The Mapper Algorithm

Western TDA Learning Seminar

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Preliminaries

Topological Mapper

Statistical Mapper

Sanity Checks

Applications

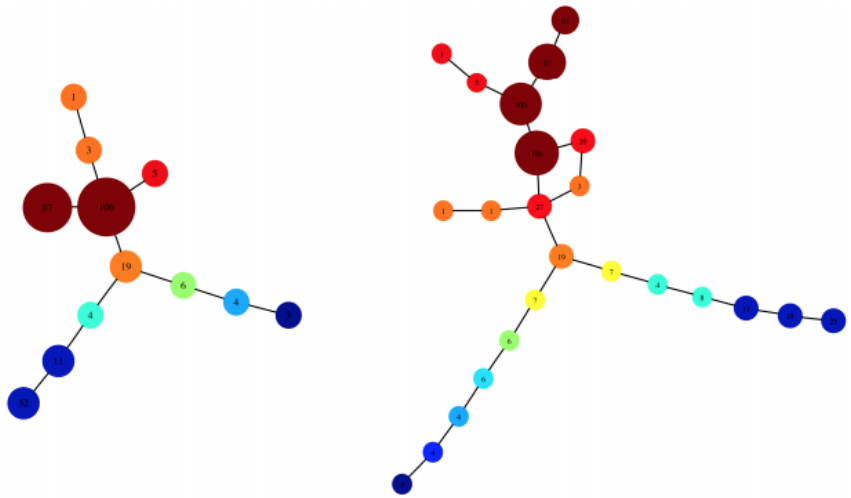
Mapper is an important tool used in TDA for data visualization.

Input

- point cloud;
- "filter function;"
- covering of a metric space;
- clustering algorithm;
- various other parameters.

Output

Graph (or higher simplicial complex) which is thought to capture aspects of the topology of the point cloud.



Developed by Singh, Mémoli, and Carlsson in [6], Mapper gives a multi-resolution, low dimensional picture of the point cloud. It's highly customizable, and has a track record of revealing structure that clustering and (linear or nonlinear) "projection pursuit" methods miss.

Image Source: Singh, Mémoli, Carlsson [6]

Notation

Let $n \geq 1$ be an integer, let $[n] := \{0, \ldots, n\}$.

- An n-**simplex** σ is the convex hull of $n+1$ affinely independent **vertices** $S = \{v^i\}_{i \in [n]}$ in $\mathbb{R}^d$ where $d \geq n$.
- A simplex τ defined by $T \subseteq S$ is called a **face**.
- A **simplicial complex** K is a finite set of simplices which meet along faces, every one of which is in K.
- Let e^0 denote the origin in $\mathbb{R}^n$ and e^i the i-th standard basis vector for $\mathbb{R}^n$.
- The **standard** n-**simplex** $\Delta^n \subset \mathbb{R}^n$ is the convex hull of $\{e^i\}_{i \in [n]}$.
- Given any subset $J \subseteq [n]$, let Δ^J be the face of Δ^n spanned by $\{e^j\}_{j \in J}$.

Nerves

Let X be a topological space and $\mathcal{U} = \{U_\alpha\}_{\alpha \in A}$ a covering of X.
The **nerve of** $\mathcal{U}$, denoted $N\mathcal{U}$, is the abstract simplicial complex with vertex set A and where $\{\alpha_0, \ldots, \alpha_k\}$ spans a k-simplex if and only if

$$U_{\alpha_0} \cap \ldots \cap U_{\alpha_k} \neq \emptyset$$

Nerve Theorem, [2]

X and $\mathcal{U}$ as above, $\mathcal{U}$ a covering by open sets which is enumerable. Suppose further that for all $\emptyset \neq S \subseteq A$ we have that $\bigcap_{s \in S} U_s$ is either empty or contractible. Then $N\mathcal{U}$ is homotopy equivalent to X.

Coverings and complexes

Suppose (X, d) metric space and fix $\varepsilon > 0$. Further suppose that $V \subseteq X$ has the property that

$$X = \bigcup_{v \in V} B_\varepsilon(v)$$

where $B_\varepsilon(v) = \{y \in X : d(v, y) < \varepsilon\}$.
Then $\{B_\varepsilon(v)\}_{v \in V}$ is a covering and has nerve $\check{C}(V, \varepsilon)$, the **Čech complex attached to** (V, ε).

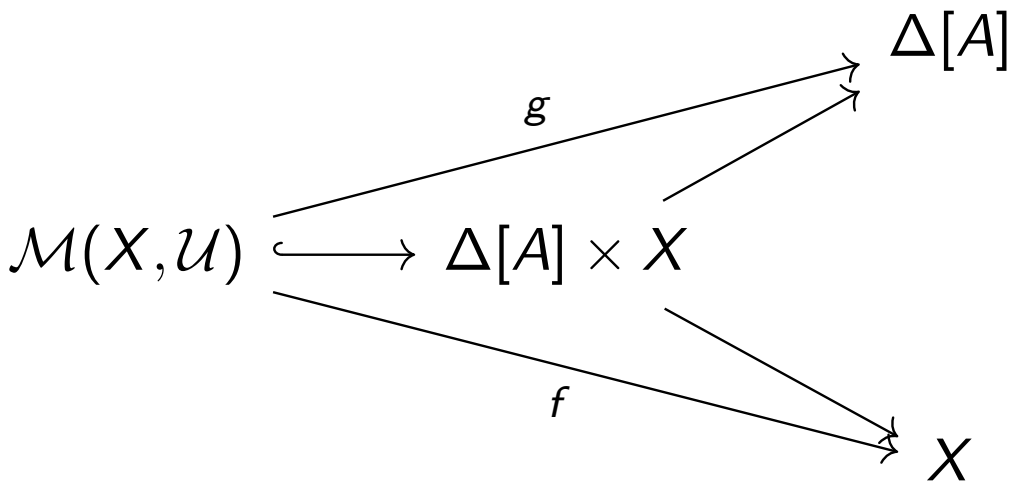
Mayer-Vietoris blowup complex

- X topological space;
- $\mathcal{U} = \{U_\alpha\}_{\alpha \in A}$ a finite covering of X;
- $\Delta[A]$ the standard simplex with vertex set A (i.e. $\Delta[A] = \Delta^{|A|-1}$ and $\dim(\Delta[A]) = |A| - 1$);
- for $\emptyset \neq S \subseteq A$, let $\Delta[S]$ be the face spanned by S;
- $X[S] := \bigcap_{s \in S} U_s \subseteq X$;

The **Mayer-Vietoris blowup complex of X associated to $\mathcal{U}$**, denoted $\mathcal{M}(X, \mathcal{U})$ is

$$\mathcal{M}(X, \mathcal{U}) = \bigcup_{\emptyset \neq S \subseteq A} \Delta[S] \times X[S] \subseteq \Delta[A] \times X$$

Mayer-Vietoris blowup complex



Natural projections satisfy the following properties:

(1) f is a homotopy equivalence when X has the homotopy type of a finite complex and $\mathcal{U}$ is an open covering. Given a partition of unity subordinate to $\mathcal{U}$, can construct an explicit homotopy inverse $\varphi : X \to \mathcal{M}(X,\mathcal{U})$ [7], [5].

(2) g is a homotopy equivalence onto its image ($\check{C}(\mathcal{U})$) when all the $X[S]$ are empty or contractible. (This is how the Nerve Theorem is proved) [2].

A better target

Obtain map

$$X \xrightarrow{\varphi} \mathcal{M}(X,\mathcal{U}) \xrightarrow{g} \check{C}(\mathcal{U})$$

But we can do even better: let $\check{C}^{\pi_0}(\mathcal{U})$ be the nerve of the covering of X by sets which are path connected components of the sets U_α. Thus covering is indexed by pairs (α, ξ) where ξ is a path component of U_α.
Projection $(\alpha, \xi) \mapsto \alpha$ induces a simplicial map

$$\check{C}^{\pi_0}(\mathcal{U}) \to \check{C}(\mathcal{U})$$

and the projections $U_\alpha \mapsto \pi_0(U_\alpha)$ induce a map

$$\mathcal{M}(X,\mathcal{U}) \to \check{C}^{\pi_0}(\mathcal{U})$$

The composite

$$\mathcal{M}(X,\mathcal{U}) \to \check{C}^{\pi_0}(\mathcal{U}) \to \check{C}(\mathcal{U})$$

is exactly the map g from before [2].

Constructing covers

How do we construct a cover of an abstract topological space?
Suppose we're given a (continuous) **reference map** $\rho : X \to Z$, Z some metric space. Given a covering $\mathcal{U}$ of Z, can pull back along ρ and obtain

$$\rho^*\mathcal{U} = \{\rho^{-1}U_\alpha\}_{\alpha \in A}$$

a covering of X.

Example: $\mathcal{U}[R, e]$

$Z = \mathbb{R}$, R, e positive real numbers. $\mathcal{U}[R, e]$ is the collection of all intervals $[kR - e, (k+1)R + e]$, $k \in \mathbb{Z}$. When $e < R/2$, it has covering dimension 1: i.e. there are no non-trivial triple intersections.

Clustering

For X a point cloud (a finite metric space), path connected components are uninteresting.
Analogue of "connected component" is "cluster." We run a clustering algorithm in order to partition a point cloud into clusters: heuristically, "points within a cluster are similar and points from distinct clusters are dissimilar."
Single-linkage clustering algorithm: (according to [2]) Let $\epsilon > 0$ and define blocks of a partition (clusters) of the point cloud as the set of equivalence classes under $\sim_\epsilon$ where

$$x \sim_\epsilon x' \iff d(x, x') \leq \epsilon$$

Notice that the set of clusters is exactly $\pi_0(VR(X, \epsilon))$, the set of connected components of the Vietoris-Rips complex on X at ϵ.

Discrete $\check{C}^{\pi_0}(\mathcal{U})$

(1) Given a point cloud X; a metric space Z; and a reference map $f : X \to Z$.

(2) Select a covering $\mathcal{U}$ of Z. (Eg. $\mathcal{U} = \mathcal{U}[R, e]$ if $Z = \mathbb{R}$).

(3) If $\mathcal{U} = \{U_\alpha\}_{\alpha \in A}$, pull back covering by the sets $X_\alpha = f^{-1}(U_\alpha)$.

(4) Fix $\epsilon > 0$, construct the set of clusters by the single linkage procedure with ϵ on each set X_α. Obtain a covering of X indexed by pairs (α, c) where $\alpha \in A$, and c is one of the clusters of X_α.

(5) Construct simplicial complex $\check{C}^{\pi_0}(\mathcal{U})$ with vertex set the collection of all pairs (α, c), and where $\{(\alpha_0, c_0), (\alpha_1, c_1), \ldots, (\alpha_k, c_k)\}$ spans a k-simplex if and only if the clusters $c_0, \ldots, c_k$ have a common point.

Discrete $\check{C}^{\pi_0}(\mathcal{U})$

Remarks

- Any clustering algorithm can be used in (4).
- If $\mathcal{U}$ has covering dimension $\leq d$ (i.e. for any family $\{\alpha_0, \ldots, \alpha_t\}$ of distinct indices with $t > d$, then $U_{\alpha_0} \cap \ldots \cap U_{\alpha_t} = \emptyset$), then $\check{C}^{\pi_0}(\mathcal{U})$ also has dimension $\leq d$.
- Choosing the parameter $\epsilon > 0$ in (4) is difficult. One can imagine contexts where ϵ should vary with α. Because clusters under single linkage are exactly connected components of $VR(X, \epsilon)$, can actually use barcodes and β_0 to analyze behavior of clusters over varying choices of ϵ and employ the "persistence philosophy". See [2] Section 3.4 for the discussion of "Scale Space."

Multi-resolution structure

$$\mathcal{U} = \{U_\alpha\}_{\alpha \in A},\ \mathcal{V} = \{V_\beta\}_{\beta \in B}$$

two coverings of a topological space Z. A **map of coverings** $\mathcal{U} \to \mathcal{V}$ is given by a set map $\theta : A \to B$ such that

$$U_\alpha \subseteq V_{\theta(\alpha)}$$

for all $\alpha \in A$.

Examples:

(1) The identity set map on $\mathbb{Z}$ yields a map of coverings $\mathcal{U}[R, e] \to \mathcal{U}[R, e']$ whenever $e \leq e'$.

(2) The map of integers $k \mapsto \lfloor k/2 \rfloor$ defines a map of coverings $\mathcal{U}[R, e] \to \mathcal{U}[2R, e]$. It's two to one in the sense that each interval in $\mathcal{U}[2R, e]$ contains two intervals from $\mathcal{U}[R, e]$.

Multi-resolution structure

A clustering algorithm is **functorial** if given an inclusion of point clouds (distance preserving injective set map) $X \hookrightarrow Y$, then the image of each cluster in X is included in one of the clusters in Y. Get induced set map

$$\{\text{clusters of } X\} \to \{\text{clusters of } Y\}$$

If clustering algorithm in (4) is functorial, we'll see that refining a covering (i.e. applying a map of coverings) refines our simplicial complex.

Multi-resolution structure

Suppose we're given:

- a point cloud X;
- $\rho : X \to Z$ a reference map to a metric space Z;
- Two coverings $\mathcal{U} = \{U_\alpha\}_{\alpha \in A}$ and $\mathcal{V} = \{V_\beta\}_{\beta \in B}$ of Z;
- a map of coverings $\theta : \mathcal{U} \to \mathcal{V}$.

By definition of the covering map,

$$U_\alpha \subseteq V_{\theta(\alpha)}$$

for all $\alpha \in A$ and therefore

$$\rho^{-1}(U_\alpha) \subseteq \rho^{-1}(V_{\theta(\alpha)})$$

for all $\alpha \in A$.

Multi-resolution structure

Applying a functorial clustering algorithm to each set $\rho^{-1}(U_\alpha)$ and $\rho^{-1}(V_\beta)$, obtain map of sets from the set of clusters in $\rho^{-1}(U_\alpha)$ to the set of clusters in $\rho^{-1}(V_{\theta(\alpha)})$, hence a map from the vertex set of $\mathcal{M}(X,\mathcal{U})$ to the vertex set of $\mathcal{M}(X,\mathcal{V})$. In fact, this induces a simplicial map

$$\Theta : \mathcal{M}(X,\mathcal{U}) \to \mathcal{M}(X,\mathcal{V})$$

Eg: obtain diagram of simplicial complexes

$$\ldots \to \mathcal{M}(X,\mathcal{U}[R/4,e]) \to \mathcal{M}(X,\mathcal{U}[R/2,e]) \to \mathcal{M}(X,\mathcal{U}[R,e])$$

Moving further to the left, the coverings give a more refined picture of $\mathbb{R}$: the simplicial complex mirrors this refinement of resolution. **Persistence philosophy!**

Mapper implemented

- **Given:** X point cloud, $|X| = N$, filter function $f : X \to \mathbb{R}$.
- Assume we can always compute inter point distances.
- Let I denote the "range" of f: explicitly $I = [m, M] \subset \mathbb{R}$ where

$$m = \min_{x \in X} f(x), \; M = \max_{x \in X} f(x)$$

- Divide I into a set S of smaller intervals (of uniform length) which overlap. Obtain two resolution controlling parameters: ℓ the length of the intervals, and p the percentage overlap between successive intervals.

Mapper implemented

(1) For each interval $I_j \in S$, let

$$X_j := \{x : f(x) \in I_j\}$$

Then the collection of all such X_j is a covering of X.

(2) For each X_j, perform a clustering algorithm to obtain clusters $\{X_{jk}\}$.

(3) Each cluster defines a vertex of our simplicial complex: draw an edge between vertices whenever $X_{jk} \cap X_{lm} \neq \emptyset$.

Example: noisy circle [6]

- The point cloud data is sampled from a noisy circle in $\mathbb{R}^2$
- filter function is $f(x) = \|x - p\|_2$ where p is the left most point in the data set.
- range of f is covered by 5 intervals, $\ell = 1$, $p = 0.20$.
- Nodes are colored by the average value of the filter function over the cluster.

Example: noisy circle [6]

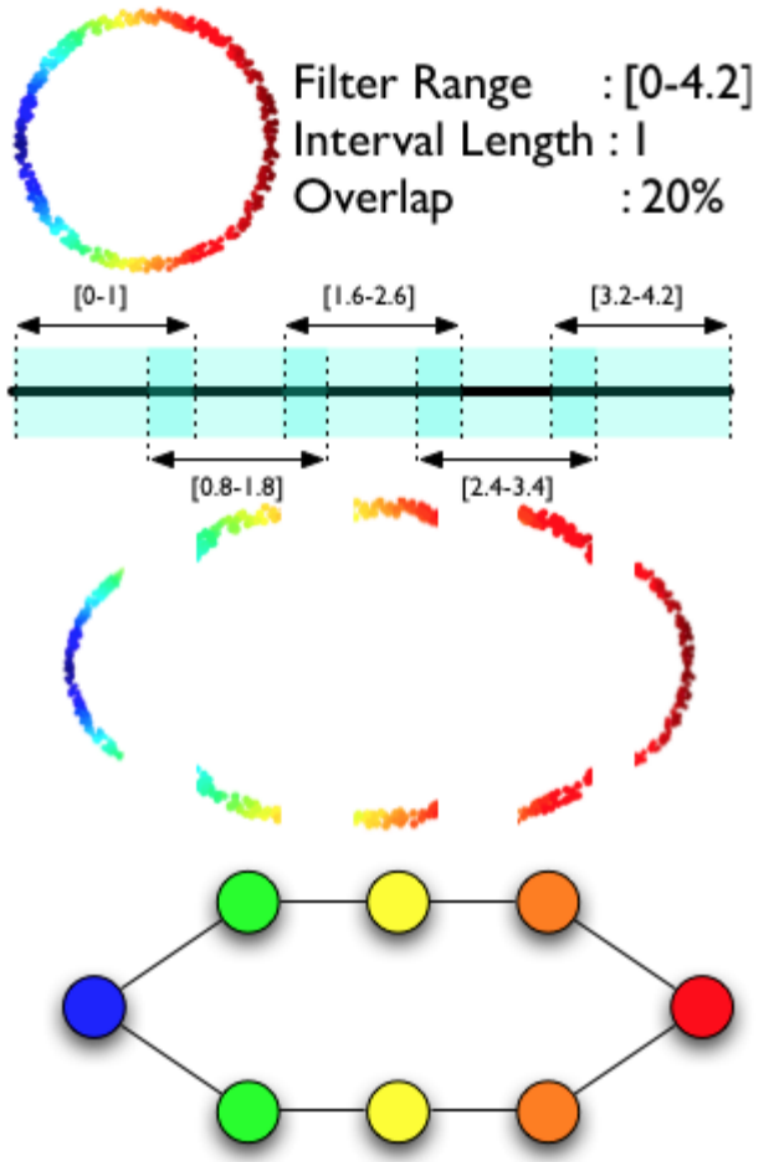


Image Source: Mémoli,Singh,Carlsson [6]

Clustering

Single linkage: $x \sim_\epsilon x'$ iff $d(x, x') \leq \epsilon$, clusters are equivalence classes.
How to choose ϵ?
Heuristically: inter-point distances within clusters should be small, with longer edge lengths required to merge clusters.
Consider $C \in \mathbb{R}^{N-1}$, vector of edge lengths at which the number of clusters successively decreases by one, and histogram of edge lengths in C. Shorter lengths (inter-cluster distances) are distributed smoothly, but edge lengths required to merge natural clusters are disjoint.

Clustering

- Suppose histogram for C has k intervals. Then we find a set of empty intervals after which lengths required to merge clusters appear. Let ϵ be the last length before empty intervals appear, and apply single linkage with that ϵ.
- Increase k to increase number of clusters and vice versa.
- Main limitation is density issues: when clusters with different densities are present, only high density clusters are selected.

Filter functions: density

For $\varepsilon > 0$ estimate the density using a Gaussian kernel

$$f_\varepsilon(x) = C_\varepsilon \sum_{y \in X} \exp\left(\frac{-d(x,y)^2}{\varepsilon}\right)$$

where $x, y \in X$ and C_ε is a constant so that $\int f_\varepsilon(x)\, dx = 1$.
"ε controls the smoothness."

Filter functions: eccentricity

Aim to identify points which are far from some intuitive/natural "center" without having identified one. For $1 \leq p < \infty$

$$E_p(x) = \left(\frac{\sum_{y \in X} d(x,y)^p}{N} \right)^{1/p}$$

and

$$E_\infty(x) = \max_{x' \in X} d(x,x')$$

Then E takes larger values on points further away from "center."

Filter functions: graph Laplacians

Construct a graph from the point cloud: it has vertex set X and edge weights given by $w(x, y) = kd(x, y)$, for k some "smoothing kernel." A **(normalized) graph Laplacian** is

$$L(x, y) = \frac{w(x, y)}{\sqrt{\sum_{z \in X} w(x, z)} \sqrt{\sum_{z \in X} w(y, z)}}$$

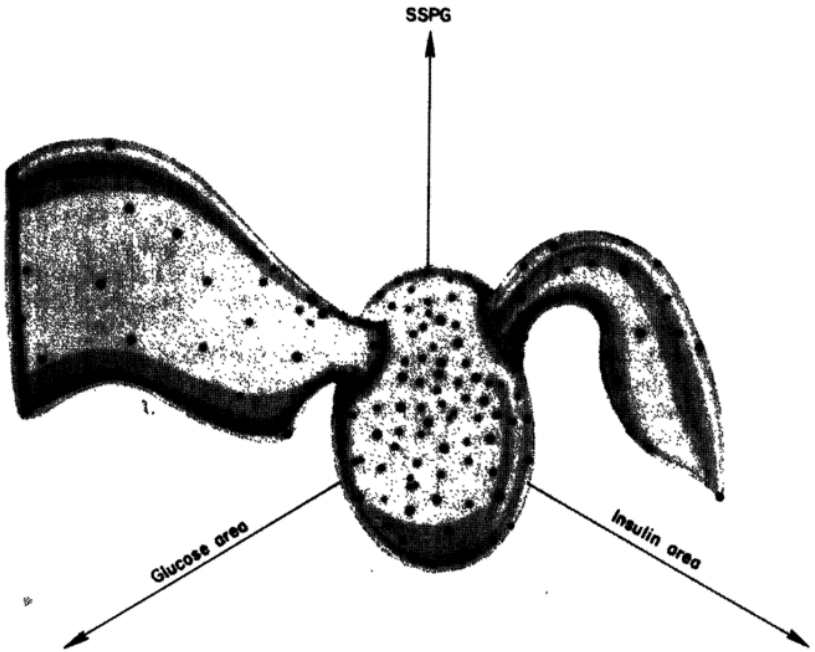
Form the graph laplacian matrix

$$[L(x, y)]_{x,y \in X}$$

and compute its eigenvectors. They're orthogonal, and encode interesting geometric features [6]: use them as filter functions!
(Discrete analogue of Laplace-Beltrami operator on a compact Riemanninan manifold...[1])

Miller-Reaven diabetes study

Applied projection methods to a data set of 145 patients with 6 clinical measurements each. Created a point cloud in $\mathbb{R}^6$ with 145 points, project into $\mathbb{R}^3$ to obtain resulting plot.



Two "flares" represent different diseases: adult and juvenile onset diabetes.

Image Source: Singh, Mémoli, Carlsson [6]

Miller-Reaven diabetes study

Density kernel estimator. On left, three intervals 50% overlap. On right, five intervals 50% overlap. Nodes colored by average density from blue to red. Size of node indicates cluster size. Note the flares!

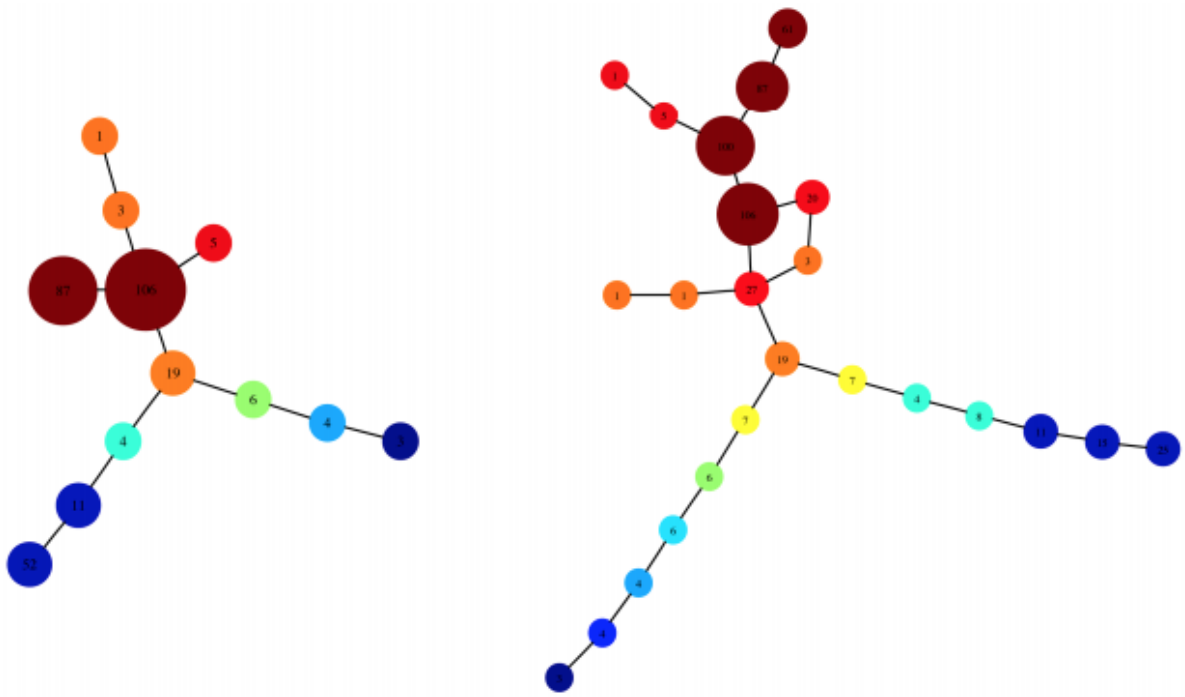


Image Source: Singh, Mémoli, Carlsson [6]

Torus

Generate 1500 evenly sampled points on torus in $\mathbb{R}^3$. Embed in $\mathbb{R}^{30}$ by padding dimensions 4 to 30 with zeros, then apply random rotation to resulting point cloud. Compute first two non-trivial eigenfunctions f_1 and f_2 of Laplacian to use as filter functions (note reference space $\mathbb{R}^2$). Eight intervals each in range of f_i with 50% overlap. Result is cluster of 325 points with 4D simplicial complex. MDS + magic to generate 3D picture (1 and 2D simplices infered from higher simplices.)

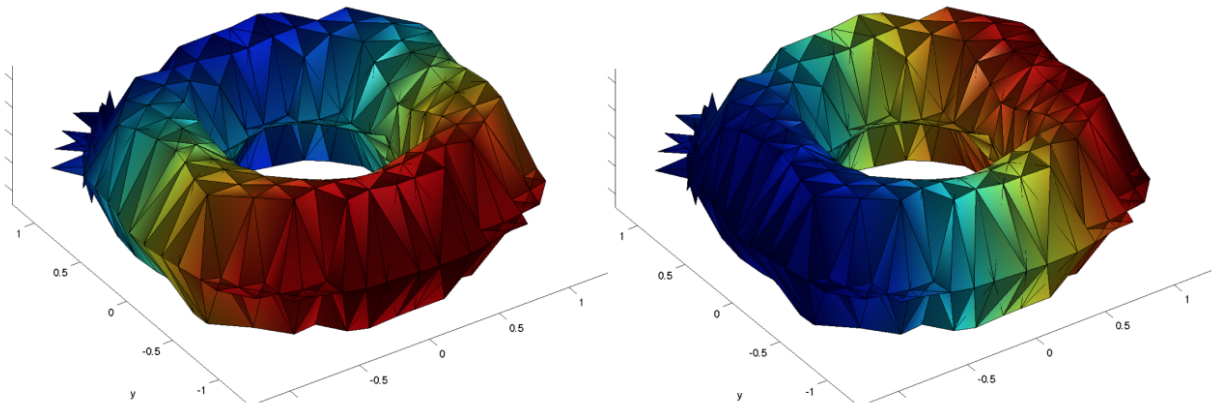


Image Source: Singh, Mémoli, Carlsson [6]

Breast cancer

Metric: correlation distance between gene expression vectors. Filter functions: L^∞ eccentricity and survival variable. Note that the two rows are **DIFFERENT DATA SETS**

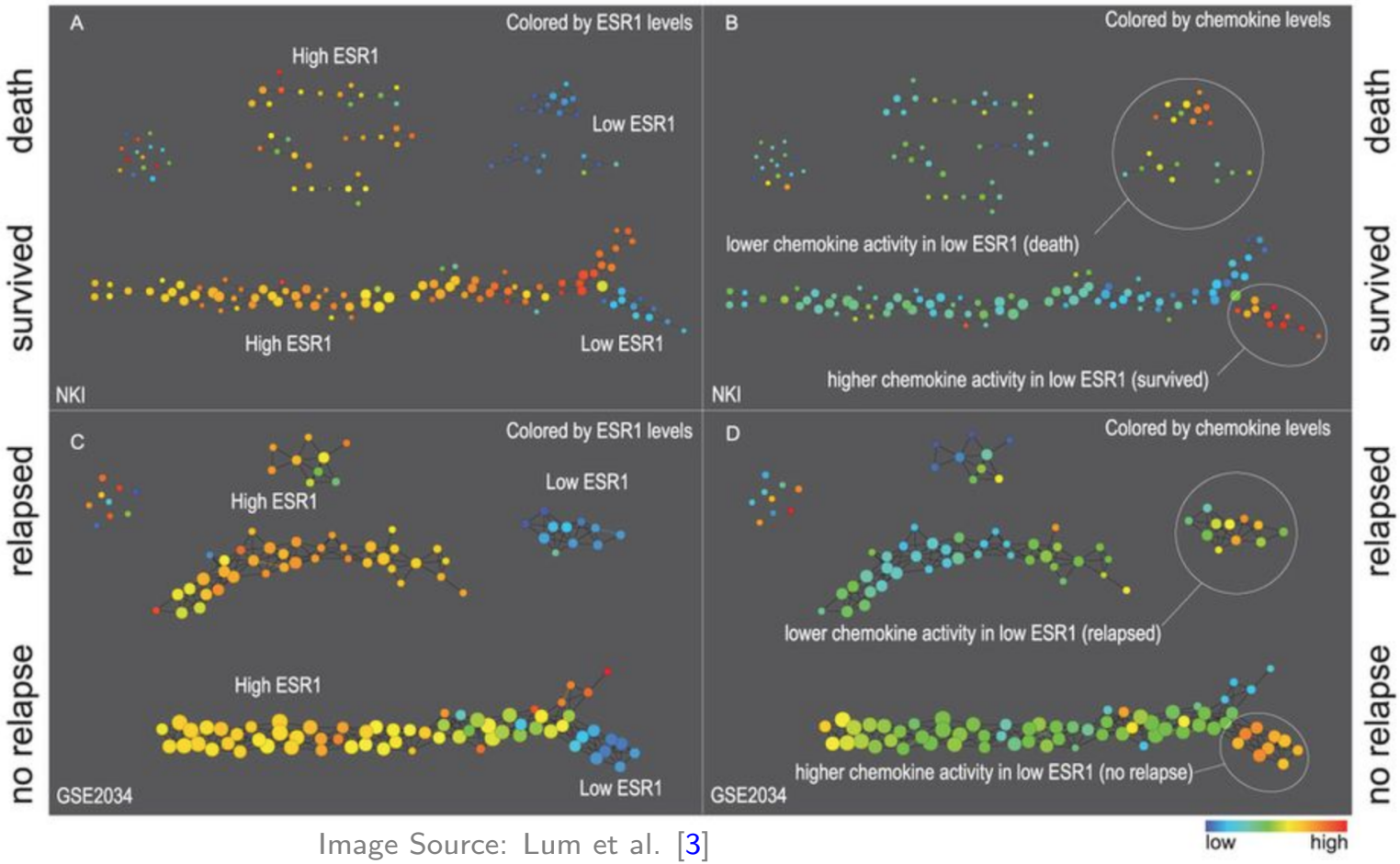


Image Source: Lum et al. [3]

Breast cancer

Mapper finds features that clustering alone misses.

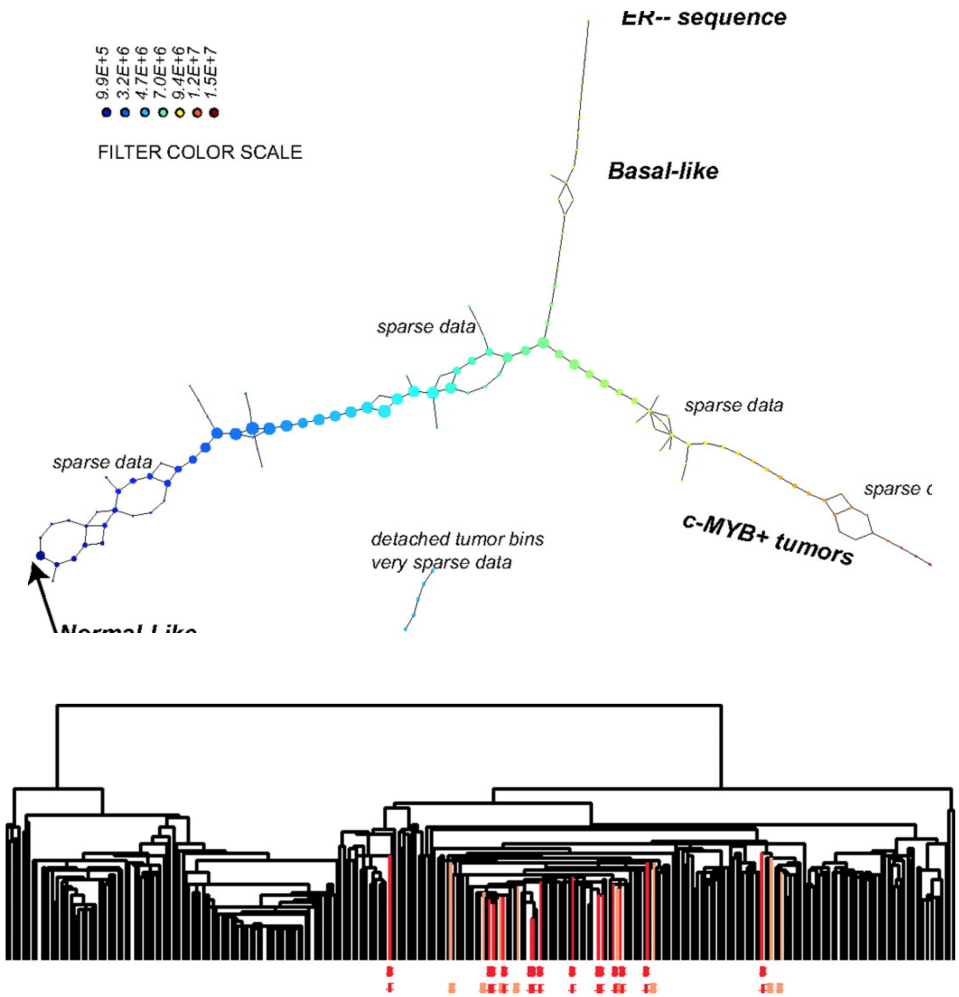


Image Source: Nicolau et al. [4]

NBA

There are more than the traditional five positions in basketball.

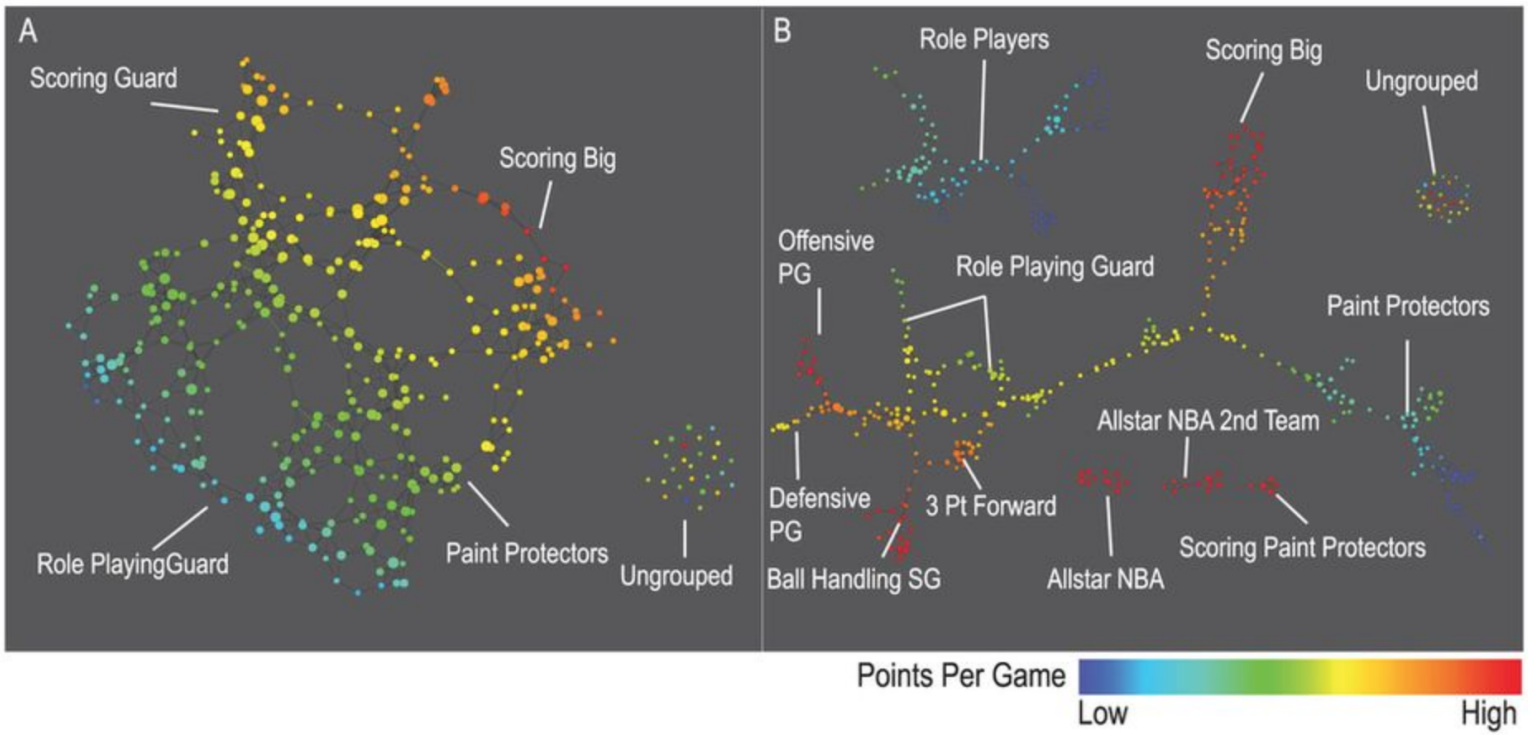


Image Source: Lum et al. [3]

Shape comparison

Triangulated mesh of different poses of the same subjects: camels cats, elephants, faces, heads, horses, and lions. Sampled "landmark points" judiciously. Filter functions E_1 eccentricity. In a statistically meaningful way, mapper outputs from same subject different pose are similar and mapper outputs between different subjects are dissimilar.

Any questions?

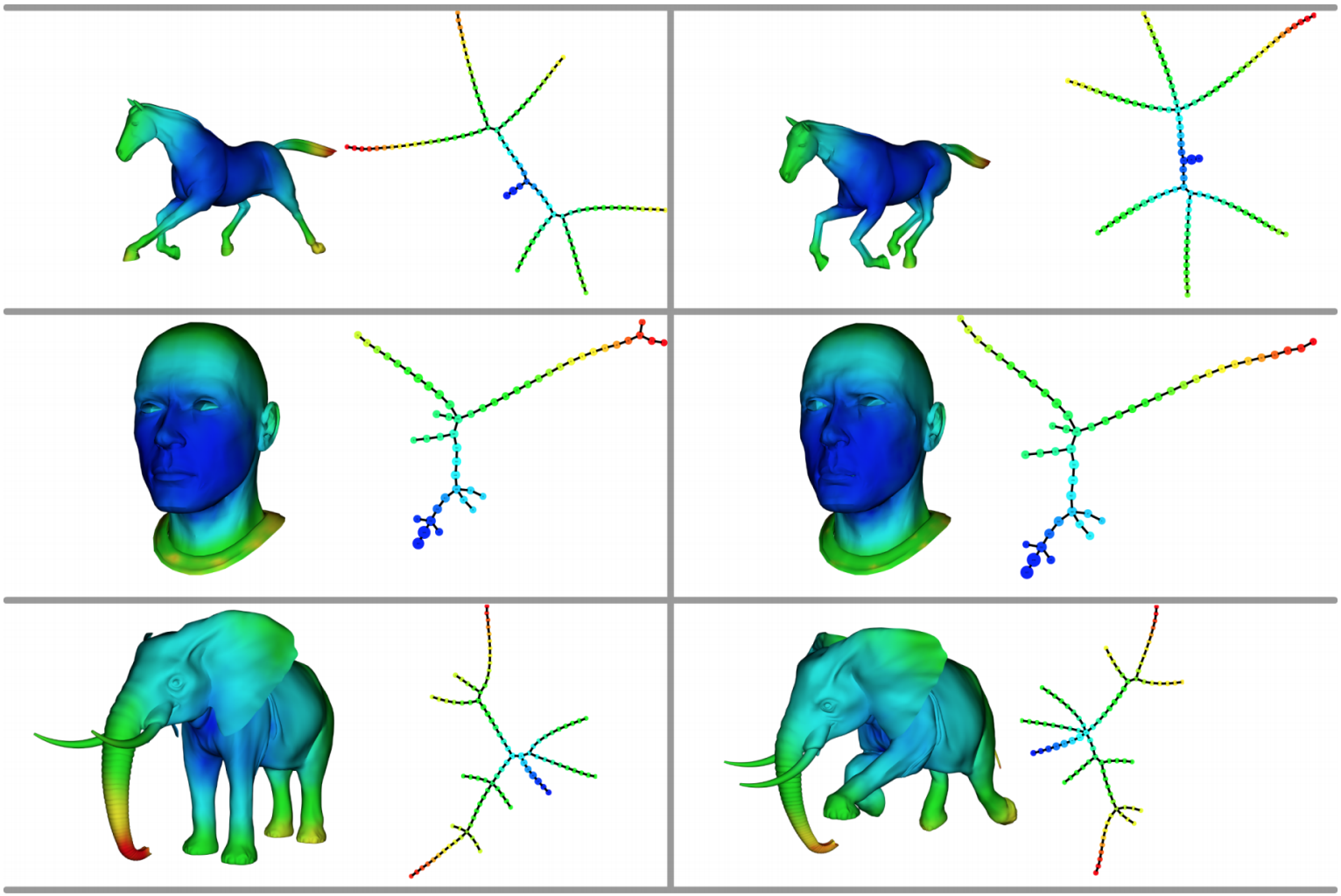


Image Source: Singh, Mémoli, Carlsson [6]

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