A combinatorial approach to assess the separability of clusters

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Given a set of entities, to what extent a particular subset X is separated from the other entities?

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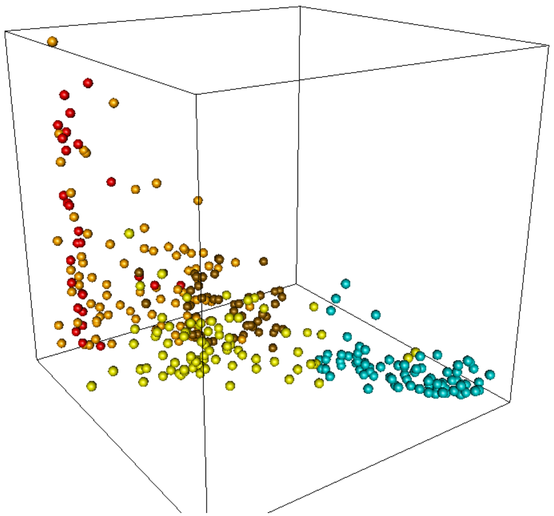
Common issue that arises in different areas

Ecology



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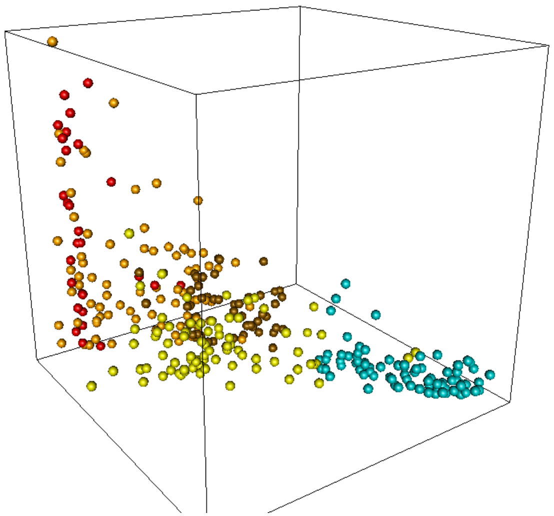
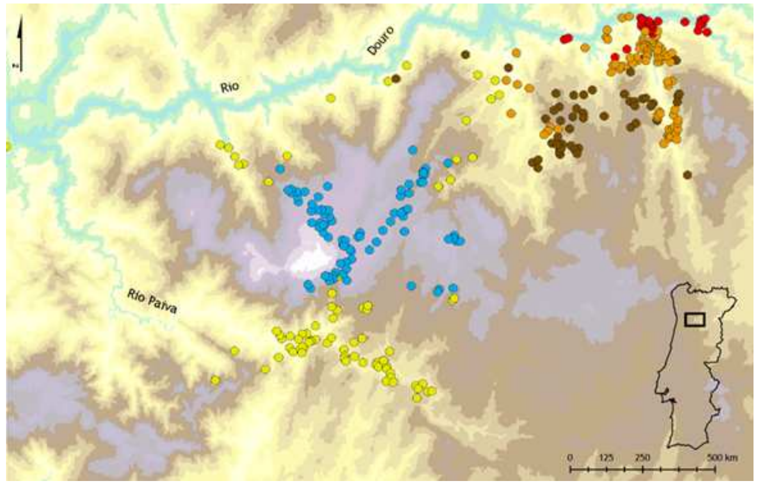
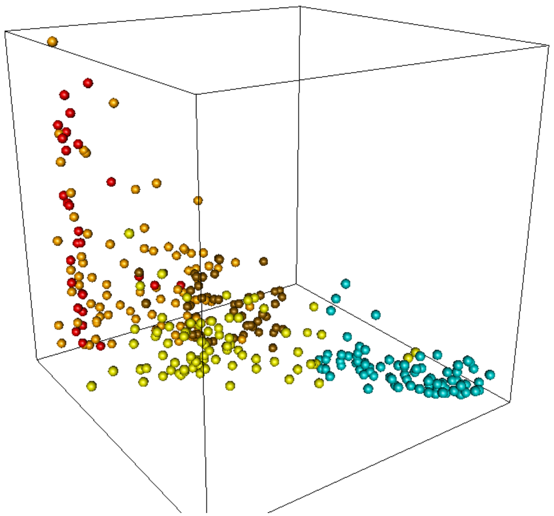
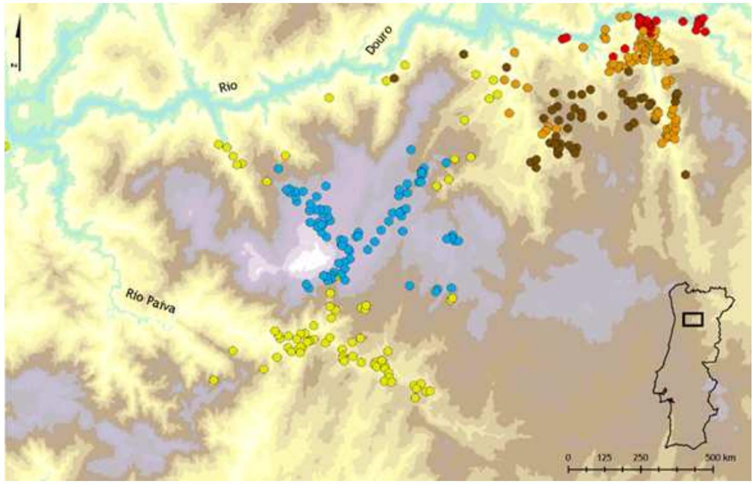




Ecology

- ▷ Introduction
- Interiority
- Separation
- Auto-interiority





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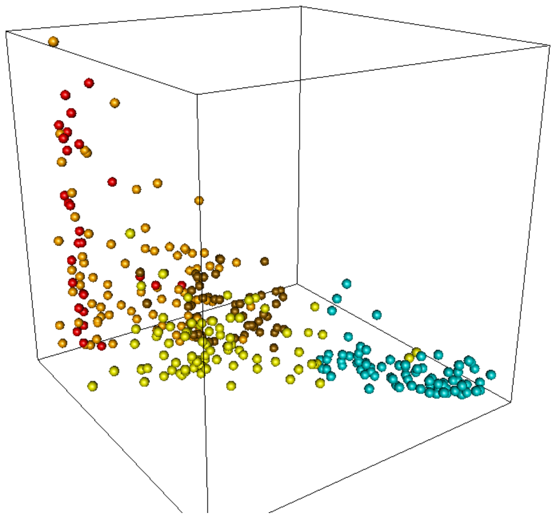

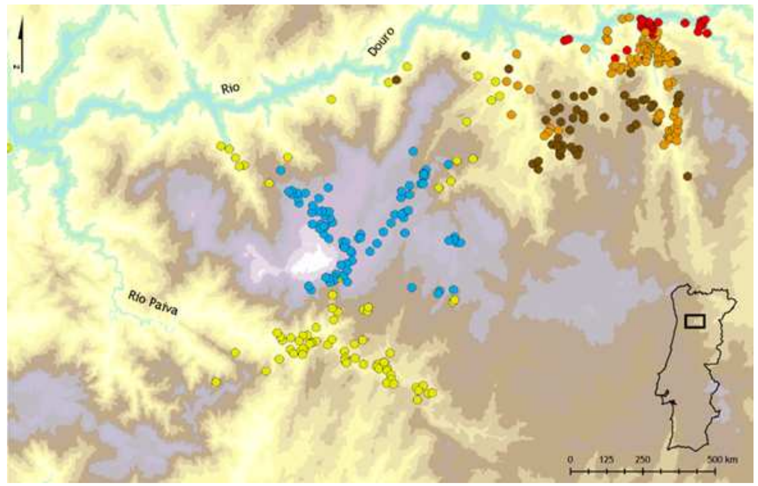

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Well separated forest types give confidence for predictive modeling, such as mapping the communities distributions

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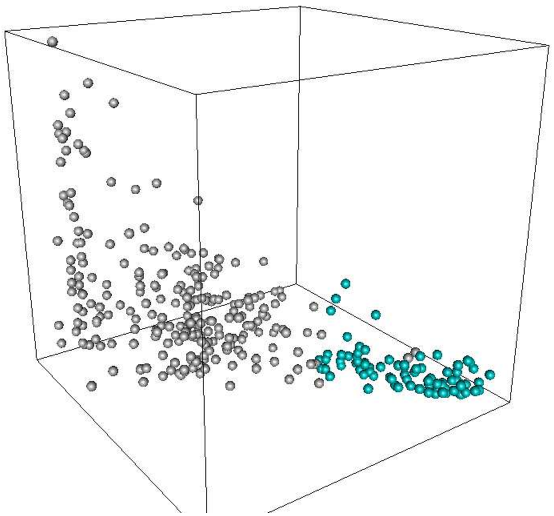

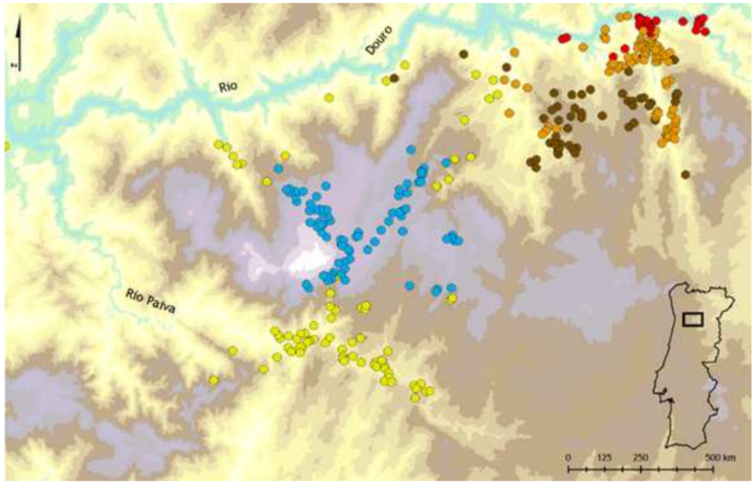

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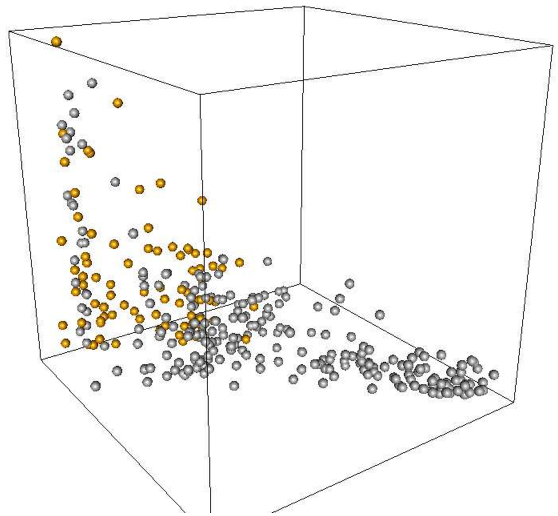

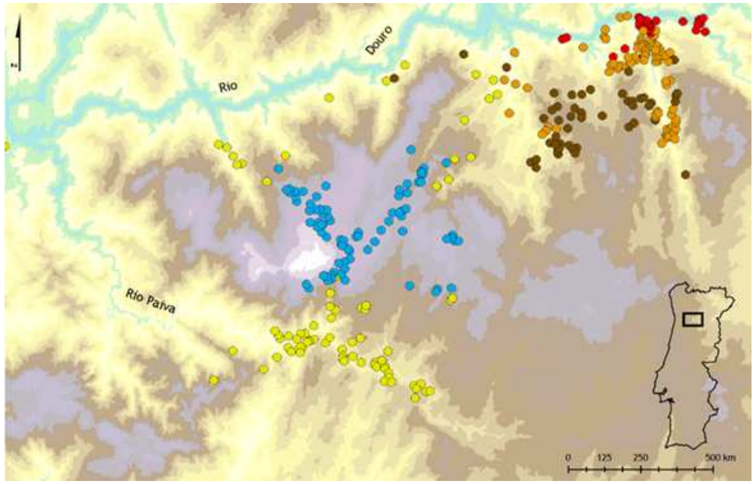

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QSAR - Quantitative Structure Activity Relationship

set of compounds with similar biological activity in a descriptor space of the chemical structure

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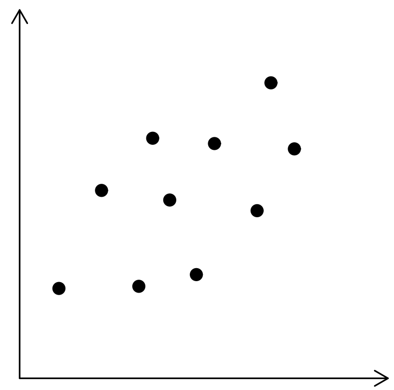

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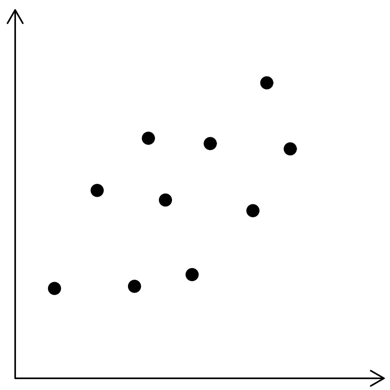

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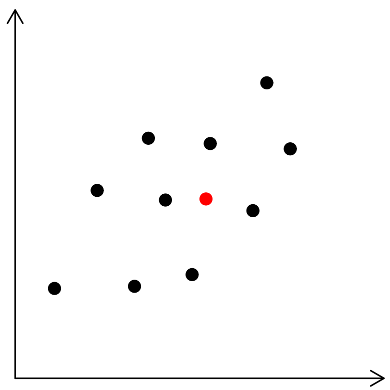

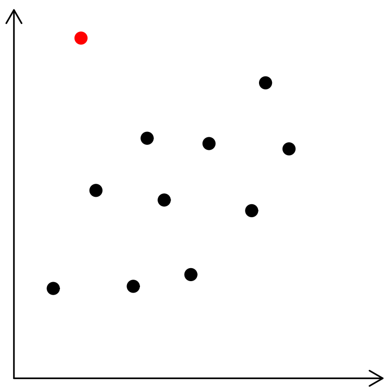

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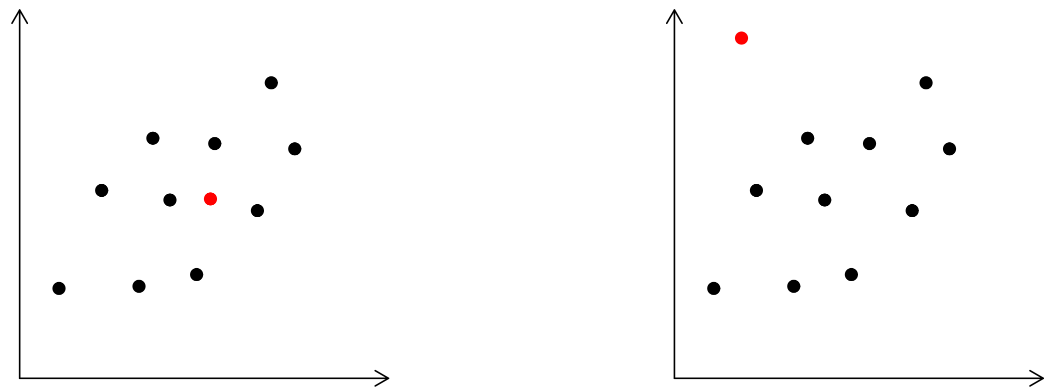

it cannot be expected to give reliable predictions to compounds *separated* from the training set to what extent a set of entities X is separated from other entities?

to what extent a set of entities X is separated from other entities?

to what extent a set of entities X is separated from <u>an</u>other entity?

to what extend $\{\bullet\}$ is separated from $\color{red}\bullet$?

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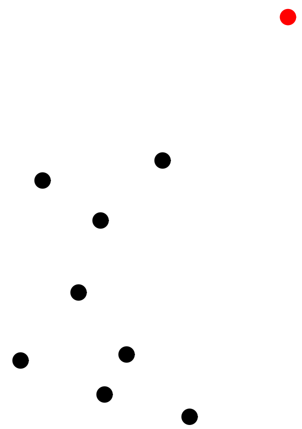

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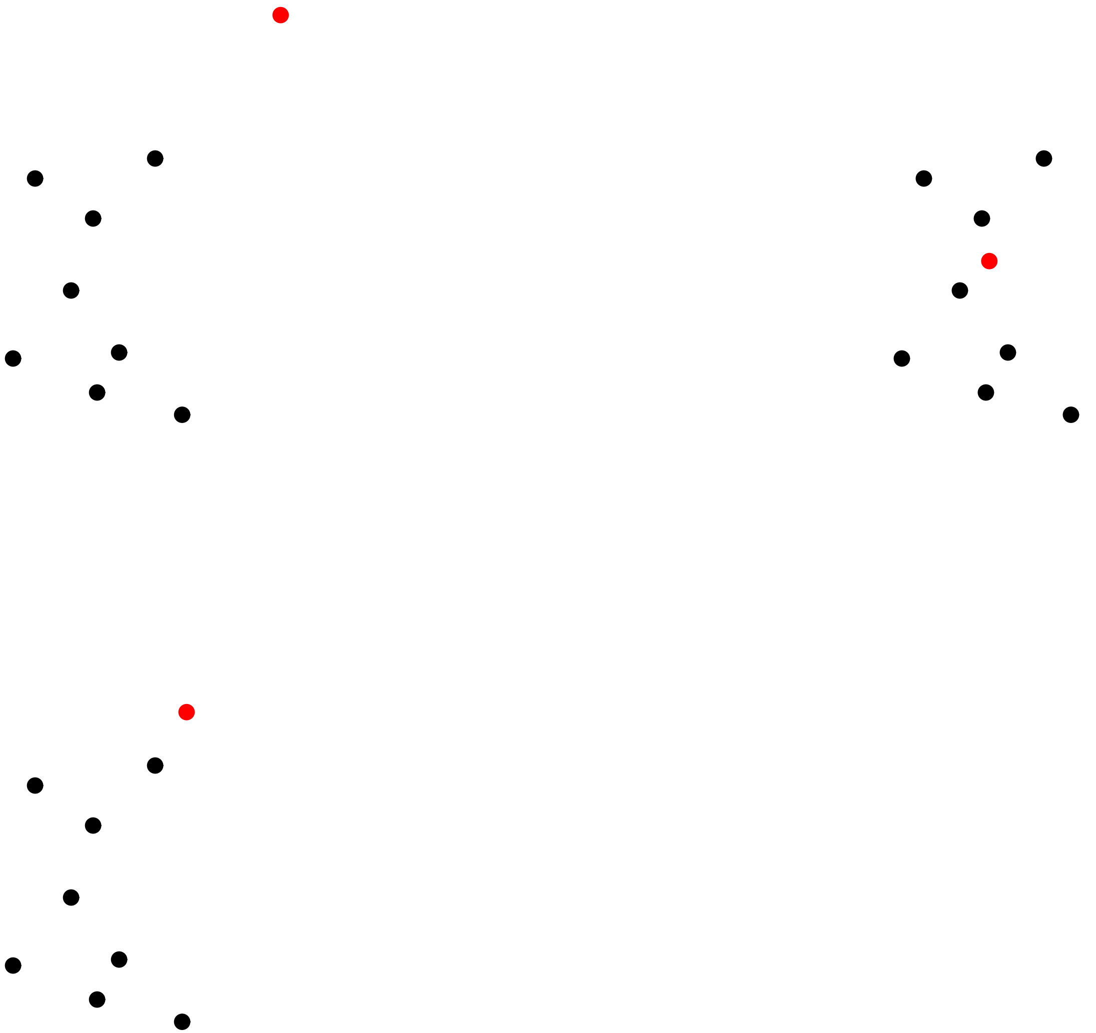

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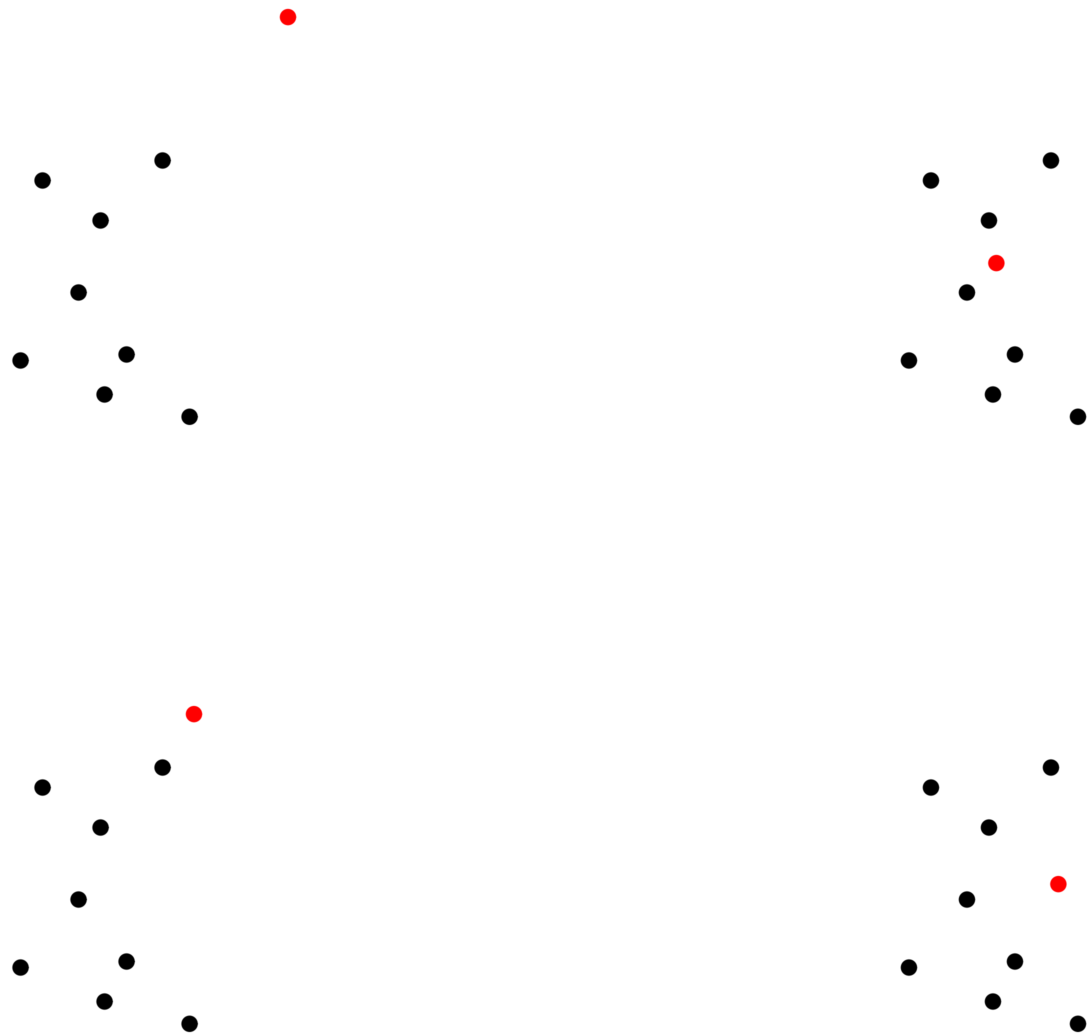

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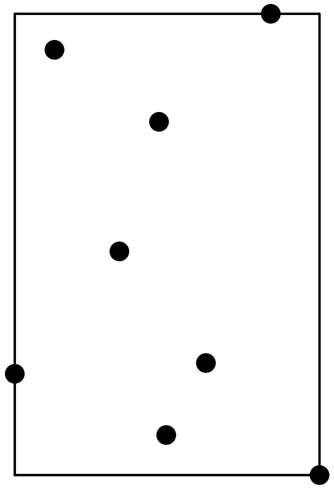

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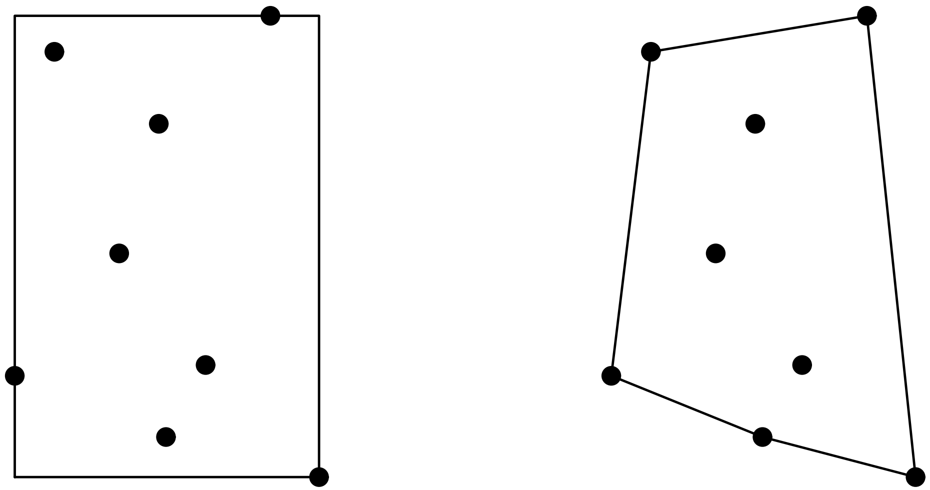

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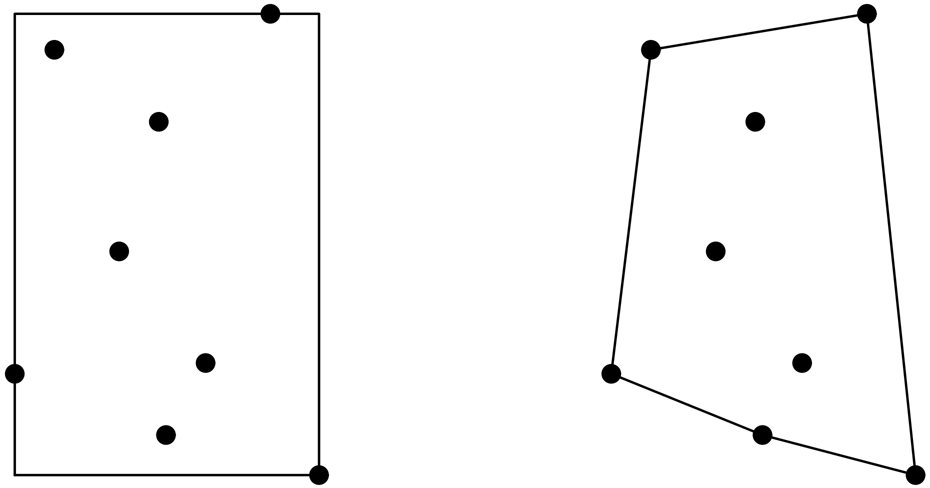

doesn't discriminate separability

to formalize separability needs fixing some aggregation criterion

i.e., a rule that identifies, for a set of entities E and $1 \leq k \leq |E|$, the k-partitions of E which are *adequately* aggregated

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entity $\bar{x}$ is k-*interior* with respect to X if for every k-partition $\mathcal{P}_k$ of X, $\mathcal{P}_k \cup \{\{\bar{x}\}\}$ is not an adequate $(k+1)$-partition of $X \cup \{\bar{x}\}$

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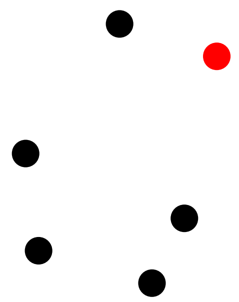

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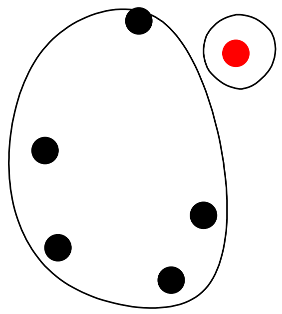

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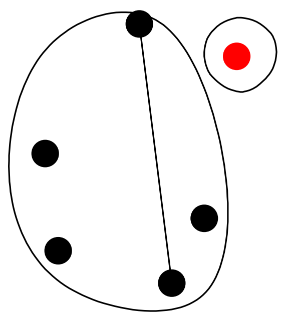

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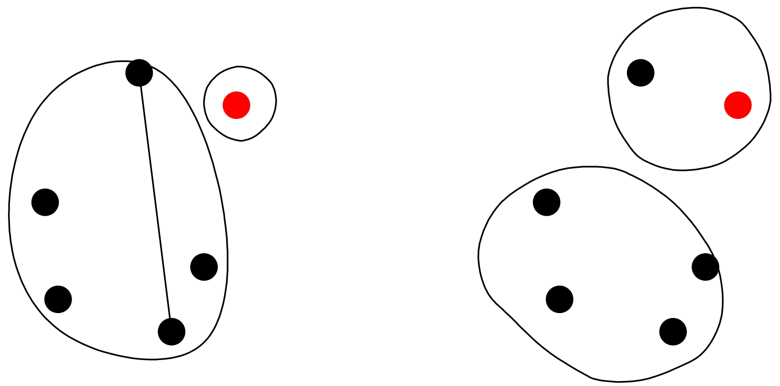

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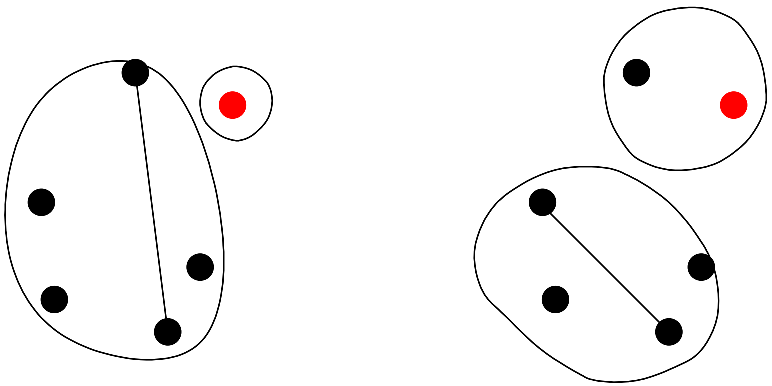

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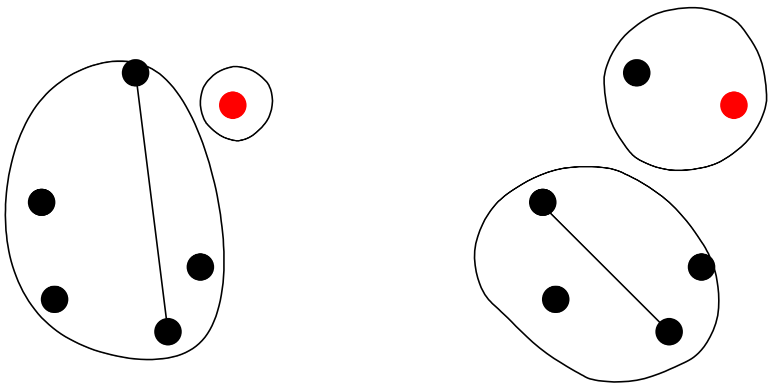

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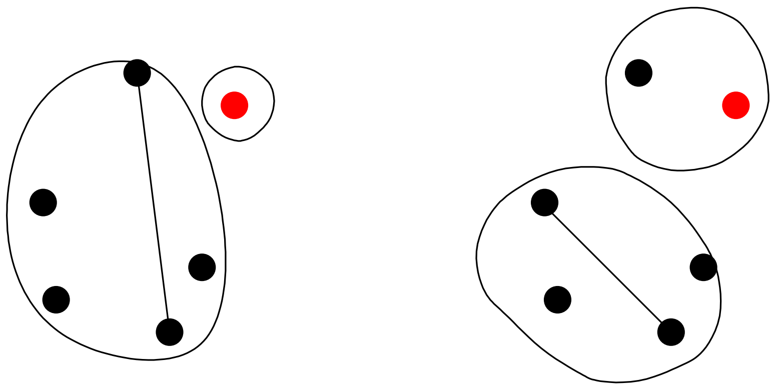

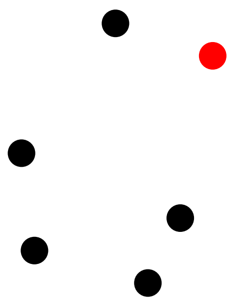

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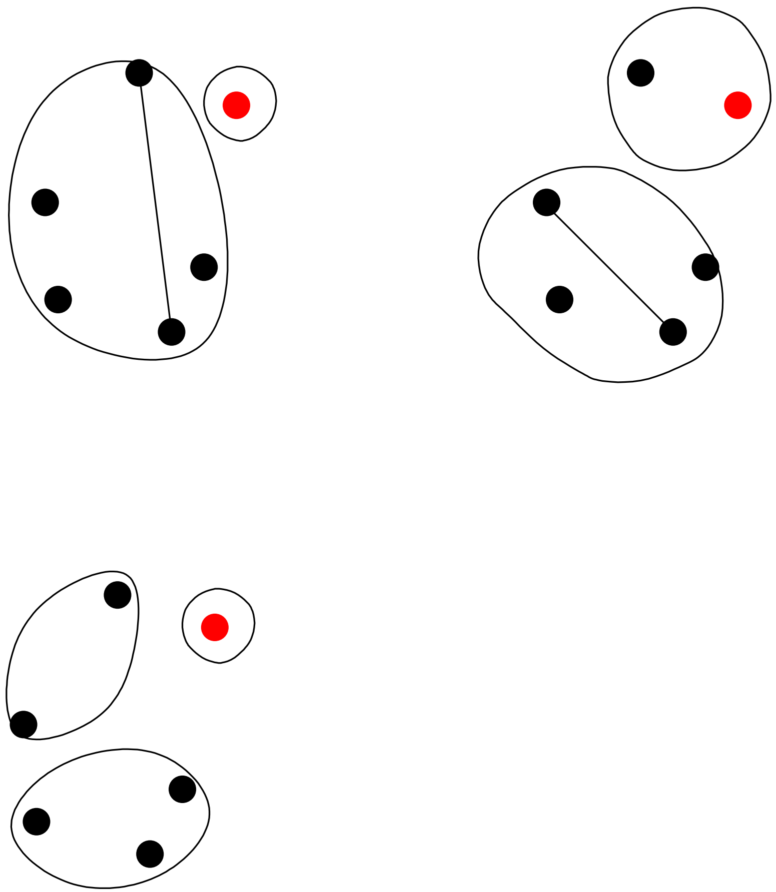

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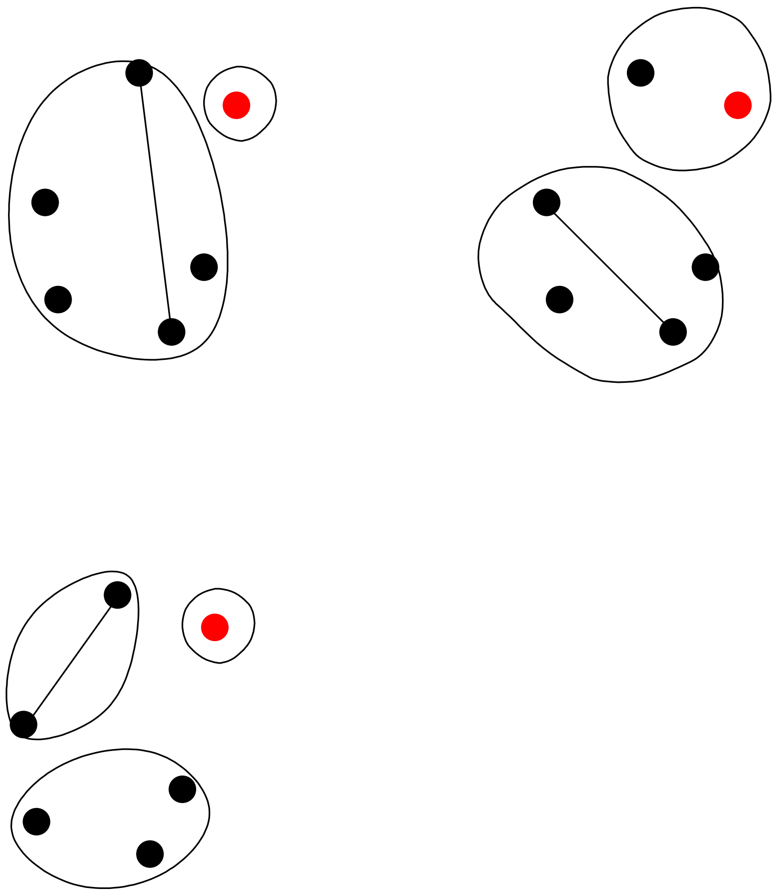

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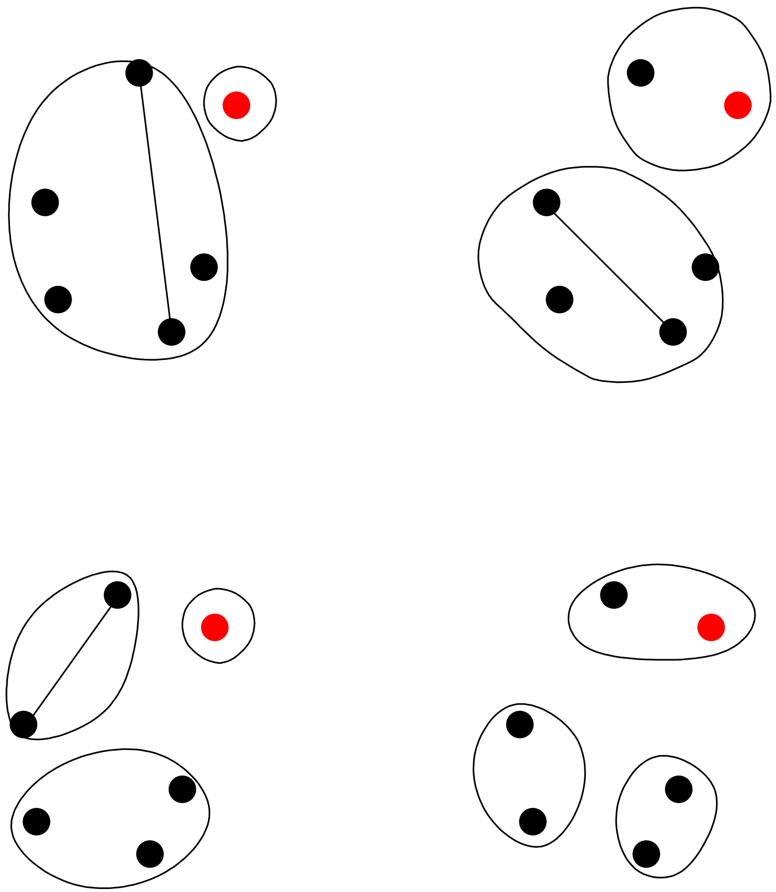

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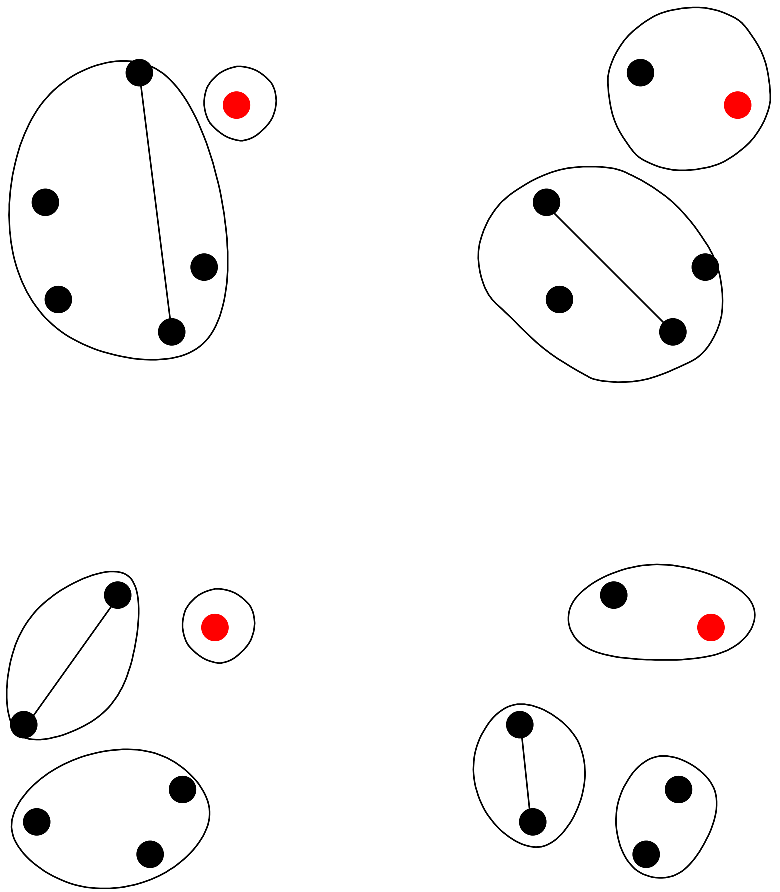

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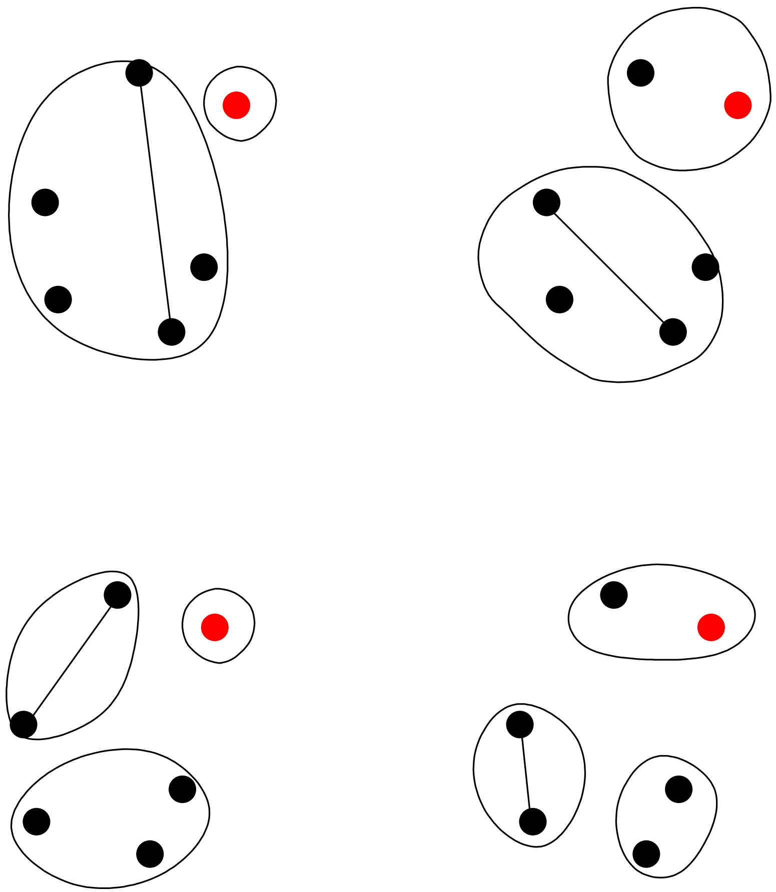

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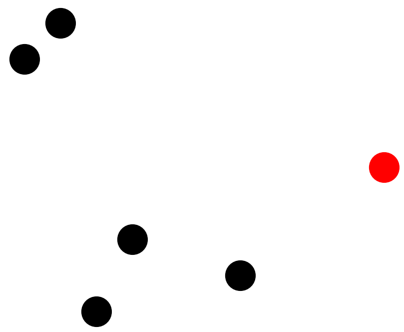

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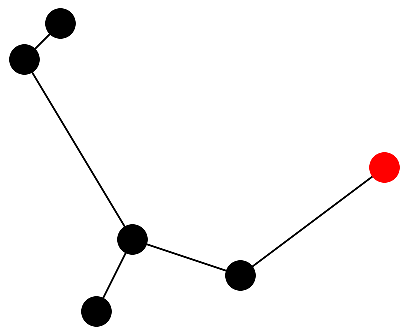

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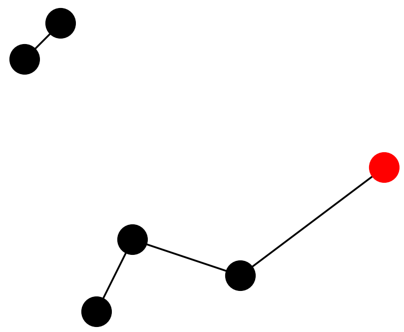

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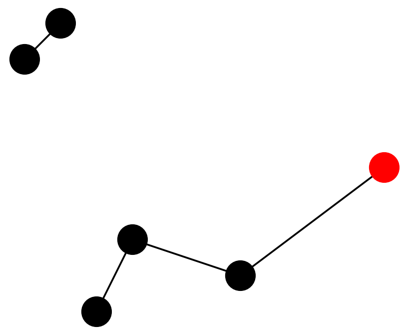

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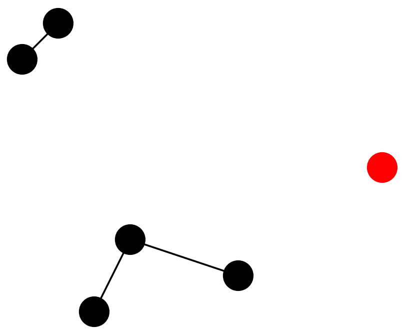

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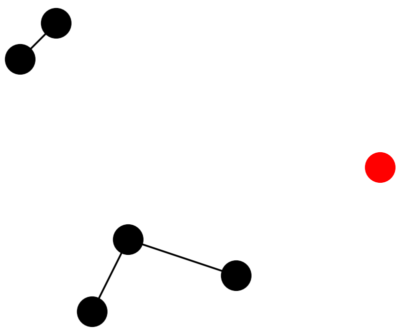

● is 1-interior but not 2-interior

interiority degree

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  - single linkage iff $\min_{x \in X} dis(\bar{x}, x) \geq \max_{\{X', X''\}} \min_{x' \in X', x'' \in X''} dis(x', x'')$, where $\{X', X''\}$ is a non trivial bipartition of X
- $d_{\bar{x}} = |X| - 1$ diameter and single linkage iff

the *interiority* degree of $\bar{x}$ is

$d_{\bar{x}} =$ the largest k such that $\bar{x}$ is k-interior

$d_{\bar{x}} = 0$ if $\bar{x}$ is not interior

- $d_{\bar{x}} = 0$
  - diameter iff $\min_{x \in X} dis(\bar{x}, x) \geq \max_{x, x' \in X} dis(x, x')$
  - single linkage iff $\min_{x \in X} dis(\bar{x}, x) \geq \max_{\{X', X''\}} \min_{x' \in X', x'' \in X''} dis(x', x'')$, where $\{X', X''\}$ is a non trivial bipartition of X
- $d_{\bar{x}} = |X| - 1$ diameter and single linkage iff

  $\min_{x \in X} dis(\bar{x}, x) < \min_{x, x' \in X} dis(x, x')$

interiority degree function

$d : \mathcal{E} \setminus X \to \{0, 1, \ldots, |X| - 1\}$ defines a partition of the entity space $\mathcal{E}$

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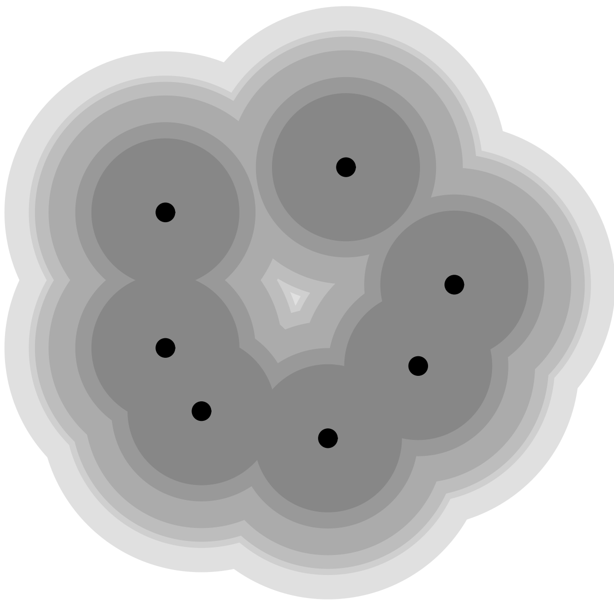

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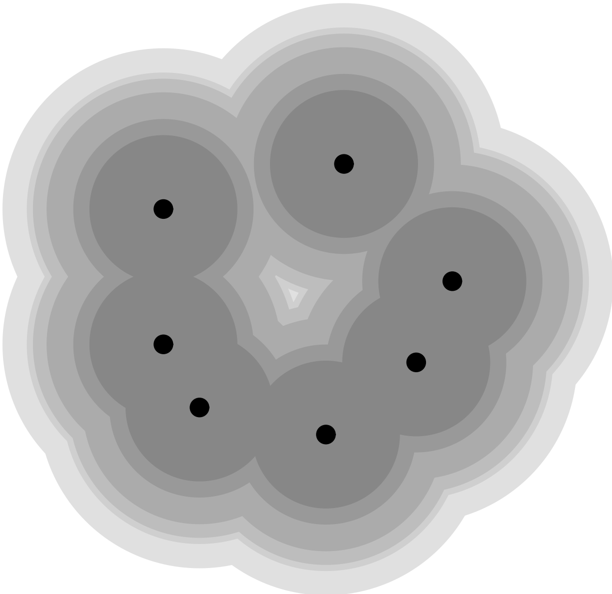
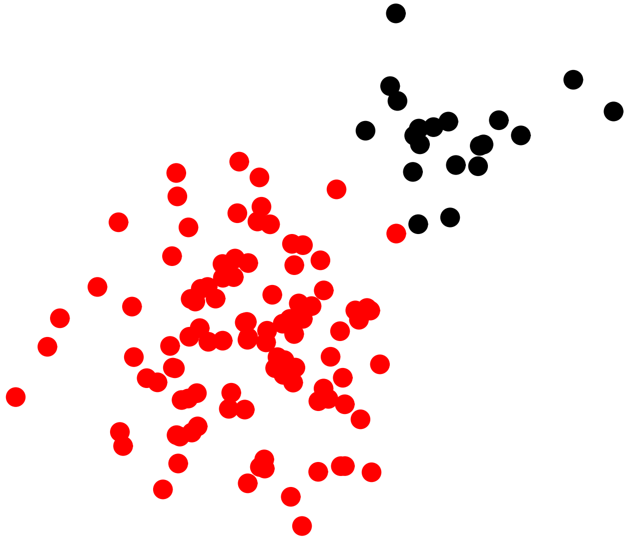
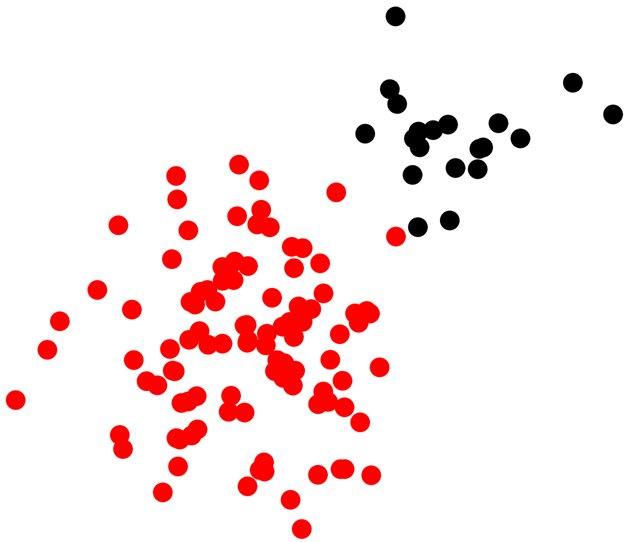


territory of discriminated levels of interiority

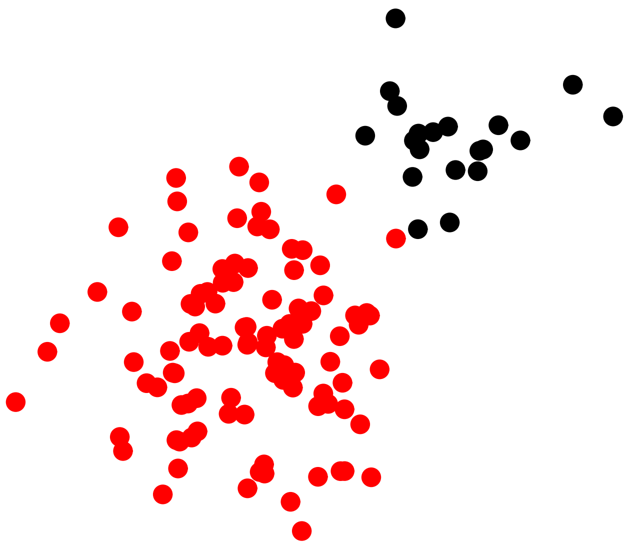
separability index





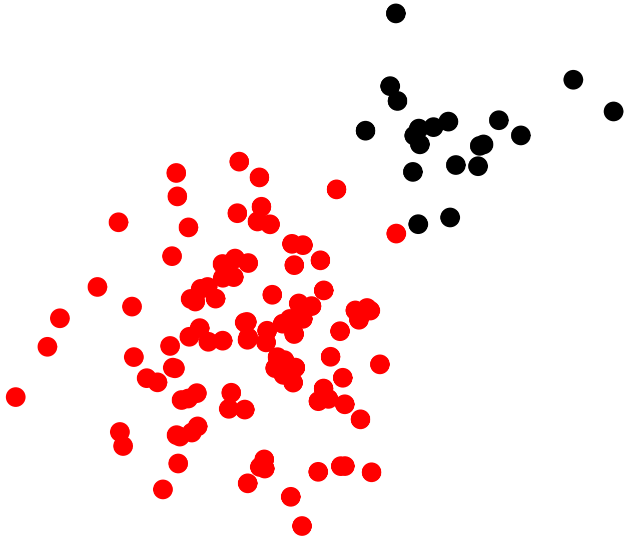
$D_{\bar{X}} = \{d(\bar{x}) : \bar{x} \in \bar{X} = \{\bullet\}\}$ *interiority* of $\bar{X}$

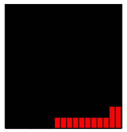
separability index



$D_{\bar{X}} = \{d(\bar{x}) : \bar{x} \in \bar{X} = \{\bullet\}\}$ *interiority* of $\bar{X}$

$D_{\bar{X}} \rightsquigarrow$ discriminate sep. index $DSI \in [0, 1]$





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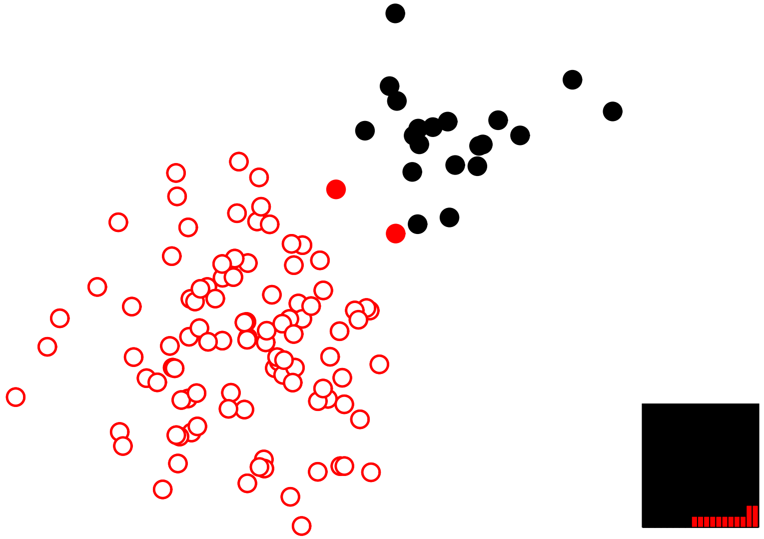

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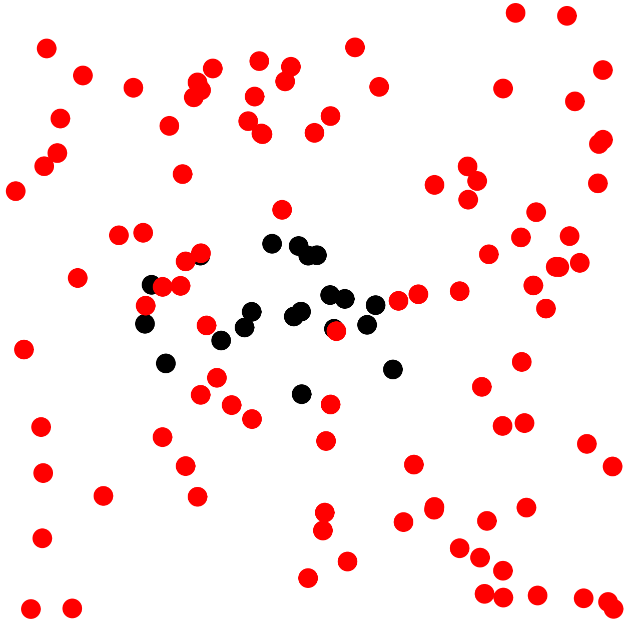

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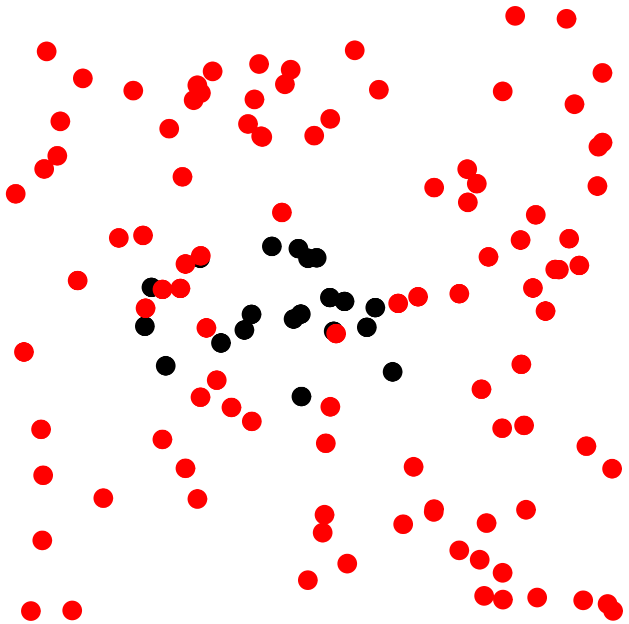

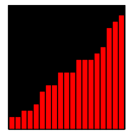

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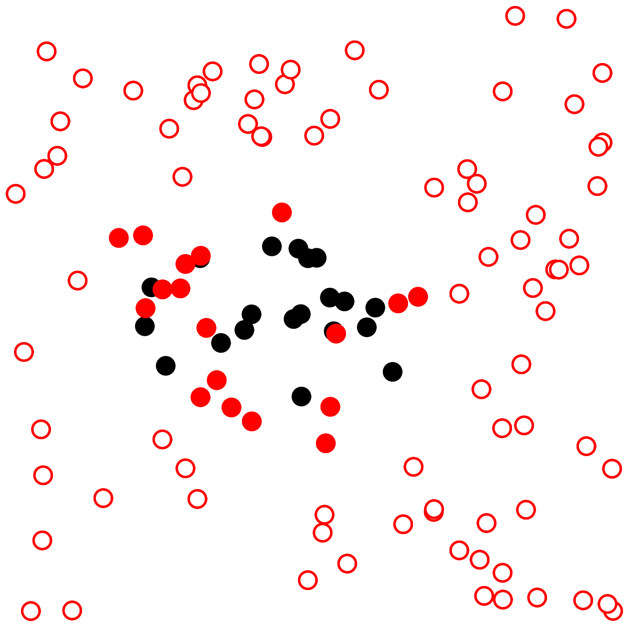

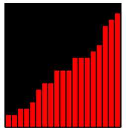

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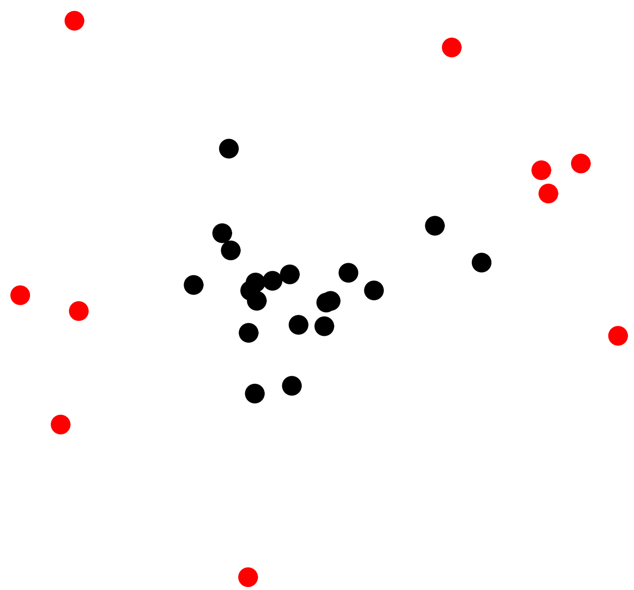

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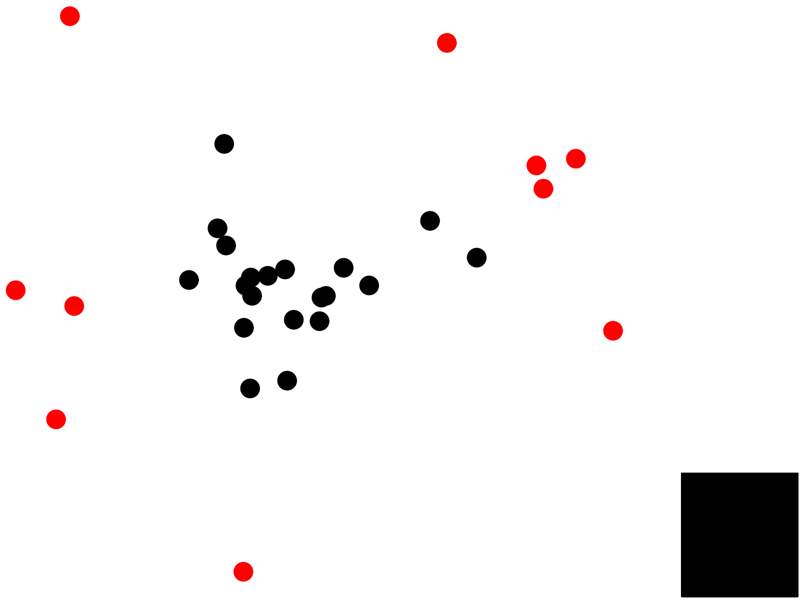

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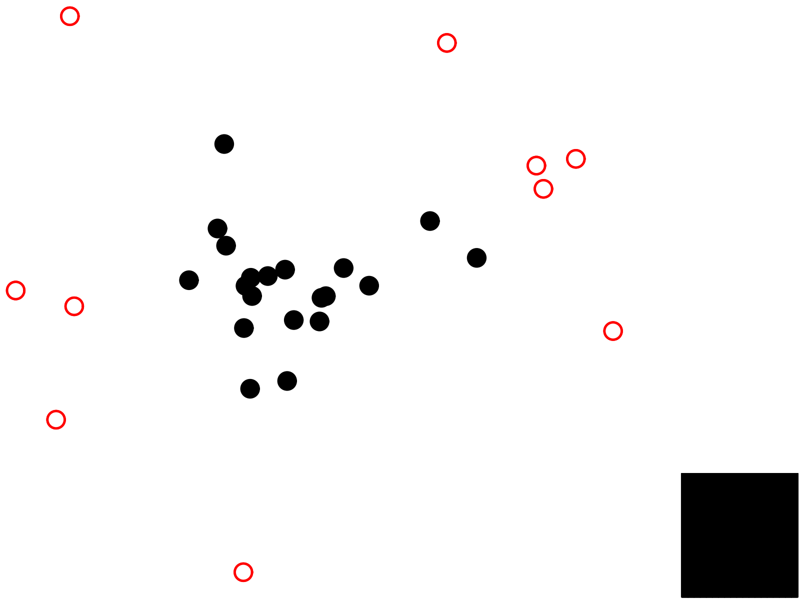

convexity criterion

a k-partition is adequate if it includes $k-1$ singletons that are not in the interior of the convex hull of the remaining points

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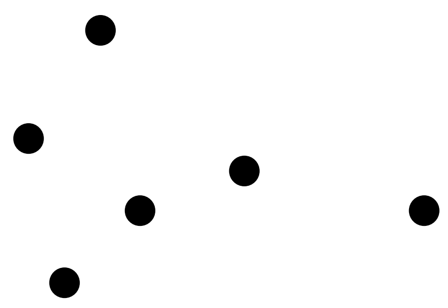

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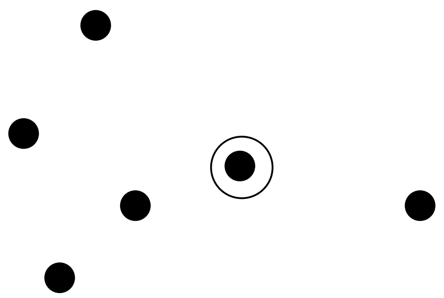

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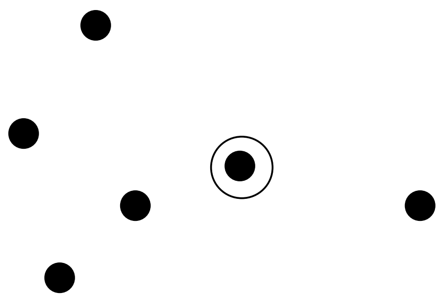

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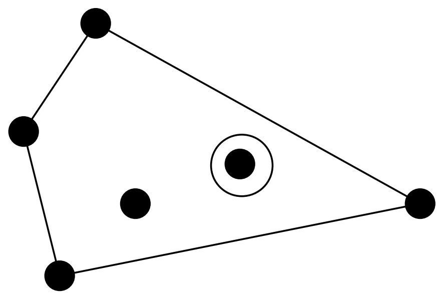

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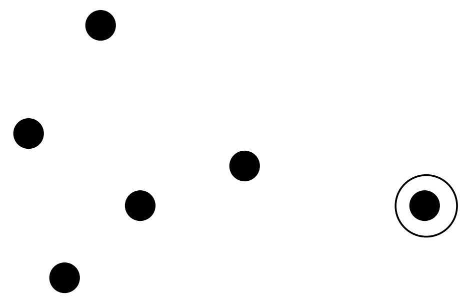

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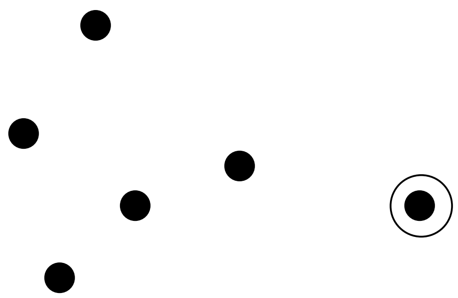

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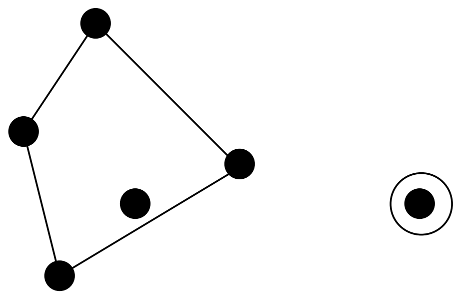

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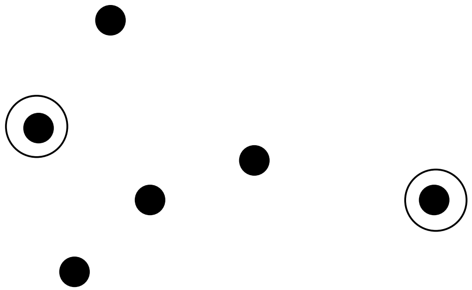

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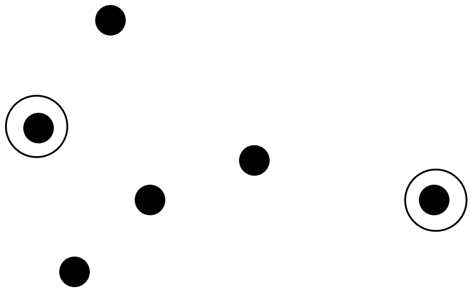

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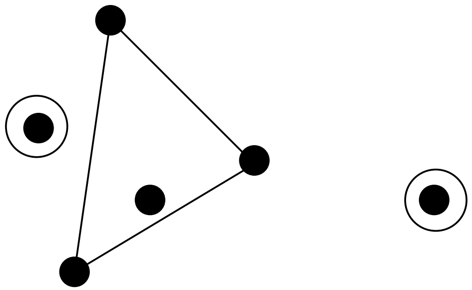

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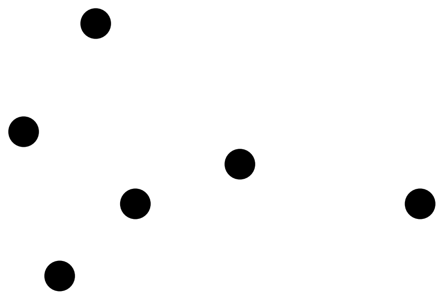

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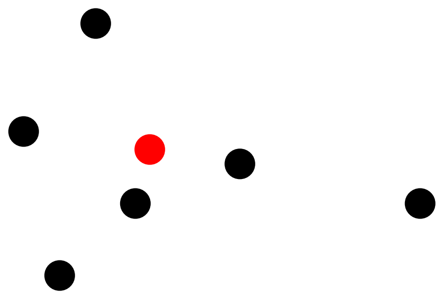

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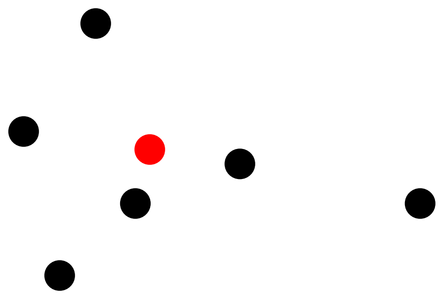

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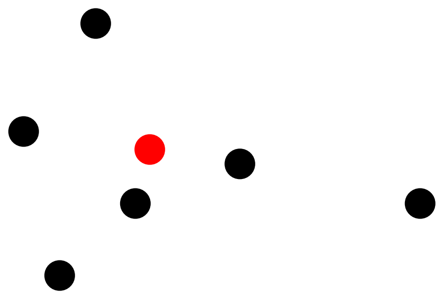

● is 1-interior, and 2-interior

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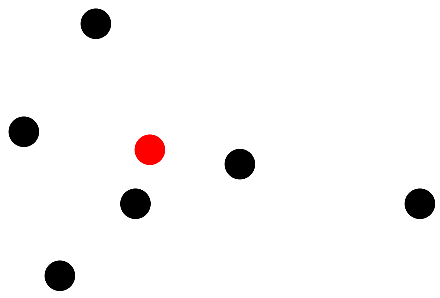

• is 1-interior, and 2-interior

d(•) is the minimum number of points to be removed from X such that • is outside conv. hull of the remaining points

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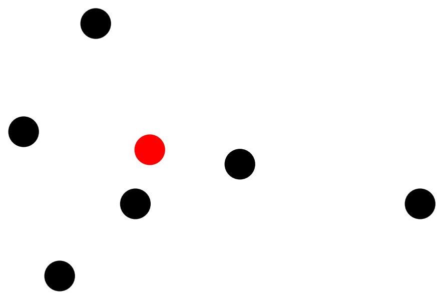
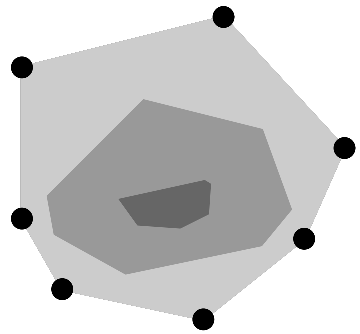


● is 1-interior, and 2-interior

d(●) is the minimum number of points to be removed from X such that ● is outside conv. hull of the remaining points

d(●) $= 2$

discriminated interiority territories



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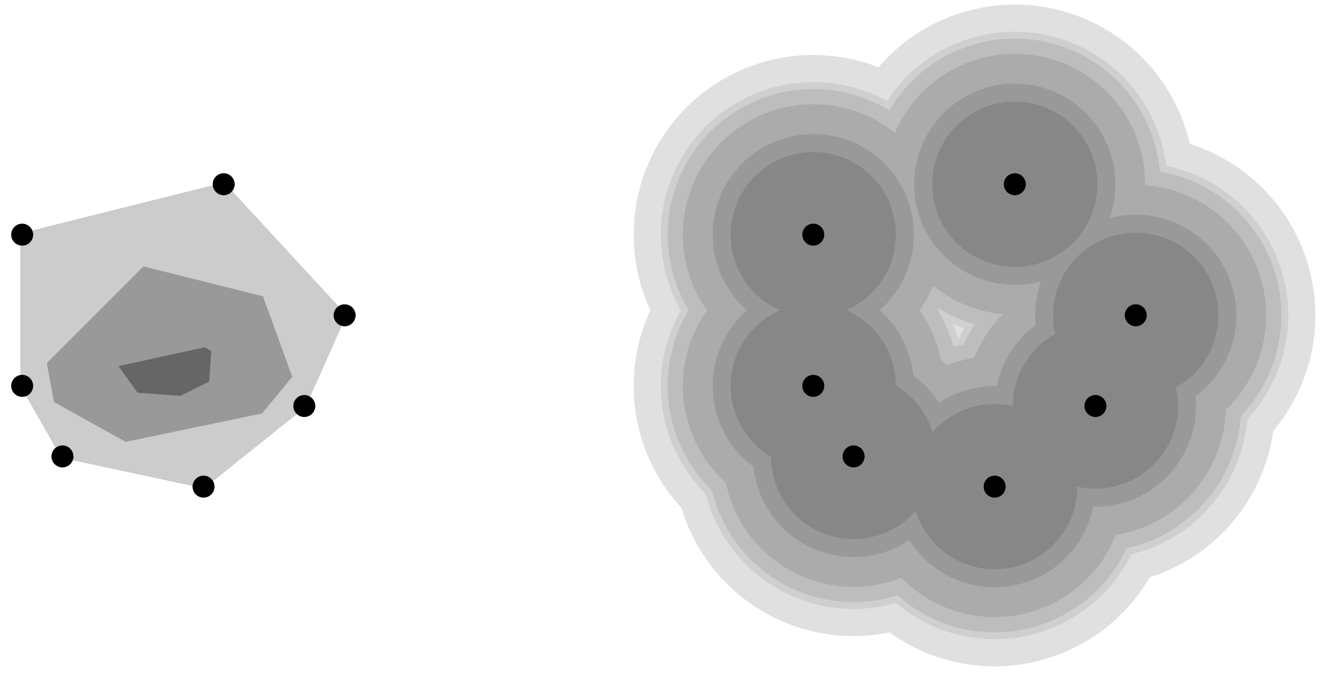

auto-interiority

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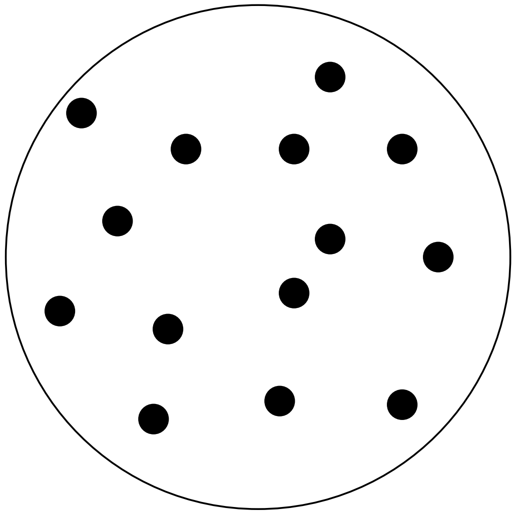
should distinguishes between configurations concentrated in the "interior" of the conv.hull, and those which occur mainly on the "margins"...

if X is uniformly distributed on an n-ball



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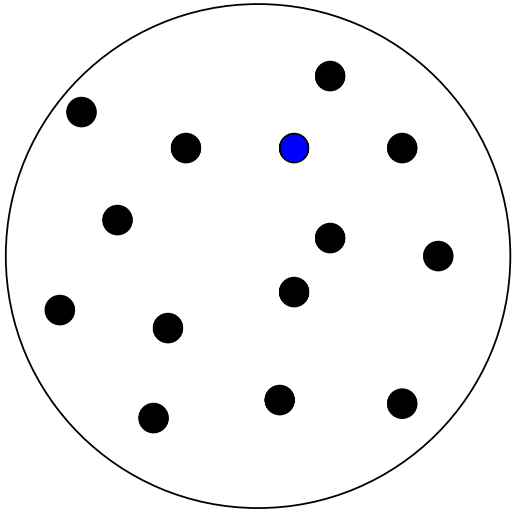
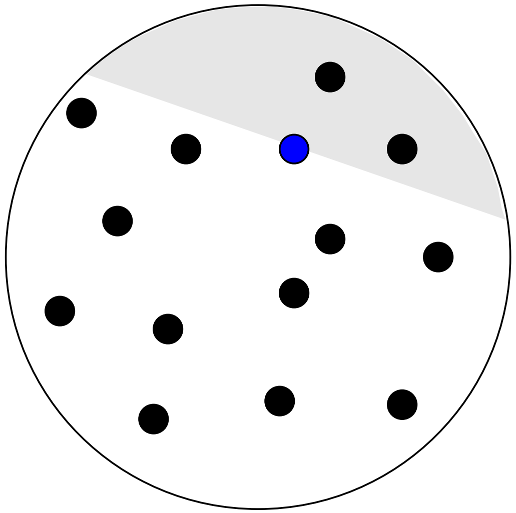


$$\frac{d(x)}{|X|} \rightsquigarrow$$

if X is uniformly distributed on an n-ball



$$\frac{d(x)}{|X|} \rightsquigarrow \frac{vol(\ \ )}{vol(B_n)} = V_r(x)$$

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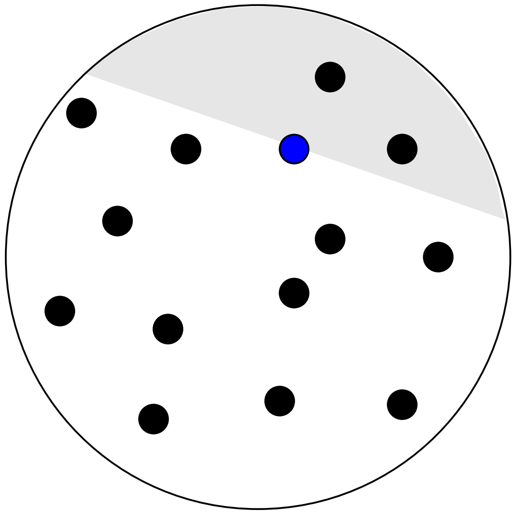

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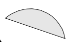

$$E[V_r(x)] = \int_{B_n} \frac{V_r(x)}{vol(B_n)}\, dx$$

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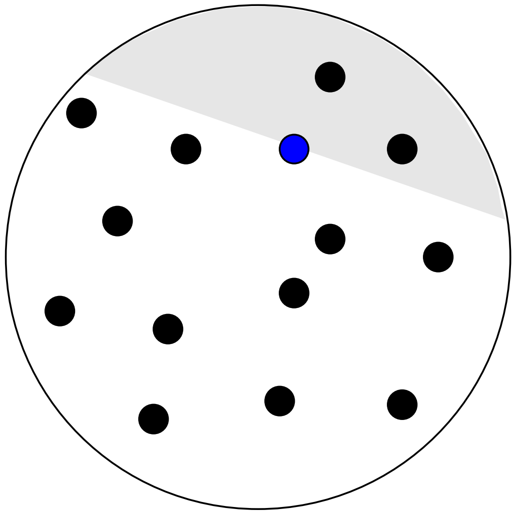

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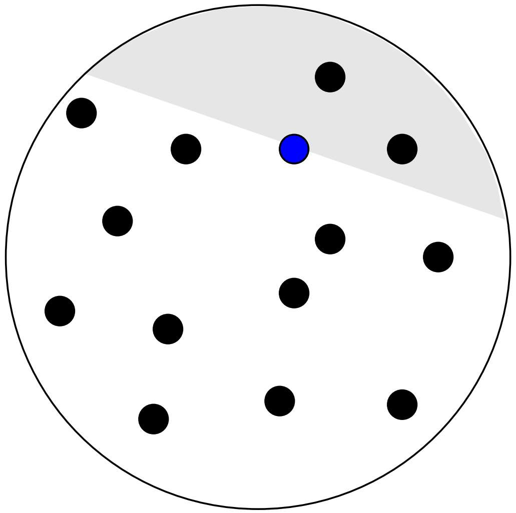

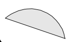

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straightforward test of the uniform distribution on a n-ball

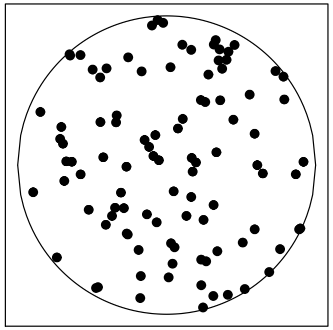
if X is uniformly distributed on an n-ball

$$E[V_r(x)] = \frac{1}{2^{n+1}}$$

if X is uniformly distributed on an n-ball

$$E[V_r(x)] = \frac{1}{2^{n+1}} \quad \Longrightarrow \quad \frac{1}{|X|}\sum_x V_r(x) \approx \frac{1}{2^{n+1}}$$

if X is uniformly distributed on an n-ball



$$\frac{1}{|X|}\sum_x V_r(x) = 0.1320314$$

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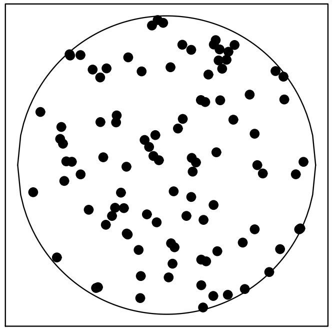

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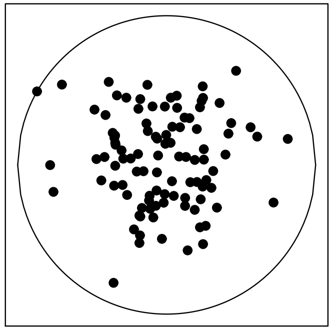

$$\frac{1}{|X|}\sum_x V_r(x) = 0.2605504$$

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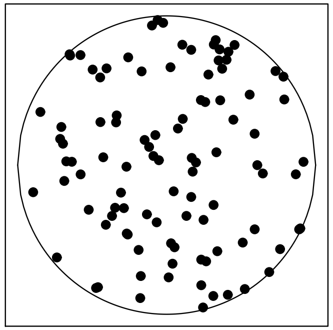
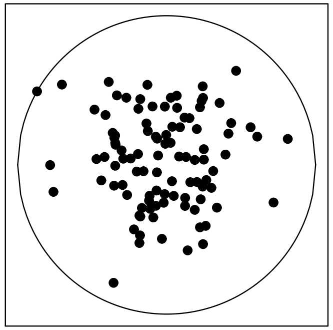


$$\frac{1}{|X|}\sum_x V_r(x) = 0.1320314$$



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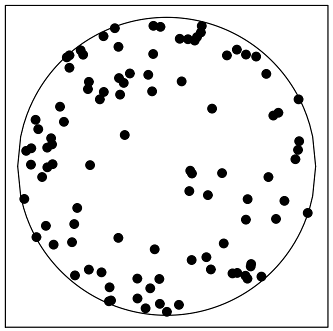

$$\frac{1}{|X|}\sum_x V_r(x) = 0.066573$$