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Steve Huntsman

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DISCRETE TOPOLOGICAL METHODS FOR CYBERSECURITY, NETWORK SCIENCE, AND MACHINE LEARNING

STEVE HUNTSMAN*

Abstract. This is an advertisement for (or a rant about) discrete topological methods—fairly new even by the standards of topological data analysis, and certainly underutilized at present—that are naturally suited to analyze (hyper)graphical data prevalent in cybersecurity applications, network science, and tasks in machine learning. As outstanding exemplars in this vein, we briefly discuss path homology and magnitude homology before paying lip service to sheaves, curvatures, and geodesics in discrete settings. Throughout, we mention new or plausible near-term applications.

Key words. topological data analysis, Dowker homology, path homology, magnitude homology

AMS subject classifications. 55N31, 55N35, 55U05

1. Introduction. The field of topological data analysis (TDA) arguably originated with the introduction of topological persistence in 2000 [25]. Since then, it has blossomed into a vast enterprise (see, e.g. [93, 24, 31, 69, 20]), albeit one that has been mostly focused on computing topological properties of structures that in some sense embody or approximate continuous objects such as spaces, probability distributions, etc. The fundamental data structure here, familiar to every student of topology, is an abstract simplicial complex. Meanwhile, the basic idea of mainstream TDA is that algebraic bookkeeping enables the construction of a filtration of abstract simplicial complexes (e.g., the computationally tractable Vietoris-Rips complexes) that adequately represents topological properties of a finite metric space across scales. Here “adequately” means that the constructions are sufficient to reconstruct many of the features of the original data, that they are resilient to noise, with quantitative error (bottleneck distance) bounds, etc.

A more peripheral branch in applied topology has an earlier origin but also ties into recent foundational developments. This branch deals with structures in which simplicial complexes are optional technical devices (if they appear at all) and are not embodiments or approximations (but are perhaps alternative representations or models) of a structure that is the direct subject of investigation. For example, in [23], Dowker showed that a relation naturally gives rise to a pair of homotopy equivalent simplicial complexes. Meanwhile, the homology over $\mathbb{F}_2$ of these complexes can be readily computed directly from the relation itself, without ever constructing either simplicial complex. That is, relations give rise directly to $\mathbb{F}_2$ -(co)chain complexes [31]. For applications (besides the implicit connection to witness complexes [18]), see, e.g. [6, 30, 32, 27, 86, 47]. More generally, bipartite graphs can be identified with a relation up to duality, and so Dowker homology could be applied to, e.g. user/computer authentication data such as [43, 51], process/file interactions, bipartite network data from [53],¹ etc. (these are exercises for the reader).²

Discrete structures such as finite topological spaces (e.g., the four-point pseudocircle) [10] and posets [89] have long been analyzed using classical methods of algebraic topology and the classical structure of a simplicial (or in some cases CW-)

*sch213@nyu.edu

¹This collection of data is presently at <http://konect.cc/>.

²Dowker complexes (and for that matter, cosheaves) also feature prominently in an effort to characterize consistency of program variants’ behavior on inputs [3, 28, 77, 79]. While topological invariants *per se* are relevant to this effort, they feature only peripherally in such work to date.

complex. More recently, hypergraphs [49] have been analyzed via the abstract simplicial complexes they generate [29]. Meanwhile, discrete versions of classical methods such as Morse theory [84] are seeing increasing use. Still, there is a sense in which the distinctly recent and computationally convenient topological techniques of *path* and *magnitude (co)homology* generalize classical techniques (though we do not specifically elaborate on the generalization aspects here) while also permitting applications to new types of data, most notably weighted digraphs and even directed hypergraphs. Because these techniques—each of which we briefly discuss in turn below—construct chain complexes directly from the data structures that they apply to, without any need to construct an intervening simplicial complex, they are particularly suited for novel applications that can give rise to new capabilities.

2. Path homology. Here we sketch the basic elements of *path homology* as treated in [36, 13].³ Let R be a ring and consider the free modules $R^X \cong R^{|X|}$ with standard basis $\{e_x : x \in X\}$; also, set $R^\emptyset := \{0\}$. Next, let $D = (V, A)$ be a loopless digraph, and consider the *non-regular boundary operator* $\partial_{[k]} : R^{V^{k+1}} \rightarrow R^{V^k}$ defined as the linear map whose action on the standard basis is

$$\partial_{[k]} e_{(v_0, \dots, v_k)} = \sum_{j=0}^k (-1)^j e_{\nabla_j(v_0, \dots, v_k)},$$

where $\nabla_j(v_0, \dots, v_k) := (v_0, \dots, v_{j-1}, v_{j+1}, \dots, v_k)$ is the result of deleting v_j from $(v_0, \dots, v_k)$. A few lines of algebra focused on index bookkeeping shows that $\partial_{[k-1]} \circ \partial_{[k]} \equiv 0$, i.e. $(R^{V^{k+1}}, \partial_{[k]})$ is a chain complex.

Path homology arises indirectly from another chain complex that is derived from $(R^{V^{k+1}}, \partial_{[k]})$. Consider the set

$$\mathcal{A}_k(D) := \{(v_0, \dots, v_k) \in V^{k+1} : (v_{j-1}, v_j) \in A, 1 \leq j \leq k\}$$

of *allowed k -paths*, with $\mathcal{A}_0 := V$, $V^0 \equiv \mathcal{A}_{-1} := \{0\}$ and $V^{-1} \equiv \mathcal{A}_{-2} := \emptyset$. Write

$$\Omega_k := \{\omega \in R^{\mathcal{A}_k} : \partial_{[k]} \omega \in R^{\mathcal{A}_{k-1}}\},$$

$\Omega_{-1} := R^{\{0\}} \cong R$, and $\Omega_{-2} := R^\emptyset = \{0\}$. Now $\partial_{[k]} \Omega_k \subseteq R^{\mathcal{A}_{k-1}}$, so $\partial_{[k-1]} \partial_{[k]} \Omega_k = 0 \in R^{\mathcal{A}_{k-2}}$ and $\partial_{[k]} \Omega_k \subseteq \Omega_{k-1}$. The *(non-regular) path complex* of D is accordingly defined to be the chain complex (Ω_k, ∂_k) , where $\partial_k := \partial_{[k]}|_{\Omega_k}$.⁴ The *(non-regular) path homology* of D is just the homology of the path complex (Ω_k, ∂_k) .⁵

A simple example illustrating the mechanics of path homology is provided by the digraphs D_1 and D_2 in Fig. 1. $\mathcal{A}_1(D_1)$ and $\mathcal{A}_1(D_2)$ are given by the digraph arcs, $\mathcal{A}_2(D_1) = \emptyset$, and $\mathcal{A}_2(D_2) = \{(w, x, z), (w, y, z)\}$. We have $\partial_{[1]}(e_{(i,j)} - e_{(i,k)} - e_{(l,j)} +$

³See also a series of papers including [37, 42, 38]. There are associated notions of cohomology [21, 22, 40, 41] and homotopy [39, 34]; the constructions of [7, 9] are closely related for the case of undirected graphs. Persistent path homology is introduced in [14] and an algorithm for computing it in dimension one is in [19]. There are extensions of path homology to (among other structures) hypergraphs [35] and directed hypergraphs [61], as well as an associated discrete Morse theory [59].

⁴The implied *regular path complex* prevents a directed 2-cycle from having nontrivial 1-homology. In our view non-regular path homology is simpler, richer, and more likely useful in applications. As a practical matter, our rationale amounts to the convention that a directed 2-cycle counts as a “hole.”

⁵For convenience, we generally replace the path complex (Ω_k, ∂_k) with its *reduction* $\dots \Omega_{k+1} \xrightarrow{\partial_{k+1}} \Omega_k \xrightarrow{\partial_k} \Omega_{k-1} \xrightarrow{\partial_{k-1}} \dots \xrightarrow{\partial_1} \Omega_0 \xrightarrow{\partial_0} R \longrightarrow 0$. Assuming the original complex is nondegenerate, this has the minor effect $\tilde{H}_0 \oplus R \cong H_0$, while $\tilde{H}_k \cong H_k$ for $k > 0$.

$e_{(l,k)} = 0$, and similarly $\partial_{[1]}(e_{(x,z)} + e_{(w,x)} - e_{(y,z)} - e_{(w,y)}) = 0$. Now $\partial_{[2]}e_{(w,x,z)} = e_{(x,z)} - e_{(w,z)} + e_{(w,x)} \notin R^{\mathcal{A}_1(D_2)}$ and $\partial_{[2]}e_{(w,y,z)} = e_{(y,z)} - e_{(w,z)} + e_{(w,y)} \notin R^{\mathcal{A}_1(D_2)}$ (because the arc $w \rightarrow z$ is not present), but

$$\begin{aligned} \partial_{[2]}(e_{(w,x,z)} - e_{(w,y,z)}) &= e_{(x,z)} - e_{(w,z)} + e_{(w,x)} - e_{(y,z)} + e_{(w,z)} - e_{(w,y)} \\ &= e_{(x,z)} + e_{(w,x)} - e_{(y,z)} - e_{(w,y)} \in R^{\mathcal{A}_1(D_2)}. \end{aligned}$$

It follows that $H_1(D_1) = R$ and $H_1(D_2) = \{0\}$, i.e., the Betti numbers are different: $\beta_1(D_1) = 1$ and $\beta_1(D_2) = 0$.

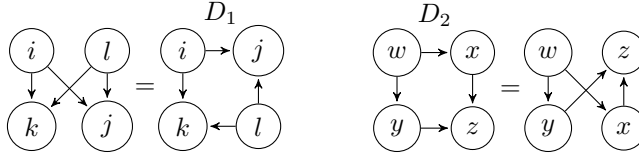


FIG. 1. The digraph D_2 has trivial path homology but the digraph D_1 does not. The nontrivial path homology of D_1 can be interpreted as a consistent and robust unidirectional flow. The trivial path homology of D_2 can be attributed to w and z appearing as “bottlenecks” that prevent robustness of the flow. This intuition is formalized by results in [12].

We note that there is good evidence that path homology provides a robust characterization of neural network architectures [12], a stronger variant of cyclomatic complexity [46], and that it can identify salient motifs and behavior in temporal networks [13]. Path homology is also phenomenologically rich, exhibiting torsion and nonvanishing homology in dimension three for various digraphs with just six vertices.

3. Magnitude homology. We follow the concise formulation of [44]. Let (X, d) be a Lawvere metric space, i.e., d is an extended quasipseudometric.⁶ A k -simplex in X is an ordered tuple $x^{(k)} := (x_0, \dots, x_k) \in X^{k+1}$ such that adjacent entries are distinct; its *length* is $\lambda(x^{(k)}) := \sum_{j=1}^k d(x_{j-1}, x_j)$. The $\mathbb{R}$ -graded *magnitude chain complex* has k -chains (where as before R is a coefficient ring)

$$MC_{k,L}(X) := R \left\{ x^{(k)} \text{ a } k\text{-simplex in } X : \lambda(x^{(k)}) = L \right\}$$

and differential $\partial_k : MC_{k,L}(X) \rightarrow MC_{k-1,L}(X)$ given by

$$\partial_k := \sum_{j=1}^{k-1} (-1)^j \partial^{(j)}$$

with

$$\partial^{(j)}(x^{(k)}) := \begin{cases} \nabla_j x^{(k)} & \text{if } d(x_{j-1}, x_{j+1}) = d(x_{j-1}, x_j) + d(x_j, x_{j+1}) \\ 0 & \text{otherwise,} \end{cases}$$

and where as before ∇_j acts on a tuple by deleting the corresponding entry. The appropriate notion of chain map is induced by distance-nonincreasing maps.

⁶Here “extended” means $d : X \times X \rightarrow [0, \infty]$; “quasi” means d need not be symmetric, and “pseudo” means that $d(x, x)$ need not be zero. A Lawvere metric space is best thought of here as a category enriched over the poset $([0, \infty], \geq)$, not least because the theory of magnitude (co)homology applies to enriched categories with a suitable notion of “size.”

The *magnitude homology* of X is the homology of the magnitude chain complex. Conveniently for a digraph D , there is a direct sum decomposition of the form

$$MC_{\bullet,L}(D) = \bigoplus_{s,t \in V(D)} MC_{\bullet,L}^{(s,t)}(D)$$

where the direct summands on the right are subcomplexes generated by simplices with initial and terminal entries s and t , respectively [5]. This provides a very specific algebraic structure and a reduction in computational complexity that makes magnitude homology particularly convenient for unweighted (or $\mathbb{Z}_+$ -weighted) digraphs.⁷

The dual theory of magnitude cohomology has an analogue of the cup product [44]. This additional ring structure allows magnitude cohomology to completely determine its underlying space up to isometry for finite extended quasi-metric spaces, such as digraphs and finite metric spaces. By comparison, trees on the same number of vertices have isomorphic magnitude (co)homology *groups*.

These constructs all generalize to the setting of enriched categories, and we sketch a slightly nontrivial construction likely to be of interest and use. There is an enriched category of sub-flow graphs of a given flow graph in the sense of [45], and it can be shown that the topological entropy (roughly, the logarithmic rate of growth of the number of possible paths as a function of length [52]) of such a flow graph with its (unique) entry and exit identified is a suitable “size function” over the max-plus semiring. This setup dovetails nicely with the direct sum decomposition above, and a categorification of these observations would presumably yield an interesting and efficiently computable instance of magnitude (co)homology, with representatives that encode detailed structural information. Meanwhile, there are effective normalization procedures to represent control flow graphs of the sort compilers actually produce in this way, so the theory has sufficient scope for genuine applications to be possible.

Besides the notional application sketched above, another interesting situation ripe for investigation/application is a graph with probability distributions on the vertices. By computing Bregman (e.g., Kullback-Leibler) divergences between adjacent distributions, we obtain an asymmetric weighted graph suited for analysis via (blurred) magnitude homology (or even just the decategorification into *magnitude* [58, 57]).

Finally, it seems likely that magnitude homology will also be useful for characterizing DAGs, and an interesting problem is to develop a formula akin to that in [12] for the path homology Betti numbers of DAGs that correspond to densely connected multilayer perceptrons. For example, the DAG underlying a densely connected multilayer perceptron with consecutive layers of 5, 4, 3, and 2 neurons has only a single nontrivial Betti number in path homology, viz. $\beta_3 = 24$, whereas a computer calculation yields the more complicated magnitude homology Betti numbers $\beta_{1,1} = 38$, $\beta_{2,2} = 61$, and $\beta_{3,3} = 60$ (recall that the second index is for the length grading): all other Betti numbers are zero except for $\beta_{0,0}$, which is just the number of vertices.

4. Proto-topological and geometrical tools. Sheaves [31, 73], (positive) Ricci curvatures and geodesics [62, 80] each control topological properties of spaces they are associated with. These objects also have analogues in the discrete setting that inherit properties familiar from traditional continuous or smooth contexts, while also being amenable to computational implementation.⁸ As such, they are likely to

⁷Notably, magnitude homology is related to Vietoris-Rips homology via a “blurring” procedure that essentially replaces equalities of the form $\lambda = L$ in the definition of the chain complex with inequalities $\lambda \leq L$ [68, 11, 33], and it is also closely related to path homology [4].

⁸See, e.g. <https://github.com/kb1dds/pysheaf>.

find progressively more useful applications adjacent to topological invariants.

4.1. Sheaves. For heterogeneous data, sheaves are the representational framework *par excellence* [70]. Without belaboring definitions, sheaves provide the mathematical framework assembling global data from local data. In this context it is natural that they should be used to model communications networks [71, 72, 47] and the process of data fusion [74, 78, 75, 50, 76].

This data fusion process, predicated on a *consistency radius*, requires a reasonable (pseudo)metric on observations. While for many applications to cybersecurity this can be a challenging if not prohibitive obstacle, it is probably less of one in the important case of networked cyber-physical systems, where models can inform the construction of a metric on observable data [1, 56, 8, 88]. In particular, hierarchical classifications and their corresponding ultrametrics are readily constructible in practice, and these have the advantage of being realizable in Euclidean space via a Cholesky decomposition of a (finite) distance matrix. Such a construction (which we note can avoid the need for continuous models/metrics in a way analogous to how the homology theories of preceding sections avoid constructing simplicial complexes) can be lifted to sequences of observed data that could then be meaningfully fused using sheaf-theoretical techniques.

4.2. Curvatures. For a reasonably up-to-date overview of discrete notions of curvature, see [63]. Various such notions exist, e.g. the Ollivier-Ricci curvature for metric spaces [66, 67] and directed hypergraphs [26]; and Forman-Ricci curvature for directed graphs, simplicial complexes [83] and hypergraphs [55]. These yield complementary tools for network science applications [54] and jointly provide features that can statistically distinguish between different model network ensembles. Other variants of Ricci curvature have also been constructed for {weighted, directed, hyper}graphs: see, e.g. [82].

Applications of such discrete curvatures include analysis of neural network architectures [82]; graph matching [64] and community detection [65, 85]; and addressing congestion in communication [90] and power networks [48]. Coming full circle, discrete curvatures also inform the construction of persistent topological invariants [81].

4.3. Geodesics. *Gromov-Wasserstein distance* [60, 87] is a Riemannian geodesic distance on the space of (isomorphism classes of) metric measure spaces. It can be computed using optimal transport methods, and algorithms based on this insight have enabled state-of-the-art performance for matching—and meaningfully interpolating between—discrete structures such as (hyper)graphs endowed with measures [92, 91, 15, 16, 17] and (via word embeddings) unsupervised translation [2].

5. Conclusion. A recurring theme that we have sought to illustrate is that while topological and adjacent methods may have been (and likely often still are) thought of as implicitly inappropriate for fundamentally discrete data and problems, the opposite is actually true. Recently developed topological invariants and adjacent geometrical constructions are amenable to computation *in silico* and can enable new capabilities for discrete data that are ubiquitous in cybersecurity, network science, and machine learning.

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