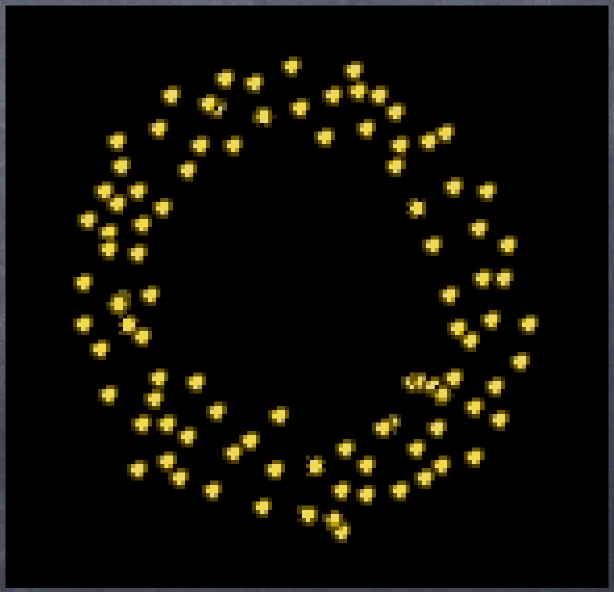
Point-cloud topology via harmonic forms

Vin de Silva, Pomona College
vin.desilva@pomona.edu

Today's goal

- Explore the use of discrete Laplacian operators...
- ...as applied to the topology of point-cloud data
- Discuss "qualitative" vs "quantitative"
- Discuss "discrete" vs "continuous"
- Run one or two demos



Thanks to my former colleagues at Stanford:

- Gunnar Carlsson
- Patrick Perry
- Afra Zomorodian
- Anne Collins
- Peter Lee

Discrete vs Continuous

Standard Pipeline (first attempt)

hidden/unknown space X

↓

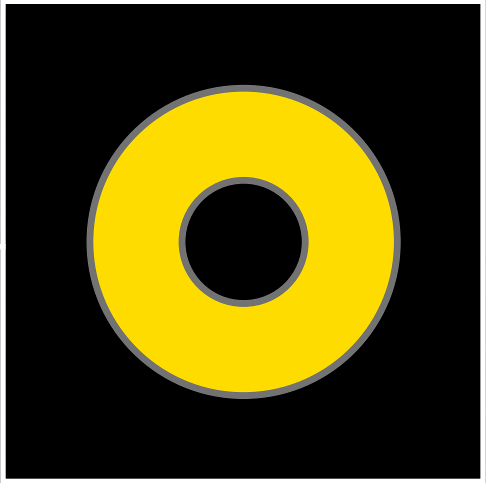
finite sample $Y \subset X$

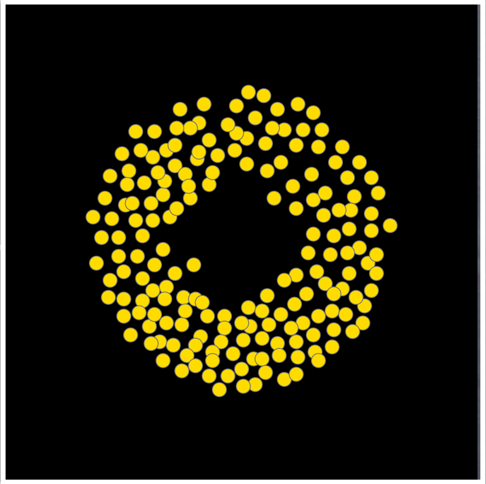
↓

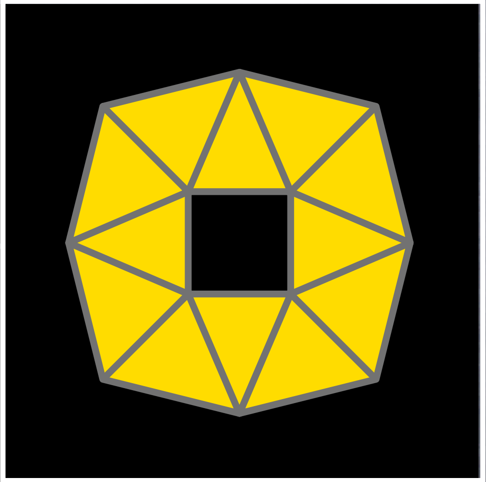
simplicial complex $S = S(Y)$

↓

homology invariants of S







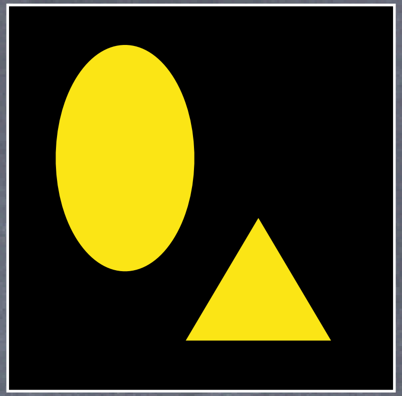
$b_0 = 1$

$b_1 = 1$

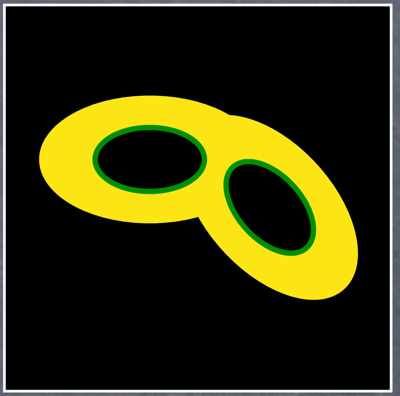
$b_2 = 0$

Betti numbers ↔ features

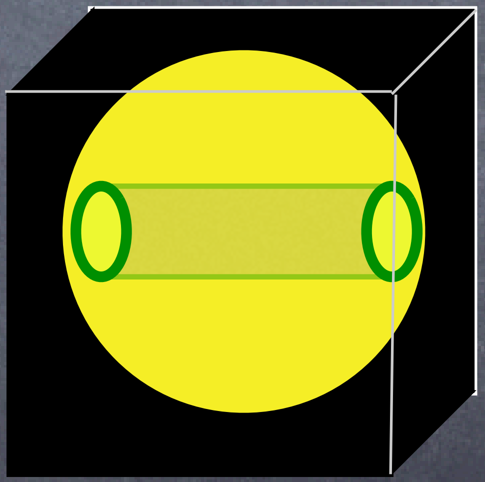
- For an object in 2D space
  - b_0 is the number of components
  - b_1 is the number of holes
- For an object in 3D space
  - b_0 is the number of components
  - b_1 is the number of tunnels or handles
  - b_2 is the number of voids
- (and so on, in higher dimensions)



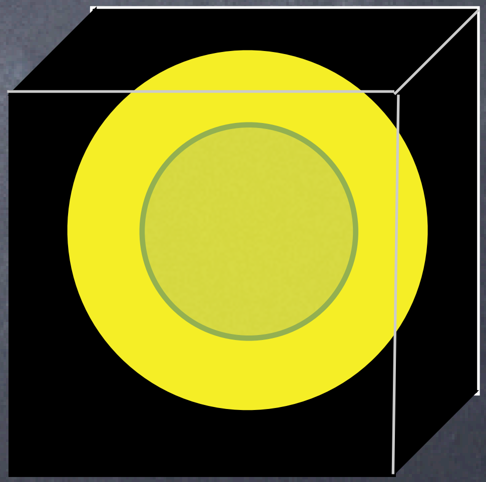
$b_0 = 2, b_1 = 0$



$b_0 = 1, b_1 = 2$



$b_0 = 1, b_1 = 1, b_2 = 0$



$b_0 = 1, b_1 = 0, b_2 = 1$

Reconstruction theorems

- Various constructions for S(Y)
  - Cech complex (folklore)
  - Rips-Vietoris complex (folklore)
  - α-shape complex (Edelsbrunner, Mücke)
  - strong/weak witness complexes (Carlsson, dS)
- Desire theorems of the form:

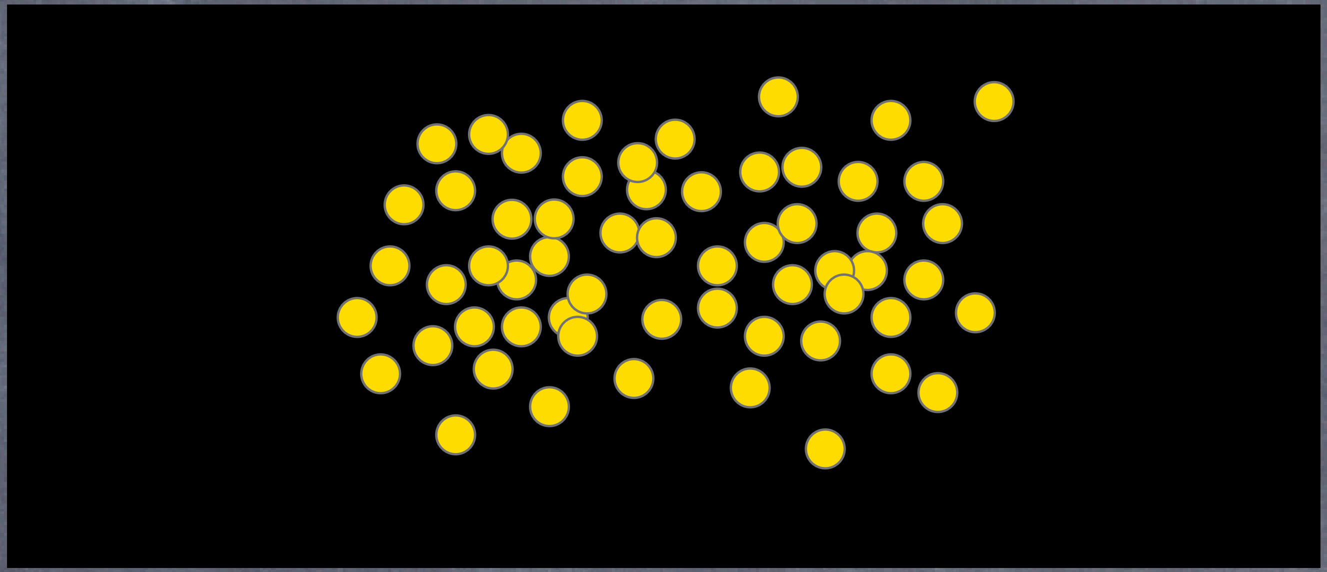
> If Y is well-sampled from X
> then $S(Y) \approx X$

- e.g. Niyogi-Smale-Weinberger (2004), Cech complex

Discrete vs continuous

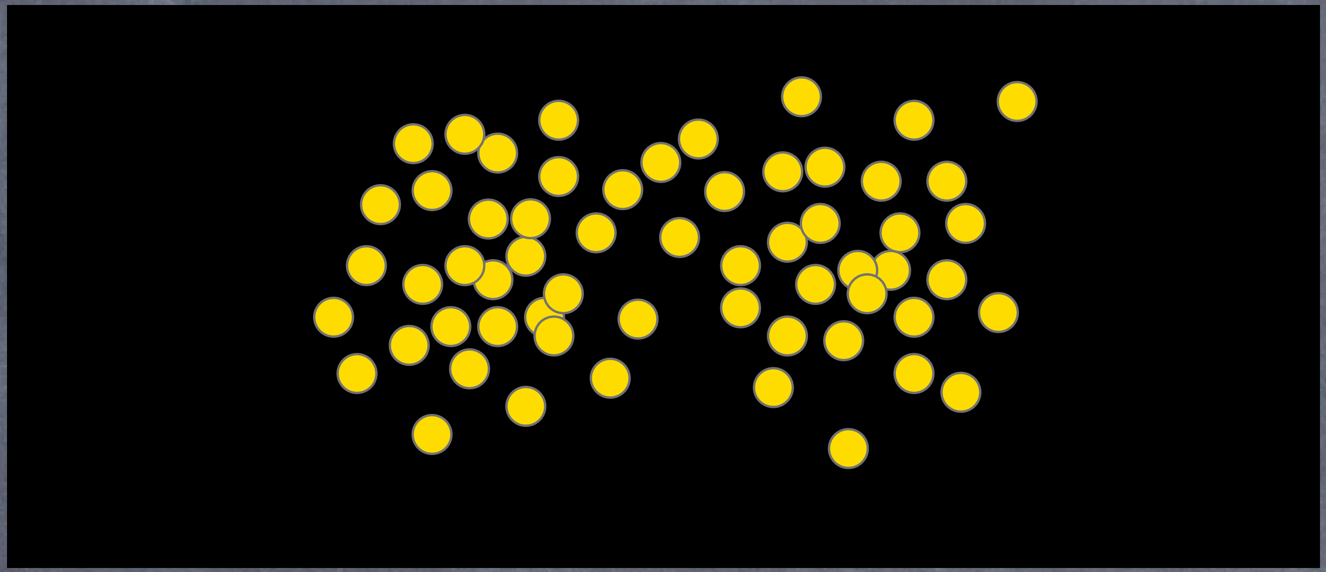
- Betti numbers are discrete
- Topological spaces
  - topological spaces are continuous
  - the space of topological spaces is discrete
- Finite point-clouds
  - point-clouds are discrete
  - the space of point-clouds is continuous
- Therefore, raw Betti numbers are
  - ✔ very handy for topological spaces
  - ✘ a bit dangerous for point-clouds

One lump or two?



At which parameter value does the number of components change?

One lump or two?



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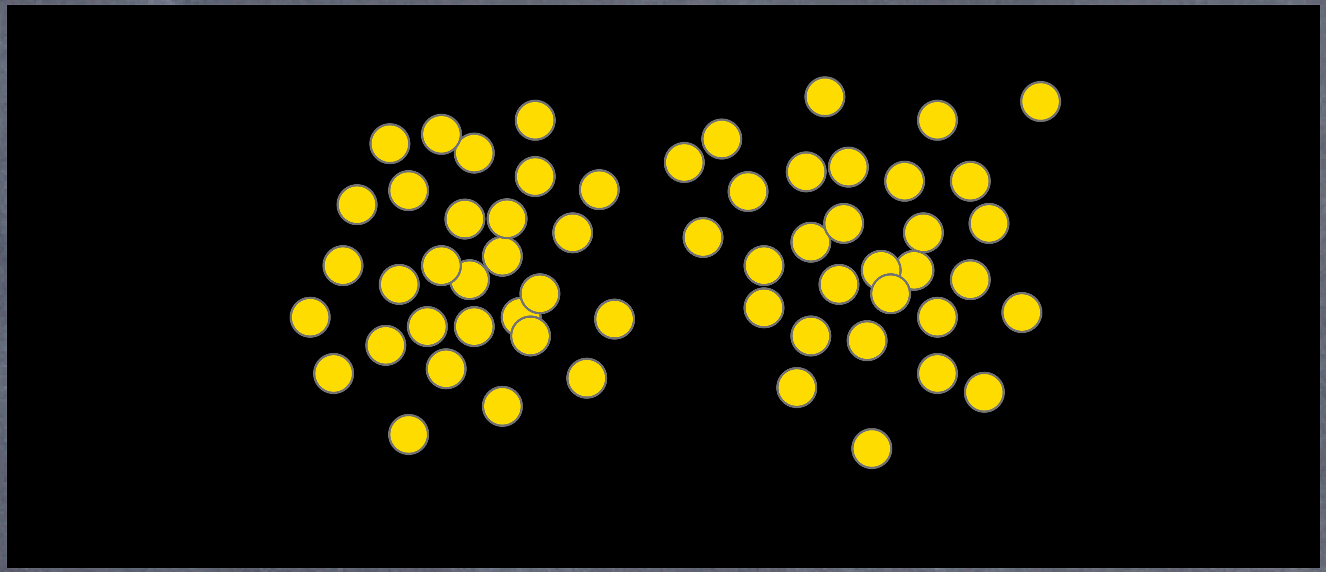

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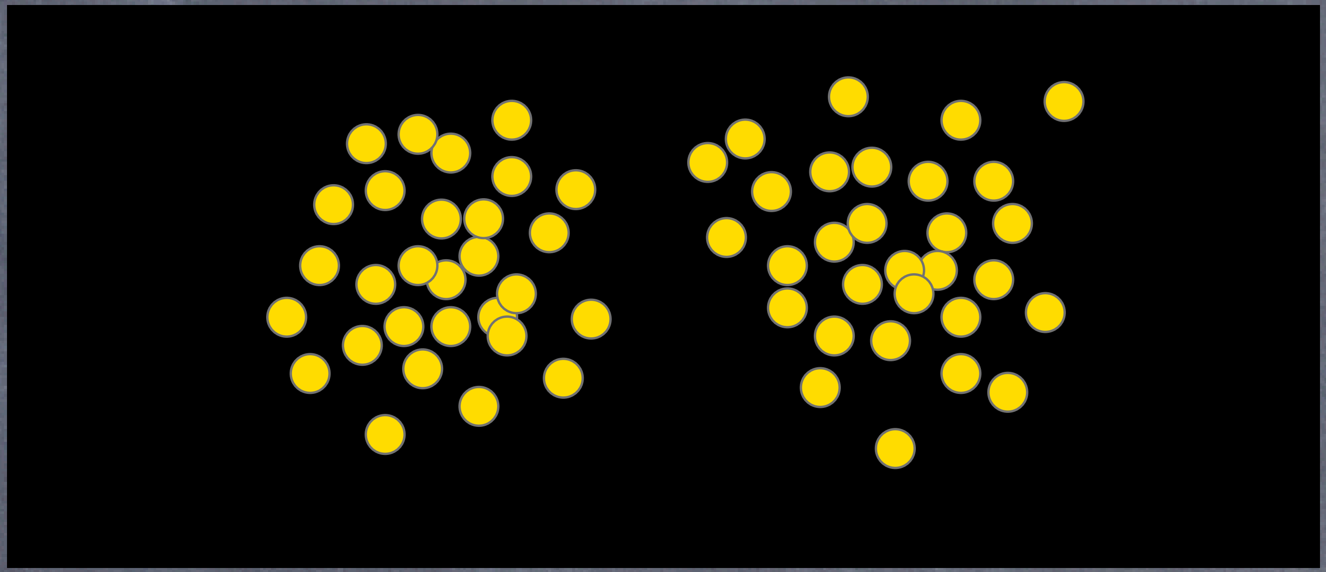
One lump or two?



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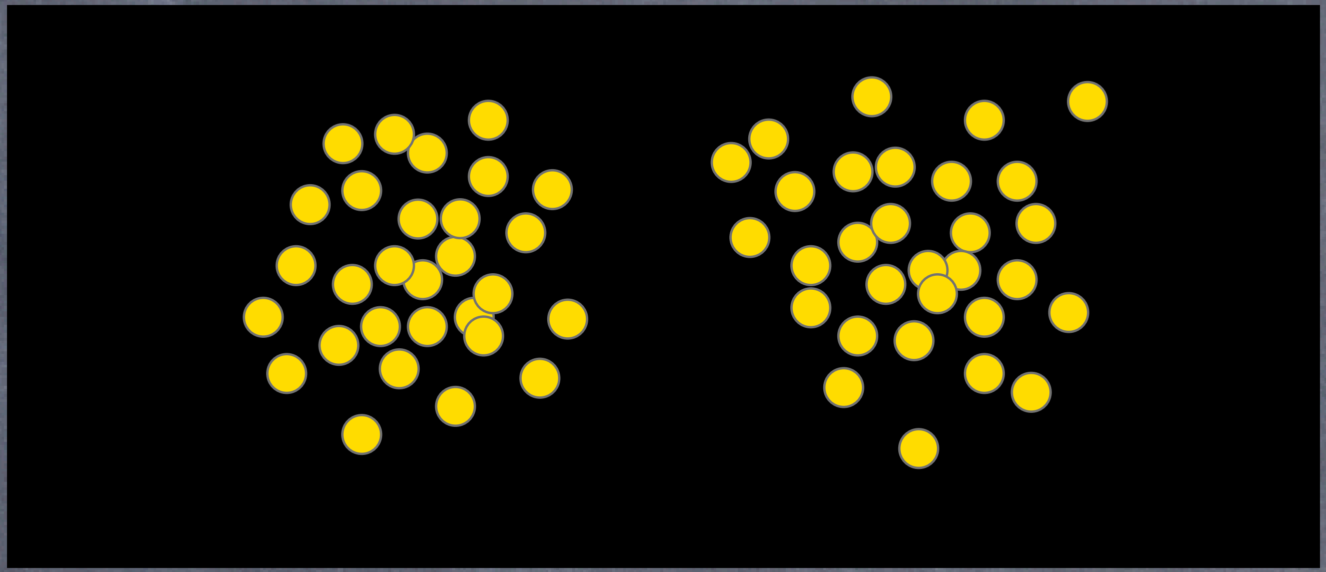

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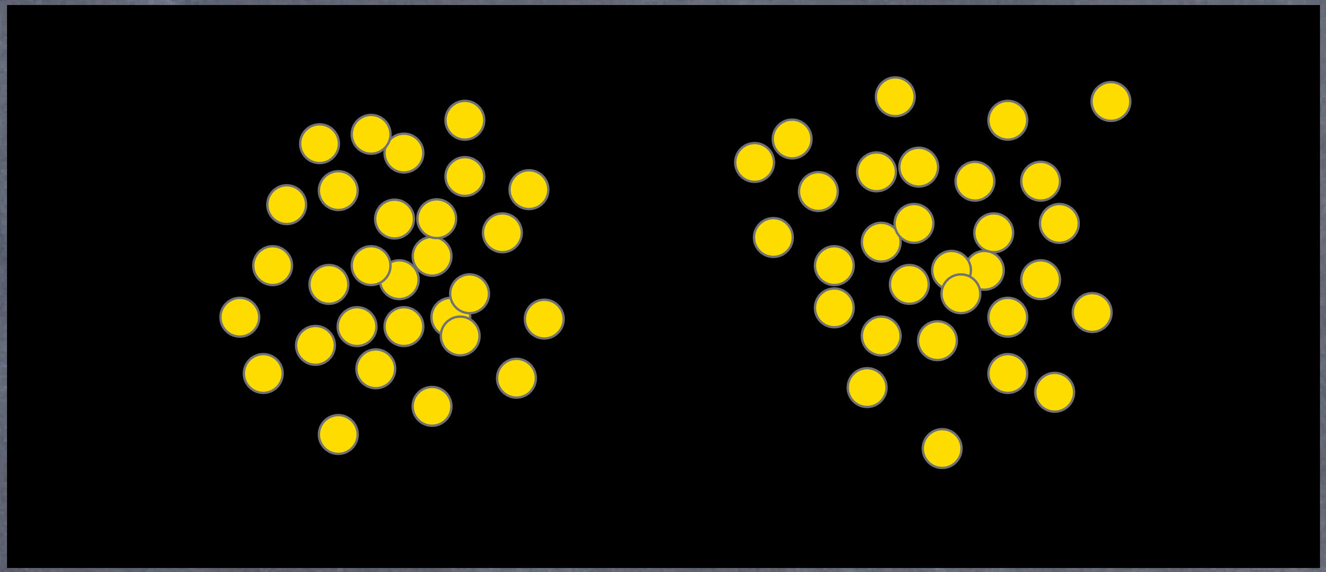
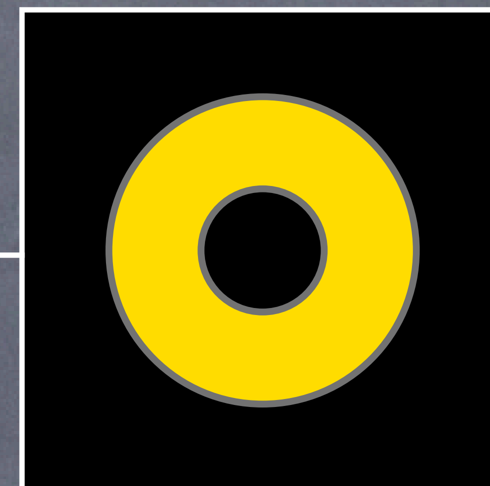


At which parameter value does the number of components change?

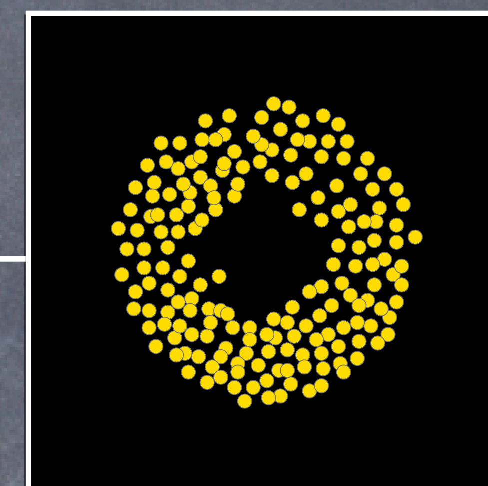
Standard Pipeline (second attempt)

hidden/unknown space X



↓

finite sample $Y \subset X$



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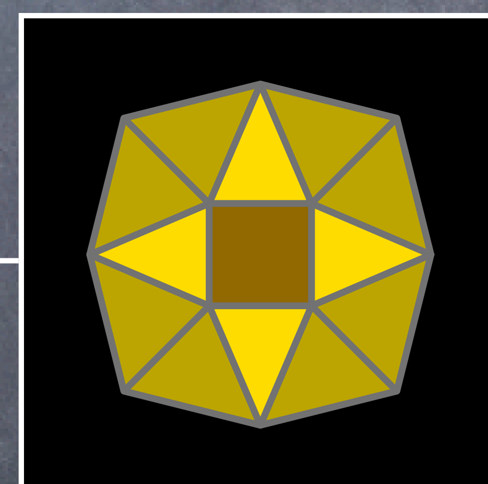
labelled complex $S(r) = S(Y,r)$



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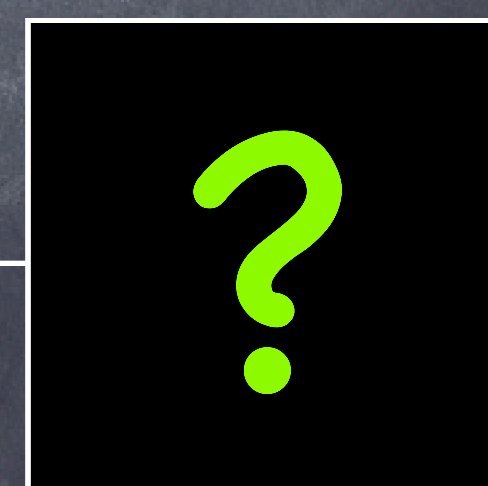
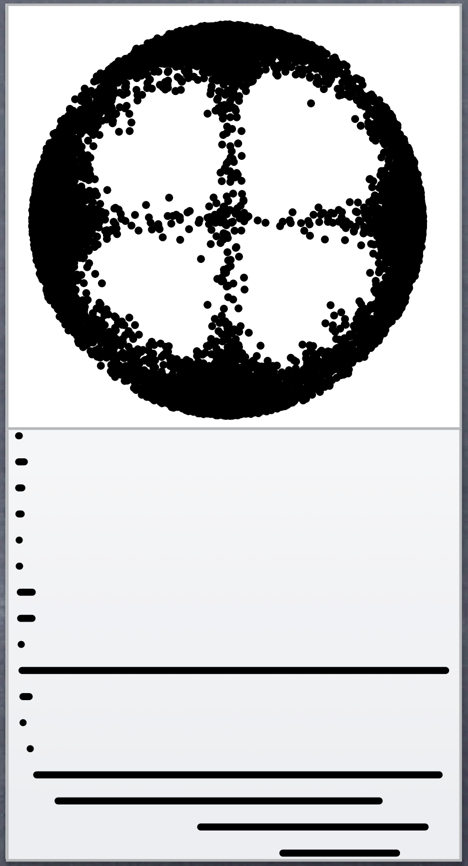
quantitative topology



Example: Persistence

Persistent homology

- Edelsbrunner, Letscher, Zomorodian (2000)
  - effective algorithm for persistence in 3-space
- Carlsson, Zomorodian (2005)
  - general theory of persistent homology
- Cells of S(Y) labelled by "time of birth"
- Bar-codes indicate feature lifetimes
- Continuous measurements (interval length) coupled to discrete information (number of intervals)



Persistence pipeline

hidden/unknown space X

↓

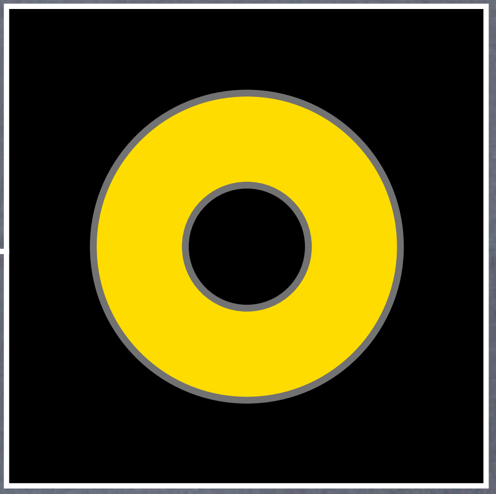
finite sample $Y \subset X$

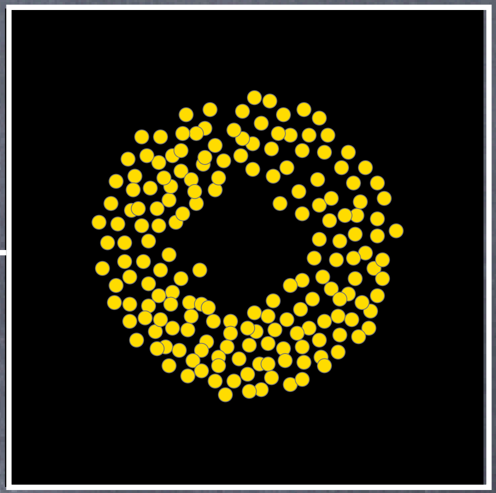
↓

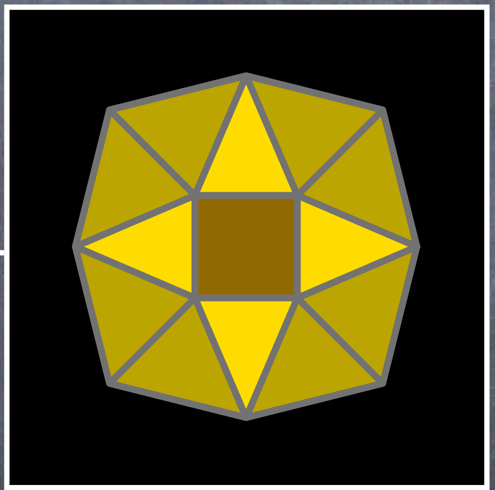
filtered complex $S(r) = S(Y,r)$

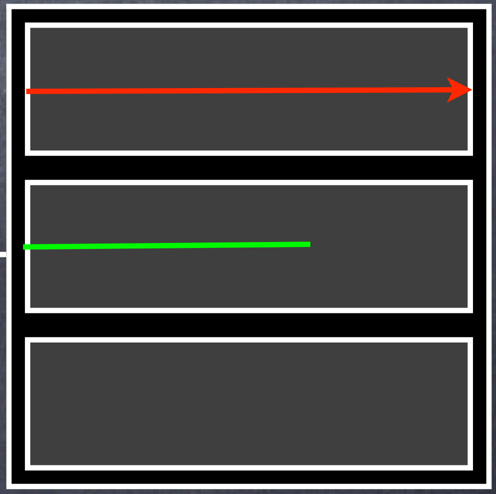
↓

persistent homology of $S(r)$









Discrete Laplacians

Δ_k

- C_k = { real-valued functions on k-simplices of S(Y) }
  - floating point rather than exact arithmetic
- Define discrete Laplacian operators $\Delta_k : C_k \to C_k$
- Consider the harmonic spaces $H_k = \mathrm{Ker}(\Delta_k)$
  - H_k is isomorphic to standard homology of X
- Consider eigenspaces $\{ f : \Delta_k f = \lambda f \}$ for λ small
  - "almost homology" or "ϵ-homology"
- Information derived from the ranks of these spaces (Betti numbers) and the eigenfunctions themselves

Constructing Δ_k

Given a chain complex over the real numbers...

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

homology is defined using a chain complex

...and an inner product on each C_k, we can form the dual cochain complex:

$$\cdots C_{k-1} \xrightarrow{\partial_k^*} C_k \xrightarrow{\partial_{k+1}^*} C_{k+1} \cdots$$

cohomology is defined using a cochain complex

The discrete Laplacian is defined...

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

...and one can easily prove (in the finite dimensional case):

harmonic space

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

homology

Aside: Hodge theory

For a 3-dimensional domain:

$$\underset{\text{scalar fields}}{\Omega^0} \xrightarrow[\text{grad}]{\nabla} \underset{\text{vector fields}}{\Omega^1} \xrightarrow[\text{curl}]{\nabla\times} \underset{\text{vector fields}}{\Omega^2} \xrightarrow[\text{div}]{\nabla\cdot} \underset{\text{scalar fields}}{\Omega^3}$$

$$\Omega^0 \xleftarrow{-\nabla\cdot} \Omega^1 \xleftarrow{\nabla\times} \Omega^2 \xleftarrow{-\nabla} \Omega^3$$

For example:

$$\begin{aligned} \Delta_0 f &:= -\nabla\cdot(\nabla f) &&= -\sum_{i=1}^3 \frac{\partial^2 f}{\partial x_i^2} \\ \Delta_1 \vec{f} &:= \nabla\times(\nabla\times\vec{f}) - \nabla(\nabla\cdot\vec{f}) &&= -\sum_{i=1}^3 \frac{\partial^2 \vec{f}}{\partial x_i^2} \end{aligned}$$

Proof that $\mathrm{Ker}(\Delta_k) = H_k$ is much more difficult.

ϵ-Betti numbers

Structure theorem for homology and ϵ-homology

For every nonnegative integer k, and $\epsilon > 0$:

Integers b_k "Betti numbers"

Integers $b_{k+½}(\epsilon)$ "ϵ-Betti numbers"

such that:

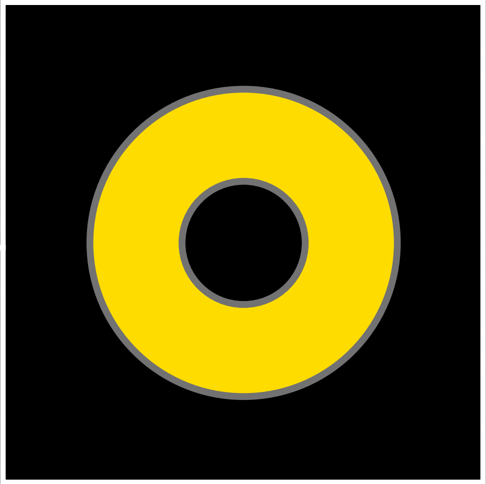
$\dim(\mathrm{Ker}(\Delta_k)) = b_k$

$\dim(\mathrm{Eig}(\Delta_k,\epsilon)) = b_{k-½}(\epsilon) + b_k + b_{k+½}(\epsilon)$

space spanned by eigenfunctions with eigenvalue less than ϵ

Laplacian pipeline

hidden/unknown space X



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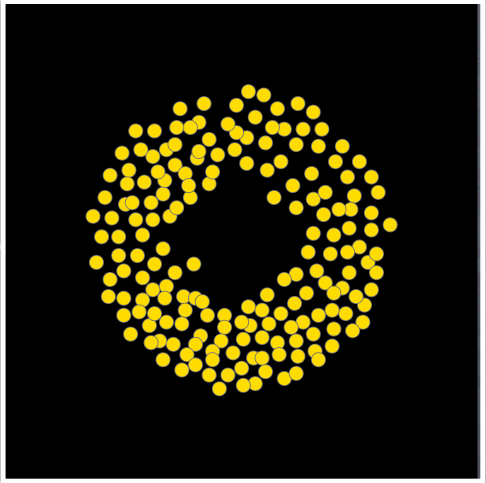
finite sample $Y \subset X$



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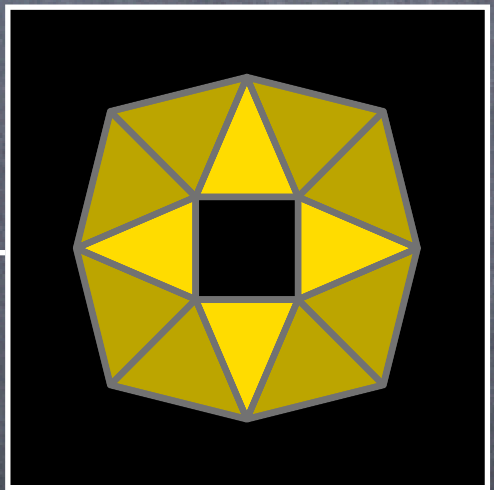
weighted complex $S = S(Y)$, $f: S \to R$



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ϵ-harmonic forms

$b_0 = 1$

$b_{0.5}(\epsilon) = ?$

$b_1 = 1$

$b_{1.5}(\epsilon) = ?$

$b_2 = 0$

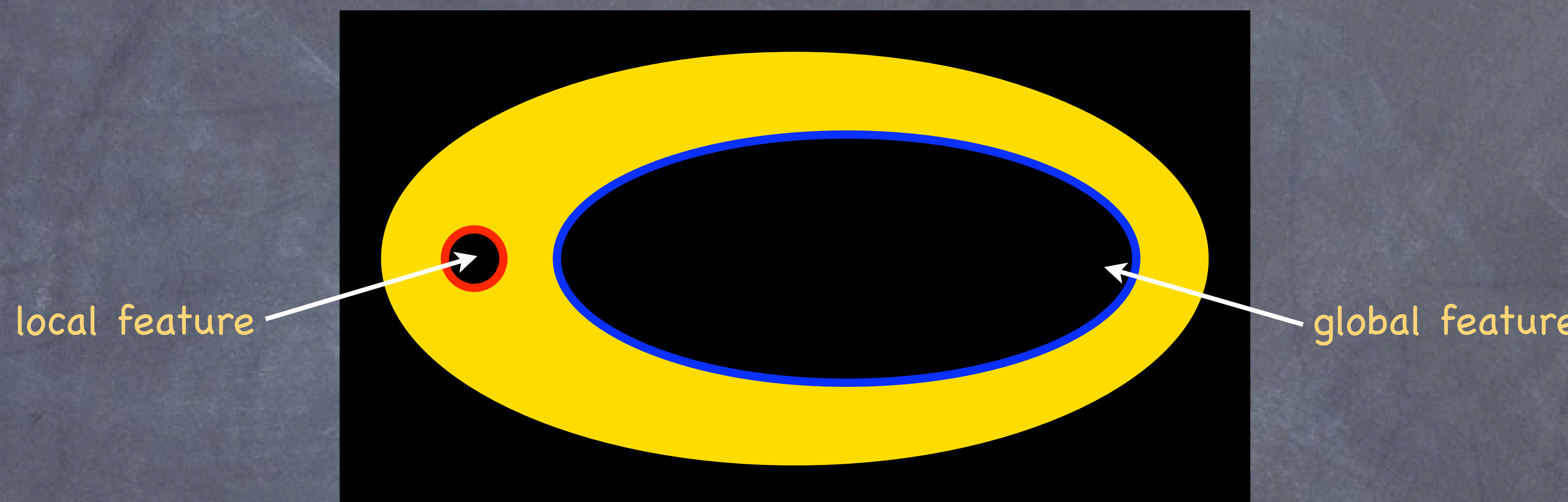
Pros and cons

- ✔ Several ways to incorporate continuous parameters
  - meaning of "λ is close to zero" — how close?
  - simplices can be weighted prior to construction of Δ_k
- ✔ Harmonic cycles have global optimality properties
  - localising features/minimal cycle problem
- ✔ Non-zero eigenfunctions encode subtle relationships between cells of adjacent dimensions
- ✘ More expensive than persistent homology
- ✘ Theory somewhat underdeveloped
  - (except graph Laplacians, see "Spectral Graph Theory" by Chung)

Entropy

Local vs global features

Homological features can be local or global to varying degrees:

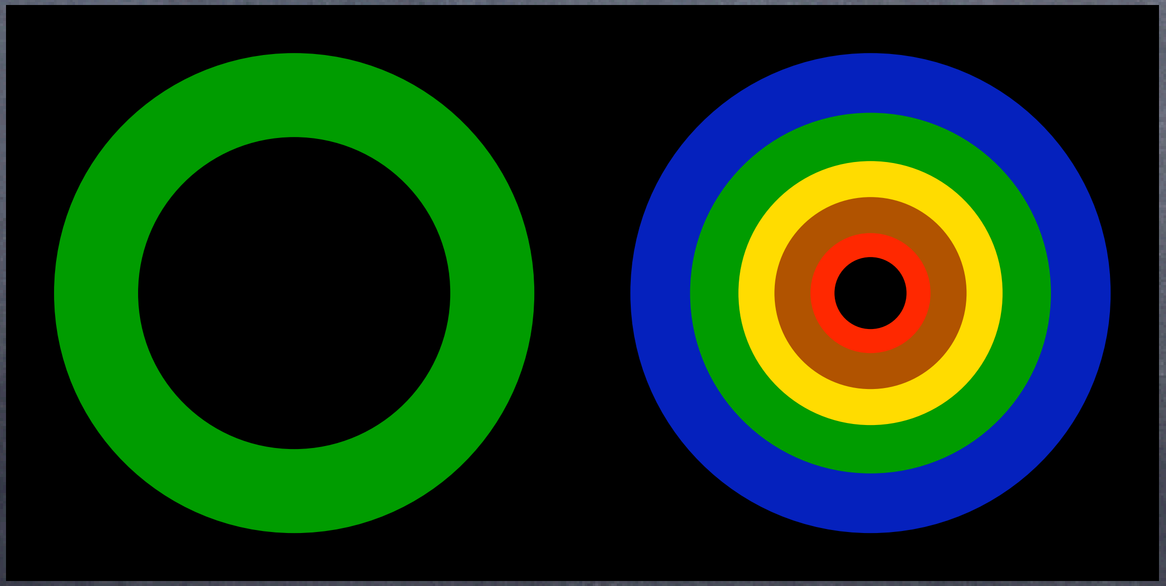


This example has a 2-dimensional space of harmonic 1-forms.
Can we pick out 1-forms representing the two features?

persistent homology
can do this very easily

Concentration

- Heuristic arguments suggest that harmonic cycles concentrate energy...
  - ...weakly along global features
  - ...strongly along local features



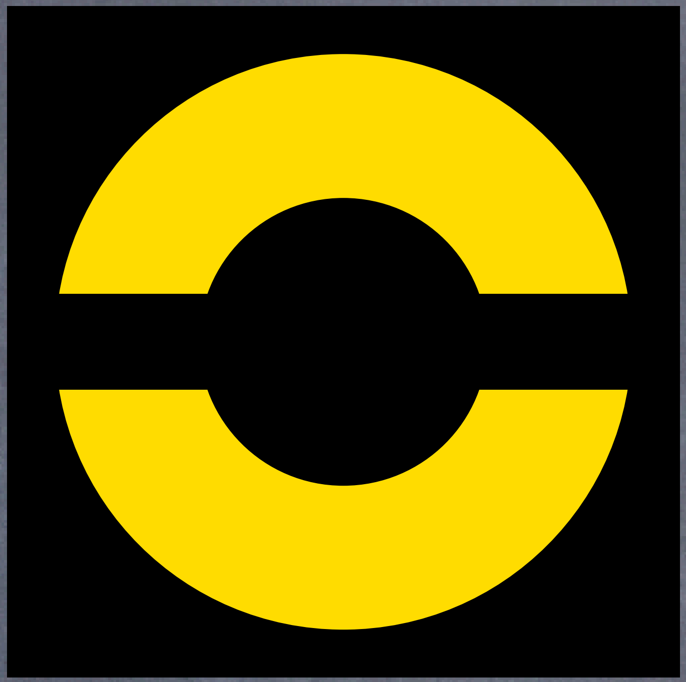
Entropy & L^p comparison

- How to detect whether a cycle is highly concentrated in some region?
- Some measure of entropy is called for
  - high entropy ↔ flat distribution ↔ global feature
  - low entropy ↔ peaked distribution ↔ local feature
- Simple estimate: compare L^1 and L^2 norms
  - $E[f] := ||f||_1 \,/\, ||f||_2$
  - E[f] large ↔ global feature
  - E[f] small ↔ local feature

DEMO!!!

Betti numbers: examples

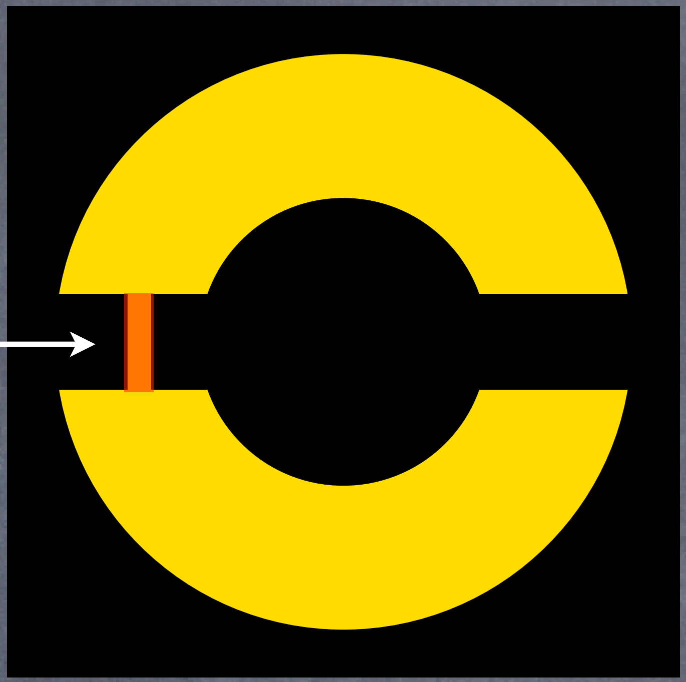
Examples



b_0	$b_{0.5}(\epsilon)$	b_1	$b_{1.5}(\epsilon)$	b_2
2	0	0	0	0

Examples

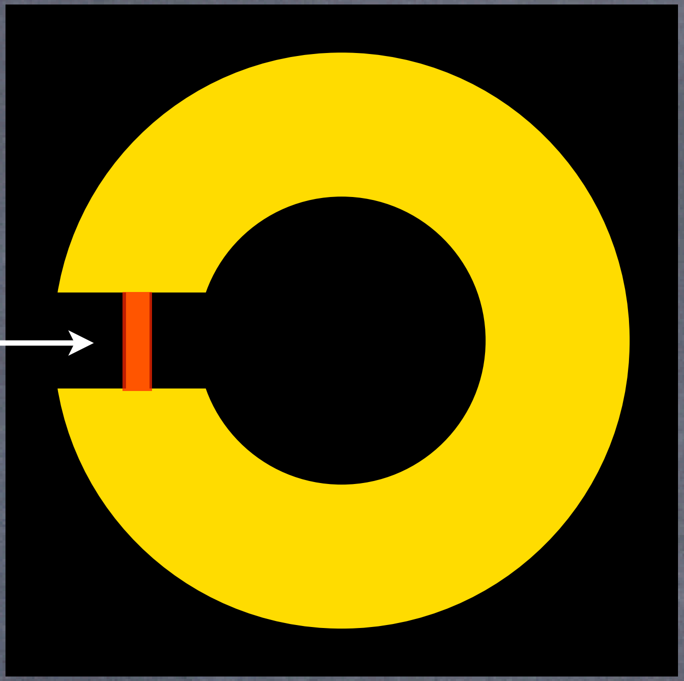
hot spot for 1-chain j, where $\Delta_1 j = \lambda j$



b_0	$b_{0.5}(\epsilon)$	b_1	$b_{1.5}(\epsilon)$	b_2
1	1	0	0	0

Examples

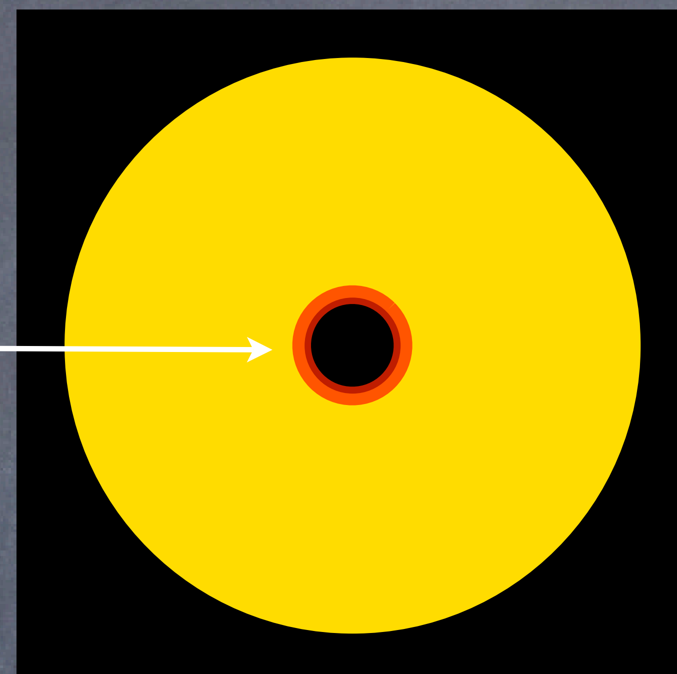
hot spot for 1-cycle j, where $\Delta_1 j = 0$



b_0	$b_{0.5}(\epsilon)$	b_1	$b_{1.5}(\epsilon)$	b_2
1	0	1	0	0

Examples

hot spot for 1-cycle j,
where $\Delta_1 j = 0$



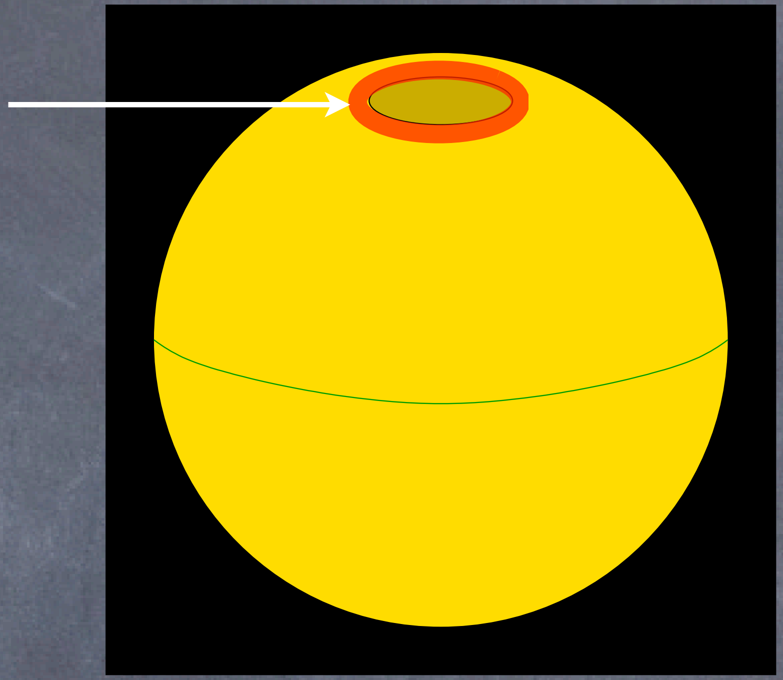
annulus

b_0	$b_{0.5}(\epsilon)$	b_1	$b_{1.5}(\epsilon)$	b_2
1	0	1	0	0

Examples

hot spot for 1-cycle j, where $\Delta_1 j = \lambda j$

hot spot for 2-chain k, where $\Delta_2 k = \lambda k$

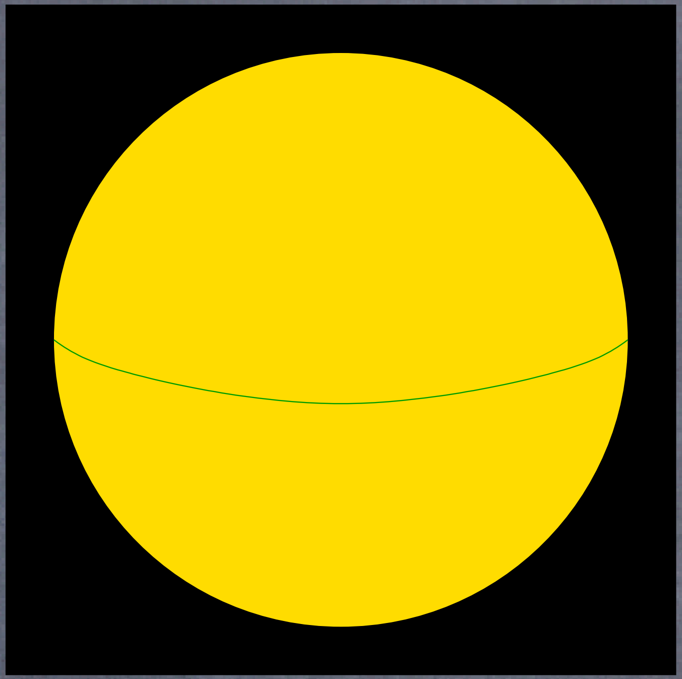


punctured sphere

DEMO!!!

b_0	$b_{0.5}(\epsilon)$	b_1	$b_{1.5}(\epsilon)$	b_2
1	0	0	1	0

Examples

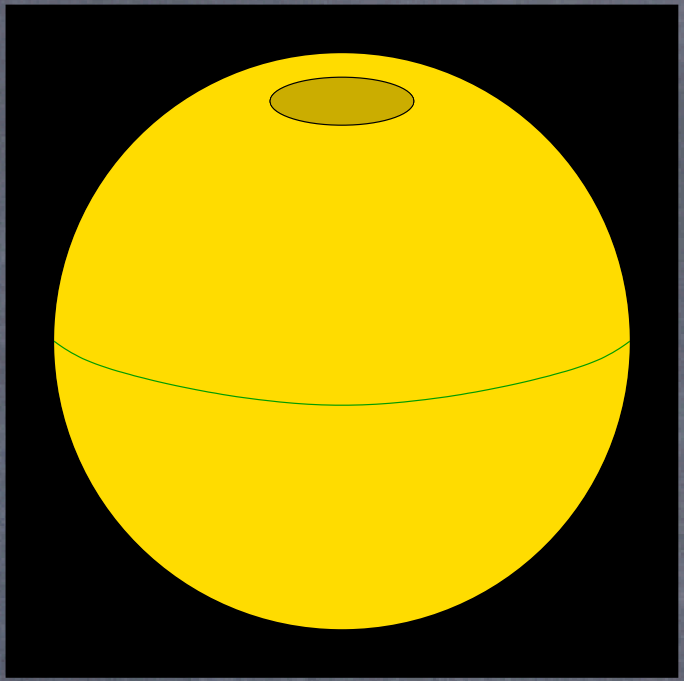


sphere

b_0	$b_{0.5}(\epsilon)$	b_1	$b_{1.5}(\epsilon)$	b_2
1	0	0	0	1

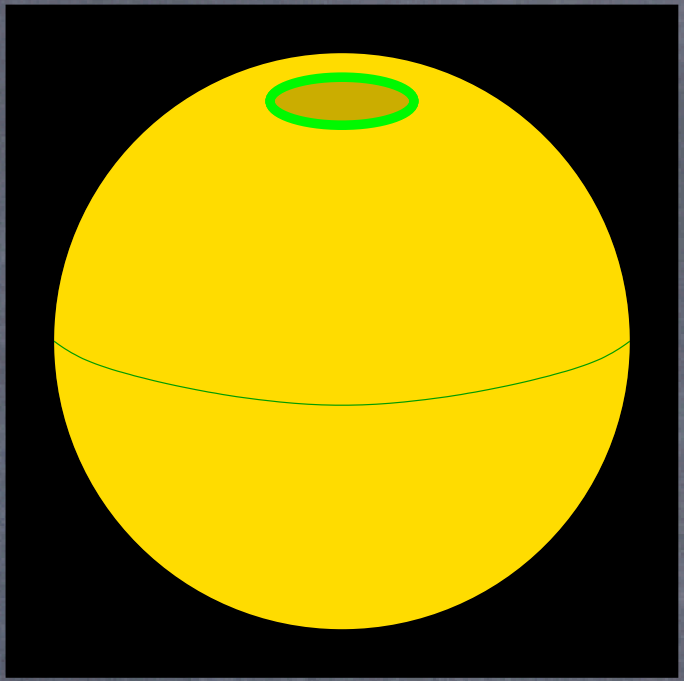
Take-home message

What is a (1.5)-D feature?



punctured sphere

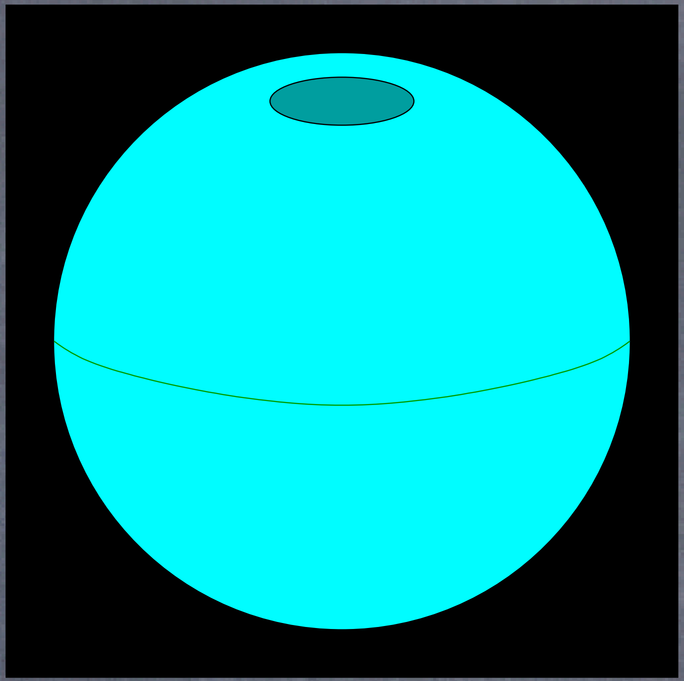
What is a (1.5)-D feature?



punctured sphere

A 1-D cycle which is a boundary (but only just)

What is a (1.5)-D feature?

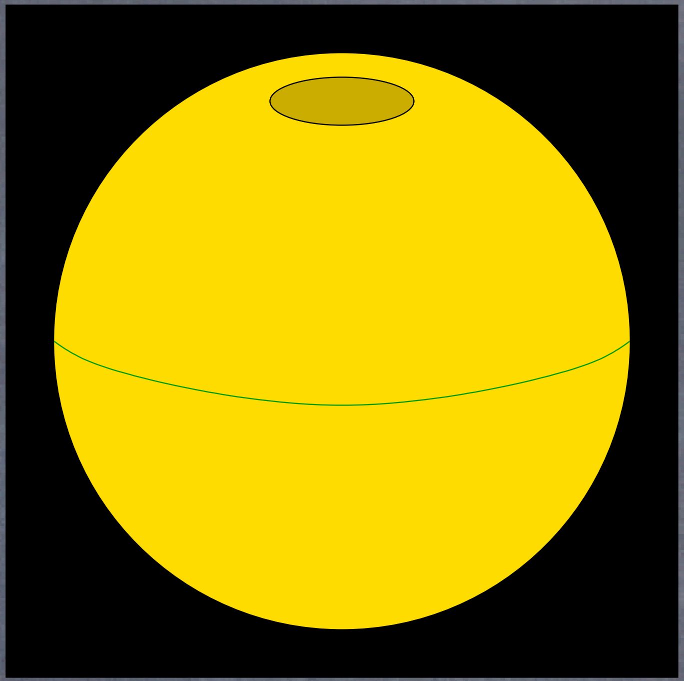


punctured sphere

A 1-D cycle which is a boundary (but only just)

A 2-D chain which is almost (but not quite) closed

What is a (1.5)-D feature?



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A 1-D cycle which is a boundary (but only just)

A 2-D chain which is almost (but not quite) closed

Thank you