
A combinatorial approach to assess the separability of clusters

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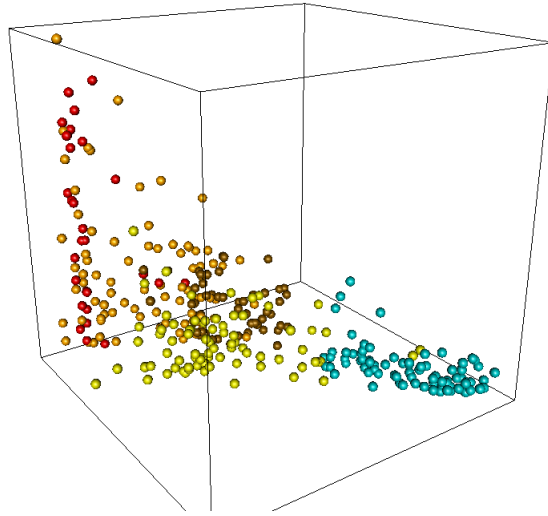
Given a set of entities, to what extent a particular subset X is separated from the other entities?

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Common issue that arises in different areas

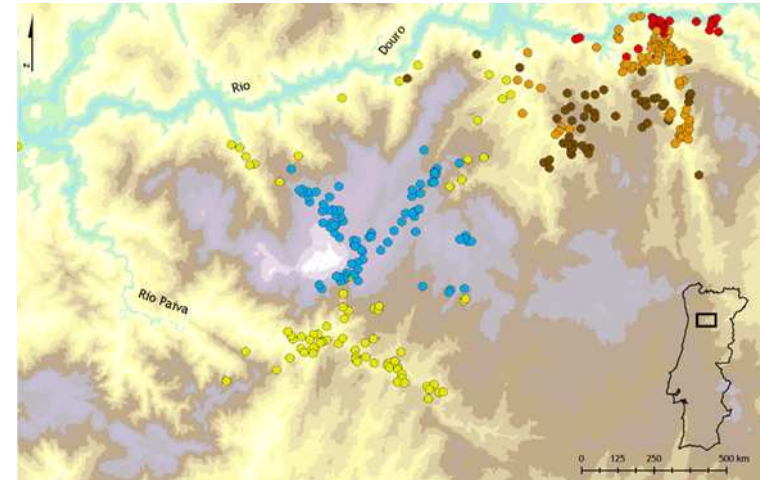
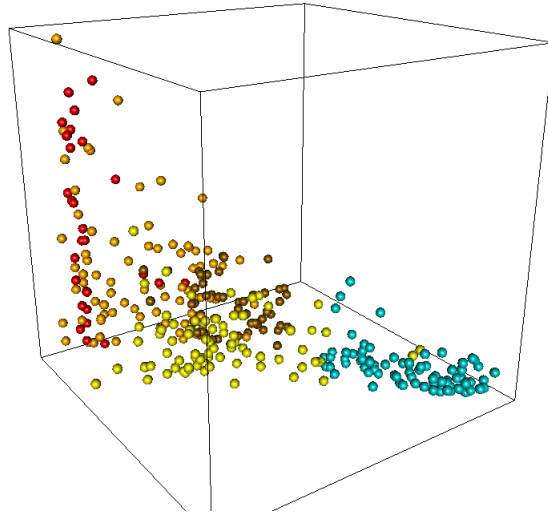
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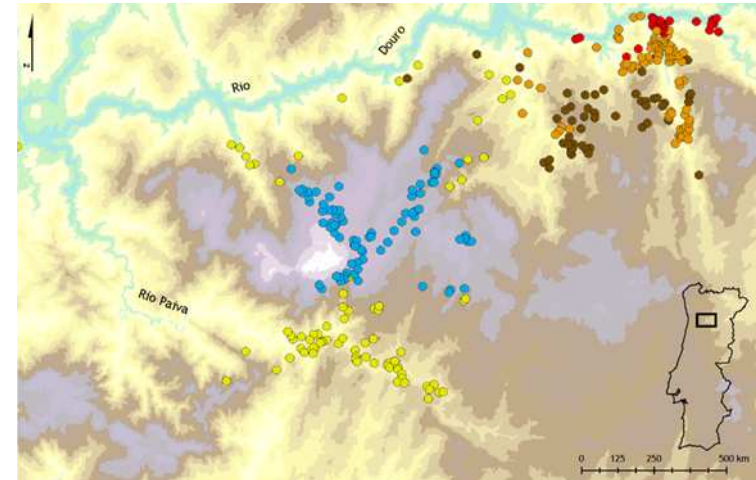
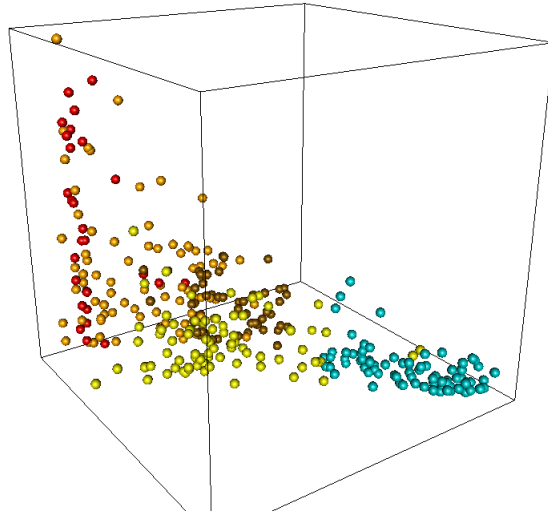
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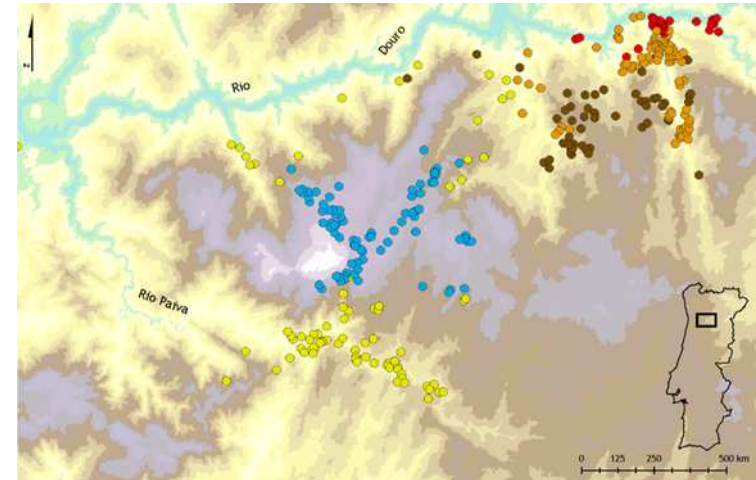
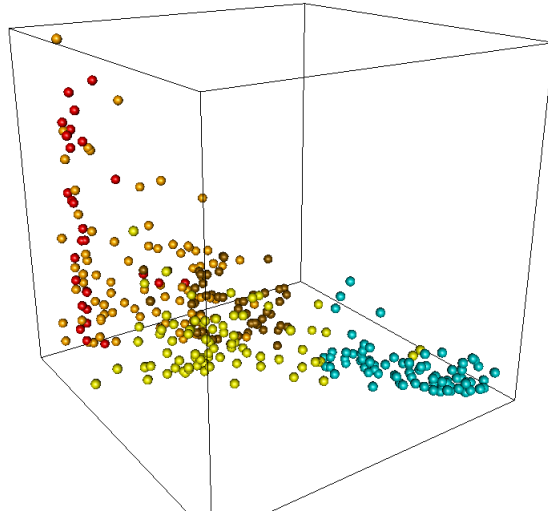


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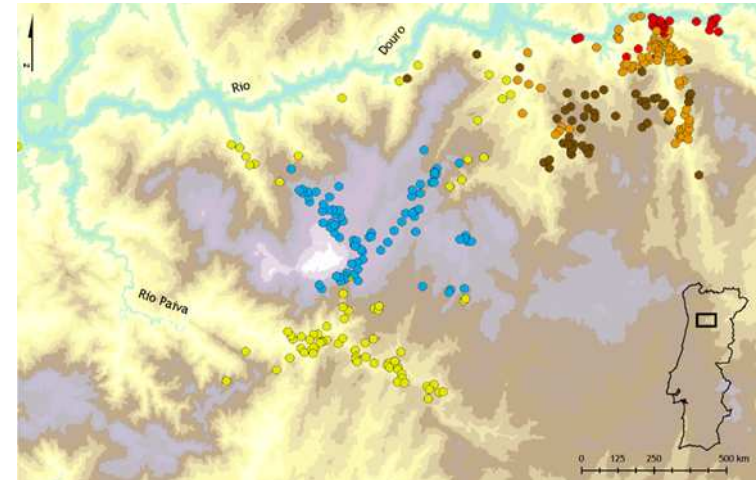
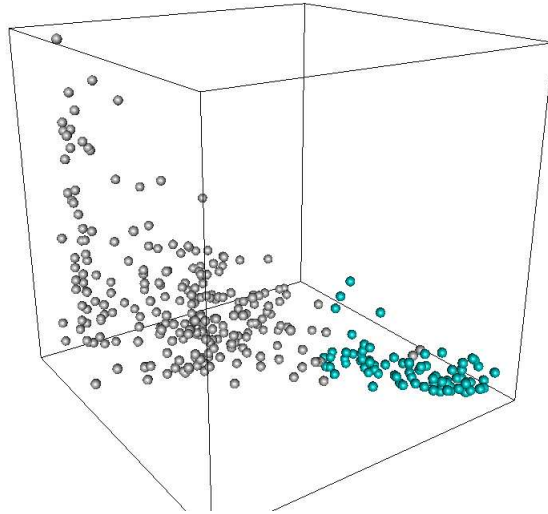


it is relevant to estimate how well the forest types are separated



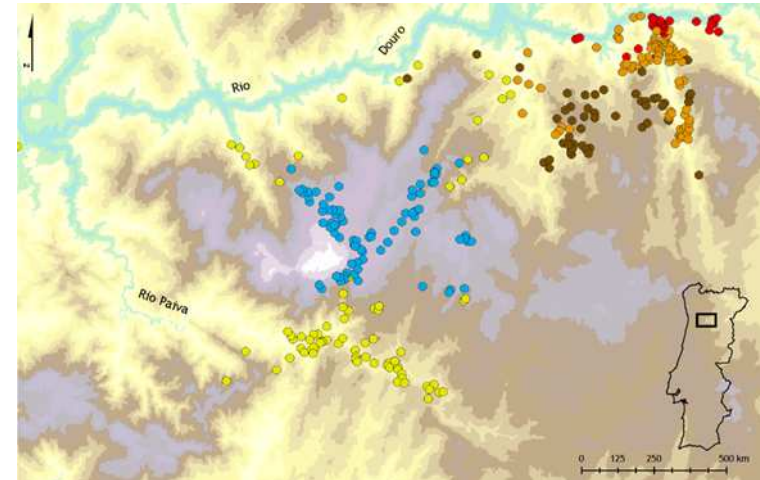
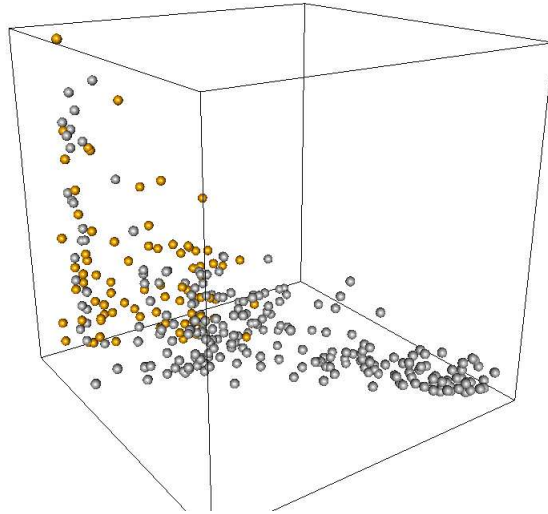
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Well separated forest types give confidence for predictive modeling, such as mapping the communities distributions



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QSAR - Quantitative Structure Activity Relationship

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QSAR - Quantitative Structure Activity Relationship

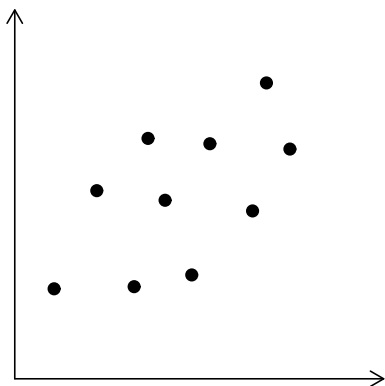
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set of compounds with similar biological activity in a descriptor space of the chemical structure

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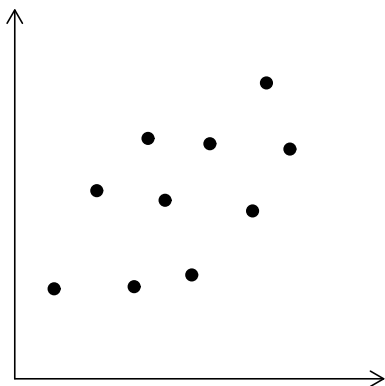


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similar molecules have similar activities

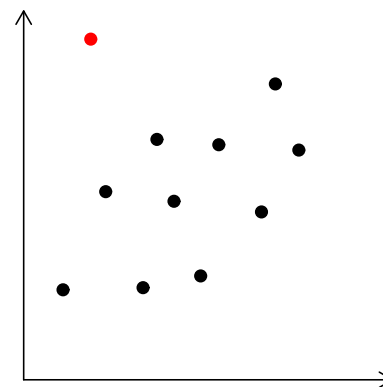
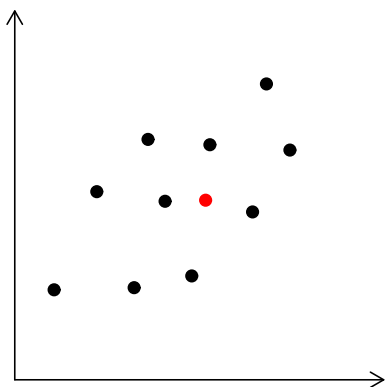


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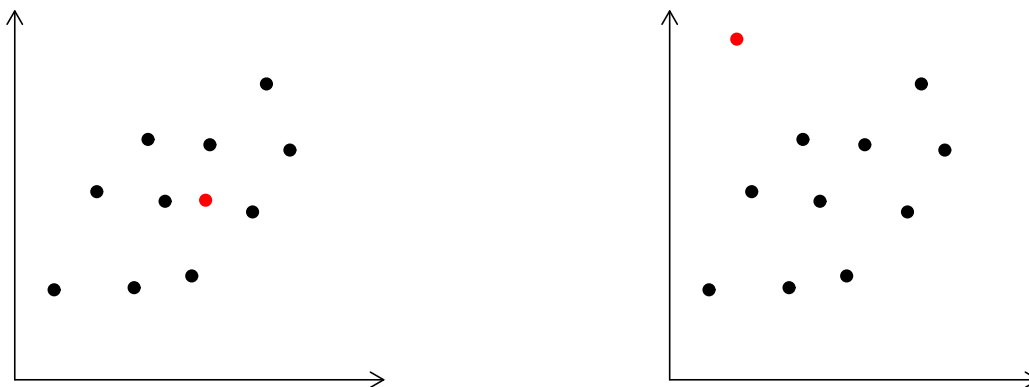


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set of compounds with similar biological activity in a descriptor space of the chemical structure

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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?

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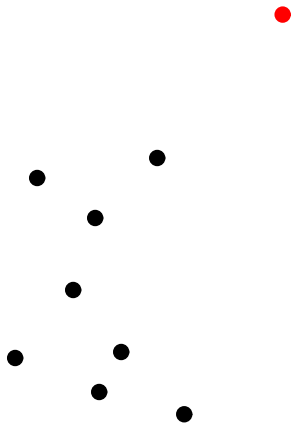
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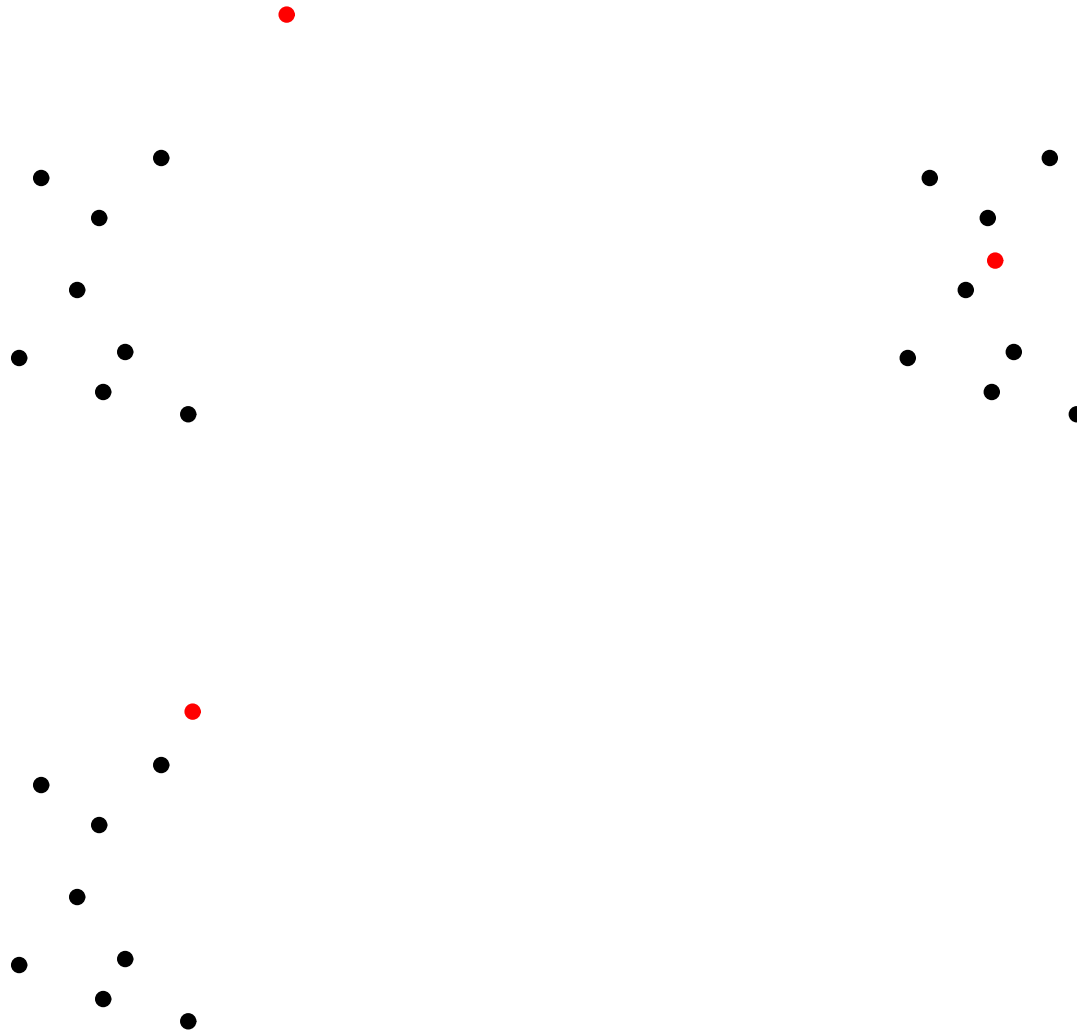
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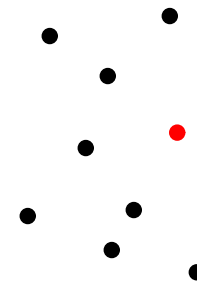
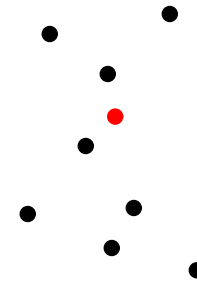
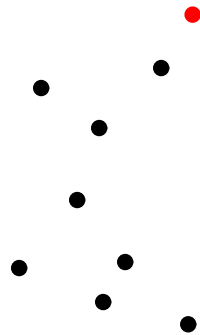
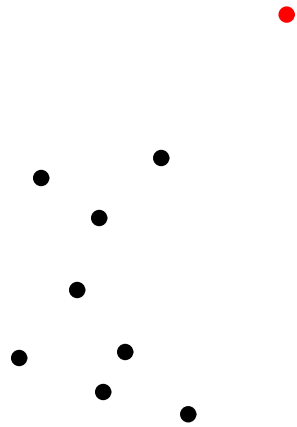
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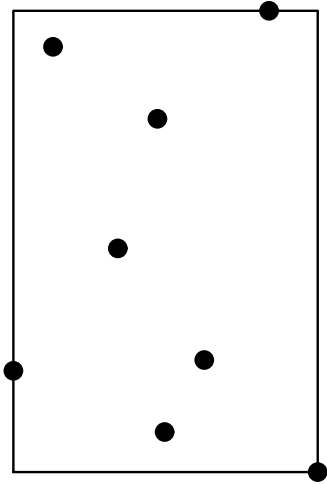


some proposals rely on a notion of *territory*

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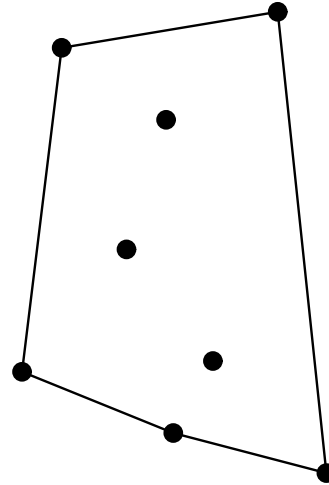
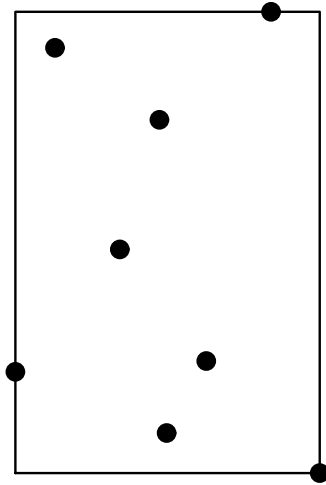
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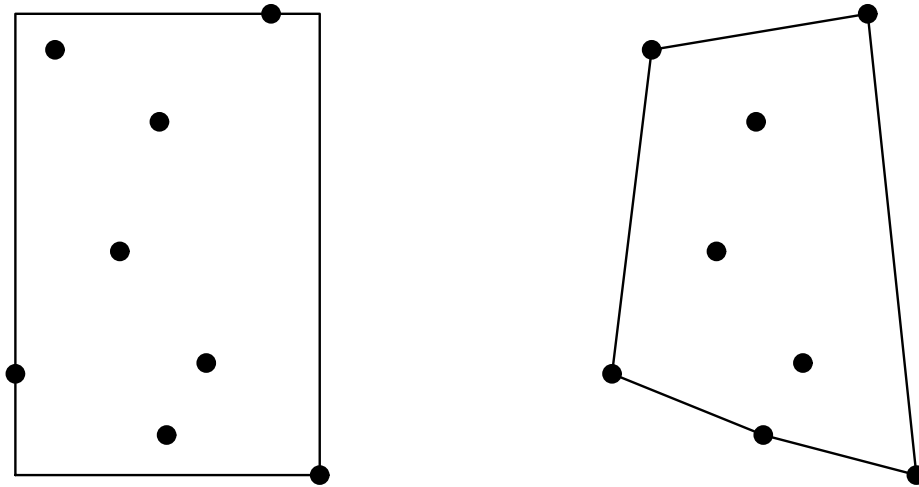
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doesn't discriminate separability

to formalize separability needs fixing some aggregation criterion

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to formalize separability needs fixing some aggregation criterion

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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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P_k is adequate

to formalize separability needs fixing some aggregation criterion

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- if the sum of distances from each point to its cluster center is minimum

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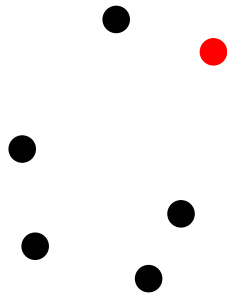
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k -interior

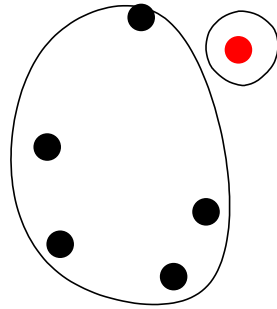
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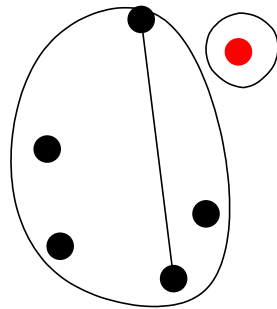
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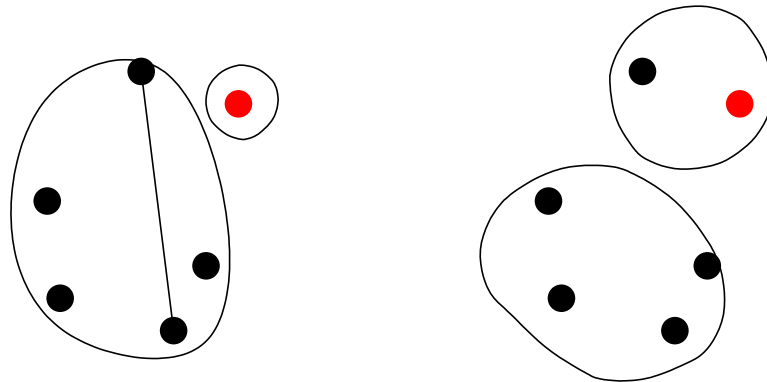
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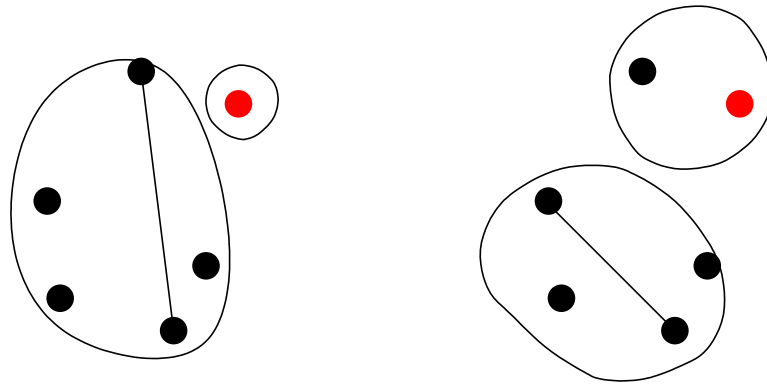
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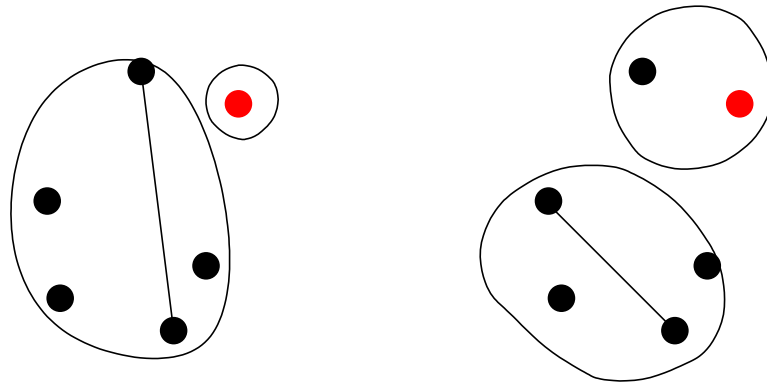
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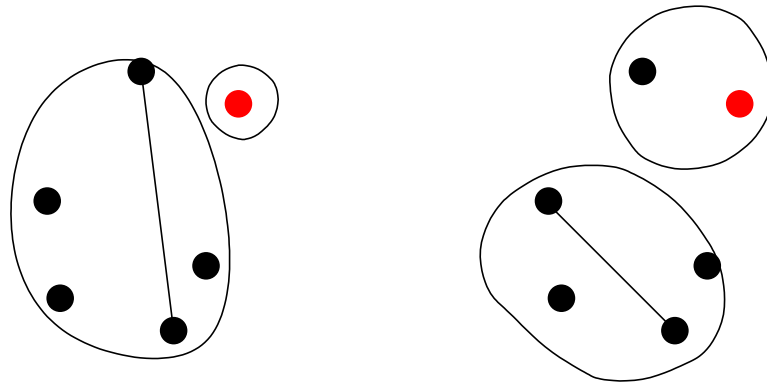


● is 1-interior

k -interior

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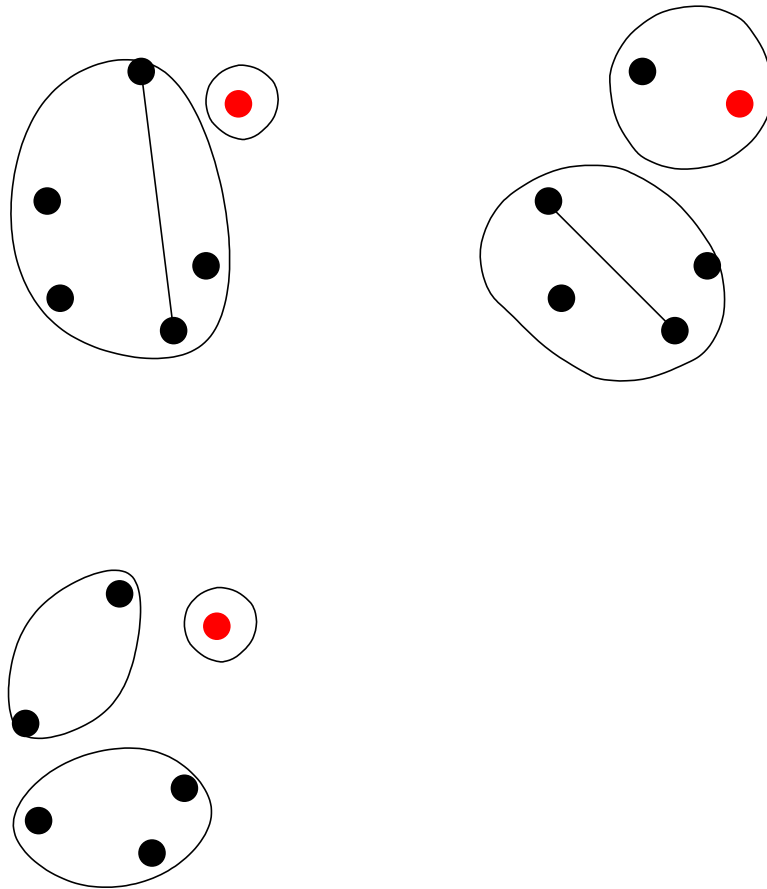


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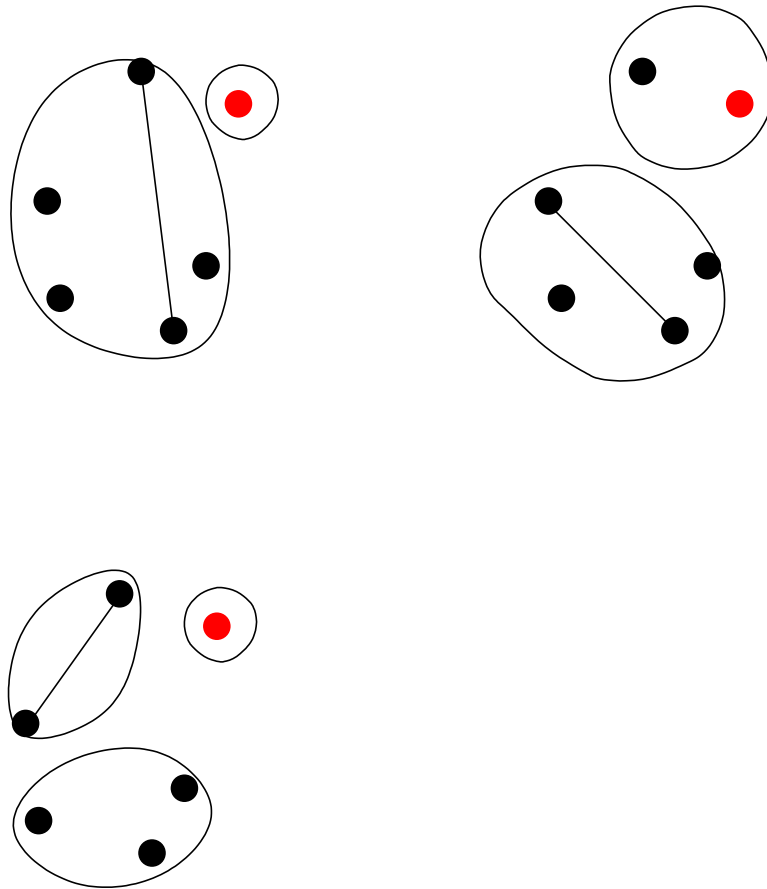


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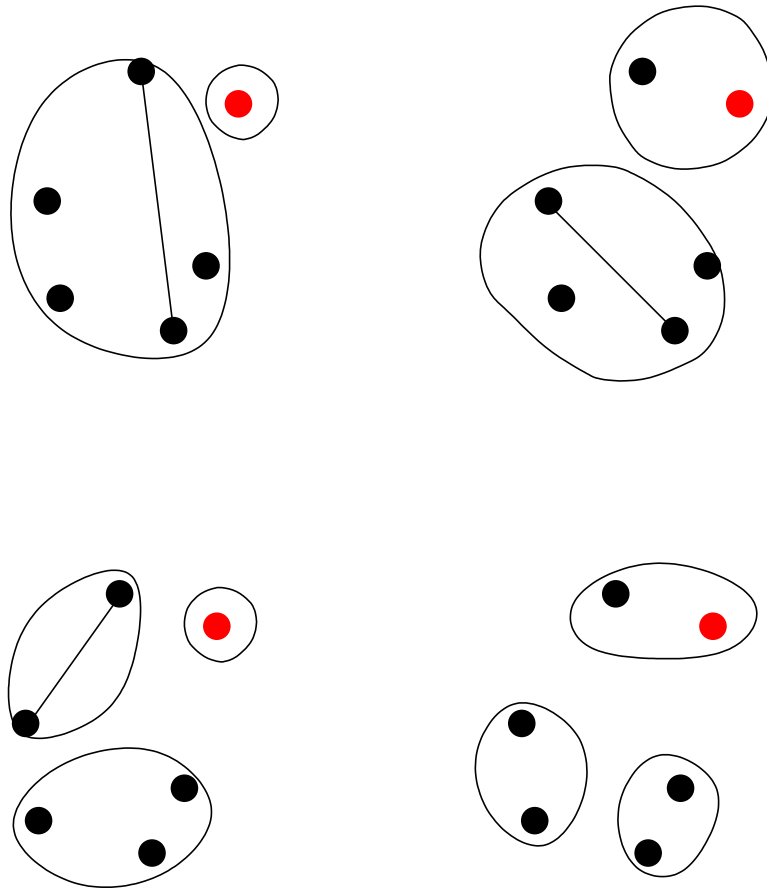


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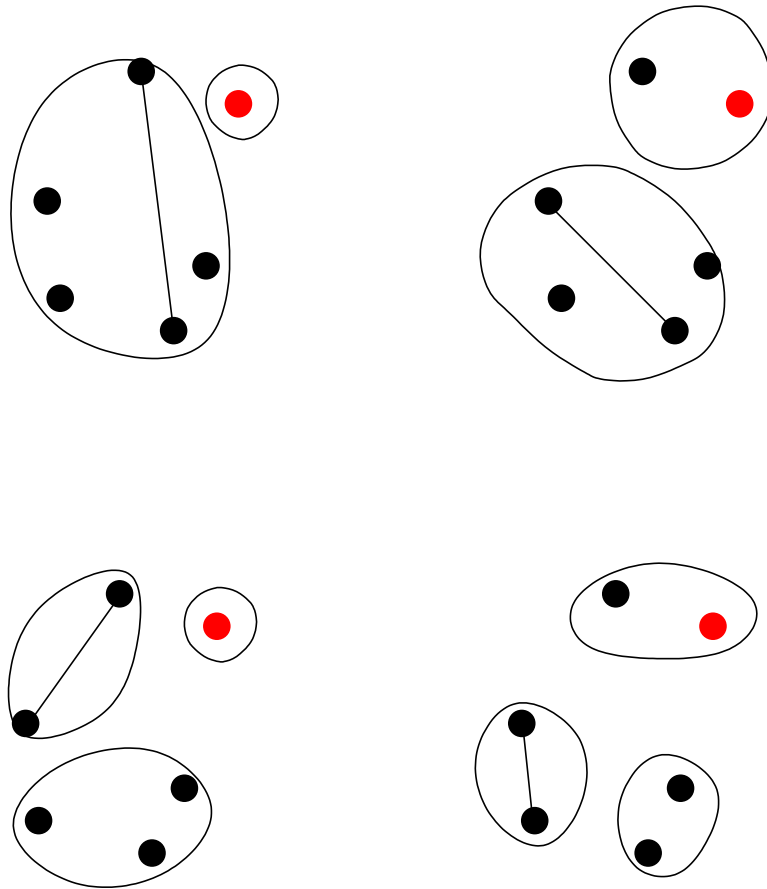


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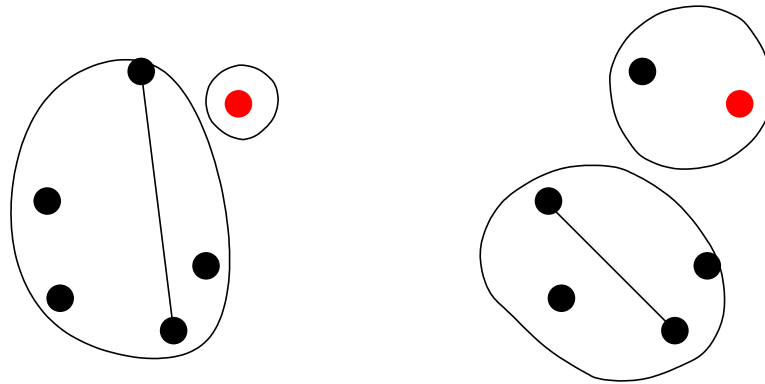


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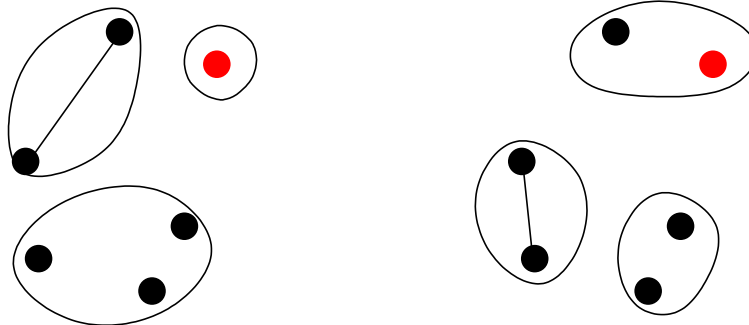
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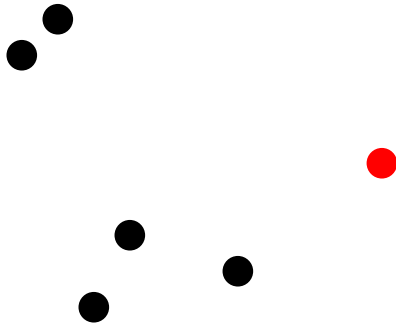


• is 1-interior



• is 2-interior

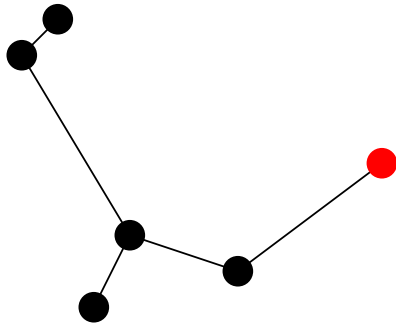
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k -interior

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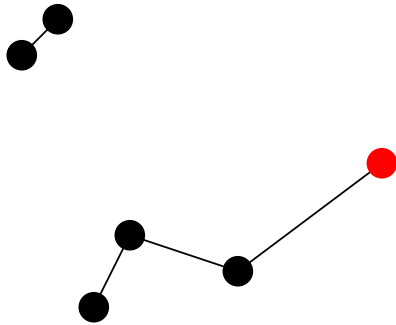
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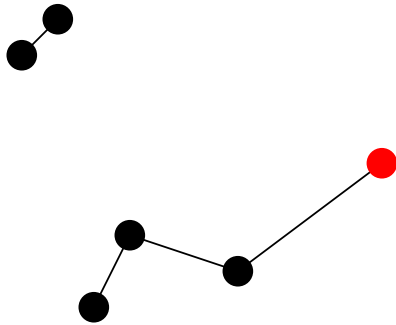
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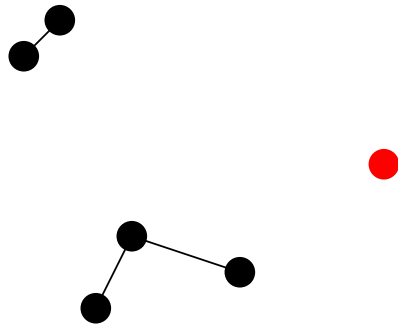
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● is 1-interior

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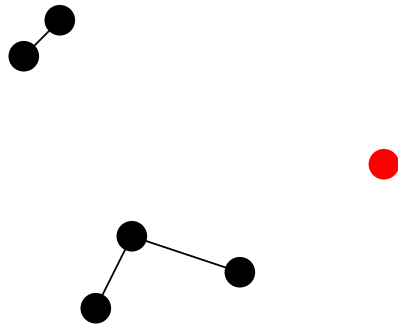


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• is 1-interior but not 2-interior

interiority degree

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interiority degree

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

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

interiority degree

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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

interiority degree

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$$\square d_{\bar{x}} = 0$$

interiority degree

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□ $d_{\bar{x}} = 0$

– diameter iff

interiority degree

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– diameter iff $\min_{x \in X} dis(\bar{x}, x) \geq \max_{x, x' \in X} dis(x, x')$

interiority degree

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□ $d_{\bar{x}} = 0$

– diameter iff $\min_{x \in X} dis(\bar{x}, x) \geq \max_{x, x' \in X} dis(x, x')$

– single linkage iff

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

$$\square d_{\bar{x}} = 0$$

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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

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□ $d_{\bar{x}} = |X| - 1$ diameter and single linkage iff

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$$\square d_{\bar{x}} = |X| - 1 \quad \text{diameter and single linkage iff}$$

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

interiority degree function

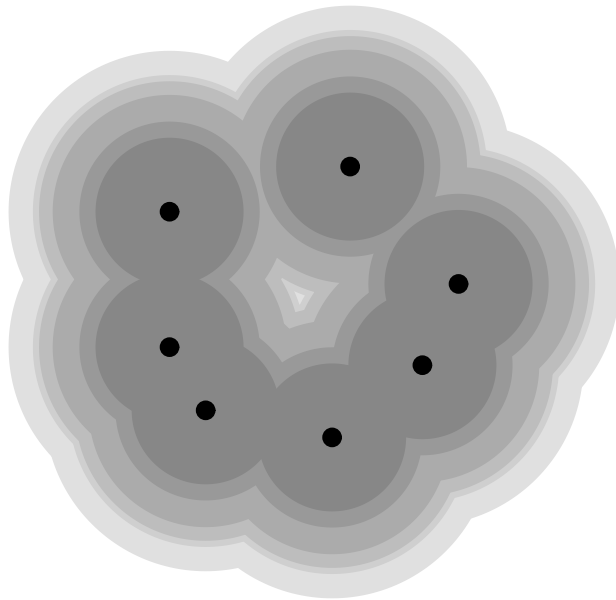
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$d : \mathcal{E} \setminus X \rightarrow \{0, 1, \dots, |X| - 1\}$ defines a partition of the entity space \mathcal{E}

interiority degree function

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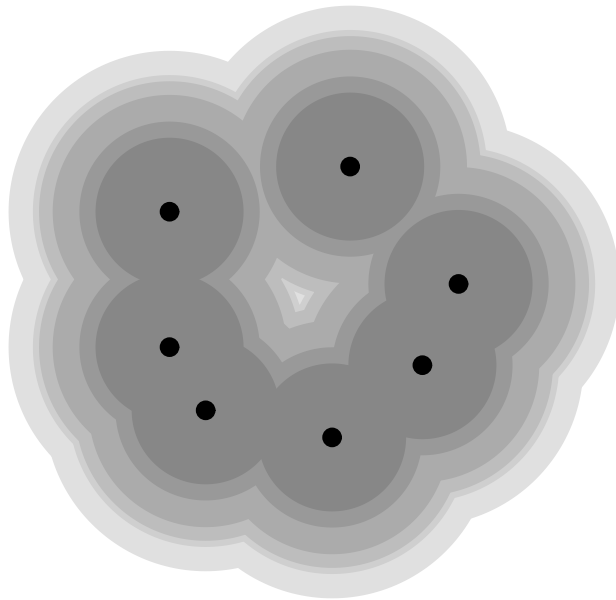
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interiority degree function

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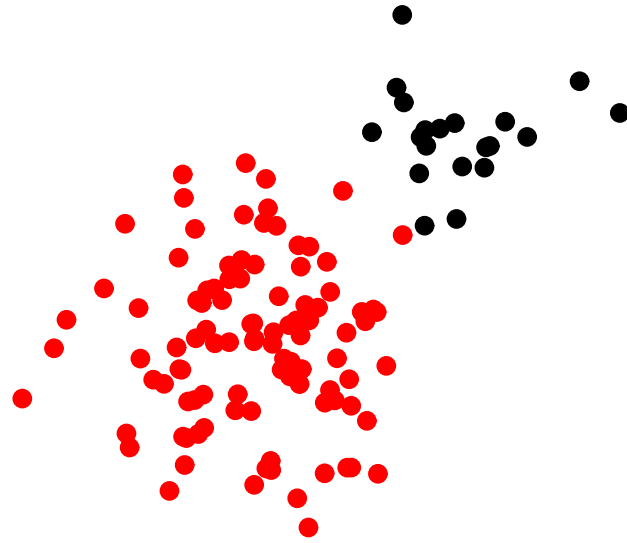
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territory of discriminated levels of interiority

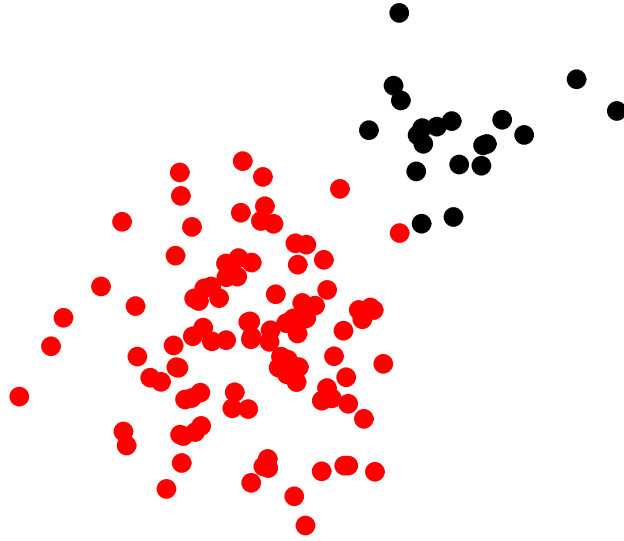
separability index

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separability index

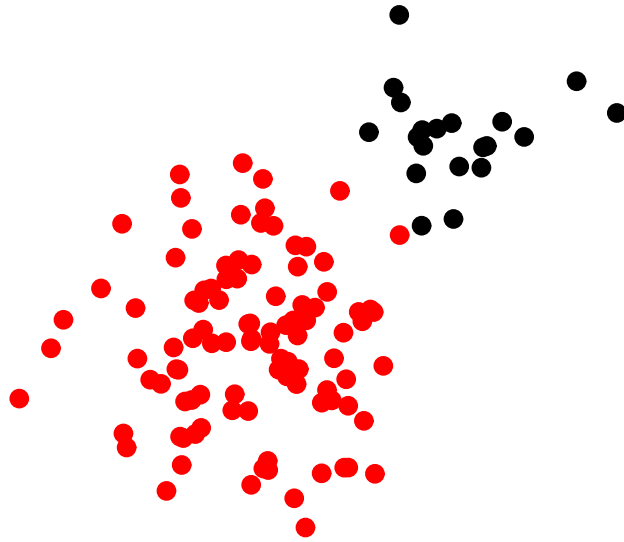
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$$D_{\bar{X}} = \{d(\bar{x}) : \bar{x} \in \bar{X} = \{\bullet\}\} \quad \textit{interiority of } \bar{X}$$

separability index

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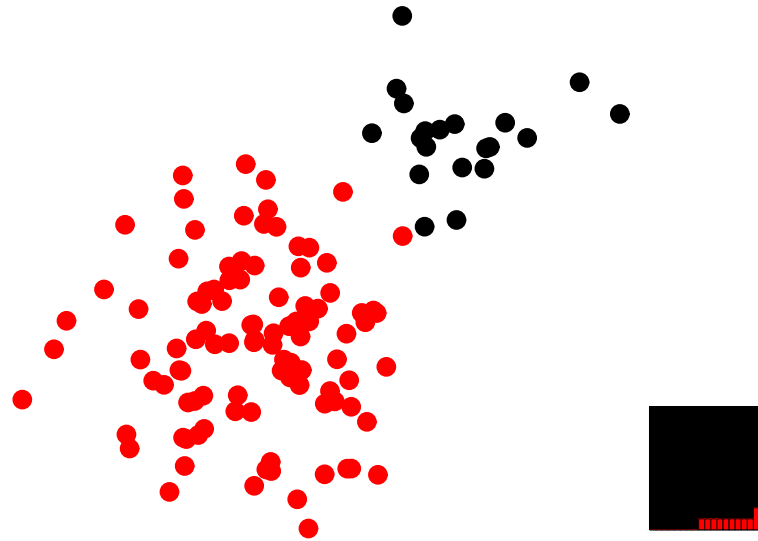


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$$D_{\bar{X}} \rightsquigarrow \textit{discriminate sep. index } DSI \in [0, 1]$$

separability index

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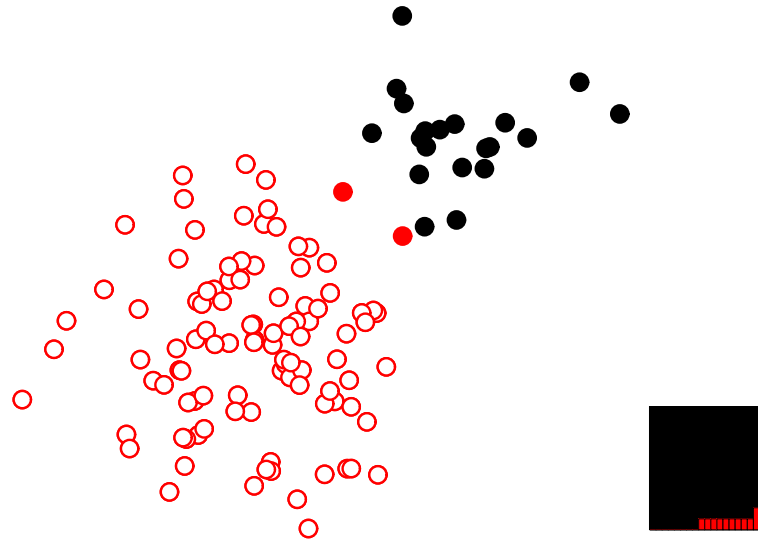


$$D_{\bar{X}} = \{d(\bar{x}) : \bar{x} \in \bar{X} = \{\bullet\}\} \quad \text{interiority of } \bar{X}$$

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separability index

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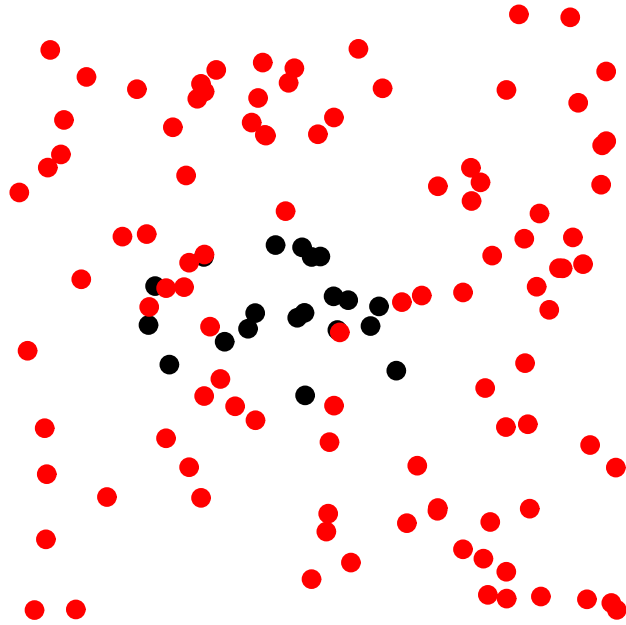


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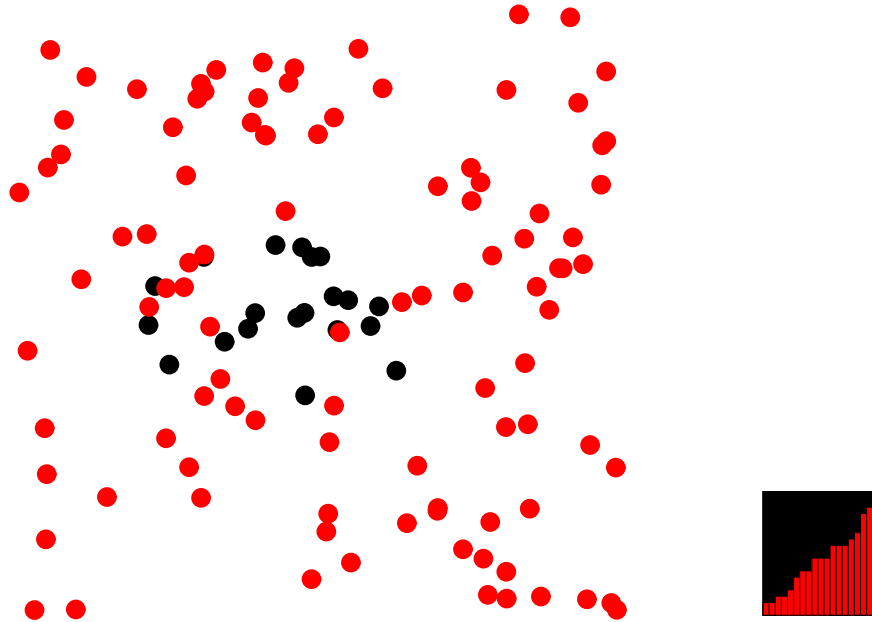
$$DSI = \text{black} / (\text{black} + \text{red})$$

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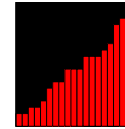
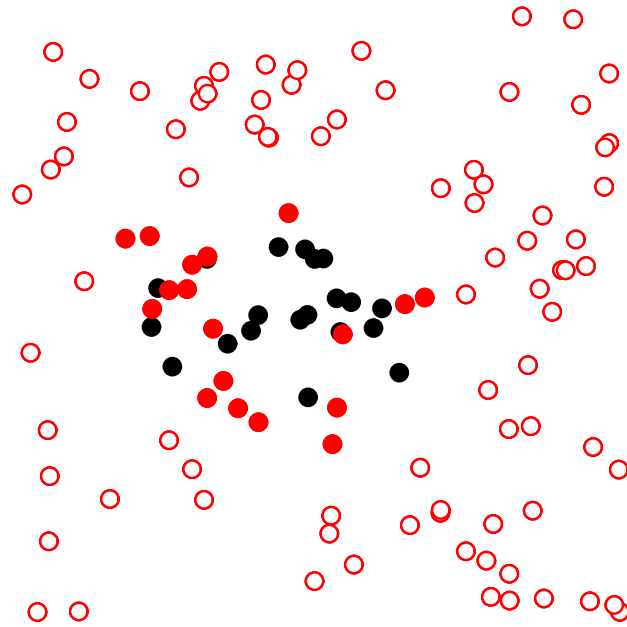
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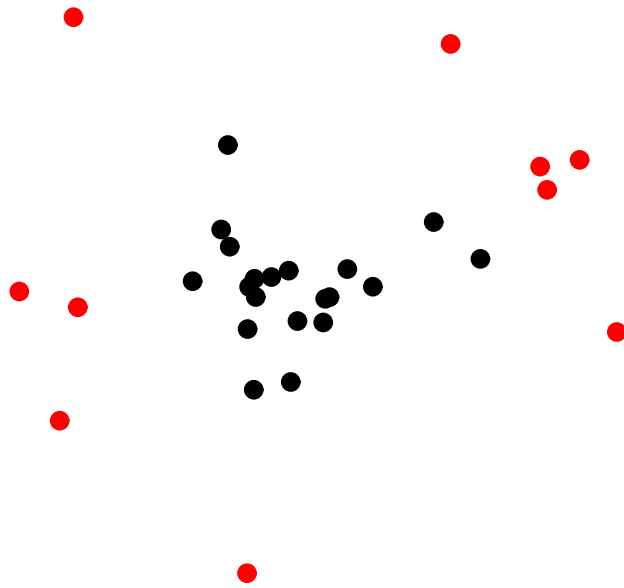
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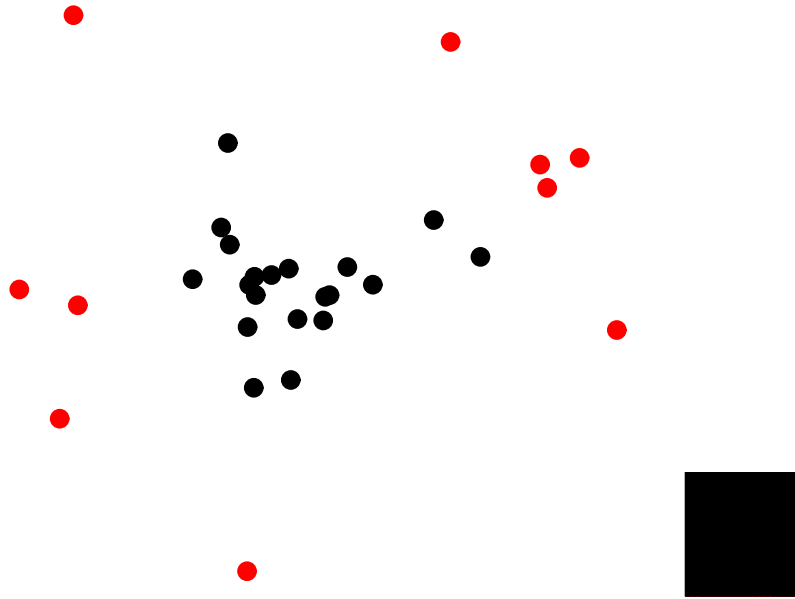
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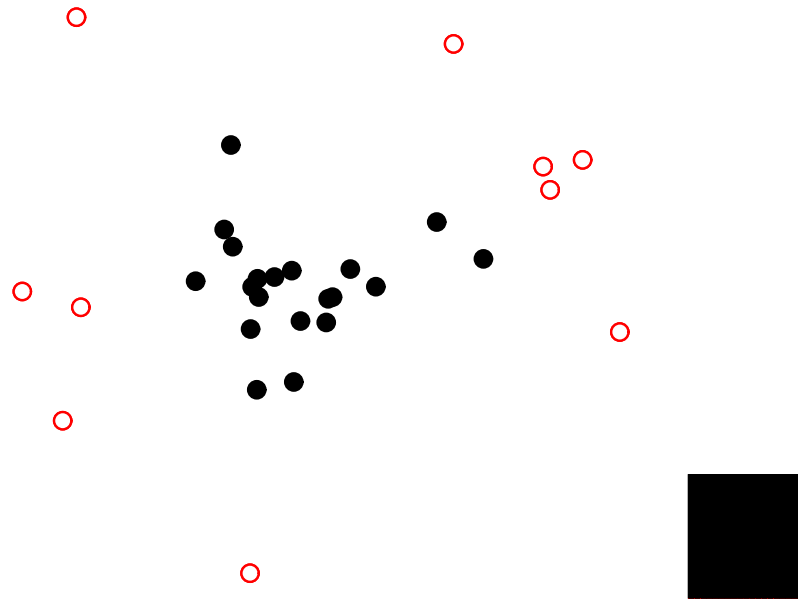
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$$DSI = \text{black} / (\text{black} + \text{red})$$

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convexity criterion

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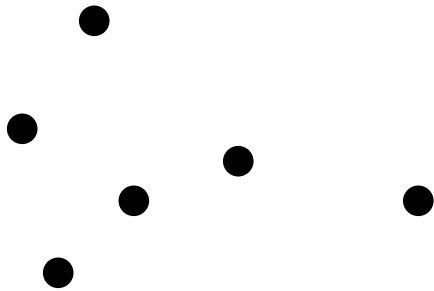
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a k -partition is adequate if it includes $k - 1$ singletons that are not in the interior of the convex hull of the remaining points

convexity criterion

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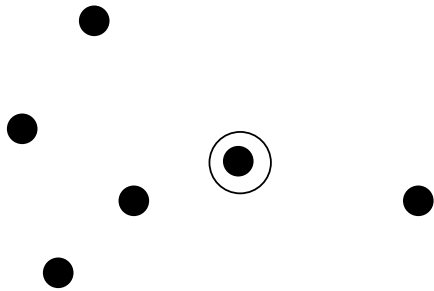
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convexity criterion

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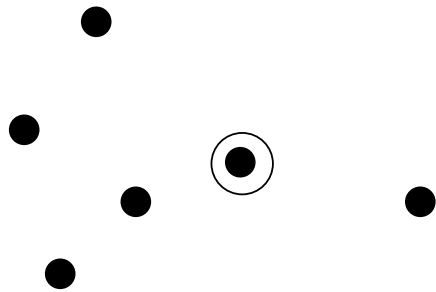
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convexity criterion

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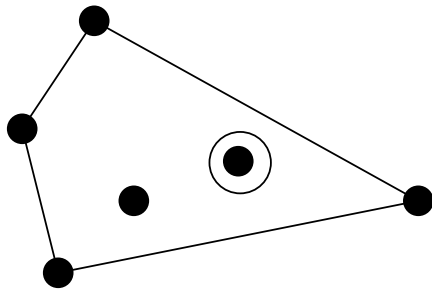


not adequate

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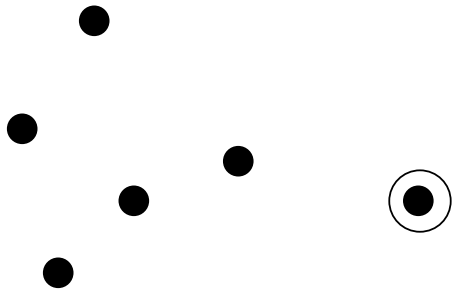


not adequate

convexity criterion

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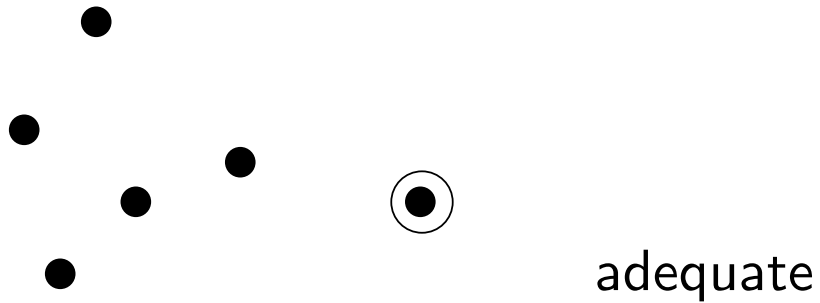
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convexity criterion

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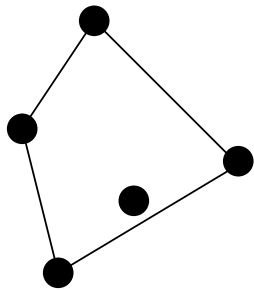
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convexity criterion

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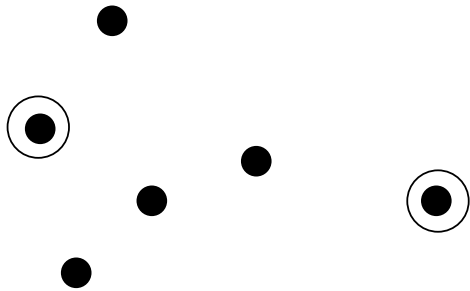


adequate

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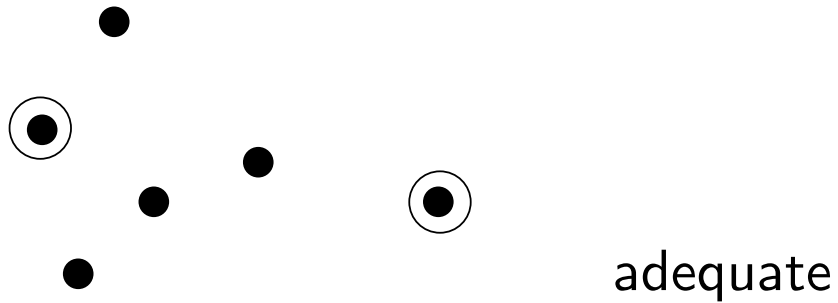
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convexity criterion

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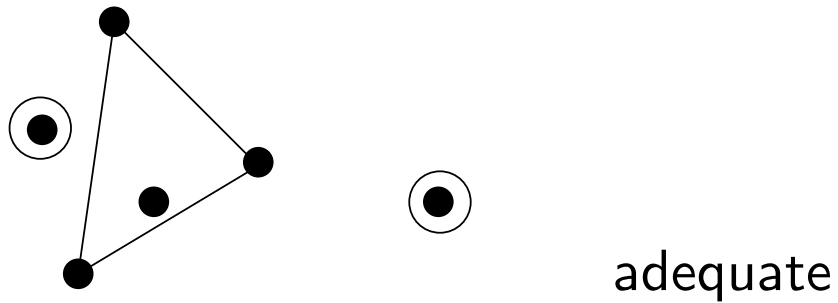
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convexity criterion

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convexity criterion

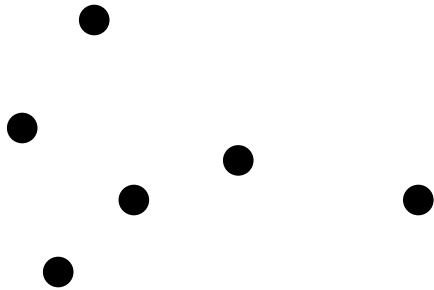
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\bar{x} is k -interior if it is inside the convex hull of any $|X| - k + 1$ points of X

convexity criterion

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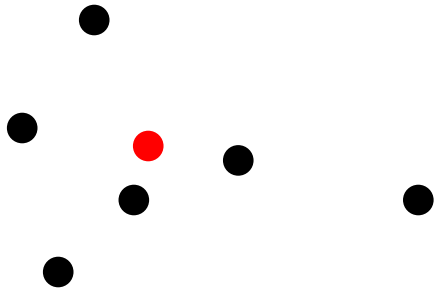
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convexity criterion

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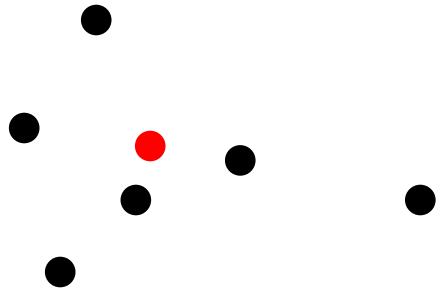
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convexity criterion

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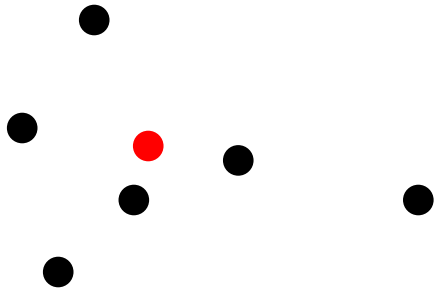


● is 1-interior

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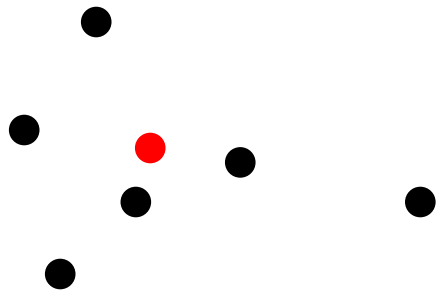


• is 1-interior, and 2-interior

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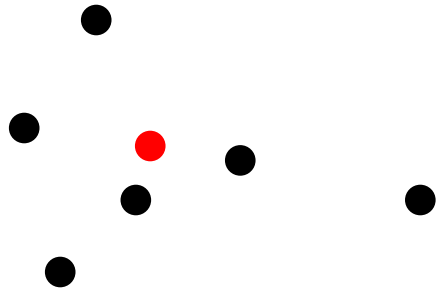
• is 1-interior, and 2-interior

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

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\bar{x} is k -interior if it is inside the convex hull of any $|X| - k + 1$ points of X



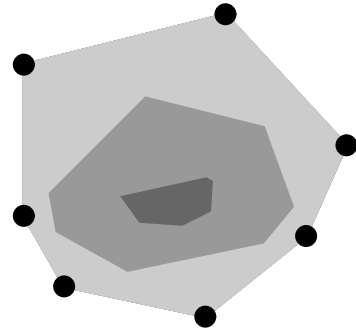
• is 1-interior, and 2-interior

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

$$d(\bullet) = 2$$

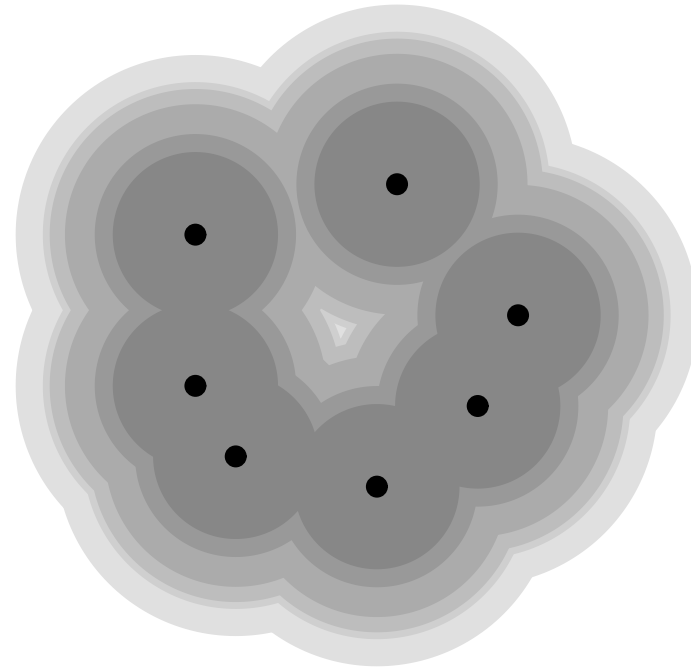
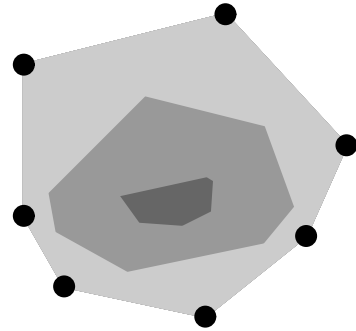
discriminated interiority territories

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discriminated interiority territories

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for $x \in X$, $d(x)$ is the minimum number of points to be removed from X such that x is outside the conv.hull of the remaining points

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$d(x) = 1$ iff x is a vertex of the conv.hull(X)

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$D_X = \{d(x) : x \in X\}$ *auto-interiority* of X

for $x \in X$, $d(x)$ is the minimum number of points to be removed from X such that x is outside the conv.hull of the remaining points

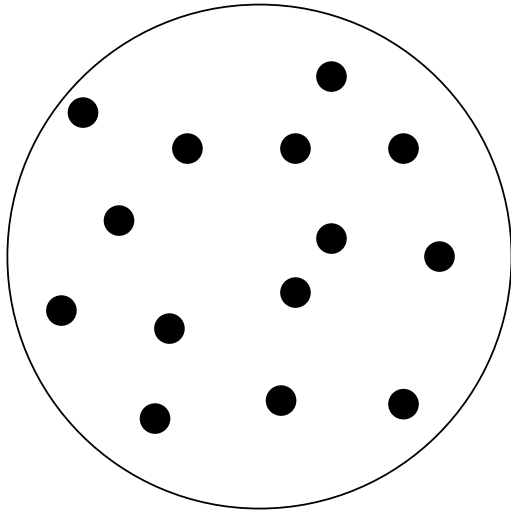
$d(x) = 1$ iff x is a vertex of the conv.hull(X)

$D_X = \{d(x) : x \in X\}$ *auto-interiority* of X

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

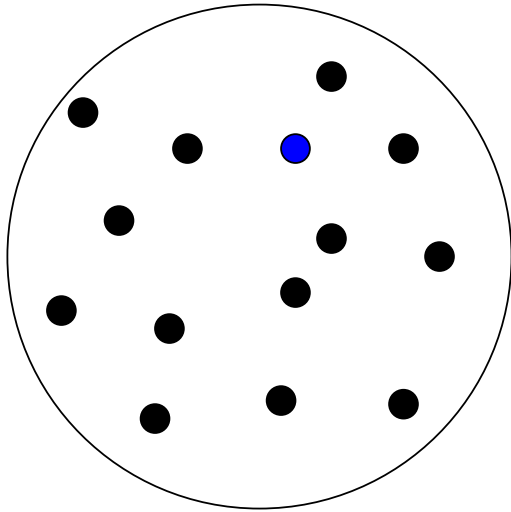
if X is uniformly distributed on an n -ball

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if X is uniformly distributed on an n -ball

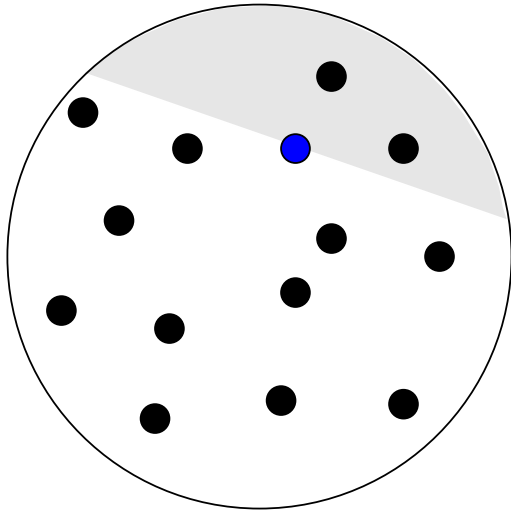
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$$\frac{d(x)}{|X|} \rightsquigarrow$$

if X is uniformly distributed on an n -ball

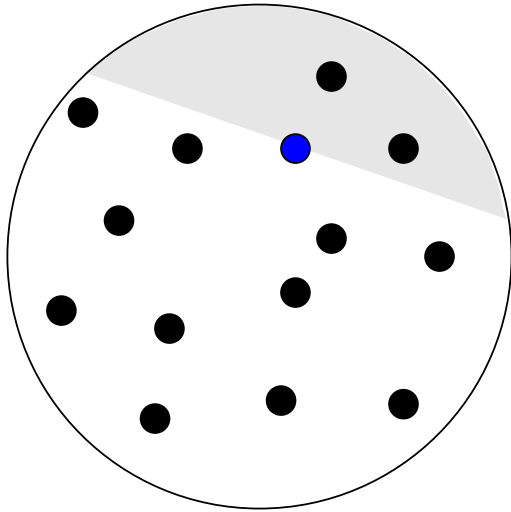
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$$\frac{d(\mathbf{x})}{|X|} \rightsquigarrow \frac{\text{vol}(\text{shaded region})}{\text{vol}(B_n)} = V_r(\mathbf{x})$$

if X is uniformly distributed on an n -ball

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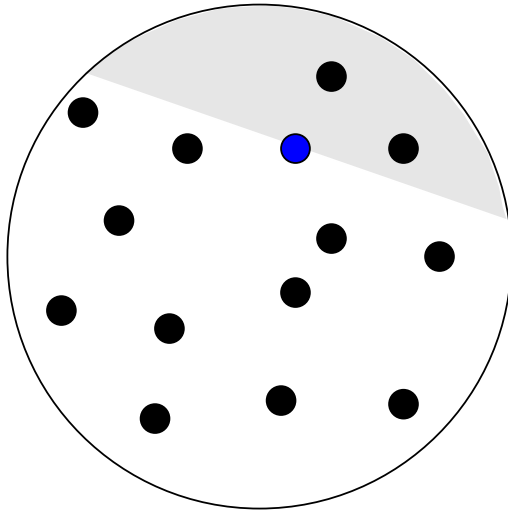


$$\frac{d(x)}{|X|} \rightsquigarrow \frac{\text{vol}(\text{sector})}{\text{vol}(B_n)} = V_r(x)$$

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

if X is uniformly distributed on an n -ball

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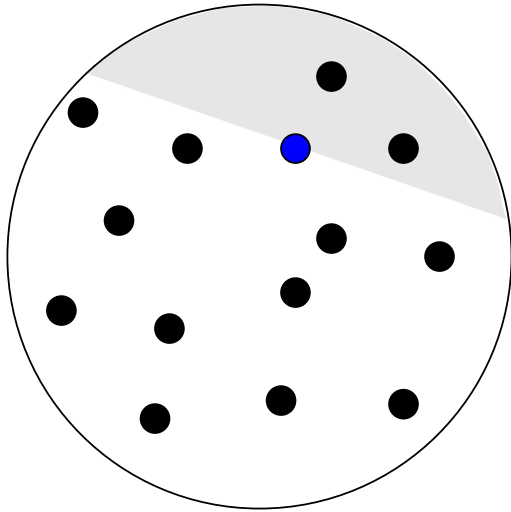


$$\frac{d(x)}{|X|} \rightsquigarrow \frac{\text{vol}(\text{shaded region})}{\text{vol}(B_n)} = V_r(x)$$

$$E[V_r(x)] = \int_{B_n} \frac{V_r(x)}{\text{vol}(B_n)} dx = \frac{1}{2^{n+1}}$$

if X is uniformly distributed on an n -ball

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

$$E[V_r(\mathbf{x})] = \int_{B_n} \frac{V_r(\mathbf{x})}{\text{vol}(B_n)} d\mathbf{x} = \frac{1}{2^{n+1}}$$

straightforward test of the uniform distribution on a n -ball

if X is uniformly distributed on an n -ball

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

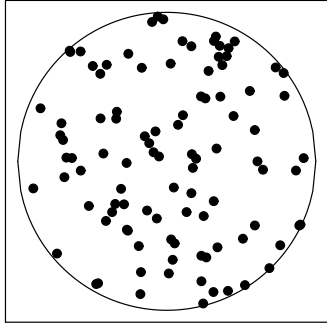
if X is uniformly distributed on an n -ball

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

if X is uniformly distributed on an n -ball

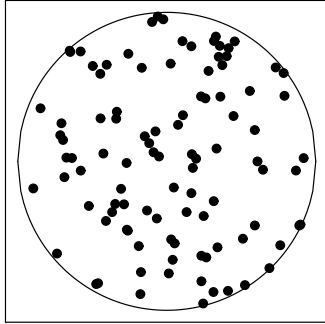
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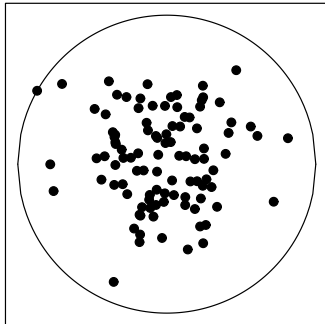
$$\frac{1}{|X|} \sum_x V_r(x) = 0.1320314$$

if X is uniformly distributed on an n -ball

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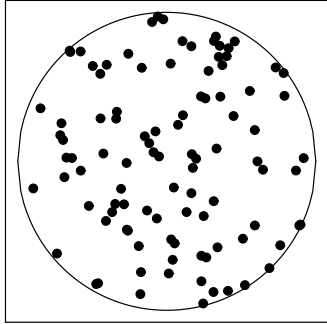
$$\frac{1}{|X|} \sum_x V_r(x) = 0.1320314$$



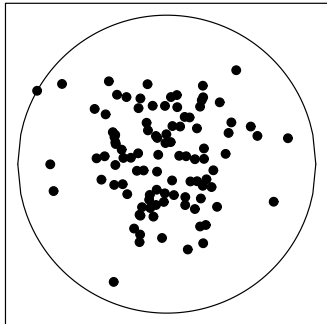
$$\frac{1}{|X|} \sum_x V_r(x) = 0.2605504$$

if X is uniformly distributed on an n -ball

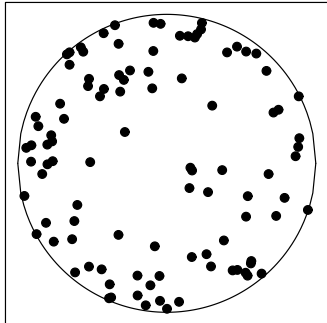
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$$\frac{1}{|X|} \sum_x V_r(x) = 0.1320314$$



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



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