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Network Topology vs. Geometry: From persistent Homology to Curvature

by

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NETWORK TOPOLOGY VS. GEOMETRY: FROM PERSISTENT HOMOLOGY TO CURVATURE

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ABSTRACT. We propose our method based on Forman's discretization of Ricci curvature, as an alternative, in the case of Complex Networks, to persistent homology. We show that the proposed method has, among other advantages, the simplicity and efficiency of computations. In addition, we gain both expressiveness and computational efficiency by taking into account only those higher dimensional faces that model higher order correlations. In this setting it also has the supplementary advantage of having the capacity of recognizing geometric structures up to homotopy.

We show that the proposed method can be applied also to weighted data, obtained via the geometric, (generalized) Ricci curvature sampling, from manifolds with density. Moreover, we show that the resulting networks can be naturally equipped with the Forman-Ricci curvature, thus representing accurate samplings of the metric, measure and geometric structures of the original weighted manifold.

In addition, we suggest as a method for inferring the real dimension of the data sampled from a geometric object that lacks a manifold structure, the notion of local and statistical dimensions due to Y. Ollivier.

1. Introduction – Forman Curvature

Among the methods for data analysis, and mainly for the understanding of the shape of the data, as obtained by sampling of some underlying structure (the intended final object of such a study) the so called *persistent homology* has gained an ever increasing popularity, since its introduction in 2002 by Edelsbrunner, Letscher and Zomorodian [7]. Given its mathematical foundation and computational capability, [3],[31], it is little wonder that it has risen towards prominence amongst such methods and was applied to a variety of fields [4], [2] and not least among them, to the study of Complex Networks [11], [22], [23].

However, beyond its merits, persistent homology also suffers from a number of drawbacks, that are not popularized by its proponents, who might be only partially aware of them, due to the numerous successes of the method. Amongst these less advantageous features, first and foremost one has to number the fact, that as its very name proclaims, this approach allows, by its very definition, for the recognition and reconstruction of (data) manifolds only up to *homology*. However, as it is well known in Algebraic Topology, the knowledge of the *homotopy* would endow us with a more powerful tool (see, e.g. [16]).

We suggest here an approach that, at least in the case of networks, is preferable to the persistent homology from more than one viewpoint. The proposed method is based on our adaptation and extension of Forman's Ricci curvature [8] to the case of complex networks [30], [35], [36]. Recall that, for proper

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(1-dimensional) networks, its expression is very simple:

$$\mathrm{Ric_F(e)} = \omega(\mathrm{e})\left(\frac{\omega(\mathrm{v_1})}{\omega(\mathrm{e})} + \frac{\omega(\mathrm{v_2})}{\omega(\mathrm{e})} - \sum_{\substack{e_{v_1} \sim e \\ e_{v_2} \sim e}}\left[\frac{\omega(\mathrm{v_1})}{\sqrt{\omega(\mathrm{e})\omega(\mathrm{e_{v_1}})}} + \frac{\omega(\mathrm{v_2})}{\sqrt{\omega(\mathrm{e})\omega(\mathrm{e_{v_2}})}}\right]\right) . \tag{1.1}$$

While the full force of Forman's curvature resides precisely in its ability do deal with weighted vertices and edges at the same time, the combinatorial case, namely $\omega(e) = \omega(v) = 1,\ e \in E(G), v \in V(G)$ is, however, extremely important since it is still employed by many scientist, especially in the Social and Biological Networks communities. Since, in this case, $\#\{\hat{e}|\hat{e}\|e\} = \deg(v_1 \sim e) + \deg(v_2 \sim e)$, we immediately obtain

$$\mathrm{Ric_F}(e) = 2 - \sum_{v\sim e}\deg(v) . \tag{1.2}$$

For the case of 2-dimensional complexes, the formula is somewhat more complicated:

$$\mathrm{Ric_F}(e) = \omega(e)\left[\left(\sum_{e\sim f}\frac{\omega(e)}{\omega(f)} + \sum_{v\sim e}\frac{\omega(v)}{\omega(e)}\right) - \sum_{\hat{e}\|e}\left|\sum_{\hat{e},e\sim f}\frac{\sqrt{\omega(e)\cdot\omega(\hat{e})}}{\omega(f)} - \sum_{v\sim e, v\sim\hat{e}}\frac{\omega(v)}{\sqrt{\omega(e)\cdot\omega(\hat{e})}}\right|\right] ; \tag{1.3}$$

where $\sigma < \tau$ means that σ is a face of τ, and where $||$ denotes parallelism, i.e. it means the two cells have a common "*parent*" (higher dimensional face) or a common "*child*" (lower dimensional face), but not both a common parent and common child. In the special case of unweighted networks, i.e. $\omega(f) = \omega(e) = \omega(v) = 1,\ \forall f \in F(G), e \in E(G), v \in V(G)$, the terms simplify to merely the counting of adjacent parents and children, respectively. We get

$$\begin{aligned}\mathrm{Ric_F}(e) &= \#\{f > e\} + \underbrace{\#\{v < e\}}_{=2} - \left(\#\{\hat{e}|\hat{e}\|e\} - \underbrace{\#\{v|v \sim e, v \sim \hat{e}\ , e||\hat{e}\}}_{=0}\right) \\ &= \#\{f > e\} - \#\{\hat{e}|\hat{e}\|e\} + 2 .\end{aligned} \tag{1.4}$$

While the markedly combinatorial nature of Forman's curvature is somewhat confusing to the classical differential geometer, the formula for the 1-dimensional case clearly reveals that Forman's Ricci curvature captures and discretizes the quantification of the *geodesics dispersal* aspect of the classical Ricci curvature. The formulas above show the first advantage of using Forman's curvature: It is very simple, inexpensive and straightforward to compute. We still have, however, to show why, at least in the networks setting, it is preferable to the Persistent Homology approach. We dedicate the next section to the answer to this question.

2. Forman Curvature vs. Persistent Homology

As we alluded above, one essential such advantage resides in the fact that, for 2-and higher dimensional complexes X, Forman's curvature captures not only homology, but also the fundamental (i.e. first homotopy) group – see [8]. More precisely, if $\mathrm{Ric_F}(e) > 0$ for every edge e of X, the first homotopy group $\pi_1(X)$ is finite. However, this assertion should be somewhat nuanced:

This result is of practical importance, since it allows us to distinguish, via the simple knowledge of the sign of the Forman curvature, between the basic topology of structures that behave, essentially, like social networks, and those that have potential infinite growth, such as communication networks (see also [17]).

Another problem with persistent homology resides precisely in the very feature that makes it attractive to the applications-inclined user, namely the (industrial, automatic) barcodes associated with the persistent homology [9], and on which its application is largely based. While seemingly ideal for experimentation, such barcodes require special attention at certain critical radii. More precisely, at tangency points, some homology group may appear or disappear and, moreover, such points are difficult to locate precisely. Therefore, different choices of the incrementation step of the radii may omit shorter barcodes, thus failing to take into account part of the topological structure. Since in most applications, this scale is associated with noise, this problem is thus solved. (A smoothing procedure, that produces structures with low absolute value of curvature/*reach* – see, e.g. [7] – automatically eliminates such topological noise.) However, for certain types of data, such as ultrasound images, the distinction between noise and the data itself is problematic, thus rendering persitent homology a rather inefficient method in such cases. Thus, in practice the result might strongly depend on the chosen radii incrementation step. In contrast, the Forman based approach is deterministic and its outcome is definite: Once the data (the network/complex) is imputed, the result of the computation is clear and unequivocal.

This brings us to the next advantage of using Forman's curvature: This notion of curvature is applicable to general polyhedral complexes. In truth, the use of simplicial complexes, while a classical and preferential construct of Algebraic Topology is also somewhat restrictive and, as such limited in its modeling capability, since raw data may very well not admit a simplicial complex structure, as it is often the case, for instance in Biological Networks (see [36]). In contrast, Forman curvature is defined for the large class of (*regular*) *weighted CW complexes* [8] (that includes, as special cases, the ubiquitous graphs/networks, as well as polygonal and polyhedral meshes of importance in Graphics and Imaging).

Here yet another advantage of our approach is revealed: One can either operate with the data "as is", or by adding higher dimensional faces in the manner detailed below. However, even when adding simplices, the process is much more economical, effective and lacking any arbitrariness. Indeed, even when one adds higher dimensional simplices to a network, this is not done in an arbitrary or automatic manner, bur rather, as we suggested in [36], this should be done only to model correlations of higher order (edges encoding correlations between couples of nodes/data points).

As we have noted above, Forman curvature based analysis outperforms persistent homology in a number of crucial aspects. In addition, we should emphasize a number of further advantages of the approach proposed above: It is applicable both to directed and undirected networks (in case this is the intended object of study); comes coupled with a Laplacian (thus standard spectral methods can also be extracted out from it); it comes equiped with a Ricci flow, both in the "pure" network case, as well as for the augmented, higher dimensional one, see [35], [36]; and, last, but certainly not least, it incorporates the analytic power not only of (Algebraic) Topology, but also of Geometry, thus gaining more expressive power and analytic force.

3. From Weighted Manifolds to Networks and Back

A legitimate question is whether the method above is restricted to data obtained, typically, by sampling objects endowed solely with a "simple" geometric structure, such as arising typically in Imaging and Graphics, or whether it can be extended to more general structures. An indication of the wider applicability of the Forman-Ricci curvature based approach is given by the fact that it can be defined,

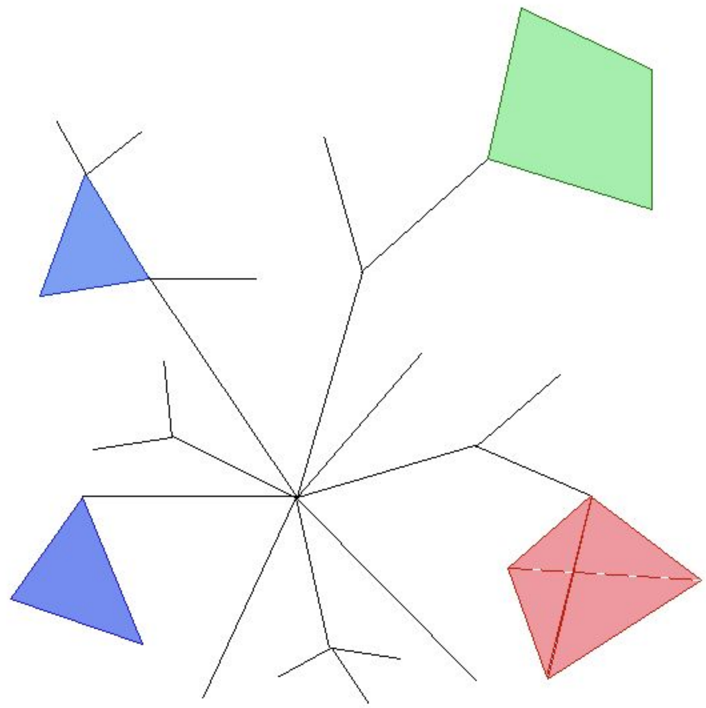

FIGURE 1. Higher order correlations in networks modeled as faces of dimension $\neq 2$ in a polyhedral complex: Triple correlations considered as triangles (2-simpleces); 4-gon modeling a quadruple of nodes (e.g. genes) that are pairwise correlated; order 4 correlations viewed as a tetrahderon (3-simplex).

as we have already seen, not just for simple combinatorial structures, nor to pure metric graphs, but also the very general weighted (both on the nodes and on the edges) graphs.

Indeed, "weighted" data arises in many context, where the weights in question might represent probability distributions or measures, inherent in the very process of acquisition (s.a. in the case of many types of MRI images, where their density equals to the very proton density); quantifying uncertainty or noise; describing certain features of texture in natural images, but also introduced as ad hoc tools in Graphics and Imaging that are employed at various stages of the implementation of a variety of tasks, such as smoothing, (elastic) registration, warping, segmentation, etc.

Such phenomena are usually modeled as *weighted manifolds*, (a.k.a. as *manifolds with densities* or *smooth metric measure spaces*). However, given that the data is, in truth, acquired via a sampling process, the natural question arises whether there exists a simple and efficient method of sampling the metric and the measure at the same time. More precisely one would like to an effective computation of the necessary and optimal sampling density (akin to the Nyquist rate in classical Signal Processing). Given that such methods, in Differential Geometry [10], Manifold Learning [18], Graphics and related fields [5], [Eu], and Communications and Information Theory [29] are based on curvature, one is conduced to the question whether there exist a proper notion of curvature for manifolds with densities, that permits for the generalization of the classical, unweighted methods.

It turns out that one classical notion of curvature generalizes particularly well to case of weighted manifolds, namely the so called *Ricci curvature*, a concept that quantifies both the growth of volumes and the dispersion of geodesics. Using the growth of volumes aspect, a number of related notions of *generalized Ricci curvature* for manifolds with densities were developed [14] and [32], and, using a somewhat different approach, in [15]. Since in the classical case sampling by the rate prescribed by (the inverse of) Ricci curvature produces a discretization of the original manifold that allows for its reconstruction up to *homotopy equivalence* (even smooth homotopy – apart from dimension 3) [10], one is naturally induced to ask whether, *mutatis mutandis* the same holds for weighted manifolds, with the generalized Ricci curvature *en lieu* of the classical one.

Fortunately enough, this proves to be the case (measures replacing volumes, naturally) [25], [26], and, moreover, the approximation is good in the metric, geometric (i.e. curvature related) and topological senses. Moreover, this a result easy adaptable to practice in Imaging and its related fields [13] (see Figure 2).

In fact, by employing the (generalized) Ricci curvature, one has an additional benefit: While more traditional sampling methods, based on more common notions of curvature, permit the reconstruction of a manifold only up to *homology* (see, e.g. [18]), the method of Grove end Peterson [10] – and its generalization to weighted manifolds – allows, as we have noted above, for reconstruction up to *homotopy type*, which represents a stronger results (see, e.g. [16]).

As we have already mentioned, the graphs (technically called ε*-nets*) obtained via the sampling and approximation technique sketched above (see [25], [26] for details, as well as Figure 3) allow for good (geo-)metrical and topological approximation of the original space. The natural question is whether such schematic approximations/backbones can also carry a significant (differential) geometric structure, that ideally would also approximate/sample the original one. If one restricts himself to the case of classical Riemannian manifolds, i.e. to "pure" differential geometric structure, then the answer is positive, and more than one solution has been given, depending on the type of curvature one would attempt to recover. (The literature on this subject is too vast for any catalogue on the subject, however brief, to be included here, therefore we suggest only [28] and the bibliography therein.) In contrast, for the case we are concerned with, namely with approximations and discretizations of weighted manifolds, no answer seems to exist in the literature.

However, a simple and direct way of producing a meaningful curvature, that captures both the metric and the measure aspect of the given structure presents itself naturally in the form of Forman-Ricci curvature. Indeed, by incorporating both node and edge weights, this represents a notion of curvature ideally suited for discretizations of metric measure spaces, where the edge weights are abstractizations of lengths, whereas node weights quantify the measure (concentrated at the atoms = nodes). In particular, if one starts from a simple geometric context, these weights can represent e.g. volumes (concentrated at the center of a Voronoi cell, for instance), or curvature measures (the very curvatures used in the sampling process – see for instance [26], or associated to the star of a vertex in a polygonal mesh – see, e.g. [33]). Note also that, if a better reconstruction (in the sense of dimensionality preservation) of the original structure is required, one can make appeal to the original formula of Forman's Ricci curvature [8]. (See also [36] for the special case of simplicial complexes.)

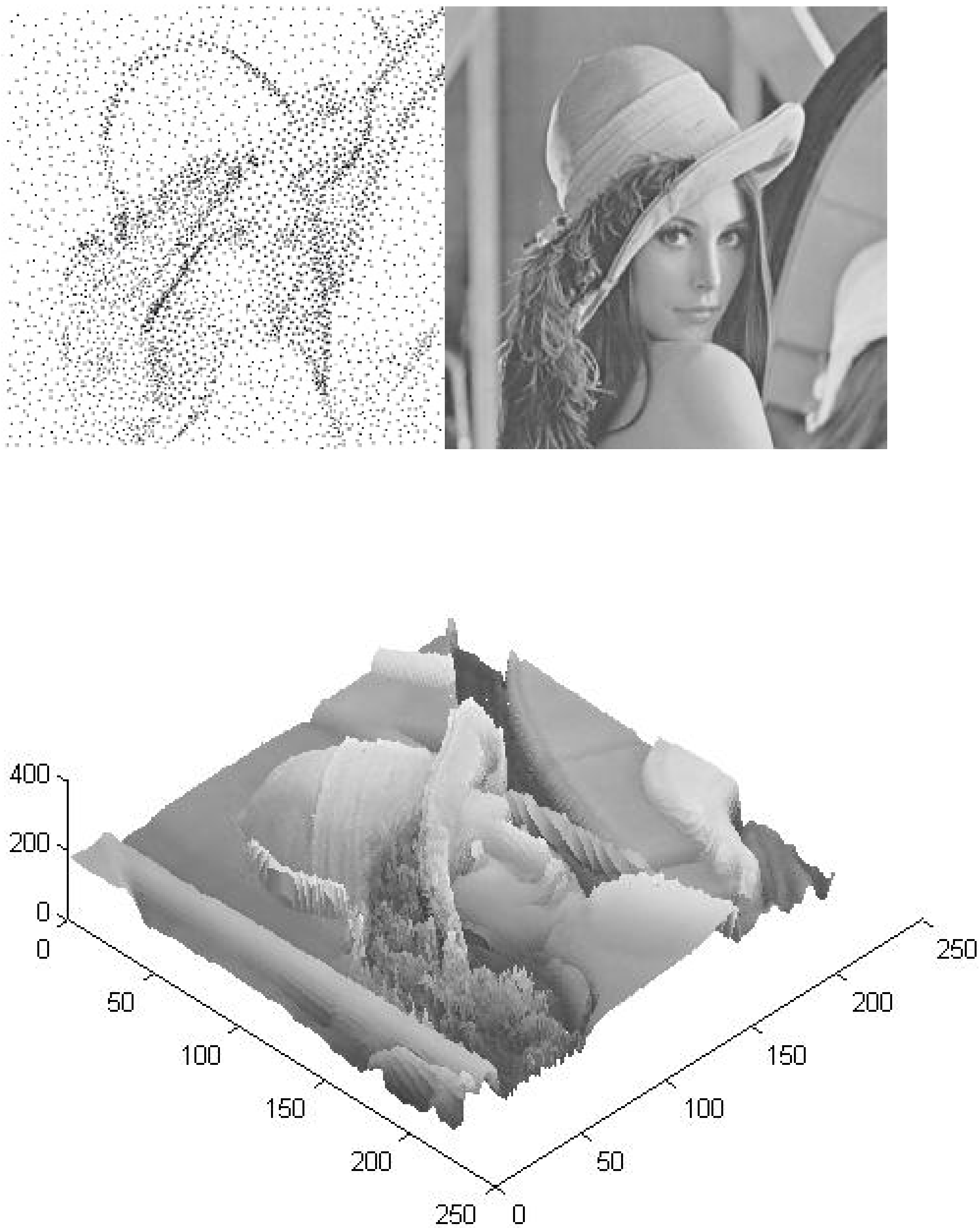

FIGURE 2. Curvature based sampling – above, left (cf. [13]) of standard test image, viewed as a smooth distribution over a square (below).

Thus this process allows, by using the generalized Ricci curvature, to pass from a weighted manifold to a discrete structure, namely to a graph/network that captures both the essential metric and measure properties of the given space. Furthermore, the obtained weighted network can be geometrized using the Forman-Ricci curvature, to obtain a discretization of the original weighted manifold, that quantizes its metric, measure, as well as curvature properties. Moreover, by adding the relevant higher dimensional faces, one can better recapture the dimensionality, as well as interplay between the geometry and the topology of the given underlying manifold. A further advantage of this approach resides in the fact that the parameter ε allows for scaling (an important feature that is shared with persistent homology).

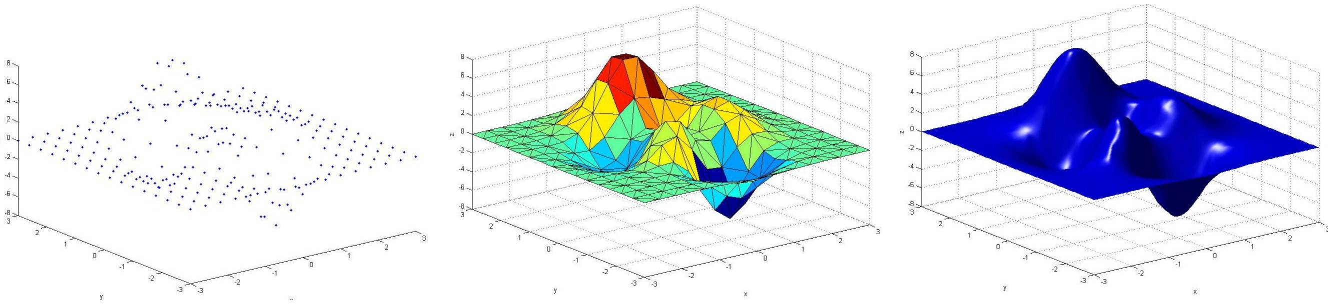

Figure 3. The curvature based sampling (left), of a smooth distribution over a square (middle), and the network ε-*net* – the edges of triangulated surface, as well as the "augmented" network, i.e. the simplicial surface induced by it (right).

Remark 3.1. A natural question is whether the quantification, so to say, of a given manifold, through the process of sampling using the generalized Ricci curvature, the production of the induced weighted graph and the computation of its Forman-Ricci curvature, represents only a coarse approximation or whether, in the case of unweighted manifolds (i.e for which the weights reduce to the natural volume form), they also have "nice" convergence properties. At this stage, this represents work in progress.

4. Data Dimensionality

The capability of taking into account faces of various – not necessarily the same – dimension, represents yet another crucial, advantage of the Forman curvature approach, and at a fundamental level: Since the very beginning of acceptance and adoption by the relevant communities of the geometric approach to understanding and handling high-dimensional data [24], [34], the manifold assumption has been essential. However, as is by now well known in the field, and as it is so well illustrated by the already famous (or rather infamous) swiss-roll example, one can not, in general, deduce or obtain unequivocally the dimension of the data, without some prior knowledge or arbitrary assumptions or decisions. (For instance, in the swiss-roll case [24], [34], the data can be interpreted – or can really represent – noisy sampling/representation of a planar curve, a surface, or a volume is space, as well as some other, more complicated and less easier to define possibilities – see also the discussion below.)

We propose a solution to this problem, that is based on Y. Ollivier's definition [19], [20], [21] of *local* and *statistical dimension*. We first must, however, bring some preparatory definitions for our setting. (For further details and background material, see, e.g. [10].)

Let (X, d) be a *Polish space*, that is a complete, separable metric space equipped with its Borel σ-algebra. Consider the *random walk* $\{m_x(\cdot)\}$, where m_x are probability measures such that (i) m_x is measurable as a function of x and (ii) m_x has finite first moments; and let $\sigma(x)$, $\sigma(x) = \left(\int\int d(y,z)dm_x(y)dm_x(z)\right)^{\frac{1}{2}}$, denote the *spread* of the *Markov chain* defined with transition probability from x to y, in n steps, given by

$$dm_x^{*n}(y) = \int_{z\in X} dm_x^{*(n-1)}(z)dm_x(y)\,;\; m_x^{*1} = m_x\,.$$

(In addition, let $\sigma_\infty(x) = \frac{1}{2}\text{diam Supp}\, m_x$, $\sigma_\infty = \sup_x \sigma_\infty(x)$.)

We can now bring the first fundamental definition:

Definition 4.1. The *local dimension* at $x \in X$ (of the random walk) is defined as follows:

$$n_x = \frac{\sigma^2(x)}{\sup\{Var_{m_x} f \mid f \text{ is } 1-\text{Lipschitz}\}}\,; \tag{4.1}$$

where $f : \mathrm{Supp}(m_x) \to \mathbb{R}$.

Also, define:

$$n = \inf_x n_x\,. \tag{4.2}$$

(Here $Var_{m_x} f$ denotes, as usual, the *variance* of the function f with respect to the measure m_x.)

Remark 4.2. We bring a couple of essential observations regarding the definitions above:

(1) $n_x \geq 1$.
(2) The meaning of the definition above is that, if the local dimension is n, then the typical variation of a Lipschitz function is $1/\sqrt{n}\times$ the typical distance between two points.

Examples 4.3. *Let us also bring a number of basic examples, to help better understand the notion introduced above:*

(1) *For the simple random walk on a graph,* $n_x \approx 1$.
(2) *For the discrete Brownian motion on a (smooth, complete) Riemannian manifold of dimension* N*, given by randomly jumping in a ball of radius* ε*, centered at* x*, we have that* $n_x \approx N$.
(3) *For discrete geometric data, such as one might expect in Manifold Learning, Pattern Recognition, Imaging, etc., the natural random walk one should consider is the one given by proximity (as extracted, say, by the k-nearest neighbors algorithm, or already encoded in the data given as a mesh/network – see* [1]*, respectively* [12]*).).*

Before proceeding further, let us observe that, at first sight, one might dismiss the locality condition as superfluous, at least in the context we are interested in. However, the manifold approach to learning (in all its aspects and applications in various fields) hides a concealed assumption that is crucial for the method, but also deeply problematic. This veiled – or rather so obvious that people fail to notice – assumption resides in the existence of an implicit manifold structure of the data. However, while a convenient and expedient tool, so natural that it is presumed implicitly even in more critical views of the method (such as [6], [27]), this hypothesis is far from evident and even fallacious in many instances. (See Figure 4 for a typified such geometric structure.) Without going in details concerning types of data for which no true determination of dimensionality and structure is possible so far, such as in Astronomy and Cosmology, one is confronted with this problem in everyday Medical Imaging practice, when a volumetric element on a hidden surface (e.g. colon) might be a tumor or a result of noise and faulty preprocessing – see Figure 3.

To address this problem, we invoke Ollivier's notion of *statistical dimension* of a metric measure space (X, d, μ):

$$\mathrm{StatDim(X,d,\mu)} = \frac{\frac{1}{2}\int\int d(y,z)dm_x(y)dm_x(z)}{\sup\{Var_\mu f \mid f \text{ is } 1-\text{Lipschitz}\}} \tag{4.3}$$

Note that, in general, the two notions of dimension introduced above do not coincide. Indeed, we have the following example: If (X, d, μ) is the discrete cube $\{0,1\}^N$ with the Gaussian measure, then $n_x \approx 1$, while $\mathrm{StatDim(X,d,\mu)} \approx N$.

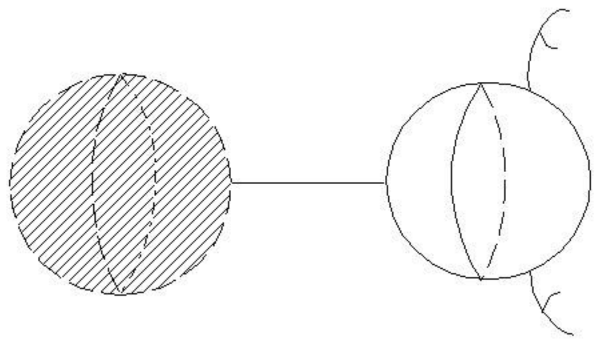

FIGURE 4. A typified geometric object for which the manifold structure – hence uniqueness of dimension – fails to hold.

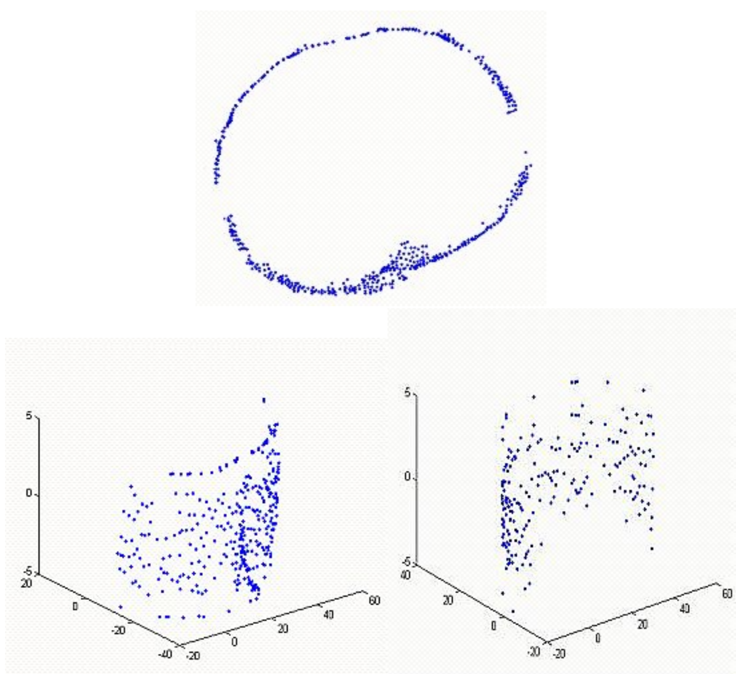

FIGURE 5. The data points in the figure above, can be interpreted as a nosy approximation to a curve, the sampling thin annular surface or a tubular shape, or a mixture of samples of, surface and volumetric data (due to the enlarge "bump" in the lower part of the figure.) However, under proper orientation, the data reveals itself to represent the two half of CT obtained samples of a highly folded part of the human colon.

To summarize, the approach we proposed above allows us to ascertain the true (though perhaps hidden) dimensionality of the data, without imposing the strong assumption of manifold structure, thus of uniqueness of dimension (and of the identity between local and global dimension) and without presuming some extraneous, "*deus ex machina*" knowledge regarding the data and its presumed dimensionality.

Remark 4.4. Since, by their very definitions, bot the local and statistical dimension necessitate the computation of the variance of all the Lipschitz functions (from a given space), the computations of the said quantities requires, in practice, some non-trivial optimization procedure.

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Appendix

We bring here the definition of ε-nets mentioned in the text

Definition 4.5. Let (X,d) be a metric space and let $p_1,\ldots,p_{n_0}$ be points $\in X$, satisfying the following conditions:

(1) The set $\{p_1,\ldots,p_{n_0}\}$ is an ε-net on X, i.e. the balls $\beta^n(p_k,\varepsilon)$, $k=1,\ldots,n_0$ cover X;
(2) The balls $\beta^n(p_k,\varepsilon/2)$ are pairwise disjoint.

Then the set $\{p_1,\ldots,p_{n_0}\}$ is called a *minimal ε-net* and the packing with the balls $\beta^n(p_k,\varepsilon/2)$, $k=1,\ldots,n_0$, is called an *efficient packing*. The set $\{(k,l)\,|\,k,l=1,\ldots,n_0 \text{ and } \beta^n(p_k,\varepsilon)\cap\beta^n(p_l,\varepsilon)\neq\emptyset\}$ is called the *intersection pattern* of the minimal ε-net (of the efficient packing).

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