The Representation Theory of Filtered Hierarchical Clustering

Ulrich Bauer (TUM)

Workshop Topology in Data Analysis and Beyond

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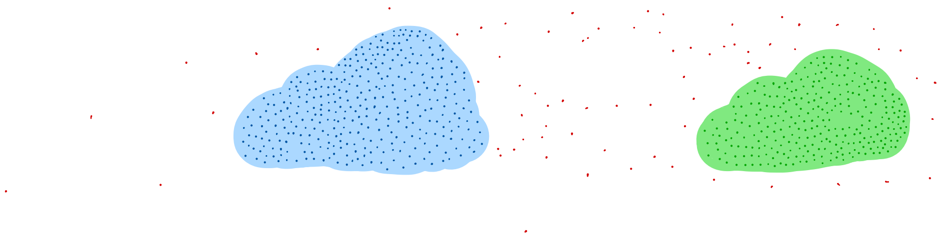
joint work with:

Magnus Botnan / Steffen Oppermann / Johan Steen



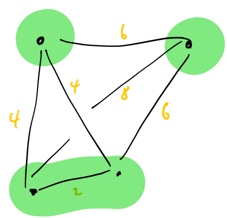
CLUSTERING FUNCTIONS

X : finite set

Clustering function φ :

maps a metric $d : X \times X \to \mathbb{R}$ (distance matrix)

to a partition of X.

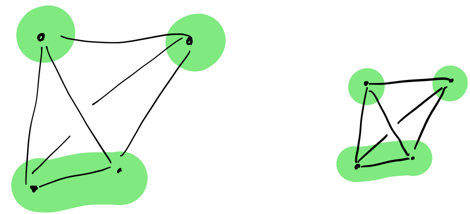


KLEINBERG'S AXIOMS

Desirable properties

- scale invariance:

$$\varphi(d) = \varphi(\lambda \cdot d).$$



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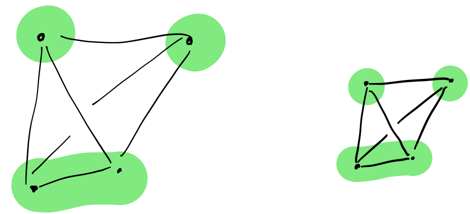

- richness:

every partition is obtained from some d.

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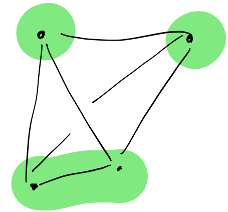
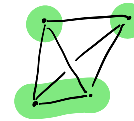


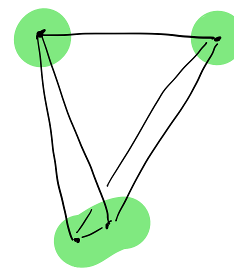


- **richness:**

every partition is obtained from some d.

- **consistency:**

decreasing d within clusters /
increasing d across clusters
does not change the result.



KLEINBERG'S IMPOSSIBILITY THEOREM

Thm [Kleinberg 2002] No clustering function satisfies

- scale-invariant,
- richness, and
- consistency.

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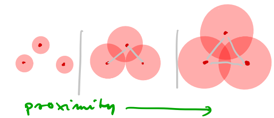
Motivates the use of a scale parameter

⇝ hierarchical clustering

CLUSTERING FROM CONNECTED COMPONENTS

proximity graph

- filter edges by proximity



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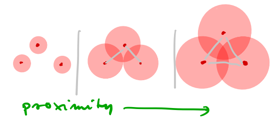
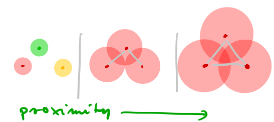
π_0 (connected components)





single-linkage clustering

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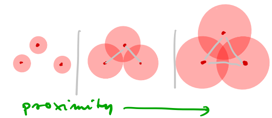

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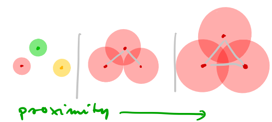


single-linkage clustering

H_0 (homology in deg. 0 with coeffs in K)

$$K^3 \to K \to K$$

proximity

persistent homology

$H_0 = F \circ \pi_0$

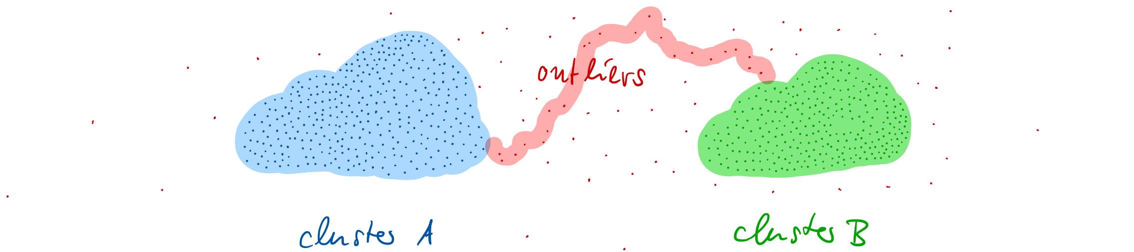
HIERARCHICAL CLUSTERING: EXISTENCE & UNIQUENESS

Thm [Carlsson, Mémoli 2010] Single-linkage clustering is the unique hierarchical clustering method satisfying [... certain axioms similar to Kleinberg's].

But ...

CHAINING EFFECT

Single-linkage clustering is sensitive to outliers

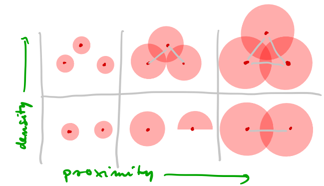


→ not used much in practice!

2-PARAMETER CLUSTERING

density-proximity graph

- filter points by density
- filter edges by proximity



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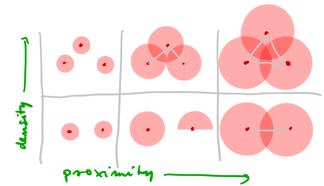

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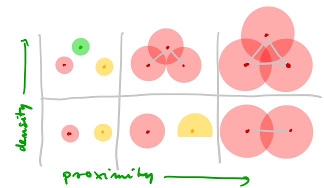

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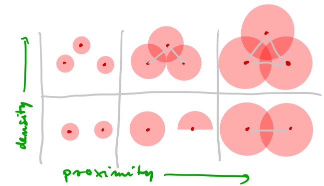

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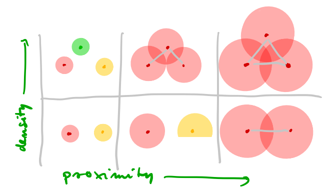

H_0 (homology in deg. 0
with coeffs in K)

$$\begin{tikzcd}
K^3 \arrow[r] & K \arrow[r] & K \\
K^2 \arrow[r] \arrow[u] & K^2 \arrow[r] \arrow[u] & K \arrow[u]
\end{tikzcd}$$

density

proximity

DECOMPOSING DIAGRAMS OF VECTOR SPACES

$$\begin{array}{ccc} V & \xrightarrow{f} & W \\ \wr\| & & \\ \ker f & \longrightarrow & 0 \\ \oplus & & \\ \operatorname{im} f & \longrightarrow & \operatorname{im} f \\ \oplus & & \\ 0 & \longrightarrow & \operatorname{coker} f \end{array}$$

TWO MAPS

$$
\begin{tikzcd}
U \arrow[r, "g"] & V \arrow[r, "f"] & W \\[-1em]
\cong & & \\
K^a \arrow[r] & 0 \arrow[r] & 0 \\
\oplus & & \\
0 \arrow[r] & K^b \arrow[r] & 0 \\
\oplus & & \\
0 \arrow[r] & 0 \arrow[r] & K^c \\
\oplus & & \\
K^d \arrow[r] & K^d \arrow[r] & 0 \\
\oplus & & \\
0 \arrow[r] & K^e \arrow[r] & K^e \\
\oplus & & \\
K^f \arrow[r] & K^f \arrow[r] & K^f
\end{tikzcd}
$$

SEQUENCES OF MAPS

$$V: \quad V_0 \to V_1 \to V_2 \to \cdots \to V_n$$

decomposes into summands of the form

$$\cdots \to 0 \to \underbrace{K \to \cdots \to K}_{i \qquad\qquad j} \to 0 \to \cdots$$

$V \cong$ "collection of intervals"

$\rightsquigarrow$ persistence barcode.

DROZD'S TRICHOTOMY

Given a finite indexing poset P. (k : algebr. closed)

What are the indecomposable diagrams with shape P ?

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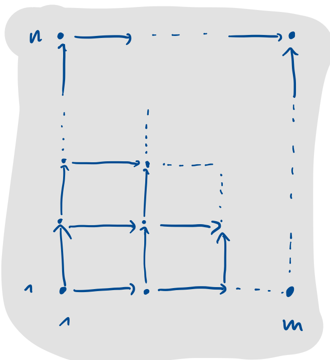
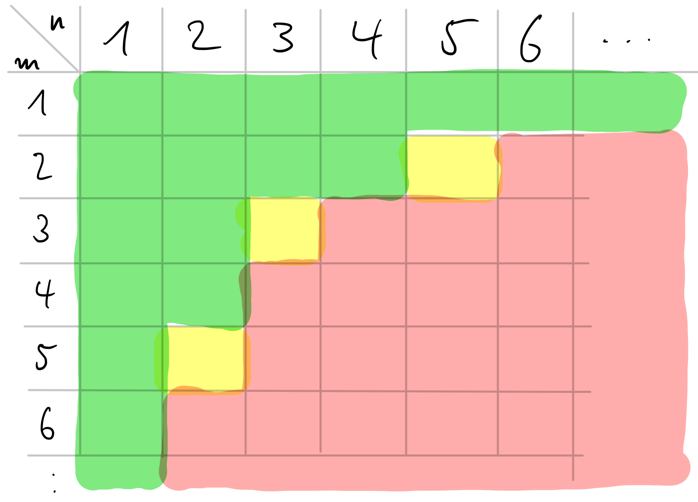
ⓑ A finite list (of 1-param. families). tame

ⓒ It's complicated. wild

(as complicated as modules over any finite-dim. algebra; including undecidable problems)

REPRESENTATION TYPES OF COMMUTATIVE GRIDS



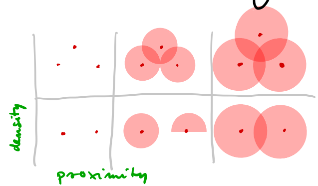


- finite type
- tame
- wild

$\left.\begin{array}{l}\text{finite type}\\ \text{tame}\\ \text{wild}\end{array}\right\}$ for $(m-1)(n-1) \left\{\begin{array}{c} < \\ = \\ > \end{array}\right\} 4$.

GRID DIAGRAMS FROM CLUSTERING

consider again 2-parameter clustering (proximity / density)



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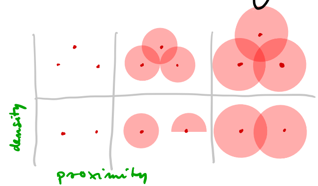

This yields diagrams of the form

$$\begin{tikzcd}
\vdots & \vdots & & \\
\bullet \arrow[u] \arrow[r, two heads] & \bullet \arrow[u] & \cdots & \\
\bullet \arrow[u] \arrow[r, two heads] & \bullet \arrow[u] \arrow[r, two heads] & \bullet \arrow[r, two heads] & {}
\end{tikzcd}$$

Horizontal maps are surjective!

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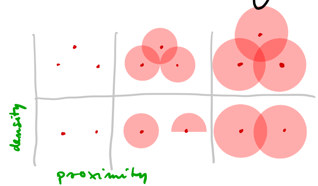

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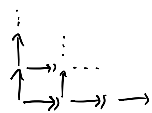
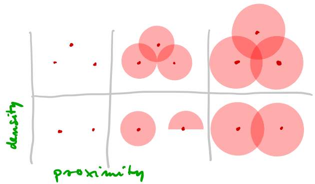


Horizontal maps are surjective !

Does this simplify the picture ?

EPIMORPHISMS

Lemma $\mathrm{Rep}^{\twoheadrightarrow}(m,2)$ is finite type.



$$H_0 \rightsquigarrow \begin{tikzcd} K^3 \arrow[r, two heads, "(1\ 1\ 1)"] & K \arrow[r, two heads] & K \\ K^2 \arrow[u, "\begin{pmatrix}1&0\\0&1\\0&0\end{pmatrix}"] \arrow[r, two heads] & K^2 \arrow[u, "(1\ 1)"'] \arrow[r, two heads, "(1\ 1)"'] & K \arrow[u] \end{tikzcd}$$

$$\cong \begin{tikzcd} K \arrow[r, two heads] & K \arrow[r, two heads] & K \\ K \arrow[u] \arrow[r, two heads] & K \arrow[u] \arrow[r, two heads] & K \arrow[u] \end{tikzcd} \oplus \begin{tikzcd} K \arrow[r, two heads] & 0 \arrow[r, two heads] & 0 \\ K \arrow[u] \arrow[r, two heads] & K \arrow[u] \arrow[r, two heads] & 0 \arrow[u] \end{tikzcd} \oplus \begin{tikzcd} K \arrow[r, two heads] & 0 \arrow[r, two heads] & 0 \\ 0 \arrow[u] \arrow[r, two heads] & 0 \arrow[u] \arrow[r, two heads] & 0 \arrow[u] \end{tikzcd}$$

- $\mathrm{Rep}(m,n)$: all commutative dgms over $m \times n$ grid
- $\mathrm{Rep}^{\twoheadrightarrow}(m,n)$: epis in horizontal direction
- $\mathrm{Rep}^{\twoheaduparrow\twoheadrightarrow}(m,n)$: epis in both directions.

EPIC GRIDS & WILD THINGS

Thm [B, Botnan, Oppermann, Steen 19]

$$\begin{array}{ccc}
\mathrm{Rep}^{\twoheaduparrow \twoheadrightarrow}(m, n) & \sim & \mathrm{Rep}^{\twoheaduparrow}(m, n-1) \\
\wr & & \wr \\
\mathrm{Rep}^{\twoheadrightarrow}(m-1, n) & \sim & \mathrm{Rep}(m-1, n-1)
\end{array}$$

same representation type

Corollary $\mathrm{Rep}^{\twoheadrightarrow}(m, n)$ is

- finite type
- tame
- wild

for $(m-1)(n-2) \left\{ \begin{array}{c} < \\ = \\ > \end{array} \right\} 4.$

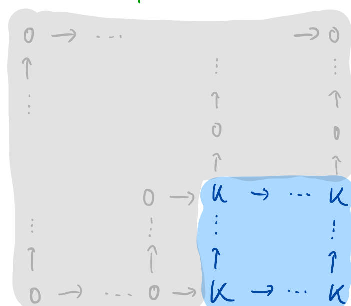
Behind the Scenes

equivalence of categories

$$\frac{\mathrm{Rep}^{\twoheadrightarrow}(m,n)}{\mathrm{Rep}^{\hat{\imath}\twoheadrightarrow}(m,n)} \simeq \mathrm{Rep}(m,n-1)$$

additive quotient $\frac{A}{B}$: identify morphisms in A whose difference factors through B

indecomposables are of the form



$\Rightarrow$ finite type

REALIZATIONS

Thm [Carlsson, Zomorodian] Any Rep(m, n) (m × n diagram of $\mathbb{Z}_2$-vector spaces) can be realized as pth-homology (H_p of an m × n diagram of top. spaces), for any $p > 0$.

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What about H_0?

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What about H_0?

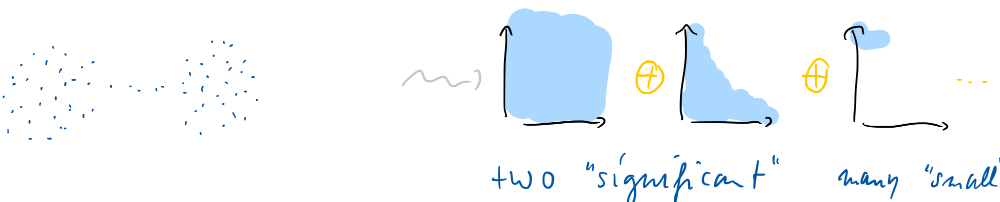
Thm [BBOS]
Not every $\mathrm{Rep}^{\uparrow \twoheadrightarrow}(m,n)$ can be realized as $\tilde{H}_0$, not even as a summand (explicit counterexample).

INDECOMPOSABLES VS CLUSTERS

- Indecomposables of H_0 from density/proximity do not correspond directly to clusters
- Rather: "linear combinations of components"

INDECOMPOSABLES VS CLUSTERS

- Indecomposables of H_0 from density/proximity do not correspond directly to clusters
- Rather: "linear combinations of components"
- Topological features, help to survey parameter space
- Typical example:



CHALLENGES

- COMPUTATION (OF INDECOMPOSABLES)
- CLASSIFICATION (OF REPS ARISING FROM CLUSTERING)
- INFERENCE (OF COMPONENTS IN THE PRESENCE OF NOISE)

FURTHER READING

U. Bauer, M. Botnan, S. Oppermann, J. Steen

Cotorsion Torsion Triples and the Representation Theory of Filtered Hierarchical Clustering

Advances in Mathematics 369, 107171 (2020)

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Funding:

DFG TR-109 Discretization in geometry & dynamics

NRC 250006 Representation theory via subcategories

NRC 231000 Clusters, combinatorics & computations in algebra

$\square$