SIAM AG / Applications of Magnitude and Magnitude Homology to Network Analysis

Prospects for applications of magnitude homology

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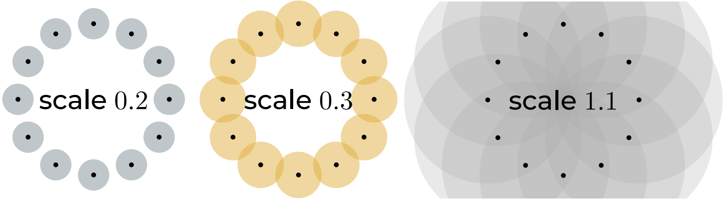
Contents

1. **Context** from mainstream topological data analysis to discrete tools
2. **Magnitude homology** with the briefest nod towards cyber applications
3. **Examples** in the vein of neural stuff (feedforward nets and actual brains)

Mainstream TDA has a playbook

- Approximate $\{X_j\}_{j=1}^n \subset (\mathbb{R}^d)^n$ at various scales
- Compute a topological invariant of each approximation
- Highlight invariants that persist across scales
- E.g., 12 equispaced points on the unit circle (half-distance $\Delta \approx 0.2588$)
  - $\beta_0 = 12 \cdot 1_{[0,\Delta)} + 1_{[\Delta,1)} + 1_{[1,\infty)}$
  - $\beta_1 = 1_{[\Delta,1)}$



We are going to play a simpler game

CATEGORY CAPITAL

- Data that interests us is fundamentally discrete
  - Approximate **nothing** (via representation or model if need be)
  - Compute a (co)chain complex **directly from the data**: simplicial complexes are optional technical devices
  - Highlight any persistence **incidentally**: it often won't apply

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- Archetype: Dowker homology
  - Relation corresponds to a pair of homotopy equivalent simplicial complexes
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- Many well known discrete tools are underutilized
  - Finite topological spaces *per se*
  - Simplicial complexes generated by posets/hypergraphs
  - Discrete Morse theory
  - ...

This simpler game has practical relevance

- Dowker applications:
    - Witness complexes
    - Systems/sociology
    - Robotics
    - Neuroscience
    - Privacy
    - Software engineering
    - ...
    - Exercises for audience: cyber interactions like user/computer; process/file; etc

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- Magnitude homology for digraphs is suited for novel applications…
  - …that can give rise to new capabilities
  - Cf. path homology, which is related but lacks *ab initio* source/target specificity

Magnitude homology is readily constructed

CATEGORY CAPITAL

- Let (X, d) be a Lawvere metric space $\Leftrightarrow$ d = extended quasipseudometric
  - $d : X \times X \to [0, \infty]$ (extended)
  - d need not be symmetric (quasi-)
  - $d(x, x)$ need not be zero (pseudo-)
  - (X, d) best thought of here as a category enriched over the poset $([0, \infty], \geq)$

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- A k-*simplex* in X is an ordered tuple $x^{(k)} := (x_0, \ldots, x_k) \in X^{k+1}$ s.t. $x_j \neq x_{j-1}$
- The *length* of $x^{(k)}$ is $\lambda(x^{(k)}) := \sum_{j=1}^{k} d(x_{j-1}, x_j)$

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The $\mathbb{R}$-graded *magnitude chain complex* (as before R is a coefficient ring):

- k-chains: $MC_{k,L}(X) := R\left\{x^{(k)} \text{ a } k\text{-simplex in } X : \lambda(x^{(k)}) = L\right\}$
- differential: $\partial_k : MC_{k,L}(X) \to MC_{k-1,L}(X)$ given by $\partial_k := \sum_{j=1}^{k-1} (-1)^j \partial^{(j)}$
  - $\partial^{(j)}(x^{(k)}) := \nabla_j x^{(k)}$ if $d(x_{j-1}, x_{j+1}) = d(x_{j-1}, x_j) + d(x_j, x_{j+1})$ and $:= 0$ otherwise
- Appropriate notion of chain map is induced by d-nonincreasing maps

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The *magnitude homology* of X…

…is the homology of the magnitude chain complex

MH has attractive features

CATEGORY CAPITAL

- For a digraph D, there is a decomposition of the form

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

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- *Magnitude cohomology* has an analogue of the cup product
  - Ring structure determines the space for finite extended quasi-metric spaces
    - E.g., digraphs; finite metric spaces
  - Meanwhile, tree magnitude (co)homology *groups* only depend on #(vertices)

MH generalizes to enriched categories

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- Consider enriched category of sub-flow graphs of a given flow graph
  - For semicartesianness, take a specific category $\mathbf{F}$ of “two-terminal graphs”
    - Presents some technical issues for decomposition (probably surmountable)
  - The topological entropy is a “size function” over the max-plus semiring
    - Recall this is log rate of growth of possible paths as a function of length
  - This setup dovetails with the source-target direct sum decomposition
  - A categorification might be interesting and efficiently computable
    - Representatives might encode nice structure
  - Possibility to connect to useful cyber applications via compilers
- More ambitiously, consider $\mathbf{F} \times \mathbf{M}$ where $\mathbf{M}$ is a “matrix category” of data
  - Size function may be something like the zeta function of a Markov chain
- Suitable data obtainable from program analysis
  - Simpler initial goal: use hitting probabilities metric of Boyd *et al.* (this is vanilla)

MH measures nonconvexity

Let $P_{p,n}$ be the DAG formed from p parallel paths of n arcs from 1 to $(n-1)p+2$

Then all the Betti numbers are zero except for

$$\beta(P_{p,n})_{0,0} = |V(P_{p,n})| = (n-1)p+2;$$

$$\beta(P_{p,n})_{1,1} = |A(P_{p,n})| = np,$$

and

$$\beta(P_{p,n})_{2,n} = p-1;$$

i.e., there are $p-1$ “convexity defects” of length n in homology dimension 2

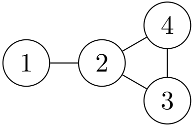
Measuring nonconvexity may be useful from the PoV of flows/routing

Besides information/transportation networks, neural stuff is also interesting

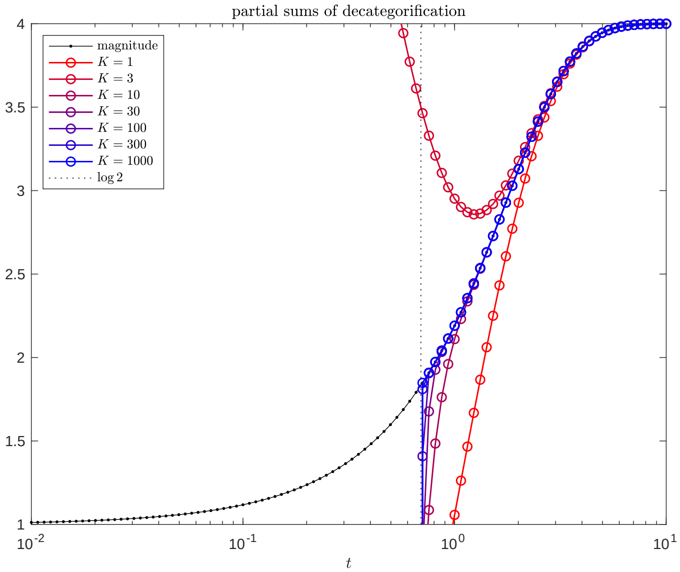
Categorification helps analyze magnitude

CATEGORY CAPITAL

Magnitude homology of



decategorifies like magnitude as shown



Categorification helps analyze weighting

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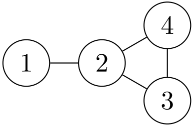

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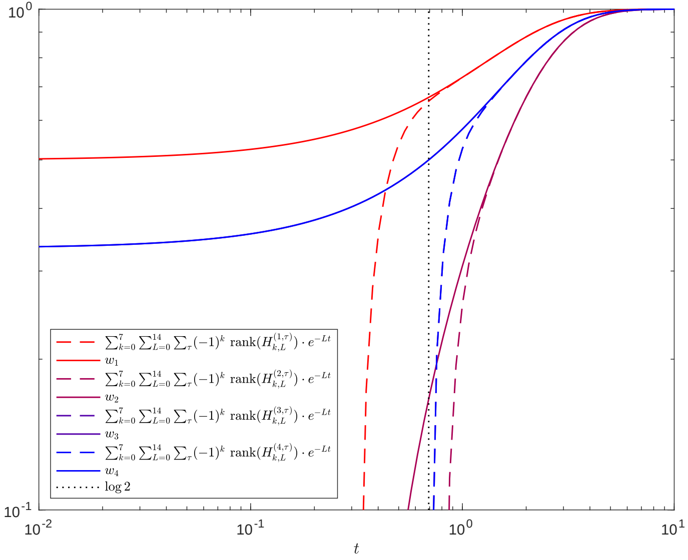
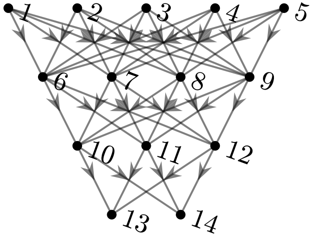


DAGs are very nicely handled

Magnitude homology of *multilayer perceptron* (MLP) $K^{\rightarrow}_{5,4,3,2}$



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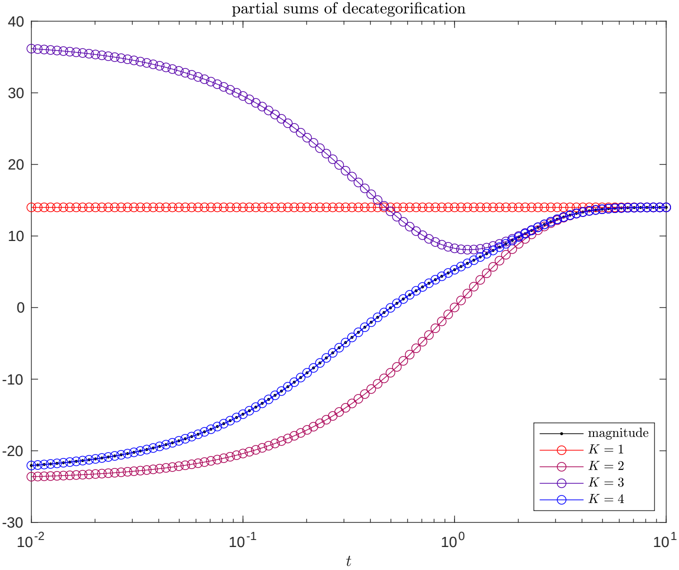

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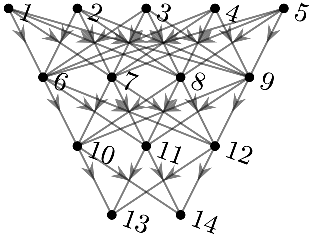
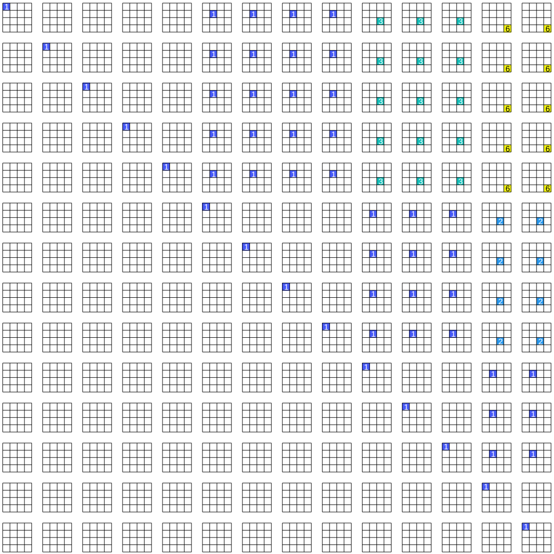


has Betti numbers shown



Fully connected MLPs have simple MH

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- Let $N_\ell := \sum_{i=1}^{\ell} n_i$, $e_{(\ell)} := \sum_{j=N_{\ell-1}+1}^{N_\ell} e_j$, and $B[x_1, \ldots, x_{L-k}; n] := \sum_{\ell=1}^{L-k} x_\ell e_{(\ell)}^T e_{(\ell+k)}$
  - E.g. $A = B[1_1, \ldots, 1_{L-1}; n]$

The preceding slide's mechanics suggest the conjecture (exercise)

For $k > 1$, $\beta_{k+1,m}^{(s,t)}(K_{n_1,\ldots,n_L}^{\rightarrow}) = \delta_{k+1,m} \cdot \left(B\left[\prod_{\ell=2}^{k+1}(n_\ell - 1), \ldots, \prod_{\ell=L-k}^{L-1}(n_\ell - 1); n\right]\right)_{st}$

Note that we automatically have $\beta_{0,m}^{(s,t)} = \delta_{0m}\delta_{st}$ and $\beta_{1,m}^{(s,t)} = \delta_{1m}A_{st}$

Examples:

$\beta(K_{5,4,3,2}^{\rightarrow}) = \text{diag}(14, 38, 61, 60, 0, 0, \ldots)$
$\beta(K_{2,11,3,7,5}^{\rightarrow}) = \text{diag}(28, 111, 304, 940, 1200, 0, 0, \ldots)$
$\beta(K_{10,2,8,4,6}^{\rightarrow}) = \text{diag}(30, 92, 280, 532, 1260, 0, 0, \ldots)$

Sparsely connected MLPs are more relevant

Sparsity arises via (e.g.) pruning small edge weights in trained networks

"Lottery tickets" exhibit hierarchical modularity [Patil, Michael, and Dovrolis]

Magnitude homology might usefully indicate structure...

...insofar as it manifests as "convexity defects" that differ from a null model

We provide some *very preliminary* supporting evidence

Sparse interconnections of MLPs and sparsification of a single MLP both induce off-diagonal magnitude homology, but differently

Sparse interconnections ⇒ off-diagonals

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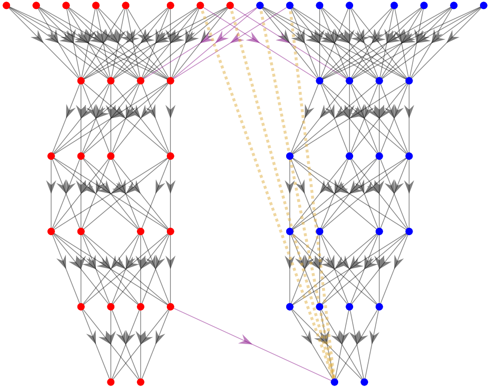
$$\beta = \begin{pmatrix} 52 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 182 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 436 & 0 & 0 & 4 & 0 & \cdots \\ 0 & 0 & 0 & 1020 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 2196 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 2646 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$



Off-diagonal contributions indicated by dotted lines from sources to targets

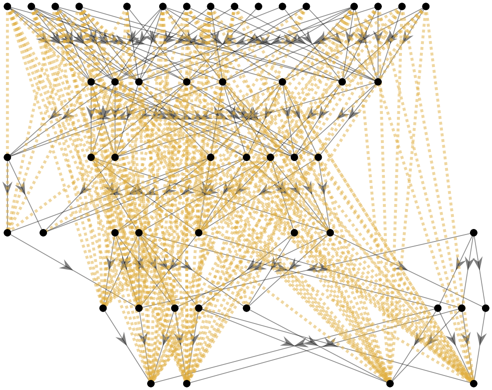
Vertices colored by undirected Fiedler vector (i.e., spectral) bipartition; traversing arcs are purple

Sparsification ⇒ off-diagonals (differently)

$$\beta = \begin{pmatrix} 52 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 143 & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 164 & 44 & 5 & 0 & 0 & \dots \\ 0 & 0 & 0 & 71 & 71 & 38 & 0 & \dots \\ 0 & 0 & 0 & 0 & 2 & 47 & 0 & \dots \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Off-diagonal contributions indicated by dotted lines from sources to targets

Keeping $\approx 2/5$ of arcs in $K^{\rightarrow}_{16,8,8,8,8,4}$



This may be useful in practice

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Deep neural networks are functionally sparsified and modular

Weight filtrations (for sparsity) and quantizations (for efficiency) are common

A "null model" of IID arc weights may actually be fairly realistic

Neural networks are initialized randomly; training finds one of many extrema

For a DAG the dimensions of simplices and lengths are bounded

In this case numerics largely suffice: e.g. the (de)categorification formula

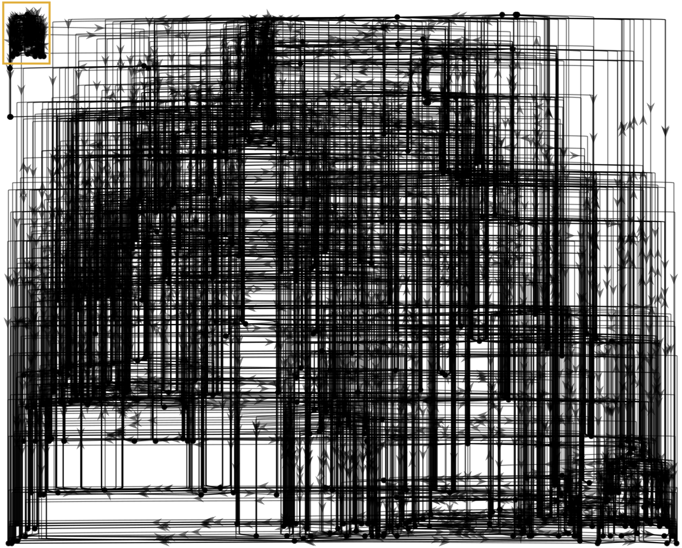
$$((\exp[-\tau d])^{-1})_{st} \overset{\tau \gg 0}{=} \sum_{k,L} (-1)^k \text{rank}\left(MH_{k,L}^{(s,t)}\right) \exp(-\tau L) = \sum_L \chi_{\bullet,L}^{(s,t)} \exp(-\tau L)$$

can exactly produce $\chi_{\bullet,L}^{(s,t)}$ via Laplace transform *without ever computing* MH

Consider a whole-animal connectome

Whole-animal chemical connectome of hermaphroditic *Caenorhabditis elegans* (nematode) is a digraph with 454 vertices and 4879 arcs (see https://wormwiring.org)

The pharynx subconnectome with 50 vertices and 242 arcs is in the box at upper left



The pharynx has off-diagonal 2-homology

CATEGORY CAPITAL

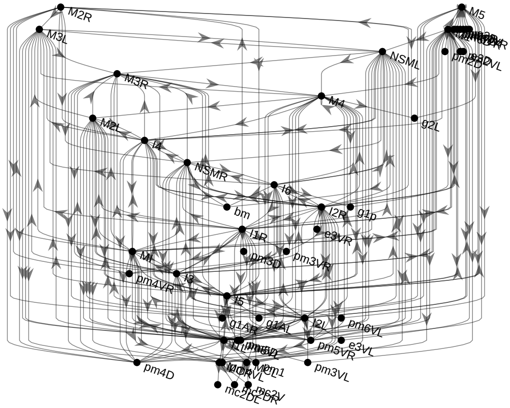
$$\beta = \begin{pmatrix} 50 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 241 & 0 & 0 & 0 & 0 & 0 & 0 & \dots \\ 0 & 0 & 1290 & 11 & 0 & 9 & 13 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Off-diagonal 2-homology is intricate

The subconnectome is not Menger convex or geodetic; it has 4-cuts

Exercise: ∃ biological significance?

E.g., 10/11 reps for $(k, L) = (2, 3)$ either have source neurons M2R, M3R, or NSML, or have target neuron MCR



Takeaways

CATEGORY CAPITAL

Magnitude homology might be considered too abstract for real applications

But this would be a mistake

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Magnitude homology is amenable to computation *in silico*

It can enable new capabilities for fundamentally discrete data and problems that are ubiquitous in network science, machine learning, and cybersecurity

Thanks

MATLAB code at
https://github.com/SteveHuntsman/MagnitudeHomology