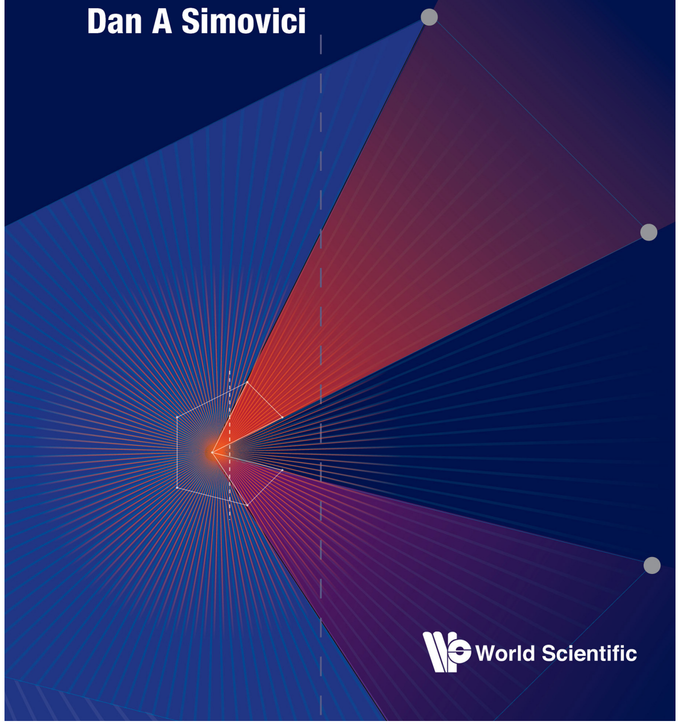
CLUSTERING

Theoretical and Practical Aspects

Dan A Simovici



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Unlike the union, the intersection is defined only for collections that consist of subsets of a set S.

If $\mathcal{C}$ is a collection of subsets of S, that is, if $\mathcal{C} \subseteq \mathcal{P}(S)$ then the intersection of $\mathcal{C}$ is the set of all elements of S that belong to every set of $\mathcal{C}$. The intersection of $\mathcal{C}$ is denoted by $\bigcap \mathcal{C}$.

If $\mathcal{C}$ and $\mathcal{C}'$ are two collections of subsets of a set S and $\mathcal{C} \subseteq \mathcal{C}'$, then $\bigcap \mathcal{C}' \subseteq \bigcap \mathcal{C}$.

If $\emptyset$ is the empty collection of subsets of S, we define $\bigcap \emptyset = S$.

Definition 2.7. A *closure system on the set* S is a collection $\mathcal{K}$ of subsets of S such that for every collection of subsets $\mathcal{C}$ such that $\mathcal{C} \subseteq \mathcal{K}$ we have $\bigcap \mathcal{C} \in \mathcal{K}$.

Note that if $\mathcal{K}$ is a closure system on a set S, then $S \in \mathcal{K}$ because S is the intersection of the empty collection of subsets of $\mathcal{K}$.

Definition 2.8. Let $\mathcal{K}$ be a closure system on a set S and let T be a subset of S. The *closure of* T *relative to the closure system* $\mathcal{K}$ is the set $\mathbf{K}(T) = \bigcap \{U \in \mathcal{K} \mid T \subseteq U\}$.

For every set T the collection $\mathcal{C}_T = \{U \in \mathcal{K} \mid T \subseteq U\}$ is non-empty because it includes at least S. The set $\bigcap \mathcal{C}_T$ is denoted by $\mathbf{K}(T)$ and is referred to as the *closure* of T.

To emphasize that the closure of T is computed relative to the closure system $\mathcal{K}$ we may denote this closure by $\mathbf{K}_{\mathcal{K}}(T)$.

Example 2.7. A subset E of $\mathbb{R}$ is said to be symmetric if $x \in E$ if and only if $-x \in E$.

Let $\{E_i \mid i \in I\}$ be a collection of symmetric subsets of $\mathbb{R}$. It is easy to see that $\bigcap \{E_i \mid i \in I\}$ is a symmetric set. Note that $\mathbb{R}$ itself is symmetric. Thus, the collection $\mathcal{E}$ of symmetric subsets of $\mathbb{R}$ is a closure system. For a subset T of $\mathbb{R}$ the set $\mathbf{K}_{\mathcal{E}}(T)$ is the smallest symmetric set that includes T.

The notion of *closure operator* can be defined independently.

Definition 2.9. A *closure operator* on set S is a mapping $\mathbf{K} : \mathcal{P}(S) \longrightarrow \mathcal{P}(S)$ that has the following properties:

(i) $X \subseteq \mathbf{K}(X)$ (extensivity);

(ii) $\mathbf{K}(X) = \mathbf{K}(\mathbf{K}(X))$ (idempotency);

(iii) $X \subseteq X'$ implies $\mathbf{K}(X) \subseteq \mathbf{K}(X')$ (monotonicity).

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The *intersection of* M *and* N is the multiset $M \cap N$ defined by

$$(M \cap N)(x) = \min\{M(x), N(x)\}$$

for $x \in S$.

The *sum of* M *and* N is the multiset $M + N$ given by

$$(M + N)(x) = M(x) + N(x)$$

for $x \in S$.

Let S be a multiset and let U be a sub-multiset of S. The *complement* of U relative to S is the sub-multiset $V = S - U$ of S defined by $m_V(x) = m_S(x) - m_U(x)$ for $x \in S$.

Example 2.6. Let $m, n \in \mathbb{N}$ be two numbers that have the prime factorizations

$$m = p_{i_1}^{k_1} \cdots p_{i_r}^{k_r},$$

$$n = p_{j_1}^{h_1} \cdots p_{h_s}^{h_s},$$

and let M_m, M_n be the multisets of their prime divisors, as defined in Example 2.5. Denote by $\gcd(m, n)$ the greatest common divisor of m and n, and by $\mathrm{lcm}(m, n)$ the least common multiple of these numbers.

We have

$$M_{\gcd(m,n)} = M_m \cap M_n,$$
$$M_{\mathrm{lcm}(m,n)} = M_m \cup M_n,$$
$$M_{mn} = M_m + M_n,$$

as the reader can easily verify.

Definition 2.6. Let M be a multiset. Its *cardinality* is the number $|\{x \in S | M(x) \geqslant 0\}$; its size is $|M| = \sum\{M(x) \mid x \in S\}$.

A multiset on the set $\mathcal{P}(S)$ is referred to as a *multicollection* of sets on S.

2.5 Closure Systems

Let $\mathcal{C} = \{S_i \mid i \in I\}$ be a collection of sets. Its union is the set U defined as

$$U = \bigcup_{i \in I} S_i.$$

Note that $\mathcal{C} \subseteq \mathcal{C}'$ implies $\bigcup \mathcal{C} \subseteq \bigcup \mathcal{C}'$.

Example 2.5. Let PRIMES be the set of prime numbers:

$$\mathsf{PRIMES} = \{2, 3, 5, 7, 11, \ldots\}. \tag{2.3}$$

A number is determined by the multiset of its prime divisors in the following sense. If $n \in \mathbb{N}$, $n \geqslant 1$, can be factored as a product of prime numbers, $n = p_{i_1}^{k_1} \cdots p_{i_\ell}^{k_\ell}$, where p_i is the i^{th} prime number and $k_1, \ldots, k_\ell$ are positive numbers, then the multiset of its prime divisors is the multiset $M_n : \mathsf{PRIMES} \longrightarrow \mathbb{N}$, where $M_n(p)$ is the exponent of the prime number p in the product (2.3).

For example, M_{1960} is given by

$$M_{1960}(p) = \begin{cases} 3 & \text{if } p = 2, \\ 1 & \text{if } p = 5, \\ 2 & \text{if } p = 7. \end{cases}$$

Thus, $carr(M_{1960}) = \{2, 5, 7\}$.

Note that if $m, n \in \mathbb{N}$, we have $M_m = M_n$ if and only if $m = n$.

We denote a multiset by using square brackets instead of braces. If x has the multiplicity n in a multiset M, we write x a number of times n inside the square brackets. For example, the multiset of Example 2.5 can be written as $[2, 2, 2, 5, 7, 7]$.

Note that while multiplicity counts in a multiset, order does not matter; therefore, the multiset $[2, 2, 2, 5, 7, 7]$ could also be denoted by $[5, 2, 7, 2, 2, 7]$ or $[7, 5, 2, 7, 2, 2]$. We also use the abbreviation $n * x$ in a multiset to mean that x has the multiplicity n in M. For example, the multiset M_{1960} can be written as $M_{1960} = [3 * 2, 1 * 5, 2 * 7]$.

The multiset M on the set S defined by $M(x) = 0$ for $x \in S$ is the *empty multiset*.

Let U and V be two multisets on a set S. U is a sub-multiset of V if $U(x) \leqslant V(x)$ for every $x \in S$.

Multisets can be combined to construct new multisets. Common set-theoretical operations such as union and intersection have natural generalizations to multisets.

Definition 2.5. Let M and N be two multisets on a set S.

The *union of M and N* is the multiset $M \cup N$ defined by

$$(M \cup N)(x) = \max\{M(x), N(x)\}$$

for $x \in S$.

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To my wife Doina,
and to the memory of my parents,
Adelina and Avram Simovici

The sequence $\mathbf{s}_n$ is the *state* of S at moment n.

Example 2.4. Let $A = \{a, b, c\}$, $\mathbf{q}_0 = \lambda$. By pushing a, b, b, c starting from $\mathbf{s}_0 = \lambda$ we obtain

$$\begin{aligned}
\mathbf{s}_1 &= \mathsf{push}(\mathbf{s}_0, a) = (a),\\
\mathbf{s}_2 &= \mathsf{push}(\mathbf{s}_1, b) = (b, a),\\
\mathbf{s}_3 &= \mathsf{push}(\mathbf{s}_2, b) = (b, b, a),\\
\mathbf{s}_4 &= \mathsf{push}(\mathbf{s}_3, c) = (c, b, b, a).
\end{aligned}$$

When the pop operation is applied, elements are extracted from the left end of the sequence. This yields:

$$\begin{aligned}
&\mathsf{pop}(\mathbf{s}_4) = (\mathbf{s}_5, c), \mathbf{s}_5 = (b, b, a)\\
&\mathsf{pop}(\mathbf{s}_5) = (\mathbf{s}_6, b), \mathbf{s}_6 = (b, a)\\
&\mathsf{pop}(\mathbf{s}_6) = (\mathbf{s}_7, b), \mathbf{s}_7 = (a)\\
&\mathsf{pop}(\mathbf{s}_7) = (\mathbf{s}_8, a), \mathbf{s}_8 = \lambda.
\end{aligned}$$

Note that the elements of the stack are extracted in the reverse order of their push on the stack, c, b, b, a.

Thus, the working of a stack can be described by “first-in last-out” rule.

2.4 Multisets

Multisets generalize the notion of a set by allowing multiple copies of an element. Formally, we have the following definition.

Definition 2.4. A *multiset* on a set S is a function $M : S \longrightarrow \mathbb{N}$. Its *carrier* is the set $carr(M) = \{x \in S \mid M(x) > 0\}$.

The *multiplicity* of an element x of S in the multiset M is the number $M(x)$.

The set of all multisets on S is denoted by $\mathcal{M}(S)$.

Note that a subset T of S can be regarded as a multiset $T : S \longrightarrow \mathbb{N}$, where

$$T(x) = \begin{cases} 1 & \text{if } x \in T,\\ 0 & \text{otherwise,}\end{cases}$$

for $x \in S$.

Sequences allow us to define two algorithmic concepts, namely, queues and stacks.

Definition 2.2. Let A be a set. A *queue* on A is a triple $\mathbf{q} = (Q, e, d)$, where Q is a sequence of sequences of A,

$$Q = (\mathbf{q}_0, \mathbf{q}_1, \ldots),$$

$e : A \times Q \longrightarrow Q$ is the enqueing operation and $d : Q \longrightarrow Q \times A$ is the dequeing operation are two functions that satisfy the following conditions:

(i) $e(a, \mathbf{q}) = (a)\mathbf{q}$,

(ii) $d(\mathbf{q})$ is defined on non-null sequence and $d(\mathbf{q}) = (\mathbf{q}', a)$ if $\mathbf{q} = \mathbf{q}'(a)$.

Example 2.3. Let $A = \{a, b, c\}$, $\mathbf{q}_0 = \lambda$. By enqueueing the a, b, b, c starting from $\mathbf{q}_0 = \lambda$ we obtain

$$\begin{aligned}
\mathbf{q}_1 &= e(\mathbf{q}_0, a) = (a),\\
\mathbf{q}_2 &= e(\mathbf{q}_1, b) = (b, a),\\
\mathbf{q}_3 &= e(\mathbf{q}_2, b) = (b, b, a),\\
\mathbf{q}_4 &= e(\mathbf{q}_3, c) = (c, b, b, a).
\end{aligned}$$

When the dequeuing operation is applied, elements are extracted from the right end of the sequence. This yields the sequence

$$\begin{aligned}
d(\mathbf{q}_4) &= (\mathbf{q}_5, a), \mathbf{q}_5 = (c, b, b)\\
d(\mathbf{q}_5) &= (\mathbf{q}_6, b), \mathbf{q}_6 = (c, b)\\
d(\mathbf{q}_6) &= (\mathbf{q}_7, b), \mathbf{q}_7 = (c)\\
d(\mathbf{q}_7) &= (\mathbf{q}_8, c), \mathbf{q}_8 = \lambda.
\end{aligned}$$

Note that the working of a queue can be described by the syntagm "first-in first-out". Indeed, the order in which elements are produced by the dequeuing operation is the same as the order these elements were enqueued: a, b, b, c.

Definition 2.3. Let A be a set. A *stack* on A is a triple $\mathbf{s} = (S, e, d)$, where S is a sequence of sequences of A,

$$S = (\mathbf{s}_0, \mathbf{s}_1, \ldots),$$

$\mathsf{push} : A \times S \longrightarrow S$ is the push operation and $\mathsf{pop} : S \longrightarrow S \times A$ is the popping operation are two functions that satisfy the following conditions:

(i) $\mathsf{push}(a, \mathbf{s}) = (a)\mathbf{d}$,

(ii) $\mathsf{pop}(\mathbf{s})$ is defined on non-null sequence and $\mathsf{pop}(\mathbf{s}) = (\mathbf{s}', a)$ if $\mathbf{s} = (a)\mathbf{s}'$.

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Preface

Clustering is a part of machine learning that seeks to identify groups into sets of objects such that objects that belong to the same group are as similar as possible, and objects that belong to two distinct groups are as dissimilar as possible. In general, clustering exploration is based on computing similarities (or dissimilarities) between objects but does not provide the reasons for the existence of these groupings.

Various notions of dissimilarities are considered among objects ranging from simple dissimilarities, metrics on linear spaces, ultrametrics, and extensions of these measures to sets. Studying these measures requires incursions in a variety of mathematical disciplines ranging from linear algebra and optimization to functional analysis and topology.

The results of clusterings are evaluated using a variety of criteria allowing users to choose clusterings that are desirable from the point of view of these criteria.

Clustering use is widespread, ranging from genomics, epidemiology, medicine, economics and many other disciplines. The intended readership of this volume consists of researchers and graduate students who work in data mining and pattern recognition, or apply those in their domain of interest. I strived to make this volume as self-contained as possible. Appendices, exercises, and supplements are provided to help readers in their search of mathematical tools useful for clustering.

Boston and Brookline

Dan A. Simovici
May 2021

2.3 Sequences

Definition 2.1. Let S be a set. A *sequence of length n on S* is a mapping $\mathbf{s} : \{1, \ldots, n\} \longrightarrow S$. The set of sequences of length n on S is denoted by $\mathbf{Seq}_n(S)$.

An *ordered pair* on S is a sequence of length 2 on S; a *singleton* is a sequence of length 1.

If $\mathbf{s}$ is a sequence of length n on S and $\mathbf{s}(i) = x_i$ for $1 \leqslant i \leqslant n$, we write $\mathbf{s} = (x_1, \ldots, x_n)$. The elements $x_1, \ldots, x_n$ are the *components* of $\mathbf{s}$.

The length of a sequence $\mathbf{s}$ is denoted by $|\mathbf{s}|$.

Example 2.1. A sequence of natural numbers of length 6 is $\mathbf{s} = (6, 5, 2, 4, 9, 6)$. Note that in a sequence the same element of S may occur on multiple positions.

If S is a finite set containing m elements, then there are m^n sequences of length n for any $n \geqslant 1$. We extend the definition of sequences on S be defining the *null sequence on S* as the sequence λ that has no components, $\lambda = ()$. Note that there exists exactly one such sequence on S and this is consistent with the fact that $m^0 = 1$ for every $m \geqslant 1$.

The *set of sequences of elements of S* is the set

$$\mathbf{Seq}(S) = \bigcup \{\mathbf{Seq}_n(S) \mid n \geqslant 0\}.$$

If $\mathbf{s} = (s_1, s_2, \ldots, s_n)$ is a sequence in S, we refer to the sequence $\tilde{s} = (s_n, \ldots, s_2, s_1)$ as the *reversal* of the sequence s. Clearly $\tilde{\lambda} = \lambda$.

If $\mathbf{s} = (s_1, \ldots, s_n)$ and $\mathbf{t} = (t_1, \ldots, t_m)$ are two sequences on a set S, their *concatenation* is the sequence $\mathbf{st} = (s_1, \ldots, s_n, t_1, \ldots, t_m)$. For the null sequence we define $\lambda\mathbf{s} = \mathbf{s}\lambda = \mathbf{s}$ for every $\mathbf{s} \in \mathbf{Seq}(S)$. Note that $|\mathbf{st}| = |\mathbf{s}| + |\mathbf{t}|$ for all sequences $\mathbf{s}, \mathbf{t} \in \mathbf{Seq}(S)$.

Note that sequence concatenation is not a commutative operation in general.

Example 2.2. Let $\mathbf{s} = (1, 2, 3), \mathbf{t} = (4, 5)$. We have

$$\mathbf{st} = (1, 2, 3, 4, 5) \text{ and } \mathbf{ts} = (4, 5, 1, 2, 3),$$

so $\mathbf{st} \neq \mathbf{ts}$.

We leave to the reader to verify that sequence concatenation is an associative operation on $\mathbf{Seq}(S)$, that is $(\mathbf{st})\mathbf{u} = \mathbf{s}(\mathbf{tu})$ for every $\mathbf{s}, \mathbf{t}, \mathbf{u} \in \mathbf{Seq}(S)$.

$\oplus$	0	1
0	0	1
1	1	0

$\cdot$	0	1
0	0	0
1	0	1

Let S be a set and let $\mathsf{GF}(2)$ be the two element field defined in earlier. Define the scalar multiplication of a subset T of S by an element of the field as

$$0 \cdot T = \emptyset \text{ and } 1 \cdot T = T$$

for every $T \in \mathcal{P}(S)$.

The sum of two subsets U and V is defined as their symmetric difference

$$U + V = (U - V) \cup (V - U).$$

With these definitions the set $\mathcal{P}(S)$ of subsets of S is an $\mathsf{GF}(2)$-linear space, as the reader can easily verify.

The set of subsets $\mathcal{P}(S)$ of a finite set $S = \{x_1, \ldots, x_n\}$ can be organized as a $\mathsf{GF}(2)$-linear space by defining the sum of two subsets U, V as their symmetric difference

$$U \oplus V = (U - V) \cup (V - U).$$

Note that $U \oplus \emptyset = \emptyset \oplus U = U$.

Multiplication with scalars in $\{0, 1\}$ is defined as

$$0\, U = \emptyset \text{ and } 1\, U = U,$$

for every $U \in \mathcal{P}(S)$.

A basis in the $\mathsf{GF}(2)$-linear space of subsets of the set $S = \{x_1, \ldots, x_n\}$ is the collection $\{\{x_1\}, \ldots, \{x_n\}\}$. Every subset U of S can be uniquely written as

$$U = a_1\{x_1\} \oplus \cdots \oplus a_n\{x_n\},$$

where

$$a_i = \begin{cases} 1 & \text{if } x_i \in U, \\ 0 & \text{if } x_i \not\in\in U, \end{cases}$$

for $1 \leqslant i \leqslant n$. Thus, the $\mathsf{GF}(2)$-linear space of subsets of S is of dimension n.

The inner product of two vectors $\mathbf{u}, \mathbf{v} \in \mathsf{GF}(2)^n$ is

$$(\mathbf{u}, \mathbf{v}) = \mathbf{u}'\mathbf{v} = \oplus_{i=1}^{n} u_i v_i.$$

Note that if $\mathbf{u} \in \mathsf{GF}(2)^n$, where n is an even number, we have $(\mathbf{u}, \mathbf{u}) = 0$, even if $\mathbf{u} \neq \mathbf{0}_n$.

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Contents

have

$$A \oplus B = (A - B) \cup (B - A).$$

For set inclusion we write $A \subseteq B$ to denote that each element x of A also belongs to B.

Note that $A = B$ if and only if $A \oplus B = \emptyset$.

For a set S we denote by $\mathcal{P}(S)$ the set of its subsets. The collection of subsets of S that contain k elements is denoted by $\mathcal{P}_k(S)$. The sets in $\mathcal{P}_2(S)$ are the *unordered pairs* of S.

A subset A of a set S is completely described by its *characteristic function* $\mathbf{1}_A : S \longrightarrow \{0,1\}$ defined as

$$\mathbf{1}_A(x) = \begin{cases} 1 & \text{if } x \in A, \\ 0 & \text{otherwise} \end{cases}$$

for $x \in S$.

If $A, B, C \in \mathcal{P}(S)$ we have:

$$A \oplus B = (A \oplus C) \oplus (C \oplus B). \tag{2.1}$$

This equality can be verified by considering all cases determined by the membership of an element x in A, B and C. These are summarized by the following table, where 1 indicates that x belongs to the set and 0 means that x is not a member of the set that labels the each column.

A	B	C	$A \oplus B$	$A \oplus C$	$C \oplus B$	$(A \oplus C) \oplus (C \oplus B)$
0	0	0	0	0	0	0
0	0	1	0	1	1	0
0	1	0	1	0	1	1
0	1	1	1	1	0	1
1	0	0	1	1	0	1
1	0	1	1	0	1	1
1	1	0	0	1	1	0
1	1	1	0	0	0	0

In all cases, the entries of the column $A \oplus B$ coincide with the entries of the column $(A \oplus C) \oplus (C \oplus B)$ proving Equality (2.1). This equality implies immediately

$$|A \oplus B| \leqslant |A \oplus C| + |C \oplus B| \tag{2.2}$$

for $A, B, C \in \mathcal{P}(S)$.

We will use frequently to two-element field $\mathsf{GF}(2)$ known as the 2-element Galois field, $\mathsf{GF}(2) = \{0,1\}$. Addition "$\oplus$" and multiplication "$\cdot$" in this field are defined by the following tables:

Chapter 2

Set-Theoretical Preliminaries

2.1 Introduction

We begin with sets, sequences, collection of sets and set-theoretical operations. Closure systems and their connection to closure operators are presented as they facilitate an elegant presentation of future mathematical results.

Set partitions are very important to clusterings (which, in most cases, are partitions of sets of objects). This topic is discussed in the context of relations and, especially, of equivalence relations.

A presentation of partially ordered sets and a detailed study of the partially ordered set of partitions provides the mathematical underpinnings of families of clusterings.

The chapter concludes with a discussion of Galois connections that relate formal concept analysis to biclustering.

We assume that the reader is familiar with the notions of Cartesian product of sets, relations, and function, that are part of many texts.

2.2 Sets and Set Operations

For a finite set S the number of elements of S is denoted by $|S|$. The empty set is denoted by $\emptyset$.

We write $x \in S$ to denote the fact that x is an element of the set S. The usual symbols are used to denote set-theoretical operations: $A \cup B$ is the union of the sets A and B, $A \cap B$ is the intersection of the sets A and B, and $A - B$ is the difference of the sets A and B.

The *symmetric difference* of the sets A and B is denoted by $A \oplus B$. We

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Machine learning algorithms struggle to match the human performance. Many clustering algorithms require the number of clusters to be provided as an input parameter, which forces these algorithms to combine of split natural clusters, or produce clusters that do not exist naturally in data. The pursuit of clusterings with a prescribed number of clusters is an ill-posed problem because a set of points can be clustered in many ways. Even if a data set has no meaningful structure, a clustering algorithm may find some partition of the data.

For the data set shown in Figure 1.1 a clustering algorithm that starts with a prescribed number of two clusters may split this data into two arbitrary clusters defined by the separating line ℓ (see Figure 1.3).

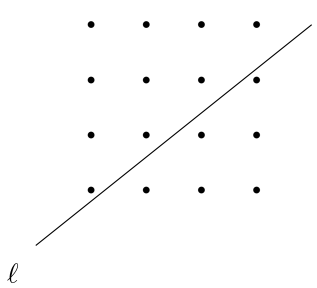

Fig. 1.3 Line separating the data set into two arbitrary clusters.

A clustering algorithm acting on the data set shown in Figure 1.2 may find two clusters or three clusters depending on the decision to fuse or not the two leftmost point groupings (which are very close).

There are many types of clustering algorithms, many of them are covered in this text. The most important are:

- partitional algorithms (represented by the k-means algorithm and its variants);
- hierarchical algorithms (which include agglomerative and divisive algorithms);
- other classes include density-based clustering, grid-based clustering, spectral clustering;
- specialized algorithms have been developed for clustering categorical data, for stream data, for collections of documents and multimedia data, for time series, etc.

ing, is very much work in progress. Various clustering algorithms applied to the same data set may produce distinct types of clusterings and no general principles to guide algorithm selection exist.

Studying clustering requires a broad spectrum of mathematical disciplines ranging from combinatorics, topology, linear algebra, optimization theory, etc. We strived to make the book as self contained as possible, including some preliminary chapters, as well as a number of appendices.

Treating clustering as an optimization problem is difficult because for each type of clustering there are objective function that fail to have optimal properties; additionally, most optimization problems are intractable and the users must contend with approximate algorithms.

The existence of clusters in data, that is, data clusterability is hard to formalize due to the variety in data distribution and the inadequacy of certain basic notions of clustering.

Humans are very good ar identifying groupings of objects, at least in the case of uni-, bi-, or even tri-dimensional sets of objects. An examination of the data shown in Figure 1.1 shows that there is no obvious grouping of objects.

On other hand, the data shown in Figure 1.2 contains some "natural" groupings.

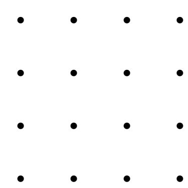

Fig. 1.1 Data set without an obvious grouping structure.

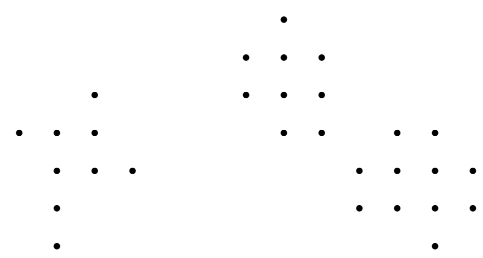

Fig. 1.2 Data that displays some grouping tendency.

Chapter 1

Introduction

Clustering is the process of grouping a set of objects into subsets referred to as clusters according to some dissimilarity measure between objects. The goal is to group together similar objects, and to ensure that objects placed in distinct groups are dissimilar.

Supervised machine learning makes use of labelled data and creates a model of the data that allows predicting the label for a yet unseen piece of data. In contrast, clustering belongs to the area of unsupervised machine learning defined as the task of discovering hidden structure from "unlabelled" data. Data items are not pre-categorized or labelled, which makes the evaluation of unsupervised learning algorithm difficult.

Supervised machine learning begins with a sample of data about which we have prior knowledge and tries to extrapolate this knowledge to larger volumes of data. Unsupervised learning, on the other hand, does not have prior knowledge, so its goal is to infer the "natural" structure present within data.

Typical supervised learning activities include classification and regression; typical unsupervised activities include clustering and density estimation. Machine learning has been successful in the realm of supervised learning by providing significant understanding of various tasks, in constructing algorithmic tools to address them, insights about the alternative machine learning paradigms and their parameter settings, and initiating the development of new algorithmic approaches. No comparable successes are yet available in clustering which is a major unsupervised learning activity.

In general, unsupervised learning, utilizing the huge amounts of raw data available, is widely recognized as one of the most important challenges facing machine learning nowadays.

The unsupervised machine learning domain, and in particular cluster-

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