Harmonic methods in computational topology

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  ATMCS II, 2004-July-20

- Ideas arising from work with Gunnar Carlsson at Stanford University

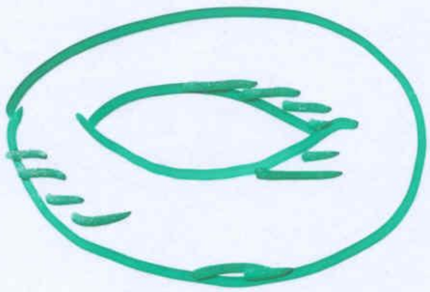
Today's goal

- Persistent homology is a successful and robust framework for studying the topology of point cloud data sets.

- I wish to develop an alternative framework based on discrete Laplacian matrices.

- Humble intentions: no desire to overthrow persistent homology; simply to explore some other ideas.

Topology for point-cloud data

-  If X is a space, ← eg torus we can use algebraic topology to describe its qualitative features.

- Invariants: $\pi_1(X)$, $H_*(X)$, $b_*(X)$

  fundamental group — homology — betti numbers

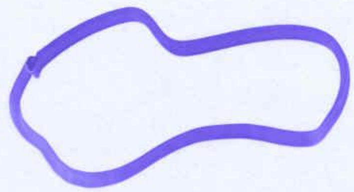
- 

  point-cloud torus

  Can we compute these invariants from a finite sample of points?

Standard Pipeline (FIRST ATTEMPT)

hidden space X

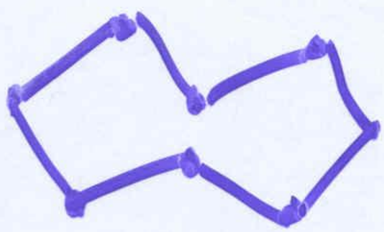


$\downarrow$

sample $Y \subset X$

$\downarrow$

Simplicial complex $S(Y)$



$\downarrow$

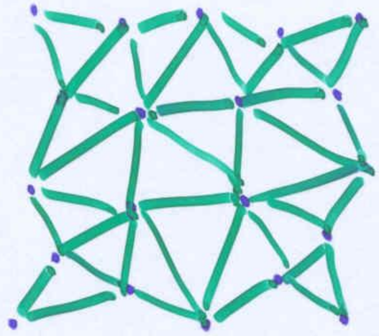
Betti numbers $b_n(S(Y))$

$b_0 = 1$
$b_1 = 1$
$b_n = 0 \quad (n > 1)$

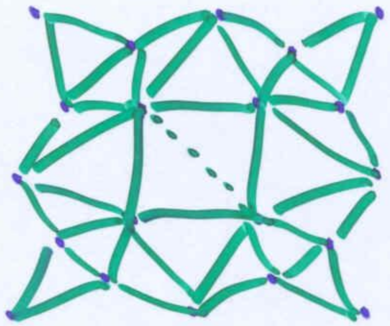
Fundamental problem

Betti numbers are DISCRETE.

Point-cloud sampling is CONTINUOUS



No hole

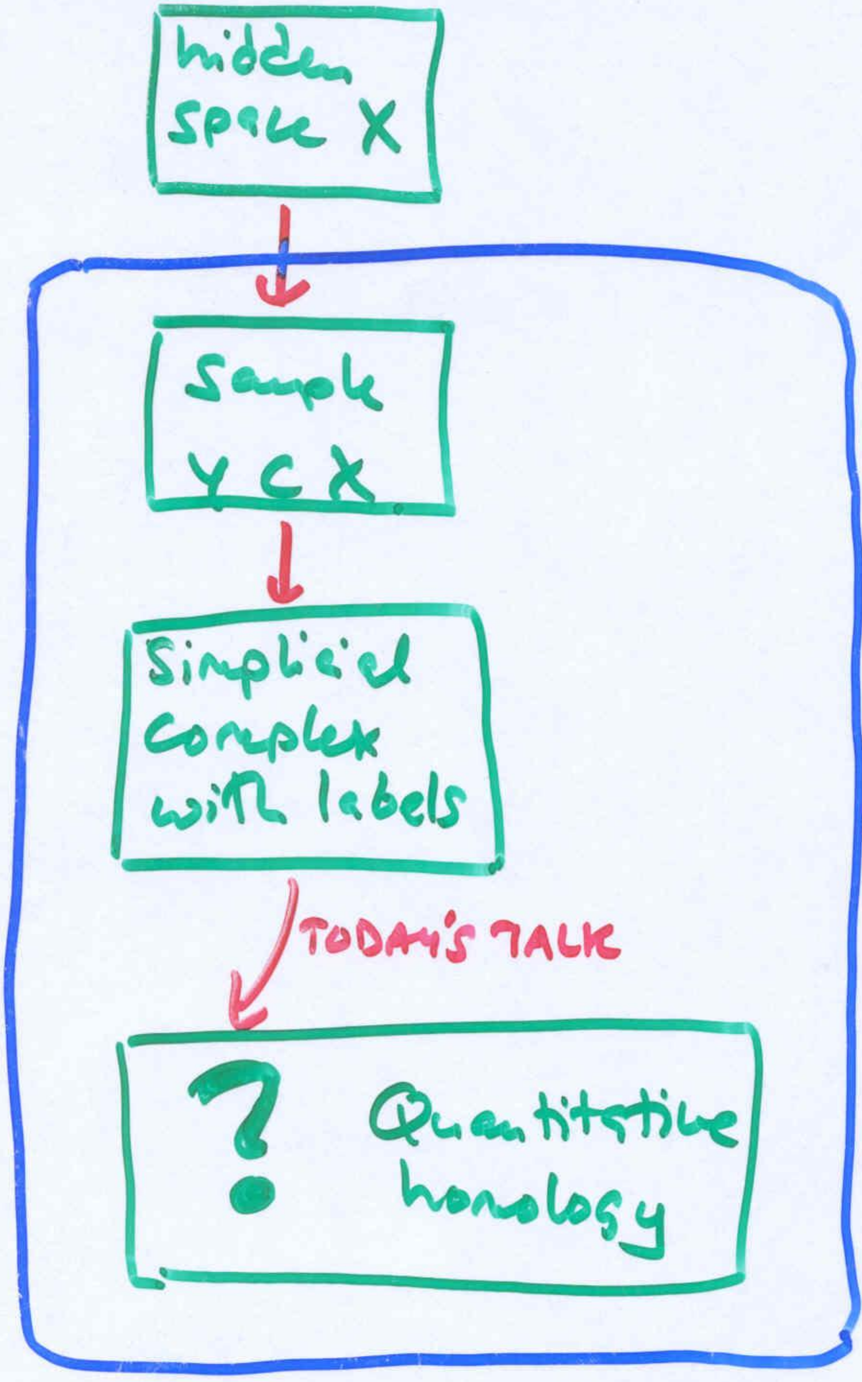


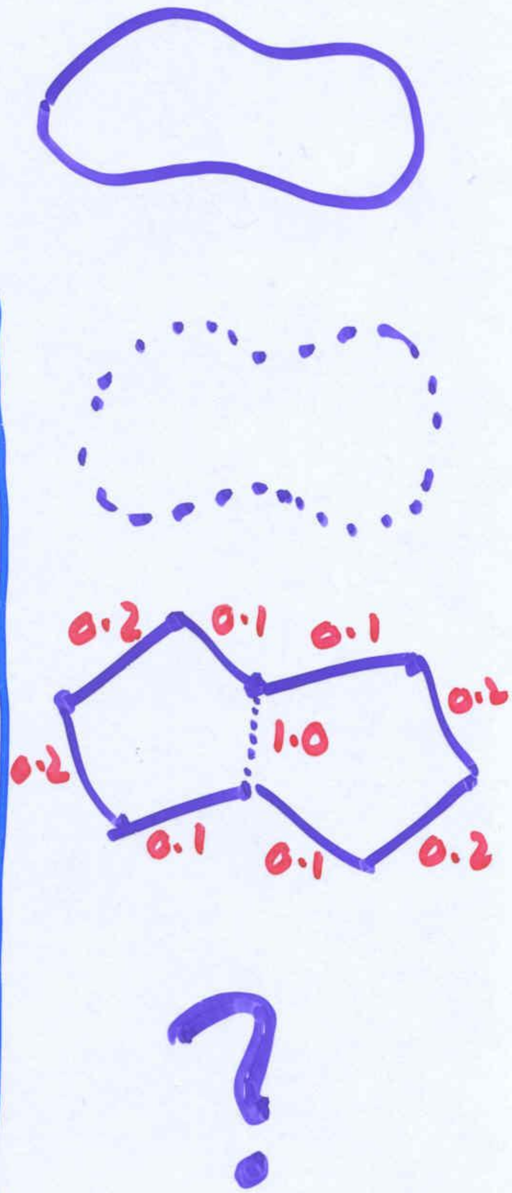
hole?

Hole!

Standard Pipeline

(REVISED ATTEMPT)





What form should "quantitative homology" take?

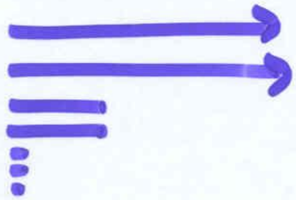
Superb Example

- Labels : the "diameter" of each cell
- Interpret labels as "time of birth".
- Persistent homology.

  [Edelsbrunner, Letscher, Zomorodian]

- Output : bar codes

  eg :



- Continuous parameters (interval length):

  Good feature / bad feature

rather than just :

feature

Today : Harmonic methods.

Basic idea :

- Discrete Laplacian Δ_k
- $\mathcal{H}_k := \operatorname{Ker}(\Delta_k) \cong H^k$
- harmonic cycles carry geometric information
- Also consider eigenfunctions

$$\Delta_k f = \lambda f$$

where λ is close to 0.

"near miss" homology

cf. (Kac) "Can one hear the shape of a drum?"

- Definition of Δ_k can be made to depend on weights.

Constructing the Laplacian

- Given a chain complex over $\mathbb{R}$:

$$\cdots\ C_{k-1} \xleftarrow{\partial_k} C_k \xleftarrow{\partial_{k+1}} C_{k+1}\ \cdots$$

- Given an inner product structure on each C_k we can form adjoints $\partial_k^* =: \delta_k$ for each k.

- Thus:

$$\cdots\ C_{k-1} \underset{\partial_k^*}{\overset{\partial_k}{\rightleftarrows}} C_k \underset{\partial_{k+1}^*}{\overset{\partial_{k+1}}{\rightleftarrows}} C_{k+1}\ \cdots$$

- Define the Laplacian

$$\Delta_k = \partial_k^* \partial_k + \partial_{k+1} \partial_{k+1}^*$$

- Claim: $\mathcal{H}_k := \mathrm{Ker}(\Delta_k) \cong \dfrac{\mathrm{Ker}(\partial_k)}{\mathrm{Im}(\partial_{k+1})} =: H_k$

Proof:

- In general, $A^*Ax = 0 \iff Ax = 0$

  Why? $\langle A^*Ax, x\rangle = \langle Ax, Ax\rangle = \|Ax\|^2$

  So if $A^*Ax = 0$ then $\|Ax\| = 0 \Rightarrow Ax = 0$.

- In general, $(A^*A + B^*B)x = 0$

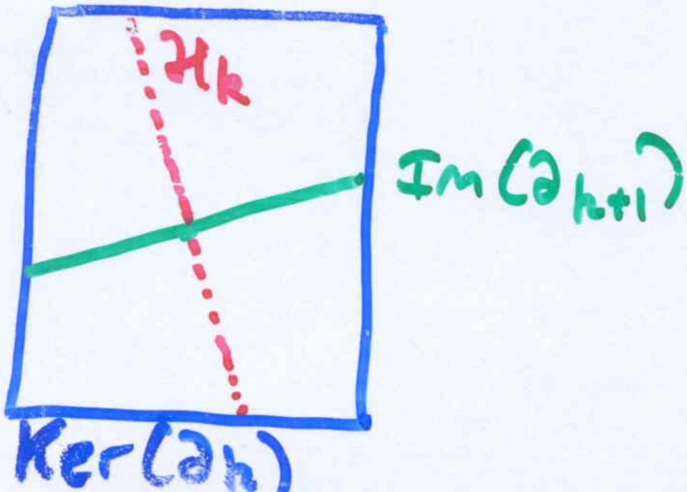
  $\iff Ax = 0$ and $Bx = 0$

  Why? $\langle (A^*A + B^*B)x, x\rangle$

  $= \|Ax\|^2 + \|Bx\|^2$ etc.

- Thus: $\Delta_k x = 0 \iff \partial_k x = 0$ & $\partial_{k+1}^* x = 0$

  $x \in \mathrm{Ker}(\partial_k)$ $\qquad$ $x \perp \mathrm{Im}(\partial_{k+1})$



- If C_k is finite dimensional, then we are done. $\square$

Aside: Classical Hodge theory.

- de Rham Complex

$$\Omega^0(M) \xrightarrow{d_0} \Omega^1(M) \xrightarrow{d_1} \cdots$$

Define $\Delta_k = d_k^* d_k + d_{k-1} d_{k-1}^*$

- In three dimensions, $U \subset \mathbb{R}^3$

$$C^\infty(U, \mathbb{R}) \xrightarrow{\nabla} C^\infty(U, \mathbb{R}^3) \xrightarrow{\nabla\times} \cdots$$

$$C^\infty(U, \mathbb{R}^3) \xrightarrow{\nabla\cdot} C^\infty(U, \mathbb{R})$$

(grad, curl, div)

- $\Delta_0 := -\nabla\cdot\nabla = -\sum_{i=1}^{3} \frac{\partial^2}{\partial x_i^2}$
- $\Delta_1 := \nabla\times\nabla\times\_ - \nabla(\nabla\cdot\_) = -\nabla\cdot(\nabla\_)$
- Proof that $\mathrm{Ker}(\Delta_k) \cong H_k$ is harder.

In the finite setting:

- Compute homology as ~~[illegible]~~

  $$\mathrm{Ker}(\Delta_k) =: \mathcal{H}_k = \langle f_1, \dots, f_b \rangle$$

  orthonormal, $b = b_k$

Attractions of this idea

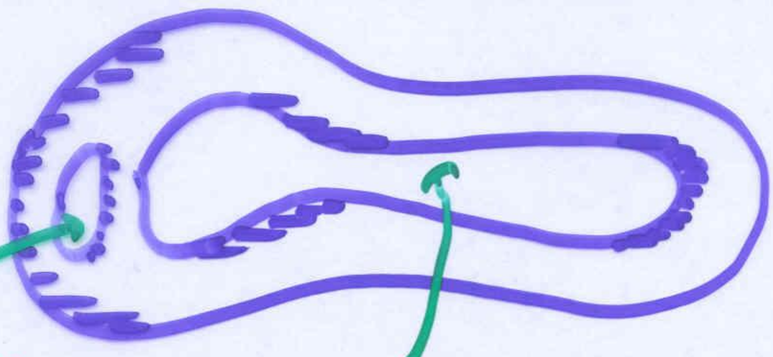
- No need to form "quotient".
- Given any k-cycle g, in homology g is equivalent to:

  $$P_{\mathcal{H}} g := \sum_{i=1}^{b} \langle g, f_i \rangle f_i$$

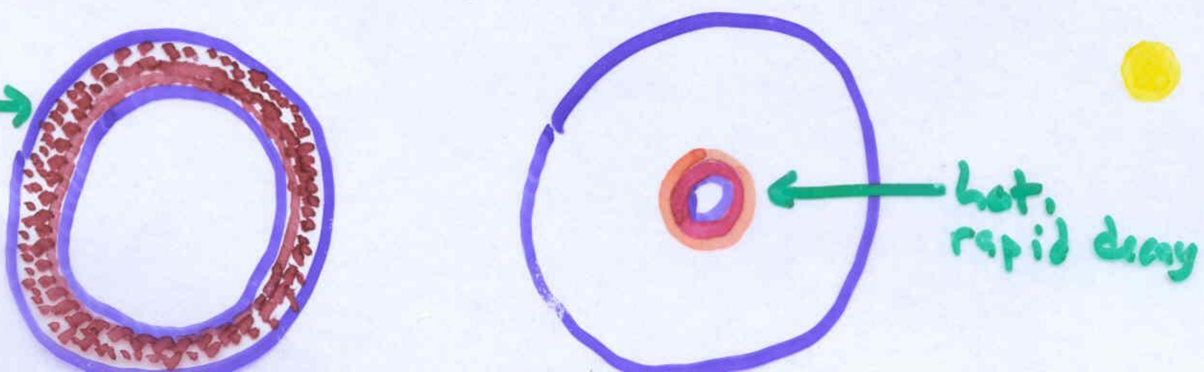
- (Wave hands) the harmonic cycles are geometrically "natural" and carry "useful" information.

Local features and Global features

- Homological features can be local or global, to different degrees.



- It turns out (empirical evidence, suggestive calculations with differential forms) ... that harmonic cycles concentrate their energy
  - strongly, along local features
  - weakly, along global features



L^p-comparison

Let f be a k-cycle.

If σ is a k-cell, $f(\sigma) \in \mathbb{R}$.

When is f locally concentrated?

- Define L^p-norm

$$\|f\|_p := \left[\sum_\sigma |f(\sigma)|^p\right]^{1/p}$$

- If $1 \leq p < q$, then consider ratio:

$$\left(\frac{\|f\|_p}{\|f\|_q}\right) \quad \begin{array}{l} \underline{\text{small}} \longleftrightarrow \underline{\text{localized}} \\ \underline{\text{large}} \longleftrightarrow \underline{\text{global}} \end{array}$$

- Example: $f_n = (1, 0, \ldots, 0) \in \mathbb{R}^n$

$$g_n = \left(\tfrac{1}{\sqrt{n}}, \tfrac{1}{\sqrt{n}}, \ldots, \tfrac{1}{\sqrt{n}}\right) \in \mathbb{R}^n$$

Then $\|f_n\|_2 = \|g_n\|_2 = 1$ (L^2-norm)

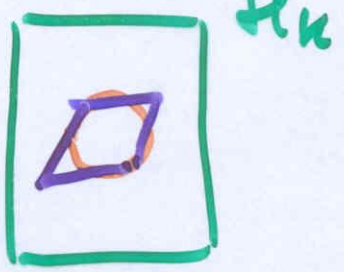
$$\|f_n\|_1 = 1, \qquad (L^1\text{-norm})$$
$$\|g_n\|_1 = \sqrt{n}$$

$\Rightarrow$ L^1-L^2 comparison.

Use of L^p-L^q comparisons

Let S be a simplicial complex,

and $\mathcal{H}_k := \mathrm{Ker}(\Delta_k(S))$.



- maximise L^1-norm over unit L^2-sphere
  - $\Rightarrow$ global feature - largest cycle
  - use this to find a good projection onto low-dimensional space
- minimise L^1-norm over unit L^2-sphere
  - $\Rightarrow$ highly concentrated cycle
  - locate features

☆ Could use L^2-L^4 if optimising solver prefers smooth functions.

Eigenvalues $\lambda \neq 0$

Graph Laplacians (∃ rich literature)

G graph

$C_0 = \langle \vec{e}_v : v \in V(G) \rangle$

Inner product $\langle f, g \rangle := \sum_v \underset{\text{degree}}{d(v)} f_v g_v$

or (unweighted version)

$\langle f, g \rangle := \sum_v f_v g_v$

$C_1 = \langle \vec{e}_e : e \in E(G) \rangle$

Inner product $\langle \alpha, \beta \rangle = \sum_e \alpha_e \beta_e$

Construct $\Delta_0 = d_1 d_1^*$ ← adjoint w.r.t. chosen inner product

d_1 is the boundary map

- Eigenvalues/eigenvectors of Δ_0 relate to:
  - random walk convergence
  - isoperimetric inequalities
  - electrostatics
  - "diffusion distance", heat equation

⋮

Connected components

- $[\Delta_0 f]_v = 0$

$$\Rightarrow \min_w f_w \le f_v \le \max_w f_w$$

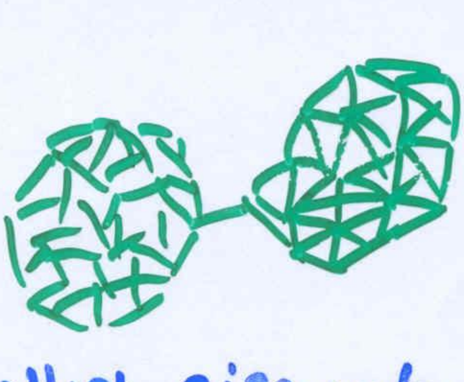
min, max taken over neighbours of v.

(MAXIMUM PRINCIPLE)

- $\Rightarrow$ If $\Delta_0 f \equiv 0$ Then f is locally constant

$\Rightarrow$ $\dim(\mathcal{H}_0)$ = # connected components

Much studied fact (see references in "Spectral Graph Theory", Fan Chung.):



Thin neck connects two otherwise separate components.

Smallest eigenvalue $\lambda_0 = 0$

-eigenvector v_0 is constant

Next eigenvalue $\lambda_1 \simeq 0$

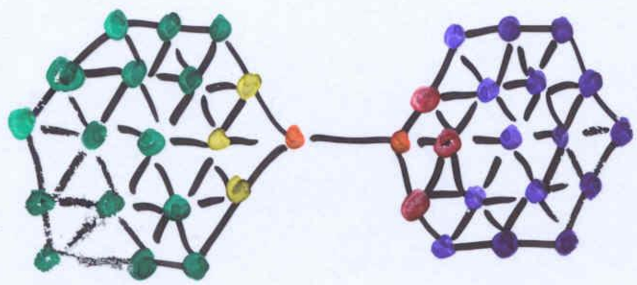
eigenvector v_1 is almost const. on each piece

Dual interpretations

0) $\boxed{\begin{array}{l} f: V \to \mathbb{R} \\ \sum_v f_v = 0 \\ \Delta_0 f = \lambda_1 f \end{array}}$ $\Longleftrightarrow$ 1) $\boxed{\begin{array}{l} \alpha: E \to \mathbb{R} \\ \text{1-Laplacian} \\ \Delta_1 \alpha = \lambda_1 \alpha \end{array}}$

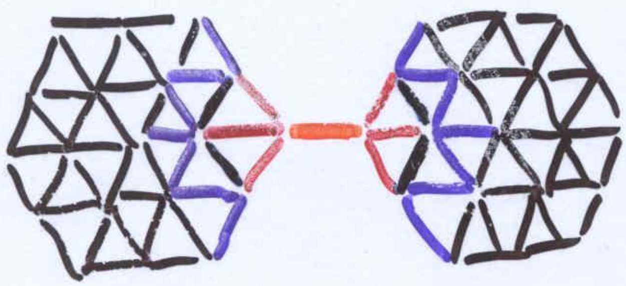
"$\longrightarrow$" : Define α by $\alpha(E) = f(x) - f(y)$ when $E = xy$. (fix orientations).

0)



vertices coloured by f

1)



edges coloured by α

"Almost Homology in dimension $k+\frac{1}{2}$"

Chain complex with adjoints:

$$\cdots \quad C_{k-1} \underset{\partial_k^*}{\overset{\partial_k}{\leftrightarrows}} C_k \underset{\partial_{k+1}^*}{\overset{\partial_{k+1}}{\leftrightarrows}} C_{k+1} \quad \cdots$$

If $f \in C_k$ and $\Delta_k f = \lambda f$, $\lambda \neq 0$,

Then $f = f^+ + f^-$, so that:

$$\partial_k f^+ = 0, \quad \partial_{k+1}^* f^+ =: g^+$$

$$\partial_k f^- =: g^-, \quad \partial_{k+1}^* f^+ = 0$$

and

$$\Delta_{k-1} g^- = \lambda g^-$$

$$\Delta_{k+1} g^+ = \lambda g^+.$$

Usually only one of f^+, f^- is nonzero.

$\Rightarrow$ $(f, f^+) \hookleftarrow$ "almost homology in dim $k+\frac{1}{2}$"

$(f, f^-) \hookleftarrow$ "almost homology in dim $k-\frac{1}{2}$"

Kernel of Laplacian $\longleftrightarrow$ homology in dimension k

$\lambda \neq 0$ Eigenspaces of Laplacian $\longleftrightarrow$ almost homology features in two adjacent dimensions

Examples to follow.

<u>Proof/Explanation</u>

$$C_k \cong \underbrace{\overbrace{K_k}^{\mathrm{Im}(\partial_{k+1})} \oplus H_k}_{\mathrm{Ker}(\partial_k)} \oplus \overbrace{K'_k}^{\mathrm{Im}(\partial^*_k)}$$

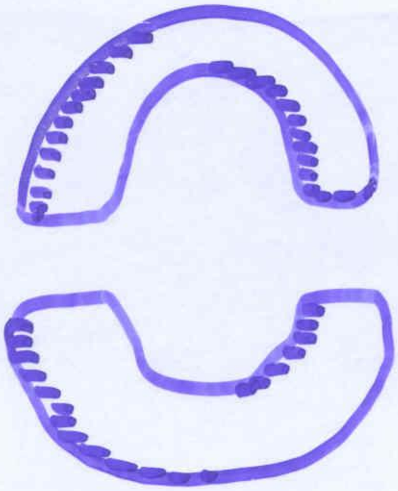
$\mathrm{Ker}(\partial^*_{k+1})$

(Orthogonal decomposition).

$$\begin{tikzcd}
K_{k-2} \arrow[ddddr, "\partial^*_{k-1}"'] & K_{k-1} \arrow[ddddr, "\partial^*_{k}"'] & K_k \arrow[ddddr, "\partial^*_{k+1}"'] & K_{k+1} \arrow[ddddr, "\partial^*_{k+2}"'] & K_{k+2} \\
\oplus & \oplus & \oplus & \oplus & \oplus \\
H_{k-2} & H_{k-1} & H_k & H_{k+1} & H_{k+2} \\
\oplus & \oplus & \oplus & \oplus & \oplus \\
K'_{k-2} & K'_{k-1} \arrow[uuuul, "\partial_{k-1}"] & K'_k \arrow[uuuul, "\partial_k"] & K'_{k+1} \arrow[uuuul, "\partial_{k+1}"] & K'_{k+2} \arrow[uuuul, "\partial_{k+2}"]
\end{tikzcd}$$

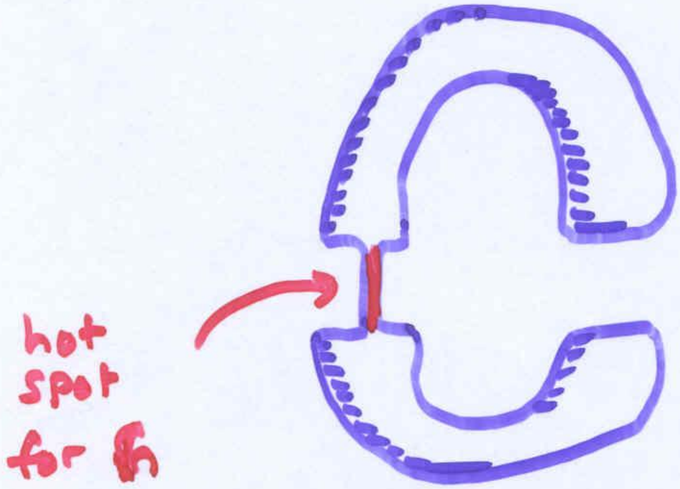
Examples:

A)



$b_0 = 2$

B)



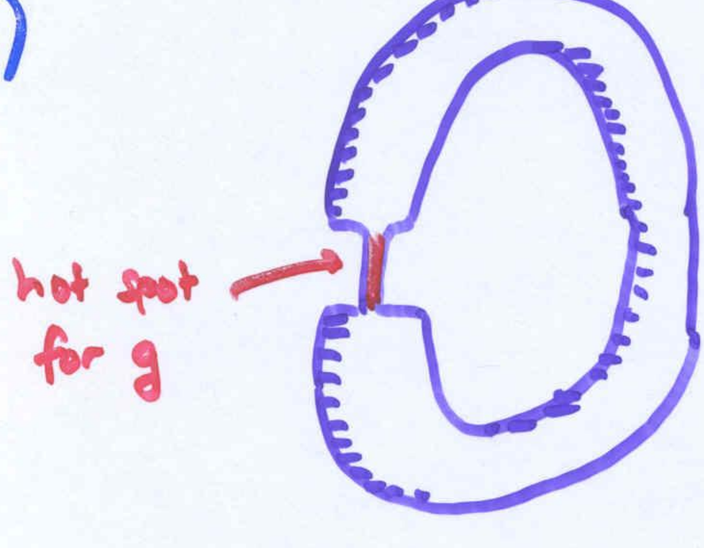
$b_0 = 1$

$b_{\frac{1}{2}}(\varepsilon) = 1$

$\Delta_0 f = \lambda f \,,\ \lambda \leq \varepsilon$

$\Leftrightarrow \Delta_1 h = \lambda h \,,\ \lambda \leq \varepsilon$

C)



$b_0 = 1$

$b_1 = 1$

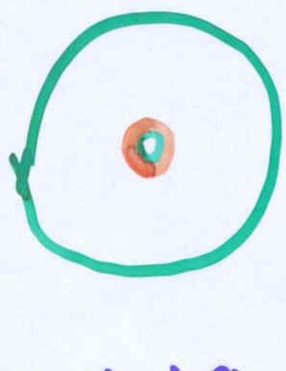
$\Delta_1 g = 0$

What is a $1\frac{1}{2}$-dimensional feature?

- A 1-dimensional closed cycle which is a boundary, but only 'just'.
- A 2-dimensional chain which is almost, but not quite, closed.

Punctured Sphere

→ If we had a punctured disk, then there is a non-bounding 1-cycle.

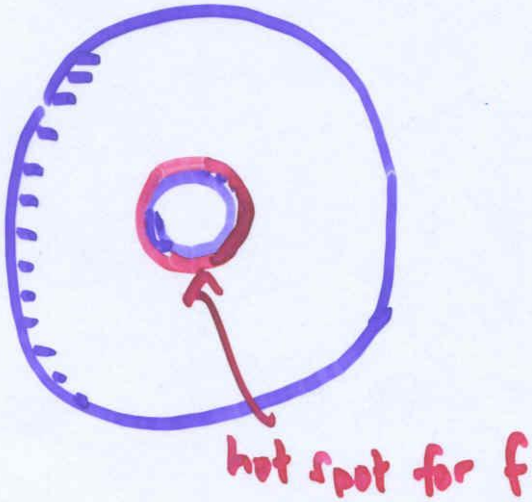


Its harmonic representative decays to 0 towards the outer boundary.

"Can't tell difference between disk and sphere".

Examples

D)

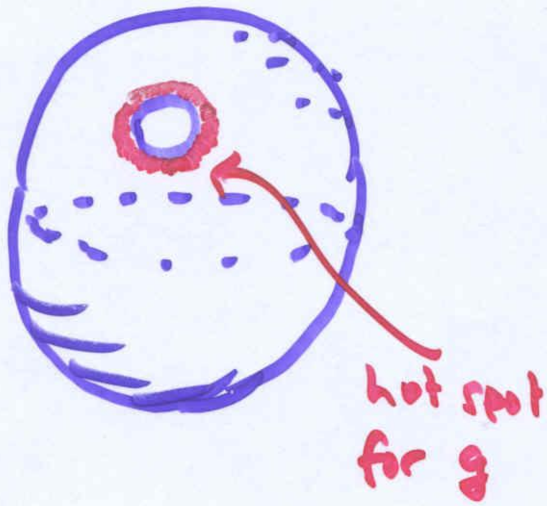


Punctured disk

$b_1 = 1$

$\Delta_1 f = 0$

E)



Punctured sphere

$b_{1,\frac{1}{2}}(\varepsilon) = 1$

$\Delta_1 g = \lambda g \, , \quad \lambda \leq \varepsilon$

$\Leftrightarrow \Delta_2 h = \lambda h \, , \quad \lambda \leq \varepsilon$

F)

Sphere

$b_2 = 1$

$\Delta_2 k = 0$

Closing Thoughts

- Formal treatment of some of these heuristic ideas – future work!
- Eigenfunctions are "geometrically natural".
- Local concentration can be used to identify features directly.

Distant hope:

→ A framework for probabilistic homology.

- S simplicial complex
- $\forall \sigma \in S$, $p_\sigma = \mathbb{P}(\sigma \text{ exists} \mid \partial\sigma \text{ exists})$
- For a cycle α, what is:

$$\mathbb{P}(\exists \beta : \alpha = \partial\beta \mid \alpha \text{ exists}) ?$$