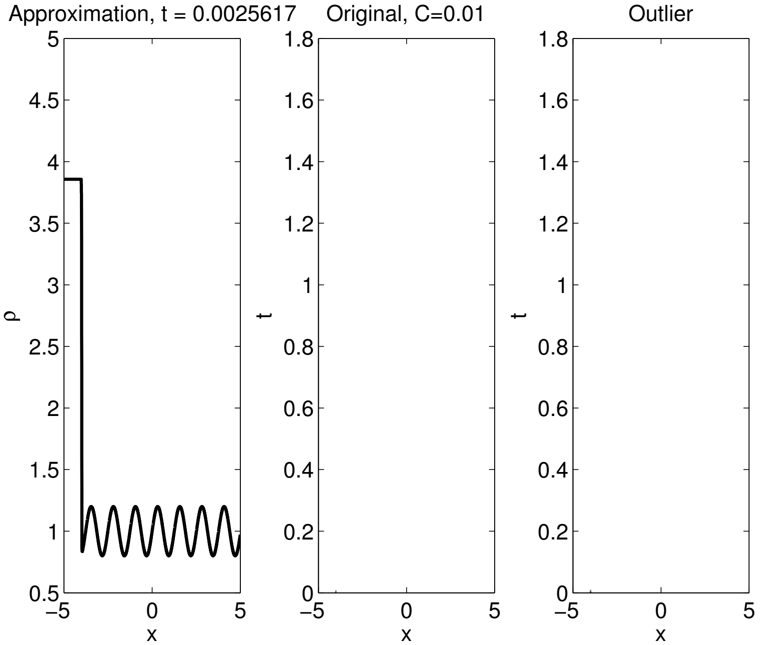
Applications

- Apply original indicator with optimal parameter C
- Compare with outlier-detected results (no parameter)
- Euler equations: Sod, sine-entropy wave



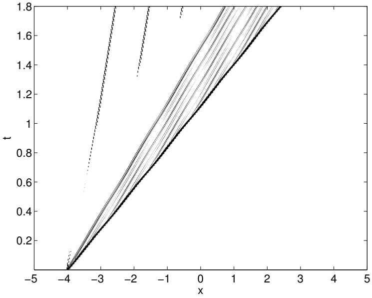
Approximation, t = 0.012058
Original, C=0.1
Outlier
ρ
t
t
x
x
x
1
0.8
0.6
0.4
0.2
0
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
−5
0
5


Approximation, t = 0.0025617
Original, C=0.01
Outlier
ρ
t
t
x
x
x

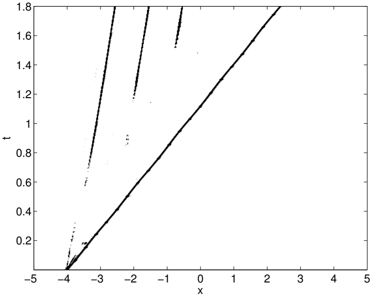
Minmod-based TVB indicator

$$u^{-}_{j+\frac{1}{2}} = \bar{u}_j + \tilde{u}_j, \quad \tilde{u}_j = \sum_{\ell=1}^{k} u_j^{(\ell)} \phi_\ell(1)$$

$$u^{+}_{j-\frac{1}{2}} = \bar{u}_j - \tilde{\tilde{u}}_j, \quad \tilde{\tilde{u}}_j = -\sum_{\ell=1}^{k} u_j^{(\ell)} \phi_\ell(-1)$$



$M = 100$

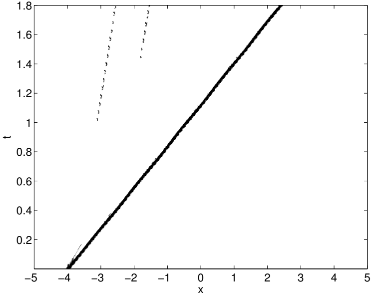


Outlier

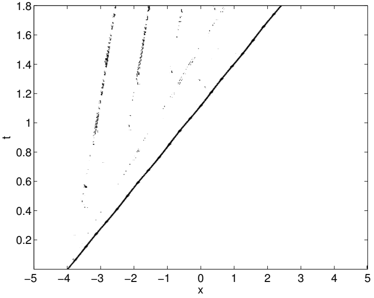
KXRCF detector

Jump across inflow edge:

$$\mathcal{I}_j = \left| \int_{\partial I_j^-} (u_h|_{I_j} - u_h|_{I_{n_j}}) ds \right|$$



Threshold equal to 1



Outlier

Computation times

	Multiwavelets		KXRCF		Minmod	
	Original	Outlier	Original	Outlier	Original	Outlier
Sod	2.772	2.987	3.224	3.232	3.752	3.833
Lax	3.928	4.292	4.596	4.621	5.395	5.603
blast wave	10.539	11.045	13.505	12.313	14.776	14.855
Shu-Osher	5.683	5.845	6.520	6.512	7.669	7.973

Computation time in seconds

Conclusion and future research

- Original troubled-cell indicator: problem-dependent parameter
- Outlier-detection technique using boxplots
- Local-vector approach
- Parameters no longer needed!

- Include spatial information (collaboration with Mahsa Mirzagar)
- General meshes

(Vuik and Ryan, arXiv:1504.05783)