Analysis of Singular Zones in Multidimensional Discrete Data

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  - Homology computation

Cubical grids

A *cubical grid* $\mathscr{K}^d$ is a collection of *elementary cubes* of the form

$$Q = I_1 \times I_2 \times \cdots \times I_d$$

where $I_j = [k, k+1]$ or $I_j = [k] = \{k\}$.
We denote the subset of $\mathscr{K}^d$ containing the elementary cubes Q of dimension k by $\mathscr{K}^d_k$, or if d is obvious, by $\mathscr{K}_k$.
Given cubical subgrids $\mathscr{A} \subset \mathscr{X} \subset \mathscr{K}^d$ and their associated *cubical sets* $X = |\mathscr{X}|$ and $A = |\mathscr{A}|$, we will consider their relative homology $H_*(X, A)$.

Combinatorial wrap

Definition

Let A be a bounded set in $\mathbb{R}^d$. The combinatorial *wrap* of A is a subset of $\mathscr{K}$ defined by

$$wrap(A) = \{P \in \mathscr{K}_d \mid P \cap A \neq \emptyset\}.$$

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$$wrap(A) = \{P \in \mathscr{K}_d \mid P \cap A \neq \emptyset\}.$$

We will denote its carrier (a cubical subset of $\mathbb{R}^d$) by

$$\mathrm{wrap}(A) = |wrap(A)|.$$

Combinatorial boundary

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Given a finite set $\mathscr{A} \in \mathscr{K}_d$, its combinatorial *outer boundary* is defined by

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We shall rescale the cubical grids before building neighbourhoods and boundaries.

Cubic subdivisions

Let $\mathscr{K}$ be a cubical grid, and consider the *rescaling isomorphism* $\Lambda^k : \mathbb{R}^d \to \mathbb{R}^d$,

$$\Lambda^k(x_1, x_2, \ldots, x_d) = (kx_1, kx_2, \ldots, kx_d),$$

where $k \in \mathbb{Z}$ is a *rescaling factor*. The corresponding refined grid is the image of $\mathscr{K}$ under the *inverse rescaling* $\Lambda^{1/k} = (\Lambda^k)^{-1}$. Given $\mathscr{A} \subset \mathscr{K}_d$, the *k-th subdivision* of $\mathscr{A}$ is given by

$$\mathrm{sd}^k \mathscr{A} := \{Q \in \Lambda^{1/k} \mathscr{K}_d \mid Q \subset A\}.$$

Scaled wraps and boundaries

Definition

The *factor k scaled wrap* of A is the subset of $\Lambda^{1/k}\mathscr{K}$ defined by

$$wrap^k(A) = \{P \in \Lambda^{1/k}\mathscr{K}_d \mid P \cap A \neq \emptyset\}.$$

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$$wrap^k(A) = \{P \in \Lambda^{1/k}\mathscr{K}_d \mid P \cap A \neq \emptyset\}.$$

Its carrier with respect to the refined grid is denoted $\mathrm{wrap}^k(A)$.
The *factor k scaled outer boundaries* of $\mathscr{A}$ and $A = |\mathscr{A}|$ are the sets

$$bd^k(\mathscr{A}) = wrap^k(A) \setminus \mathrm{sd}^k(\mathscr{A}),$$

and

$$\mathrm{bd}^k(A) = |bd^k(\mathscr{A})|.$$

Isolating neighbourhoods

Theorem (Allili)

Given a cubical set A and a scaling factor $k \geq 3$, the inclusion $A \hookrightarrow \mathrm{wrap}^k(A)$ induces an isomorphism in homology.

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Given a cubical set A and a scaling factor $k \geq 3$, the inclusion $A \hookrightarrow \mathrm{wrap}^k(A)$ induces an isomorphism in homology.

This provides a way to construct a cubical set that is an isolating neighbourhood of A and that preserves its topological properties.

Wraps

Definition

Let $\mathscr{X}_d \subset \mathscr{K}_d$. Consider a function $f : \mathscr{X}_d \to \mathbb{R}$ and an elementary cube $Q \in \mathscr{X}_d$ such that $wrap(Q) \subset \mathscr{X}_d$. We define the *upper wrap*, *lower wrap* and *level wrap* of Q as, respectively,

$$\overline{wrap}(Q) = \{P \in \ wrap(Q) \mid f(P) > f(Q)\},$$
$$\underline{wrap}(Q) = \{P \in \ wrap(Q) \mid f(P) < f(Q)\},$$
$$wrap_z(Q) = \{P \in \ wrap(Q) \mid f(P) = f(Q)\}.$$

Wraps (next)

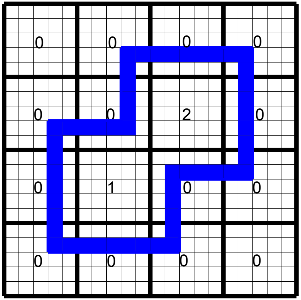
Definition

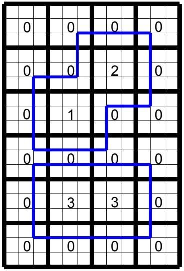
We can define wraps for cubical sets $A = |\mathscr{A}|$ by ensuring that the inequalities be satisfied locally:

$$\overline{wrap}(A) = \{P \in bd(\mathscr{A}) \mid f(P) > f(Q) \forall Q \in \mathscr{A} \cap bd(P)\},$$
$$\underline{wrap}(A) = \{P \in bd(\mathscr{A}) \mid f(P) < f(Q) \forall Q \in \mathscr{A} \cap bd(P)\},$$
$$wrap_z(A) = bd(\mathscr{A}) \setminus \left(\underline{wrap}(A) \cup \overline{wrap}(A)\right).$$

We will denote the carriers of $\overline{wrap}$ and $\underline{wrap}$ by $\overline{\mathrm{wrap}}$ and $\underline{\mathrm{wrap}}$. We will use a terminology and notation analogous as for the factor k scaled wraps.

Wraps (example)





Existence

Theorem (Ważewski)

Let S be an isolated invariant set and (N, L) an index pair for S. The homology $H_*(N, L)$ is called the *homological Conley index* of S, denoted $CH_*(S)$. Let N be an isolating neighbourhood and suppose that

$$CH_*(\mathrm{Inv}\, N) \ncong 0.$$

Then $\mathrm{Inv}\, N$ is nonempty.
More generally, if L is a closed subset of ∂N and $H_*(N, L)$ is non-trivial, then N contains a nonempty invariant set in its interior. Our algorithm will make use of this property.

Singular cubes

Definition

Let $\mathscr{X}_d \subset \mathscr{K}_d$ and $k \geq 5$. Consider a function $f : \mathscr{X} \to \mathbb{R}$ and an elementary cube $Q \in \mathscr{X}_d$ such that $wrap(Q) \subset \mathscr{X}_d$. Define

$$\begin{aligned} N &= \mathrm{wrap}^k(\mathrm{wrap}^k(Q)), \\ L_p &= \overline{\mathrm{wrap}}(Q) \cap \mathrm{bd}^k(\mathrm{wrap}^k(Q)), \\ L_n &= \underline{\mathrm{wrap}}(Q) \cap \mathrm{bd}^k(\mathrm{wrap}^k(Q)), \\ L_z &= \mathrm{wrap}_z(Q) \cap \mathrm{bd}^k(\mathrm{wrap}^k(Q)). \end{aligned}$$

The elementary cube Q is called *ordinary* if $H_*(N, L_p) = 0$ and $H_*(N, L_n) = 0$. Otherwise, it is called *singular*.

Singular components

Definition

Let $\mathscr{X}_d \subset \mathscr{K}_d$ and $k \geq 5$, and consider a function $f : \mathscr{X}_d \to \mathbb{R}$. A set $\mathscr{C}$ of elementary cubes in $\mathscr{K}_d$ is called an *isolated singular component* if

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- $\mathrm{wrap}\,(C) \subset X$;
- $C = |\mathscr{C}|$ is connected;
- $\mathscr{C}$ is *isolated*, that is, every $P \in bd\,(\mathscr{C})$ is ordinary.

Isolating neighbourhoods of components

Definition

We define the *isolating neighbourhood* of $C = |\mathscr{C}|$ and its *upper*, *lower* and *level sets* as

$$
\begin{aligned}
N &= \operatorname{wrap}^k(\operatorname{wrap}^k(C)),\\
L_p &= \overline{\operatorname{wrap}}(Q) \cap \operatorname{bd}^k(\operatorname{wrap}^k(C)),\\
L_n &= \underline{\operatorname{wrap}}(Q) \cap \operatorname{bd}^k(\operatorname{wrap}^k(C)),\\
L_z &= \operatorname{wrap}_z(Q) \cap \operatorname{bd}^k(\operatorname{wrap}^k(C)).
\end{aligned}
$$

Critical components

Definition

An isolated singular component $\mathscr{C}$ is called *regular* if $H_*(N, L_p) = 0$ and $H_*(N, L_n) = 0$. Otherwise it is a *critical component*. A cube Q is called *critical* if it belongs to a critical component; otherwise it is *regular*. An ordinary cube is regular by definition.

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We suppose that $\mathscr{C}$ is a critical component.

- If $L_p = L_z = \emptyset$, then $\mathscr{C}$ is a maximum,

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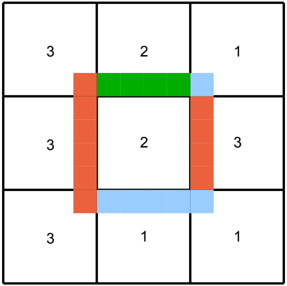
We suppose that $\mathscr{C}$ is a critical component.

- If $L_p = L_z = \emptyset$, then $\mathscr{C}$ is a maximum,
- if $L_p = L_z = \emptyset$, then $\mathscr{C}$ is a minimum,
- otherwise $\mathscr{C}$ is a saddle component.

Remark on criticality



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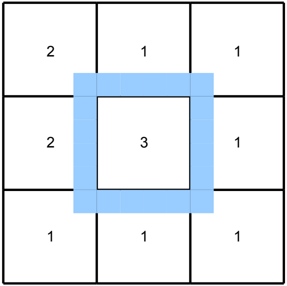

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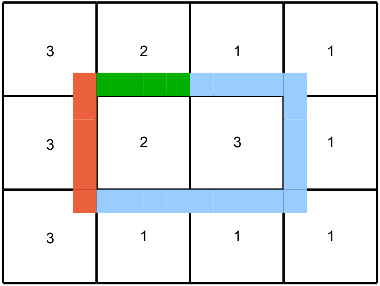

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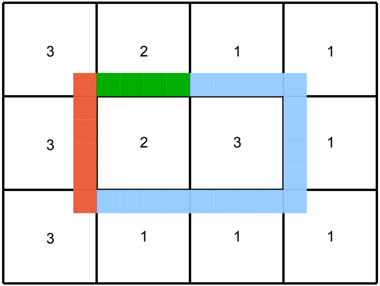


Non-critical singular components may be said to correspond to *removable singularities* in analysis.

Critical circle

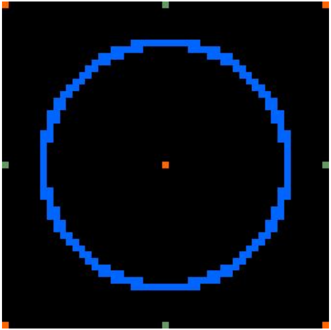
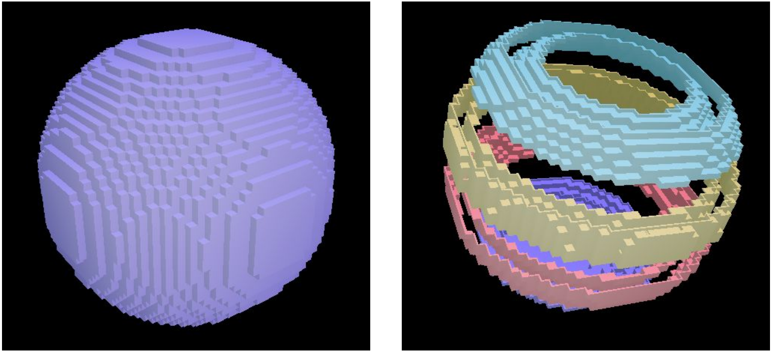


Figure: Critical components of $f(x,y) = (x^2 + y^2 - 5)^2$ over the domain $X = [-3,3] \times [-3,3]$ discretized in 51×51 2-cubes, with the function's range discretized over 2048 levels. A minimum circle, a maximum pixel in the centre, as well as four saddles and four maxima on the boundary are visible.

Critical sphere



(a) (b)

Figure: N and a few slices of L_p for the minimal sphere of $f(x,y,z) = (x^2+y^2+z^2-5)^2$ over the domain $[-3,3]^3$ discretized in 51^3 3-cubes, with the range of f discretized over 8192 levels. L_p includes two concentric spheres. The colors are used to facilitate viewing.

Torus

Consider the following function defined in polar coordinates on the unit disc:

$$\bar{f}(r,\theta) = r^2(1 - 2\sin^2(\theta)).$$

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Now consider the toroid in $\mathbb{R}^3$ obtained by revolution of the disc D_{r_1,r_2} given by

$$(x - r_2)^2 + z^2 \leq r_1^2, y = 0$$

around the z-axis ($0 \leq r_1 \leq r_2$), and on this toroid the following function defined in toric coordinates:

$$f(r,\theta,\phi) = r^2(1 - 2\sin^2(\theta - \phi/2)).$$

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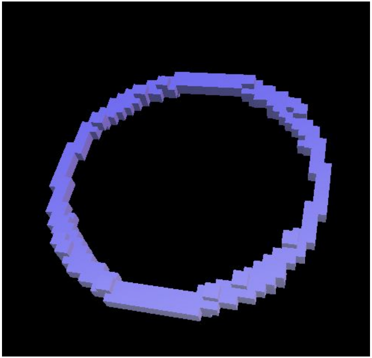
The function f is $\bar{f}$ defined on each revolved disc, but with a twist of half the revolution angle applied. Therefore, it has for a saddle component the circle obtained by revolution of D_{r_1,r_2}'s centre.

Torus (next)



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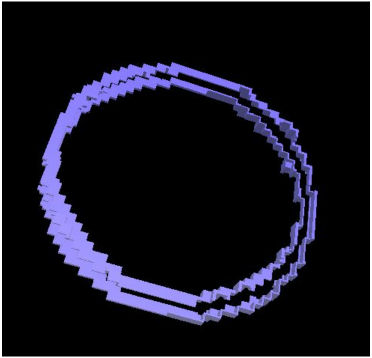

(b)

Figure: N and L_p for the critical (saddle) circle of the preceding function over $[-3,3]^2 \times [-4/5, 4/5]$ discretized in $51^2 \times 19$ 3-cubes, with range discretized over 16383 levels. L_p does a half-rotation around N for every revolution around the z-axis. Notice that L_p (and by symmetry, L_n) is connected, but the component is not regular.

Upcoming research

- Multiresolution
    - Persistance of topological artifacts across different resolutions
    - Resolution of domain and image

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  - Persistance of topological artifacts across different resolutions
  - Resolution of domain and image
- More rigorous use of the Conley index and isolating block theory
- Euler-Maxwell-Morse formula
  - Can be used (even enforced) as a condition of validity for a classification of critical points
  - Needs to be generalized to critical components