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The Minimum Code Length for Clustering Using the Gray Code

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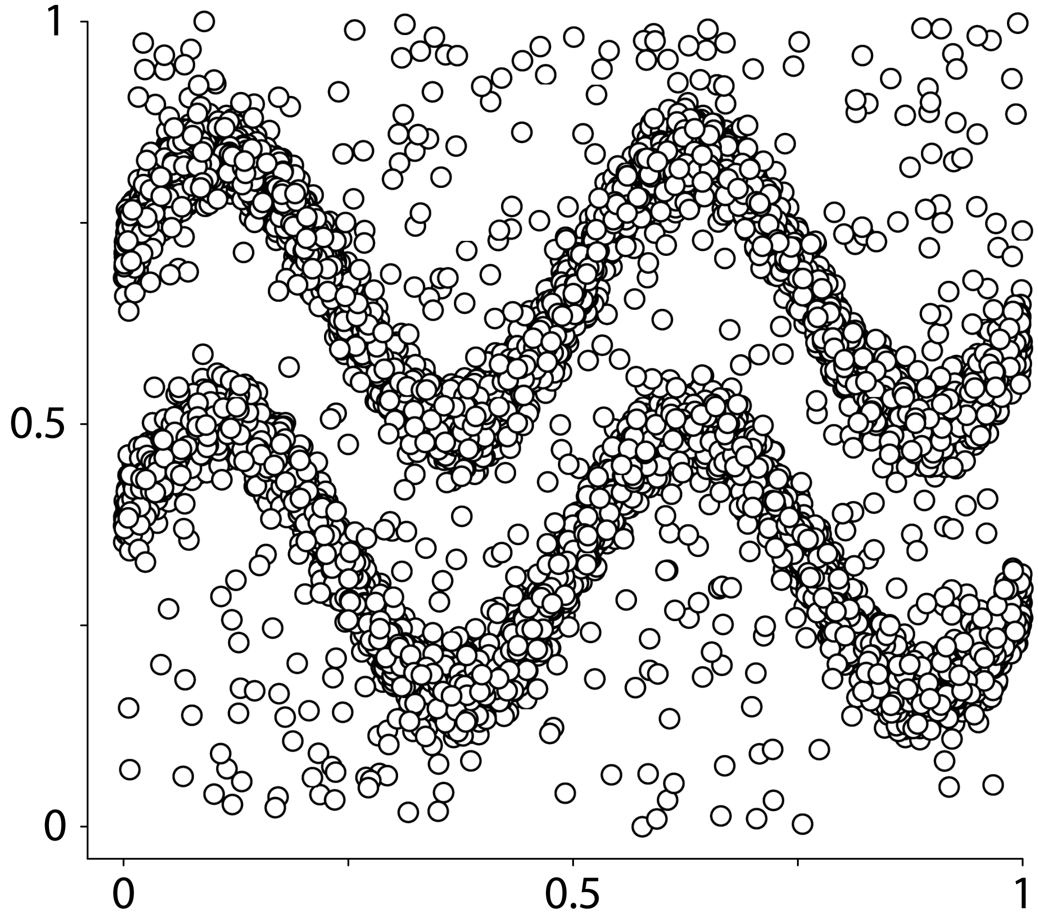
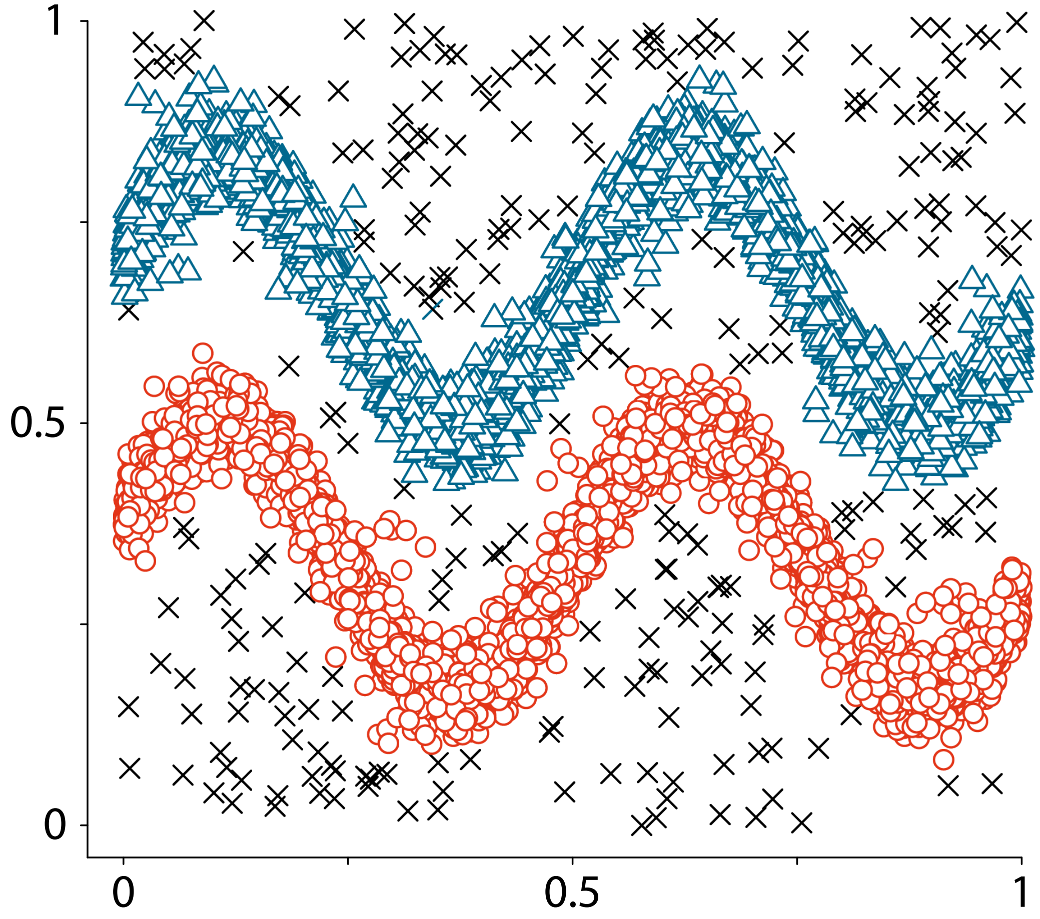
Contributions

1. ***The MCL (Minimum Code Length)***
   - A new measure to score clustering results
   - Needed to distinguish each cluster under some fixed encoding scheme for real-valued variables
2. ***COOL (COding-Oriented cLustering)***
   - A general clustering approach
   - Always finds the best clusters (*i.e.*, the global optimal solution) which minimizes the MCL in $O(nd)$
   - Parameter tuning is not needed
3. ***G-COOL (COOL with the Gray code)***
   - Achieves internal cohesion and external isolation
   - Finds arbitrary shaped clusters

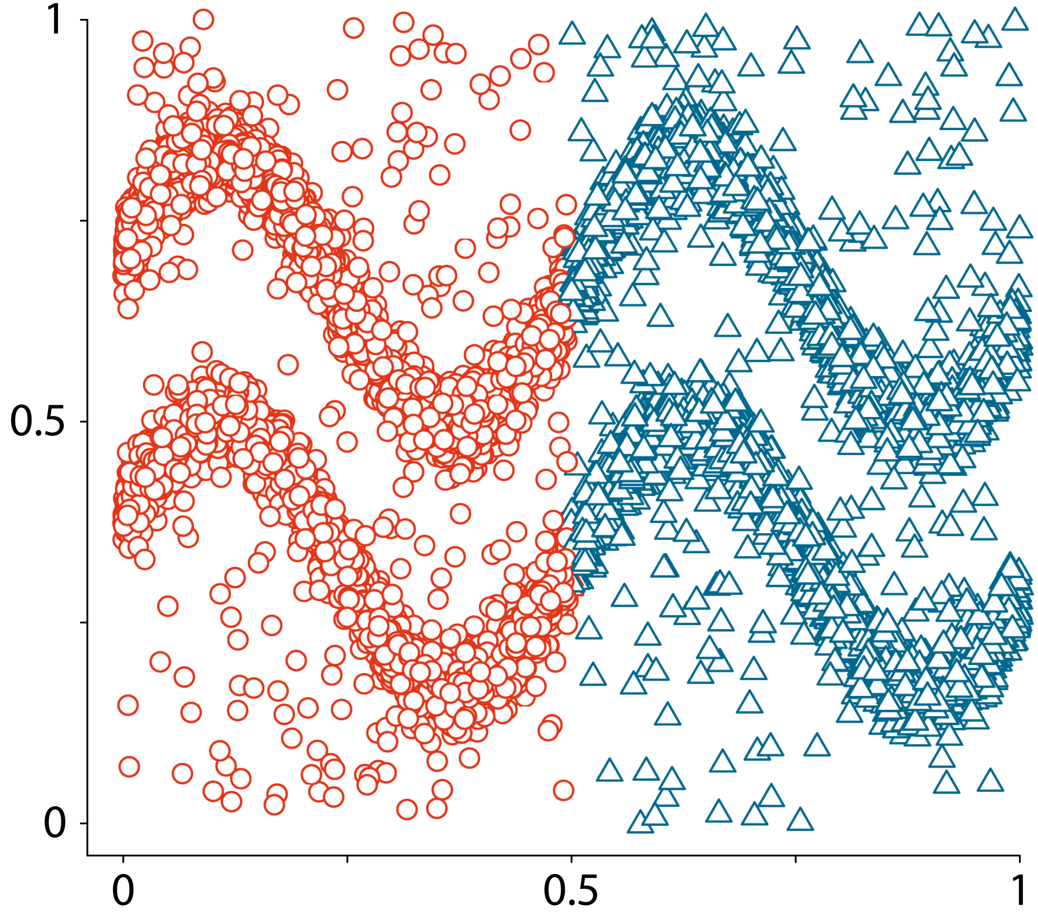
Demonstration (Synthetic Dataset)



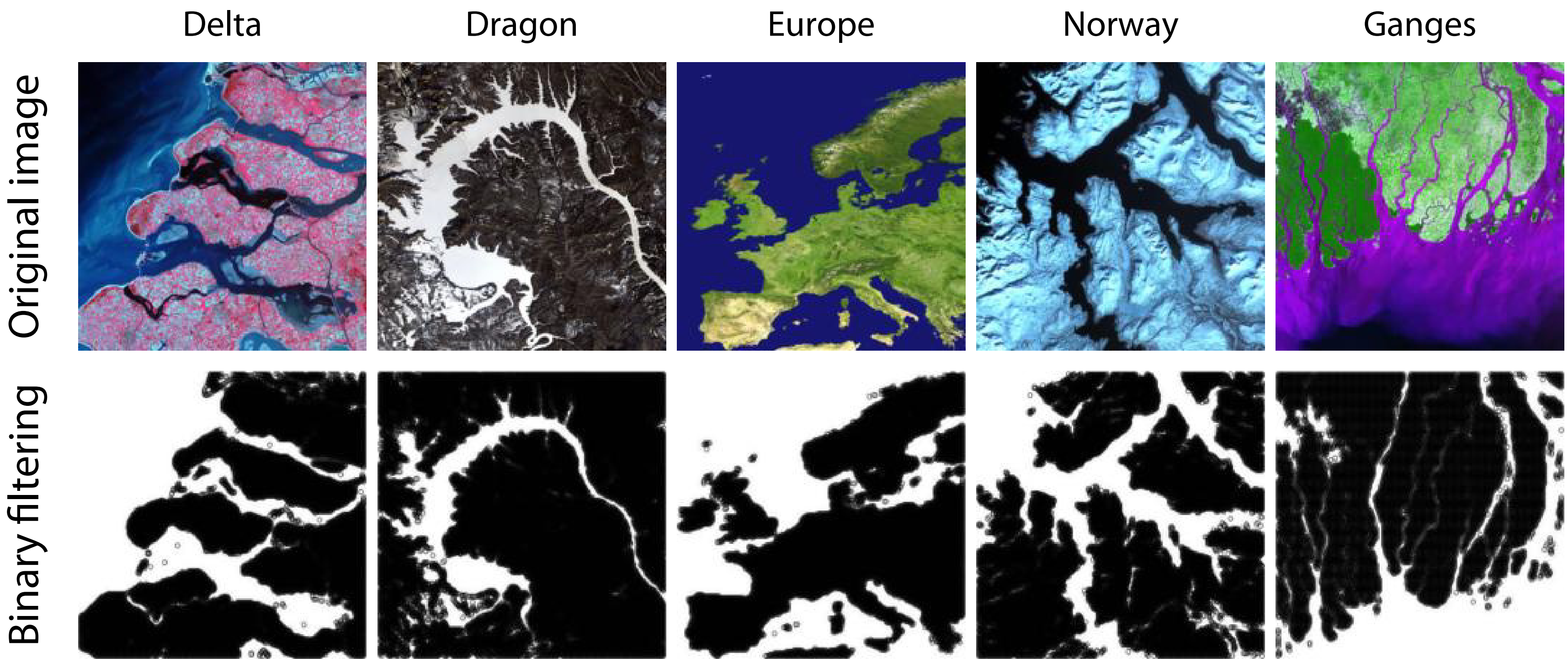
G-COOL



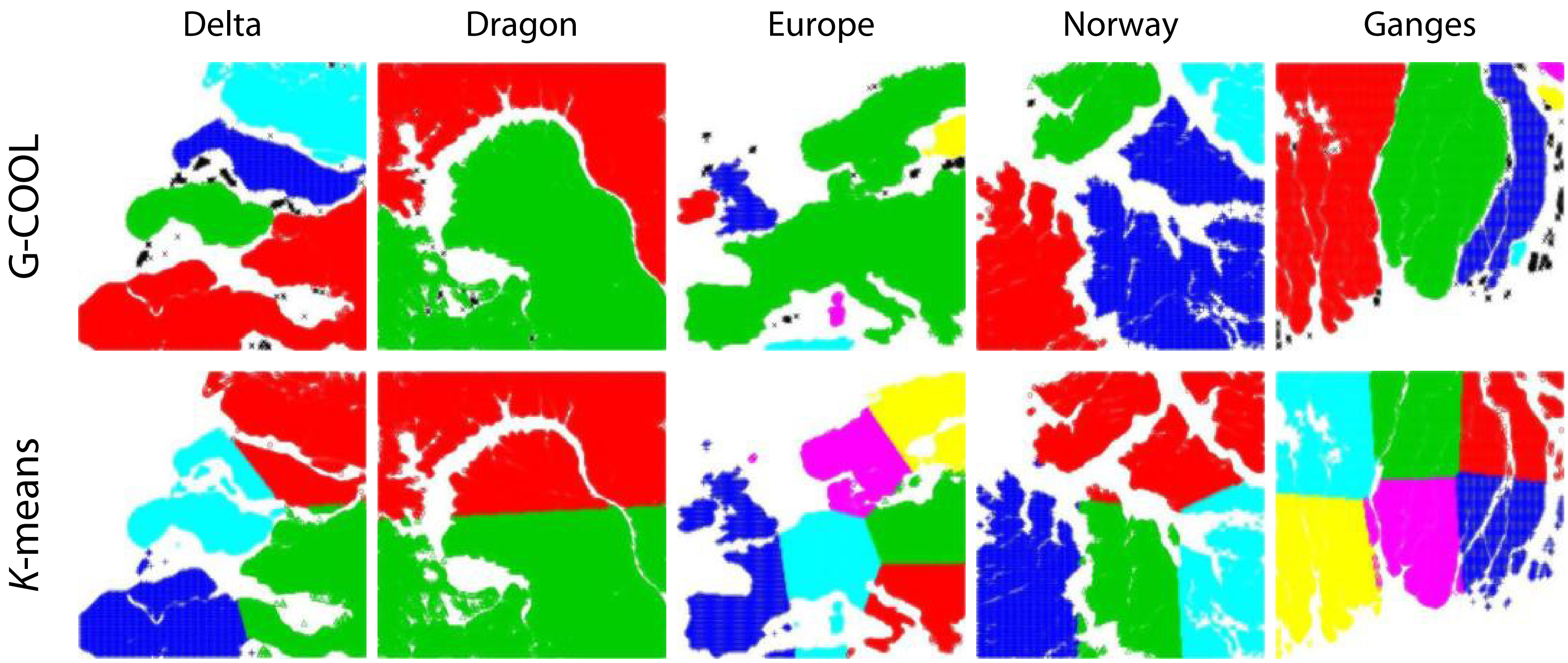
K-means



Results (Real datasets)



Results (Real datasets)



Outline

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0. Overview
1. Background and Our Strategy
2. MCL and Clustering
3. COOL Algorithm
4. G-COOL: COOL with the Gray Code
5. Experiments
6. Conclusion

Clustering Focusing on Compression

- The MDL approach [Kontkanen *et al.*, 2005]
  - Data encoding has to be optimized
    - All encoding schemes are (implicitly) considered
    - The time complexity $\geqslant O(n^2)$
- The Kolmogorov complexity approach [Cilibrasi, 2005]
  - Measures the distance between data points based on compression of finite sequences
    - Difficult to apply multivariate data
  - Actual clustering process is the traditional agglomerative hierarchical clustering
    - The time complexity $\geqslant O(n^2)$
- Both approaches are not suitable for massive data

Our Strategy

- *Requirements:*
  1. Fast, and linear in the data size
  2. Robust to changes in input parameters
  3. Can find arbitrary shaped clusters

Our Strategy

- *Requirements:*
  1. Fast, and linear in the data size
  2. Robust to changes in input parameters
  3. Can find arbitrary shaped clusters
- *Solutions:*
  1. Fix an encoding scheme for continuous variables
     - Motivated by *Computable Analysis* [Weihrauch, 2000]
  2. Clustering = Discretizing real-valued data
     - Always finds the best results w.r.t. the MCL
  3. Use the Gray code for real numbers [Tsuiki, 2002]
     - Discretized data points are overlapped and adjacent clusters are merged

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MCL (Minimum Code Length)

- The MCL is the code length of the maximally compressed clusters by using a fixed encoding scheme
- The MCL is calculated in $O(nd)$ by using radix sort
  - n and d are the number of data and dimension, resp.

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  - n and d are the number of data and dimension, resp.

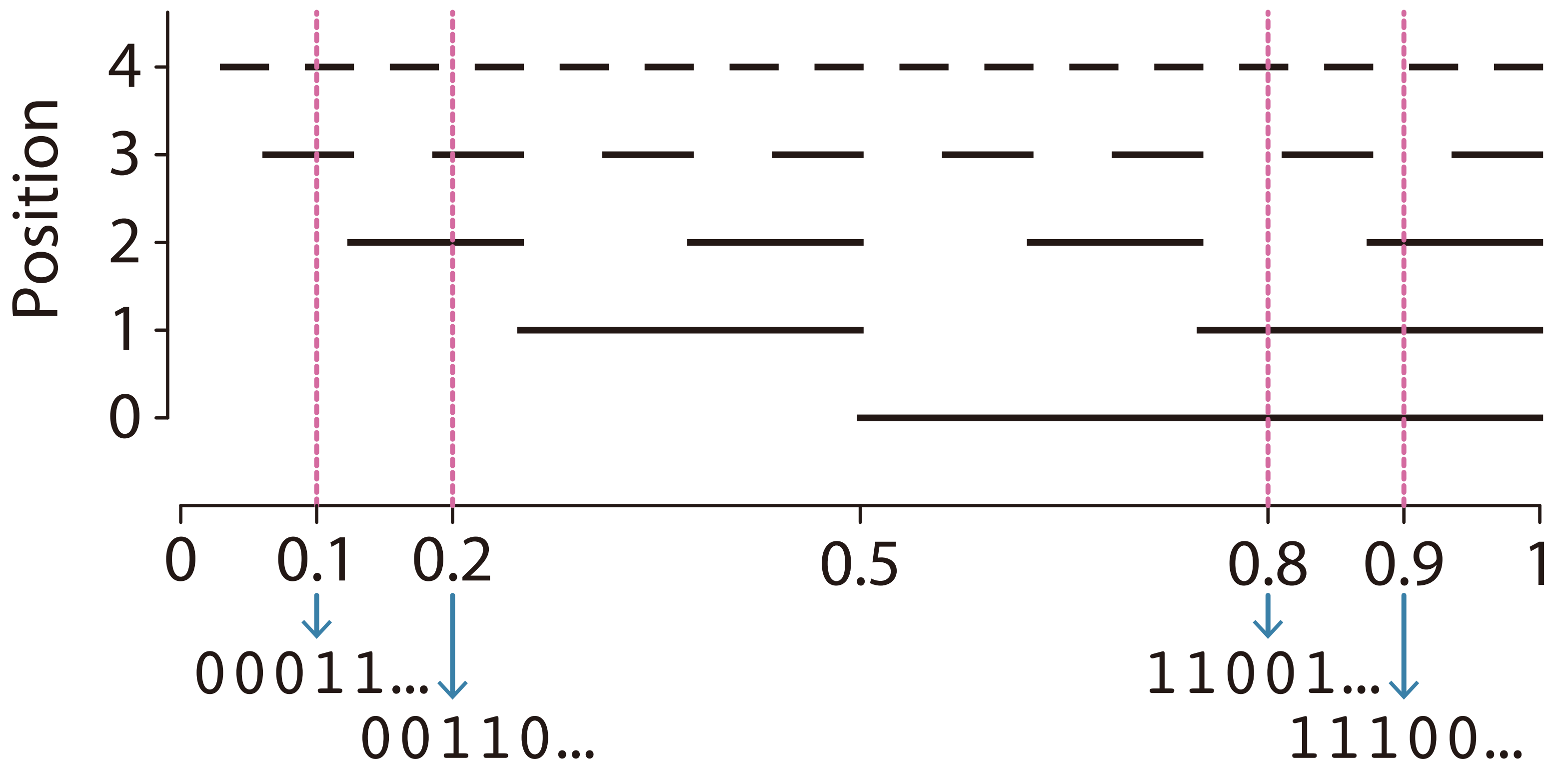
Example: $X = \{0.1, 0.2, 0.8, 0.9\}$,

$$\mathscr{C}_1 = \{\{0.1, 0.2\}, \{0.8, 0.9\}\}$$

$$\mathscr{C}_2 = \{\{0.1\}, \{0.2, 0.8\}, \{0.9\}\}$$

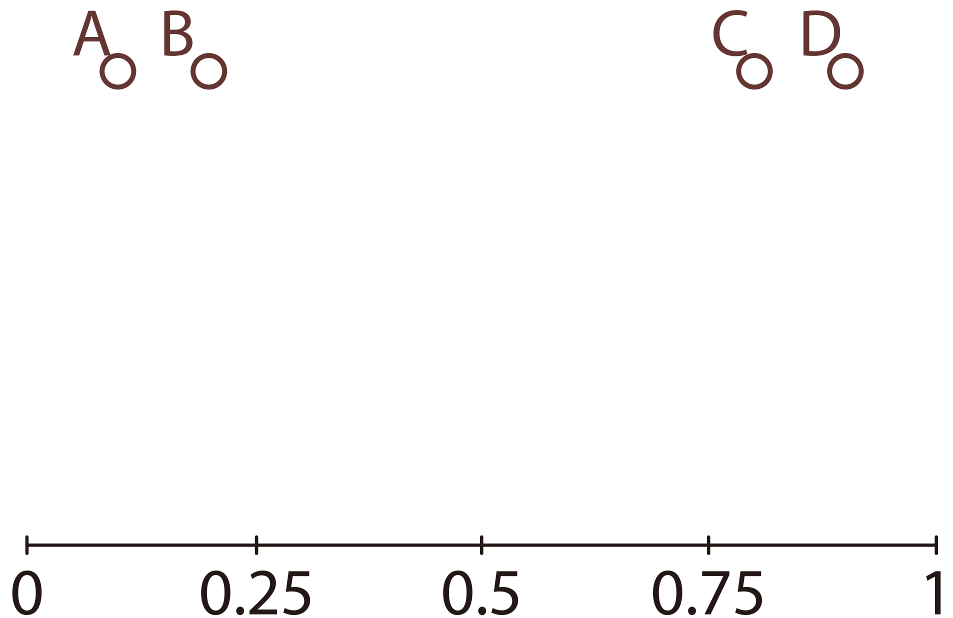
- Use binary encoding
- Which is preferred?

Binary Encoding



MCL with Binary Encoding

id	value
A	0.1
B	0.2
C	0.8
D	0.9



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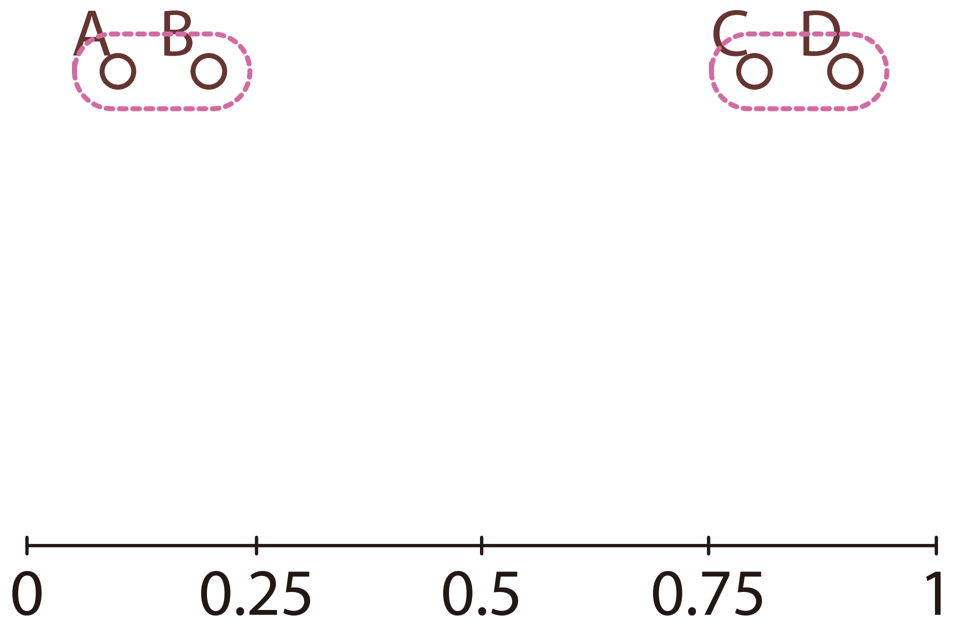

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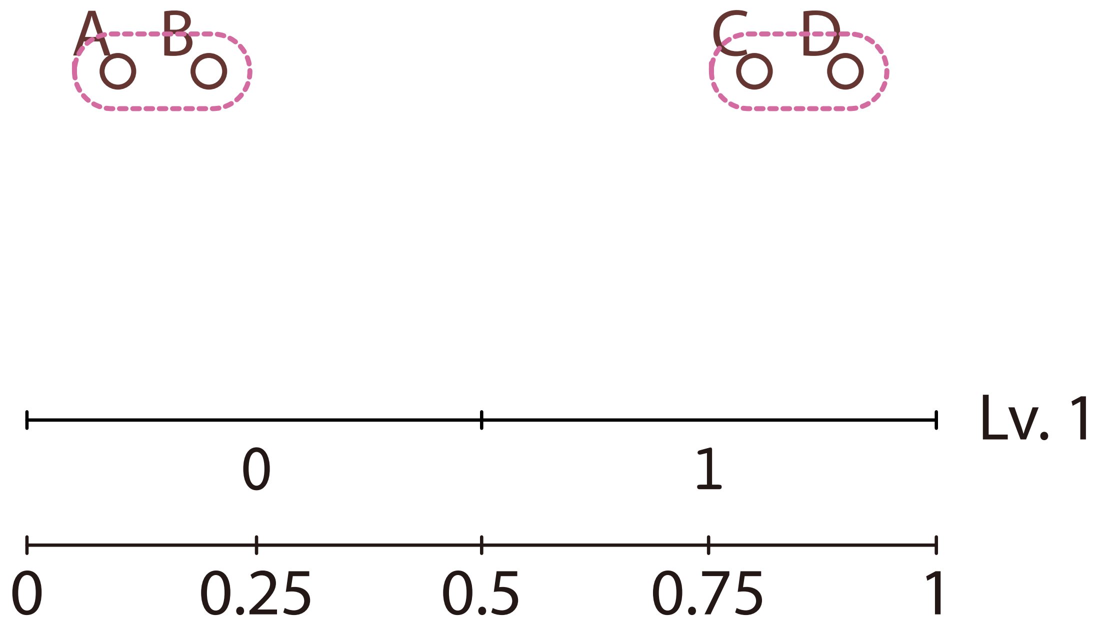

MCL = 1 + 1 = 2

MCL with Binary Encoding

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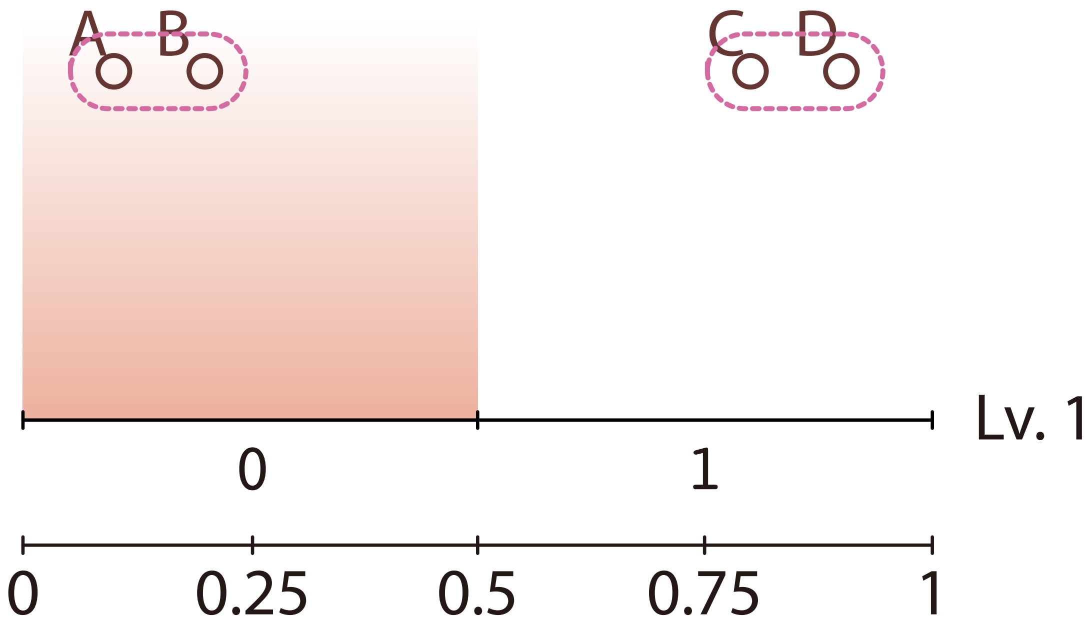
D	0.9



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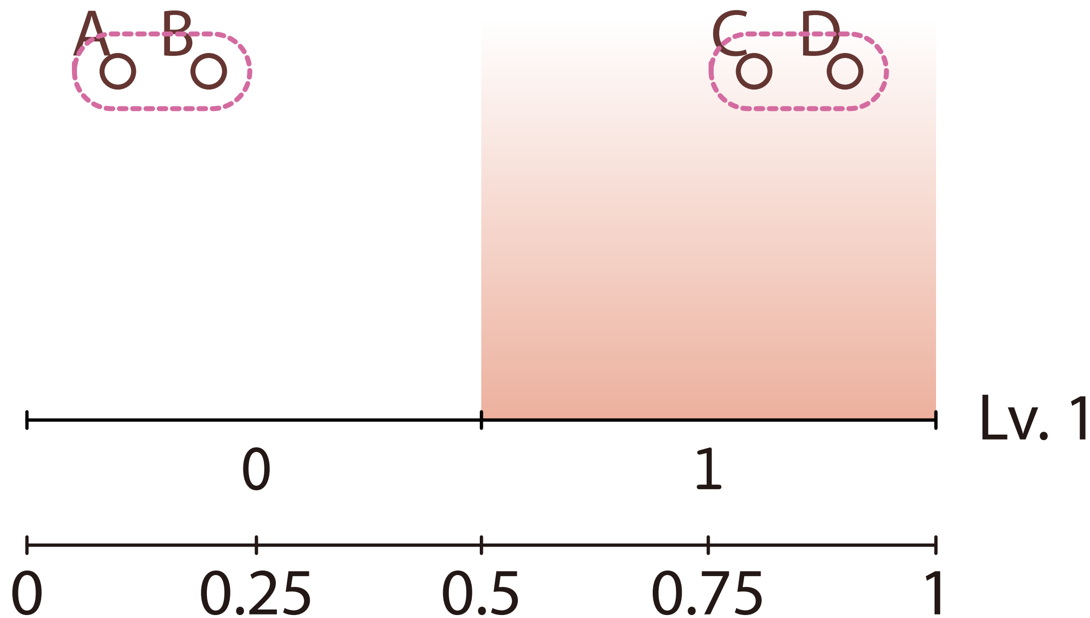

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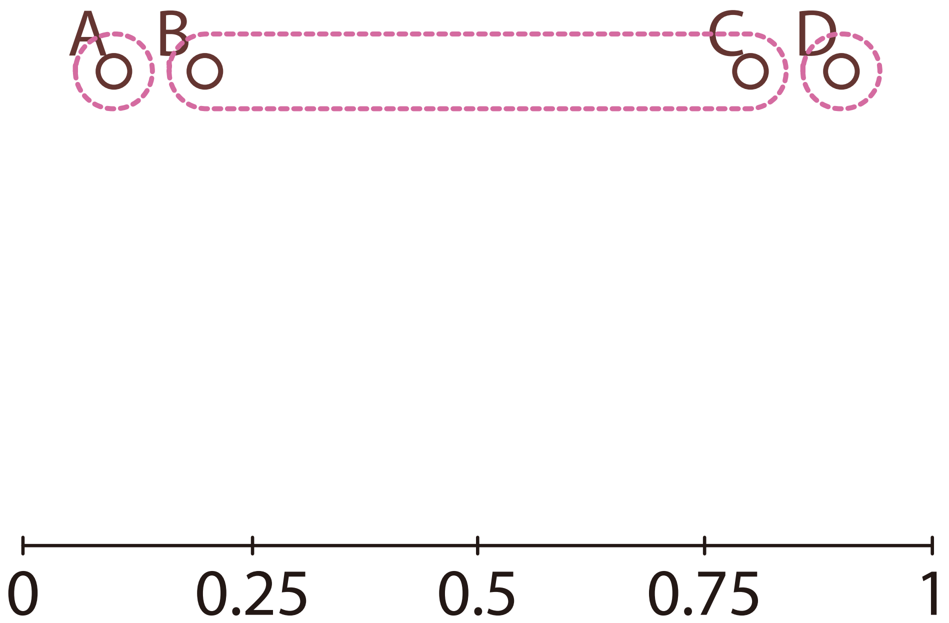

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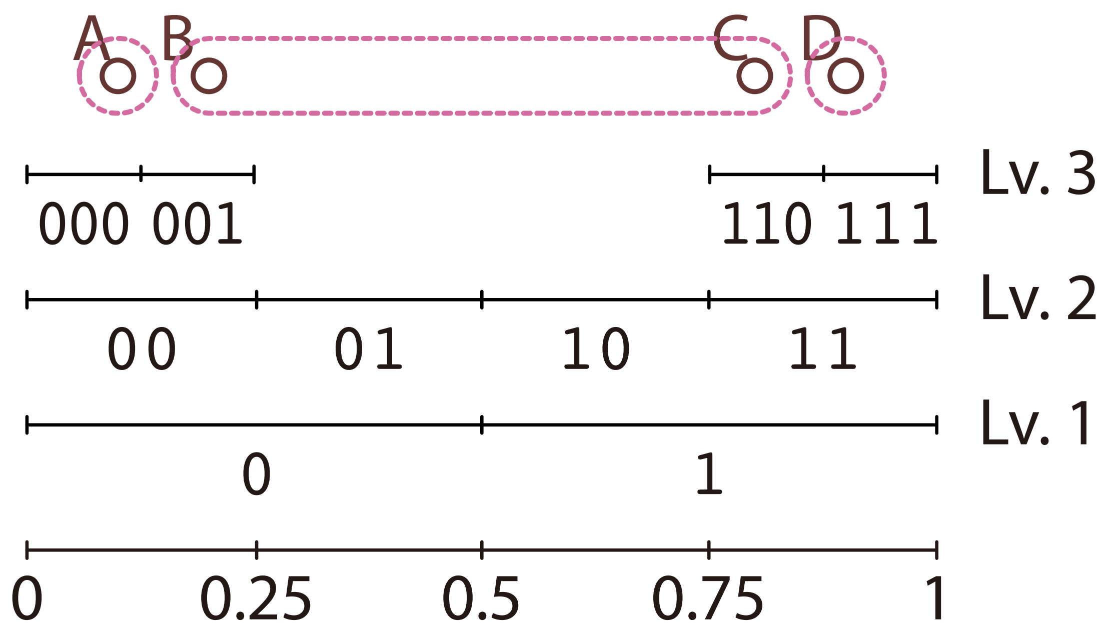

$MCL = 3 \cdot 4 = 12$

MCL with Binary Encoding

id	value
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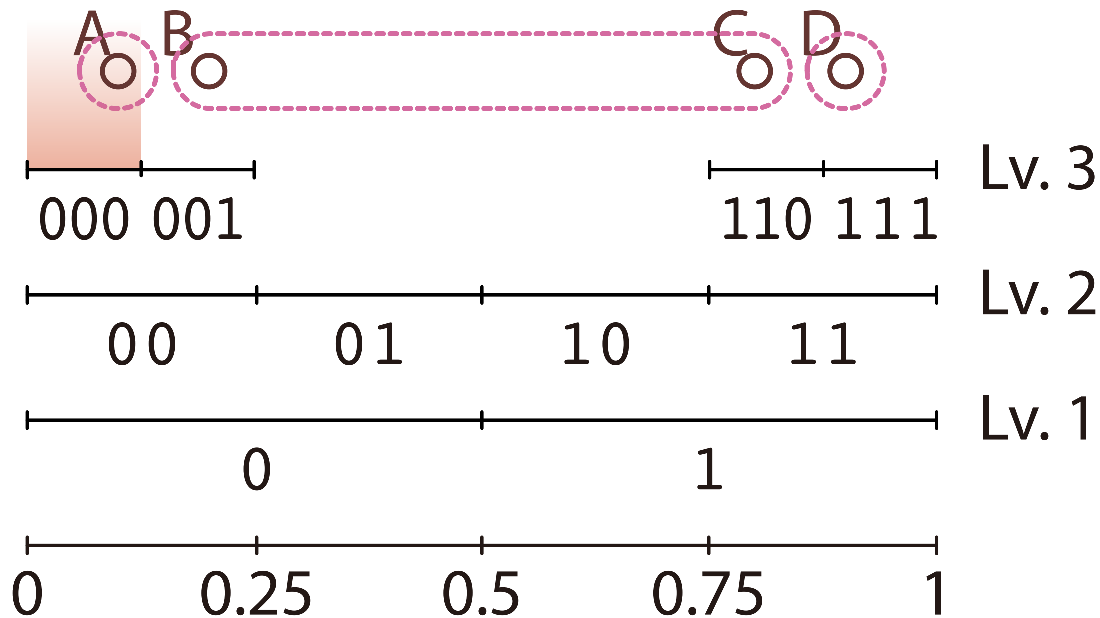

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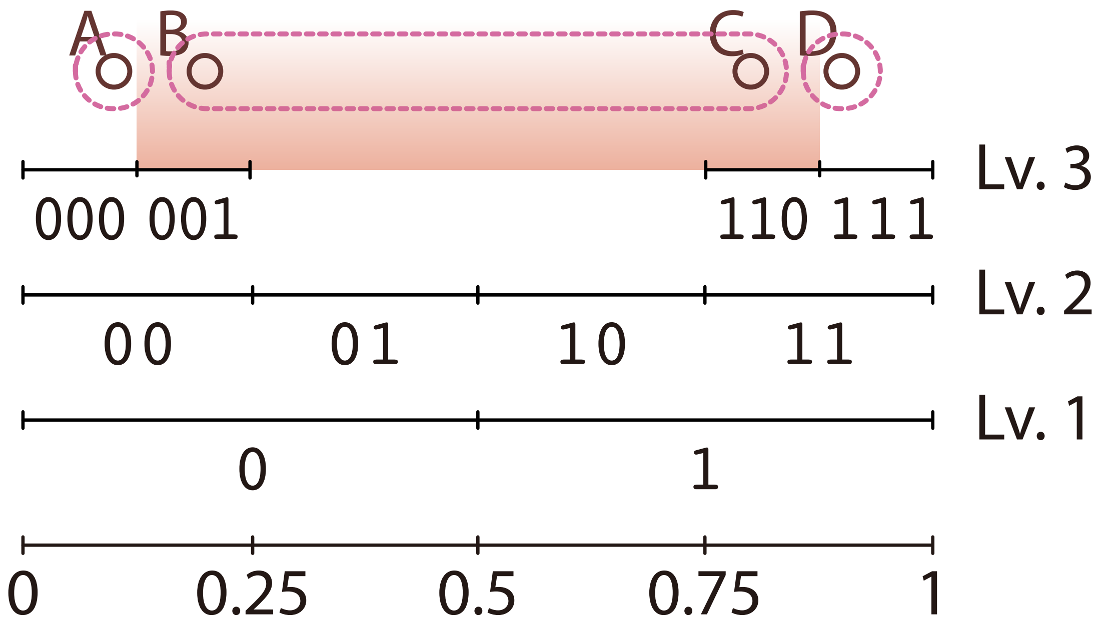

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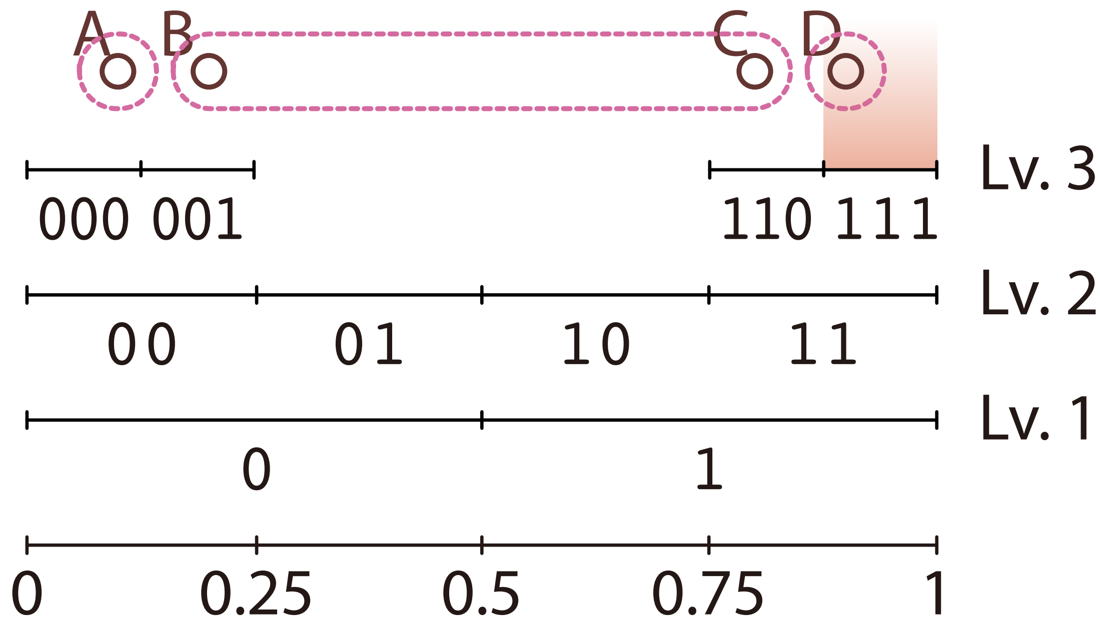

$MCL = 3 \cdot 4 = 12$

Definition of MCL

- Fix an embedding $\gamma : \mathbb{R}^d \to \Sigma^\omega$ ($\Sigma = \{0, 1\}$ usually)
- For $p \in \mathrm{range}(\gamma)$ and $P \subset \mathrm{range}(\gamma)$, define

$$\Phi(p \,|\, P) := \left\{ w \in \Sigma^* \,\middle|\, \begin{array}{l} p \in {\uparrow}w \text{ and } P \cap {\uparrow}v = \varnothing \text{ for all } v \\ \text{such that } |v| = |w| \text{ and } p \in {\uparrow}v \end{array} \right\}$$

  - Each element in $\Phi(p \,|\, P)$ is a prefix that discriminates p from P

For a partition $\mathscr{C} = \{C_1, \dots, C_K\}$ of a data set X,

$\mathrm{MCL}(\mathscr{C}) := \sum_{i \in \{1,\dots,K\}} L_i(\mathscr{C})$, where

$$L_i(\mathscr{C}) := \min \left\{ |W| \,\middle|\, \begin{array}{l} \gamma(C_i) \subseteq {\uparrow}W \text{ and} \\ W \subseteq \bigcup_{x \in C_i} \Phi(\gamma(x) \mid \gamma(X \setminus C_i)) \end{array} \right\}$$

Minimizing MCL and Clustering

Clustering under the MCL criterion is to find the global optimal solution that minimizes the MCL

- Find $\mathscr{C}_{\mathrm{op}}$ such that

  $$\mathscr{C}_{\mathrm{op}} \in \operatorname*{argmin}_{\mathscr{C} \in \mathscr{C}(X)_{\geqslant K}} \mathrm{MCL}(\mathscr{C}),$$

  where $\mathscr{C}(X)_{\geqslant K} = \{\, \mathscr{C} \text{ is a partition of } X \mid \#C \geqslant K \,\}$

- We give the lower bound of the number of clusters K as a input parameter
  - $\mathscr{C}_{\mathrm{op}}$ becomes one set $\{X\}$ without this assumption

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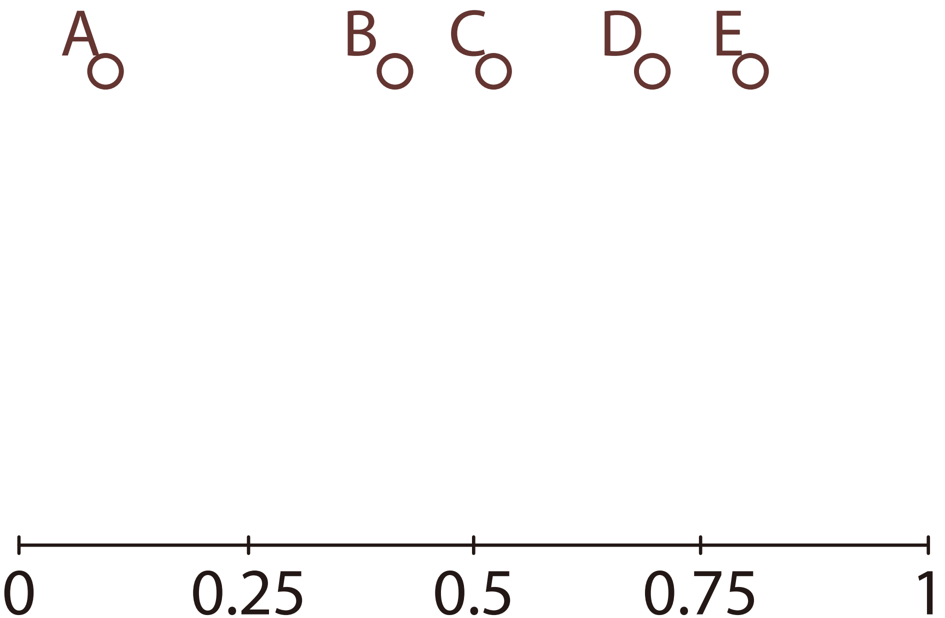
Optimization by COOL

- COOL solves the optimization problem in $O(nd)$
  - n and d are the number of data and dimension, resp.
    - The naïve approach takes exponential time and space
  - Computing process of the MCL becomes clustering process itself via discretization
- COOL is level-wise, and makes the level-k partition $\mathscr{C}^k$ from $k = 1, 2, \dots,$ which holds the following condition:
  - For all $x, y \in X$, they are in the same cluster $\iff$ $v = w$ for some $v \sqsubset \gamma(x)$ and $w \sqsubset \gamma(y)$ with $|v| = |w| = k$
    - Level-k partitions form hierarchy
    - For $C \in \mathscr{C}^k$, there exists $\mathscr{D} \subseteq \mathscr{C}^{k+1}$ such that $\bigcup \mathscr{D} = C$
- For all $C \in \mathscr{C}_{\mathrm{op}}$, there exists k such that $C \in \mathscr{C}^k$

COOL with Binary Encoding

id	value
A	0.113
B	0.398
C	0.526
D	0.701
E	0.796



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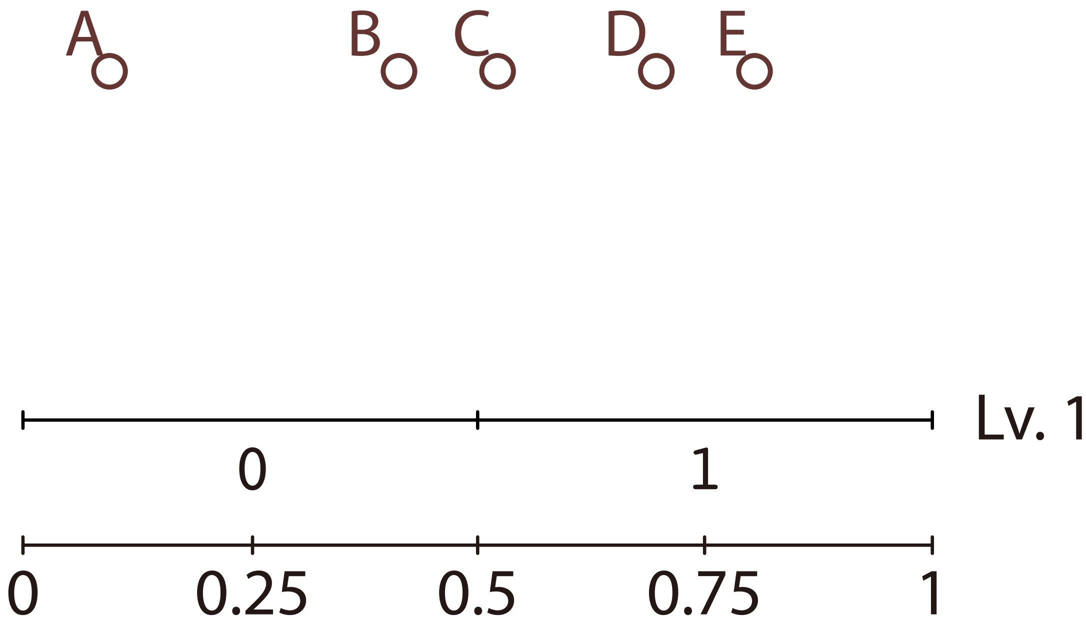
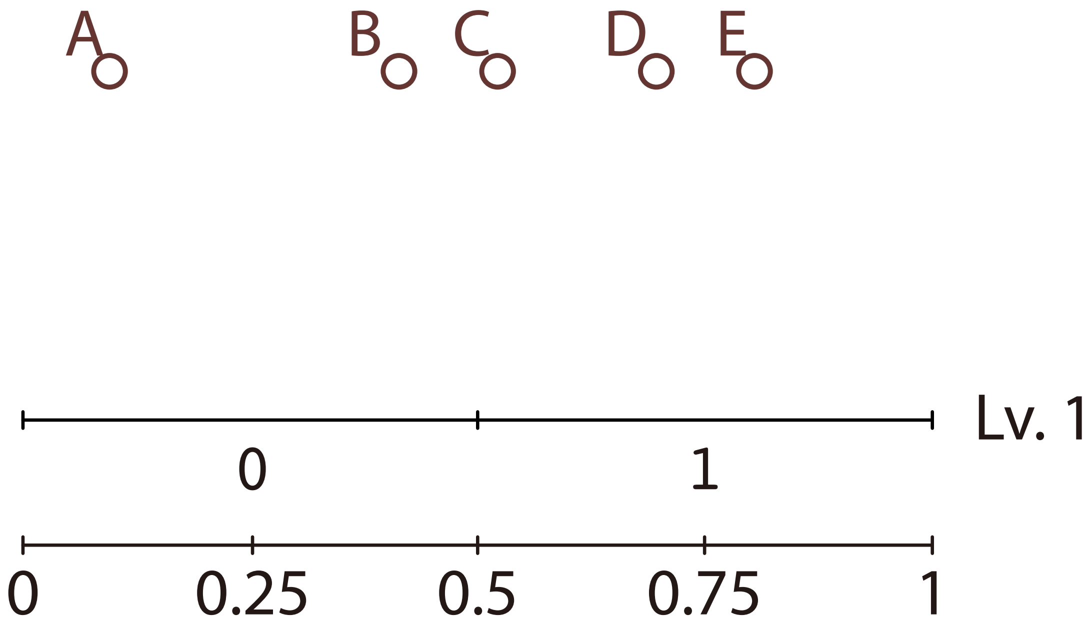


COOL with Binary Encoding

id	value
A	0
B	0
C	1
D	1
E	1



COOL with Binary Encoding

id	value
A	0
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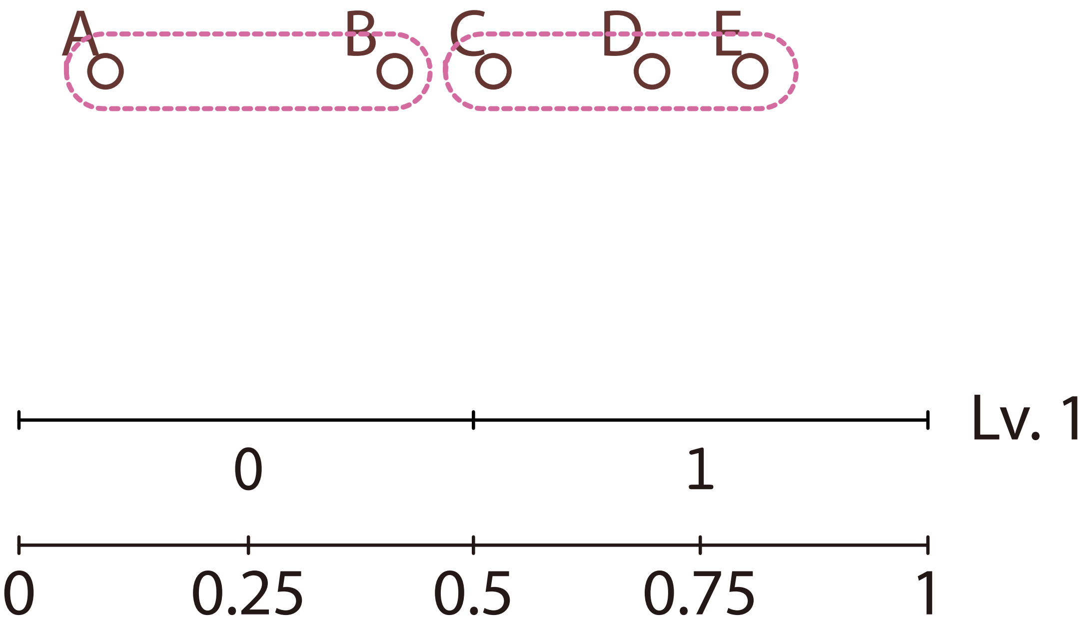
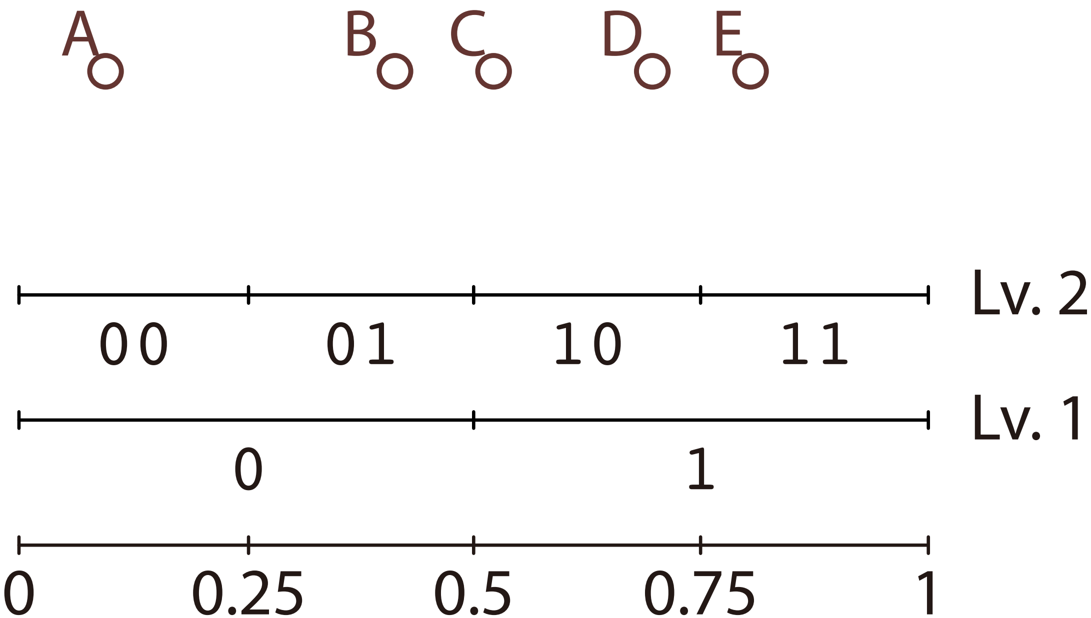


MCL = 1 + 1 = 2

COOL with Binary Encoding

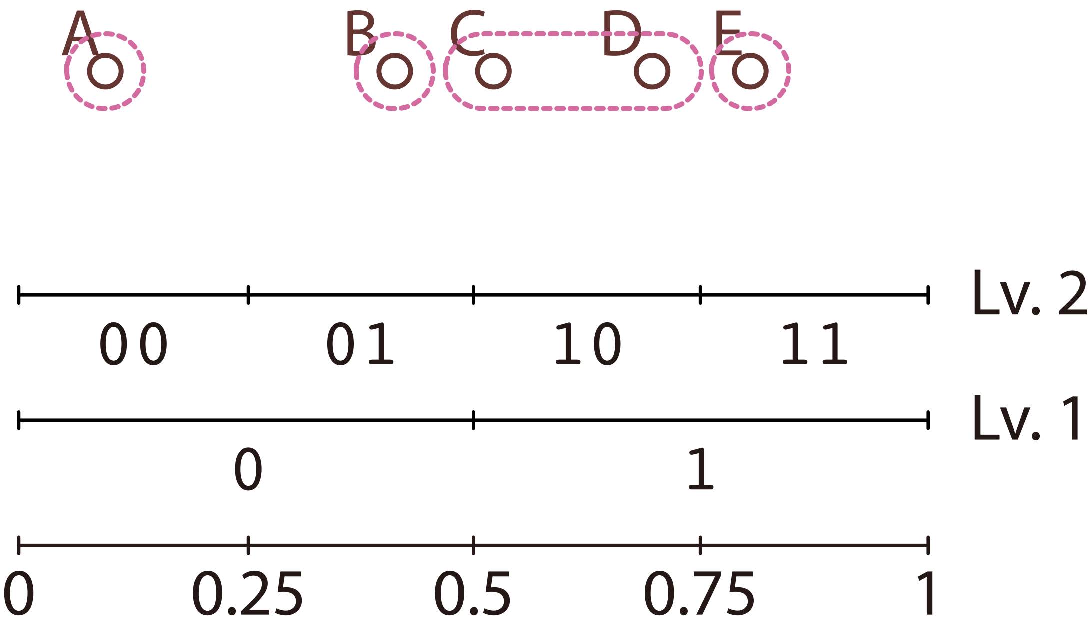
id	value
A	00
B	01
C	10
D	10
E	11



COOL with Binary Encoding

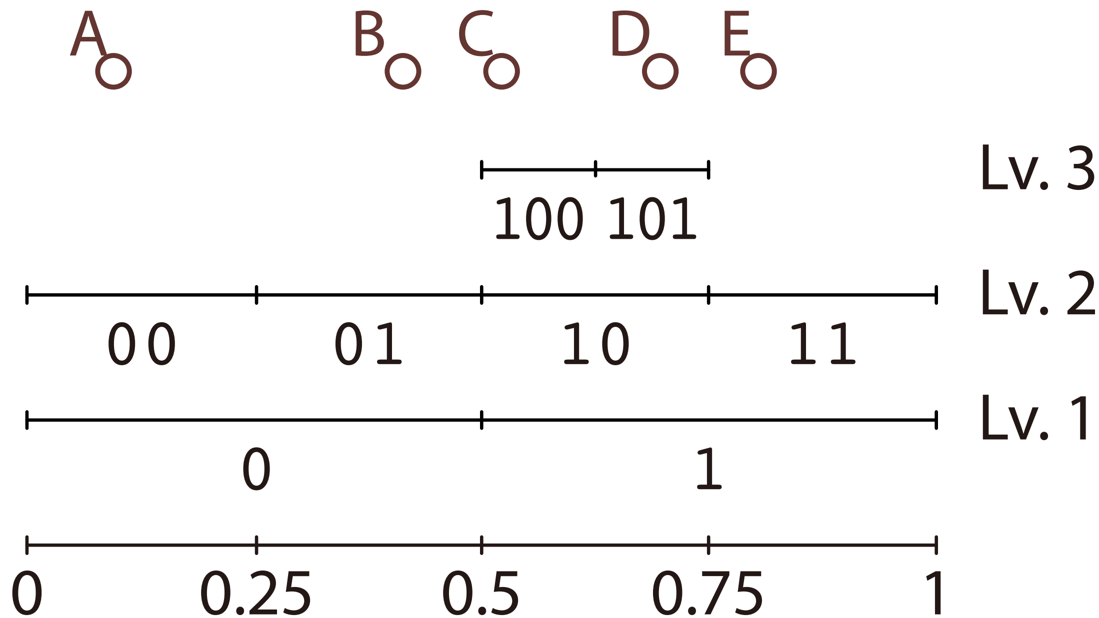
id	value
A	00
B	01
C	10
D	10
E	11

MCL = 2 · 4 = 8



COOL with Binary Encoding

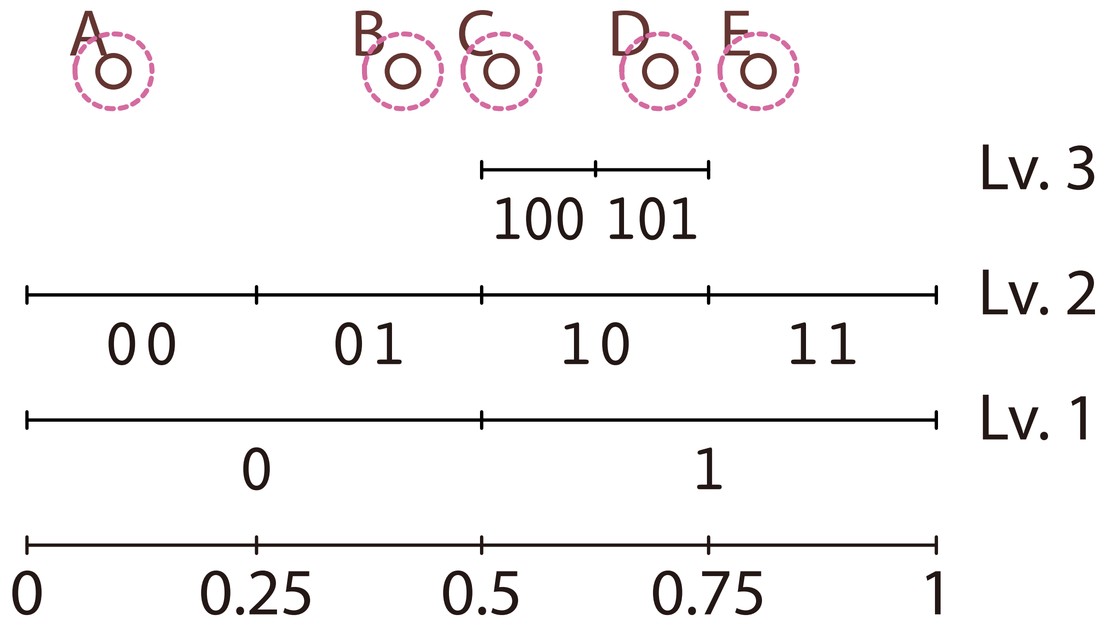
id	value
A	00
B	01
C	100
D	101
E	11



COOL with Binary Encoding

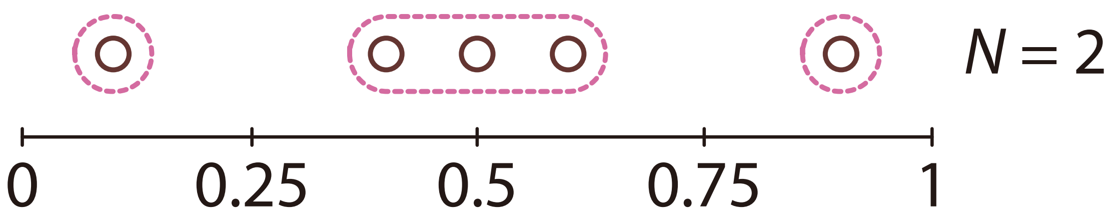
id	value
A	00
B	01
C	100
D	101
E	11

MCL = 6 + 6 = 12



Noise Filtering by COOL

- Noise filtering is easily implemented in COOL
- Define $\mathscr{C}_{\geqslant N} := \{C \in \mathscr{C} \mid \#C \geqslant N\}$ for a partition $\mathscr{C}$
  - See a cluster C as noises if $\#C < N$
- Example: Given $\mathscr{C} = \{\{0.1\}, \{0.4, 0.5, 0.6\}, \{0.9\}\}$
  - $\mathscr{C}_{\geqslant 2} = \{\{0.4, 0.5, 0.6\}\}$, and 0.1 and 0.9 are noises
- We input the lower bound N of the cluster size as a input parameter



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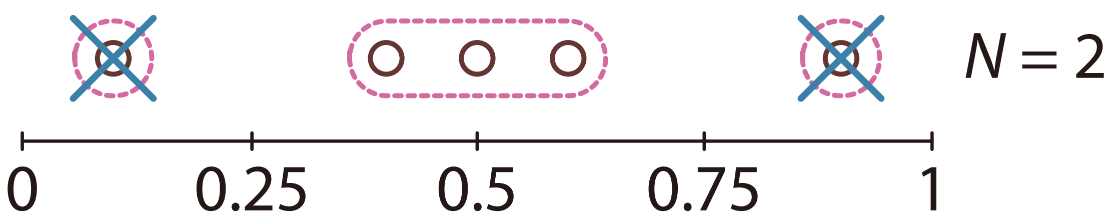

Algorithm of COOL

Input: A data set X, two lower bounds K and N
Output: The optimal partition $\mathscr{C}_{\text{op}}$ and noises

function $\textsc{Cool}(X, K, N)$

```
Find partitions 𝒞^1_{≥N}, ..., 𝒞^m_{≥N} such that ||𝒞^{m−1}_{≥N}|| < K ≤ ||𝒞^m_{≥N}||
(𝒞_op, MCL(𝒞_op)) ← FindClusters(X, K, {𝒞^1_{≥N}, ..., 𝒞^m_{≥N}})
return (𝒞_op, X \ ⋃ 𝒞_op)
```

function $\textsc{FindClusters}(X, K, \{\mathscr{C}^1, \dots, \mathscr{C}^m\})$

```
Find k such that ||𝒞^{k−1}|| < K and ||𝒞^k|| ≥ K
𝒞_op ← 𝒞^k
if K = 2 then return (𝒞_op, MCL(𝒞_op))
for each C in 𝒞^1 ∪ ... ∪ 𝒞^{k−1}
    (𝒞, L) ← FindClusters(X \ C, K − 1, {𝒞^1, ..., 𝒞^k})
    if MCL(𝒞 ∪ C) < MCL(𝒞_op) then 𝒞_op ← C ∪ 𝒞
return (𝒞_op, MCL(𝒞_op))
```

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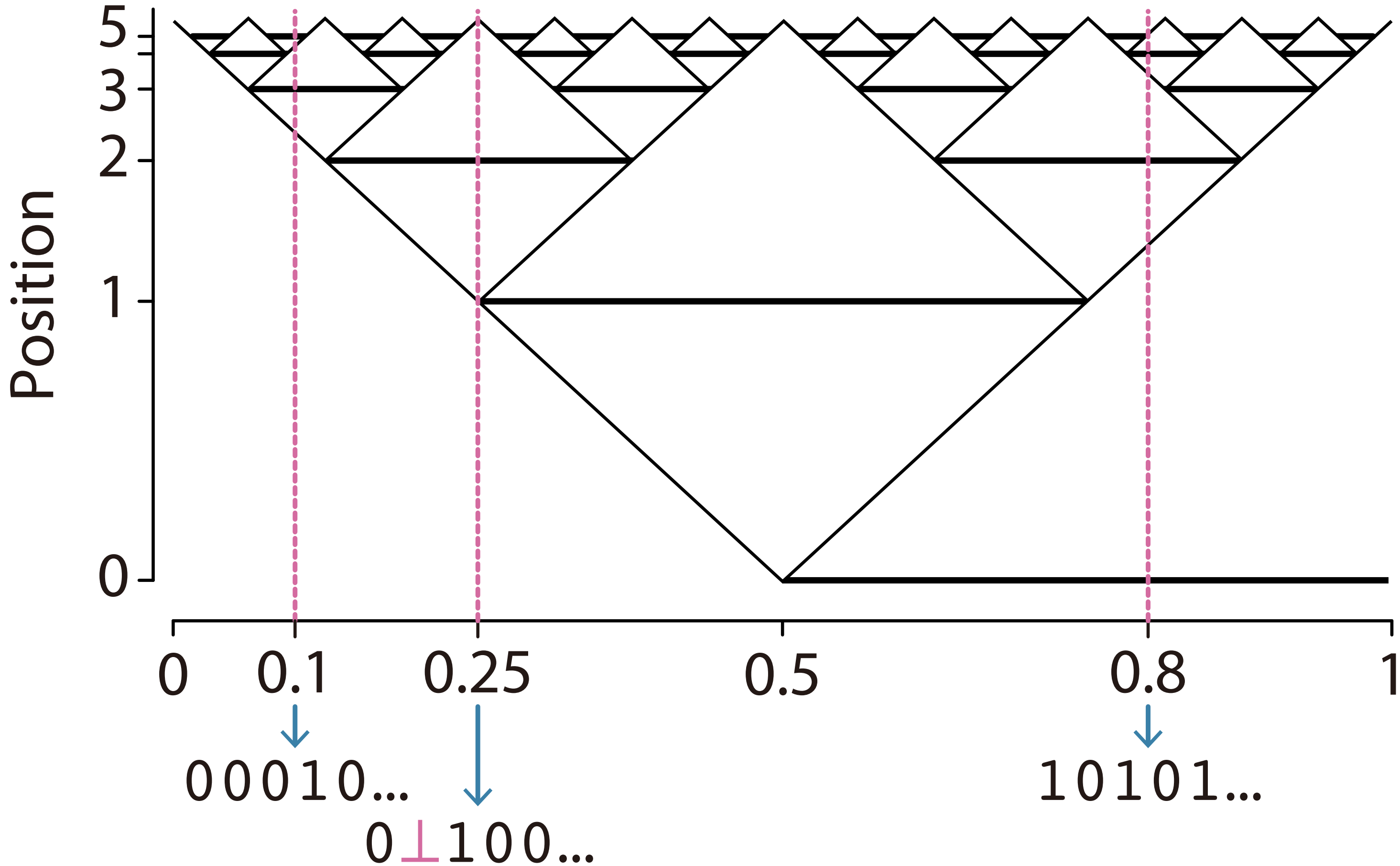
Gray Code

- Real numbers in [0, 1] are encoded with 0, 1, and $\perp$
  Binary: $0.1 \to \texttt{00011}\ldots, 0.25 \to \texttt{00111}\ldots$
  Gray: $0.1 \to \texttt{00010}\ldots, 0.25 \to \texttt{0}\perp\texttt{100}\ldots$
- Originally, another binary encoding of natural numbers
  - Especially important in applications of conversion between analog and digital information [Knuth, 2005]

The Gray code embedding is an injection γ_{G} that maps $x \in [0, 1]$ to an infinite sequence $p_0 p_1 p_2 \ldots$, where

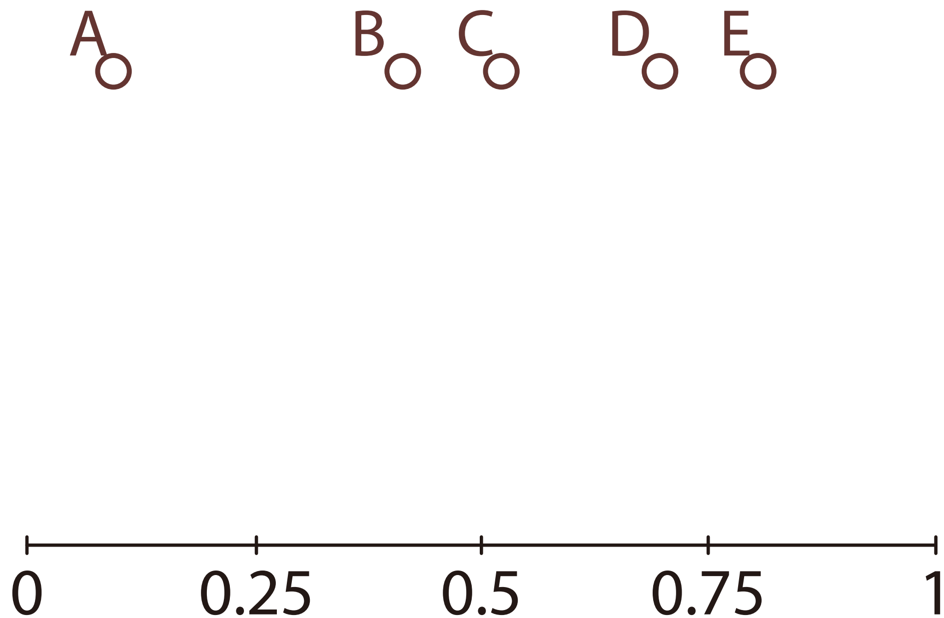
- $p_i := 1$ if $2^{-i}m - 2^{-(i+1)} < x < 2^{-i}m + 2^{-(i+1)}$ for an odd m, $p_i := 0$ if the same holds for an even m, and $p_i := \perp$ if $x = 2^{-i}m - 2^{-(i+1)}$ for some integer m
- For a vector $\boldsymbol{x} = (x^1, \ldots, x^d)$, $\gamma_{\mathrm{G}}(\boldsymbol{x}) = p_1^1 \ldots p_1^d p_2^1 \ldots p_2^d \ldots$

Gray Code Embedding



COOL with Gray Code (G-COOL)

id	value
A	0.113
B	0.398
C	0.526
D	0.701
E	0.796



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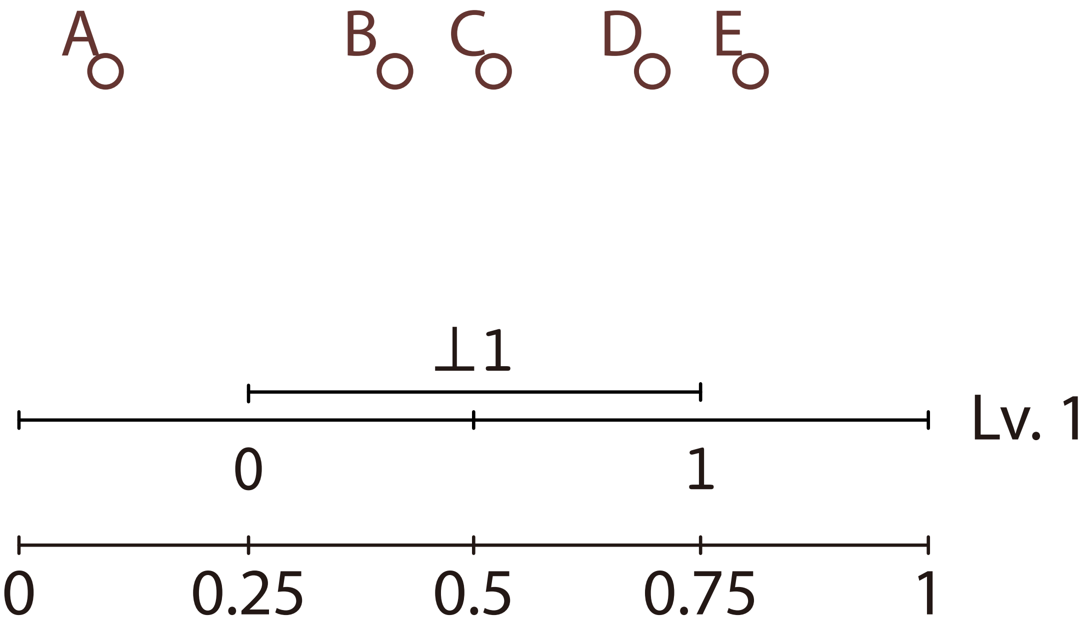
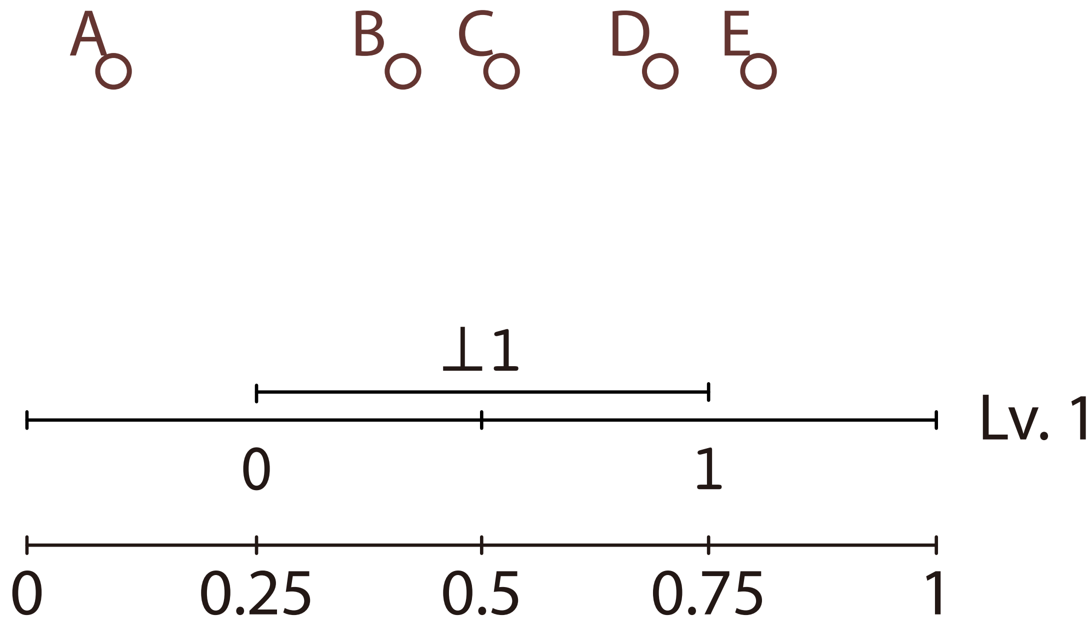


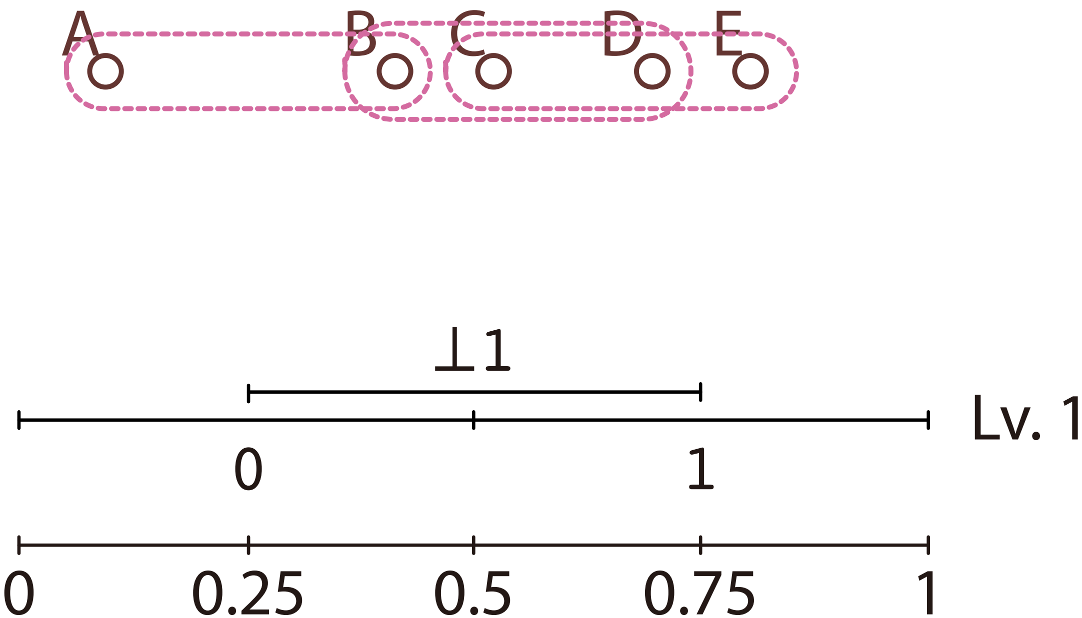
COOL with Gray Code (G-COOL)

id	value
A	0
B	0, ⊥1
C	1, ⊥1
D	1, ⊥1
E	1



COOL with Gray Code (G-COOL)

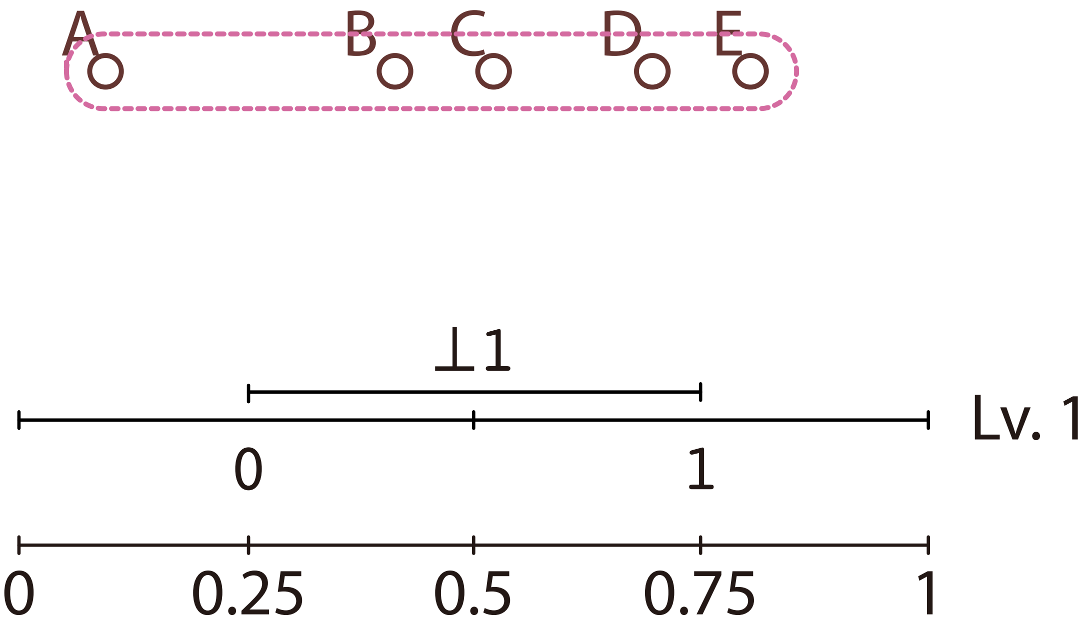
id	value
A	0
B	0, ⊥1
C	1, ⊥1
D	1, ⊥1
E	1



COOL with Gray Code (G-COOL)

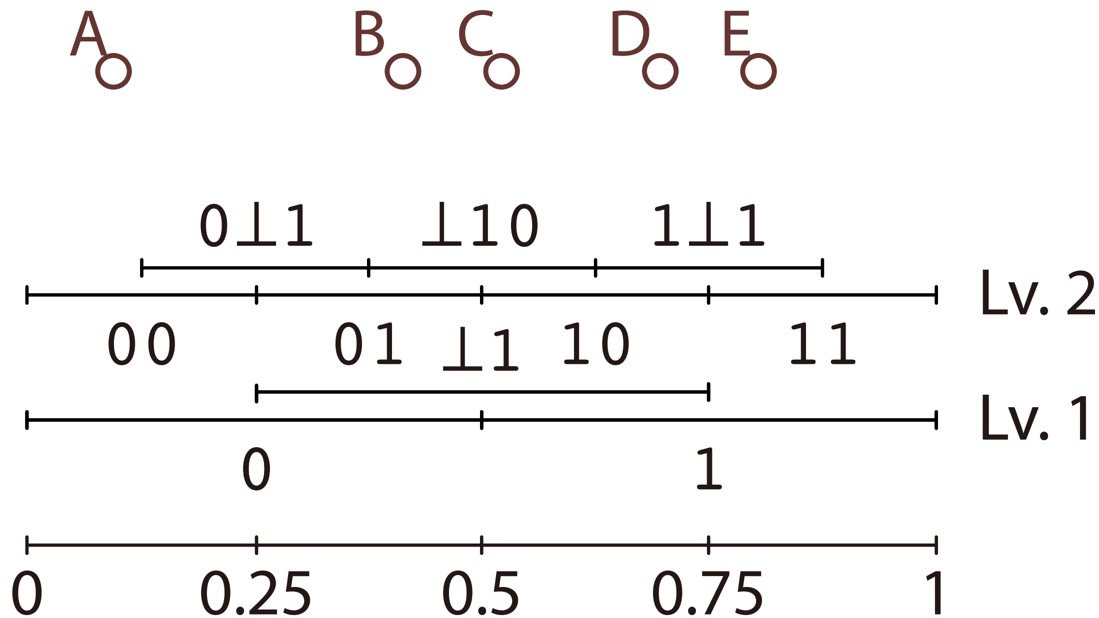
id	value
A	0
B	0, ⊥1
C	1, ⊥1
D	1, ⊥1
E	1

MCL = 1 · 2 = 2



COOL with Gray Code (G-COOL)

id	value
A	00
B	01, ⊥10
C	10, ⊥10
D	10, 1⊥1
E	11, 1⊥1



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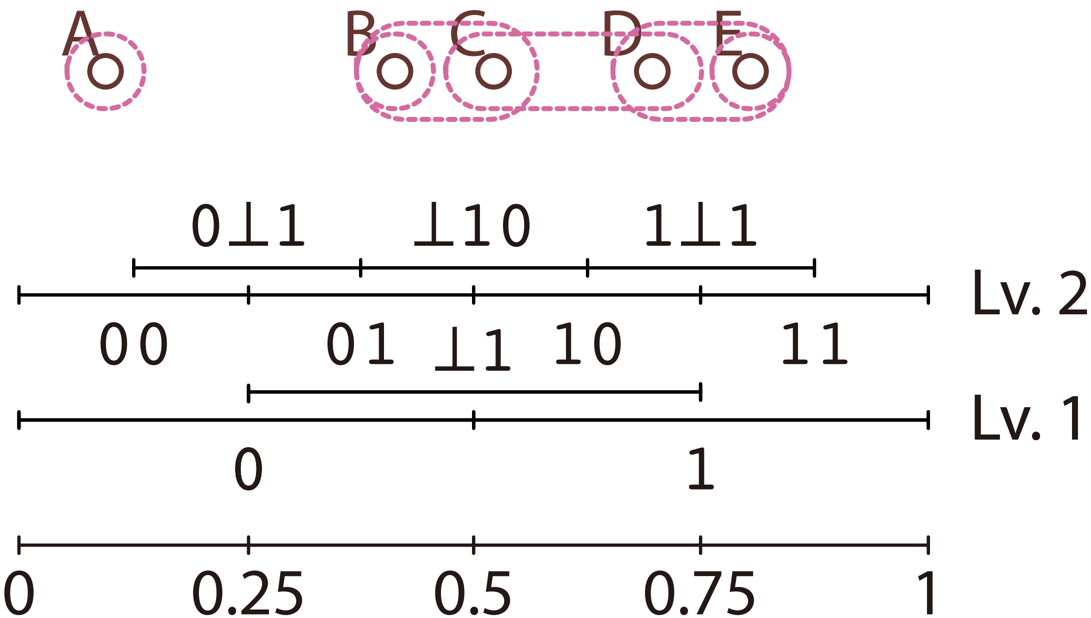

COOL with Gray Code (G-COOL)

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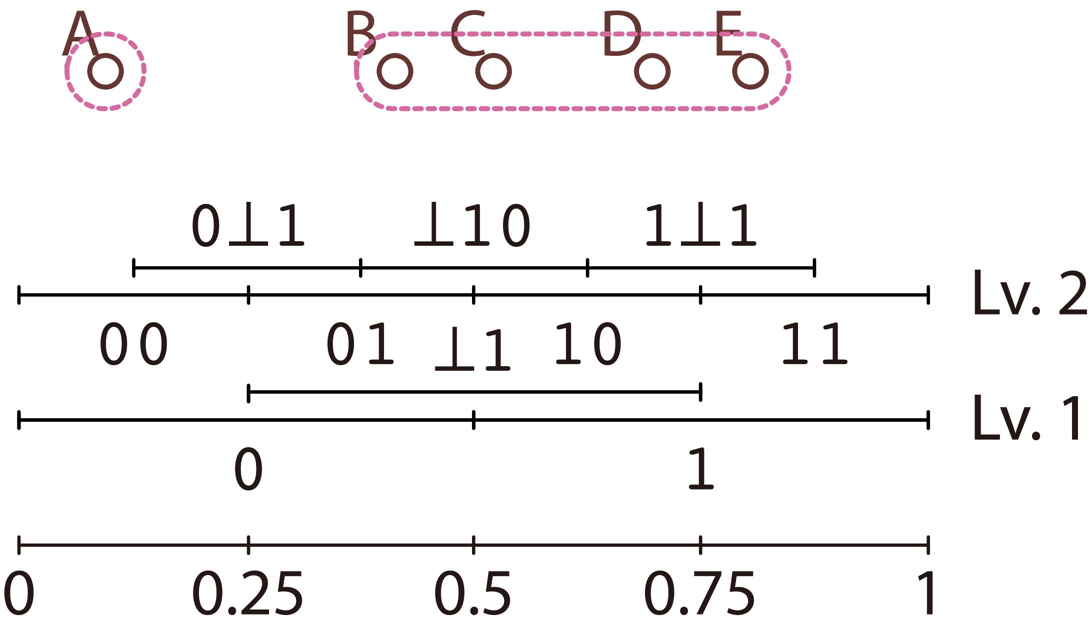
D	10, 1⊥1
E	11, 1⊥1

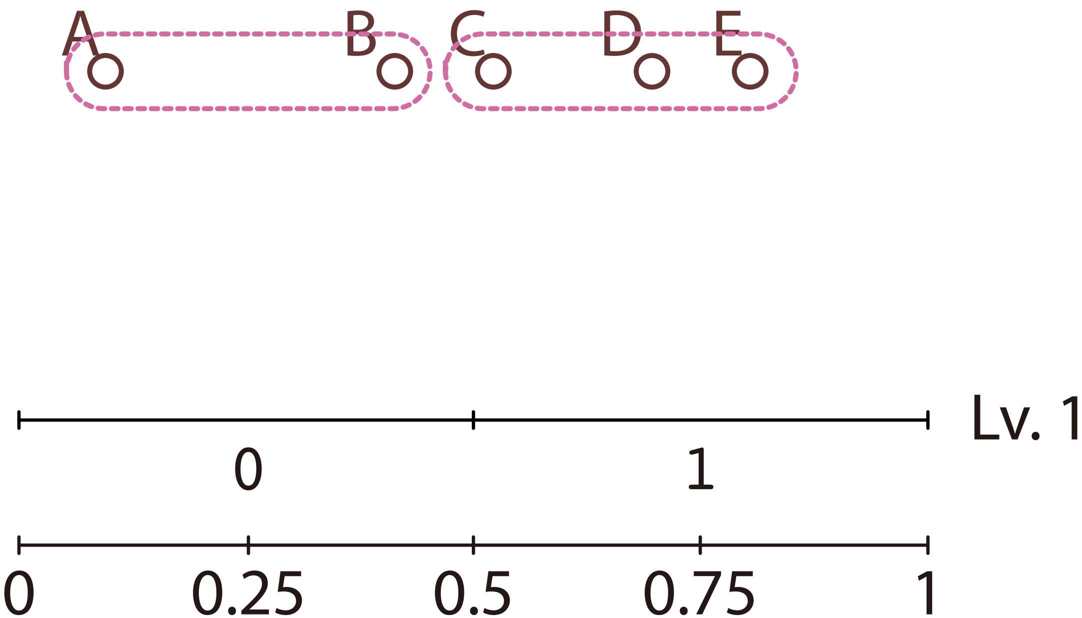
MCL = 2 · 3 = 6



COOL with Binary Encoding

id	value
A	0
B	0
C	1
D	1
E	1

MCL = 1 + 1 = 2

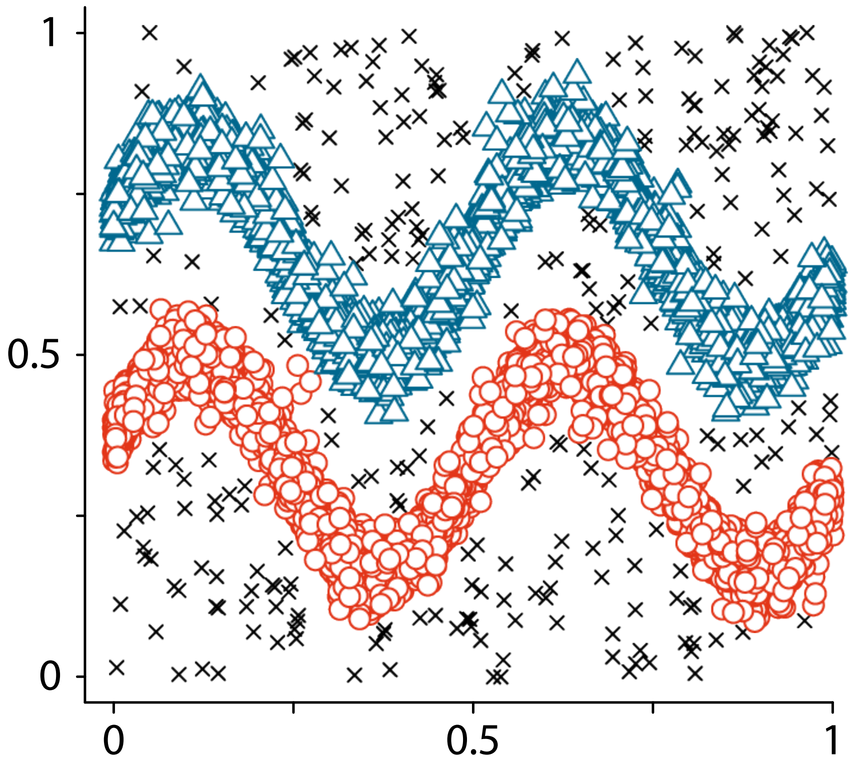


Theoretical Analysis of G-COOL

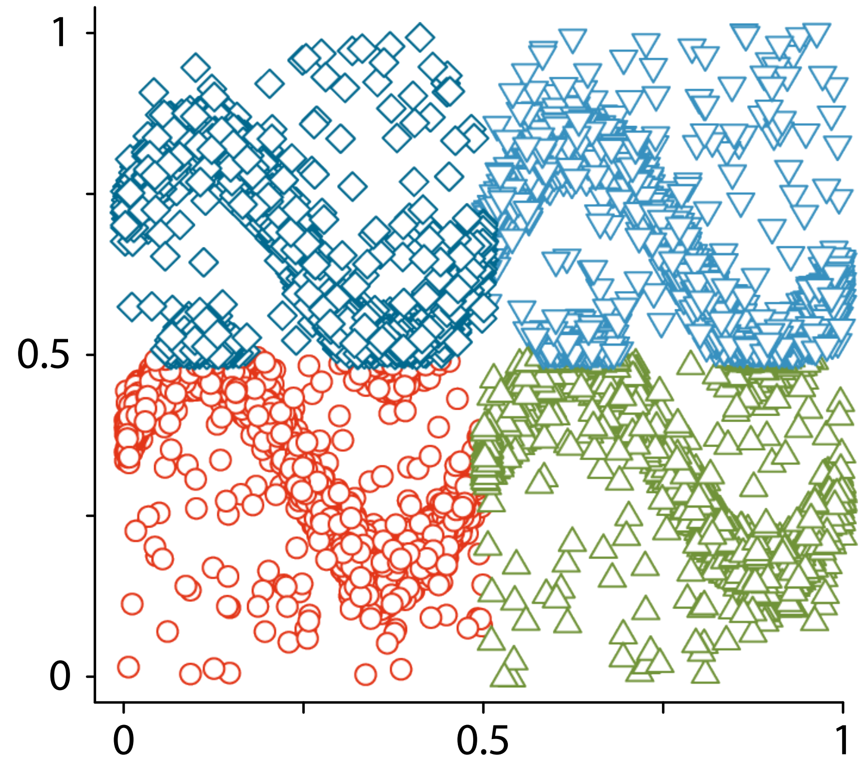
- Use the Gray code as a fixed encoding in COOL
  - It achieves internal cohesion and external isolation
- ***Theorem:*** ***For the level-k partition $\mathscr{C}^k$, $x, y \in X$ are in the same cluster if $d_\infty(x, y) < 2^{-(k+1)}$***
  - Thus x, y are in the different clusters only if $d_\infty(x, y) \geqslant 2^{-(k+1)}$
  - $d_\infty(x, y) = \max_{i \in \{1,\dots,d\}} |x_i - y_i|$ (L_∞ metric)
    - Two adjacent intervals overlap and they are agglomerated
- ***Corollary:*** ***In the optimal partition $\mathscr{C}_{op}$, for all $x \in C$ ($C \in \mathscr{C}_{op}$), its nearest neighbor $y \in C$***
  - y is nearest neighbor of $x \iff y \in \operatorname{argmin}_{y \in X} d_\infty(x, y)$

Demonstration of G-COOL

G-COOL



COOL with the binary encoding



Outline

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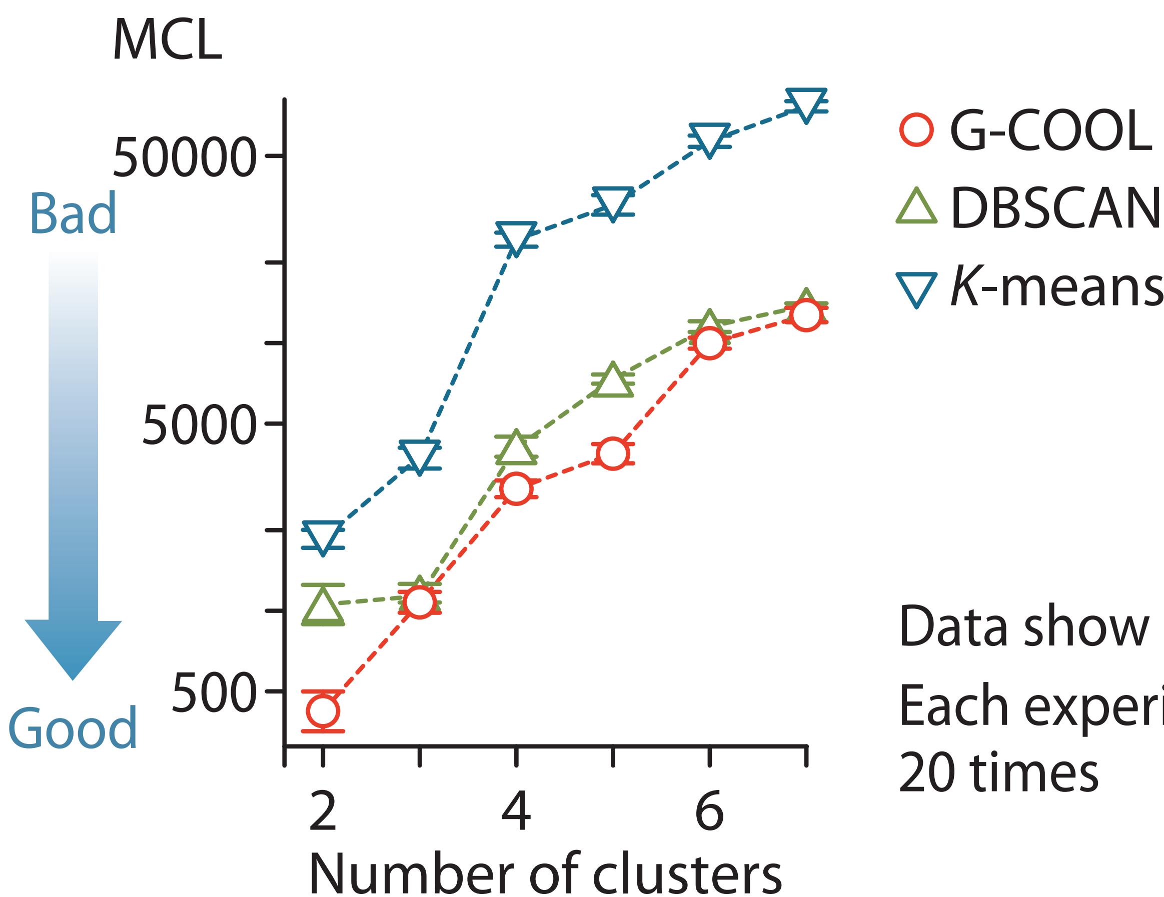
Experimental Methods

- Analyze G-COOL empirically with synthetic and real datasets compared to DBSCAN and *K*-means
  - Synthetic datasets were generated by the R package *clusterGeneration* [Qiu and Joe, 2006]
    - $n = 1,500$ for each cluster and $d = 3$
  - Real datasets were geospatial images from Earth-as-Art
    - reduced to 200×200 pixels, translated into binary images
  - All data were normalized by min-max normalization
- G-COOL was implemented by R (version 2.12.1)
- Internal and External measure were used
  - Internal: MCL, connectivity, Silhouette width
  - External: adjusted Rand index

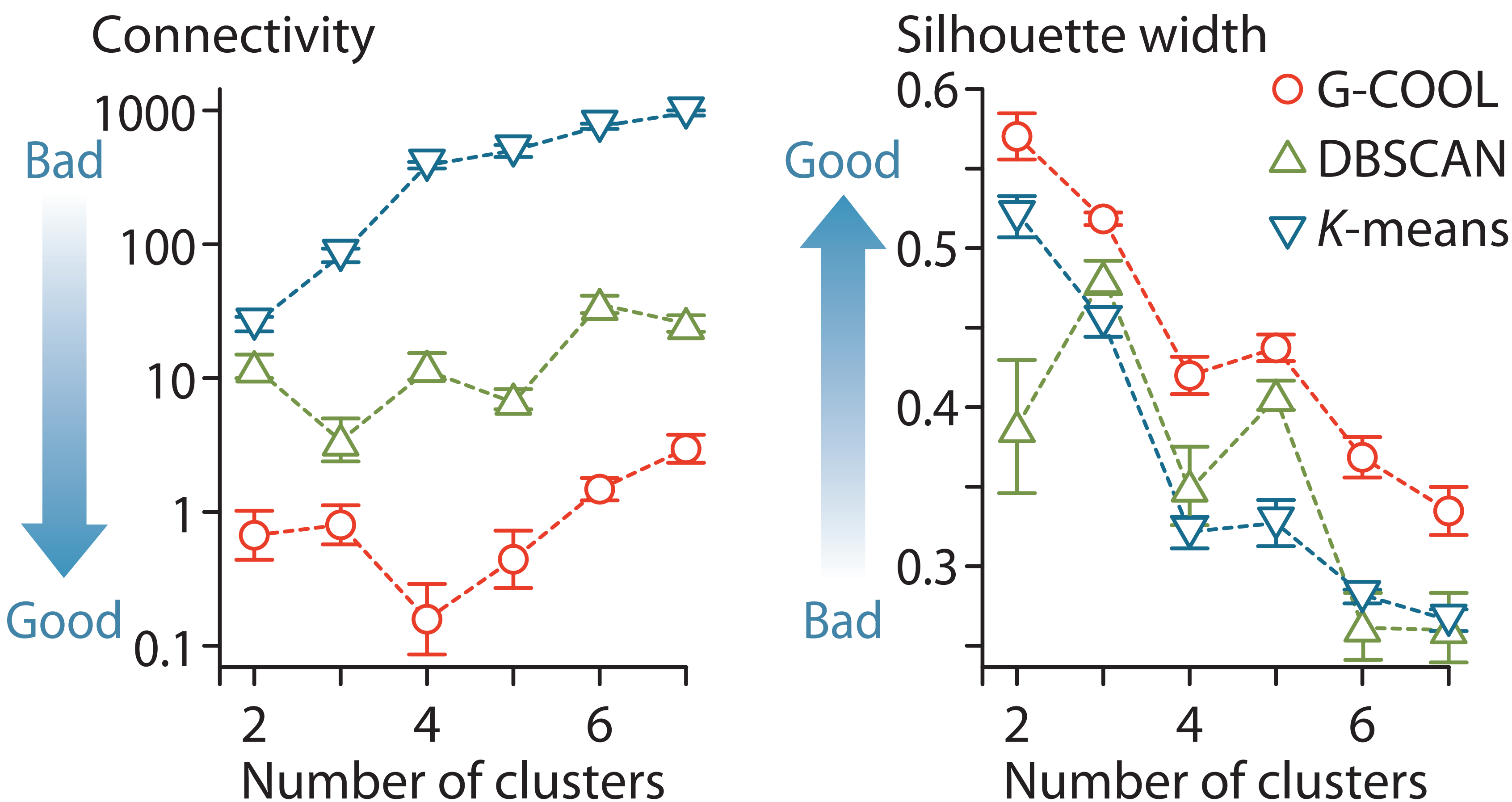
Results (Synthetic datasets)



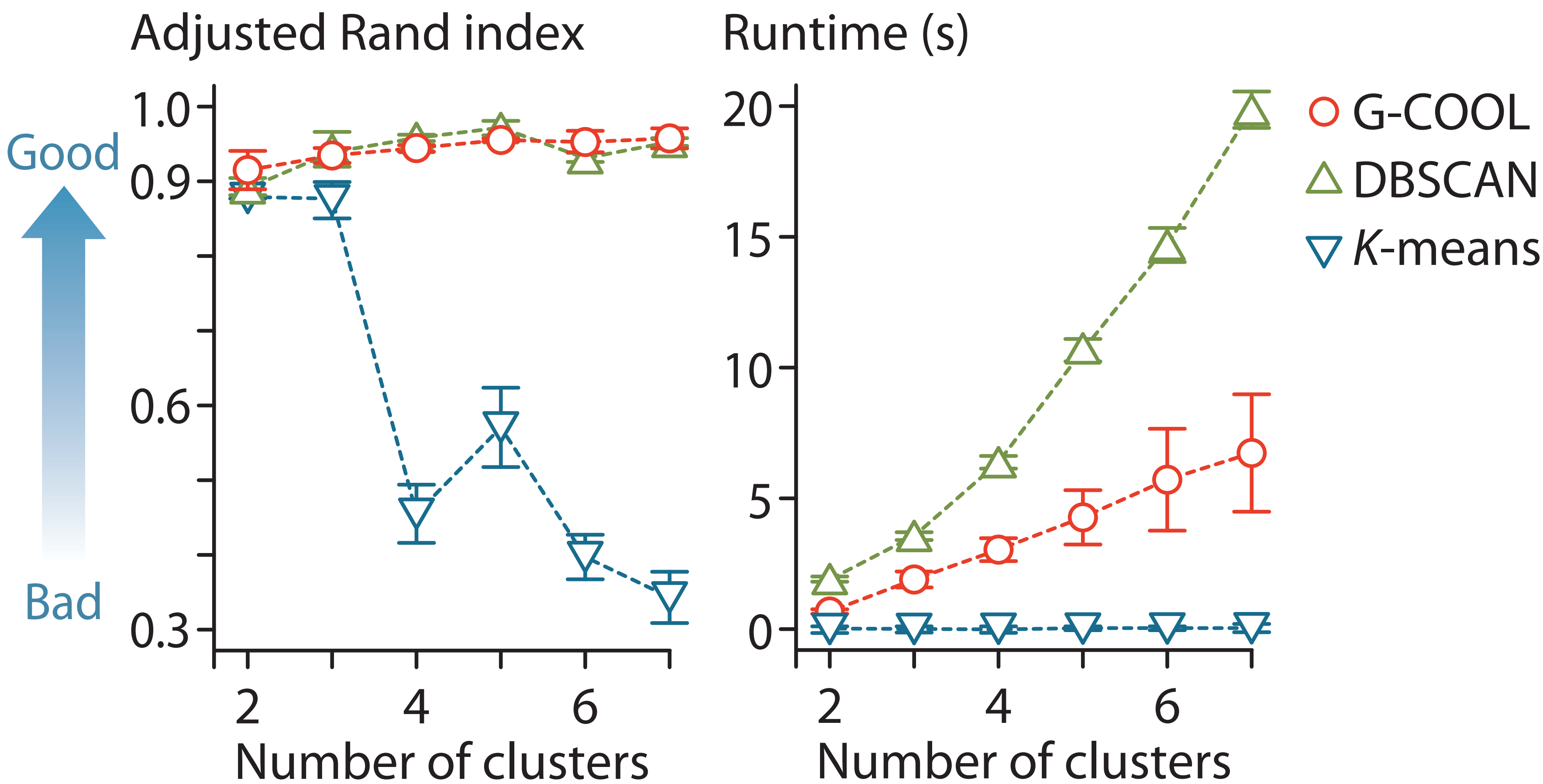
Data show mean ± s.e.m.

Each experiment was performed 20 times

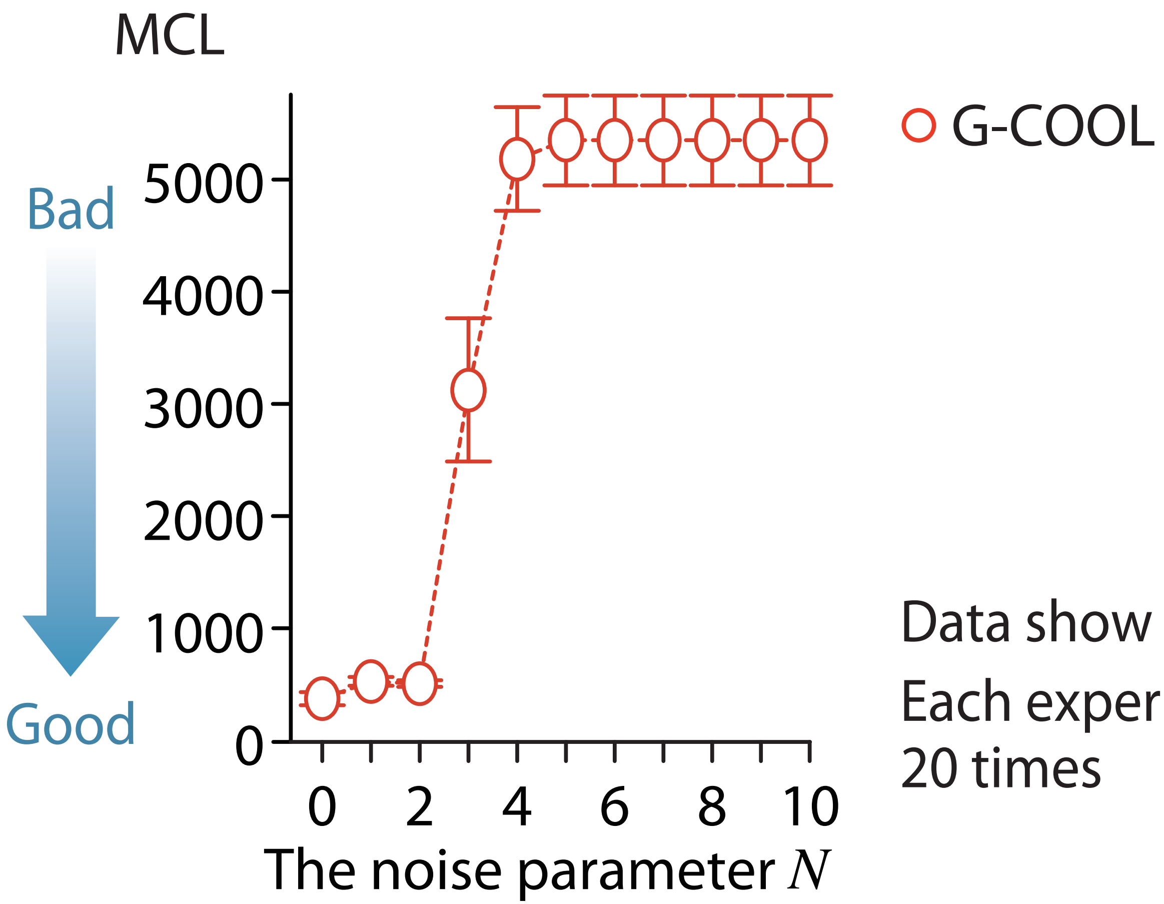
Results (Synthetic datasets)



Results (Synthetic datasets)



Results (Synthetic datasets)



Data show mean ± s.e.m.

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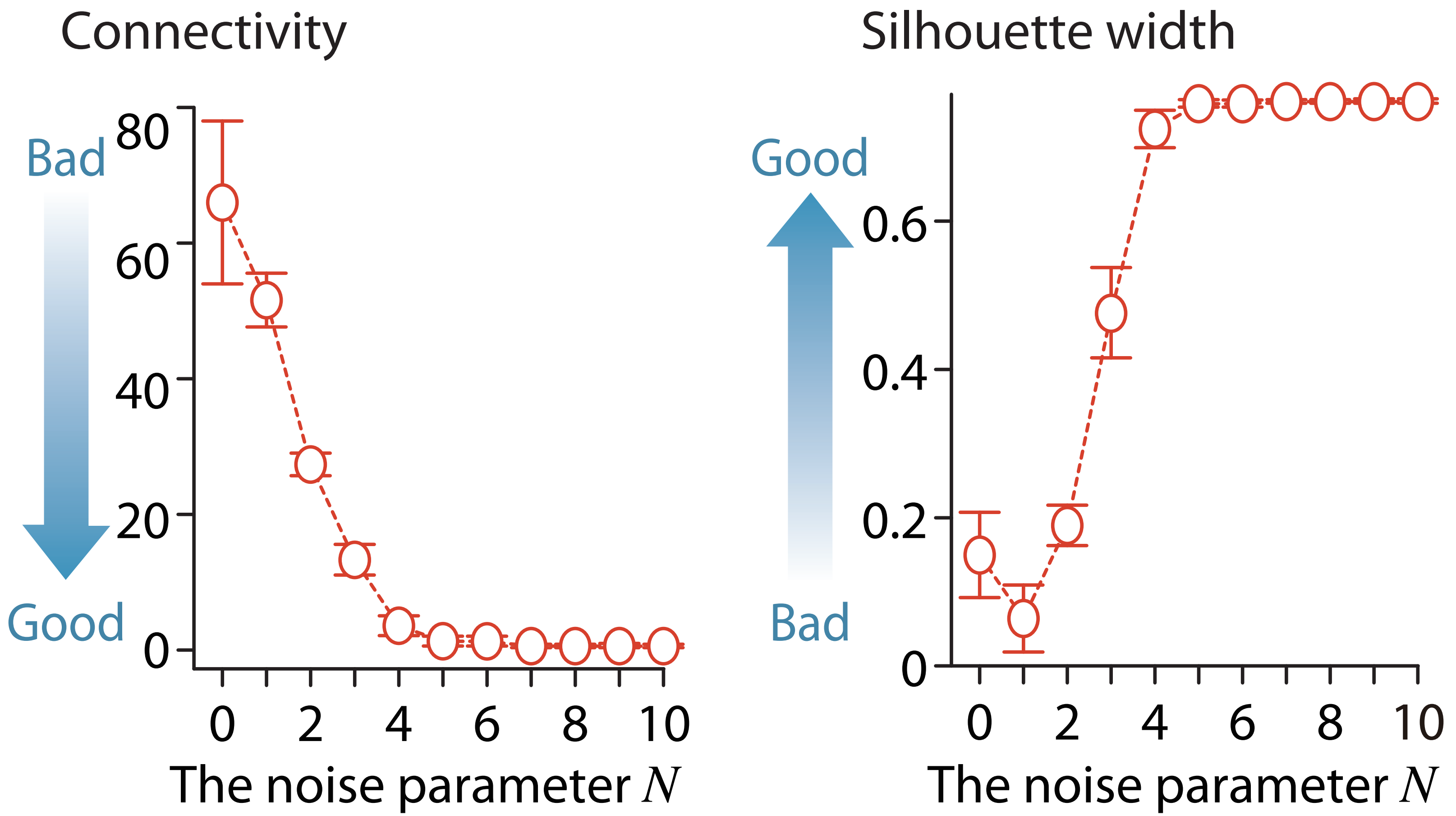
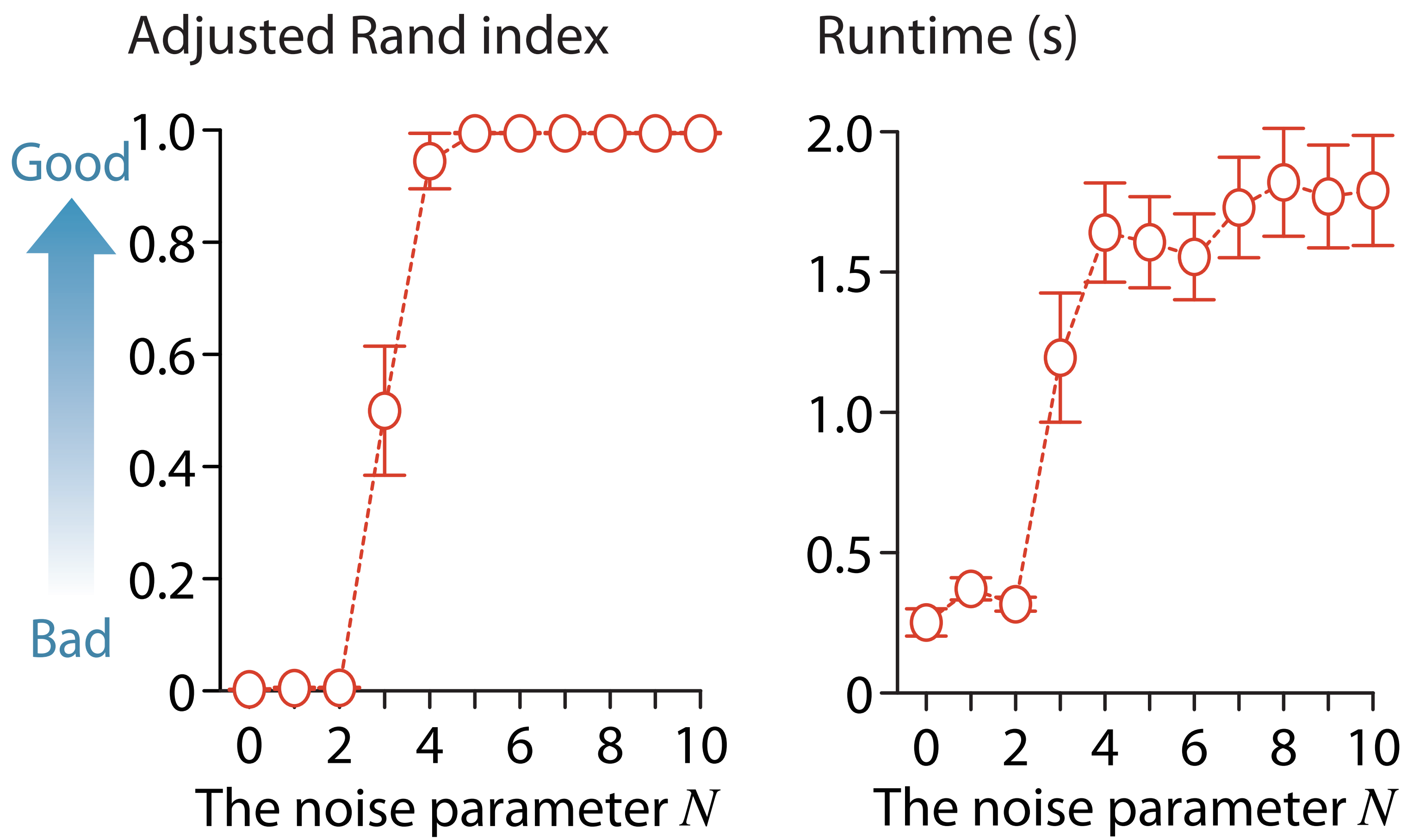
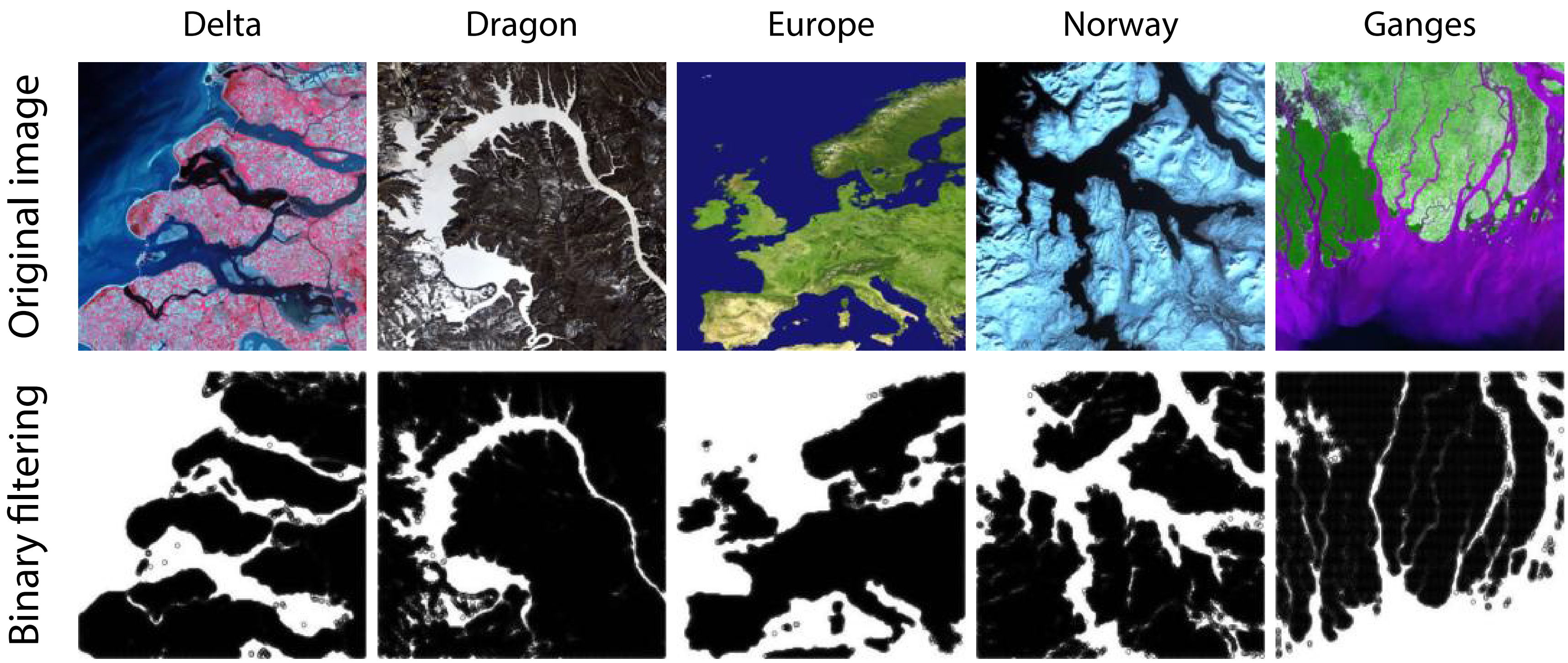
Results (Synthetic datasets)



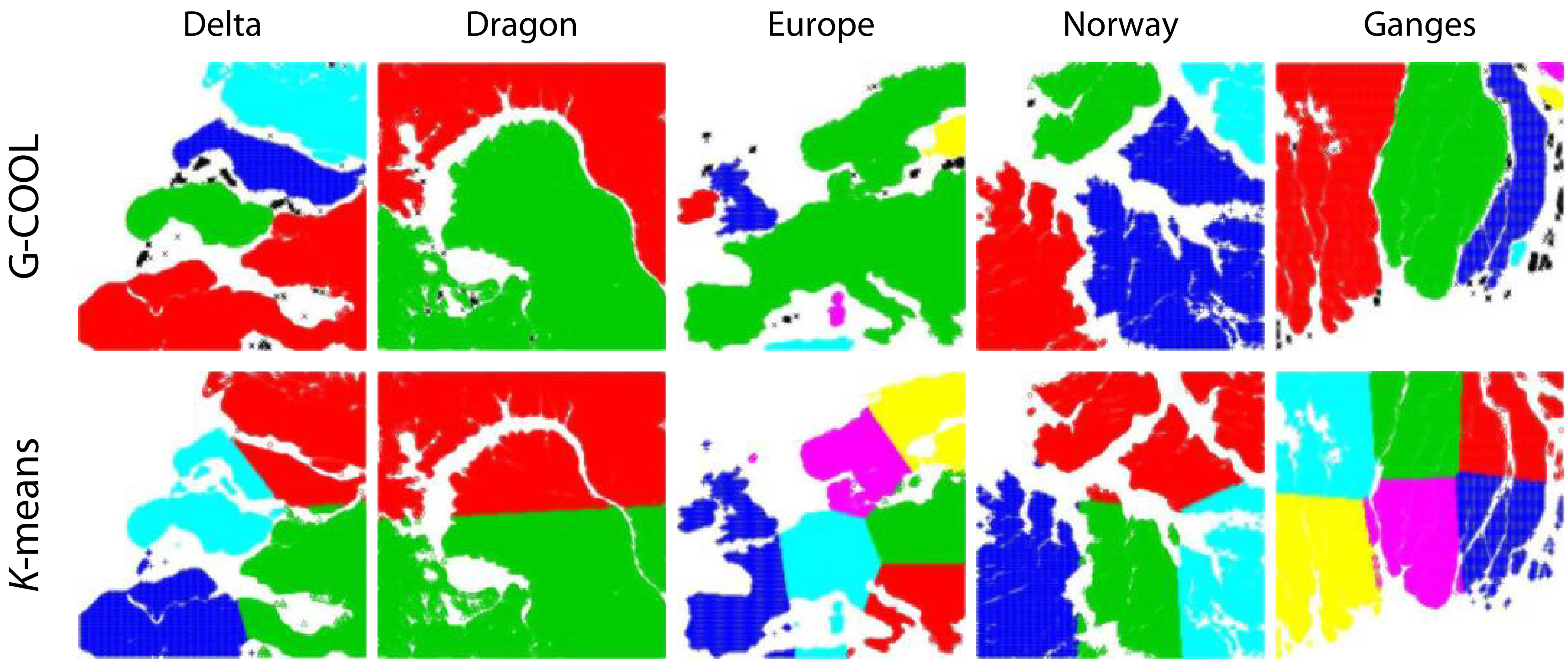
Results (Synthetic datasets)



Results (Real datasets)



Results (Real datasets)



Results (Real datasets)

Name	n	K	Running time (s)		MCL	
			GC	KM	GC	KM
Delta	20748	4	1.158	0.012	4010	4922
Dragon	29826	2	0.595	0.026	3906	7166
Europe	17380	6	2.404	0.041	2320	12210
Norway	22771	5	0.746	0.026	1820	6114
Ganges	18019	6	0.595	0.026	2320	12526

GC: G-COOL, KM: K-means

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Conclusion

- Integrate clustering and its evaluation in the coding-oriented manner
  - An effective solution for two essential problems, how to measure goodness of results and how to find good clusters
    - No distance calculation and no data distribution
- ***Key ideas:***

1. ***Fix of an encoding scheme for real-valued variables***
   - Introduced the MCL focusing on compression of clusters
   - Formulated clustering with the MCL, and constructed COOL that finds the global optimal solution linearly
2. ***The Gray code***
   - We showed efficiency and effectiveness of G-COOL by theoretically and experimentally

Appendix

Notation (1/2)

- A datum $\boldsymbol{x} \in \mathbb{R}^d$, a data set $X = \{x_1, \dots, x_n\}$
  - $\#X$ is the number of elements in X
  - $X \setminus Y$ is the relative complement of Y in X
- Clustering is partition of X into K subsets (clusters) $C_1, \dots, C_K$
  - $C_i \neq \emptyset$ and $C_i \cap C_j = \emptyset$
  - We call $\mathscr{C} = \{C_1, \dots, C_K\}$ a partition of X
  - $\mathscr{C}(X) = \{\mathscr{C} \mid \mathscr{C}$ is a partition of $X\}$
- The set of finite and infinite sequences over an alphabet Σ are denoted by Σ^* and Σ^ω, resp.
  - The length $|w|$ is the number of symbols other than $\perp$
    - If $w = 11\perp100\perp\perp\dots$, then $|w| = 5$
  - For a set of sequences W, $|W| = \sum_{w \in W} |w|$

Notation (2/2)

- An embedding of $\mathbb{R}^d$ is an injective function γ from $\mathbb{R}^d$ to Σ^ω
- For $p, q \in \Sigma^\omega$, define $p \leqslant q$ if $p_i = q_i$ for all i with $p_i \neq \bot$
  - Intuitively, q is more concrete than p
- For $w \in \Sigma^*$, we write $w \sqsubset p$ if $w\bot^\omega \leqslant p$
  - $\uparrow w = \{p \in \mathrm{range}(\gamma) \mid w \sqsubset p\}$ for $w \in \Sigma^*$
  - $\uparrow W = \{p \in \mathrm{range}(\gamma) \mid w \sqsubset p \text{ for some } w \in W\}$ for $W \subseteq \Sigma^*$
- The following monotonicity holds
  - $\gamma^{-1}(\uparrow v) \subseteq \gamma^{-1}(\uparrow w)$ iff $v\bot^\omega \geqslant w\bot^\omega$

Optimization by COOL (cont.)

- The optimal partition $\mathscr{C}_{\text{op}}$ can be constructed by the level-k partitions

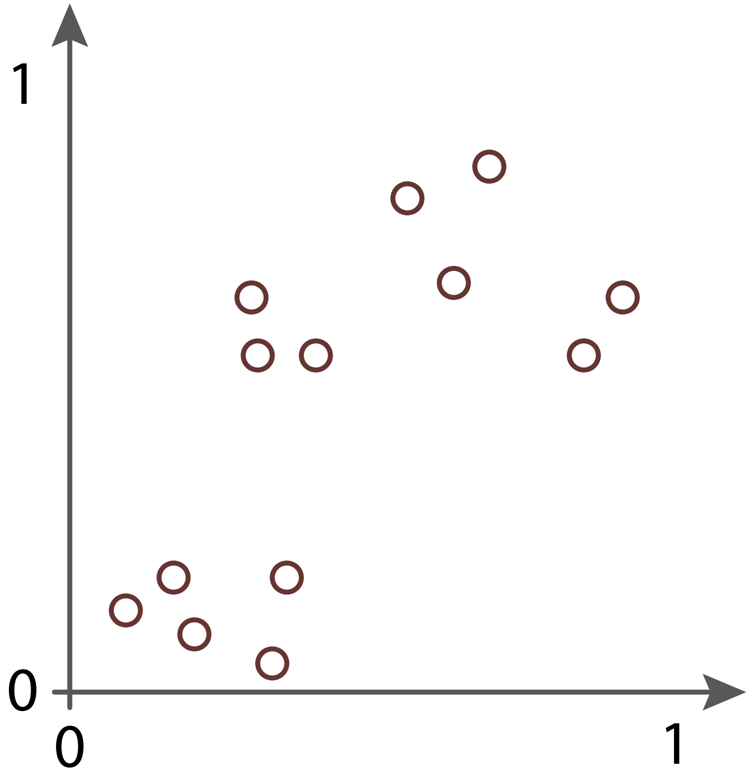
> For all $C \in \mathscr{C}_{\text{op}}$, there exists k such that $C \in \mathscr{C}^k$

- The level-k partitions have the hierarchical structure
  - For each $C \in \mathscr{C}^k$ we have $\bigcup \mathscr{D} = C$ for some $D \subseteq \mathscr{C}^{k+1}$
  - COOL is similar to divisive hierarchical clustering

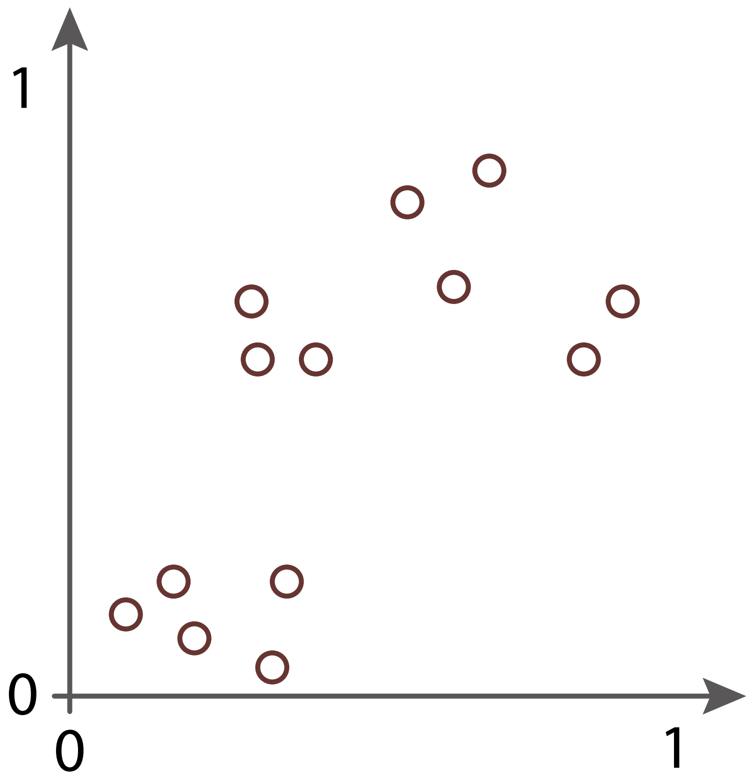
> COOL always outputs the global optimal partition $\mathscr{C}_{\text{op}}$

- The time complexity is $O(nd)$ (best) and $O(nd + K!)$ (worst)
  - Usually $K \ll n$ holds, hence $O(nd)$

Clustering Process of COOL

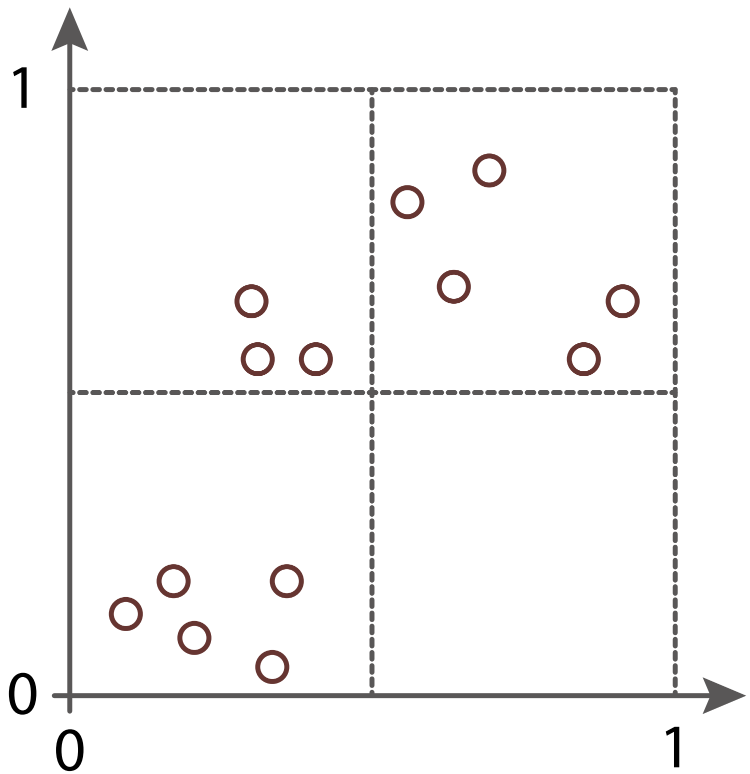


Clustering Process of COOL



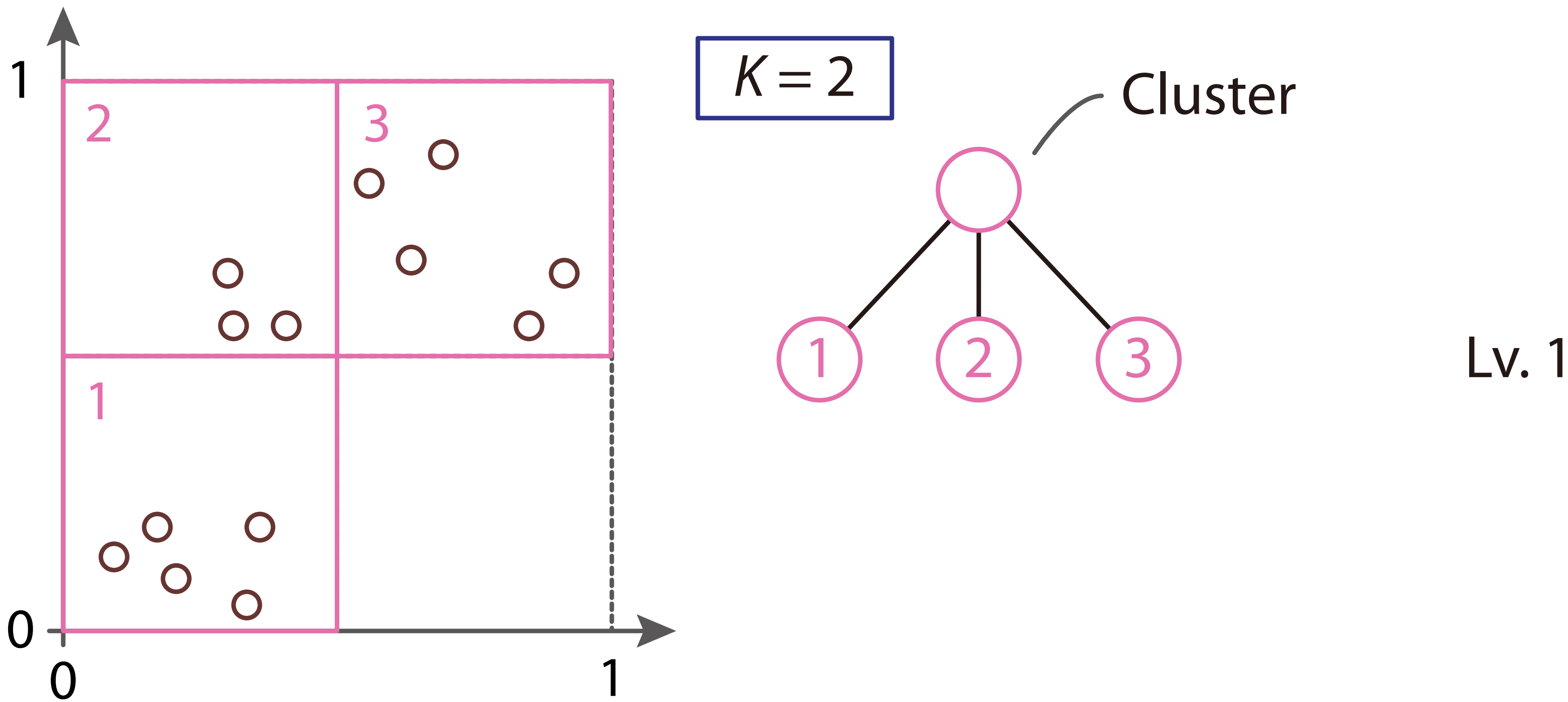
$K = 2$

Clustering Process of COOL

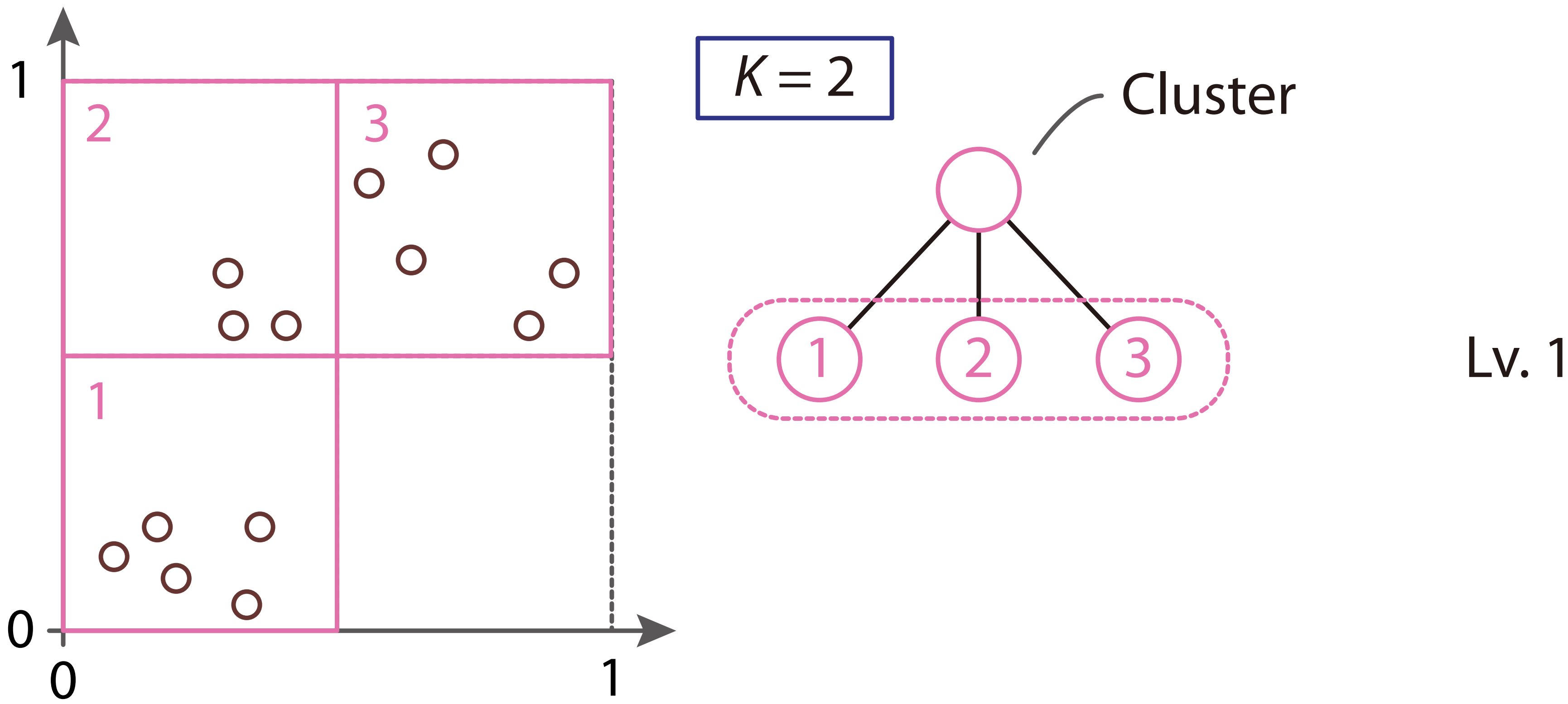


$K = 2$

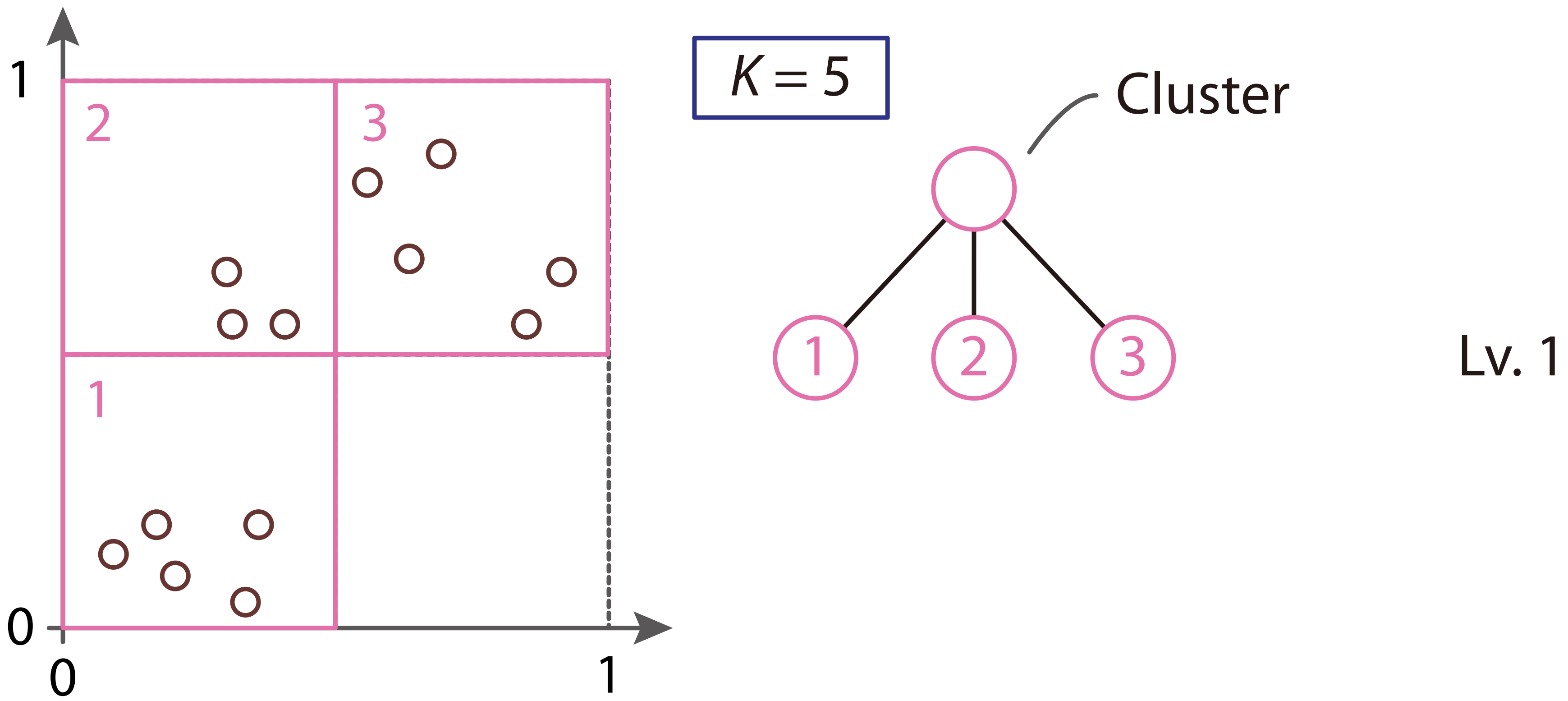
Clustering Process of COOL



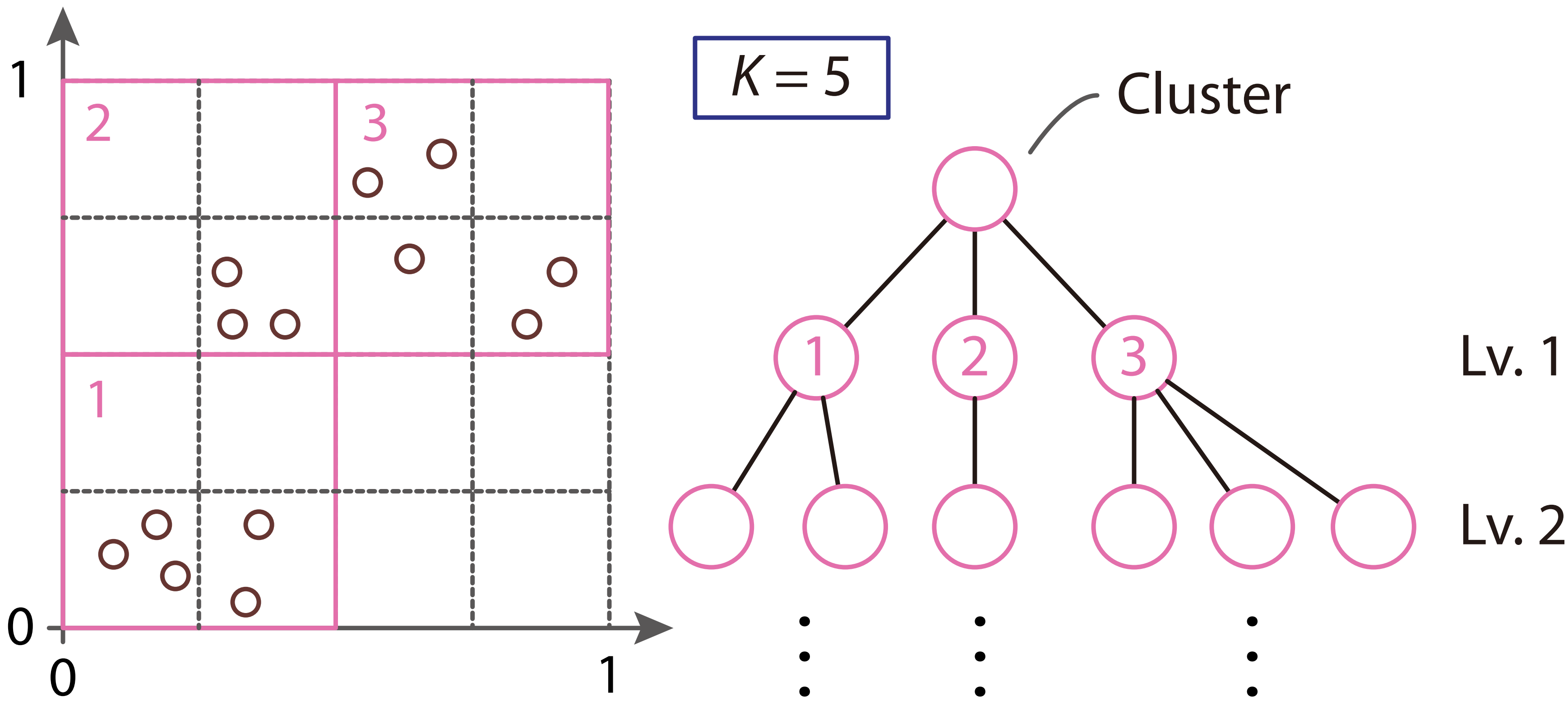
Clustering Process of COOL



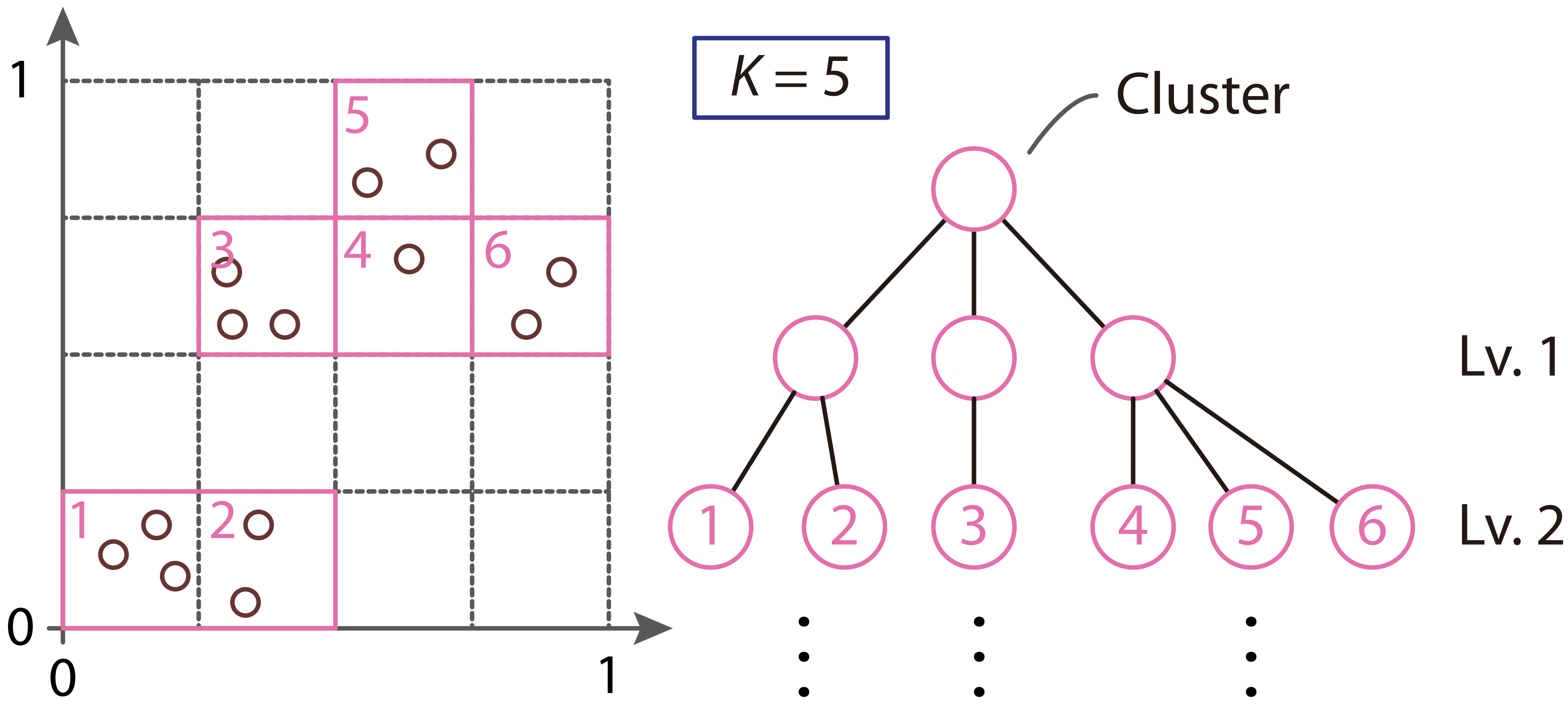
Clustering Process of COOL



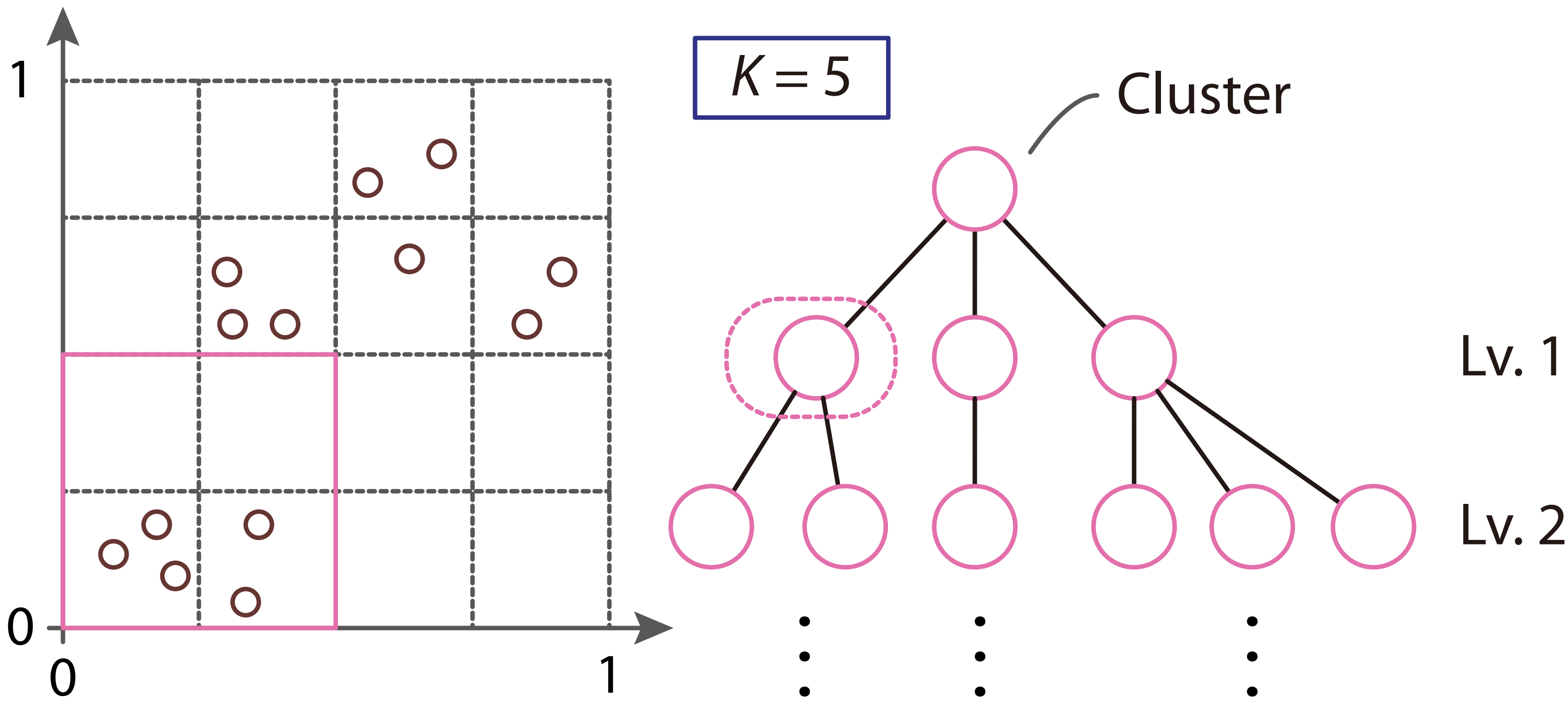
Clustering Process of COOL



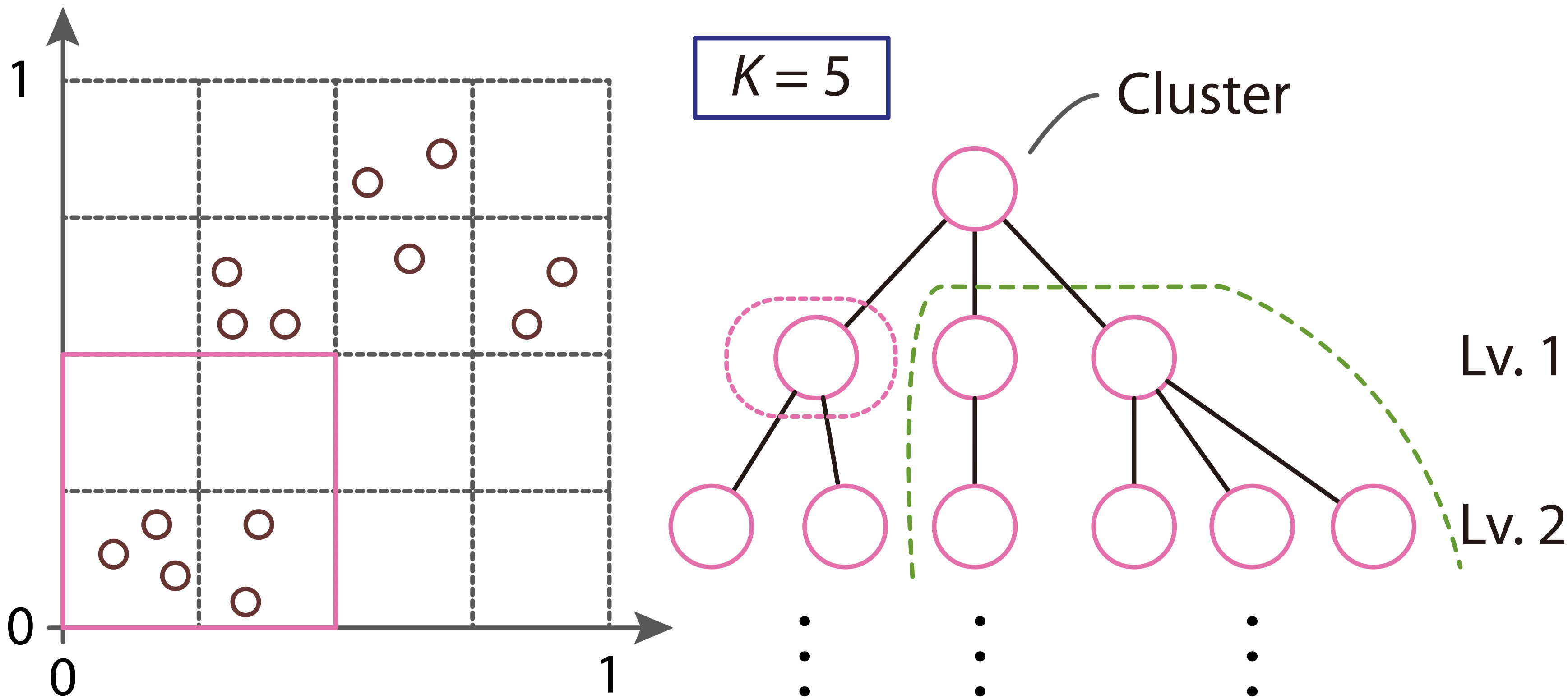
Clustering Process of COOL



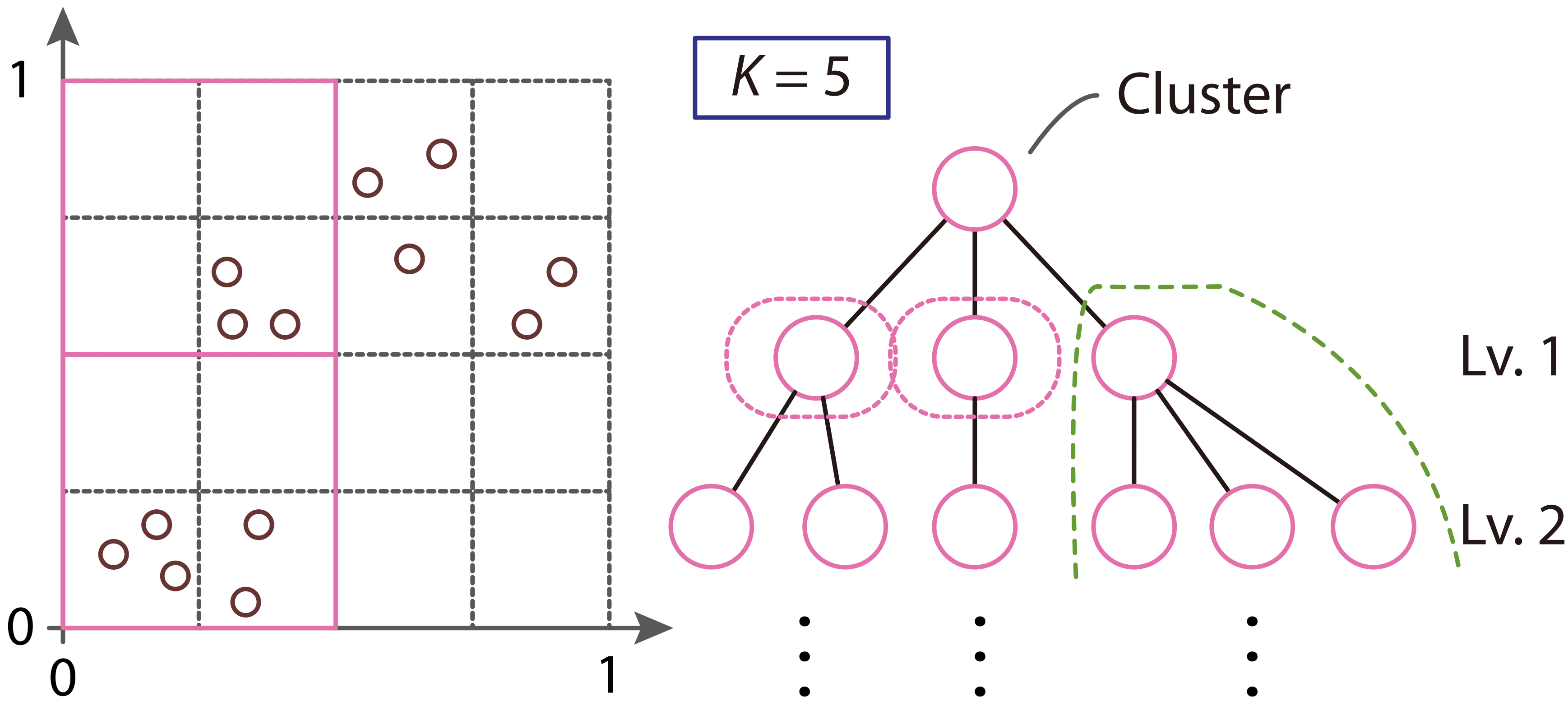
Clustering Process of COOL



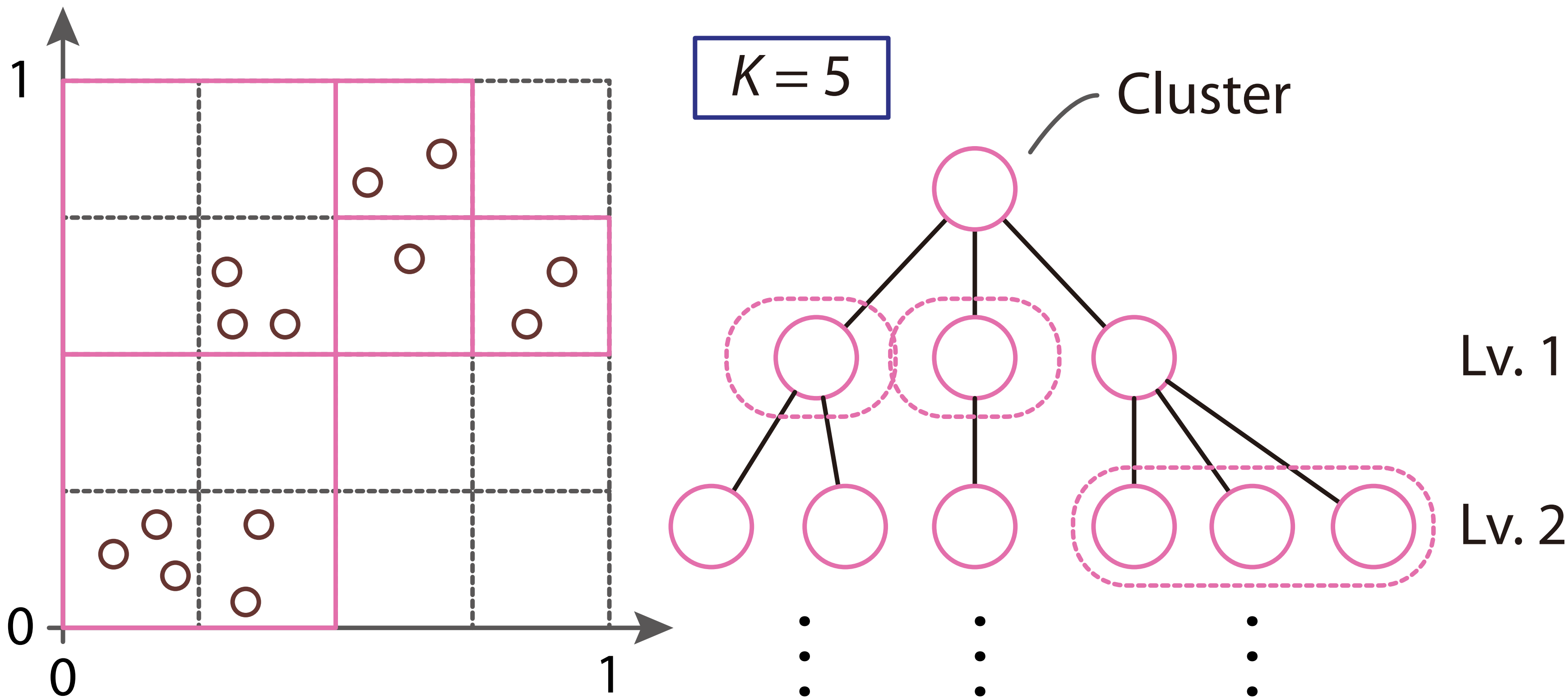
Clustering Process of COOL



Clustering Process of COOL



Clustering Process of COOL



The Multi-Dimensional Gray Code

- Use the wrapping function $\varphi(p^1, \dots, p^d) := p^1_1 \dots p^d_1 p^1_2 \dots p^d_2 \dots$

> Define the d-dimensional Gray code embedding $\gamma^d_{\mathrm{G}} \colon \mathscr{I} \to \Sigma^\omega_{\perp,d}$ by $\gamma^d_{\mathrm{G}}(x_1, \dots, x_d) := \varphi(\gamma_{\mathrm{G}}(x_1), \dots, \gamma_{\mathrm{G}}(x_d))$

- We abbreviate d of γ^d_{G} if it is understood from the context

Internal Measures

- Connectivity [Handl et al., 2005]
  - $Conn(\mathscr{C}) = \sum_{x \in X} \sum_{i=1}^{M} f(x, nn(x, i))/i$
    - $nn(x, j)$ is the i-th neighbor of x, $f(x, y)$ is 0 if x and y belong to the same cluster, and 1 otherwise
    - M is an input parameter (we set as 10)
  - Takes values from 0 to ∞, should be minimized
- Silhouette width
  - The average of Silhouette value $S(x)$ for each x
    $S(x) = (b(x) - a(x)/\max(b(x), a(x)))$
    - $a(x) = \|C\|^{-1} \sum_{y \in C} d(x, y)$ $(x \in C)$
    - $b(x) = \min_{D \in \mathscr{C} \setminus C} \|D\|^{-1} \sum_{y \in D} d(x, y)$
  - Takes values from -1 to 1, should be maximized

External Measures

- Adjusted Rand index
  - Let the result be $\mathscr{C} = \{C_1, \ldots, C_K\}$ and the correct partition be $\mathscr{D} = \{D_1, \ldots, D_M\}$
  - Suppose $n_{ij} := \|\{x \in X \mid x \in C_i, x \in D_j\}\|$. Then

$$\frac{\sum_{i,j\ n_{ij}} C_2 - (\sum_{i\ \|C_i\|} C_2 \sum_{h\ \|D_j\|} C_2) / {}_n C_2}{2^{-1}(\sum_{i\ \|C_i\|} C_2 + \sum_{h\ \|D_j\|} C_2) - (\sum_{i\ \|C_i\|} C_2 \sum_{h\ \|D_j\|} C_2) / {}_n C_2}$$

Discussion

- Results for synthetic datasets
  - Best performance under the internal measures
  - (nearly) Best performance under the internal measures
  - G-COOL is efficient and effective
    - DBSCAN is sensitive to input parameters
  - The MCL works well as an internal measure
- Results for real datasets
  - not good, and not bad
    - There are no clear clusters originally
- G-COOL is a good clustering method

Related Work

- Partitional methods [Chaoji *et al.*, 2009]
- Mass-based methods [Ting and Wells, 2010]
- Density-based methods (DBSCAN [Ester *et al.*, 1996])
- Hierarchical clustering methods
  (CURE [Guha *et al.*, 1998], CHAMELEON [Karypis *et al.*, 1999])
- Grid-based methods
  (STING [Wang *et al.*, 1997], WaveCluster [Sheikholeslami *et al.*, 1998])

Future Works

- Speeding up by using tree-structures such as BDD
- Apply to anomaly detection
- Theoretical analysis, in particular relation with Computable Analysis
  - Admissibility is a key property

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