Classifying Clustering Schemes

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joint with Gunnar Carlsson

IMA, 2014

What is data clustering?

A (standard/flat) **clustering scheme** assigns to any finite set X a partition P_X of that set.

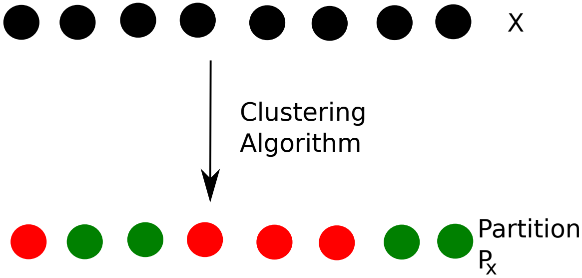

Figure : **Elements with the same color are in the same block**

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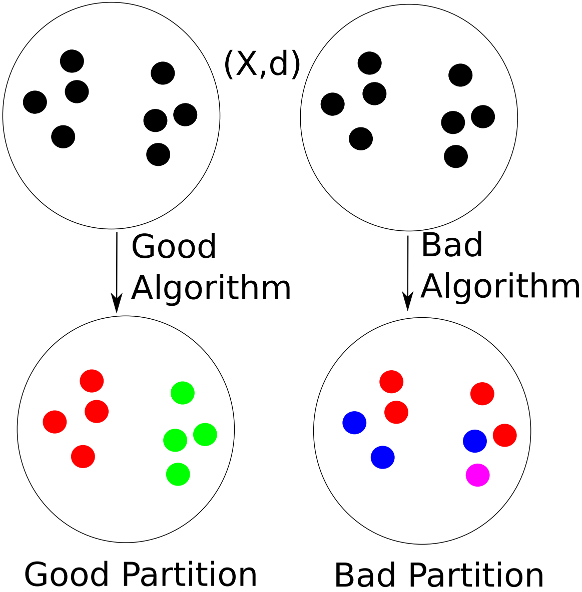
A **standard clustering scheme** is a map:

$$\begin{aligned} \mathfrak{C} : \mathcal{M} &\longrightarrow \mathcal{P} \\ (X, d_X) &\mapsto (X, P_X) \end{aligned}$$

Goal of data clustering



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Kleinberg's theorem was the inspiration for this work.

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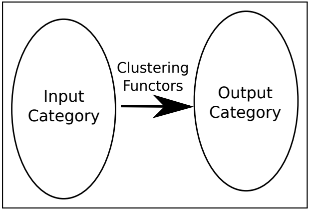
3. Study "functors" between categories (respecting this structure)



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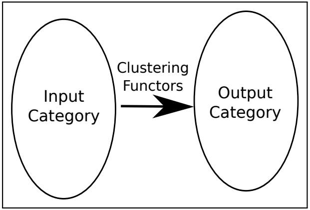

We provide a range of input categories (small to large) and show analogues of Kleinberg's theorem in each.

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- **Composition operations**:
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- **Identity morphisms**: special morphisms $X \to X$, $\mathrm{id}_X \in \mathrm{Mor}_{\mathcal{C}}(X, X)$ for each X *(think self loops/ identity maps)* such that if $f \in \mathrm{Mor}_{\mathcal{C}}(X, Y)$ then $\mathrm{id}_Y \circ f = f \circ \mathrm{id}_X = f$

Examples of categories

Example (category $\underline{3}$)

The category $\underline{3}$ has exactly three objects A, B and C and six morphisms: the identities for A, B,C, and three more morphisms, $\mathrm{Mor}_{\underline{3}}(A, B) = f$, $\mathrm{Mor}_{\underline{3}}(B, C) = g$ and $\mathrm{Mor}_{\underline{3}}(A, C) = h$:

$$\begin{tikzcd}
A \arrow[loop left, "id_A"] \arrow[rr, "f"] \arrow[dr, "h"'] & & B \arrow[loop right, "id_B"] \arrow[dl, "g"] \\
& C \arrow[loop below, "id_C"] &
\end{tikzcd}$$

In order to satisfy composition: $h = g \circ f$.

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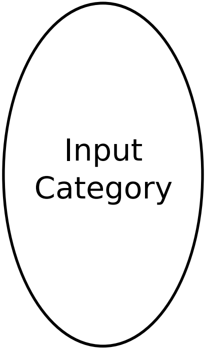

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Consider $(X, d_X), (Y, d_Y) \in \mathcal{M}$, where $\mathcal{M}$ is the collection of all finite metric spaces.

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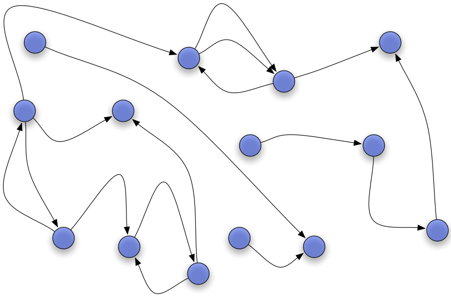
$\mathcal{M}$ will denote any of these categories

Nested categories: same object set, but filter morphisms



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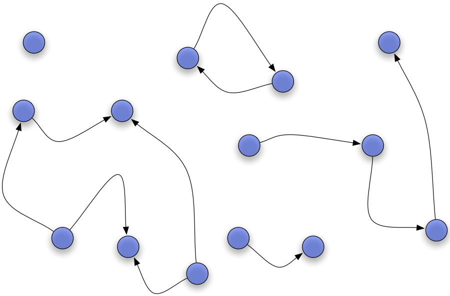

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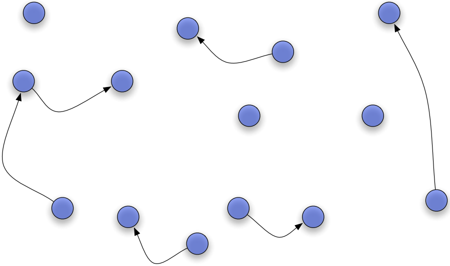

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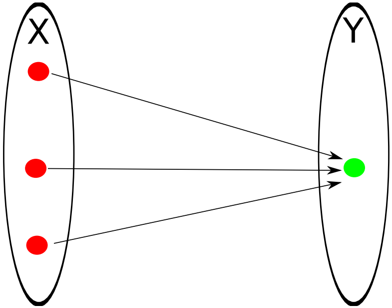

Figure : Constant maps are always distance non-increasing. Hence, $\mathcal{M}^{gen}$ is fully connected! Thus, can always have diagram $X \to Y \to X$ in $\mathcal{M}^{gen}$.

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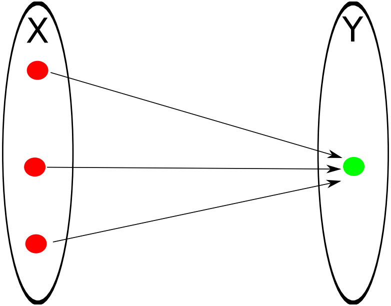

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This property fails in $\mathcal{M}^{inj}$ and $\mathcal{M}^{iso}$, since morphism ϕ could not send two different elements in X, to one element in Y.

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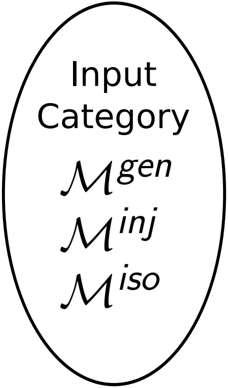

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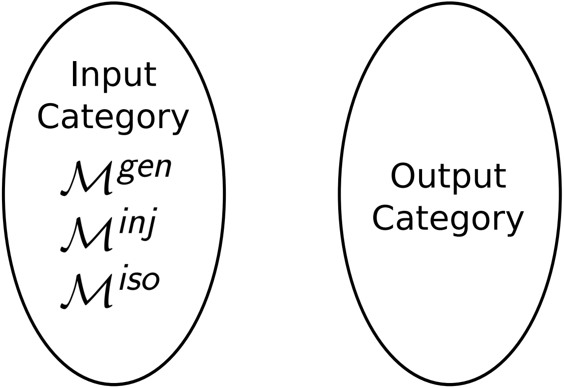

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- $\mathrm{Mor}_{\mathcal{P}}\big((X, P_X), (Y, P_Y)\big)$ is the set of all maps $f : X \to Y$ where P_X is a refinement of $f^*(P_Y)$.

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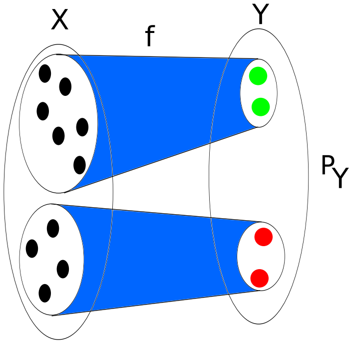

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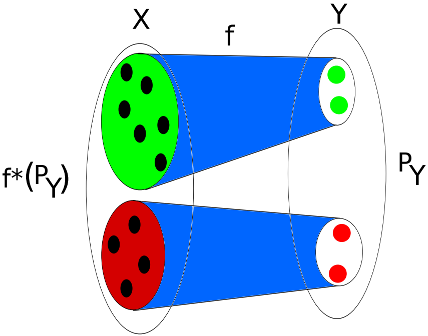

Morphisms in $\mathcal{P}$

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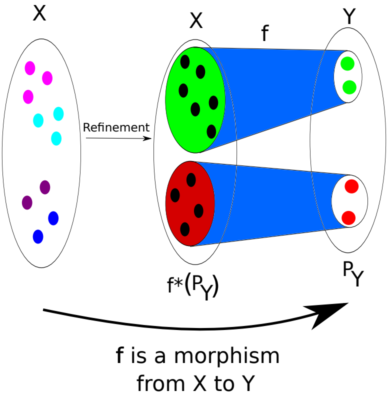

Figure : P_X refines $f^*(P_Y)$

For a finite set X we denote by $\mathbf{P}(X)$ the set of all partitions of X.

Definition ($\mathcal{P}$, a category of outputs of standard clustering schemes)

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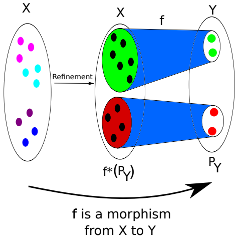
- $\mathrm{ob}(\mathcal{P})$ equal to all possible pairs (X, P_X) where X is a finite set and $P_X \in \mathbf{P}(X)$.
- $\mathrm{Mor}_{\mathcal{P}}\big((X, P_X), (Y, P_Y)\big)$ is the set of all maps $f : X \to Y$ where P_X is a refinement of $f^*(P_Y)$.



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- Let $f \in \mathrm{Mor}_{\mathcal{P}}\big((X,P_X),(\{a,b\},\{\{a\},\{b\}\})\big)$. Then,

  $f(x) \neq f(x')$, implies that x, x' must be in <u>different</u> blocks of P_X.

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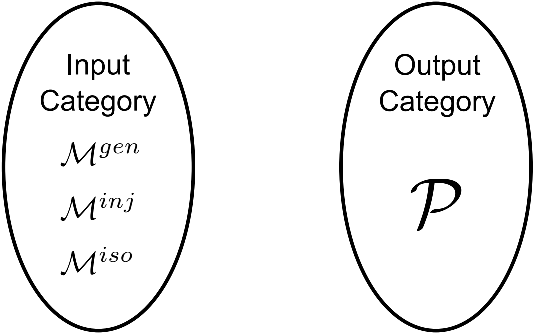

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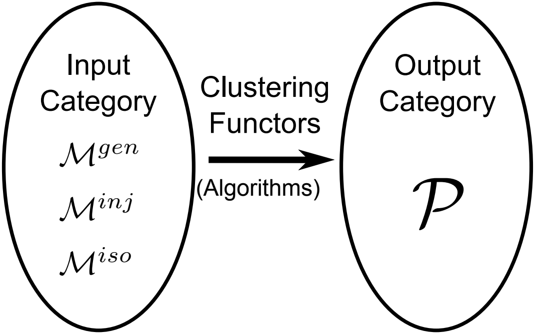

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- Notice that it is more difficult to find functors $\mathcal{M}^{gen} \to \mathcal{P}$ than to find functors $\mathcal{M}^{inj} \to \mathcal{P}$, than to find functors $\mathcal{M}^{iso} \to \mathcal{P}$.

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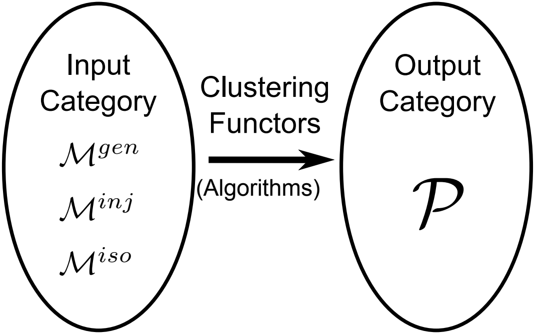

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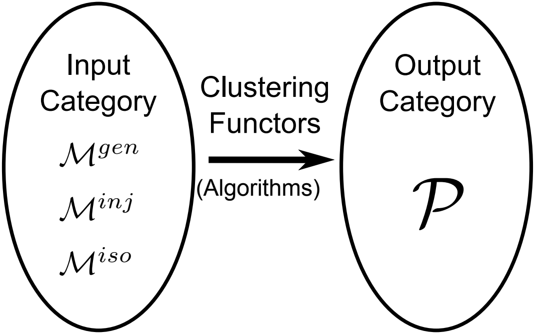

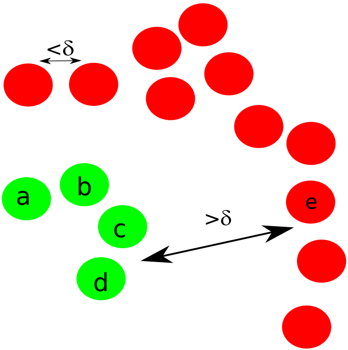

Definition

On $(X, d_X) \in \mathcal{M}$, for each $\delta \geq 0$, define the **equivalence relation** $\sim_\delta$, where $x \sim_\delta x' \iff$ there is a sequence $x_0, x_1, \ldots, x_k \in X$ so that $x_0 = x, x_k = x'$, and $d_X(x_i, x_{i+1}) \leq \delta$ for all i. Let $\mathbf{P_X}(\delta)$ be the resulting partition.

$\mathcal{M}^{gen}$ functorial clustering algorithms

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For each $\delta \geq 0$ define

$$\mathfrak{R}_\delta : \mathcal{M}^{gen} \to \mathcal{P}$$

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Functoriality is equivalent to:

$\phi \in \mathrm{Mor}_{\mathcal{M}^{gen}}(X, Y)$, then $x \sim_\delta x'$ in X, implies $\phi(x) \sim_\delta \phi(x')$ in Y.

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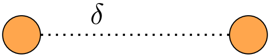
Let $\Delta_2(\delta)$ be the metric space of two points, where $d(x, y) = \delta$:



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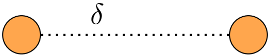

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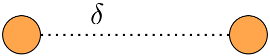

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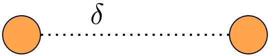

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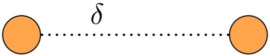

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Then, $\mathfrak{C}$ is the Vietoris-Rips functor with parameter $\delta_{\mathfrak{C}}$. i.e.
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- To what degree do these properties hold for the VR/SL functor?

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A similar theorem holds in $\mathcal{M}^{inj}$.

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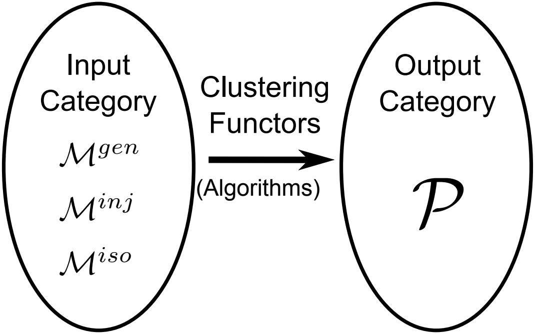

A property for functorial algorithms

Definition (Excisive clustering functors)

We say that a clustering functor $\mathfrak{C}$ is **excisive** if for all $(X, d_X) \in \mathrm{ob}(\mathcal{M})$, if we write $\mathfrak{C}(X, d_X) = (X, \{X_\alpha\}_{\alpha\in A})$, then $\mathfrak{C}\left(X_\alpha, d_{X|_{X_\alpha\times X_\alpha}}\right) = (X_\alpha, \{X_\alpha\})$ for all $\alpha \in A$.

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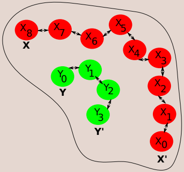

Metric Space
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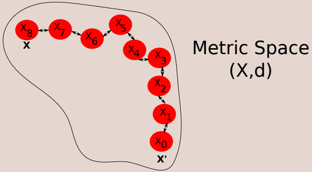

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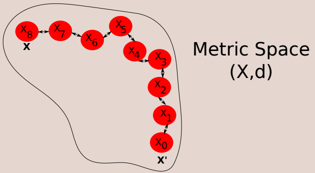

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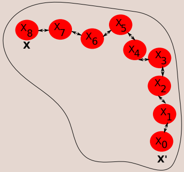

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Do non-excisive methods exist? Definitely not in $\mathcal{M}^{gen}$!

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Indeed, assume that $\phi \in \mathrm{Mor}_{\mathcal{M}^{inj}}(X, Y)$, then for all $x \neq x'$:

$$d_X(x, x') \geq d_Y(\phi(x), \phi(x')) \boxed{\geq} \min_{y \neq y'} d_Y(y, y') = \mathrm{sep}(Y).$$

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That this indeed defines a functor in $\mathcal{M}^{inj}$ follows from:

$$\mathrm{Mor}_{\mathcal{M}^{inj}}(X, Y) \neq \emptyset \Longrightarrow \mathrm{sep}(X) \geq \mathrm{sep}(Y).$$

Indeed, assume that $\phi \in \mathrm{Mor}_{\mathcal{M}^{inj}}(X, Y)$, then for all $x \neq x'$:

$$d_X(x, x') \geq d_Y(\phi(x), \phi(x')) \boxed{\geq} \min_{y \neq y'} d_Y(y, y') = \mathrm{sep}(Y).$$

Then, $\mathrm{sep}(X) \geq \mathrm{sep}(Y)$, and since $\mathfrak{R}_\delta$ is functorial and $\eta(Y) \geq \eta(X)$,

$$x \sim_{\eta(X)} x' \Longrightarrow \phi(x) \sim_{\eta(X)} \phi(x') \Longrightarrow \phi(x) \sim_{\eta(Y)} \phi(x').$$

Excisiveness in $\mathcal{M}^{inj}$

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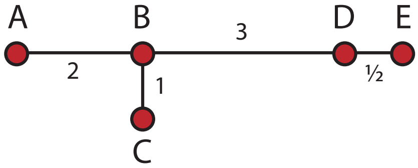

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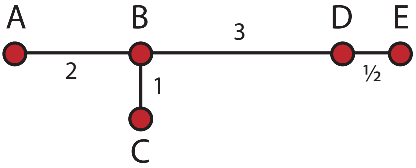

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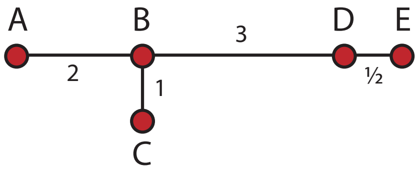

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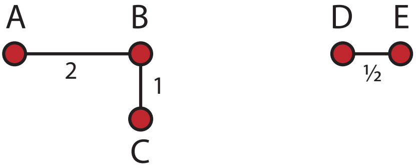

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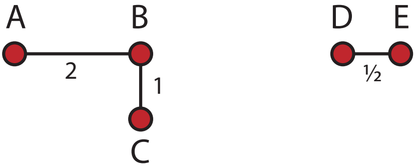

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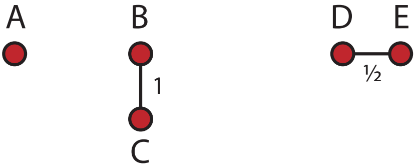

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a factory of monsters

Let $\iota : \mathcal{M}^{inj} \to (\mathbb{R}, \geq)$ by any non-constant contra-variant functor:

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Indirectly: $X \to Y \to X$ is always a possible diagram on $\mathcal{M}^{gen}$.
Apply ι and get $\iota(X) = \iota(Y)$.

And now something completely different..

Generalize single linkage clustering

Notice the following: given $\delta \geq 0$, $(X, d_X) \in \mathcal{M}$ and $x, x' \in X$,

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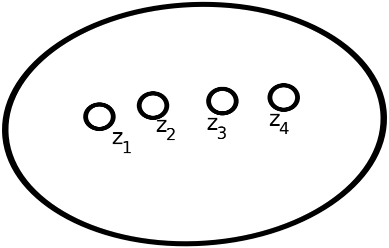

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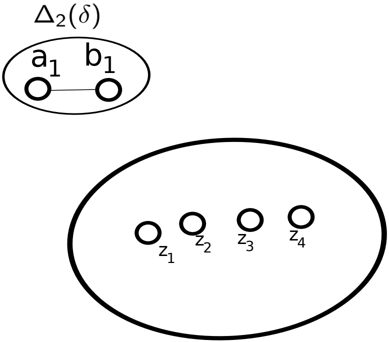

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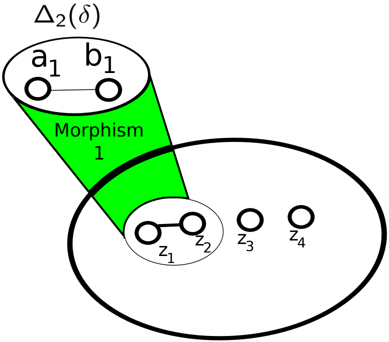

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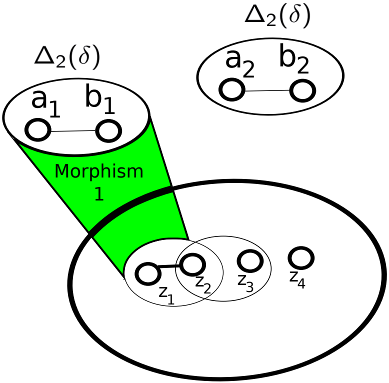

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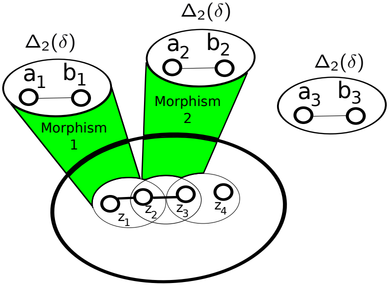

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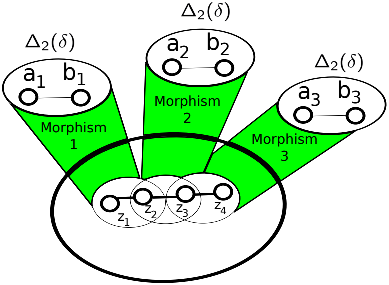

What if we use something else instead of $\Delta_2(\delta)$?

Generalize single linkage clustering

Definition (representable functors)

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Clustering in $\mathcal{M}^{inj}$ (and $\mathcal{M}^{gen}$)

Theorem (Excisive $=$ Representable)

A clustering functor is excisive if and only if it is representable.

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$$\mathfrak{T}^\Omega : \mathcal{M} \to \mathcal{M}$$

.

Excisive clustering functors in $\mathcal{M}^{inj}$

Our factorization theorem suggests how to change metrics to account for **density**– ameliorate SL's **chaining effect**.

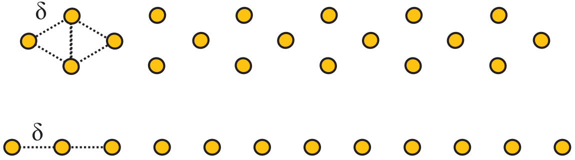

Figure : $\mathfrak{C}^{\Omega}$, with $\Omega = \{\Delta_n(\delta)\}$ for increasing n, requires more and more density.

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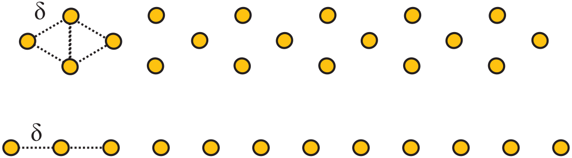

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Related to **DBSCAN** (network clustering, and database mining)!

More generality in $\mathcal{M}^{inj}$

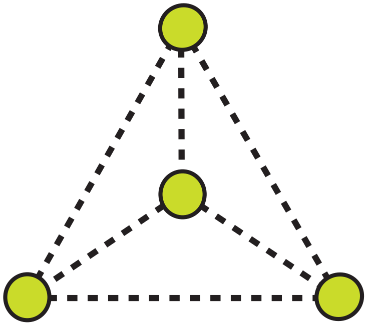


Figure : A metric space that encodes a notion of "density" different from that provided by $\Delta_3(\delta)$.

Same thing for HC methods

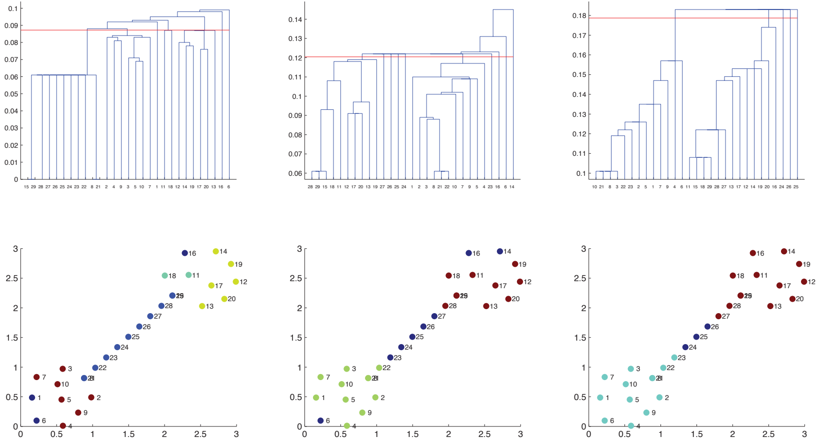
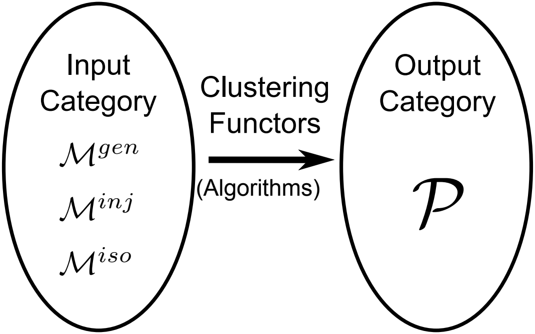


Figure : Dendrograms arising from $\mathfrak{R}^{\Delta_m}$ applied to a randomly generated points in $\mathbb{R}^2$. Top: from left to right we show dendrograms corresponding to $\mathbf{m} = \mathbf{2}, \mathbf{3}$ and $\mathbf{4}$. Bottom: partitioning induced on data by each dendrogram using parameters corresponding to red lines shown over dendrograms.

Roadmap for classification

- Motivation
- Categories
- Framework
  - Input Categories
  - Output Categories
- Functors
- Results
  - $\mathcal{M}^{iso}$ (small)
  - $\mathcal{M}^{gen}$ (large)
  - $\mathcal{M}^{inj}$ (medium)
- **Discussion**



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- In context of HC: metric structures on $\mathcal{M}$ lead to **stability** and **convergence** (Gromov-Hausdorff distances).
- Paper in FoCM, 2013. Also JMLR, 2010.
- Ongoing work on extending to **networks**. Joint with Carlsson, Ribeiro, Segarra. Some unexpected results.

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Any questions?