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| Luciano da Fontoura Costa. An Introduction to Multisets (CDT-63). 2021. hal-03388935v1

HAL Id: hal-03388935

<https://hal.science/hal-03388935v1>

Preprint submitted on 20 Oct 2021 (v1), last revised 13 May 2022 (v3)

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An Introduction to Multisets

(CDT-63)

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15th Oct 2021

Abstract

Multisets are sets that allow repetition of elements, therefore account for their frequency of observation. As such, multisets pave the way to a number of interesting possibilities of both theoretical and applied nature. In the present work, after revising the main aspects of traditional sets, we introduce some of the main concepts and characteristics of multisets, which is followed by their generalization to take into account vectors, matrices, functions, scalar fields, and densities. The potential of multisets in pattern recognition and deep learning is also briefly characterized and illustrated.

‘In the bag, long ago gathered seashells resound.’

LdaFC

1 Introduction

Multisets can be informally understood as sets capable of incorporation of repeated entries of the same element (e.g. [1, 2, 3, 4, 5, 6]).

In the present work, we aim at providing an introduction to this interesting area, while also briefly covering the Jaccard index adapted to multiset, and applications to pattern recognition.

We start by reviewing the main concepts and properties of traditional sets, and then present the concept of multisets, as well as some of their simpler properties. The challenges implied by the definition of a universe set for multisets is briefly characterized and discussed. It is also argued that the operations of sum and subtraction between multisets correspond to one of the main distinction between multiset and set theories.

The possibility to generalized multisets to several other mathematical structures including vectors, matrices, functions, scalar and vector fields, as well as probability densities are approached next, including several examples. In particular, the extension of msets as representations of functions and scalar fields paves the way for obtaining hybrid expressions involving combinations of the the set operations of union and intersection with

algebraic expressions involving sum, subtraction, product and division of sets.

The Jaccard index, as well as its extension to multisets and multiple arguments, is then briefly presented as an interesting manner to compare any of the mathematical structures mentioned above after they have been transformed into respective multisets.

The application of multisets and the Jaccard index to quantify the relationship between two or more clusters is then described with respect to an example related to the iris dataset. The measurement of the separation between clusters corresponds to an important issue in both pattern recognition (e.g. [7, 8]), deep learning (e.g. [9, 10, 11]), and modeling (e.g. [12, 13])

For simplicity’s sake, the term multisets are henceforth abbreviated as *msetmset*.

2 Traditional Sets

A *set* is an unordered collection of items, or *elements*, which are not allowed to be repeated. A set A with elements a , b , and c is typically represented as:

$$A = \{a, b, c\}$$

The two essential properties of sets therefore are that the elements appear in any order, which distinguish sets from vectors, and that the elements cannot be repeated.

The number of elements in a set is called its *cardinality* or *size*, being represented as $|A|$.

A *subset* B of a given set A consists of a set so that any of its elements are contained in A . If A contains N elements, there will be $|A| = 2^N$ possible subsets that can be derived from it. The set containing all possible subsets of A is called its *power set* P^A .

An important point about sets that is sometimes overlooked regards the fact that they always refer to a respective *universe set* Ω . More specifically, once this set is established, any possible set needs to be a subset of Ω . Observe that Ω can have any type of element, though the situation where the elements are homogenous is of particular interest.

In case some sets are given but the universe set is not provided, it is possible to estimate the respective universe set (within hypotheses and subject to incompleteness in case new sets appear) as corresponding to the union of the supplied sets.

The universe set is of fundamental importance because the operation of *complement* of a set is defined with respect to the universe set. More specifically, the complement of a set A consists of all elements of Ω that are not part of A . The complement of a set is henceforth represented as A^C , being implicit that the operation refers to a given Ω .

Sets can be finite or infinite, as well as discrete or continuous. A *finite set* is any set A so that $|A| < \infty$. A *discrete set* is characterized by having all its elements corresponding to isolated points p , in the sense that each of these points possesses a neighborhood which when united with the universe set yields only p . Any continuous set is infinite, but discrete sets can be finite or infinite.

An interesting point regards the relationship between an element, let's say 'a' and the set $\{a\}$. These two mathematical structures are not identical because it is possible to include an element into $\{a\}$, but not into 'a'.

The *empty set*, represented as $\phi = \{\}$ is a subset of any possible set.

Given two sets A and B , their *union* consists of a third set C containing all elements from A and B . The *intersect* of these two sets corresponds to a set C containing all elements that are in both A and B . A subset B of A can therefore be understood as to be so that $A \cap B = B$. Any set is a subset of itself.

The *difference* between two sets A and B , indicated as $A - B$, corresponds to the set C containing all elements that are in A but are not in B .

Given three sets A , B , and C derived from a given Ω ,

the following properties are satisfied:

$$A \cup A^C = \Omega \quad (1)$$

$$A \cap A^C = \phi \quad (2)$$

$$A \cup \phi = A \quad (3)$$

$$A \cap \phi = \phi \quad (4)$$

$$A \cup A = A \quad (5)$$

$$A \cap A = A \quad (6)$$

$$A \cup B = B \cup A \quad (7)$$

$$A \cap B = B \cap A \quad (8)$$

$$A \cup (B \cap C) = (A \cup B) \cap C \quad (9)$$

$$A \cap (B \cup C) = (A \cap B) \cup C \quad (10)$$

$$A \cap (B \cup C) = (A \cap B) \cup (A \cap C) \quad (11)$$

$$A \cup (B \cap C) = (A \cup B) \cap (A \cup C) \quad (12)$$

$$(A \cup B)^C = A^C \cap B^C \text{ (De Morgan)} \quad (13)$$

$$(A \cap B)^C = A^C \cup B^C \text{ (De Morgan)} \quad (14)$$

3 Multisets

Basically, *msets* are sets allowing the *repetition* of elements, which is understood as their *multiplicity* or *frequency*. As with sets, the order of the elements is immaterial. Examples of mset include:

$$A = \{a, a, b, b, d\};$$

$$B = \{1, 2, 1, 2, 1, 2, 1\} = \{1, 1, 1, 1, 2, 2, 2\};$$

$$C = \{1, a, 2, b, b, 3, c, c, c, 1, d, 2, a, a\} = \\ = \{1, 1, 2, 2, 3, a, a, a, b, b, c, c, c\};$$

$$D = \{a, a, b, d\}.$$

Observe the different symbol adopted henceforth in this work in order to emphasize the distinction between a traditional set ($\{\}$), and a mset ($\{\!\!\{\}$).

A more compact representation of a mset A can be obtained by using 2-tuple or pairs $[a, m(a)]$, where 'a' is an element and $m(a)$ its multiplicity, i.e. the number of times it appear in A . In the case of the above examples, we have:

$$A = \{a, a, b, b, d\} = \{[a, 2]; [b, 2]; [d, 1]\};$$

$$B = \{1, 1, 1, 1, 2, 2, 2\} = \{[1, 4]; [2, 3]\};$$

$$C = \{1, 1, 2, 2, 3, a, a, ab, b, c, c, c\} = \\ = \{[1, 2]; [2, 2]; [3, 1]; [a, 3]; [b, 2]; [c, 3]\};$$

$$D = \{a, a, b, d\} = \{[a, 2]; [b, 1]; [d, 1]\}.$$

Though this type of representation of msets actually corresponds to a set, because it is impossible to have two identical entries, we shall maintain the ' $\{\!\!\{\}$ ' notation in order to emphasize that a mset is being meant.

When referring to the multiplicity of an element, it is important to specify to which mset this is being referred. This can be done by writing $m_A(a)$, meaning the multiplicity of the element a in the mset A .

The property analogous to inclusion in sets can be stated as follows. A mset A is included in another mset B whenever $m_A(a) \leq m_B(a)$. For instance, in the case of the examples above, we have $m_A(a) = 2$ and $m_C(a) = 2$.

As with sets, it is particularly important to specify the universe of mset. This can be done in an analogous manner as with sets. As an example, let's obtain a possible universe set for the two msets A and B above:

$$\Omega = \{a, b, d, 1, 2\} \quad (15)$$

It should be kept in mind that this universe is not analogous to the counterpart in sets, as it does not actually account for the possible multiplicity of the involved elements.

It is now possible to rewrite those two sets in a more complete, though redundant manner, as follows:

$$A = \{[a, 2]; [b, 2]; [d, 1]; [1, 0]; [2, 0]\};$$

$$B = \{[a, 0]; [b, 0]; [c, 0]; [1, 4]; [2, 3]\};$$

The *support* of a given mset A is defined as:

$$\mathcal{S}_A = \{x | x \in \Omega, m(x) > 0\} \quad (16)$$

As such, this set can be understood as containing all distinct elements in A . Observe that the support set provides a useful index to which symbols can be found in any of the respective msets.

4 Multiset Operations

A set A is said to be *included* into another set whenever:

$$m_A(x) \leq m_b(x), \forall x \in A \quad (17)$$

For simplicity's sake, we will indicate this operation using the same symbol as for sets, i.e. $A \subset B$, as the type of operation can be inferred from A and B being sets or msets.

In the case of the mset examples above, we can write that $D \subset A$.

The *union* C of two msets A and B can be defined as:

$$C = A \cup B = \{[x, m_C(x)], x \in A \text{ or } x \in B\},$$

$$\text{with } m_C(x) = \max \{m_A(x), m_B(x)\} \quad (18)$$

Examples considering the msets in the beginning of Section 3 include:

$$A \cup B = \{[a, a, b, b, b, d, 1, 1, 1, 1, 2, 2, 2]\} =$$

$$\{[1, 2]; [b, 2]; [d, 1]; [1, 4]; [2, 3]\}$$

$$A \cup D = \{[a, a, b, d]\} = \{[a, 4]; [b, 4]; [d, 2]\}$$

It is interesting to observe that the resulting multiplicity of each element does *not* correspond to the *sum* of the respective multiplicities, but to the *maximum* between them. This is a particularly important point that deserves further contemplation, so we will be back to it after presenting the concept of *sum* of two msets.

Let A and B be msets. The *sum* of these two sets, henceforth represented as $C = A + B$, is defined as:

$$C = A + B = \{[x, m_C(x)], x \in A \text{ or } x \in B\},$$

$$\text{with } m_C(x) = m_A(x) + m_B(x) \quad (19)$$

Figure 1 illustrates the two different ways in which the common elements of two msets A and B are collected into the respective union and sum msets.

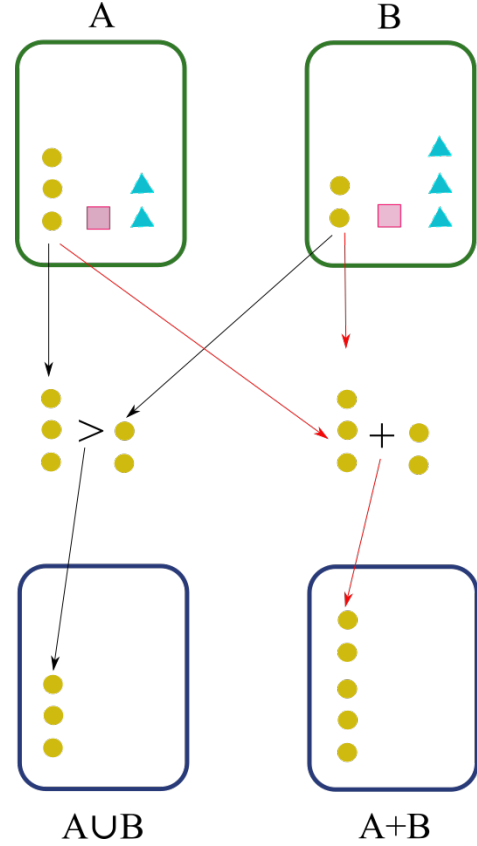


Figure 1: The union (a) and sum (b) of two msets A and B typically yield quite different resulting msets. In the case of the union operation, each of the elements of the same type are compared, with the elements with the maximum multiplicity being incorporated into C . The sum of the two msets incorporates all the $m_A(x_i) + m_B(x_i)$ elements into C .

Examples respective to the msets in the beginning of Section 3 include:

$$A + B = \{[a, a, b, b, b, d, 1, 1, 1, 1, 2, 2, 2]\} =$$

$$\{[1, 2]; [b, 2]; [d, 1]; [1, 4]; [2, 3]\}$$

$$A + D = \{[a, a, a, a, b, b, b, b, d, d]\} = \{[a, 4]; [b, 4]; [d, 2]\}$$

Thus, we have that the mset operations of union and sum are related in the sense that both collect the same elements from the two msets, but the way in which this is done is quite different, with the cardinality of the mset obtained by union becoming necessarily smaller or equal than that of the mset obtained by sum.

Observe that $m_{A \cup B}(x_i) \leq m_{A+B}$. It is interesting to consider these two operations in the context of possible respective applications. The sum of the two msets ensures conservation of the total number of elements, being therefore more indicated for related situations. The union of two msets can be conceptually understood as a kind of mid point between the sum of msets and the conventional union of traditional sets. Though the union of msets will typically yield larger msets than the union, it will not guarantee conservation of the total number of elements. A typical situation in which the union of msets can be applied is when the incorporation of the elements from the two msets is performed in terms of a choice, with the larger set being taken.

The *intersection* between two msets A and B can be defined as:

$$C = A \cap B = \{[x, m_C(x)], x \in A \text{ or } x \in B\},$$

$$\text{with } m_C(x) = \min \{m_A(x), m_B(x)\} \quad (20)$$

Examples drawn from the msets in the beginning of Section 3 include:

$$A \cap B = \{\}$$

$$A \cap D = \{[a, a, b]\} = \{[a, 4]; [b, 4]; [d, 2]\}$$

$$(21)$$

The *difference* or *subtraction* between two msets is expressed as:

$$C = A - B = \{[x, m_C(x)], x \in A \text{ or } x \in B\},$$

$$\text{with } m_C(x) = \max \{m_A(x) - m_B(x), 0\} \quad (22)$$

It is interesting to observe that the restriction of not having negative values can be overlooked without great impact on the other properties and operations as addressed in the present work.

Figure 2 illustrates the intersection and difference between two msets A and B .

Respective examples include:

$$A - D = \{[b, b]\} = \{[b, 2]\}$$

$$D - A = \{\}$$

$$(23)$$

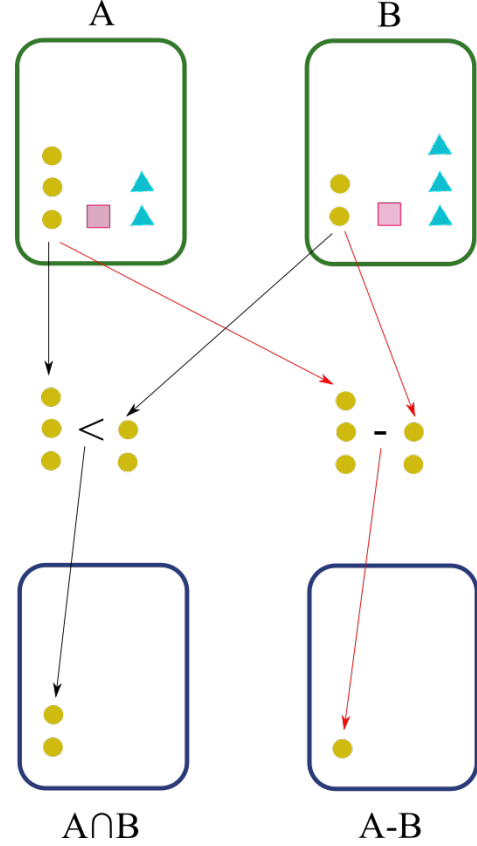


Figure 2: The intersection (a) and difference (b) of two msets A and B typically yield quite different resulting msets. In the case of the intersection operation, each of the elements of the same type are compared, with the elements with the minimum respective multiplicity being incorporated into C . The difference between A and B depends on $m_A(x_i) - m_B(x_i)$. As the result is negative in the case of the present example, no elements are incorporated into $A - B$.

5 Multisets Properties

It can be shown that msets satisfy the following properties:

$$A \cup \phi = A \quad (24)$$

$$A \cap \phi = \phi \quad (25)$$

$$A \cup A = A \quad (26)$$

$$A \cap A = A \quad (27)$$

$$A \cup B = B \cup A \quad (28)$$

$$A \cap B = B \cap A \quad (29)$$

$$A \cup (B \cup C) = (A \cup B) \cup C \quad (30)$$

$$A \cap (B \cup C) = (A \cap B) \cup C \quad (31)$$

$$A \cap (B \cup C) = (A \cap B) \cup (A \cap C) \quad (32)$$

$$A \cup (B \cap C) = (A \cup B) \cap (A \cup C) \quad (33)$$

Informally speaking, the above properties can be understood by identifying each repeated element in an mset with unique respective tags, in which case they would

behave with respect to the operation of union and intersection exactly in the same way as common sets.

So, we have that msets follow all the properties in Equations 1 to Equations 14, except those involving complementation. Indeed, the definition of the complement of an mset has been a challenging issue (e.g. [6]), which has to do with the fact that there is no bound to the size of possible msets generated by making additions between any non-empty mset. For instance, we can write:

$$\begin{aligned} A &= \{a\} \\ A + A &= \{a, a\} \\ A + A + A &= \{a, a, a\} \\ &\dots \end{aligned} \tag{34}$$

For this reason, the useful De Morgan properties, as well as other related results, do not hold for msets. In addition, there are relative few properties involving the sum and subtraction of msets.

In a sense, it is these two operations that differentiates msets from sets because, as commented above, msets behave like sets respectively to their union and intersection when the elements are tagged.

In a sense, though we gain two new operations when working with msets, these operations imply some specific challenges to be addressed. In the present work, we will simply assume that the complement of msets are not available.

6 Multisets, Vectors, Matrices

In this section we will discuss the relationship between msets and vectors. First, we recall that the elements in a vector are expected to follow a well-determined order as indicated by their indices. For instance, in the case of the vector in \mathbb{R}^5 :

$$\vec{v} = [3, 2.5, \pi, 0, -1]$$

we have five indices $i = 1, 2, \dots, 5$, so that we can specify the respective element values as $v[1] = 3$, $v[2] = 2.5$, $v[3] = \pi$, $v[4] = 0$, and $v[5] = -1$.

By understanding the values of the components of a vector as generalized multiplicities, we can immediately derive the following mset from the above vector:

$$V = \{[1, 3]; [2, 2.5]; [3, \pi]; [4, 0]; [5, -1]\}$$

Therefore, we have that an mset can be derived from any vector, but that a vector can be obtained from an mset only if their elements are ordered in some manner, e.g. by taking their respective values. As such, msets can be used to study the elements of vectors without taking into account their relative position along the vector.

It is also interesting to contemplate the relationship between the above discussion and the traditional sets. More specifically, we can write the set containing all values in the vector \vec{v} above as:

$$\tilde{V} = \{3, 2.5, \pi, 0, -1\} = \{0, 3, 2.5, -1, \pi\} = \text{etc.}$$

Though V and \tilde{V} are very similar, they are not identical because in V the *order* of the elements is maintained. This difference becomes critically important in case we want to apply the operations of addition and subtraction between msets, which would be otherwise impossible in case of sets because we would not know which element of one set should be added to which element in the other set.

By representing vectors as msets, we not only maintain the operations of subtraction and difference, but also incorporates the possibilities of defining intersections and unions between any two vectors.

Another interesting possibility is to incorporate new operators for multiplication and division into the mset framework, which can be done straightforwardly, while avoiding divisions by zero.

Interestingly, it is also possible to obtain mset representations from matrices or even other more sophisticated mathematical structures as tensors. In the case of matrices, this can be done by mapping the indices $i = 1, 2, \dots, N_i$ and $j = 1, 2, \dots, N_j$ into a single index k , e.g.:

$$k \longleftrightarrow N_i(j - 1) + i - 1 \tag{35}$$

so that the matrix becomes a vector, which can then be transformed into the respective mset as described above. Interestingly, observe that though the obtained msets would not directly provide the respective indices of the elements, they can be nevertheless obtained from the unified index.

7 Functions and Scalar Fields

The possibility to represent vectors as msets opens the way to a number of interesting possibilities. One of them is to represent discrete and continuous *functions* and *scalar fields* (vector fields can be approached as vectors of scalar fields). We develop these possibilities in the following.

We start with a discrete function as illustrated in Figure 3.

It is often interesting to represent such discrete functions in terms of sums of Dirac delta functions.

Provided that we limit the extension of this function along the horizontal axis, e.g. $i = 1, 2, \dots, N$, it can be immediately represented in terms of the vector:

$$\vec{f} = [f(x_i)] \tag{36}$$

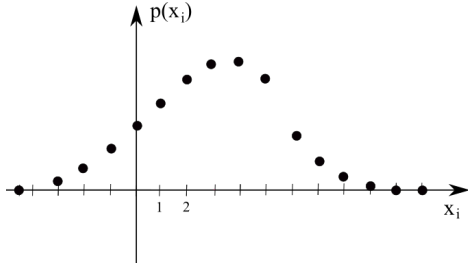


Figure 3: A generic discrete function $f(x_i)$.

which can then be transformed into the respective mset as described in the previous section.

A similar approach can be applied to transform discrete scalar fields defined on more than one variables into respective msets, involving the index mapping described above.

Now, we can approach the case of continuous functions and scalar fields simply by taking the separation between the points along the horizontal axis to the limit of 0. As a consequence, the functions and scalar fields will become associated to msets with infinite elements, but these can still be operated by the ‘max()’, ‘min()’, ‘+’ and ‘-’ operations required by the mset operations.

Let’s illustrate the above concepts and possibilities in terms of the two following functions:

$$\begin{aligned} g(x) &= e^{-10x^2} \\ h(x) &= 2e^{-10|x|} \end{aligned} \quad (37)$$

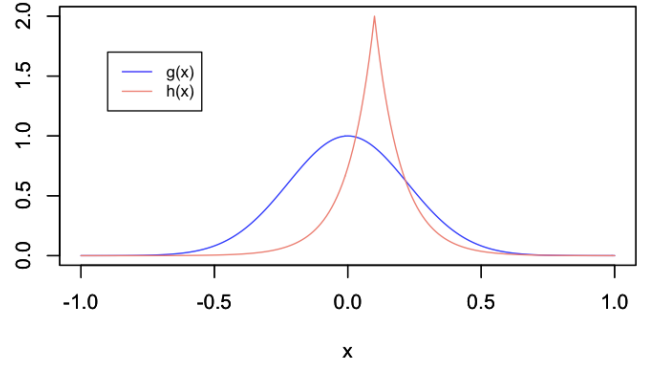
Figure 5 illustrates the two above functions as well as their union, intersection, sum, and subtraction after having been converted into respective msets.

This examples illustrates several interesting points. First, we have the transformation of functions into respective msets immediately allow them to be operated by union and intersction. In addition, we observe an example that the sum of two functions is larger or equal than their union, as well as the possibility of the subtraction operation yielding negative values.

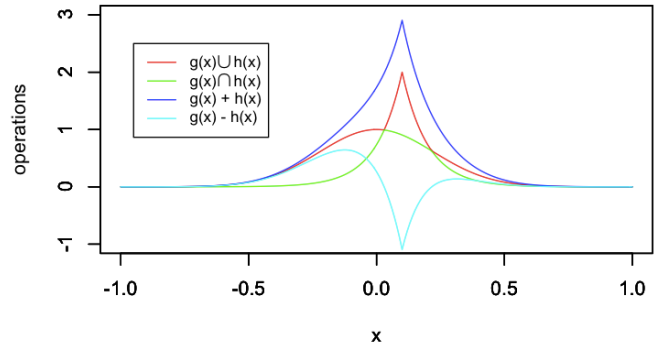
Figure 5 shows the two additional operations of product and quotient between the two functions $g(x)$ and $h(x)$ above, avoiding the divisions by zero.

It is interesting to observe that the potential of the operations of union and intersection in producing sharp derivatives and discontinuities, which contribute an interesting manner of representing an ample range of function types as combinations of these operations, not to mention the operations of sum, subtraction, product and quotient.

The above developments also allow new functions to be obtained as combinations of logic operations as the



(a)



(b)

Figure 4: Two functions $g(x)$ and $h(x)$ of a single variable (a), and their respective mset operations (b) of union, intersection, sum, and subtraction.

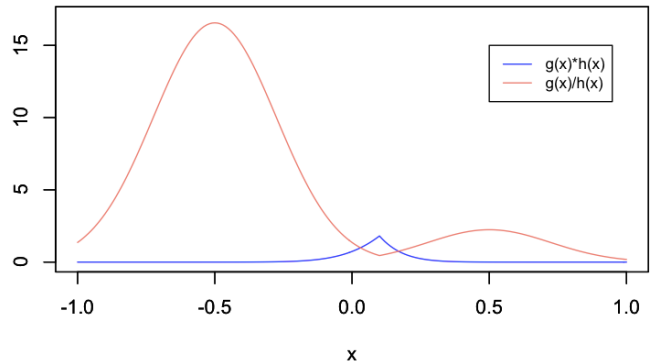


Figure 5: Two functions $g(x)$ and $h(x)$ of a single variable (a), and their respective mset operations (b) of union, intersection, sum, and subtraction.

union and intersection and numeric operations as sum, subtraction, product, and division. For instance, it be-

comes possible to write things such as:

$$\begin{aligned}
 r(x) &= (g(x) \cap h(x)) + g(x) \\
 s(x) &= (g(x) + h(x)) \cup (g(x) - h(x)) \\
 t(x) &= [g(x) \cap h(x)] - [g(x) \cup h(x)]
 \end{aligned}
 \tag{38}$$

These three functions are illustrated in Figure 6 assuming the function in Equation 37.

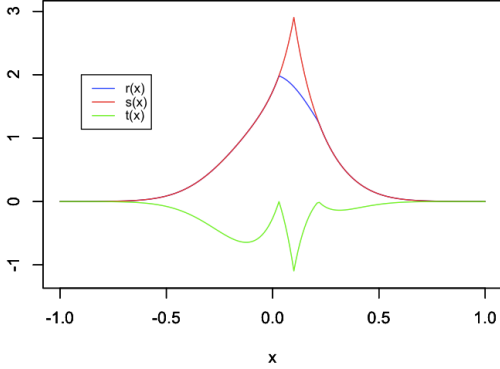


Figure 6: The functions $r(x)$, $s(x)$ and $t(x)$ obtained through mset operations.

The potential of these hybrid constructions is as large as our imagination, because it allows the incorporation of much of the concepts, structures, and properties of both arithmetic, set theory, and also logic (which is directly analogous to set theory).

8 The Multiset Jaccard Indices

The Jaccard index represents an effective and conceptually appealing manner to quantify the similarity between any two sets A and B (e.g. [14, 15, 16]), having therefore being extensively applied in a vast range of problems in several scientific and technological fields.

In its most basic form, the Jaccard index between an two sets A and B can be expressed as:

$$\mathcal{J}(A, B) = \frac{A \cap B}{A \cup B}
 \tag{39}$$

It is possible to adapt the Jaccard index to msets by making:

$$\mathcal{J}_M(A, B) = \frac{\sum_{i=1}^N \min(m(a_i), m(b_i))}{\sum_{i=1}^N \max(m(a_i), m(b_i))}
 \tag{40}$$

where a_i and b_i are the elements of the sets A and B , respectively, and N is the cardinality of the universe of those sets. We also have that $0 \leq \mathcal{J}_M(A, B) \leq 1$.

As an example, let's consider $A = \{a, b, b, c, c, c\}$ and $B = \{a, b, c, c, d\}$. Then, we have:

$$\mathcal{J}(A, B) = \frac{1 + 1 + 2 + 0}{2 + 3 + 5 + 1} = \frac{4}{11}
 \tag{41}$$

The Jaccard index has been enhanced and extended to functions, scalar fields, joint variations and more than 2 sets [16]. In particular, the latter type of Jaccard index for 3 sets A , B and C can be written as:

$$\mathcal{J}(A, B, C) = \frac{A \cap B \cap C}{A \cup B \cup C}
 \tag{42}$$

9 Multisets in Pattern Recognition

The possibility to use msets to represent any type of density paves the way to interesting applications in pattern recognition and deep learning (e.g. [7, 8, 9, 10, 11]). In this section we illustrate how msets and the Jaccard index can be readily applied in order to quantify the similarity between two (or more) clusters represented by respective density functions.

Let's consider the three sets of points in the scatterplot shown in Figure 7, which corresponds to the three species of iris flower in the frequently adopted iris dataset. Only two out of their 4 features have been chosen in the following example for simplicity's sake.

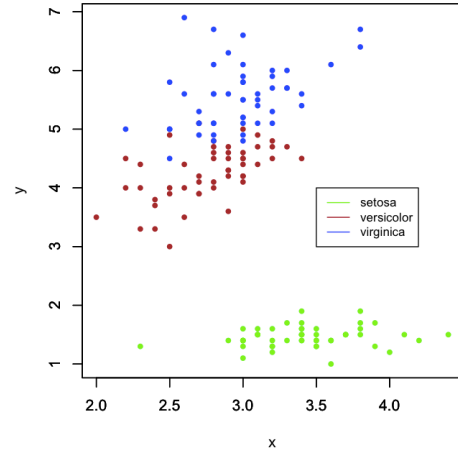


Figure 7: A scatterplot representing the distribution of three types of iris flowers represented by two respective features x and y .

The density obtained from the respective discrete samples through gaussian kernel expansion are shown in Figure 8.

The obtained multiset Jaccard index for each pairwise combination of categories are presented in Table 1.

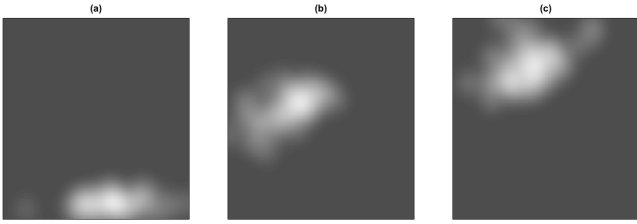


Figure 8: The three density scalar fields obtained by gaussian kernel expansion of each of the three categories.

	setosa	versicolor	virginica
setosa	1	2.6e-5	0
versicolor	2.6e-5	1	0.145
virginica	0	0.145	1

Table 1: The Jaccard indices obtained for pairwise combinations between the three iris species. The resolution has been limited to 6 digits.

The obtained results are fully compatible with the interrelationships between the three densities, or clusters, in Figure 7. In addition, the threewise Jaccard index from Equation 42 result nearly null, indicating a really small chance that the three densities correspond to the same cluster.

10 Concluding Remarks

The fascinating subject of multisets has been presented in a hopefully introductory manner.

We started with a brief review of traditional sets and their properties, which was followed by a progressive presentation of multisets and their characteristics. The possibility of obtaining multiset generalizations capable of dealing with functions, scalar fields, and densities, was then described and illustrated.

The extension of the Jaccard index, which is intrinsically related to set theory, to msets and also to allow the consideration of more than two sets were also presented, which paved the way to employing these combined concepts for the characterization of relationships between clusters in feature spaces, a problem that is common to both the areas of pattern recognition and deep learning.

The presented concepts and methods pave the way to several interesting applications, also motivating further integrations between the structures and properties between the domains of set theory, propositional logic, and analysis.

Acknowledgments.

Luciano da F. Costa thanks CNPq (grant

no. 307085/2018-0) and FAPESP (grant 15/22308-2).

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It is hoped that CDTs can also incorporate new insights and analogies concerning the reported concepts and methods. We hope these characteristics will contribute to making CDTs interesting both to beginners as well as to more senior researchers.

Each CDT focuses on a limited set of interrelated concepts. Though attempting to be relatively self-contained, CDTs also aim at being relatively short. Links to related material are provided in order to provide some complementation of the covered subjects.

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