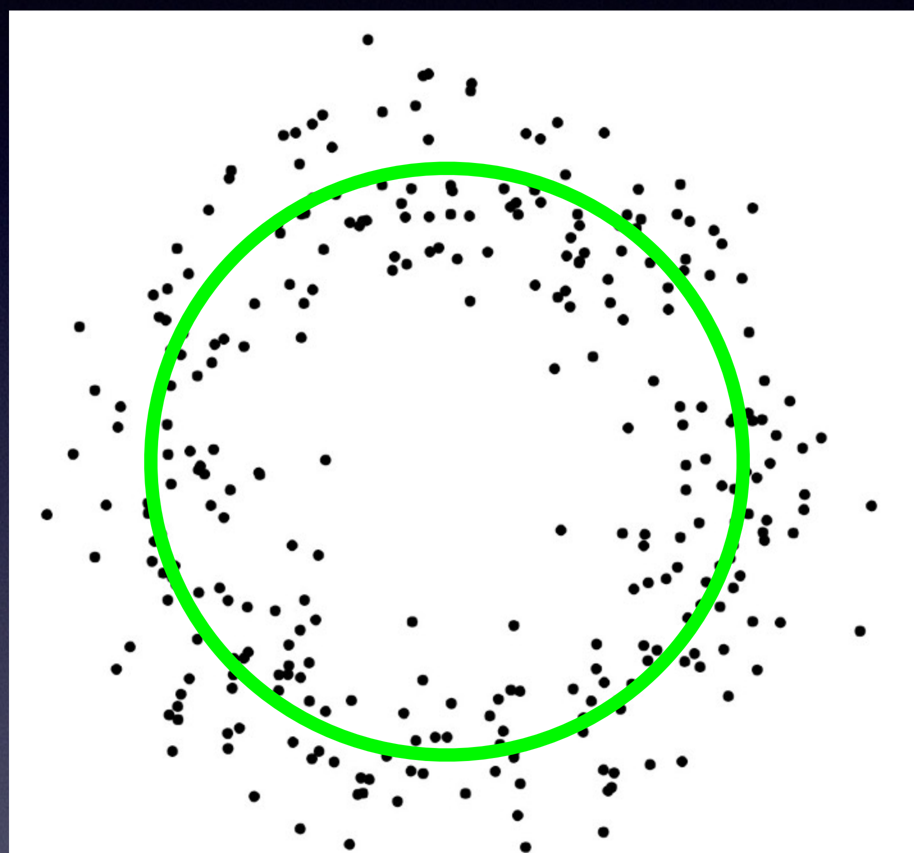
Topological Data Analysis

CBMS Lecture 4

Vin de Silva
Pomona College

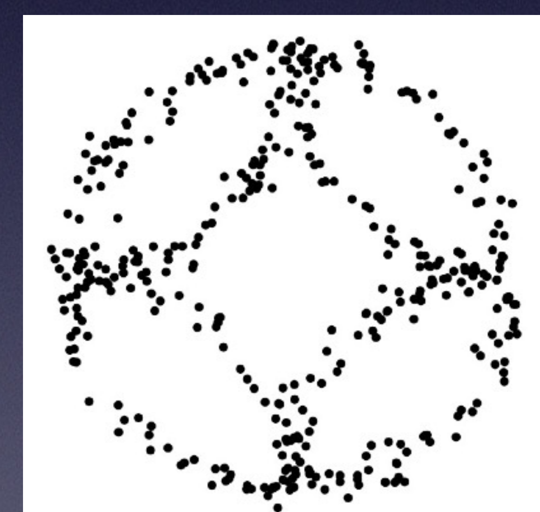
Point-cloud topology

Point-cloud topology



$b_1 = 1$

$b_1 = 3$



$b_1 = 5$

Data sampled from an unknown topological space Y.
Estimate Betti numbers of Y from the sample.

The standard pipeline

hidden/unknown space X

↓

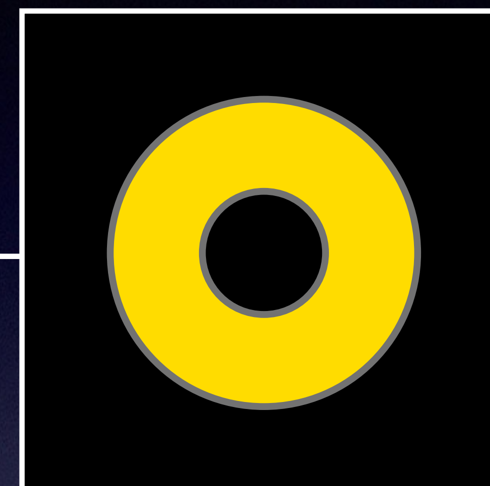
finite sample $Y \subset X$

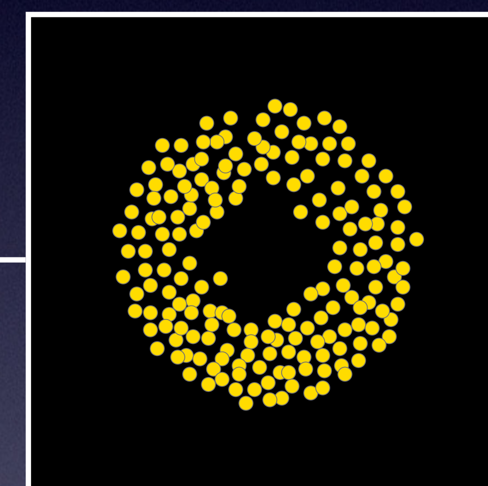
↓

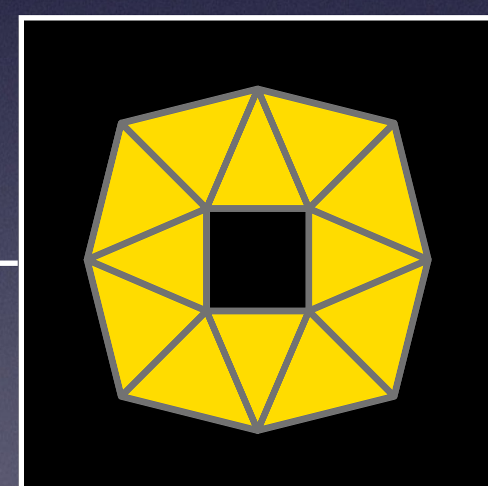
simplicial complex $S = S(Y)$

↓

homology invariants of S







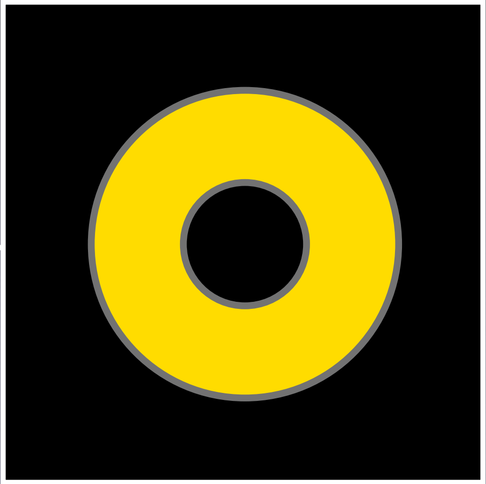
$b_0 = 1$

$b_1 = 1$

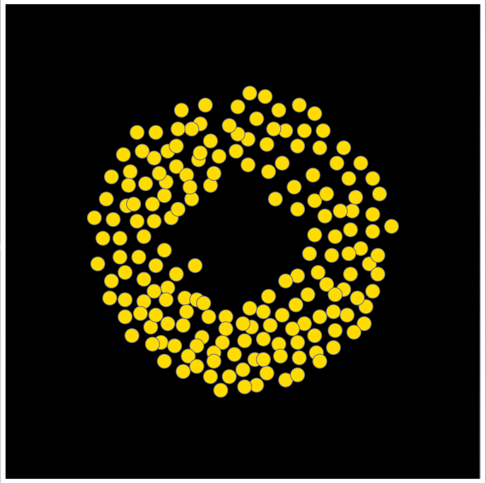
$b_2 = 0$

The standard pipeline

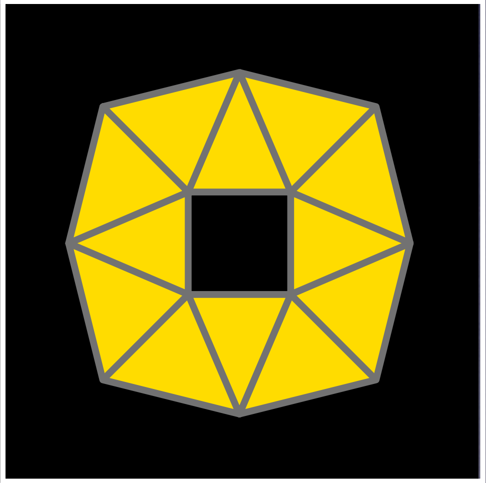
hidden/unknown space X



finite sample $Y \subset X$



simplicial complex $S = S(Y)$



homology invariants of S

$b_0 = 1$

$b_1 = 1$

$b_2 = 0$

Simplicial reconstructions

- Given a collection of points X in Euclidean space:
  - Proximity graph

$$\{\text{all vertices } [x]\} \cup \{\text{edges } [x,y] \text{ such that } \|x-y\| \leq r\}$$

  - Vietoris–Rips complex

$$\{\text{simplices } [x_0, x_1, \ldots, x_k] \text{ for which every } \|x_i - x_j\| \leq r\}$$

  - Čech complex

$$\{\text{simplices } [x_0, x_1, \ldots, x_k] \text{ whose vertices are contained in an } (r/2)\text{-ball}\}$$

  - Alpha shape (Edelsbrunner, Kirkpatrick, Seidel 1983)

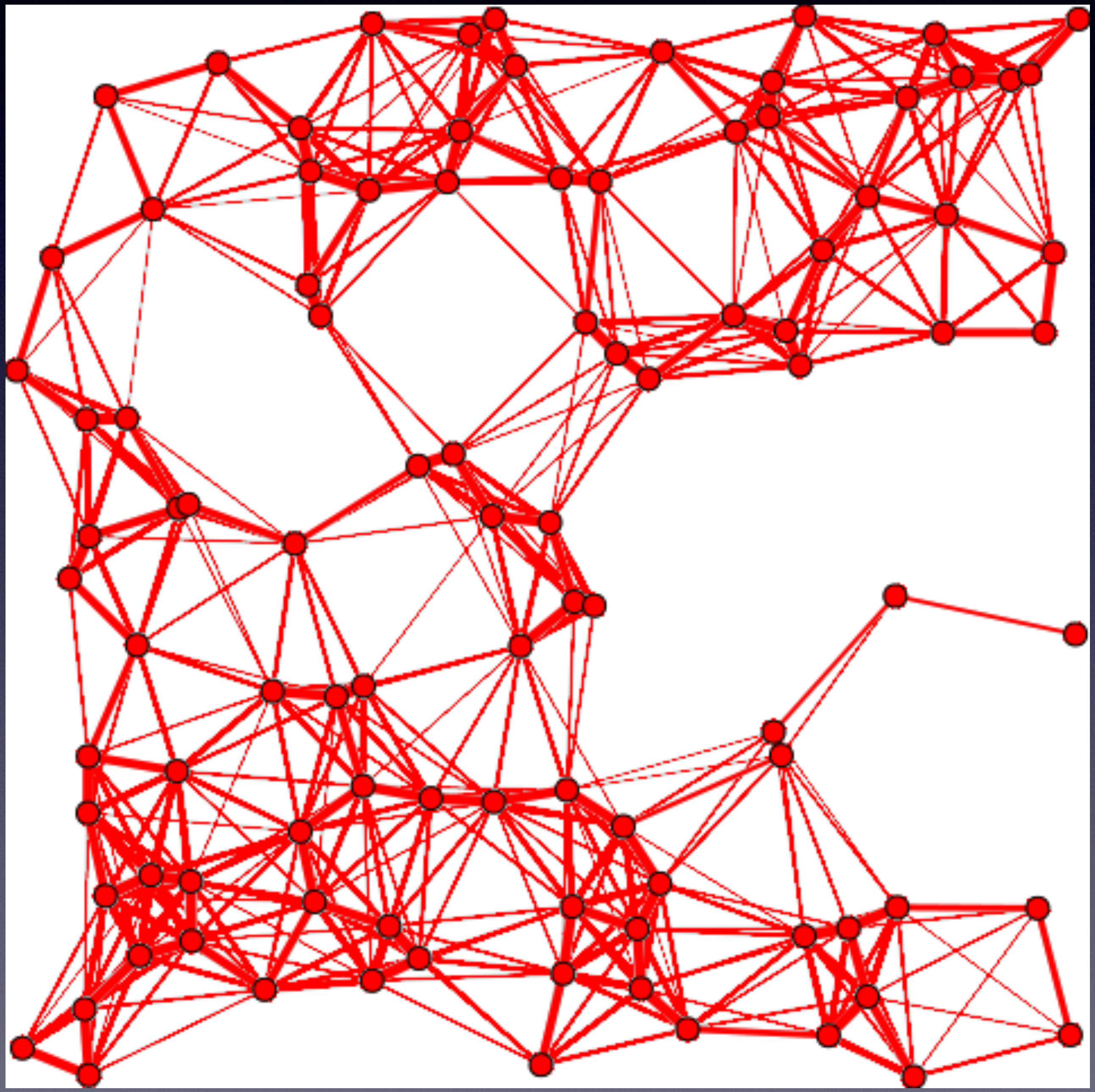
$$\left\{\begin{matrix}\text{simplices } [x_0, x_1, \ldots, x_k] \text{ whose vertices are contained in} \\ \text{an } (r/2)\text{-ball whose interior meets no other points of } X\end{matrix}\right\}$$

- Desire theorems of the form:

$$\boxed{\text{If Y is well-sampled from X then S(Y)} \approx \text{X}}$$

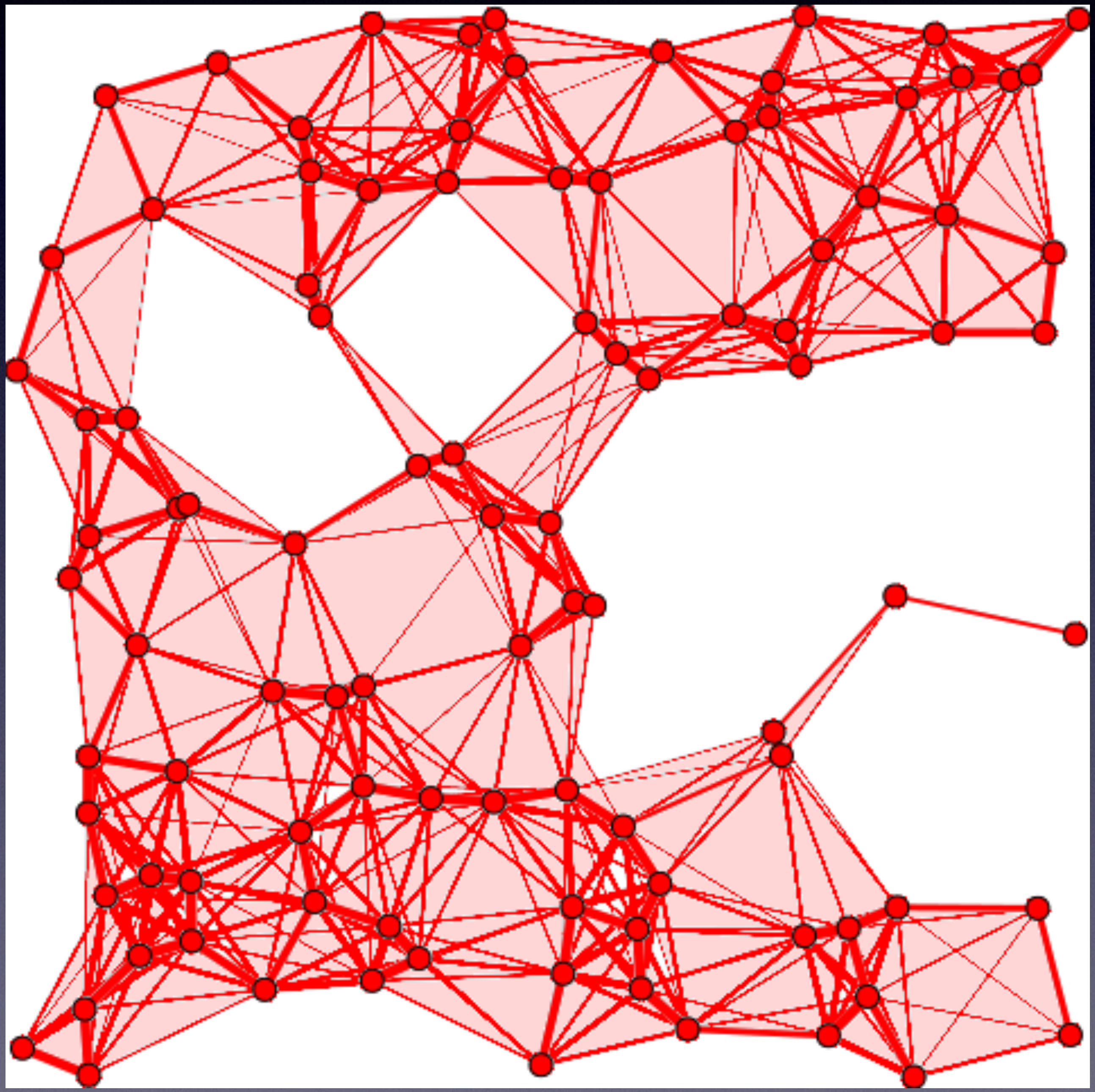
E.g. Niyogi–Smale–Weinberger (2004) for the Cech complex

Proximity Graph



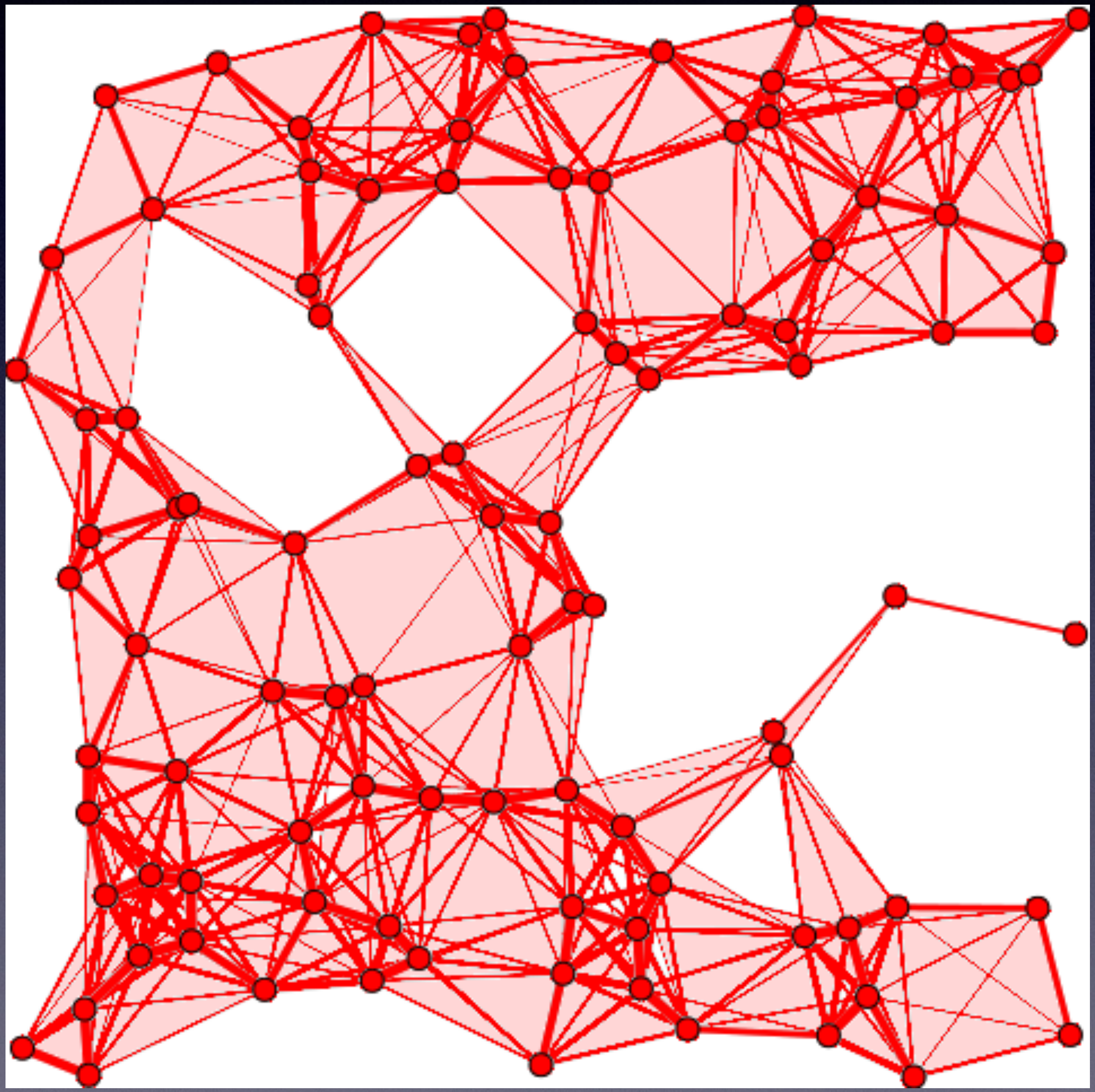
(picture credit: Elizabeth Meckes)

Vietoris–Rips complex



(picture credit: Elizabeth Meckes)

Čech complex



(picture credit: Elizabeth Meckes)

Properties

- Each complex depends on a scale parameter r
- $r=0$
  - discrete collection of vertices
- $r=\infty$
  - graph complex = the complete graph on X
  - Vietoris–Rips = the complete simplex on X
  - Čech = the complete simplex on X
  - Alpha = Delaunay triangulation of convex hull of X

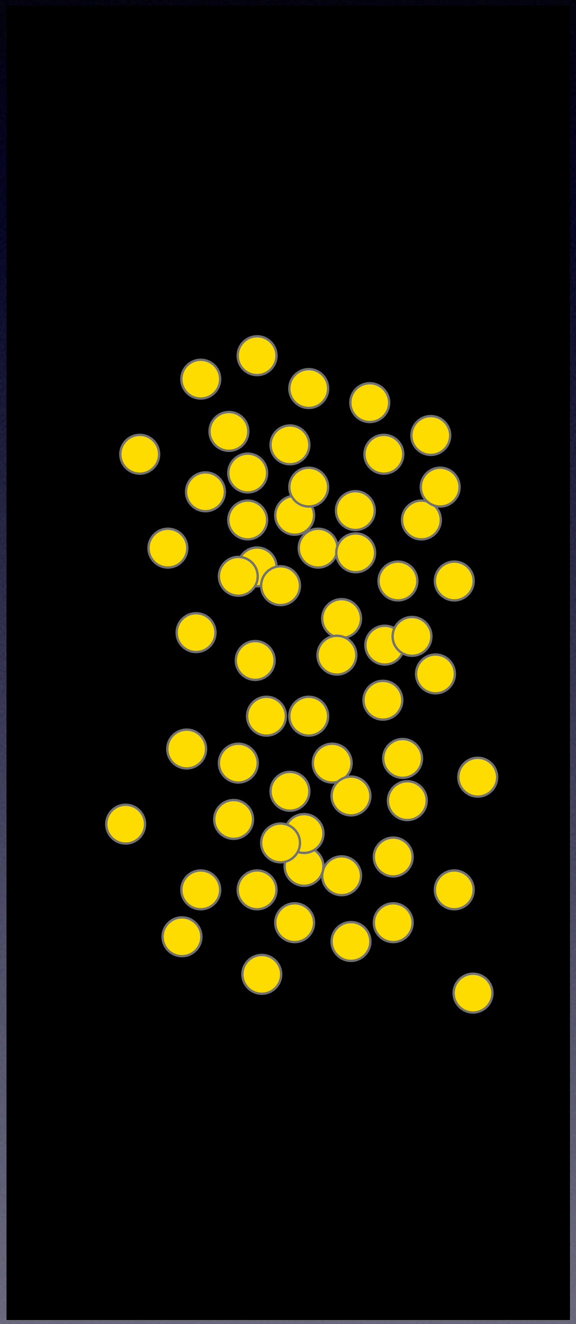
trivial topology

- Seek interesting topology in the range $0 < r < \infty$

Persistence

Instability

- 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
  - ✔ suitable for topological spaces
  - ✘ dangerous for point-clouds



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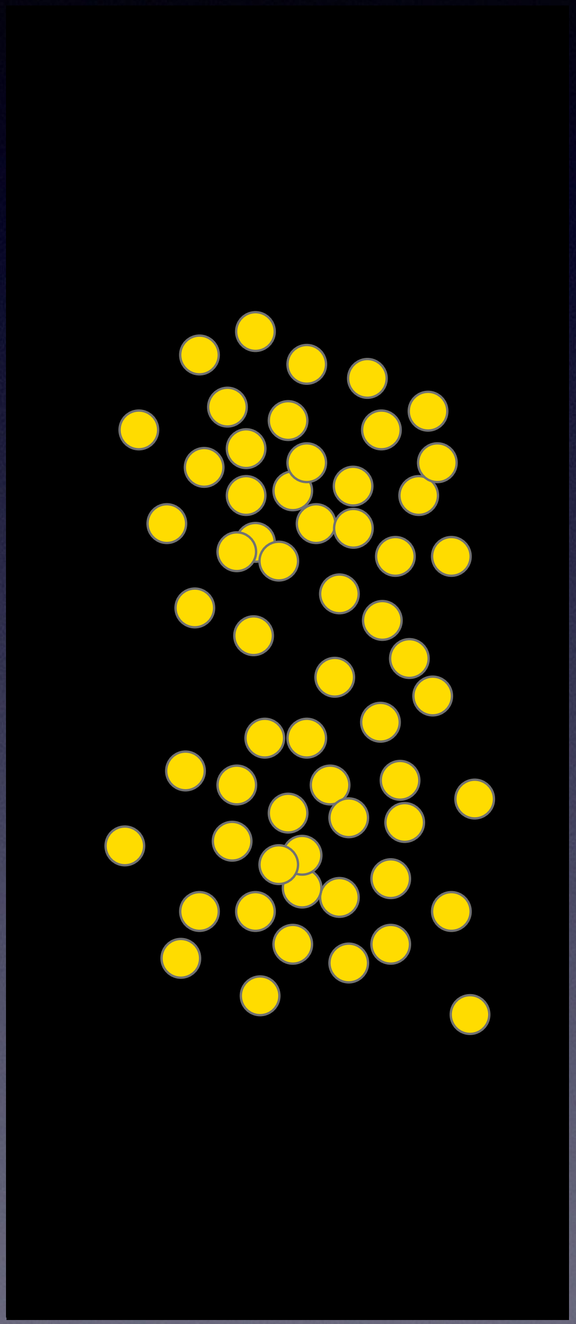

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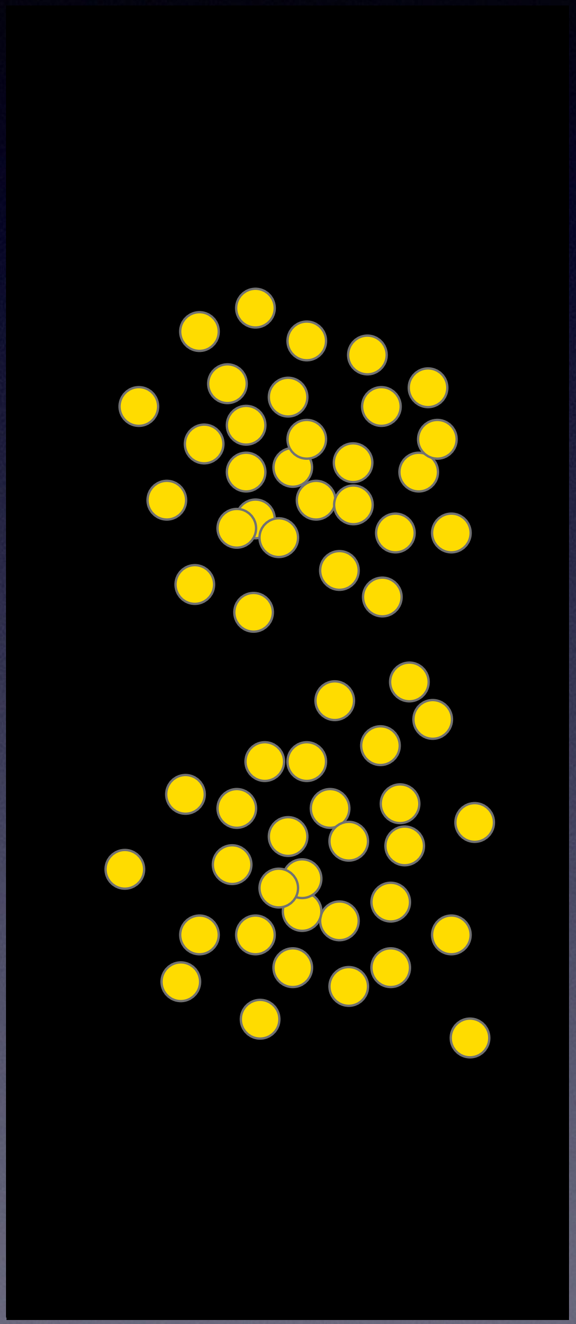
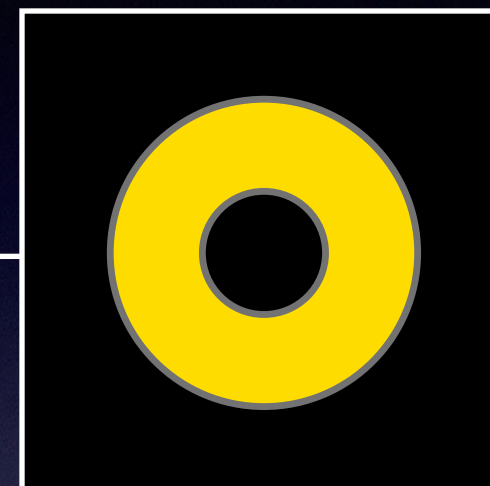
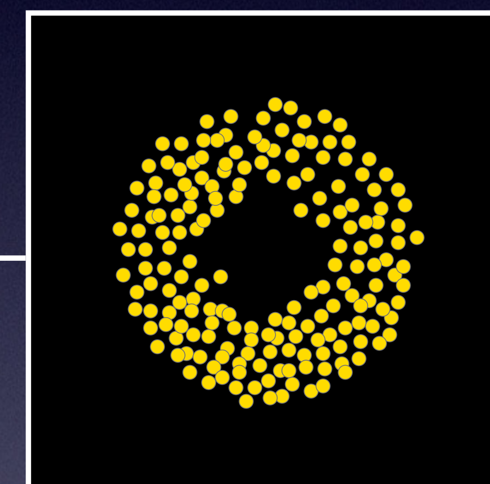


The standard pipeline (first attempt)

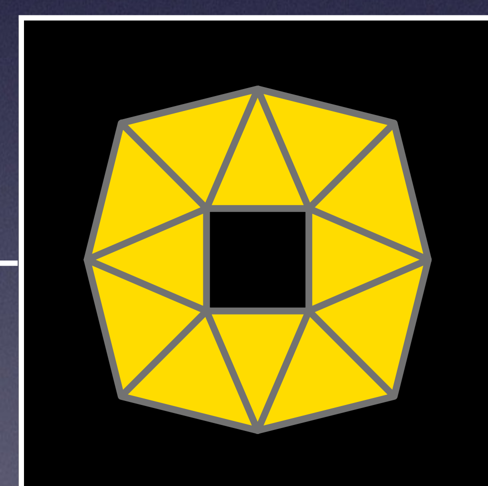
hidden/unknown space Y



finite sample $X \subset Y$



simplicial complex $S = S(X)$



homology invariants of S

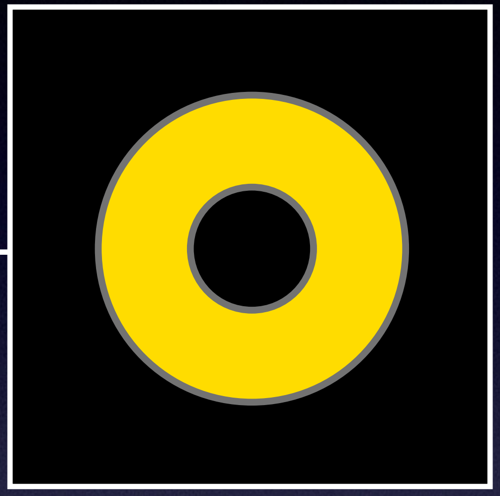
$b_0 = 1$

$b_1 = 1$

$b_2 = 0$

The standard pipeline (second attempt)

hidden/unknown
space Y



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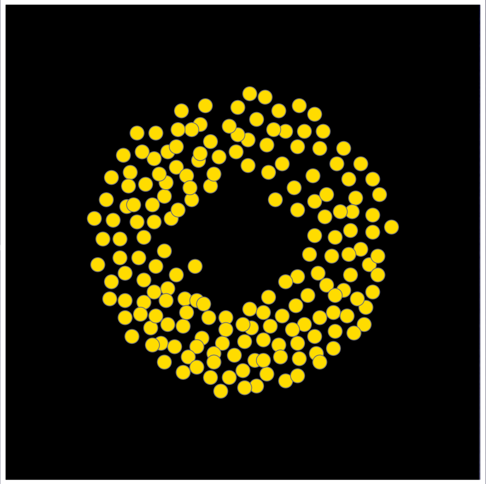
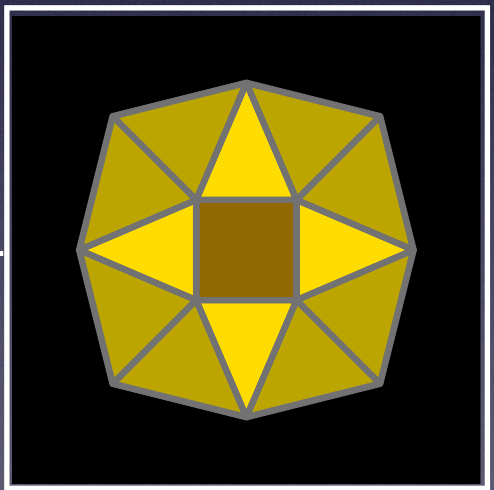
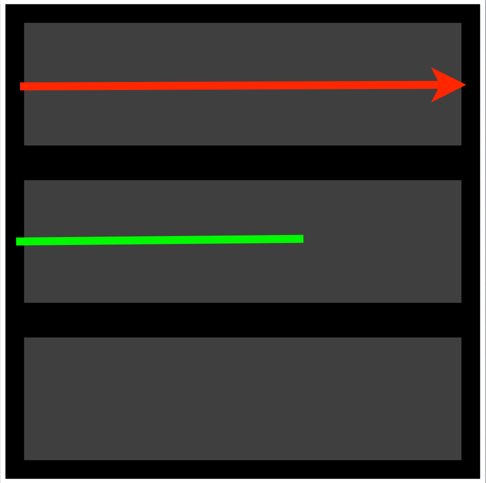


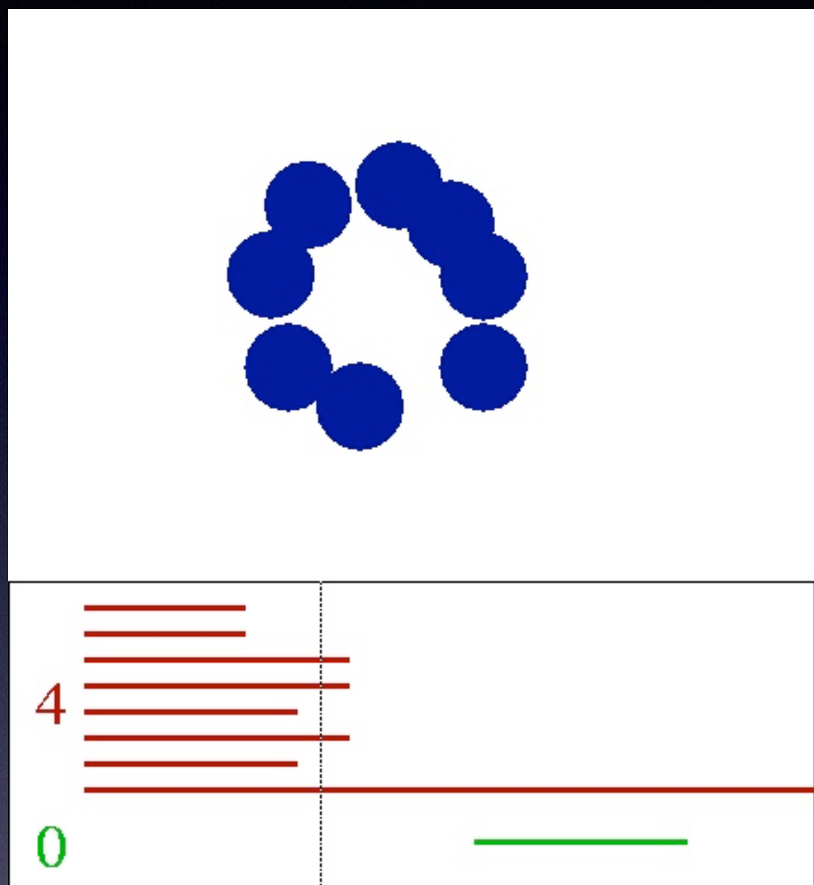
filtered complex
$S(r) = S(X, r)$



persistent homology
of $S(r)$



Persistent homology



- Homology provides functors H=H$_k$
- Construct a sequence of spaces

$$\boxed{X_0 \to X_1 \to \cdots \to X_k}$$

- Obtain a sequence of vector spaces

$$\boxed{\mathrm{H}(X_0) \to \mathrm{H}(X_1) \to \cdots \to \mathrm{H}(X_k)}$$

- Describe the structure of such a sequence
  (what are the irreducible factors?)

one vector space $\leftrightarrow$ dimension

sequence of vector spaces $\leftrightarrow$ persistence barcode

Edelsbrunner, Letscher, Zomorodian (2000)
Zomorodian, Carlsson (2002)
Cohen-Steiner, Edelsbrunner, Harer (2007)

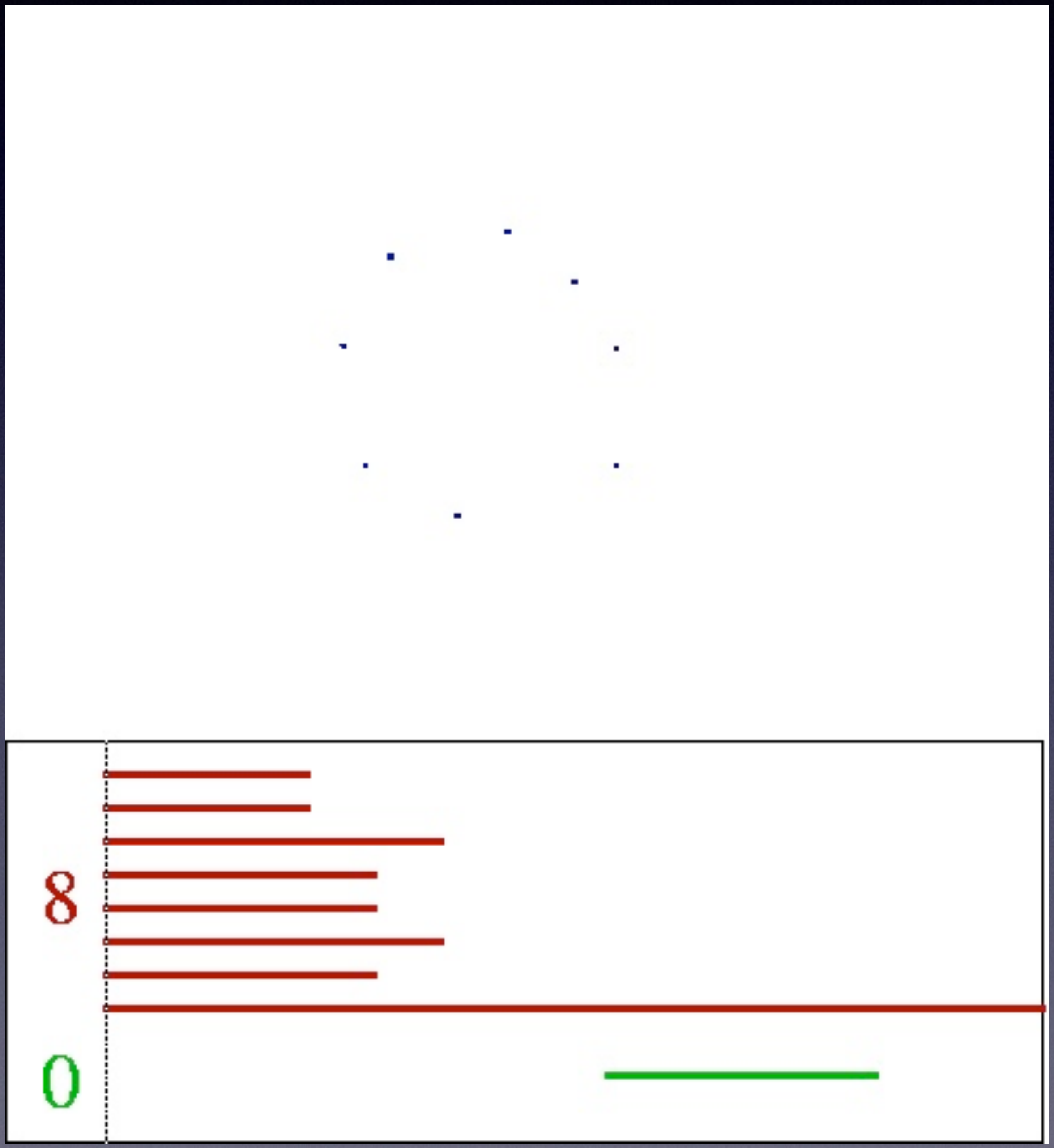
Persistence

- Algorithm (Edelsbrunner, Letscher, Zomorodian ’00)
  - barcode: finite collection of half-open intervals
  - [b,d) indicates feature lifetime: born at time b, dies at time d

- Stability theorem (Cohen-Steiner, Edelsbrunner, Harer ’07)
  - barcode depends continuously on the underlying data
  - interleaved systems have similar barcode (Chazal, Cohen-Steiner, Glisse, Guibas, Oudot ’09)
  - continuous measurements (interval length)

  & discrete information (number of intervals)

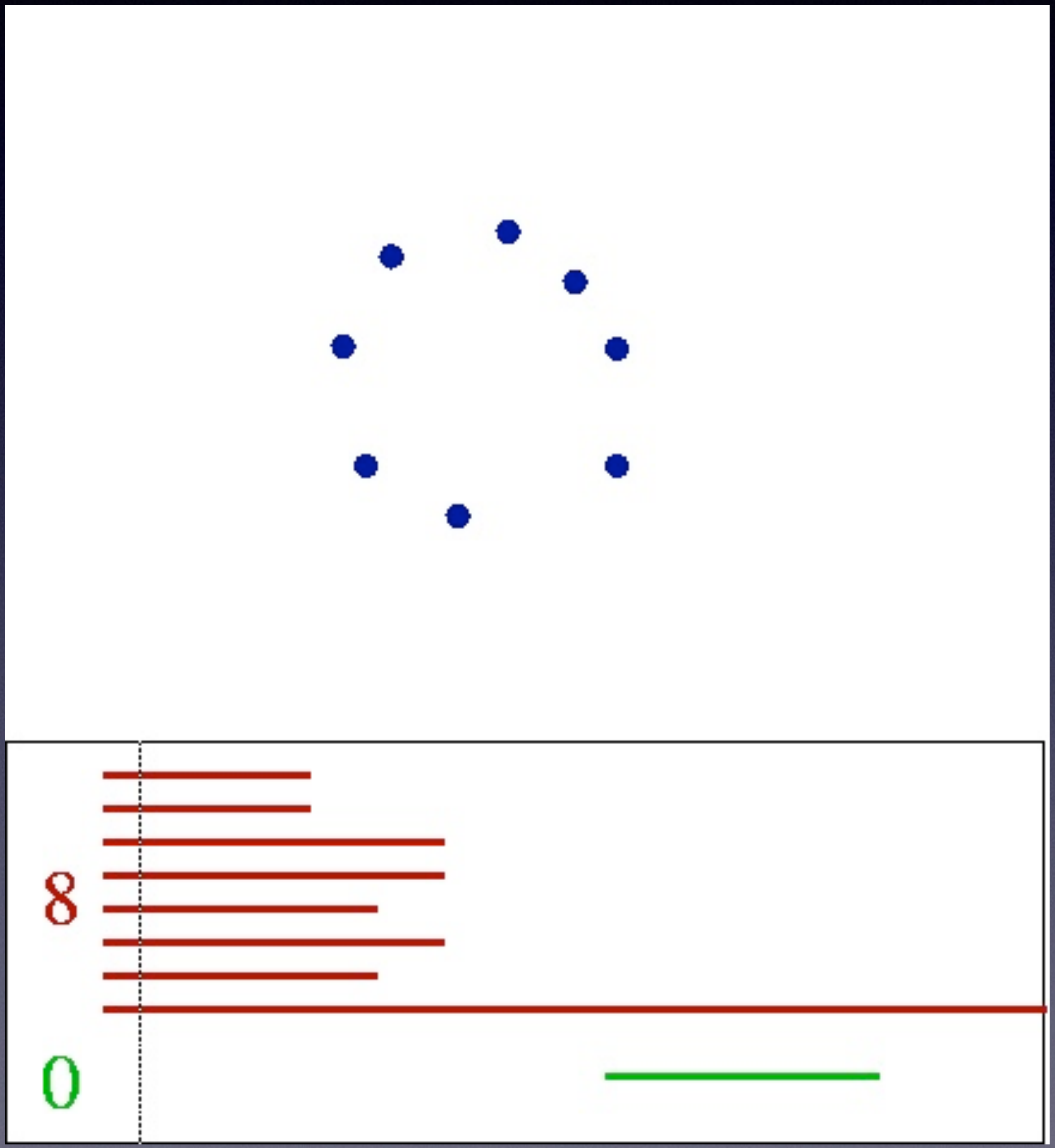
Example



b_0: (clusters)

b_1: (holes)

Example



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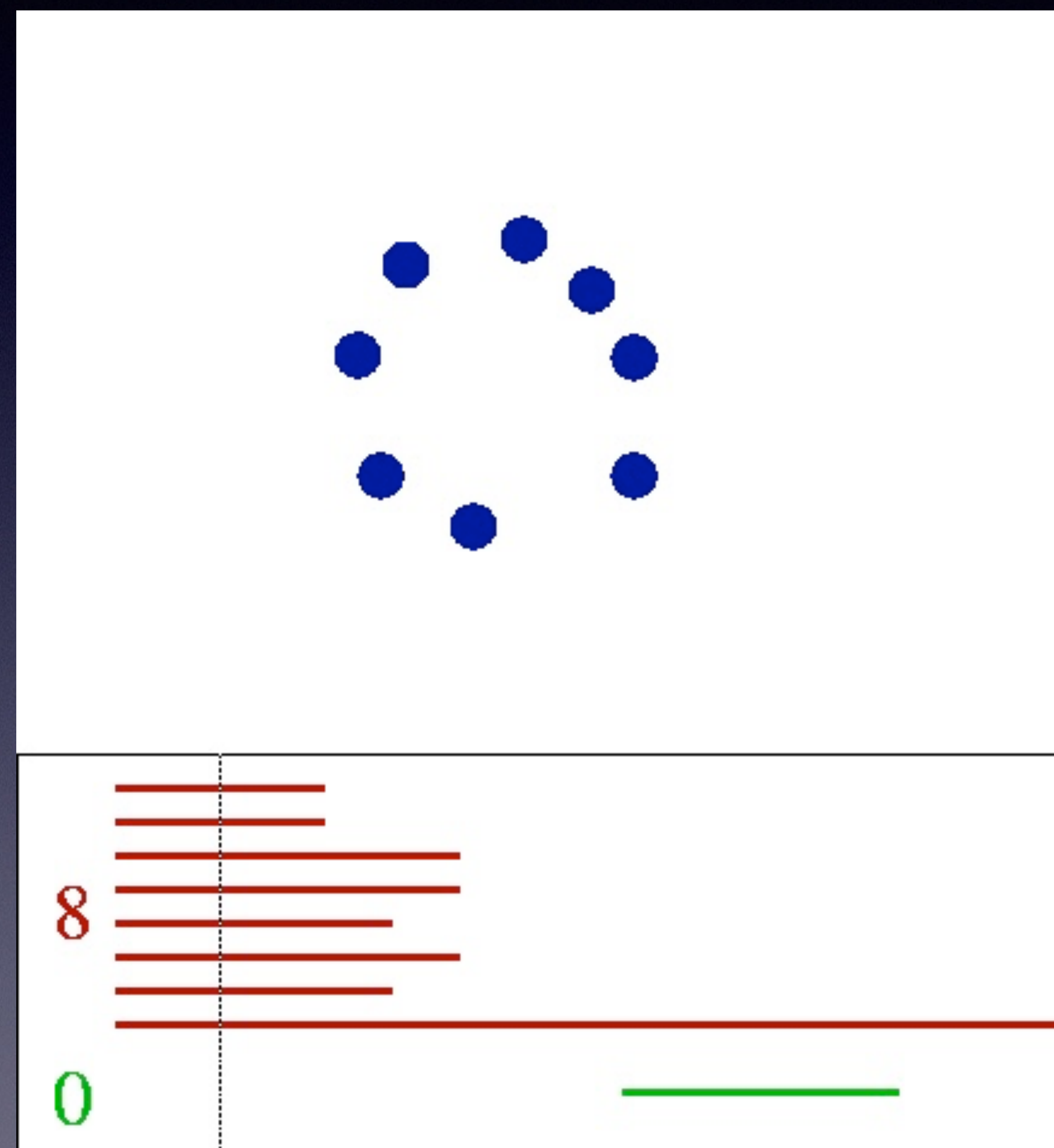

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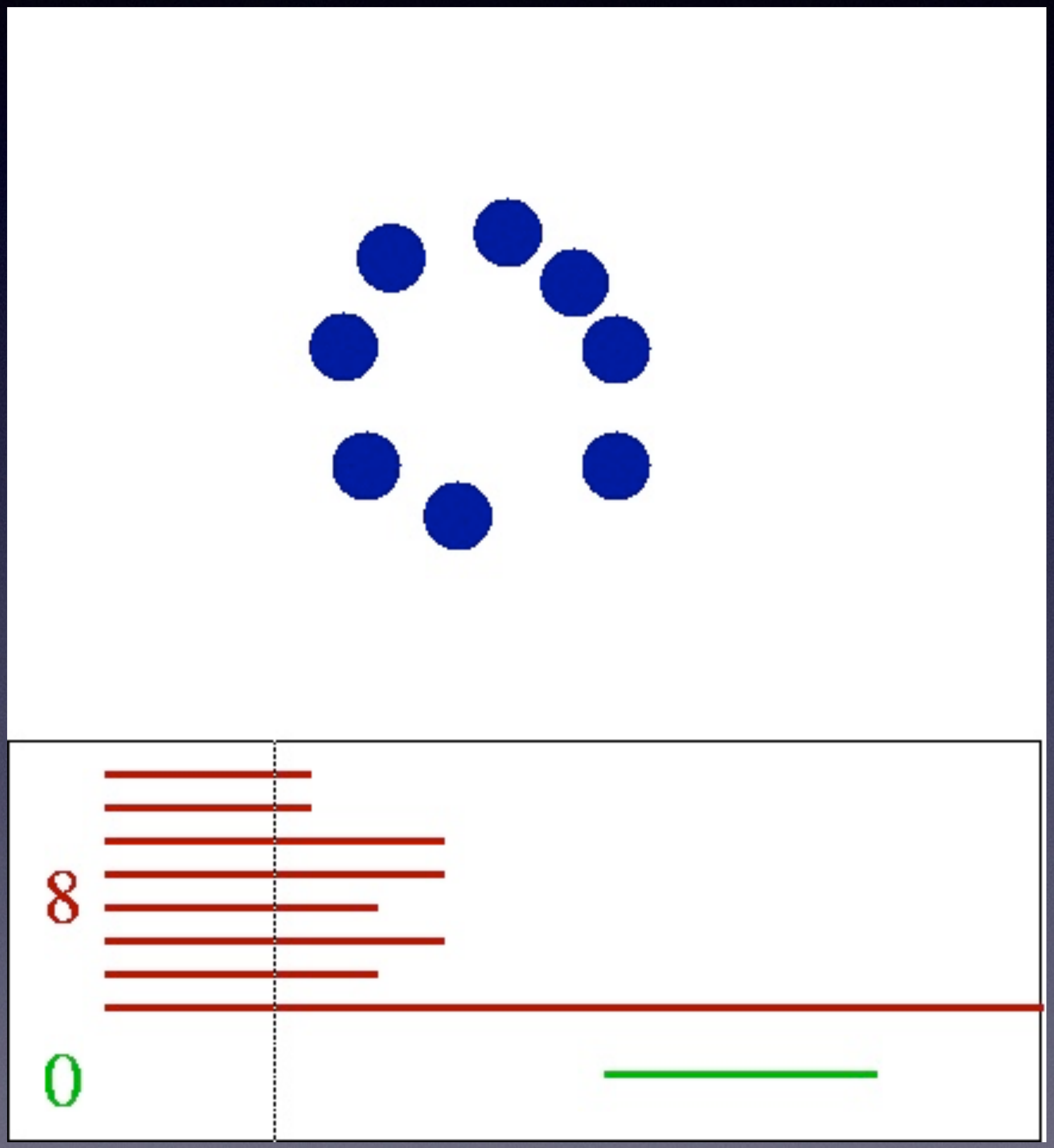

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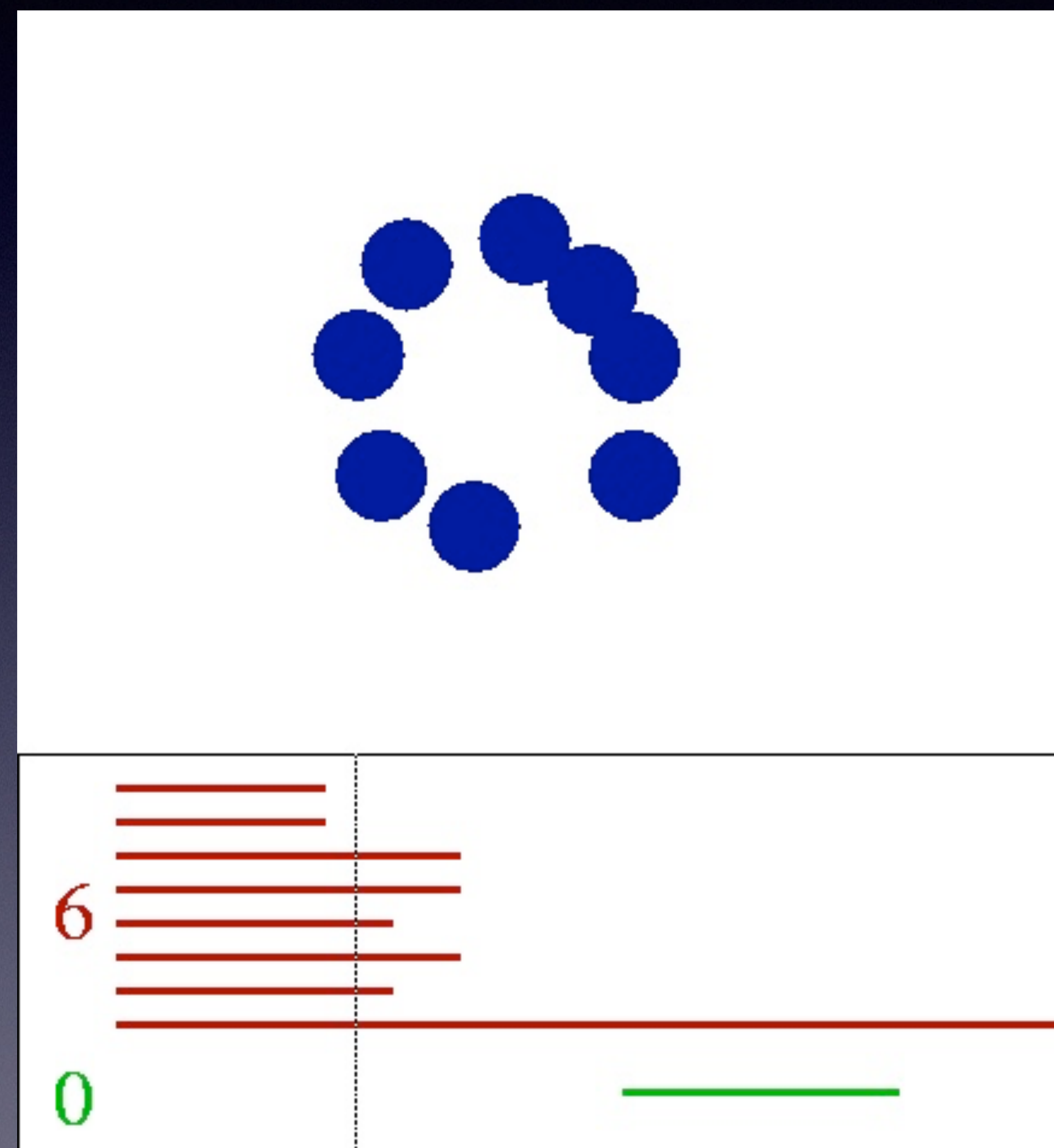

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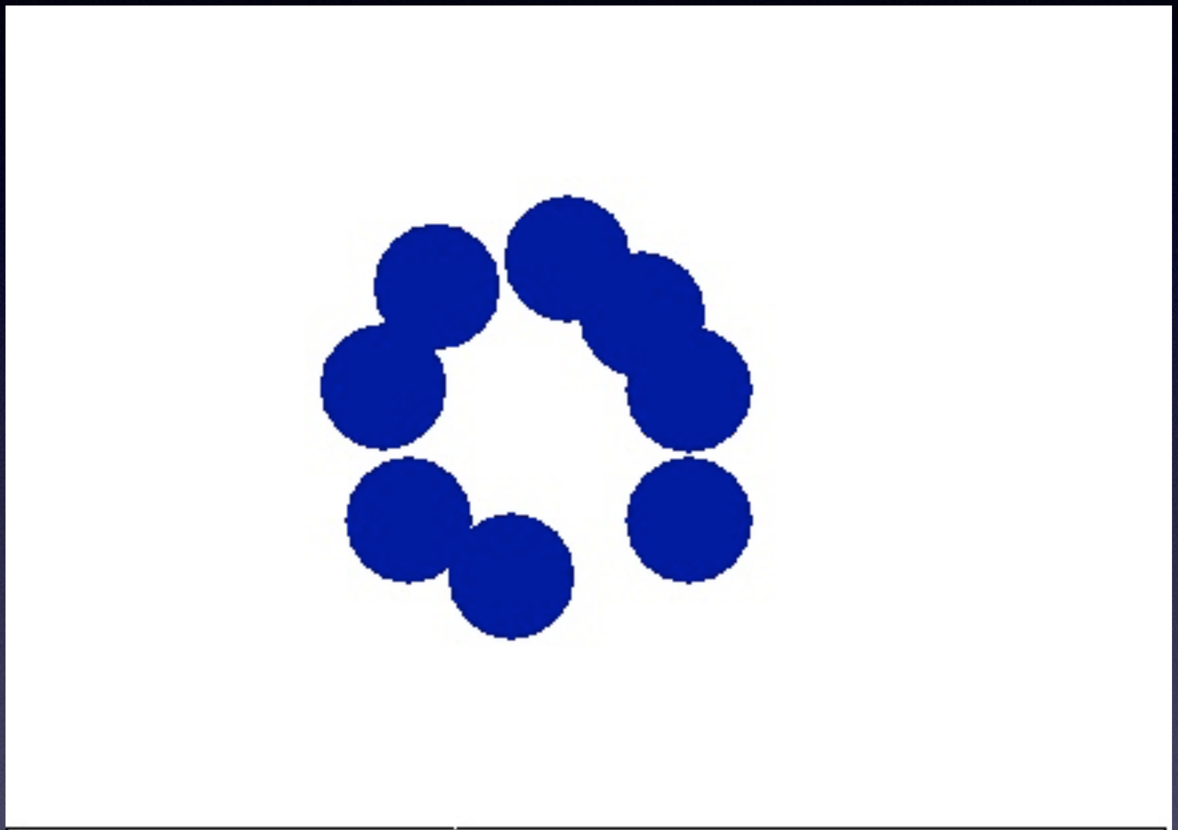

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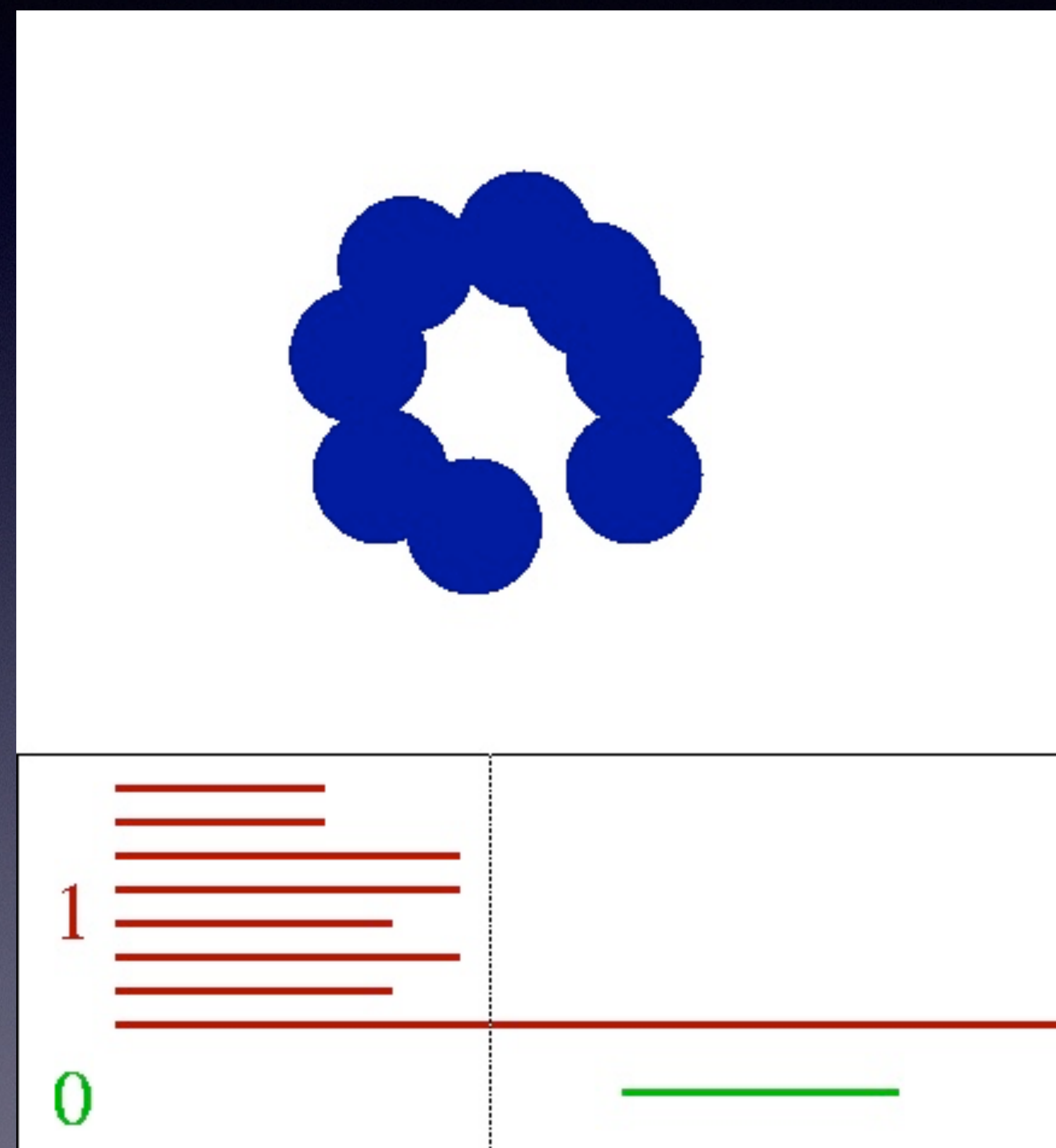

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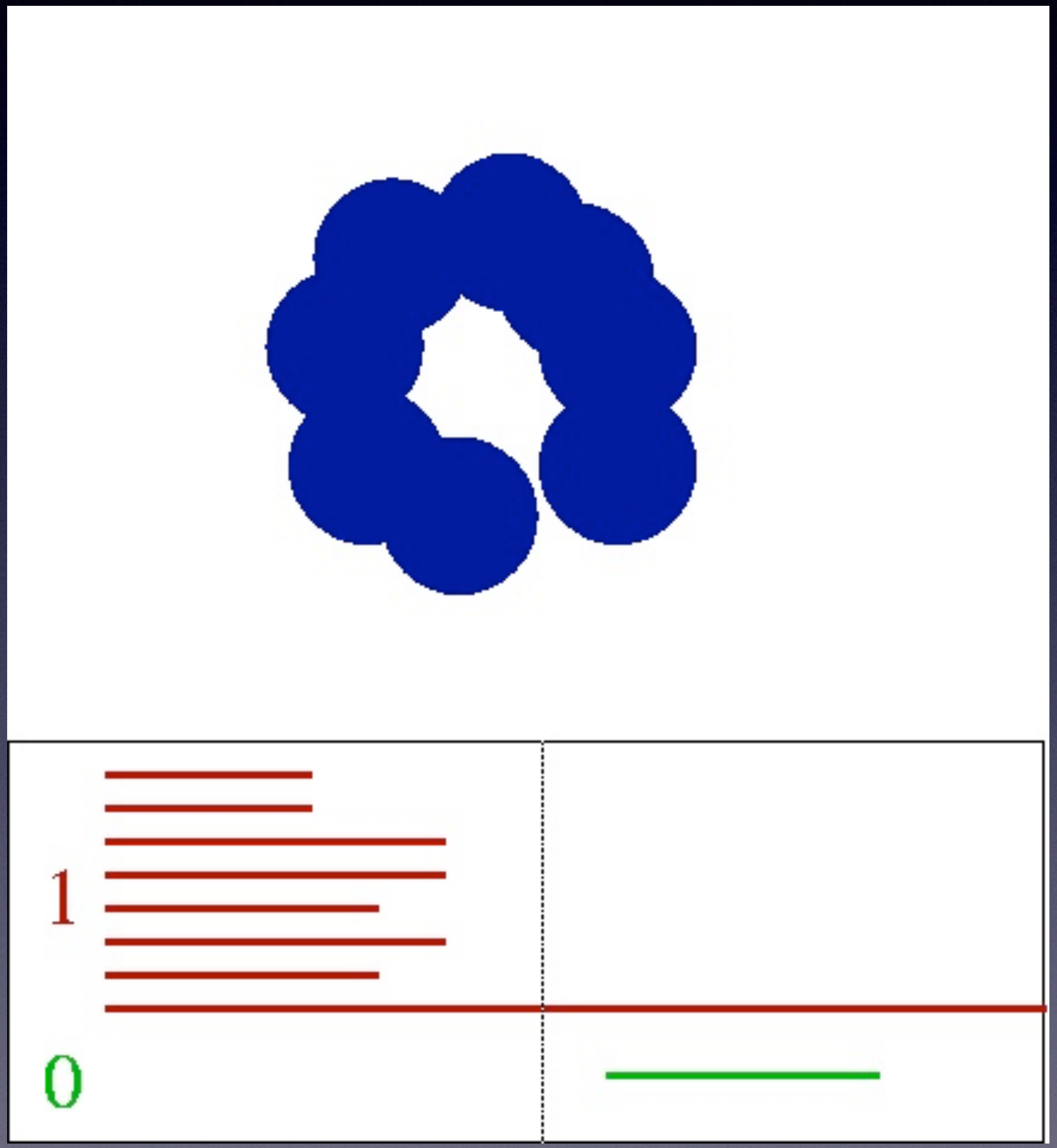

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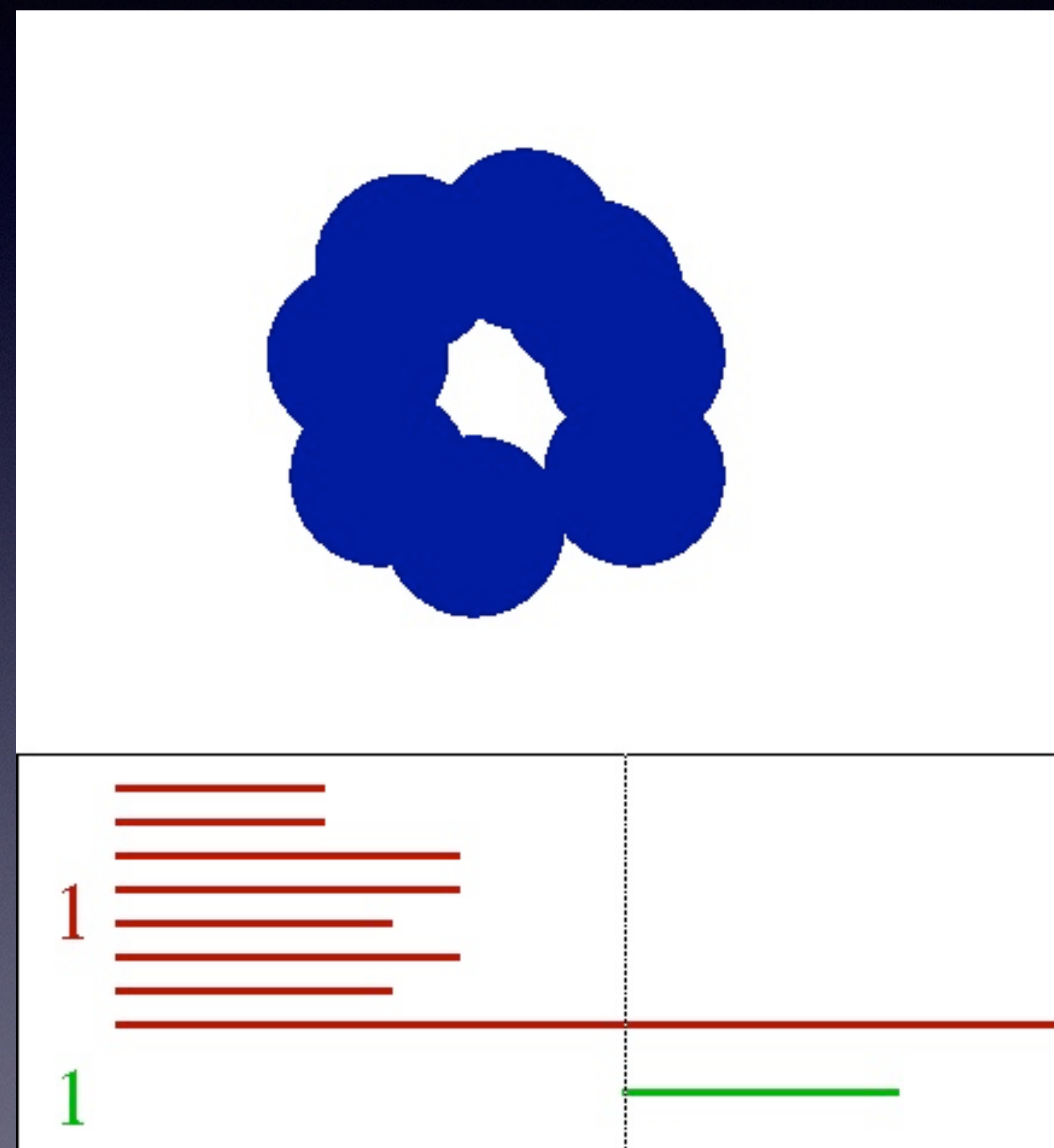

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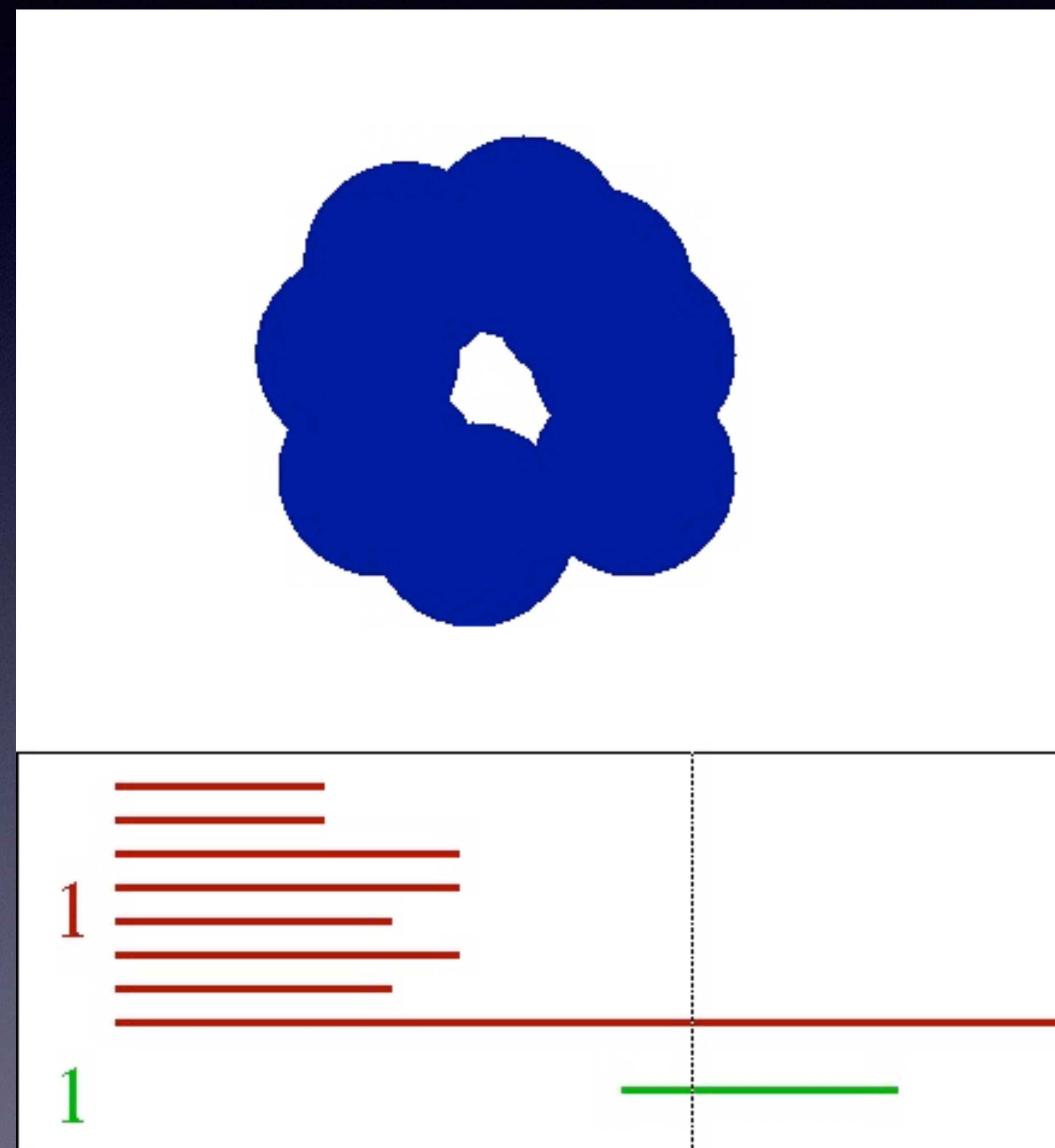

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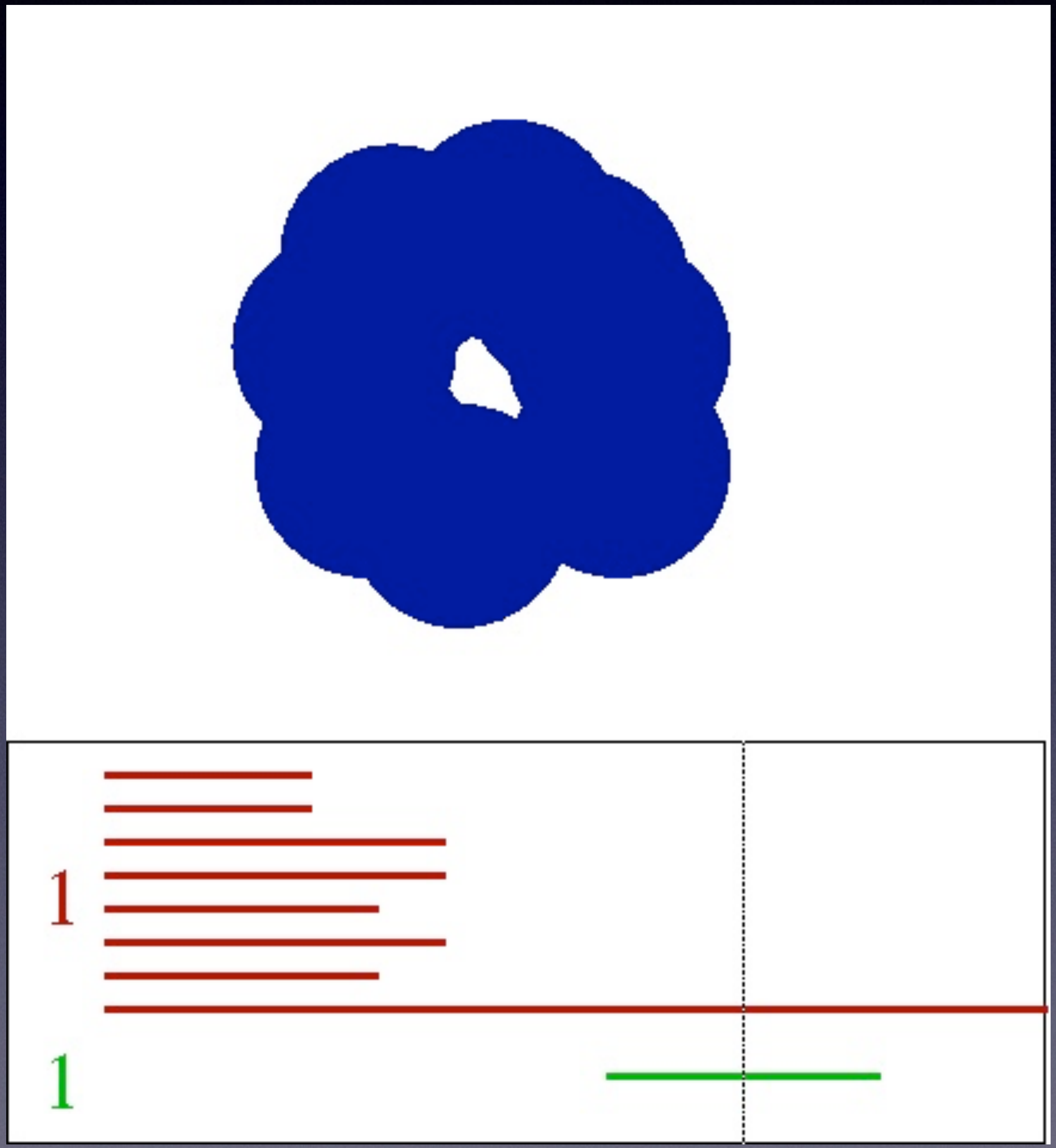

b$_0$: (clusters)

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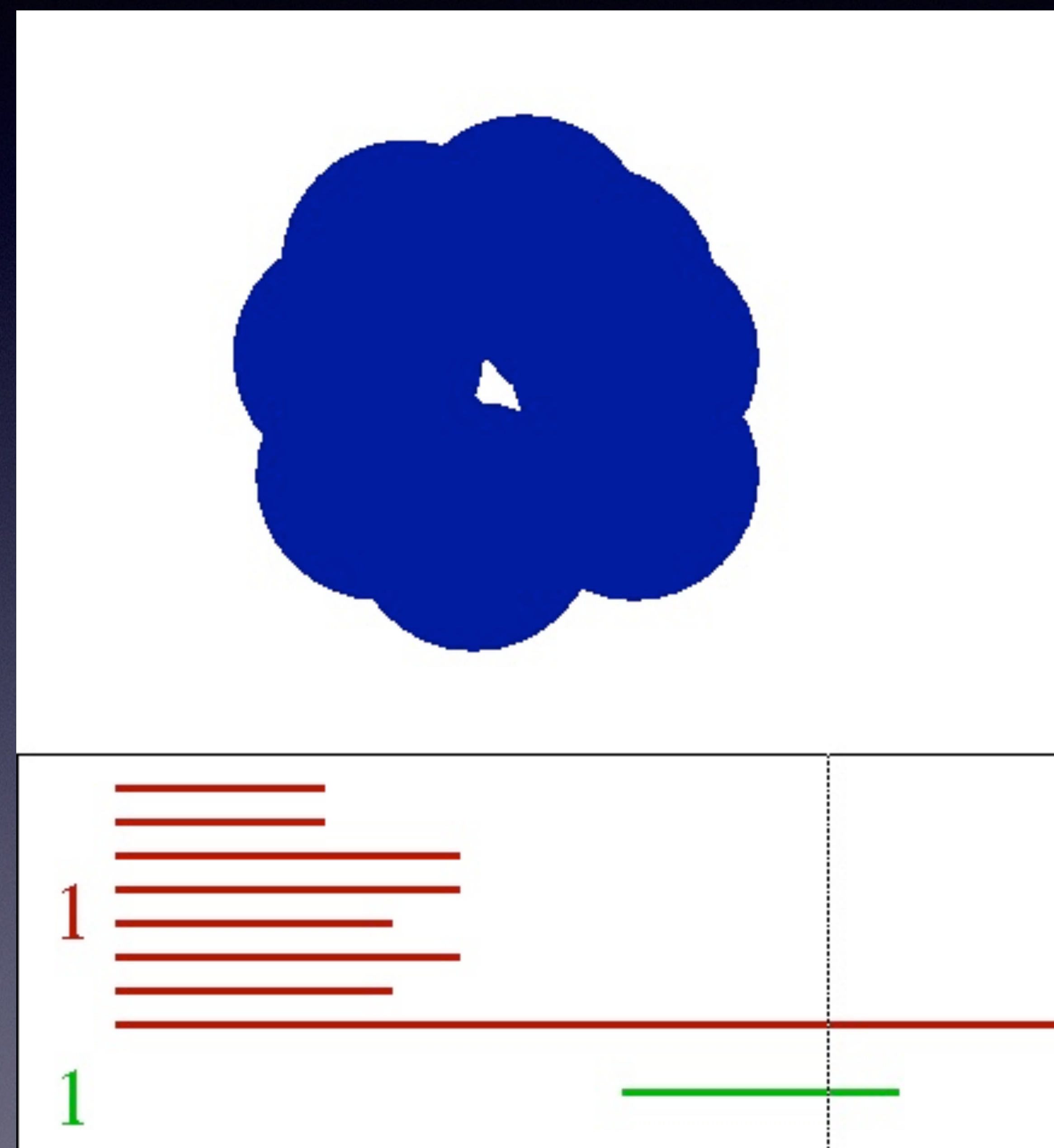

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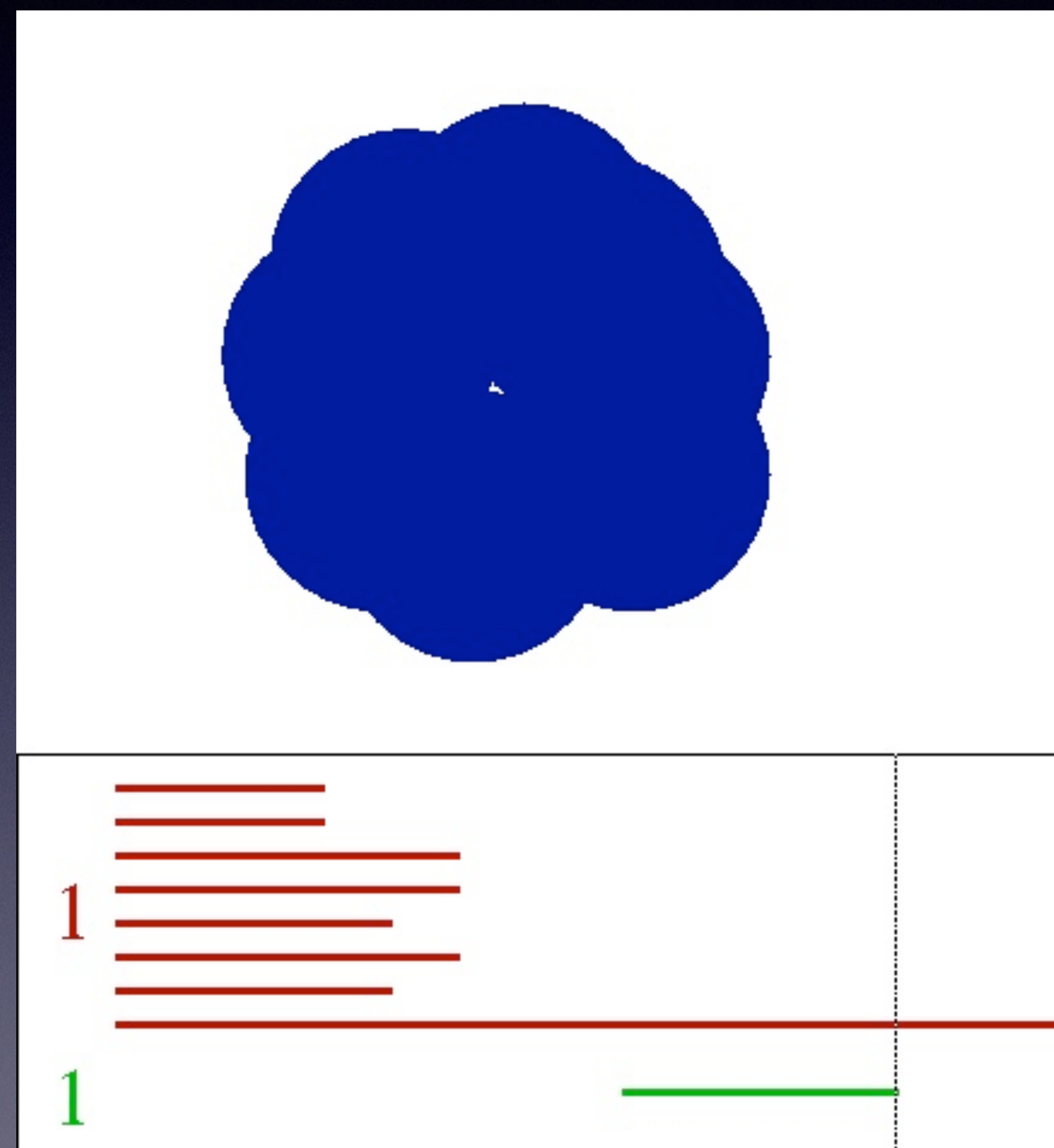

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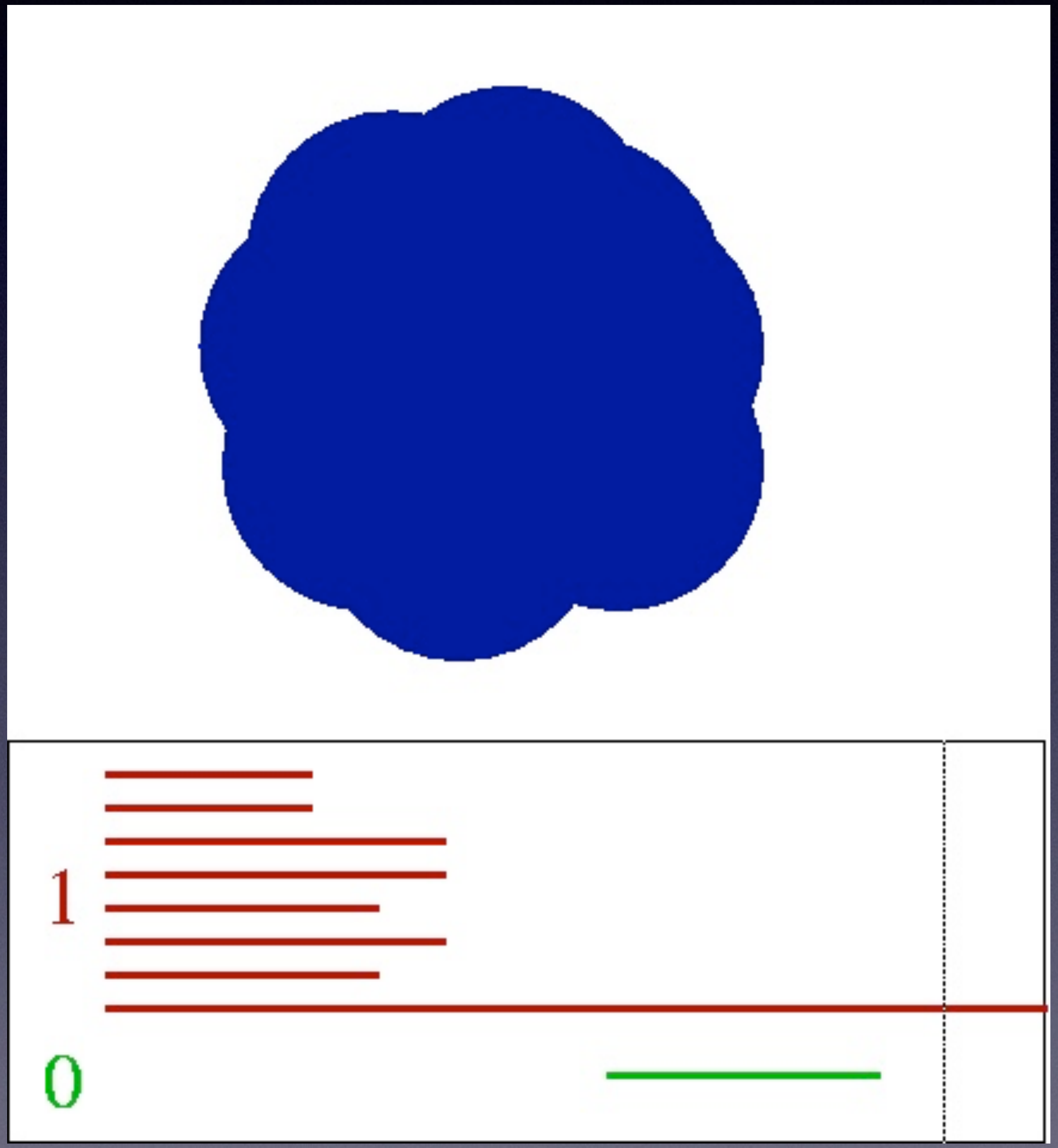

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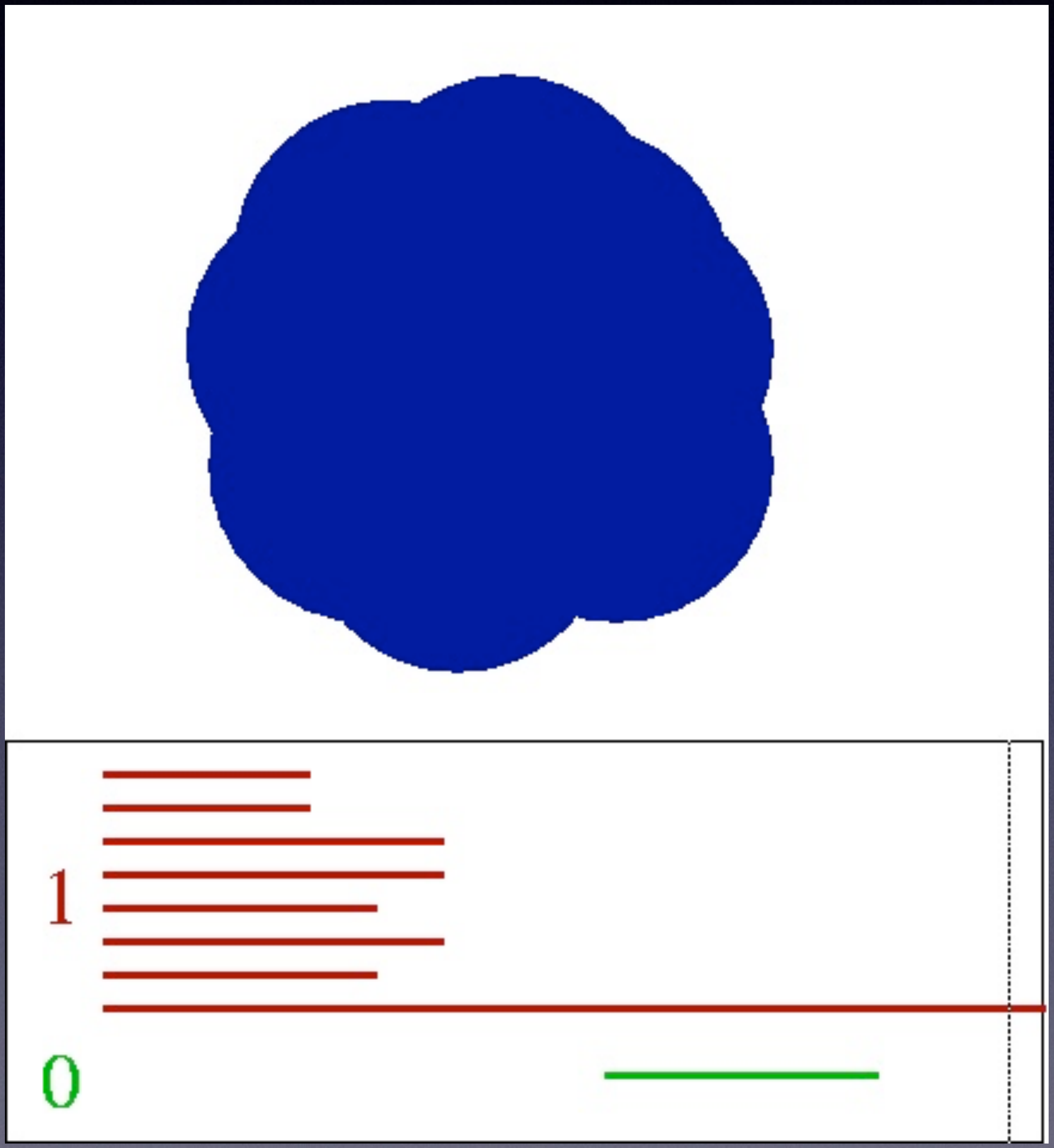

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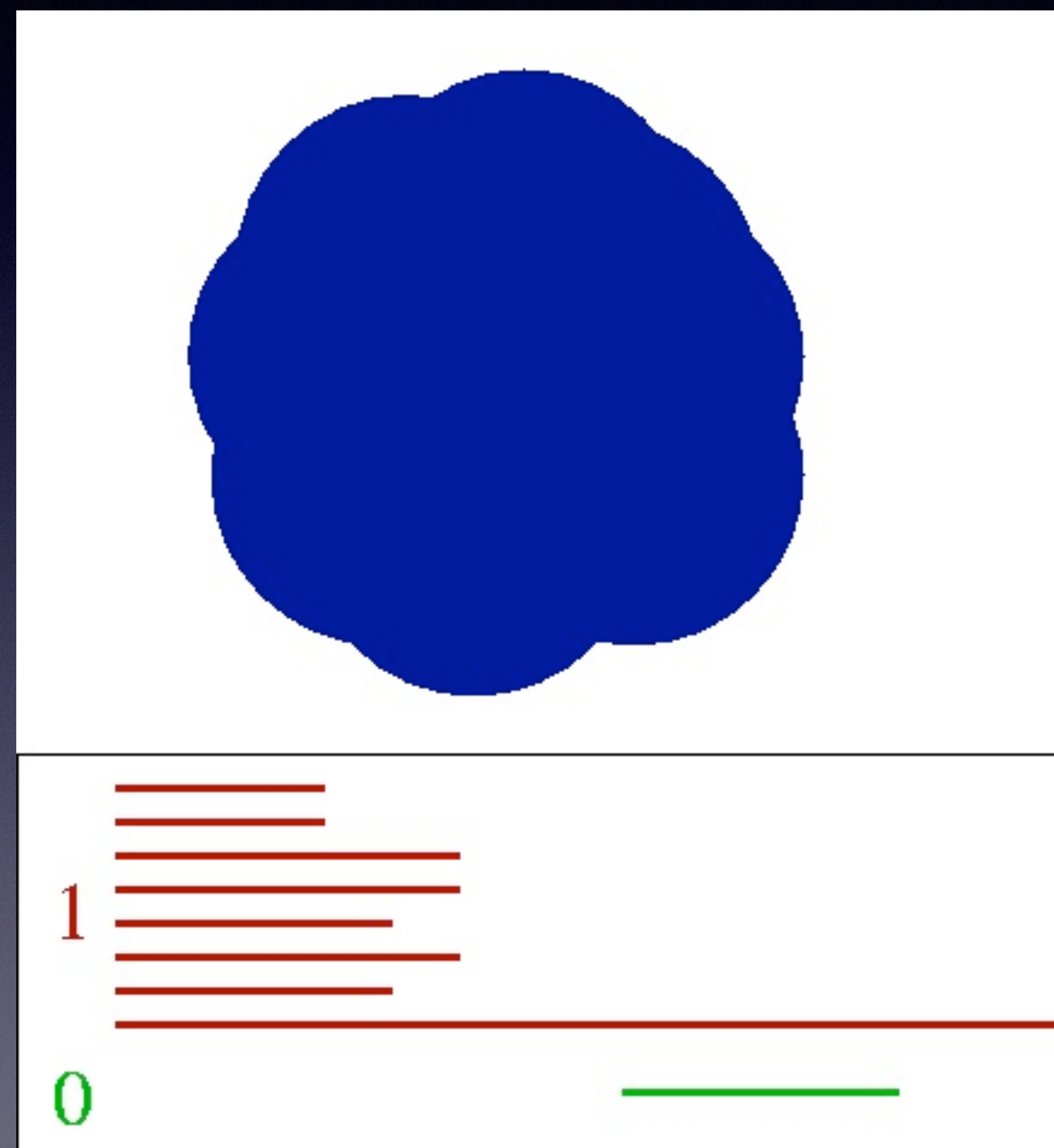

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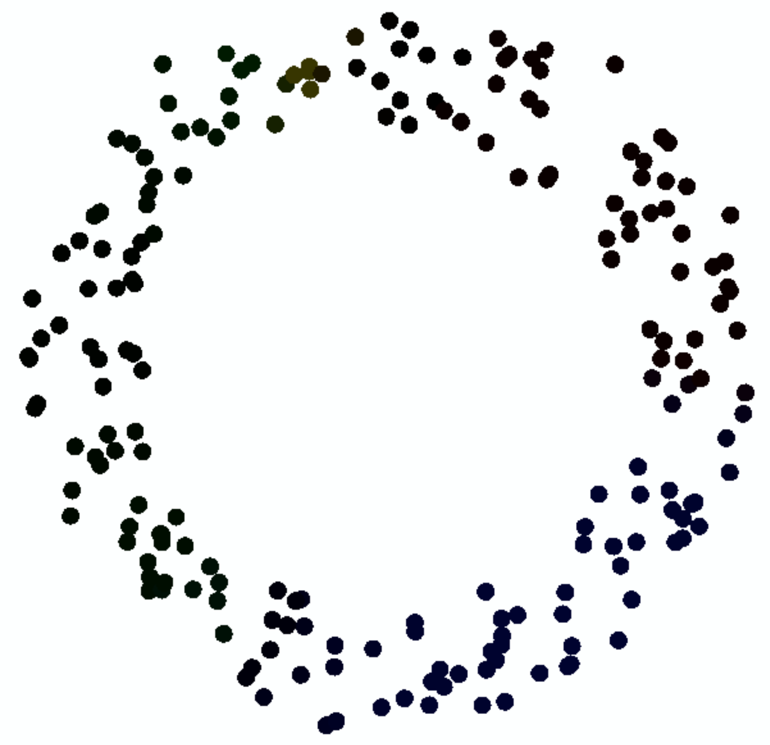
Persistence diagram



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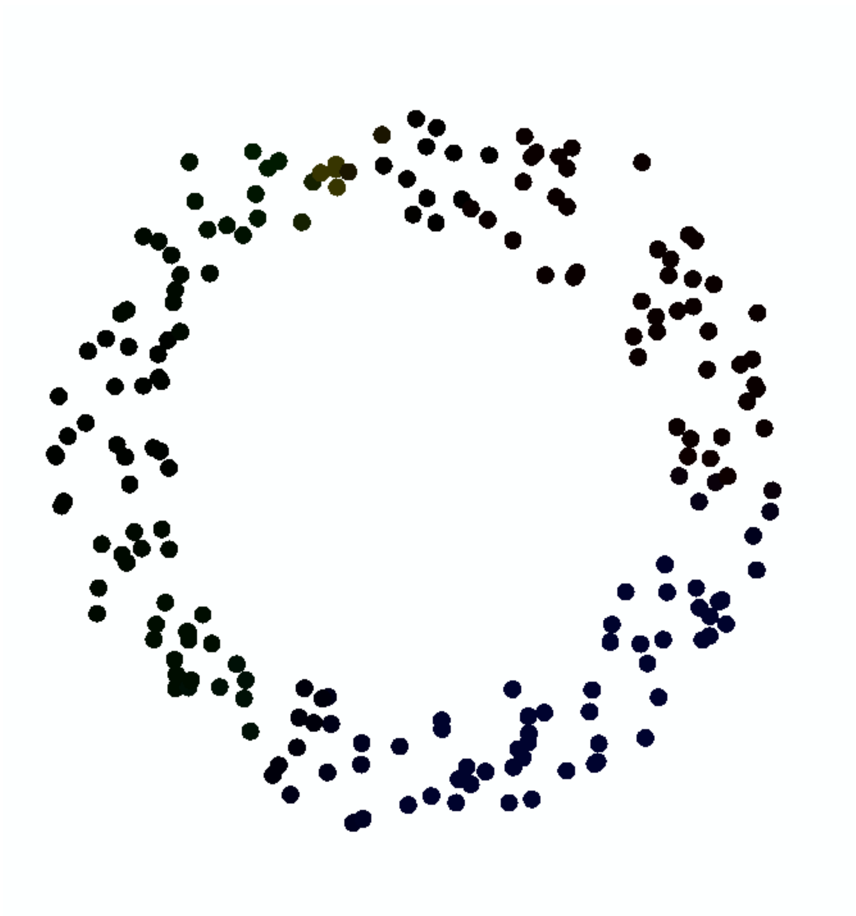
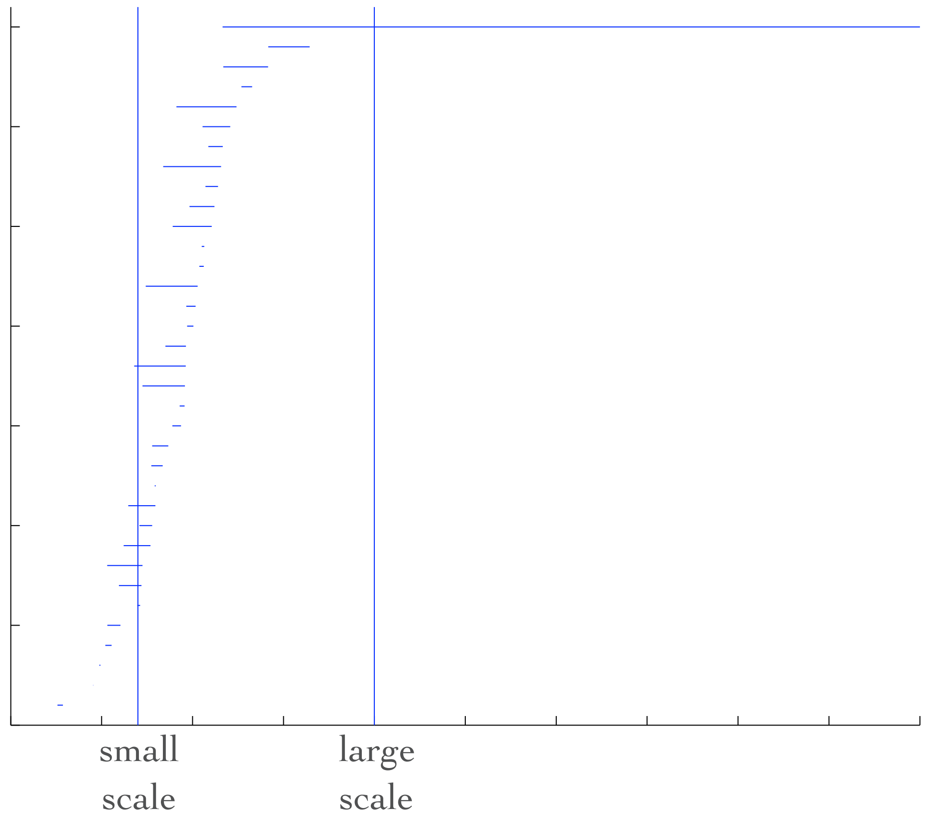
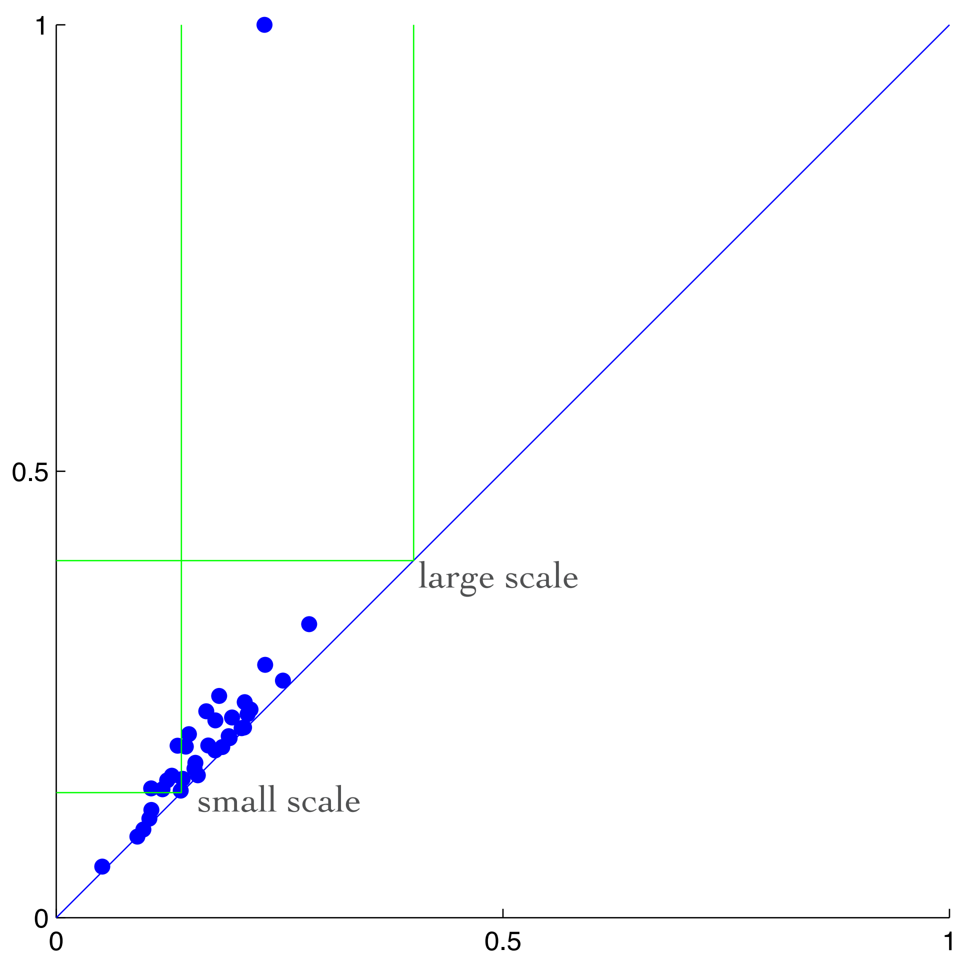
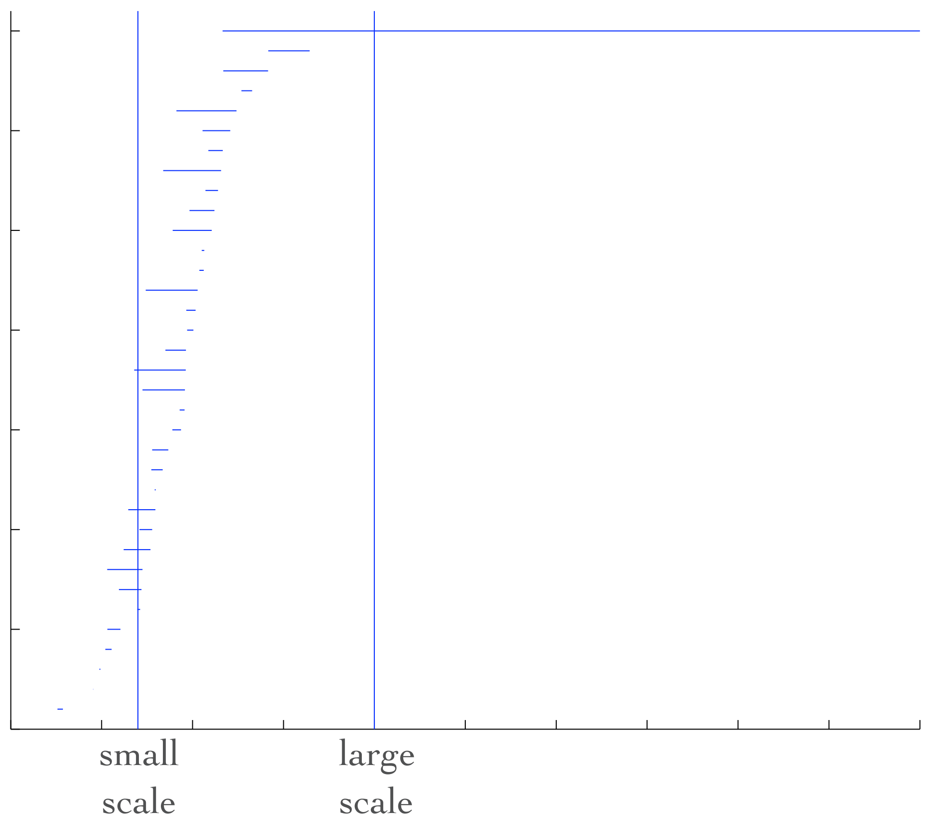




Barcode

Persistence diagram





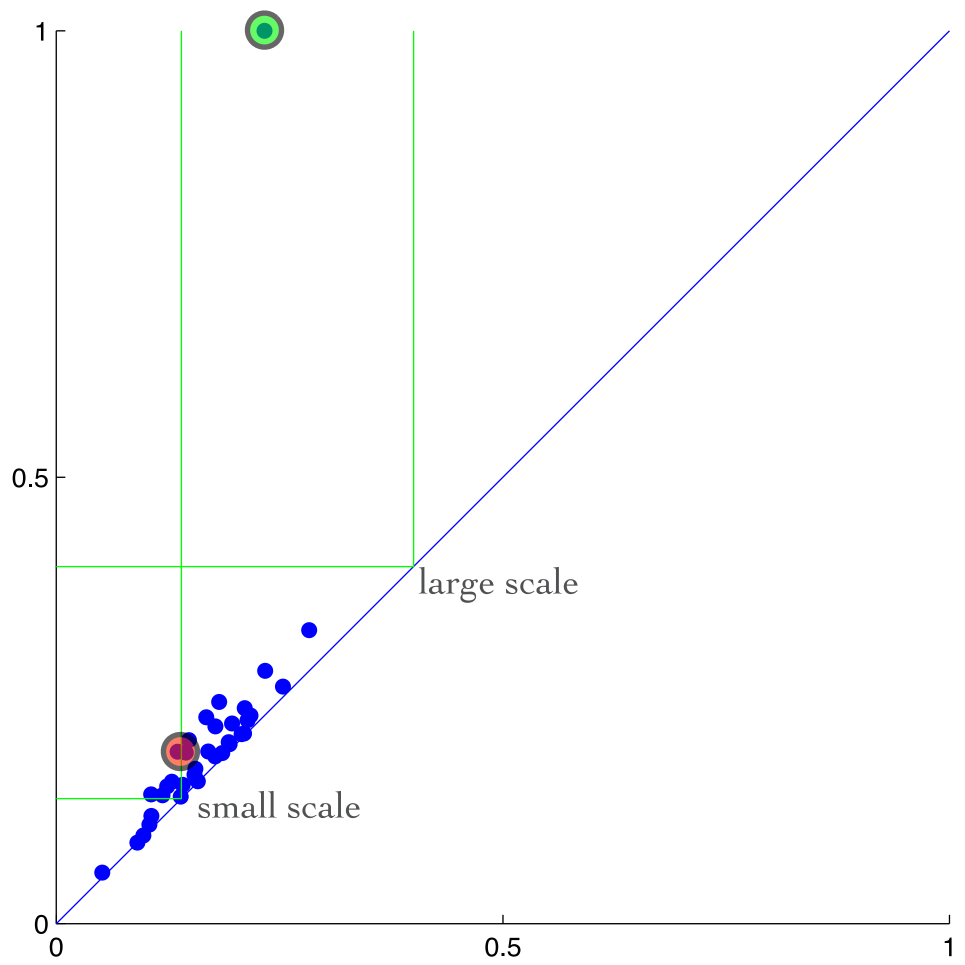
Persistence diagram

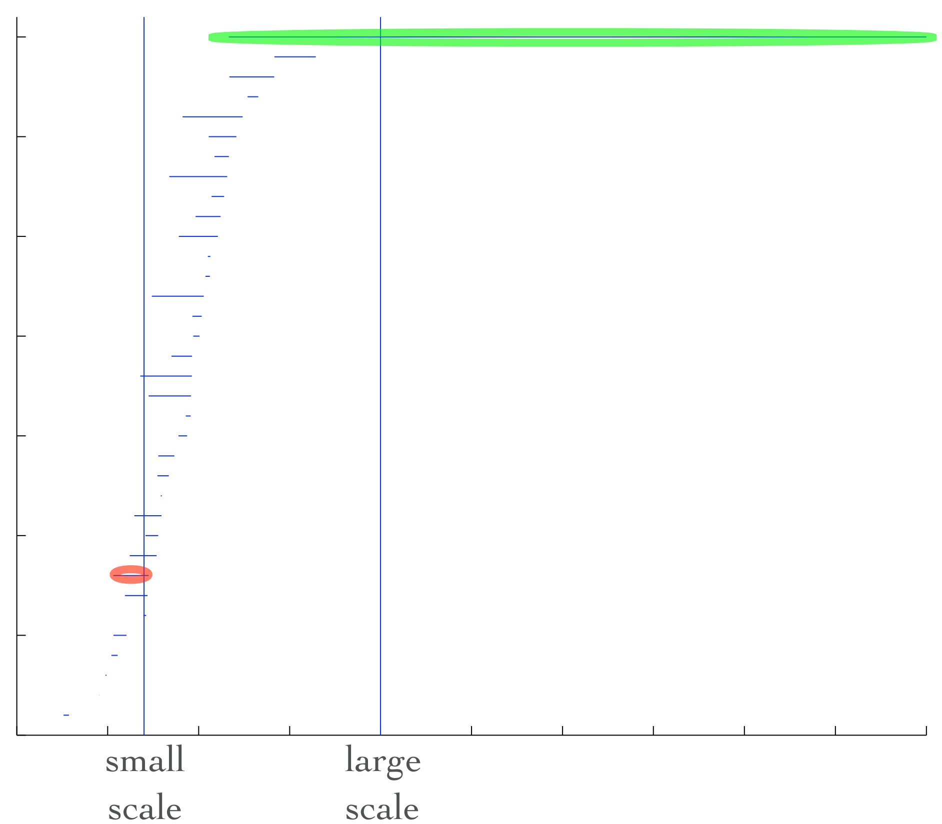
points (b,d)

Barcode

intervals [b,d)

Persistence diagram





Persistence diagram

Barcode

points (b,d) ⟷ intervals [b,d)

And the Oscar goes to...

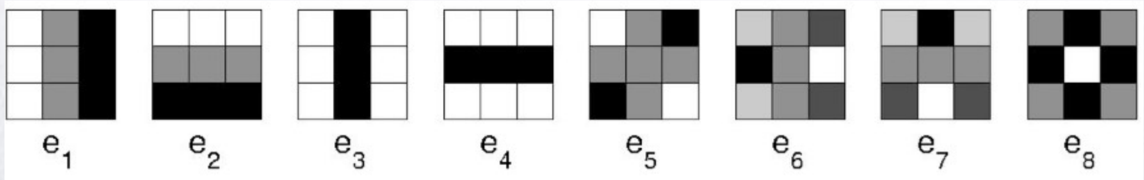
Witness Complexes -- Mumford Dataset

Vin de Silva & Gunnar Carlsson

Visual Image Patches

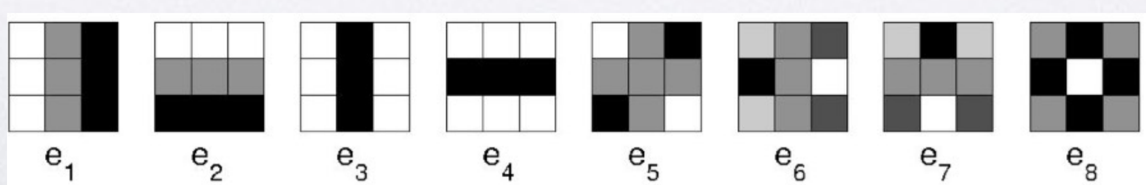
Visual image patches

- Lee, Pedersen, Mumford (2003) studied the local statistical properties of natural images (from Van Hateren's database)
- 3-by-3 pixel patches with high contrast between pixels: are some patches more likely than others?
- Carlsson, VdS, Ishkhanov, Zomorodian (2004/8): topological properties of high-density regions in pixel-patch space



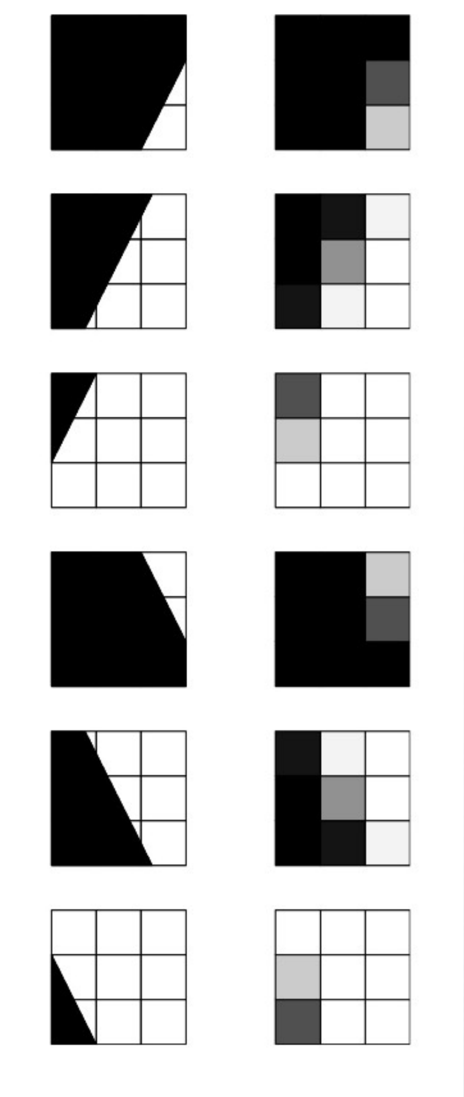
The space of image patches

- ~4.2 million high-contrast 3-by-3 patches selected randomly from images in database.
- Normalise each patch twice: subtract mean intensity, then rescale to unit norm.
- Normalised patches live on a unit 7-sphere in 8-dimensional space with the following basis:



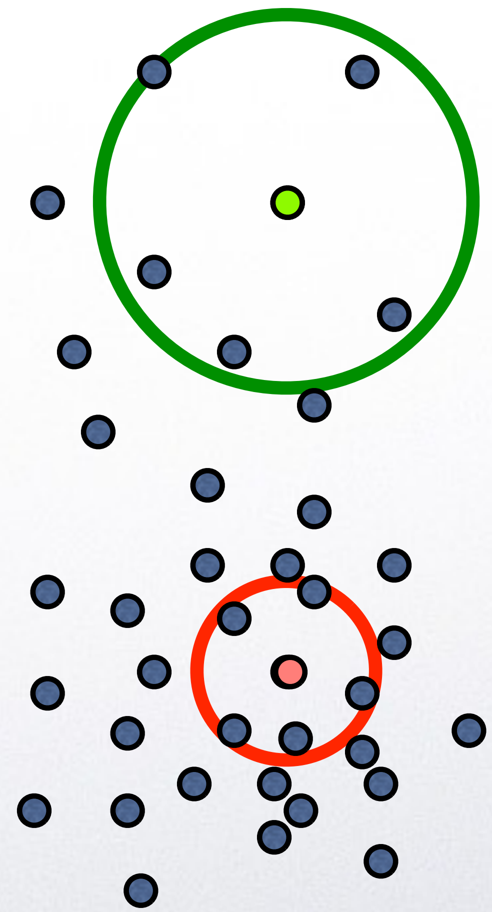
High-density regions

- LPM2003 found that the distribution of patches is dense in the 7-sphere.
- There are high-density regions:
  - edge features
- Can we describe the structure of the high-density regions?
  - threshold by k-nearest-neighbour density estimator

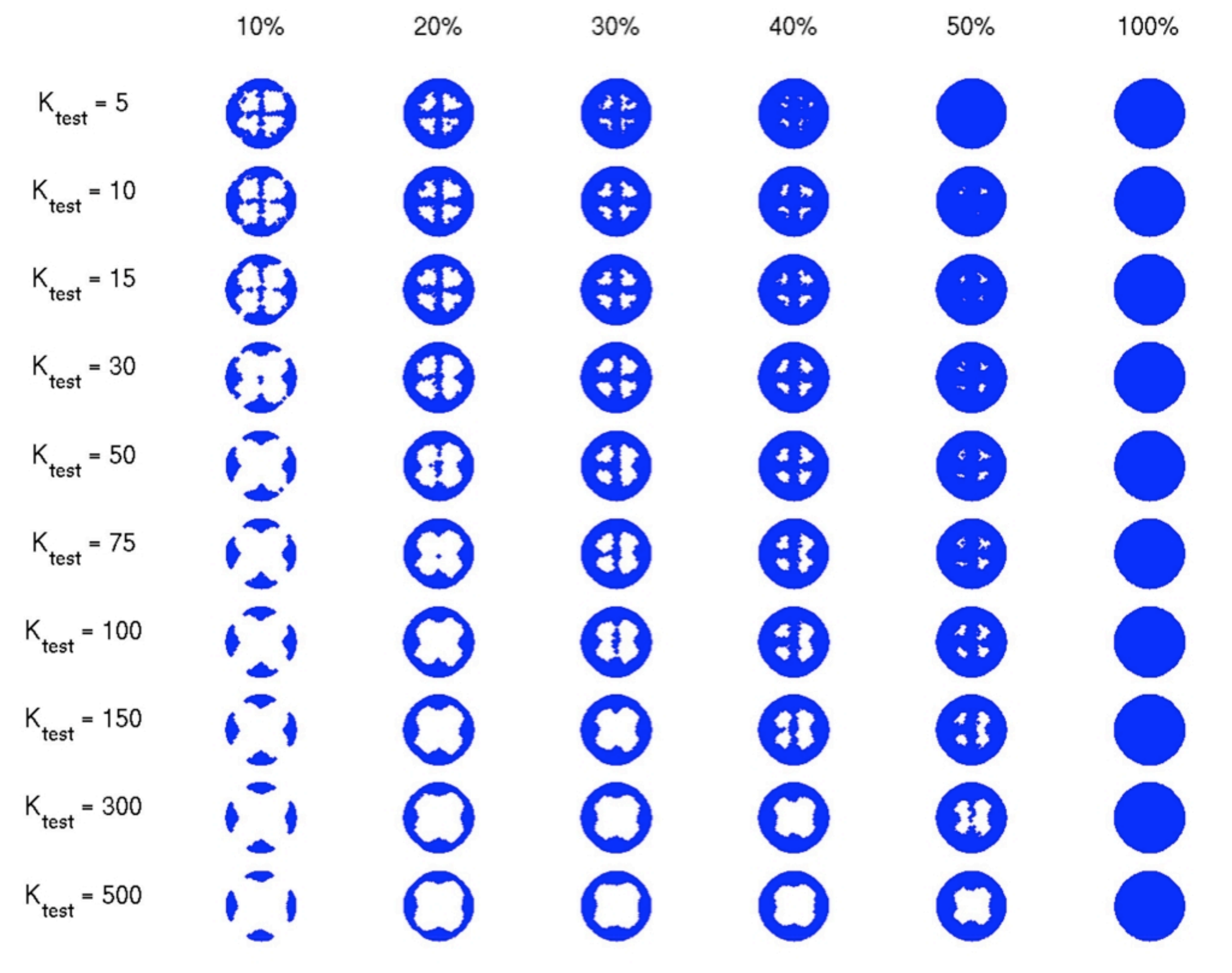


Defining "high-density"

- How do we define "high density"?
  - Select a positive integer k.
  - $r_k(x)$ = distance between x and its k-th nearest neighbour.
  - x is a high-density point ⇔ $r_k(x)$ is small.
- Select "cuts" by thresholding on $r_k(x)$.
  - k small ⇔ fine structure
  - k large ⇔ coarse structure

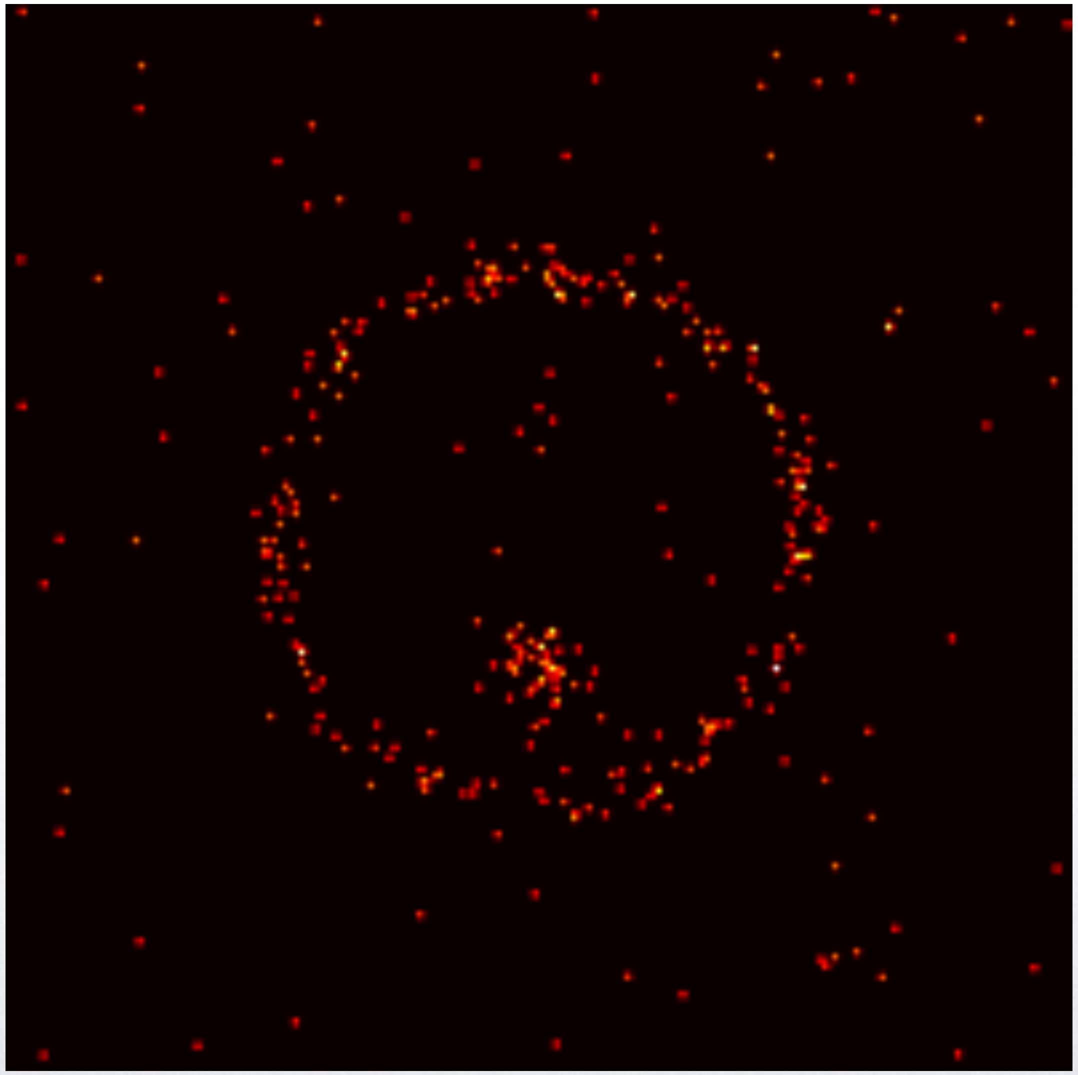


Straining a data soup



Varying the density parameter

(toy example)



Varying the density parameter

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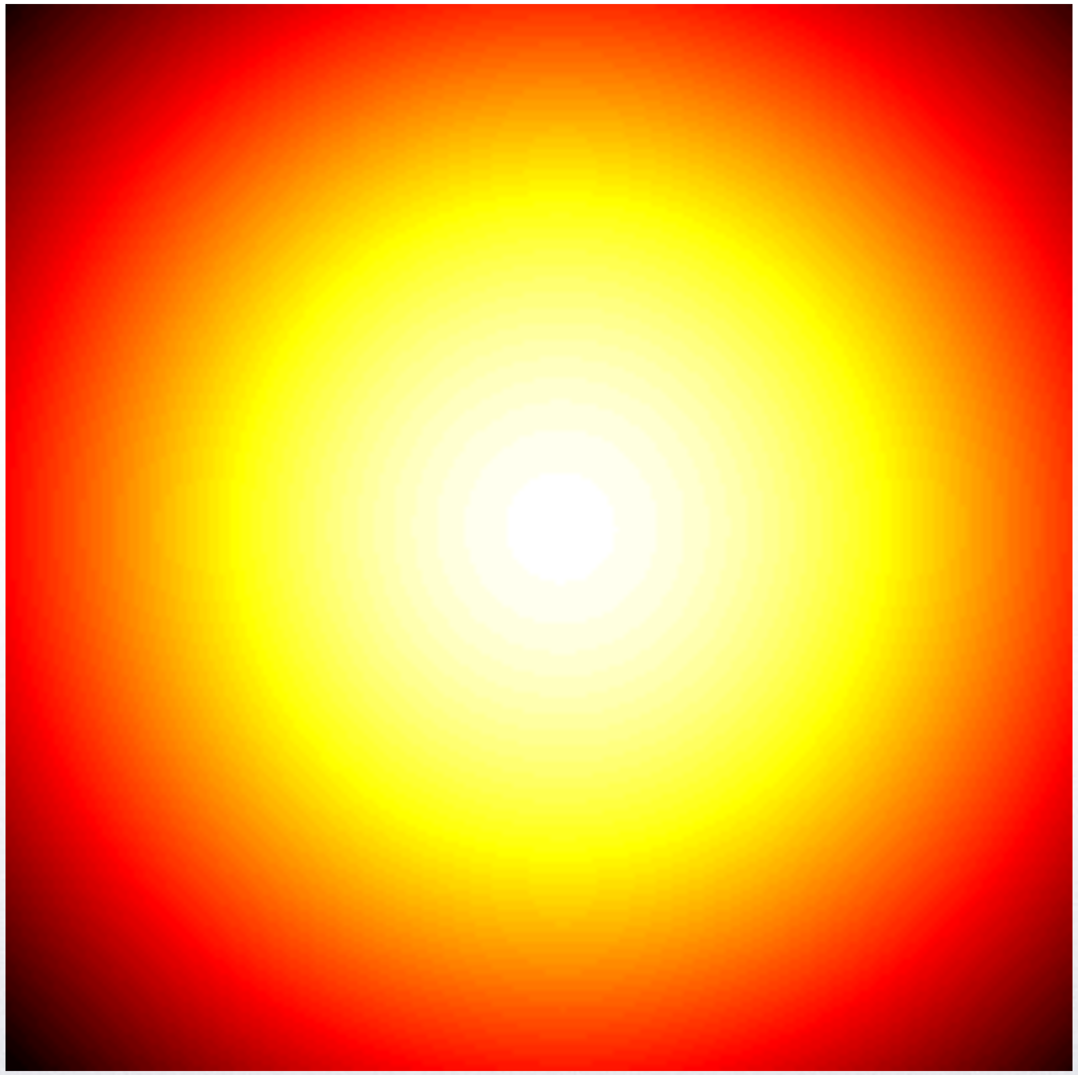
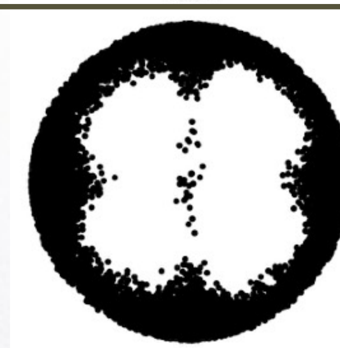
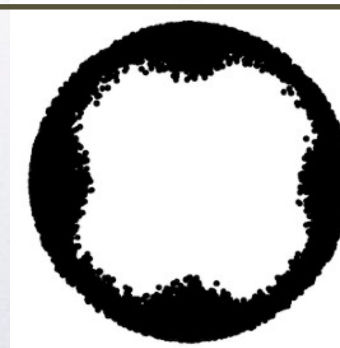
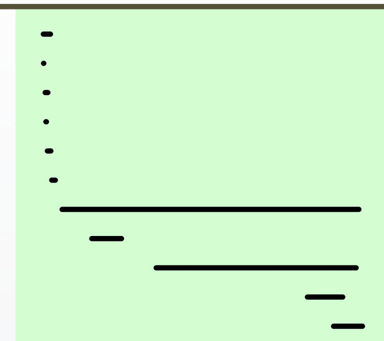
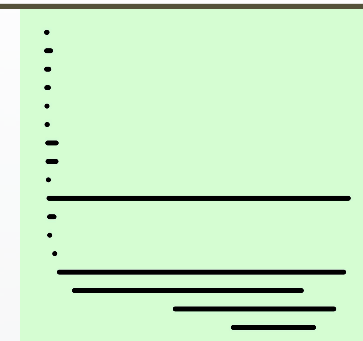
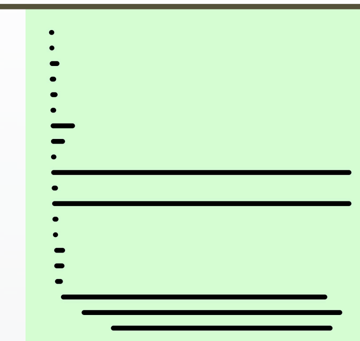
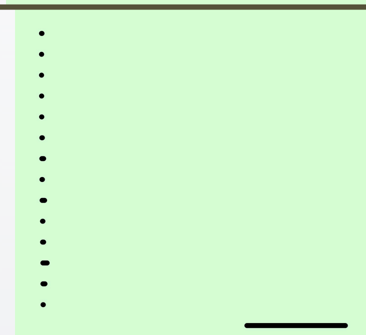
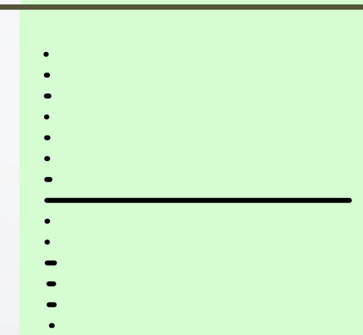
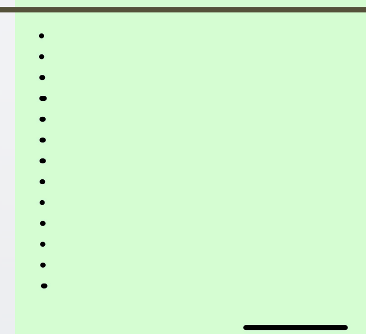
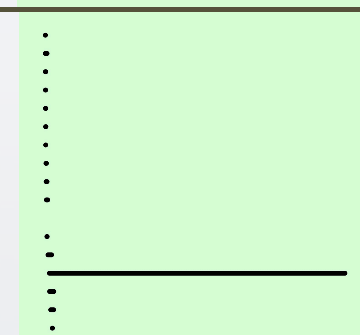
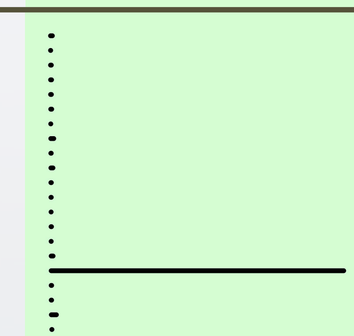


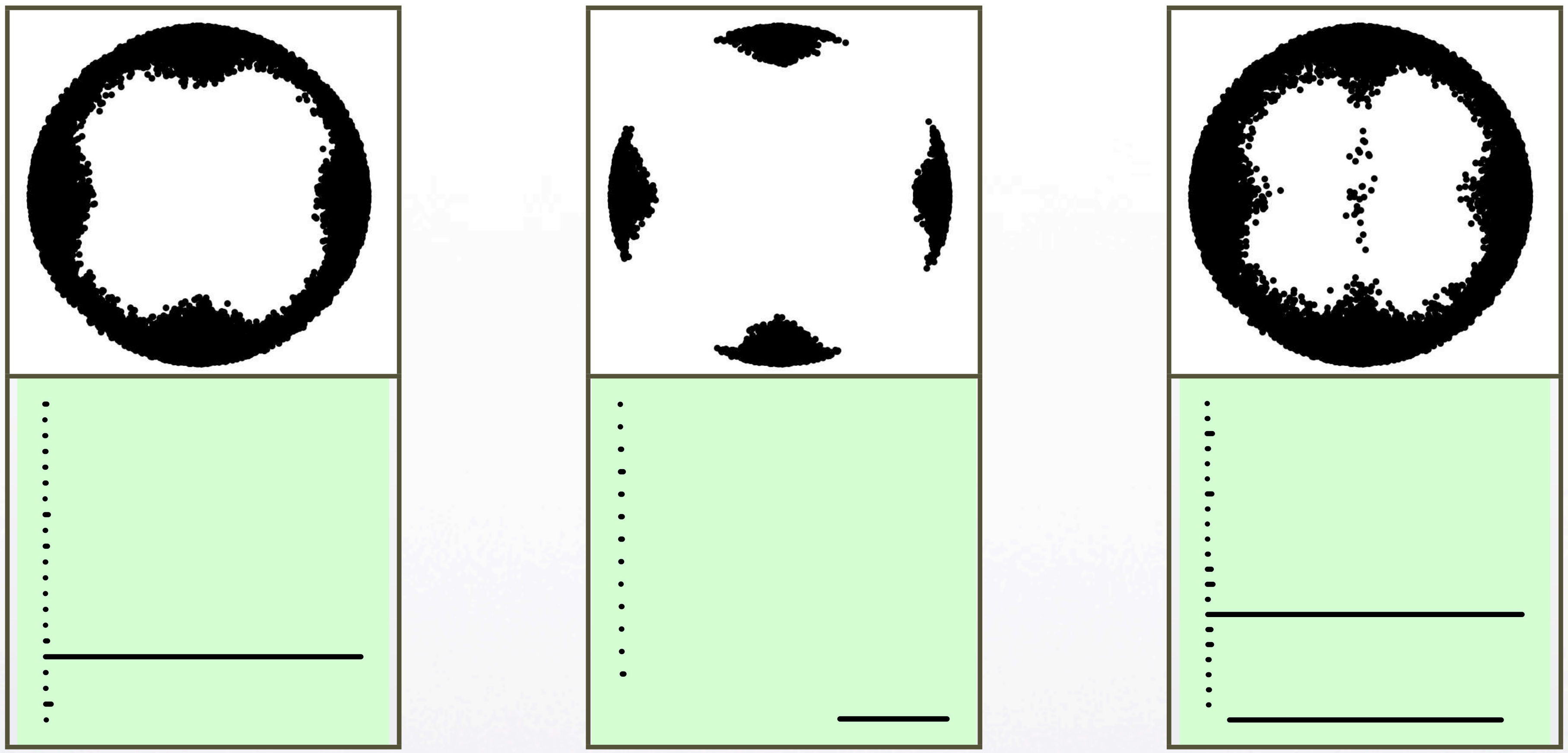
A small platter of cuts

	10%	20%	30%
K=15			
K=100			
K=300			

A small platter of cuts

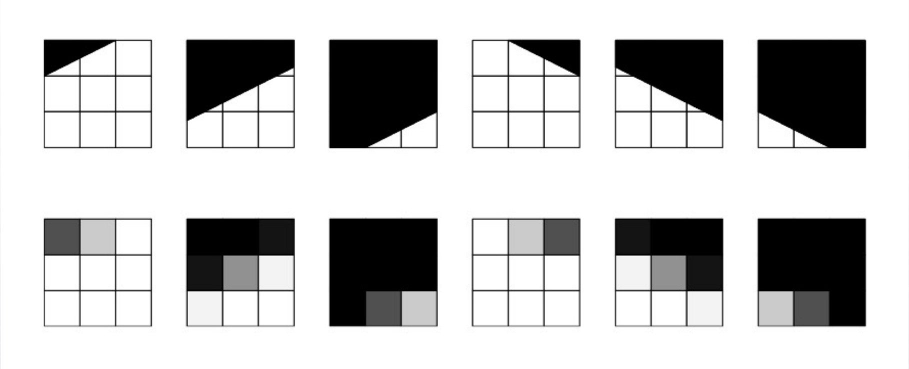
	10%	20%	30%
K=15			
K=100			
K=300			

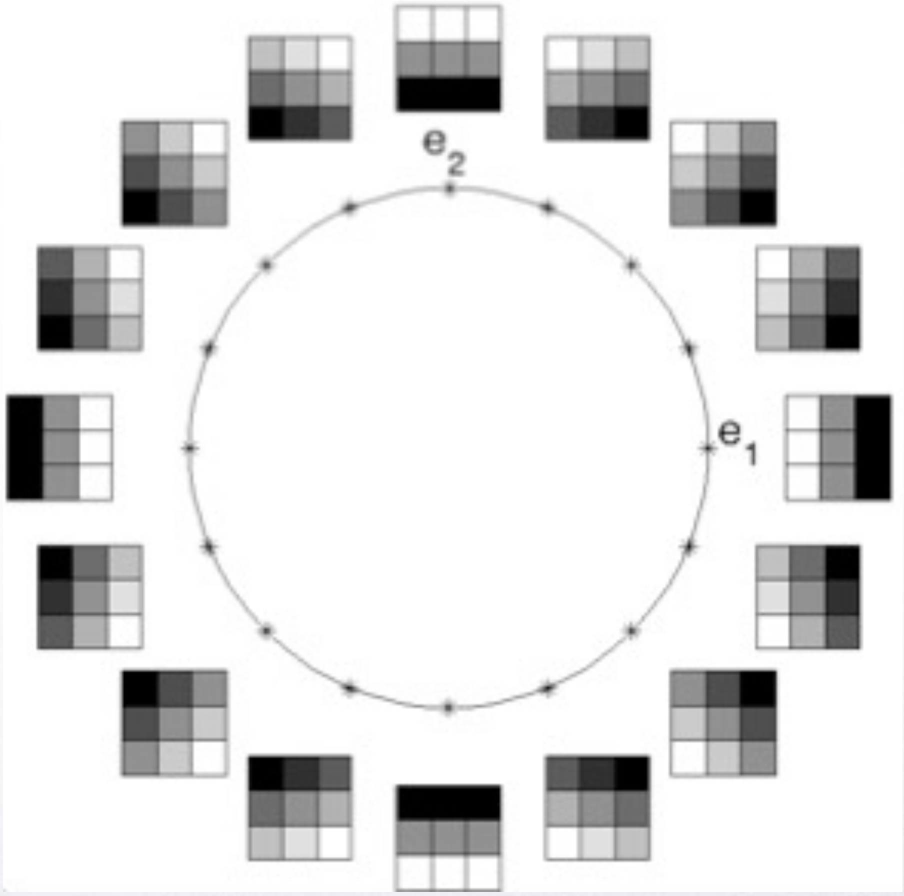
8-dimensional data



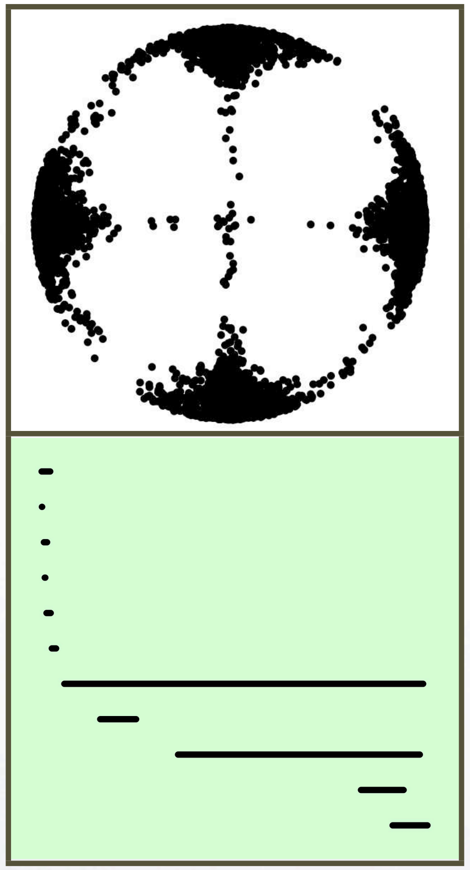
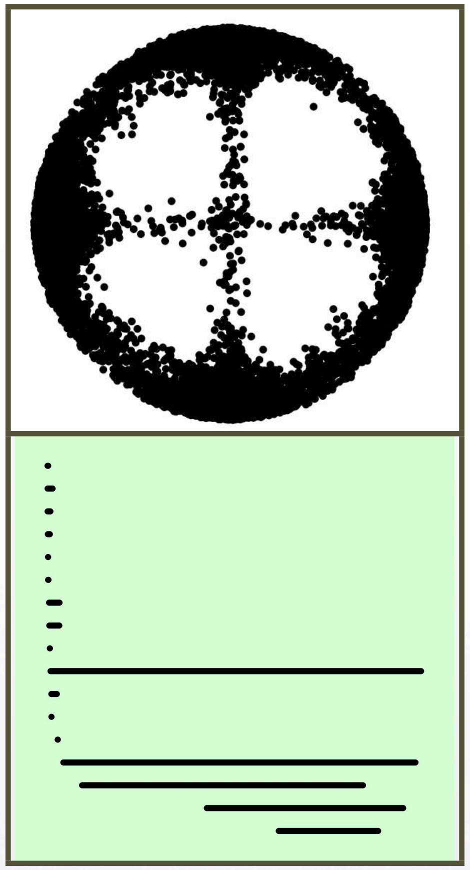
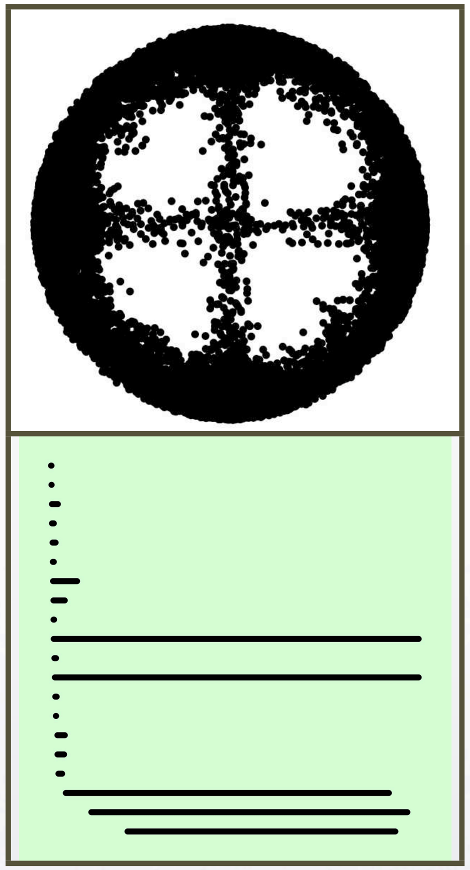
The primary circle

- The thick e_1–e_2 circle consists of linear gradient patches and their nearby edge feature patches.

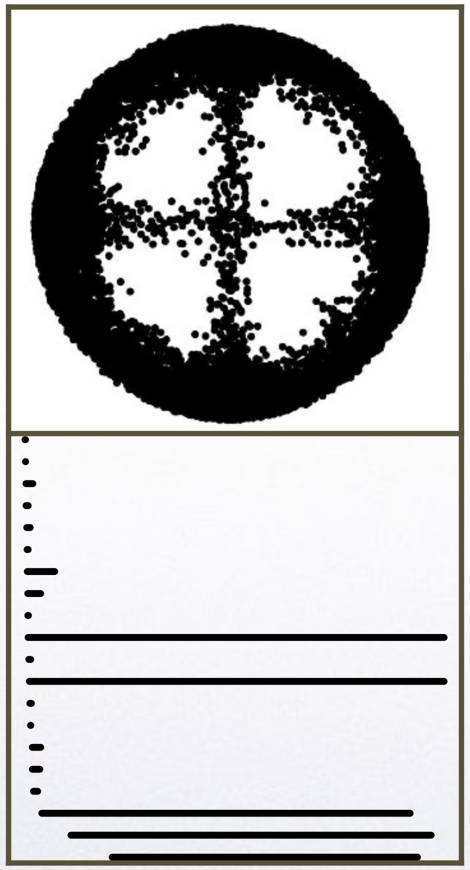


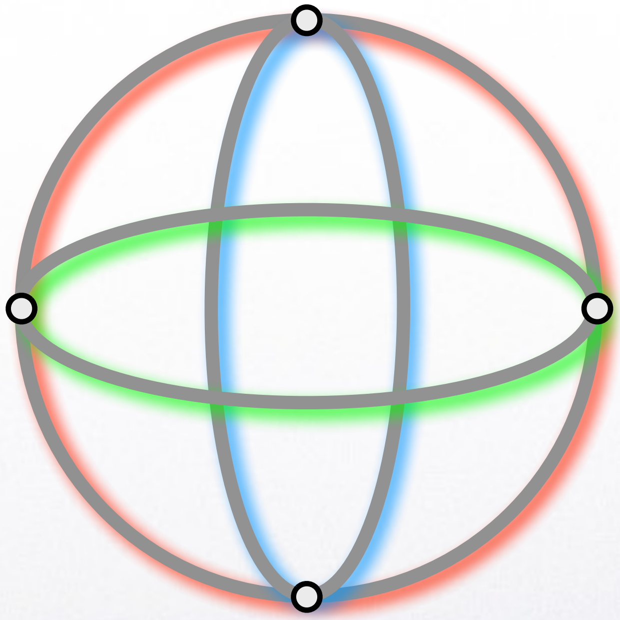


8-dimensional data

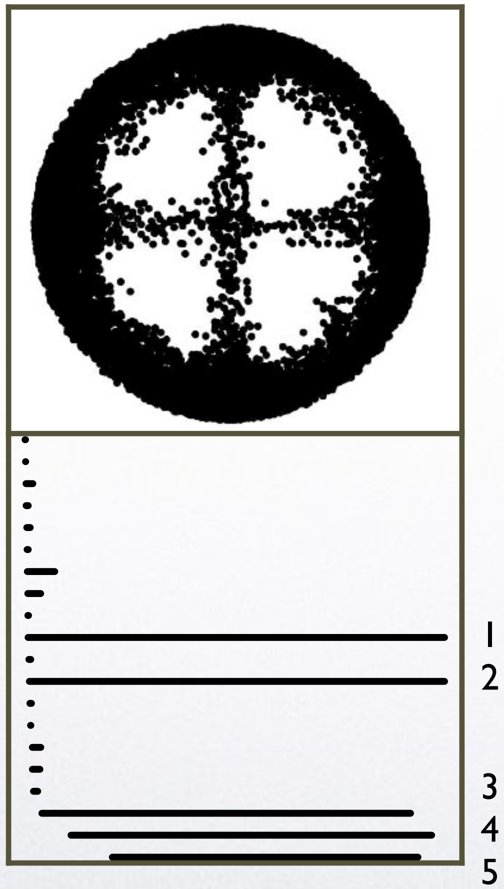




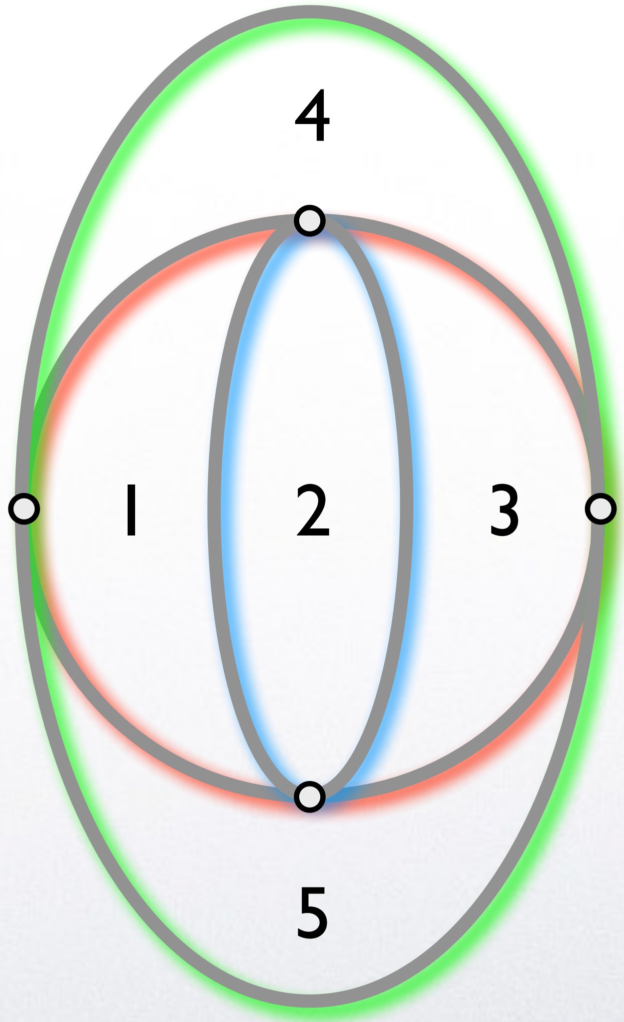
3-circles model



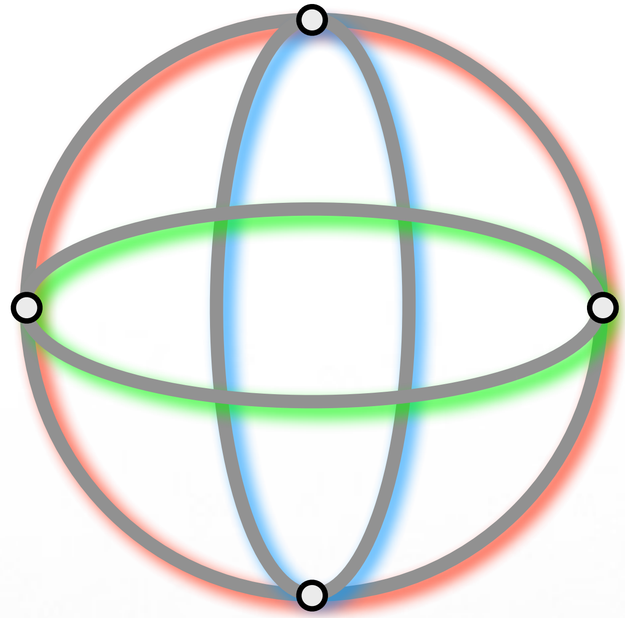


3-circles model

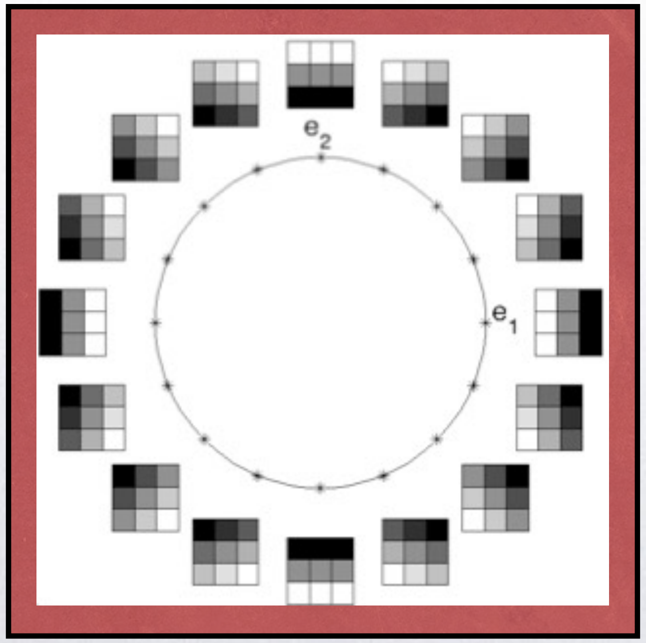




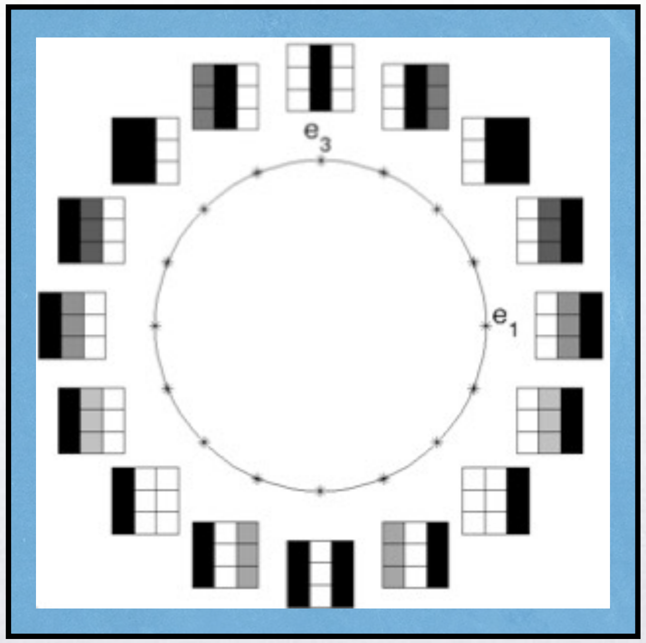
3 circles explained



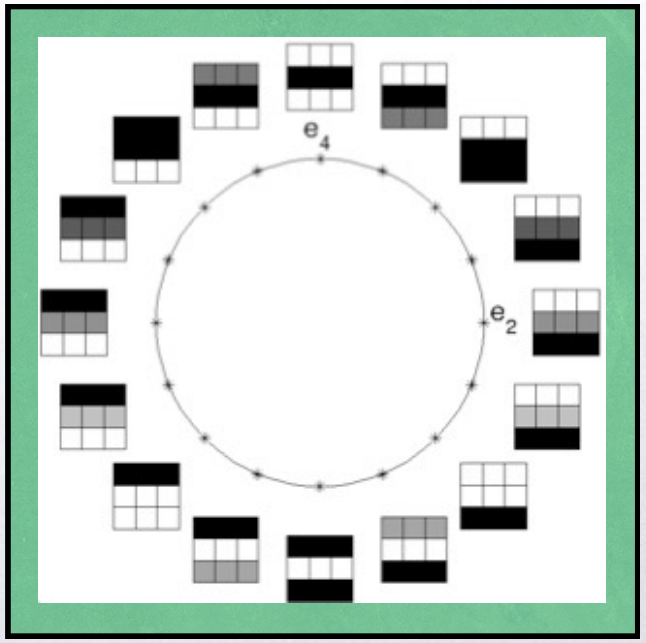
linear gradients



vertical features

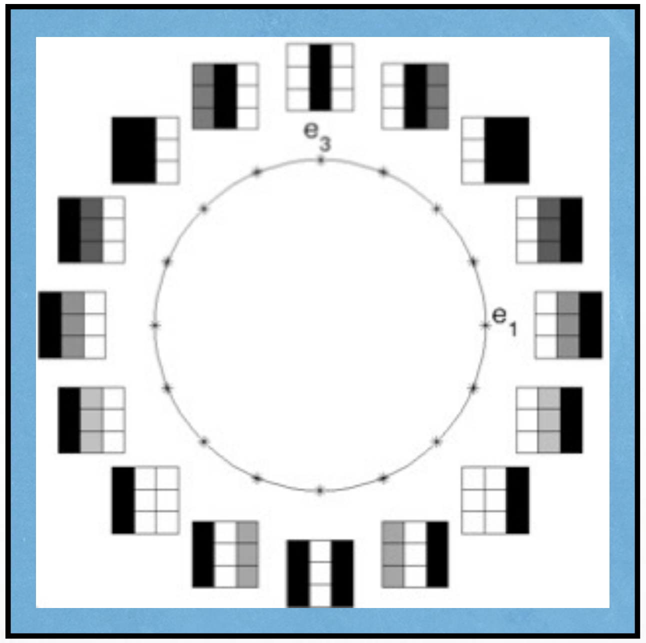


horizontal features

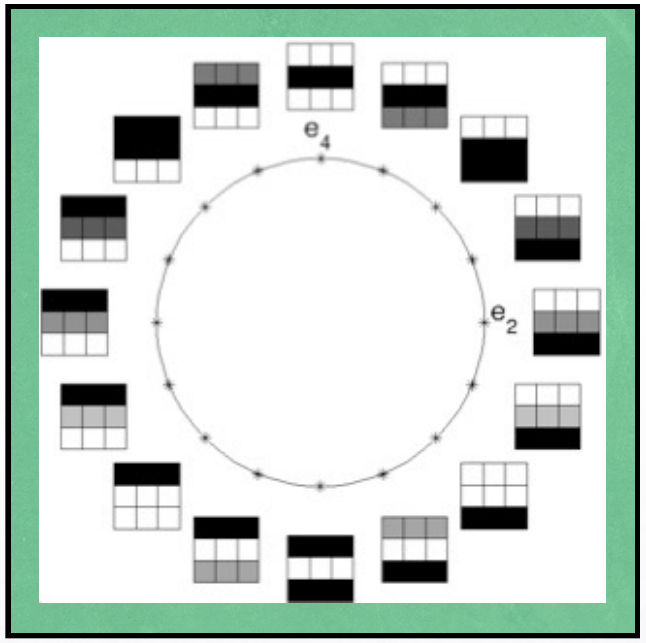


The secondary circles

vertical features



horizontal features



Why is there a predominance of vertical/horizontal local features?

Artefact of the square patch shape?
Artefact of the natural world?

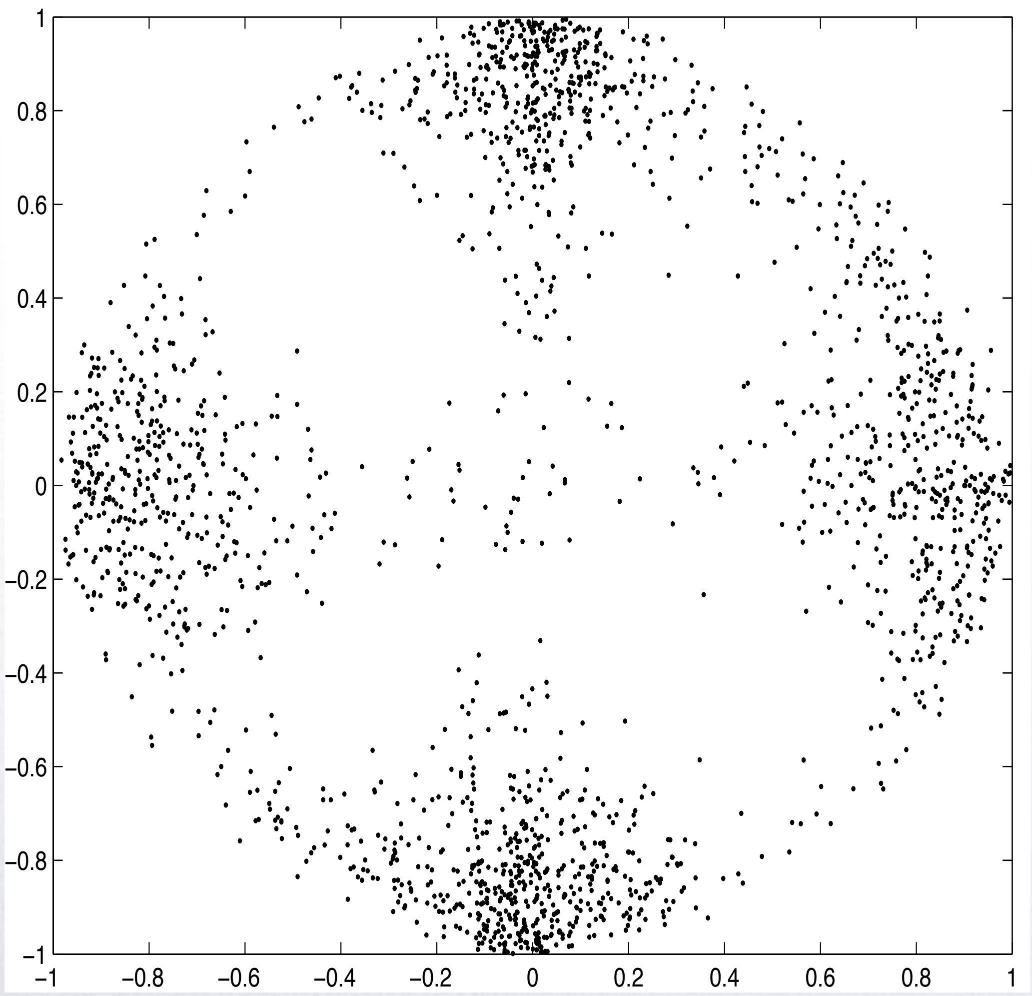
Tilting the camera

orthogonal images

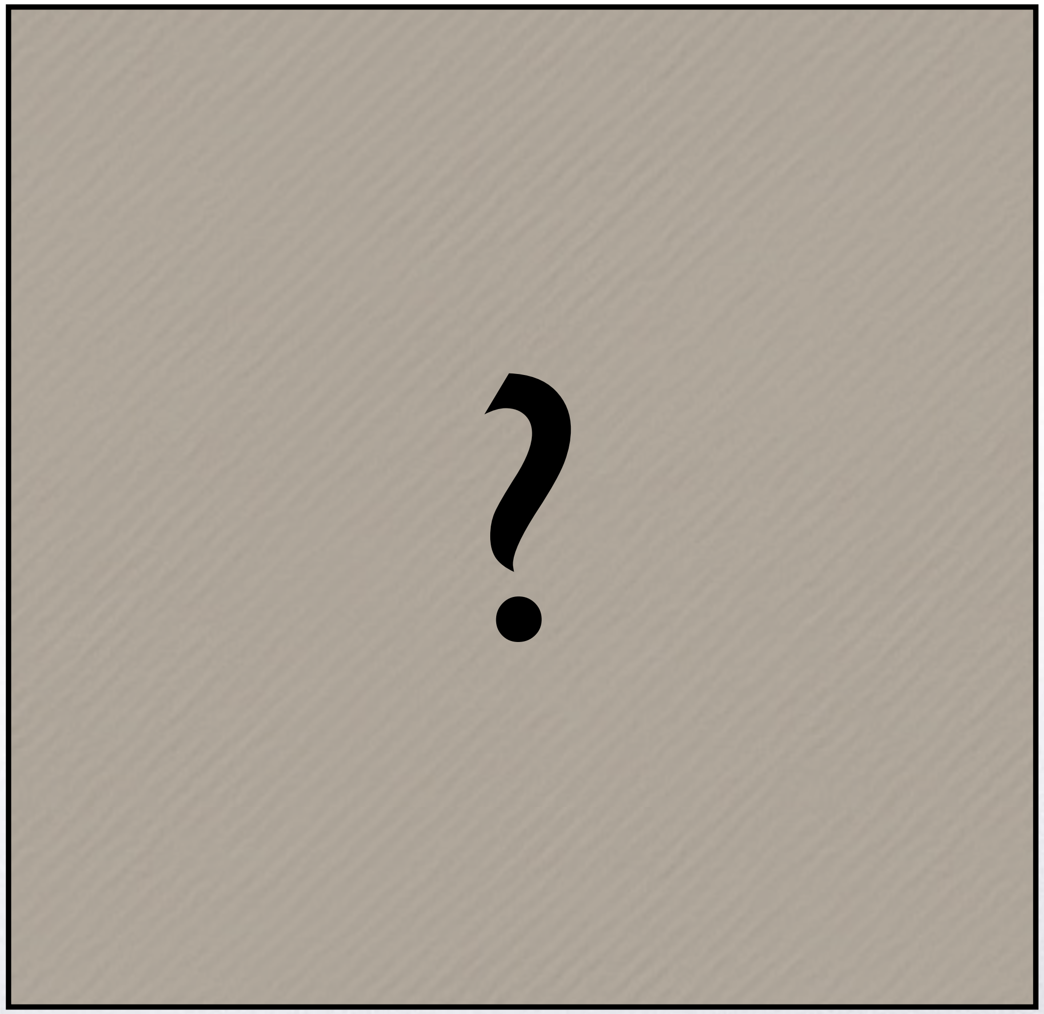
diagonal images

Tilting the camera

orthogonal images

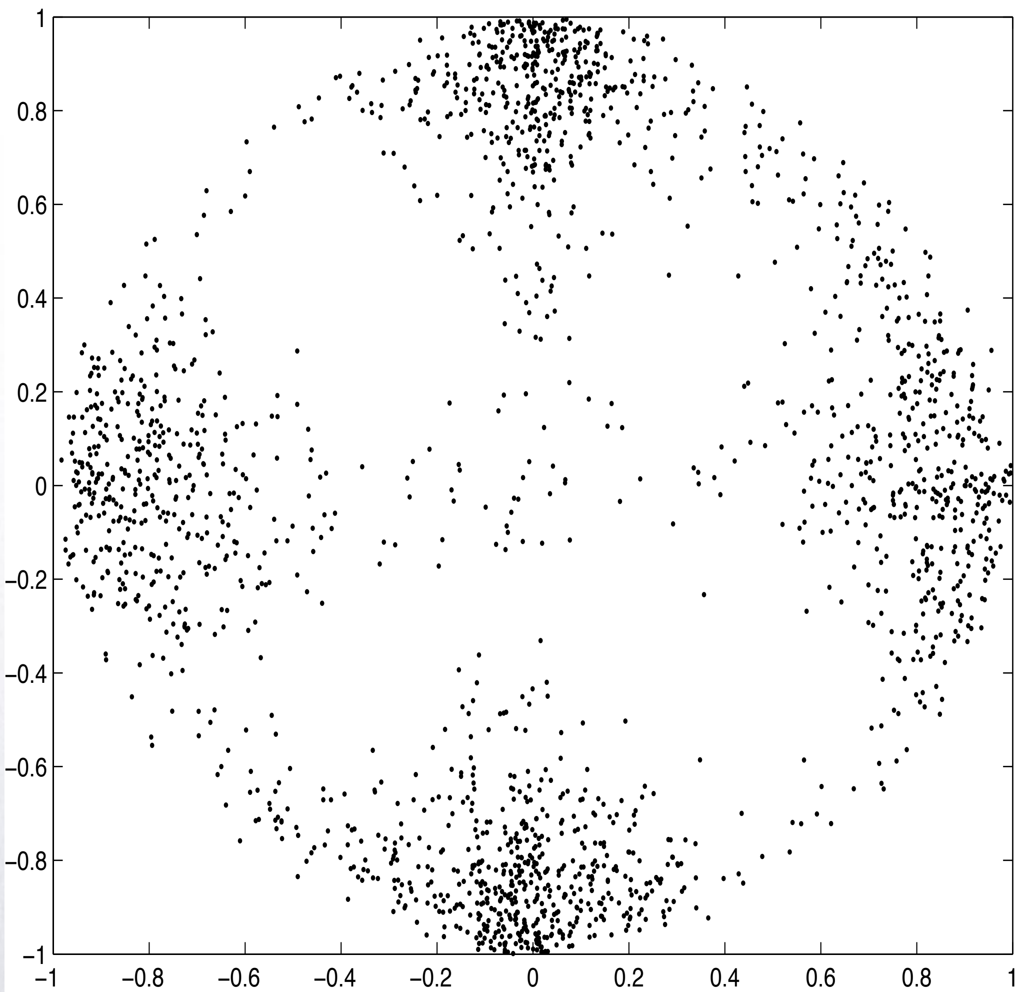


diagonal images

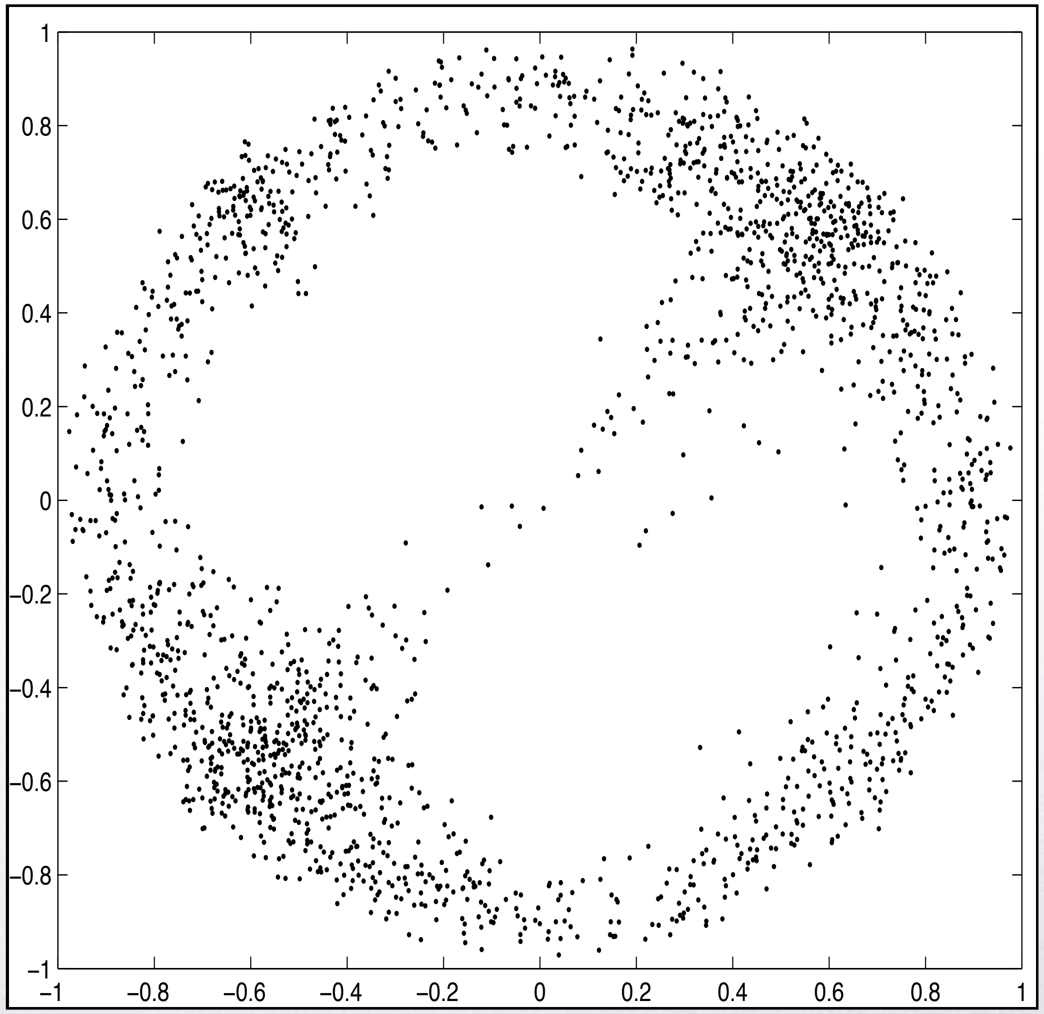


Tilting the camera

orthogonal images



diagonal images



Homogenizing over all tilt angles

- e_1-e_2 circle: arbitrary linear functions $ax+by$ in the image plane.
- e_1-e_3 circle: quadratic functions of x.
- e_3-e_4 circle: quadratic functions of y.
- What about quadratic functions of arbitrary linear functions $ax+by$?

The Klein bottle