

Directed complexes, sequence dimension
and inverting a neural network.

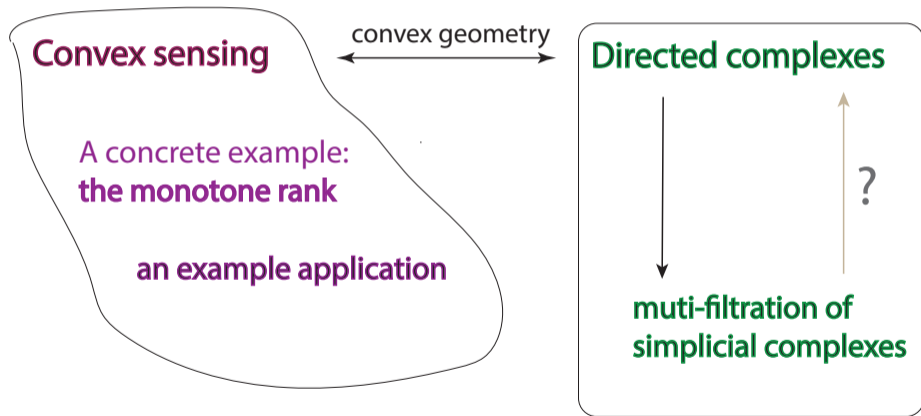
Vladimir Itskov

The Pennsylvania State University

Abel Symposium on TDA

Geiranger, Norway, June 4–8, 2018

Plan of the talk:



Directed Complexes

V is a finite set of vertices.

- A sequence in V is a simplex equipped with a total order, i.e. a tuple $s = (v_1, \dots, v_k)$, where $v_j \in V$ do not repeat.

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Directed complexes come with the usual bells and whistles:

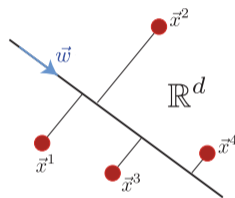
- geometric representations
- homotopy equivalence
- (co-) homology $H_*(D)$, persistence, etc.

Embedding a ~~set of sequences~~ directed complex.

An embedding problem:

Given a directed complex \mathcal{D} , on n vertices, find an arrangement of n points $x^1, \dots, x^n \in \mathbb{R}^d$ so that

$$s \in \mathcal{D} \iff (\exists w, \text{ s.t. } u <_s v \iff w \cdot x^u < w \cdot x^v)$$

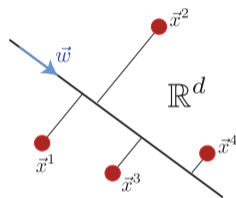


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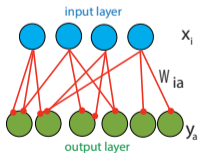
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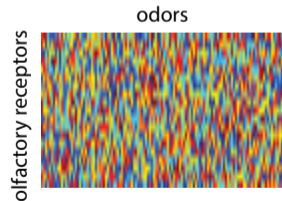
Definition. The monotone rank, $\text{mrank}(\mathcal{D})$ of a directed complex \mathcal{D} is the minimal possible dimension of such an embedding.

Neuroscience motivation:

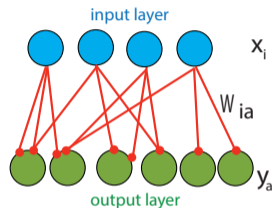
1) Feedforward networks



2) What is the dimension of the space of smells?



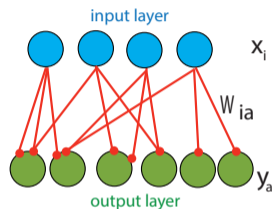
Motivation: one-layer feedforward neural networks



$$y_i = \phi_i \left(\sum_{a=1}^d W_{ia} x_a - t_i \right),$$

$\phi_i: \mathbb{R} \rightarrow \mathbb{R}_{\geq 0}$ are monotone incr.

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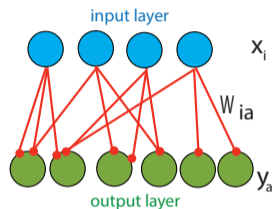
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Assume that all we know is the activity of the output layer, i.e. a collection of points $\{\vec{y}^\alpha\} \subseteq \mathbb{R}^n$

$$\vec{y}^\alpha = \vec{\Phi} (W \vec{x}^\alpha - \vec{t}) \in \mathbb{R}^n$$

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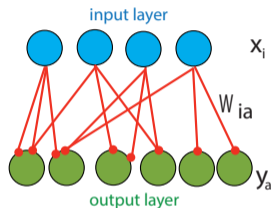
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Question: Can we use the output of a one-layer network to tell the size d of the input layer?

A non-linear matrix factorization



$$y_i = \varphi_i \left(\sum_{a=1}^d W_{ia} x_a - t_i \right),$$

$\varphi_i: \mathbb{R} \rightarrow \mathbb{R}_{\geq 0}$ are monotone incr.

Assume that all we know is the activity of the output layer, i.e. a collection of points $\{\vec{y}^\alpha\}$, $\vec{y}^\alpha \in \mathbb{R}^n$.

Think of this as an $n \times m$ matrix
 $M = [\vec{y}^1, \dots, \vec{y}^m] = \vec{\Phi}(WX - t)$.

Equivalently, find the minimal d so that the factorization

$$M_{i\alpha} = \phi_i \left(\sum_{a=1}^d W_{ia} X_a^\alpha \right),$$

is possible with some monotone increasing $\phi_i: \mathbb{R} \rightarrow \mathbb{R}$.

Here the functions ϕ_i are unknown.

The non-linear rank

$\mathcal{G} \stackrel{\text{def}}{=} \{f: \mathbb{R} \rightarrow \mathbb{R} \text{ monotone increasing, surjective} \}$

$\mathcal{M}_{m,n} \stackrel{\text{def}}{=} \{m \times n \text{ matrices} \}$

The group \mathcal{G}^m acts on rectangular matrices $\mathcal{M}_{m,n}$.

For $g = (g_1, \dots, g_m) \in \mathcal{G}^m$ and $M \in \mathcal{M}_{m,n}$,

$$(g \cdot M)_{ia} \stackrel{\text{def}}{=} g_i(M_{ia}).$$

Definition: The monotone rank of an $m \times n$ real-valued matrix M is the minimum rank of the matrices in the orbit of M , i.e.

$$\text{mrank}(M) \stackrel{\text{def}}{=} \min_{g \in \mathcal{G}^m} \text{rank}(g \cdot M).$$

Simple facts about “monotone rank”:

- $\text{mrank}(M) \leq \text{rank } M$ is determined by the ordering of each row, i.e. the directed complex $\mathcal{D}(M)$.

directed complexes

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Definition: A directed complex is a poset of sequences in V , closed under inclusion.

A pure directed complex is a directed complex whose maximal sequences have the same length.

A construction: Each matrix $M \in \mathcal{M}_{m,n}^o$ yields a set of sequences s_i in $[n]$ s.t. each sequence $s_i = (v_{i1}, v_{i2}, \dots, v_{in})$ is the total order on the i -th row:

$$M_{iv_{i1}} < M_{iv_{i2}} < \dots < M_{iv_{in}}.$$

An example:

$$\mathcal{D} \left(\begin{pmatrix} 10 & 20 & 30 & 40 \\ 11 & 13 & 14 & 12 \\ 1 & 4 & 2 & 3 \end{pmatrix} \right) = \langle (1, 2, 3, 4), (1, 4, 2, 3), (1, 3, 4, 2) \rangle$$

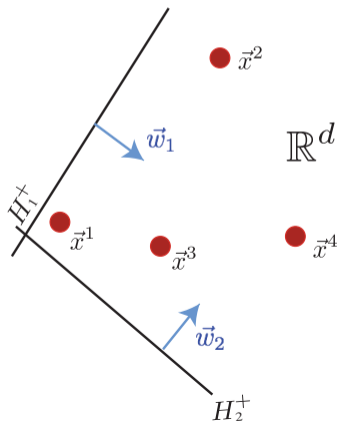
A geometric interpretation of $\mathcal{D}(M)$:

a non-linear matrix factorization \mapsto a pure directed complex

$$\begin{pmatrix} * & * & * & * \\ * & * & * & * \end{pmatrix} \mapsto \langle (1, 2, 3, 4), (1, 3, 4, 2) \rangle$$

$$M_{i\alpha} = f_i(\vec{w}_i \cdot \vec{x}^\alpha)$$

The i -th sequence is the order in which the i -th plane encounters the points \vec{x}^α .



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- $\text{mrank}(M) \leq \min\{n - 1, m\}$ for any $m \times n$ matrix.
- There are combinatorial constraints that guarantee that $\text{mrank}(M) > d$ for any prescribed d . These come from convex geometry...

a quick example: a bound on mrank via Radon's Theorem

Observation: If $M_{i\alpha} = \phi_i(\vec{w}_i \cdot \vec{x}^\alpha)$ and $s = (v_1, v_2, \dots, v_n) \in \mathcal{D}(M)$ then for every $l \in [n]$, the convex hulls do not intersect:

$$\text{conv}\{v^1, v^2, \dots, v^l\} \cap \text{conv}\{v^{l+1}, v^{l+2}, \dots, v^n\} = \emptyset.$$

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Radon's Theorem: Any set of $d + 2$ points in \mathbb{R}^d can be partitioned into two disjoint sets whose convex hulls intersect.



Corollary: If $\mathcal{D}(M)$ allows all the partitions on $[n]$ then $\text{mrank } M > n - 2$.

Example:

$$\mathcal{D}(M) = \langle 1234, 1423, 1342 \rangle \implies \text{mrank } M = 3$$

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Note: The general combinatorial constraints on the monotone rank are currently not well-understood, but the topology of $\mathcal{D}(M)$ imposes constraints in two different “good sampling” regimes.

Need for a “good sampling”

Two different regimes:

- “good sampling” of the functions
- “good sampling” of points x_a

The limit of “many/enough” functions

Given a point cloud $X = \{x_a\} \subset \mathbb{R}^d$, $|X| = n$, there are only finitely many combinatorially distinct linear functions, thus define

$$D_{\text{lin}}(X) = \{\text{all sequences in } X \text{ from linear functions } f_w(x) = w \cdot x\}$$

Theorem. Let $X \subset \mathbb{R}^d$ be a set of points in general position. Then the homology of the directed complex $D_{\text{lin}}(X)$ satisfies

$$H_k(D_{\text{lin}}(X)) = 0 \quad \forall k \in \{1, \dots, d\},$$

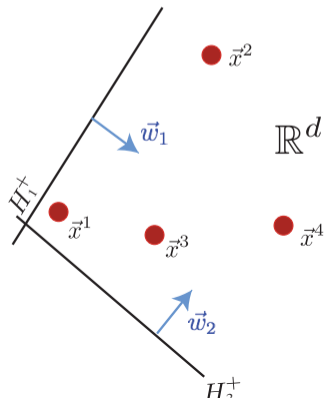
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Lemma [T. Cover, 1967] The number $Q(n, d)$ of maximal sequences in $D_{\text{lin}}(X)$ satisfies $Q(n+1, d) = Q(n, d) + nQ(n, d-1)$.



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Conjecture. Let $X \subset \mathbb{R}^d$ be a set of points in general position. Assume that either $d \leq 3$ and $n \geq d + 2$ or $d \geq 4$ and $n \geq 2d - 1$. Then the homology of the directed complex $D_{\text{lin}}(X)$ satisfies

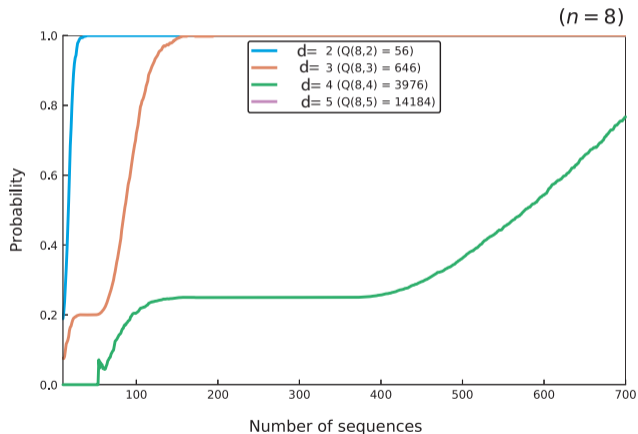
$$H_*(D_{\text{lin}}(X)) = H_*\left(\bigvee^{n-1} S^d\right).$$

Question: What happens when the sequences are (grossly) undersampled?

Answer: If the underlying dimension $d \ll n$, then d can be reliably inferred from relatively few sequences.

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The probability of a correct dimension inference.

The case of many/enough points.

The Dowker multi-filtration of a pure directed complex.

Given M is an $m \times n$ matrix.
and thresholds $\theta = (\theta_1, \dots, \theta_m)$.

Binary matrix $B_{ia} \stackrel{\text{def}}{=} (M_{ia} \leq \theta_i)$.

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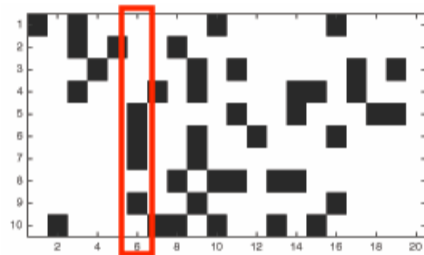
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The Dowker complex is

$$\text{Dow}(M, \theta) \stackrel{\text{def}}{=} \Delta(\sigma_1, \dots, \sigma_n)$$

where $\sigma_a \stackrel{\text{def}}{=} \{i \mid M_{ia} \leq \theta_i\}$.

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Note: An increasing chain of thresholds induces a filtration.

This is because

$$\theta_i \leq \tilde{\theta}_i \quad \forall i \in [m] \implies \text{Dow}(M, \theta) \subseteq \text{Dow}(M, \tilde{\theta})$$

A fun fact:

Theorem (C. H. Dowker, 1952)

Let B be a binary matrix, then the following two complexes are homotopy equivalent:

$$\text{Dow}(B, 1) \sim \text{Dow}(B^T, 1)$$

Question: What does Dowker complex have to do with monotone rank?

$M_{ia} = \phi_i \left(\sum_{a=1}^d W_{ia} x_a^\alpha \right)$, where ϕ_i are monotone increasing.

$$\begin{aligned}
 M_{ia} &\leq \theta_i, \\
 \phi_i \left(\sum_{a=1}^d W_{ia} x_a^\alpha \right) &\leq \theta_i, \\
 \sum_{a=1}^d W_{ia} x_a^\alpha &\leq \phi_i^{-1}(\theta_i), \\
 \vec{x}^\alpha &\in H_i^+,
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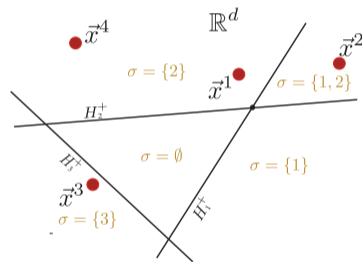
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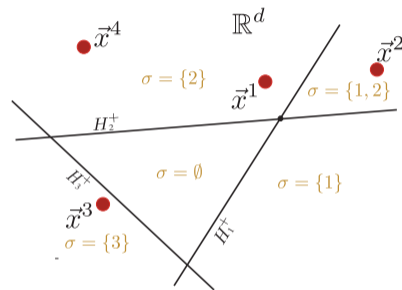
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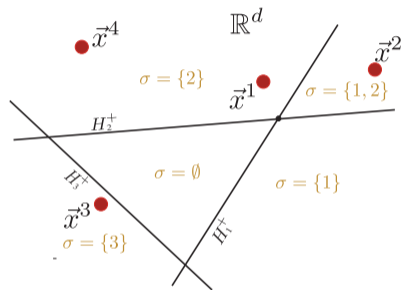
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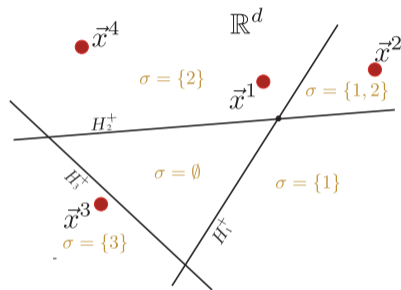
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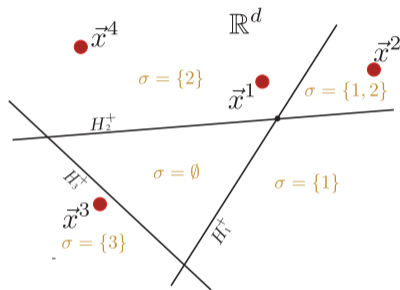
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Question: What does one do if the sampling is not perfect?



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Homological invariants of a filtered Dowker complex

Given a real $n \times m$ matrix M . An increasing sequence of threshold vectors,

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induces a sequence of simplicial complexes $\Delta_j \stackrel{\text{def}}{=} \text{Dow}(M, \vec{\theta}_j)$,

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Homological invariants:

- *Betti Curves*, $\beta_m(\theta) \stackrel{\text{def}}{=} \dim H_m(\text{Dow}(M, \theta))$
- *Persistence intervals*

Why can we infer the monotone rank from the Dowker complex?

Given M and $\Theta = (\vec{\theta}_1 < \dots < \vec{\theta}_p)$ one obtains
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$$\bar{\beta}_k(\rho) \stackrel{\text{def}}{=} \frac{1}{|\mathcal{S}_m|} \sum_{s \in \mathcal{S}_m} \beta_k^{\Theta_s}(\rho)$$

very well via random sampling of \mathcal{S}_m .

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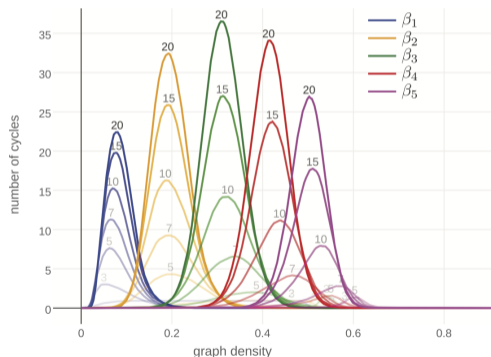
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However, one can estimate

$$\bar{\beta}_k(\rho) \stackrel{\text{def}}{=} \frac{1}{|\mathcal{S}_m|} \sum_{s \in \mathcal{S}_m} \beta_k^{\Theta_s}(\rho)$$

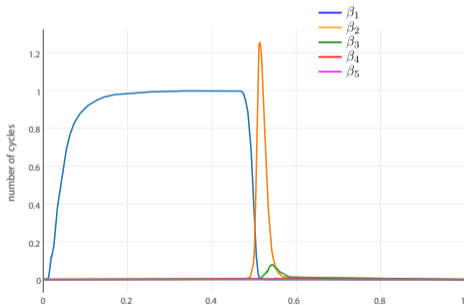
very well via random sampling of \mathcal{S}_m .

Average Betti curves $\bar{\beta}_k(\rho)$ in various ranks.

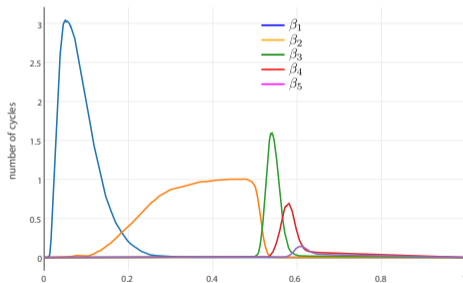


Two different ways of inferring d :

- 1) A single persistent cycle $\in H_m(\text{Dow}(M, -))$ in dimension $m = (d - 1)$.
- 2) The 'shapes' of the of the Betti curves

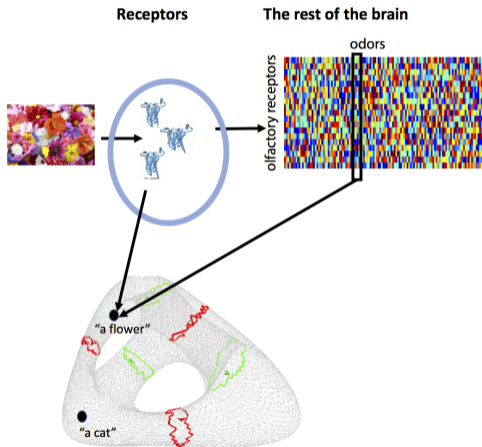


Betti curves for random matrices of $\text{mrank} = 2$



Betti curves for random matrices of $\text{mrank} = 3$

Can one estimate the dimension of the space of smells?



"Olfactory Space" that the brain can possibly perceive

A question: Can we tell the dimension of the olfactory space from OR ? ligand response map?

Answer: A "yes". *Preliminary findings:* We've found that the fly olfactory space of likely low-dimensional ($4 \leq d \leq 6$).

Quick summary

- Convex sensing problems can be best understood in terms of directed complexes.
- Natural questions about feedforward networks can be restated in terms of “nonlinear matrix factorization” and the monotone rank.
- Exact bounds on the monotone rank are still poorly understood, but there are hard constraints from geometry and topology.
- monotone rank can be estimated (with high precision) using topological tools.

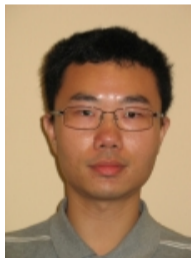
Thanks!

Takk for din oppmerksomhet.

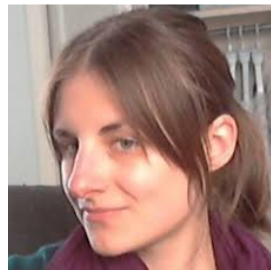
this talk:



Philip Egger



Min-Chun Wu



Aliaksandra Yarosh