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Notes on the Topology of Random Fields¹

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Abstract

The purpose of these notes is to give an understandable introduction to the topology of random fields. To this end we detail simple proofs when their understanding is deemed essential for geostatisticians, and we omit complex proofs that are too technical. Our principal effort will be in showing the main steps in the proof for the expression that gives us the expected value of the Euler characteristic, χ , of the excursion sets $Z^{-1}[u, +\infty)$, of a smooth and isotropic random field Z on \mathbb{R}^N restricted to a sub-manifold M, for the case in which Z is a Gaussian field

 $\mathbb{E}\Big[\chi\big(M\cap Z^{-1}[u,+\infty)\big)\Big]$

The principal motivation for this is the application of the concepts involved behind the study of the Euler characteristic, in particular, to applications such as the reconstruction of geological bodies. Figures will be employed in order to illustrate some of the concepts.

1. Introduction

1.1. Road Map

We begin by giving a very rough description of the path that we are going to follow. All the notions introduced here will be formalized in the later sections. Let us consider $Z = \{Z(x) : x \in D \subseteq \mathbb{R}^N, N \ge 1\}$ a Random Field (RF) defined on a fixed continuous domain of interest D of the Euclidean space \mathbb{R}^N . Here \mathbb{R} denotes the set of all real numbers. The random field itself might be real or vector valued, that is, it can take values in \mathbb{R}^k , for any $k \ge 1$. We find this type of situations, for example, when we analyze any multi-element databases (Copper, Gold, Iron and more, in different locations of the space). We will analyze, however, the case k = 1. The domain of interest D that we want to tackle, as an introductory example, is a *connected* subset of \mathbb{R}^2 . Let us take a square domain $D = [0, 20]^2$. In summary, the RF may be defined in all \mathbb{R}^2 , but will be focused in the RF on $\mathbb{R}^2 \cap [0, 20]^2$ (Fig. 1, top), and the notation for this map is:

$$Z: [0, 20]^2 \subset \mathbb{R}^2 \to \mathbb{R}$$
$$x \mapsto Z(x)$$

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1.1.1. Modeling Geology from RFs

One of the common tricks used in geological modeling is to use the RF Z to obtain geological bodies (or lithofacies). This is done by looking at the *preimage* of a given target subset $T \subset \mathbb{R}$ of values in the image of the map given by Z, $\operatorname{preim}_{Z}(T)$, where in this case

$$\operatorname{preim}_{Z}(T) := \{ x \in D \subseteq \mathbb{R}^{N} \mid Z(x) \in T \}.$$

Note that it is not accurate to define geological bodies by looking at the *inverse image* of a given set, since Z is not a bijection. However, since we are already aware of this subtlety, we are going to do some abuse of notation and call $Z^{-1}(T)$ to the preim_Z(T).

We let T take different forms. If the interval is of the type $Z^{-1}[u, \infty)$, we call it the *level set* u, which is one of the most common image sets used (Fig. 1, bottom). Also T can take the bit more general form of an interval, [a, b], with $a \leq b$, or in other cases, union (or finite intersection) $\bigcup_{j \in J} [a_j, b_j]$ ($\bigcap_{j \in J} [a_j, b_j]$) of ranges. Thus, we can build different geological bodies just by getting some $Z^{-1}[a, b)$.

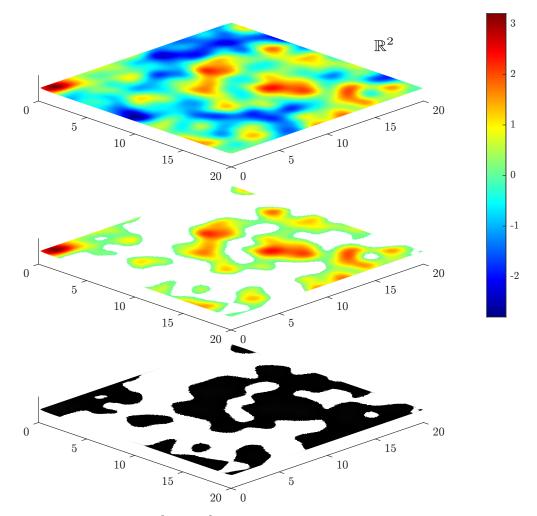


Figure 1: Example of a RF defined on $\mathbb{R}^2 \cap [0, 20]^2$ (top), and the process of defining a geological body by looking the set given by $\mathbb{R}^2 \cap \text{preim}_{\mathbb{Z}}([0, +\infty))$.

1.1.2. Triangulations and the Euler Characteristic

We notice, in particular, that $Z^{-1}[u, \infty)$ is a planar surface, or more specifically, it is formed by the disconnected union of different planar surfaces, which may or may not possess holes inside. By changing the threshold from u to v, components of $Z^{-1}[u, \infty)$ may merge and new components may be born, and possibly later merge with another of the components of $Z^{-1}[u, \infty)$, changing as a result the geometry of the level set. We are interested in following these changes in the *topology* of these sets, as a function of u. In order to achieve this objective, we need a measure that gives us direct or indirect information about the number of disjoint component and holes in the set. For this, the next step will be to define a *triangulation* on the level set u.

In the mathematical language triangulations of a set are referred as *simplicial complex*, and they come with the notion of dimension within them, with each triangle called a *simplex* of dimension k. They can be open sets, or closed. Very roughly speaking, the linearly independent points of the simplex are called *vertices* and the simplices spanned by subsets vertices called the *faces*. A 0-dimensional face of a simplex is also called a *vertex*. A 1-dimensional face of a simplex is also called an *edge*.

Definition 1. The standard 0-simplex is the point $1 \in \mathbb{R}$ This is also the standard open 0-simplex.

Definition 2. The standard 1-simplex is homeomorphic (a continuous bijection whose inverse is also continuous) to an interval. See Figs. 2 and 3.

Definition 3. The standard 2-simplex is a "triangle" with vertices at (1,0,0), (0,1,0), and (0,0,1). Figure 4 depicts a 2-simplex.

Definition 4. The standard 3-simplex is a tetrahedron with vertices at (1, 0, 0, 0), (0, 1, 0, 0), (0, 0, 1, 0), and (0, 0, 0, 1). Figure 5 depicts a 3-simplex.

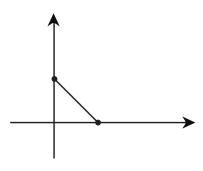


Figure 2: The standard 1-simplex.

Figure 3: A 1-simplex.

Definition 5. A 0-simplex has only itself as a face.

Definition 6. The standard 1-simplex $[v_0, v_1]$ (and hence all 1-simplices) has itself as a 1-dimensional face. It also has two 0-dimensional faces, $[v_0]$ and $[v_1]$.

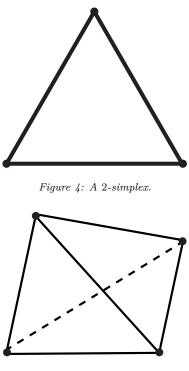


Figure 5: A 3-simplex.

Definition 7. A 2-simplex has one 2-dimensional, three 1-dimensional, and three 0-dimensional faces.

Definition 8. A 3-simplex has one 3-dimensional, four 2-dimensional, six 1-dimensional, and four 0-dimensional faces.

The notion of triangulation is formalized by defining the concept of *simplicial complex*, which is basically a map from the space of simplices to the topological target space, in our case the set $Z^{-1}[u, \infty)$. For examples of simplicial complexes, see Figs 6, 7, and 8.

The idea now is to cover the space $Z^{-1}[u, \infty)$ with a triangulation that approximately covers this set (Fig. 9). Then, one can proceed to compute the Euler Characteristic of our given set.

Definition 9. The Euler characteristic of a finite simplicial complex K of dimension k is computed via the following formula:

$$\chi(K) = \sum_{i=0}^{k} (-1)^{i} \# \{\text{simplices of dimension } i \text{ in } K\}$$

In the case of a surface or a 2-dimensional simplicial complex K, the Euler characteristic (EC) is given by $\chi(K) = V - E + F$, with vertices (V), edges (E), and faces (F). We notice that the EC takes values on the integers, i.e, $\chi(K) \in \mathbb{Z}$.

We will come back to this topics to cover more details and more general notions for Euler characteristic in the following sections, for instance, to show that the Euler characteristic is independent

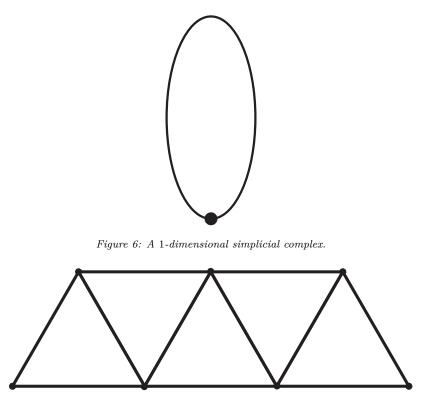


Figure 7: A 2-dimensional simplicial complex.

on the triangulation imposed to the set K, and also invariant under continuous deformations of the set.

Finally, taking several realizations of RFs Z, now we are able to compute

$$\mathbb{E}\big[\chi\big(D\cap Z^{-1}[u,+\infty)\big)\big]$$

1.1.3. Enters Morse Theory

Theoretical computations by counting the number of vertices, edges, and faces, although very intuitive and easy to follow, can not lead us too far. Indeed, it is a very primitive approach to the problem and we will have to leave it rapidly, specially since it is not clear yet how to relate directly the concept of triangulation and RFs. We will take in stead an indirect approach to the problem.

Morse Theory investigates how functions defined on a surface M (and *manifolds*, which are a generalization of the concept of surface, for higher dimensions) are related to geometric aspects of the surfaces. Surfaces are easy to visualize, and all the essential points of the theory readily appear in the case of surfaces.

1.1.3.1. Critical points of functions.

Let us consider a function z = f(x) in one variable. We assume that both x and y are real numbers. A point x_0 which satisfies

$$f'(x_0) = 0$$

is called a *critical point* of the function f. The points at which f takes its maximum or minimum values, and the inflection point of $y = x^3$, are examples of critical points. The critical points of

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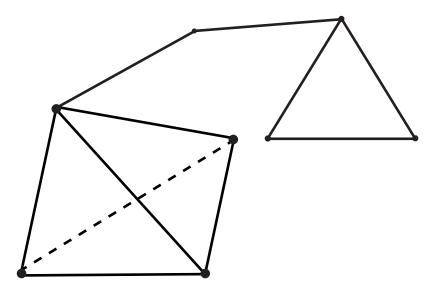


Figure 8: A 3-dimensional simplicial complex.

f fall in two classes according to the values of the second derivative of f, $f''(x_0)$. We call x_0 a non-degenerate critical point if $f''(x_0) \neq 0$, and a degenerate critical point if $f''(x_0) = 0$.

1.1.3.2. Hessian. We now move to a real-valued function

z = f(x, y)

of two variables, where x and y are both real numbers. We may think of a pair (x, y) of real numbers as a point in the xy-plane. In this way f becomes a function defined on the plane, which assigns a real number to each point in the plane. We can visualize the graph of this function in the 3-dimensional space with three orthogonal axes x, y, z = f(x, y).

Definition 10. (Critical points of functions of two variables). We say that a point $p_0 = (x_0, y_0)$ in the xy-plane is a critical point of a function z = f(x, y) if the following conditions hold:

$$\frac{\partial f}{\partial x}(p_0) = 0, \qquad \frac{\partial f}{\partial y}(p_0) = 0.$$

We assume in this definition that the function f(x, y) is of class C^{∞} (differentiable to any desired degree). Such a function is also called a C^{∞} -function or a smooth function.

Example 1. The origin 0 = (0, 0) is a critical point of each of the following three functions:

$$z = x^2 + y^2$$
, $z = x^2 - y^2$, $z = x^2 - y^2$

(see Fig. 11)

Now we need to define non-degenerate and degenerate critical points for functions of two variables. The reader may be tempted to define a critical point p_0 to be non-degenerate if it satisfies

$$\frac{\partial^2 f}{\partial x^2}(p_0) \neq 0, \qquad \frac{\partial^2 f}{\partial y^2}(p_0) \neq 0.$$
(1)

38

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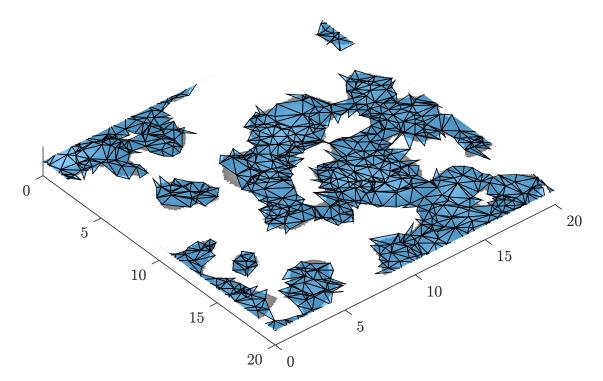


Figure 9: Example of triangulation defined on $\mathbb{R}^2 \cap \operatorname{preim}_Z([0, +\infty))$ for a given RF Z.

This is, in fact, a "bad definition", since after some coordinate changes, the condition (1) would no longer hold for the same f and p_0 in general. We want the concept of *non-degenerate critical points* or that of *degenerate critical points* to be independent of choice of coordinates. The following definition satisfies this requirement.

Definition 11. (i) Suppose that $p_0 = (x_0, y_0)$ is a critical point of a function z = f(x, y). We call the matrix

$$\begin{pmatrix} \frac{\partial^2 f}{\partial x^2}(p_0) & \frac{\partial^2 f}{\partial x \partial y}(p_0) \\ \\ \frac{\partial^2 f}{\partial y \partial x}(p_0) & \frac{\partial^2 f}{\partial y^2}(p_0) \end{pmatrix},$$

of second derivatives evaluated at p_0 , the Hessian of the function z = f(x, y) at a critical point p_0 , and denote it by $H_f(p_0)$.

(ii) A critical point p_0 of a function z = f(x, y) is non-degenerate if the determinant of the Hessian of f at p_0 is not zero; that is, p_0 is non-degenerate if we have the following:

$$\det H_f(p_0) = \frac{\partial^2 f}{\partial x^2}(p_0) \frac{\partial^2 f}{\partial y^2}(p_0) - \left(\frac{\partial^2 f}{\partial x \partial y}(p_0)\right)^2 \neq 0.$$

On the other hand, if det $H_f(p_0) = 0$, we say that p_0 is a degenerate critical point. Notice that the matrix $H_f(p_0)$ is a symmetrix matrix, since $\frac{\partial^2 f}{\partial x \partial y}(p_0) = \frac{\partial^2 f}{\partial y \partial x}(p_0)$.

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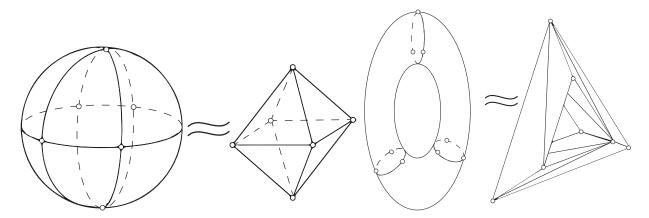


Figure 10: The EC of the two-dimensional sphere is $\chi(\mathbb{S}^2) = V - E + F = 6 - 12 + 8 = 2$ and of the two-dimensional torus $\chi(\mathbb{T}^2) = V - E + F = 9 - 27 + 18 = 0$.

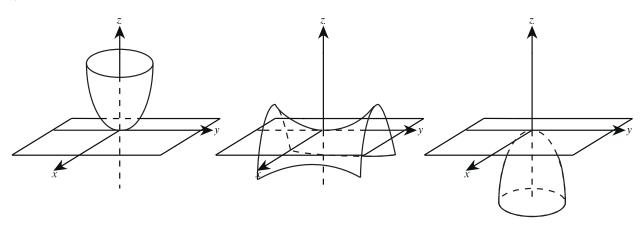


Figure 11: The graphs of $z = x^2 + y^2$, $z = x^2 - y^2$ and $z = x^2 - y^2$, respectively from the left.

Example 2. Let us compute the Hessian for each of the three functions in Example 1 evaluated at the origin 0. (i) For $z = x^2 + y^2$, the Hessian at the origin is

$$\begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}.$$

(ii) For $z = x^2 - y^2$, the Hessian at the origin is

$$\begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix}.$$

(iii) For $z = -x^2 - y^2$, the Hessian at the origin is

$$\begin{pmatrix} -2 & 0 \\ 0 & -2 \end{pmatrix}.$$

The determinant of each of these matrices is not zero, and hence the origin 0 is a non-degenerate

critical point for each of the three functions.

Example 3. Consider the function z = xy. The origin 0 is its critical point. The Hessian at 0 is

 $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$

and its determinant is not zero; hence, the origin 0 is a non-degener.ate critical point. In fact, the function z = xy is obtained from $z = x^2 + y^2$ by a coordinate change.

Example 4. The origin 0 is a critical point of the function $z = x^2 + y^3$, but the Hessian of this function at 0 is

$$\begin{pmatrix} 2 & 0 \\ 0 & 0 \end{pmatrix}$$

whose determinant is zero. Thus 0 is a degenerate critical point of $z = x^2 + y^3$.

Now we proceed to state our first theorem.

Theorem 1. (The Morse lemma) Let p_0 be a non-degenerate critical point of a function f of two variables. Then we can choose appropriate local coordinates (x', y') in such a way that the function f expressed with respect to (x', y') takes one of the following three standard forms:

(i)
$$f = x'^2 + y'^2 + c$$
 (2)

(*ii*)
$$f = x'^2 - y'^2 + c$$
 (3)

(*iii*)
$$f = -x'^2 - y'^2 + c$$
 (4)

where c is a constant $(c = f(p_0))$ and p_0 is the origin $(p_0 = (0, 0))$ in the new coordinates.

This theorem says that a function looks extremely simple near a non-degenerate critical point: for a function of two variables, a suitable coordinate change will make it one of the three simple functions we saw in Example 1.

Definition 12. (Index of a non-degenerate critical point). Let p_0 be a non-degenerate critical point of a function f of two variables. We choose a suitable coordinate system (x, y) in some neighborhood of the point p_0 so that the function f has a standard form given by Theorem 1. Then we define the index of the non-degenerate critical point p_0 of f to be 0, 1 and 2, respectively for $f = x^2 + y^2 + c$, $f = x^2 - y^2 + c$ and $f = -x^2 - y^2 + c$. In other words, the number of minus signs in the standard form is the index of p_0 .

We see immediately from the respective graphs (Fig 11) of the functions $f = x^2 + y^2$, $f = x^2 - y^2$ and $f = -x^2 - y^2$ that if the point p_0 has index 0, then f takes a minimum value at p_0 . If the index of p_0 is 1, then in some neighborhood of p_0 , f may take values strictly larger than $f(p_0)$ or it may take values strictly smaller than $f(p_0)$. If the index of p_0 is 2, then f takes a maximum value at p_0 . Thus the index of a non-degenerate critical point p_0 is determined by the behavior of f near p_0 .

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1.1.3.3. Morse functions on surfaces.

In the previous sections we limited ourselves to "local" investigation of critical points in their neighborhoods. We now turn to a "global" investigation which involves the shape of a space as a whole. In this section we consider two-dimensional spaces; that is, *surfaces*.

Some examples of closed surfaces were depicted in Fig. 10 and Fig. 12: a sphere and a torus in Fig. 10, and closed surfaces of genus two and three in Fig. 12. By the *genus* of a closed surface we mean the number of "holes" in it. The genus of a torus is one and that of a sphere is zero. We consider a closed surface of genus g for any natural number g. If one thinks of a torus as a "float", then one might think of a surface of genus two as a "float for two persons". Similarly we may think of a surface of genus g as a "float for g persons".

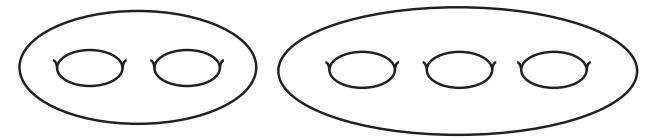


Figure 12: Closed surfaces of genus 2 and genus 3.

We denote the sphere by \mathbb{S}^2 . The superscript 2 represents the dimension of the sphere. We denote a torus by \mathbb{T}^2 . We often denote by Σ_g the closed surface of genus g, and in this case Σ_0 and Σ_1 are nothing but a sphere \mathbb{S}^2 and a torus \mathbb{T}^2 , respectively.

Let M be a surface. We call a map

$$f: M \to \mathbb{R},$$

which assigns a real number to each point p of M, a function on M. Notice that a surface is curved, so that local coordinates on it are also curved in general (cf. Fig. 13).

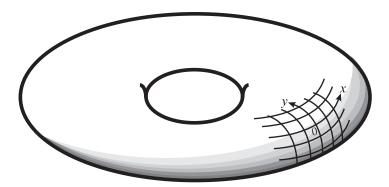


Figure 13: A local coordinate system on a surface.

We say that a function $f: M \to \mathbb{R}$ defined on a surface M is of class C^{∞} (or smooth) if it is of class C^{∞} with respect to any smooth local coordinates at each point of M. The concept of a "critical point" we saw in the previous section carries over to a function $f: M \to \mathbb{R}$ defined on a surface M with the aid of local coordinates. More precisely we say that a point p_0 of a surface M

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is a *critical point* of a function $f: M \to \mathbb{R}$ if

$$\frac{\partial f}{\partial x}(p_0) = 0, \qquad \frac{\partial f}{\partial y}(p_0) = 0.$$
 (5)

with respect to local coordinates in some neighborhood of p_0 . We saw in the first section that nondegenerate critical points are stable and have some convenient properties in contrast to degenerate critical points. Therefore the functions on a surface with only non-degenerate critical points would be *nice* ones. Based on this consideration, we define

Definition 13. (Morse functions). Suppose that every critical point of a function $f: M \to \mathbb{R}$ on M is non-degenerate. Then we say that f is a Morse function.

1.1.3.4. Critical points and the EC.

Let us come back to the example on which the surface M is the sphere or the torus. We consider the unit sphere \mathbb{S}^2 with the orthogonal coordinates (x, y, z) in three-dimensional space \mathbb{R}^3 ; that is, \mathbb{S}^2 is defined by the equation

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

Let

 $f: M \subset \mathbb{R}^3 \to \mathbb{R}$ $(x, y, z) \mapsto z$

be the nice function on \mathbb{S}^2 which assigns to each point p = (x, y, z) on \mathbb{S}^2 its third coordinate z. One might say that f is the "height function". Then f is a Morse function, with two critical points; the north pole $p_0 = (0, 0, 1)$ and the south pole $q_0 = (0, 0, 1)$ (Fig. 14). One easily sees that f has no other critical points, and in fact, it is a lemma that for a Morse function defined on a closed surface has only a finite number of critical points.

Now we are ready to state one of the most striking results, and which relates the number of critical points and the EC.

Theorem 2. (The Morse theorem) Let $f: M \to \mathbb{R}$ be a Morse function on a compact manifold M of dimension n, and denote by k_{λ} the number of critical points of f with index λ . Then the Euler characteristic of M is given by:

$$\chi(M) = \sum_{\lambda=0}^{n} (-1)^{\lambda} k_{\lambda} \tag{6}$$

The intuition behind achieving this theorem, in a very rough and informal fashion, is that we can build our compact surface M by *attaching* our nice graphs function of Fig. 11 one by one, and using continuous deformations, until we get the surface M, in what is called a "handle decomposition". The graphs function of Fig. 11 are particular cases of "handles". During this process of construction, the important geometrical changes (the topological ones) appear when the continuous deformations are close to some critical point (Fig. 15).

In order to use this theorem, we will need to study under which conditions the RFs that we will making use of have the property of being Morse functions with probability one. This will be one © Predictive Geometallurgy and Geostatistics Lab, Queen's University 43

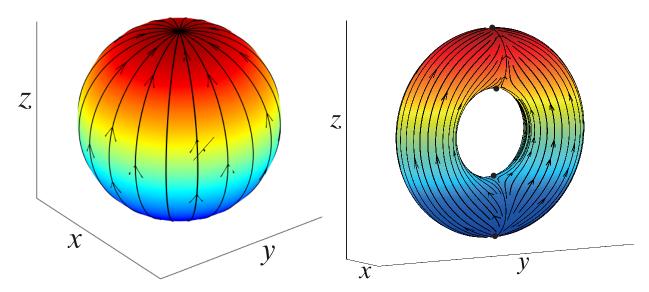


Figure 14: The height function and their gradient of the surface of \mathbb{S}^2 and \mathbb{T}^2 . The sphere has 2 critical points (north and south pole): one of index 0 and another one of index 2. Therefore, $\chi(\mathbb{S}^2) = 1 \cdot 1 - 1 \cdot 0 + 1 \cdot 1 = 2$. The torus has 4 critical points: one of index 0, two of index 1, and another one of index 2. Therefore, $\chi(\mathbb{T}^2) = 1 \cdot 1 - 1 \cdot 2 + 1 \cdot 1 = 0$.

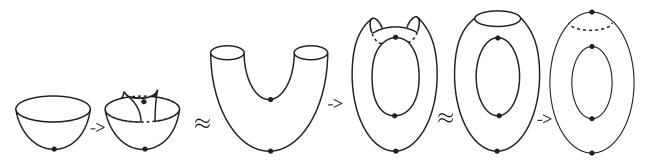


Figure 15: Building a torus by attaching "handles" to the previous ones and using continuous deformations.

of the technical issues that we must address on the second part these notes. Once this has been established, we will proceed with the following trick. We are going to use the value of the RF in our planar surface of Fig. 1 as both height and as a Morse function, i.e., f = Z.

After establishing the mentioned technical issues and others, the problem of finding the EC of the RF Z is basically reduced to find the number k_{λ} of points $p \in D$ for which:

- (i) the RF Z at p is above the desired threshold u, i.e., $Z(p) \ge u$;
- (ii) the RF Z at p is also a critical point, i.e.,

$$\frac{\partial Z}{\partial x}(p) = 0, \qquad \frac{\partial Z}{\partial y}(p) = 0;$$

(we summarize this condition by writing dZ = 0)

(iii) the index of the non-degenerate critical point p, for which we are going to see that is a function of the Hessian of Z (more precisely, equal to the number of negative eigenvalues of the Hessian of Z), i.e., the index $(H_Z(p))$ is equal to λ .

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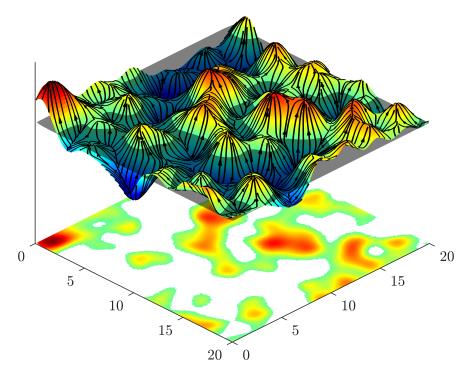


Figure 16: Schematic showing the trick used to find $\chi(Z^{-1}[u, +\infty))$: to use the RF Z as the height function in order to find critical points above the threshold u.

Then, we would like to use the Morse theorem for one realization of Z to find the value of the EC

$$\chi\bigl(Z^{-1}[u,+\infty)\bigr) = \sum_{\lambda=0}^n (-1)^\lambda \#\{Z>u, dZ=0, \mathrm{index}\bigl(H_Z\bigr) = \lambda\}.$$

Sadly, this will not be possible, but taking the expected value on both sides will be, in order to obtain first $\mathbb{E}[\chi(Z^{-1}[u, +\infty))]$. The continuation of these notes is devoted to finding the expected values on the right hand side (RHS). By working a bit more, we are going to be able to find $\mathbb{E}[D \cap \chi(Z^{-1}[u, +\infty))]$.

2. Acknowledgements

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