Detecting Critical Regions in Multidimensional Data Sets

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Abstract

We propose a new approach, based on the *Conley index theory*, for the detection and classification of critical regions in multidimensional data sets. The use of homology groups makes this method consistent and successful in all dimensions and allows to generalize visual classification techniques based solely on the notion of connectedness which may fail in higher dimensions.

1 Introduction

In the geometric study of scalar functions $f : X \to \mathbb{R}$ on a multidimensional data set X, the goal is to extract features that enhance our understanding of the measured data and allow us to represent the data in a structure that is easy to manipulate for subsequent processing. In the case of a two-dimensional data set X, f can be geometrically interpreted as a height field. The features of interest are critical points of f, that is, the points where the gradient ∇f is nul. They are interpreted as peaks, pits, or mountain passes, also called saddles. Once the critical points are extracted, different techniques are used to analyze relationships between them and to trace structures such as ridge and ravine lines, and isolines. In the case of data of higher dimensions, the geometric interpretation of critical points is more

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complex but those points play equally important role in further investigation, such as the construction of the level sets given by $f = c$. These level sets are interpreted as isolines in dimension 2, isosurfaces in dimension 3 and so on.

The mathematical tool commonly used to detect and classify critical points is the Morse theory [14], [6, Chapter 7]. This theory relies on very strong smoothness and non-degeneracy assumptions, described in Section 2, which appear not realistic in discrete models. Among the non-degeneracy assumptions is one, that critical points are isolated and have distinct critical values. This assumption fails when considering, for example, a height field of a terrain with water surfaces as minimum plateaus, sandbars near a seashore may become saddle isolines at a low tide, and ridges of volcano craters as maximum closed isolines.

In [2], we have introduced the notion of critical regions in the case of a height field for a 2-dimensional square lattice. In that case, the detection and classification of a critical region $\mathcal{C}$ can be done by studying the number of connected components of its *upper* and *lower wraps*, $\overline{wrap}\,(\mathcal{C})$ and $\underline{wrap}\,(\mathcal{C})$. These are, roughly speaking, the subsets of their immediate neighborhoods where the values of the function are respectively greater and smaller than $f(\mathcal{C})$. Our approach is to some extent influenced by a classification of critical regions for continuous but not necessarily smooth functions in $\mathbb{R}^3$ given by Weber *et al.* [20].

In many applications of the classical Morse theory to imaging science, one spends a lot of effort on forcing data so to obey the assumptions of the theory. This practice is validated by the argument, that a small perturbation of a given function can bring it to the *generic case* where all critical points are non-degenerated, isolated, and correspond to distinct critical values. Among most systematic studies of that kind one could point the work of Edelsbrunner *et al.* [9, 10]. This approach may be natural in some problems but there are many other situations where it is not applicable. One, addressed by Arnold [4, 1984], arises in the study of parameterized family of equilibrium states. A small perturbation can remove a degeneracy at one parameter value but it would create a new one at another value.

Another arises in the singularity theory [15], [4, 1993]. Critical regions of polynomial functions of several variables are extensively studied there, under the name of singular curves and surfaces. The *Whitney-Cayley umbrella* [4, 1993] given by

$$x^2 - y^2 z = 0$$

is a simple classical example of an algebraic level surface in R^3 self-intersecting at a singular curve (the z-axis). Any level set $g(x) = c$, where $x \in \mathbb{R}^d$, can be turned into a critical region of

$$f(x) = (g(x) - c)^2 h(x).$$

Thus one can easily construct critical regions with a non-trivial topology such as a circle or a wedge of several circles. Such sets arise for example in the study of *Milnor fibers* [11] of complex functions.

In computational geometry, there are well-developed methods for construction of non-singular level surfaces $f = c$. However, the mesh generation algorithms break near the singular zone $\nabla f = 0$. A particular attention is required for critical regions of saddle-type, because these are the curves where the level surface self-intersects. In singular zones, one has to investigate the local topology nearly on a pixel level, in order to determine how to locally complete the construction of the studied surface so to preserve its global properties.

Since we now work on multidimensional data, we have to be cautious about carrying over intuitions from planar geometry to higher dimensions: There is a tendency in geometric visualisation research to overlook, for example, the fact that the number of connected components may no longer be sufficient to describe changes in topology of studied sets when parameters change. One has to take into account such topological invariants as homotopy type, homotopy groups, or homology groups. We focus on homology descriptors, because there is a vast library of convenient programs computing homology such as [7], while the homotopy type is not constructive, and the computability of homotopy groups is problematic. In Section 2, we recall the basic terminology concerning the Morse and Conley indices and we give examples motivating the use of homology descriptors.

In Section 3, we propose a method for detecting and classifying critical regions of discrete functions inspired by the Conley index theory. This theory is a generalization of the Morse theory in the following sense: The Morse index discussed in Section 2, classifies the geometric nature of isolated critical points of a smooth non degenerated function f. The gradient field ∇f of that function generates a flow whose equilibrium points are the critical points of f. The Conley index applies not only to gradient flows but to arbitrary continuous flows as well as to discrete dynamical systems, and it classifies not only equilibrium points but also isolated invariant sets. In particular, a critical region can be presented as an isolated invariant set and its Conley index is a natural substitute of the Morse index. We give algorithmic definitions of regular and critical regions inspired by the Conley index theory for functions defined on a unit-size cubical grid in $\mathbb{R}^d$. This choice is well justified in practice, because many applications in 3D imaging science produce regularly gridded data by sampling scalar fields at uniform intervals of time and space. This data is given in the form of scalar functions defined on the vertices of a hypercubic decomposition of space. Regularly gridded data does not require an explicit storage of cell adjacency information, which would be necessary, if we wanted to subdivide each cube into tetrahedral grids. Thus it results in lower complexity and lower storage requirements. Note that irregularly gridded data is typically organized into tetrahedral cells using techniques such as the ones based on Voronoi diagrams and Delaunay triangulations [6]. Our method is valid in all dimensions. It requires verifying whether or not relative homology groups of certain sets are trivial. In our case, the verification is implemented at a low cost, since it reduces to so-called *elementary collapses*, see [12, Sec. 2.4].

In Section 4, we derive conclusions related to the concept of the *Morse connection graph (MCG)* introduced in [3]. This is a graph whose nodes are critical components and edges display the existence of trajectories connecting them. An new algorithm building MCG for planar images and its implementation are presented in [2]. The method is based on the construction of two multivalued maps $\mathcal{F}_+$ and $\mathcal{F}_-$, defined on a set of pixels whose values are subsets of neighboring pixels. The iterations of $\mathcal{F}_+$ and $\mathcal{F}_-$ imitate instantaneous movements of a point along a trajectory of a flow. There are some works somewhat similar in spirit to our approach e.g. Edelsbrunner [8] or Boczko *at al.* [5] on polygonal flows. The second work is motivated by applications to dynamical systems rather than imaging. Both are based on building adapted triangulations, while we are using a previously mentioned fixed cubical grid. In this paper, we reinforce the MCG Algorithm of [2], by presenting its improved and simplified formulation, extended to arbitrary dimensions.

In Section 5, we discuss some open questions and prospects for future applications to construction of isosurfaces.

2 Motivating examples from the Morse and Conley theories

Let M be a smooth manifold and $f : M \to \mathbb{R}$ a function of class C^2. At this point we do not assume that M is compact, so we may consider $M = \mathbb{R}^d$. A point $p \in M$ is *critical* if the gradient ∇f vanishes at p and it is called *regular* otherwise. The function f is called a *Morse function* if all of its critical points p are *non degenerate*. This condition implies in particular that p is an isolated critical point.

Given a Morse function f, the index of any critical point p, denoted by $\lambda(p)$, is the number of negative eigenvalues of the Hessian $H_f(p)$. If $\lambda(p) = 0$, p is a local minimum and if $\lambda(p) = d$, it is a local maximum. The values $0 < \lambda(p) < d$, characterize saddles which may topologically differ from each other when $d > 3$.

Consider a function whose critical points are still isolated but possibly degenerate. Then there may occur a critical point p of "inflection type". which is inessential in the sense that a perturbation of f in a small isolating neighborhood N of p may cause the removal of singularity from N. One of possible topological definitions may be formulated in terms of the *sublevel* and *superlevel sets*

$$N_n = \{x \in N \mid f(x) < f(p)\},$$
$$N_p = \{x \in N \mid f(x) > f(p)\},$$

The intersection of their closures is the level set

$$N_z = \{x \in N \setminus \{p\} \mid f(x) = f(p)\}.$$

Whether p is a regular point or an inessential critical point, if N is a disc, the sets N_n and N_p should be its topological half-discs. At a maximum or minimum point, one set is $N \setminus \{p\}$ and another one is empty. At a critical saddle such as $p = 0$ of the function $f(x, y) = x^2 - y^2$, each of the sets N_n and N_p consist of two disjoint wedges limited by the crossing lines $x^2 = y^2$. We may be tempted to use the numbers n_n, n_p and n_z of connected components of N_n, N_p, and N_0 respectively, to distinguish various types of topological critical points. This approach seems to work well in dimensions 2 and 3 but it fails to characterize critical points in dimensions higher than 3 even in the classical Morse setting, as the following example illustrates.

Example 2.1 Let $f : \mathbb{R}^4 \to \mathbb{R}$ be given by

$$f(x, y, z, t) = x^2 + y^2 - z^2 - t^2. \tag{1}$$

Then $p = 0$ is an isolated non-degenerate critical point with the value 0. It is a saddle point and its Morse index is $\lambda(p) = 2$. Consider its neighborhood $N = \overline{B}(0, r)$ the closed ball of radius r centered at 0. Since f is radially homogeneous, the choice of r is not important so we may assume $r = 1$, For the same reason, the radial projection of $N \setminus \{0\}$ onto the unit sphere S^3 given by

$$x^2 + y^2 + z^2 + t^2 = 1$$

is a homotopy deformation. Consider the discussed sets N_n, N_p and N_z deformed to S^3:

$$L_n = N_n \cap S^3 = \{(x, y, z, t) \in S^3 \mid x^2 + y^2 < z^2 + t^2\},$$

$$L_p = N_p \cap S^3 = \{(x, y, z, t) \in S^3 \mid x^2 + y^2 > z^2 + t^2\},$$

and

$$L_z = N_z \cap S^3 = \{(x, y, z, t) \in S^3 \mid x^2 + y^2 = z^2 + t^2\}.$$

Since L_z can be expressed by $x^2+y^2 = 1/2 = z^2+t^2$, it is a torus (product of two circles). Its complements L_n and L_p in S^3 are "donuts" that is, products of a circle by a 2-disc. All three sets are connected. The same is true for a regular point, hence the number of connected components does not permit to distinguish a saddle from a regular point in $\mathbb{R}^4$.

In the study of critical regions or, more explicitly, connected regions consisting of non-isolated critical points, the three-dimensional space is sufficient to construct examples showing that the connected components of sublevel and superlevel sets do not provide sufficient information.

Example 2.2 Let M be a "donut-shape" solid in $\mathbb{R}^3$ obtained by revolution of the disc D_{r_1,r_2} given by

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

about the z-axis, where $0 < r_1 < r_2$. Its boundary ∂M is a torus. We use toric coordinates (r, θ, ϕ) in M, that is, (r, θ) are polar coordinates for D_{r_1,r_2} and ϕ is the angle of revolution. First, we want to define $f(r, \theta, \phi)$ at $\phi = 0$ by

$$f(r, \theta, 0) = (x - r_2)^2 - z^2 = r^2(1 - 2\sin^2\theta).$$

The center of D_{r_1,r_2} is a simple saddle of this function on D. We extend this definition to M by the formula

$$f(r, \theta, \phi) = r^2 \left(1 - 2\sin^2(\theta - \phi/2)\right). \tag{2}$$

The revolution of the center of D produces a circle S of radius r_2 given by $r = 0$. Both f and ∇f vanish on S, so this circle is a singular curve of f forming the self-intersection of the isosurface $f = 0$. Moreover, all points on it are simple saddles of the function f restricted to the plane perpendicular to the circle.

Let now N be a neighborhood of S in M defined in toric coordinates by $r \leq \delta$, for any chosen $0 < \delta < r_1$. Consider the torus $T := \partial N$. At $\phi = 0$, the boundary of the disc D_{δ,r_2} is composed of four arcs limited by isolines at $\theta = \pm\pi/4, \pm 3\pi/4$, with $f > 0$ on the left and right arcs A_L, A_R, and $f < 0$, on the upper and lower arcs A_+, A_-. The arc A_L is revolved to A_R forming a band on T and, similarly, A_+ is revolved to A_-. Thus each of the sets $L_p := N_p \cap T$ and $L_n := N_n \cap T$ is a band wrapped twice around the torus T. The set $L_z := N_z \cap T$ consists of two circles separating the band L_p from L_n. By the same argument on radial projection as in the previous example, each of the sets L_p, L_n and L_z is a deformation retract of N_p, N_n, and N_z respectively, so it has the same homotopy type. Thus N_p and N_n are connected. If we wanted to use this information only, S would be classified as a regular region. In the next section, we discretise this example and show that our homology criterion classifies it as a saddle-type region.

Below we give a brief overview of the Conley index [17, 16] in the context of a flow generated by the gradient field of a C^2 function f.

A subset $S \subset X$ is called an *invariant set* of φ, if $\varphi(t, x) \in S$ for all $x \in S$ and all $t \in \mathbb{R}$. It is called *isolated* if there exists a neighborhood N such that S is the maximal invariant set in N. The main purpose of the Conley index theory of flows is to describe isolated invariant sets.

Let N be the closure of a bounded region in X and ∂N its boundary. A set $L \in N$ is called the *exit set* of N if given $x \in N$ and $t_0 > 0$ such that $\varphi(t_0, x) \notin N$, then there exists $0 \leq t_1 \leq t_0$ such that $\varphi(t_1, x) \in L$. Obviously, we must have $L \subset \partial N$. Here is a homological version of the classical Ważewski principle [19] which inspired the definition of the Conley index.

Theorem 2.3 *[12, Prop. 10.40] Suppose that L is a closed subset of ∂N. If $H_*(N, L)$ is non trivial then N contains a non-empty invariant set in its interior.*

The original Ważewski principle formulated in terms of deformation retraction gave rise to the Conley theory. Given a maximal invariant set S isolated by N, the *homotopical Conley index* $C(S)$ is the relative homotopy type $[N, L]$ of the pair (N, L). Since the homotopy type is not constructive, in modern application-oriented formulations of the Conley index theory [16], $C(S)$ tends to be replaced by computable descriptors such as the *homological Conley index* given by $CH_*(S) = H_*(N, L)$. Additional assumptions on N and L are imposed in order to make the index definition dependent only on S, and not on the choice of N, and in order to achieve desired topological properties, such as stability of the index with respect to small perturbations of the flow. We avoid introducing those assumptions here because, in our work, we will not use the Conley index literarily but only as an inspiration for the digital setting. The following well known example shows how the homological Conley index generalizes the Morse index.

Example 2.4 Let p be a non-degenerate critical point of the Morse index $\lambda(p) = m$ of a function f defined on a d–dimensional manifold. Consider the flow of the differential equation $\dot{x} = -\nabla f(x)$. Let N be an admissible isolating neighborhood for the Conley index of $\{p\}$ and L its exit set. Then

$$CH_k(\{p\}) = H_k(N, L) \cong H_k(S^m, \{s_0\}) \cong \begin{cases} \mathbb{Z} & \text{if } k = m, \\ 0 & \text{otherwise,} \end{cases}$$

where S^m is the m-dimensional sphere and s_0 is a chosen base point in S^m.

3 Critical regions of discrete functions

Our goal in this section is to introduce a discrete analogy of critical points and critical regions of functions $f : \mathbb{R}^d \to \mathbb{R}$.

The geometric structure we are going to work with is the cubical grid $\mathcal{K}$ defined in [12, Sec. 2.1]. Recall that $\mathcal{K}$ is the collection of *elementary cubes* of the form

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

where $I_j = [k, k+1]$ or $I_j = \{k\}$, $k \in \mathbb{Z}$ (the set of integers), including the empty set. We denote by $\mathcal{K}^d$ the subset of $\mathcal{K}$ consisting of d–dimensional cubes, also called *full* cubes. These are the cubes which have no degenerate intervals $I_j = \{k\}$ in their expression, equivalently, which are not proper faces of other cubes in $\mathcal{K}$. Note that $\mathcal{K}$ is a particular case of a regular cellular complex. A set $X \subset \mathbb{R}^d$ is called a *cubical set*, if it is a finite union of elements of $\mathcal{K}$, and it is called *full* if it is a finite union of elements of $\mathcal{K}^d$. We should distinguish between a finite set $\mathcal{X} \subset \mathcal{K}$ and the *support* or *polytope* of $\mathcal{X}$ which is the cubical set $X \subset \mathbb{R}^d$ given by

$$X = |\mathcal{X}| = \bigcup \mathcal{X}.$$

Given a cubical set X, $\mathcal{K}(X)$ is the restriction of the grid $\mathcal{K}$ to the cubes contained in X.

Would chosen units appear too coarse, one may apply 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 called a *scaling factor*. The corresponding refined grid is the image of $\mathcal{K}$ under the *inverse rescaling* $\Lambda^{1/k} = (\Lambda^k)^{-1}$:

$$\Lambda^{1/k}\mathcal{K} = \{\Lambda^{1/k}Q \mid Q \in \mathcal{K}\}.$$

Here is the natural extension of the concept of neighborhood to the combinatorial setting.

Definition 3.1 Let A be a bounded set in $\mathbb{R}^d$. The combinatorial unit–scale *wrap* of A is a subset of $\mathcal{K}$ defined by

$$wrap(A) = \{P \in \mathcal{K}^d \mid P \cap A \neq \emptyset\}.$$

It is a finite set, so its support denoted by $\mathtt{wrap}(A) = |wrap(A)|$ is a cubical set. The *factor k scaled wrap* of A is a subset of $\Lambda^{1/k}\mathcal{K}$ defined by

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

Its support with respect to the refined grid is denoted by $\mathtt{wrap}^{1/k}(A)$.

The study of scaled wraps is motivated by the following theorem.

Theorem 3.2 (Allili [1]) *Given a cubical set A and a scaling factor $k \geq 3$, the inclusion $A \hookrightarrow \mathtt{wrap}^{1/k}(A)$ induces an isomorphism in homology.*

Definition 3.3 The *factor k scaled exterior boundary* of a cubical set A is the topological boundary $\partial\, \mathtt{wrap}^{1/k}(A)$ of A.

In practice, the values of functions $f : \mathbb{R}^d \to \mathbb{R}$ are only known at finitely many grid points. Our approach, inspired by the combinatorial multivalued maps used in [13, 12, 18] is to define combinatorial maps on full elementary cubes rather that on their vertices. Thus we consider discrete functions[1]

$$f : \mathcal{X}^d \to \mathbb{R}, \text{ where } \mathcal{X}^d \subset \mathcal{K}^d.$$

This approach is very natural if we view the smallest objects in an image, n-pixels, as d-cells of a cubical grid $\mathcal{K}$. The passage from our definition to a vertex definition is by simple translation of coordinates $x_i \mapsto x_i + 1/2$, $i = 1, 2, \ldots d$. Conversely, if a function f is given on a cubical set $X = |\mathcal{X}^d| \subset \mathbb{R}^d$, we may define the discretization of f on $\mathcal{X}^d$ by taking its values at the center of each elementary full cube.

[1]As a matter of fact writing $f : \mathcal{X}^d \to \mathbb{R}$ is a slight abuse of notation. In fact, we consider $f : \mathcal{X}^d \to 10^{-k}\mathbb{Z}$ for a fixed $k \in \mathbb{Z}$, $\mathbb{Z}$ integers.

Definition 3.4 Let $\mathcal{X}^d \subset \mathcal{K}^d$. Consider a function $f : \mathcal{X}^d \to \mathbb{R}$ and an elementary cube $Q \in \mathcal{X}^d$ such that $wrap(Q) \subset \mathcal{X}^d$. The *upper wrap* of Q is defined by

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

Analogously, the *lower wrap* of Q is given by

$$\underline{wrap}\,(Q) := \{P \in\ wrap(Q) \mid f(P) < f(Q)\}\,,$$

and the *level wrap* of Q is given by

$$wrap_z(Q) := \{P \in\ wrap(Q) \mid f(P) = f(Q)\}\,.$$

The extension of the upper and lower wraps to cubical sets $A = |\mathcal{A}|$ is more delicate. We assume that $wrap(A) \subset \mathcal{X}$. Since the values of f may vary, we want the inequalities in the earlier formulas to be satisfied locally:

$$\overline{wrap}\,(A) := \{P \in wrap^*(A) \mid f(P) > f(Q) \text{ for all } Q \in \mathcal{A} \cap wrap^*(P)\}\,,$$

$$\underline{wrap}\,(A) := \{P \in wrap^*(A) \mid f(P) < f(Q) \text{ for all } Q \in A \cap wrap^*(P)\}\,.$$

$$wrap_z(A) := wrap^*(A) \setminus \big(\underline{wrap}\,(A) \cup \overline{wrap}\,(A)\big)$$

where $wrap^*(A) = wrap(A) \setminus \mathcal{A}$. As for wraps, the notation $\overline{\texttt{wrap}}$ and $\underline{\texttt{wrap}}$ is used for the supports of upper and lower wraps $\overline{wrap}$ and $\underline{wrap}$.

Analogous terminology and notation is carried over to the scaled wraps introduced in definition 3.1.

The upper and lower wraps are analogies of the exit set and entrance set from the Conley index theory. In [2], the algorithms detecting, first, critical pixels in $\mathbb{R}^2$ and, secondly, their critical components $\mathcal{C} \subset \mathcal{K}^2$, where based on the number of *edge-connected* components of combinatorial upper and lower wraps $\overline{wrap}\,(\mathcal{C})$ and $\underline{wrap}\,(\mathcal{C})$. We did not need to consider scaled wraps introduced above, so we need to explain why do we use them now. As we showed in the previous section, the connectivity concept is not sufficient in dimensions higher than 2. In order to compute homology groups, we need to pass to geometric carriers. Therefore, following the approach chosen in [2], the set

$$N := |wrap(\mathcal{C})| = \overline{\texttt{wrap}}\,(\mathcal{C})$$

would be a natural candidate for the isolating neighborhood of $\mathcal{C} \subset \mathcal{K}^2$, and $\overline{\texttt{wrap}}\,(\mathcal{C})$ and $\underline{\texttt{wrap}}\,(\mathcal{C})$ respectively, for its entrance and exit sets. However, there is a problem related to the fact that while the combinatorial sets

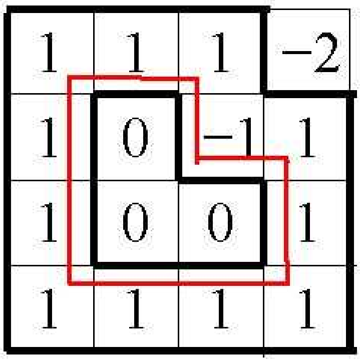

Figure 1: The region $\mathcal{C}$ of pixels with the value 0 is classified accordingly to the algorithm in [2] as regular, because both $\overline{wrap}\ (\mathcal{C})$ and $\underline{wrap}\ (\mathcal{C})$ are non-empty and edge-connected. However $\overline{\texttt{wrap}}\ (\mathcal{C})$ contains $\partial wrap(\mathcal{C})$, as in the case of a minimum.

$\overline{wrap}\ (\mathcal{C})$ and $\underline{wrap}\ (\mathcal{C})$ are disjoint, their carriers may intersect, resulting in misleading topological information. This is illustrated in Figure 3. One possible remedy to the described problem is to consider open wraps instead of the closed ones. However, computing homology of open polyhedra is a substantially more complex task than that of compact polyhedra. We shall achieve the same effect, while staying in the class of compact cubical sets, by considering a scaled wrap bounded by the contour around $\mathcal{C}$ marked in Figure 3.

Definition 3.5 Let $\mathcal{X}^d \subset \mathcal{K}^d$ and $k \geq 3$. Consider a function $f : \mathcal{X} \to \mathbb{R}$ and an elementary cube $Q \in \mathcal{X}^d$ such that $wrap(Q) \subset \mathcal{X}^d$. Define

$$N := \texttt{wrap}^{1/k}(Q),\ \ L_n := \underline{\texttt{wrap}}\ (Q) \cap \partial N\ L_p := \overline{\texttt{wrap}}\ (Q) \cap \partial N,$$

and

$$L_z := \texttt{wrap}_z(Q) \cap \partial N.$$

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

Here is the related algorithm.

Algorithm 3.6 Detecting singular cubes

For each elementary full cube Q
build $N,\ \partial N,\ L_p,\ L_n,\ L_0$
$H := H_*(N, L_p) = 0$ *and* $H_*(N, L_n) = 0$
if $H =$ *TRUE* **then** Q *is ordinary*
else Q *is singular*
endif

As it was pointed out in [2] in the planar case, the adjacent singular cells may, in a sense, cancel each other. In other words, the type of criticality of a singular cube cannot be decided without looking at neighboring cubes. This is taken care of by the following definitions.

Definition 3.7 Let $\mathcal{X}^d \subset \mathcal{K}^d$, $k \geq 3$ and consider a function $f : \mathcal{X}^d \to \mathbb{R}$. A set $\mathcal{C}$ of singular elementary cubes in $\mathcal{K}^d$ is called an *isolated singular component* if

(a) $\texttt{wrap}(C) \subset X$;

(b) $C = |\mathcal{C}|$ is connected;

(c) $\mathcal{C}$ is *isolated* in the sense that any $P \in wrap^*(C)$ is ordinary.

The *isolating neighborhood* of $C = |\mathcal{C}|$ is defined by

$$N = \texttt{wrap}^{1/k}(C).$$

The *lower*, *upper*, and *level sets* of $\mathcal{C}$ are respectively defined by

$$L_n = \underline{\texttt{wrap}}\ (C) \cap \partial N, Ł_p = \overline{\texttt{wrap}}\ (C) \cap \partial N,\ L_z = \texttt{wrap}_z(C) \cap \partial N$$

Definition 3.8 An isolated singular component $\mathcal{C}$ is called *regular* if $H_*(N, L_p) = 0$ and $H_*(N, L_n) = 0$. Otherwise it is called a *critical component.* A singular cube Q is called *critical*, if it belongs to a critical component, otherwise, it is called *regular.* An ordinary cube Q is, by definition, *regular.*

In a sense, singular-regular cubes are an analogy of an inessential or removable singularities in mathematical analysis. Given any singular cell $Q \subset \mathcal{K}^d$, the component $\mathcal{C}(Q) = \mathcal{C}$ is constructed by the following algorithm:

Algorithm 3.9 Sorting components in $\mathbb{R}^d$
For each singular cube $Q,\ \mathcal{C} := \{Q\}$
while $P \in wrap^*(\mathcal{C}) \cap X$ *is singular*
$\mathcal{C} := \mathcal{C} \cup \{P\}$

build $wrap^*(\mathcal{C})$

endwhile

build $N,\ \partial N,\ L_p,\ L_n$

do

$H := H_*(N, L_p) = 0$ *and* $H_*(N, L_n) = 0$

if $H =$ *TRUE* **then** $\mathcal{C}$ *is a regular component*

else if $L_n = \partial N$ **then** $\mathcal{C}$ *is a maximum component*

else if $L_p = \partial N$ **then** $\mathcal{C}$ *is a minimum component*

else $\mathcal{C}$ *is a saddle component*

endif

break

A practical implementation of the Algorithms 3.9 and 3.6 is a work in progress. In order to illustrate the ideas behind these algorithms, we shall construct discrete analogies of the Examples 2.1 and 2.2, in the setting of cubical grids.

Example 3.10 We come back to Example 2.1 with the unit euclidean sphere in $\mathbb{R}^4$ replaced by the unit sphere with respect to the maximum norm $||x|| = \max_{i=1\ldots 4} |x_i|$. For the convenience of presentation, we consider a cubical grid shifted so that the origin of coordinates is the center of a full elementary cube σ, and rescaled so that $N = wrap(\sigma) = [-1,1]^4$. By discretizing f so that the values of f in the centers of the 3–dimensional faces in ∂N determineed L_p, L_n and L_z, we obtained:

$$\begin{aligned} L_p &= \big(\{-1,1\} \times [-1,1] \times [-1,1]^2\big) \cup \big([-1,1] \times \{-1,1\} \times [-1,1]^2\big) \\ &= \partial[-1,1]^2 \times [-1,1]^2, \\ L_n &= \big([-1,1]^2 \times \{-1,1\} \times [-1,1]\big) \cup \big([-1,1]^2 \times [-1,1] \times \{-1,1\}\big) \\ &= [-1,1]^2 \times \partial[-1,1]^2, \\ L_z &= \emptyset. \end{aligned}$$

We used the software CHomP [7] and obtained the result:

$$H_*(N, L_p) \simeq H_*(N, L_n) \simeq \begin{cases} \mathbb{Z} & \text{if } k = 2 \\ 0 & \text{otherwise} \end{cases}$$

the Algorithms 3.6 and 3.9, the cell σ is classified as a saddle.

Example 3.11 We present a cubical analogy of Example 2.2 and use the homology program of [7] to classify the criticality of the studied region. We choose the radius $r_2 = 2$. The circle S discussed in Example 2.2 is inscribed in the cubical donut-shape region

$$C = \left([-3,3]^2 \setminus [-1,1]^2\right) \times [-1,1].$$

The values of the function f given by (2) at the centers of the cubes of $\mathcal{C} = \mathcal{K}^3(C)$ are either equal or close to 0. By means of a suitable tresholding, we obtained its discretization $\bar{f}$ with the value 0 on all cubes of $\mathcal{C}$. Next, the space has been rescaled by the factor of 10 in order to exclude the z-axis and to obtain a discrete approximation $\bar{f}$ that reflects the behavior of f in the neighborhood $N = wrap^{1/10}(C)$ of C. To avoid working with fractional grids, we redefined C as

$$C := \left([-30,30]^2 \setminus [-10,10]^2\right) \times [-10,10]$$

and N as $N := wrap(C)$. The direct implementation of the Algorithm 3.9 has confirmed that C is an isolated singular component and it generated the sets L_p and L_n. Using the software CHomP [7], we obtained the result:

$$H_*(N, L_p) \simeq H_*(N, L_n) \simeq \begin{cases} \mathbb{Z} & \text{if } k = 2 \\ \mathbb{Z} & \text{if } k = 1 \\ 0 & \text{if } k = 0 \end{cases}$$

which shows that $\mathcal{C}$ is a saddle component. The computed homology is, in fact, the homology of the wedge of the circle and the 2D sphere relatively the wedge point. The snapshots of C and of the solid-cube sets $\overline{\texttt{wrap}}\,(C)$ and $\underline{\texttt{wrap}}\,(C)$ giving rise to L_p and L_n are shown in Figure 3.11.

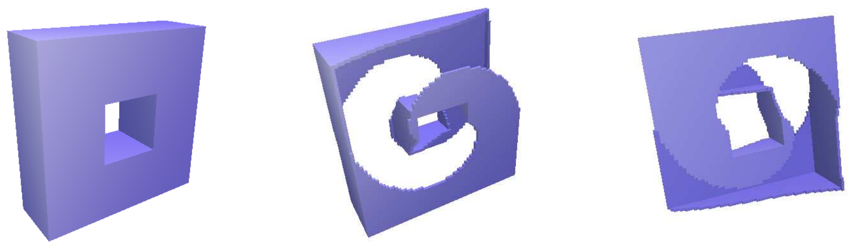

Figure 2: The sets C, $\overline{\texttt{wrap}}\,(C)$ and $\underline{\texttt{wrap}}\,(C)$ in Example 3.11.

We finish this section with several remarks.

(1) In the definition of the homological Conley index for flows, the condition $H_*(N, L_p) \neq 0$ would be sufficient for criticality, one would not need to take N_n into account. This is due to the fact, that the flow of $-\nabla f$ has the same trajectories as that of ∇f oriented in the opposite direction. In the digital case we study here, there is no such symmetry, so we need to take both L_p and L_n into consideration. Such differences between the smooth and digital case are discussed in grater detail in [2].

(2) It is possible to modify the definition of the sets L_p and L_n so to build them of full cubes rather than $(d-1)$–dimensional faces in ∂N. Namely, one can define N as the two-layer wrap of $\mathcal{C}$:

$$N := \mathtt{wrap}^{1/k}(\mathtt{wrap}^{1/k}(C)),$$

while L_p and L_n can be defined as the intersections of $\overline{\mathtt{wrap}}\,(C)$ and, respectively, $\underline{\mathtt{wrap}}\,(C)$ with the second layer of this scaled wrap. If $\mathcal{C}$ consists of a single cube, the scaling by $k = 3$ is sufficient but in general, one should use scaling by $k = 5$ for topology preservation. This approach may be convenient for the uniformity of data structure since it does not require generating faces of pixels within the program that builds the pairs (N, Lp) and (N, L_n). Note that generating faces takes place implicitly in the homology computation.

(3) The condition $H^*(N, L_p) = 0$ (and the same for L_n) in our definitions and algorithms can be replaced by a stronger condition that the homotopy type $[N, L_p]$ of the pair of spaces (N, L_p) is non-trivial. However, as already commented in the introduction, such a condition could not be verified in practice. A yet stronger but combinatorial condition would be "N collapses to L_p", which means that N can be deformed to N_p by a chain of *elementary collapses* described in [12, Sec. 2.4]. Elementary collapses preserve not only homology but also homotopy type and the algorithm *Collapse* actually is the fastest method of verifying that $H_*(X, L_p) = 0$.

(4) Note that there are many topologically distinct types of saddle components. In the case of a single elementary cube, one can characterize it as a minimum, maximum, or a k–fold saddle, $k \in \mathbb{N}$, by means of $H_*(N, L_p)$ and $H_*(N, L_p)$. For larger components $\mathcal{C}$, the topology of C may be nontrivial and one has to take into account $H{*}(C)$. An attempt of classifying all

cases that may occur would be equivalent to solving most of the challenges of the singularity theory.

4 Dynamics of a multidimensional scalar field and associated Morse Connections Graph

In [2], we gave a detailed description of the dynamics of a given height field and we associated a structure called the Morse connections Graph whose nodes are critical components of the height field and the edges show different connecting trajectories between the nodes. This graph encodes a summary of topological features of the data and makes it easy to manipulate in many imaging applications such as shape representation and retrieval. We present here a very simple reformulation of these concepts in the context of a multidimensional scalar field.

Let now $\mathcal{K}$ be the cubical grid in $\mathbb{R}^d$ and $\mathcal{X}^d \subset \mathcal{K}^d$. Consider a function $f : \mathcal{X}^d \to \mathbb{R}$. We want to introduce a multivalued map on $\mathcal{X}^d$ such that the dynamics of its iterates in the sense of [13] would exhibit the dynamical properties analogous to those of the gradient flow of a Morse function of f. First, we define the distance $\mathrm{dist}\,(Q, P)$ between two elementary cubes as the euclidean distance between their centers. Note that, if $Q, P \in \mathcal{X}^d$ intersect at a common face of dimension k, then

$$\mathrm{dist}\,(Q, P) = \sqrt{d-k}.$$

The *directional derivative* of f at Q in the direction of an adjacent cell P is defined by

$$\partial_P f(Q) = \frac{f(P) - f(Q)}{\mathrm{dist}\,(Q, P)}.$$

By convention, $\partial_Q f(Q) = 0$. Given a critical cell Q, we put

$$m(Q) = \min_{P \in \underline{wrap}\,(Q)} \partial_P f(Q) \quad \text{and} \quad M(Q) = \max_{P \in \overline{wrap}\,(Q)} \partial_P f(Q).$$

Definition 4.1 Given $f : \mathcal{X}^d \to \mathbb{R}$, the *ascending system* is the semi-dynamical system of iterates of the map $\mathcal{F} : \mathcal{X}^d \to \mathcal{P}\mathbb{R}$, which is defined on cells $Q \in \mathcal{X}^d$ as follows. If Q is critical, we put $\mathcal{F}_+(Q) = Q$. If Q is regular, we put

$$\mathcal{F}_+(Q) = \{P \in \overline{wrap}\,(Q) \mid \partial_P f(Q) = M(Q)\}.$$

The *descending system* is generated by the map $\mathcal{F}_- : \mathcal{X}^d \to \mathcal{P}\mathbb{R}$ defined as before with $\overline{wrap}\,(Q)$ replaced by $\underline{wrap}\,(Q)$ and M(Q) replaced by m(Q).

Note that the inverses of $\mathcal{F}_+$ and $\mathcal{F}_-$ may have empty values (and these two maps are not mutual inverses), hence the prefix "semi" in the name for the system.

Definition 4.2 Let $\mathcal{F} : \mathcal{X} \to \mathcal{P}\mathcal{X}$ be anyone of the two maps introduced in Definition 4.1. Consider a critical component $\mathcal{C} \subset \mathcal{X}$ and let $C = |\mathcal{C}|$. The *stable* and *unstable manifolds* of $\mathcal{C}$ relatively to $\mathcal{F}$ are defined by

$$\begin{array}{rclcl} W^u(\mathcal{C}, \mathcal{F}) & = & \mathcal{F}(wrap(C), \mathbb{Z}_+) & = & \bigcup_{Q \in wrap(C), n \geq 1} \mathcal{F}^n(Q); \\ W^s(\mathcal{C}, \mathcal{F}) & = & \mathcal{F}(wrap(C), \mathbb{Z}_-) & = & \bigcup_{Q \in wrap(C), n \geq 1} \mathcal{F}^{-n}(Q). \end{array}$$

If $\mathcal{F}$ is clear from the context, we will just write $W^s(\mathcal{C})$, $W^u(\mathcal{C})$.

The following theorems proved in [2] remain valid in arbitrary dimension:

Theorem 4.3 *Let $\mathcal{X}^d$ be finite and let $\mathcal{F}$ be anyone of the two maps introduced in Definition 4.1. If $\mathcal{C}$ and $\mathcal{D}$ are critical components such that $W^u(\mathcal{C}) \cap W^s(\mathcal{D}) \neq \emptyset$, then there exists a trajectory connecting $\mathcal{C}$ to $\mathcal{D}$ in the sense that it is issued at a cell in $wrap(C)$ and ends at a cell in $wrap(D)$.*

Theorem 4.4 *Let $\mathcal{X}^d$ be finite and let $\mathcal{F}$ be anyone of the two maps introduced in Definition 4.1. Let $\{\mathcal{C}_i\}_{i=1,2,\ldots k}$ be the set of all critical components in $\mathcal{X}^d$. Then*

$$\bigcup_{i=1}^{k} W^s(\mathcal{C}_i) = \mathcal{X}^d = \bigcup_{i=1}^{k} W^u(\mathcal{C}_i).$$

Let $\mathcal{C}$ and $\mathcal{D}$ be two critical components of $f : \mathcal{X} \to \mathbb{R}$. We say there is an *upward connection* from $\mathcal{C}$ to $\mathcal{D}$, denoted $\mathcal{C} \nearrow \mathcal{D}$, if

$$W^u(\mathcal{C}, \mathcal{F}_+) \cap W^s(\mathcal{D}, \mathcal{F}_+) \neq \emptyset.$$

There is a *downward connection* from $\mathcal{C}$ to $\mathcal{D}$, denoted $\mathcal{C} \searrow \mathcal{D}$, if

$$W^u(\mathcal{C}, \mathcal{F}_-) \cap W^s(\mathcal{D}, \mathcal{F}_-) \neq \emptyset.$$

We can now define the Morse Connection Graph as follows:

Definition 4.5 The Morse Connections Graph $MCG_f = (V_f, E_f)$ is a graph whose vertices (or nodes) V_f and edges E_f are defined as follows:

$$\begin{array}{ll} V_f & = \{\text{critical components of } f\}; \\ E_f & = \{(\mathcal{C}_i, \mathcal{C}_j) \in V_f \times V_f \ \mid \ \mathcal{C}_i \nearrow \mathcal{C}_j \text{ or } \mathcal{C}_i \searrow \mathcal{C}_j\} \end{array}$$

Equivalently, $(\mathcal{C}_i, \mathcal{C}_j)$ is an edge of the graph if

$$W^u(\mathcal{C}_i, \mathcal{F}_+) \cap W^s(\mathcal{C}_j, \mathcal{F}_+) \neq \emptyset \text{ or } W^u(\mathcal{C}_i, \mathcal{F}_-) \cap W^s(\mathcal{C}_j, \mathcal{F}_-) \neq \emptyset.$$

The algorithm constructing Morse Connections Graph based on the described multivalued maps, and experimentation on two-dimensional image data are presented in [2]. The Morse Connections Graph algorithm itself is dimension independent but an experimentation in higher dimensions has not been done yet at the time of writing this paper.

5 Directions of the future work

A natural question to rise is, weather or not our construction is stable with respect to perturbation of f or with respect to rescaling (that is, with respect to a change of resolution). Since our model assumes a discrete function as an input, and stability concerns continuous data, these questions cannot be answered within the framework of this paper, because that would involve different methods of discretizing, that is interpolating a continuous fonction. Thus interpolation methods should be integrated into the study.

Another interesting direction is to study extensions of the Euler formula in the context of our work. This formula is used (sometimes enforced) as a criterion of correctness of critical points extracted from discrete data. Our two-dimensional experiments test positively when the isolation and non-degeneracy assumptions hold and when there are no critical pixels on the boundary of the region. But the Euler formula cannot hold in presence of critical components. In fact, a critical component itself may have an Euler characteristics different than that of a point. Thus the goal is to find a suitable generalization of the Euler formula that would hold for the degenerate case.

Yet another direction is an application of our results to the problem of isosurfaces which has been the main motivation for our work. Isosurface extraction deals with the problem of generating a surface defined by the preimage of a scalar value c, called an isovalue, under a scalar function f of several variables. It is a powerful tool for visualizing and investigating volumetric scalar fields. Indeed, by varying the isovalue c and studying each corresponding isosurface, one can completely explore a given volume data, at any appropriate level of detail. Moreover, in domains such as medical image processing, many imaging modalities give images (such as CT and MRI scan data images) that are piecewise constant, because the intensity is related to tissue type. It follows that isosurfaces correspond approximately to tissue regions.

Studying the representation of all possible isosurfaces is not realistic in large scale data sets. Therefore, one needs to limit the study to isovalues where "interesting" behavior occurs. However, it is very difficult to determine which isovalues are of interest, since failing to consider certain isovalues may result in missing important features of the volume data. The analysis of the topological properties of a given discrete scalar field with appropriate methods such as the ones inspired by Morse and Conley index theories as is carried out in this work makes it possible to determine critical regions that correspond to the topological changes for which relevant isosurface behavior occurs. By determining the locations of critical components, one can track all the fundamental changes in the scalar data and reconstruct an appropriate isosurface for any given isovalue using meshing techniques and marching cubes algorithms (see [20] and the references therein).

Although a panoply of methods for reconstruction of non-singular isosurfaces are available, the techniques utilized break near the singular zones where one has to investigate the local topology nearly on a pixel level, in order to determine how to locally complete the construction of the studied surface so to preserve its global properties.

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