

Shells, point cloud huts, generalized scalar products, cosines and similarity tensor representations in vector semispaces

Ramon Carbó-Dorca · Emili Besalú

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Abstract This study provides an as complete as possible set of precise definitions, within the mathematics developed for quantum similarity purposes. The topics are embedded in the structure of vector semispaces and the possibility of constructing generalized scalar products on them. This scenario allows describing precisely several items and procedures like: (a) the concept of point clouds, (b) the holographic properties of the so called unit shells of vector semispaces, (c) the cosine of a vector set, (d) the description of point cloud huts and (e) opens the way towards the tensorial representation of molecular structures.

Keywords Quantum similarity · Vector semispaces · Generalized scalar products · Shells in vector semispaces · Point clouds · Point cloud huts · Generalized cosine of a point cloud · Tensorial representation of molecules

1 Introduction

Since the initial description of quantum similarity [1,2], the effort to provide with an appropriate theoretical background the development of its applications has given birth to a series of papers [3–27], mainly devoted to the mathematical aspects of this branch of quantum chemistry studying the possible interrelationships of molecular sets in particular and quantum objects in general.

In several instances the information which will be provided along this paper development has been previously studied from a more or less profound point of view, see for example [8, 11, 13–15, 19, 20, 22, 24]. However, the material included now here was dispersed enough among the space and time of the literature, as to feel that the systematic

R. Carbó-Dorca (✉) · E. Besalú
Institut de Química Computacional, Universitat de Girona, 17071 Girona, Catalonia, Spain
e-mail: quantumQSAR@hotmail.com

use of this material in forthcoming application papers on quantum similarity, may convert into an uncomfortable task the citation of this large list of papers in every new manuscript. Thus, the authors thought useful to write an up-to-date summary of the most employed mathematical terms and definitions, associated to quantum similarity and more generally related to the discrete and continuous description of molecular sets.

In doing so, not only appeared in front of our minds an old collection of terms linked in a logical sequential way, but new subtle ideas, which had not been described before, have appeared as a consequence of the logical ordering effort on the old knowledge.

The most interesting of these new concepts, which have developed along the building up of the present work, is the fact that within normed vector semispaces the notion of unit shell corresponds to a hologram of the whole vector semispace.

Therefore, not only individually quantum mechanical density functions appear as mathematical objects containing hologram properties [28], but some holographic properties can be also considered collectively present, when studying quantum density function sets.

On the other hand, the connection of point clouds, an idea which was used in initial work in quantum molecular similarity [3], with tagged sets [8, 13] appears also evident in the present study for the first time leading to the new concept of point cloud hut.

Finally, the notion of discrete molecular representations in a general tensorial context appears as a simple consequence of the theoretical framework developed within the present paper scheme. Such an idea encompasses the classical vectorial molecular description and opens a vast application way in both chemical modeling and molecular engineering fields.

All these new conceptual findings could not have been developed without the simple formal idea of vector semispace [13, 14]; leading the way to the possibility to define in this context extended scalar products [14, 19, 22, 27] involving point clouds. On the other hand, generalized scalar products constitute a computational structure, which is an essential building block for quantum similarity development. Therefore, in the present paper all these concepts will be actors within a general and coherent notation theater, prior to leading the way towards new ideas and advances to be published elsewhere.

Then, from this point of view the present collection of notions can be further used to avoid cumbersome repetitions within other forthcoming papers containing different subjects, for instance computational techniques which demand other kind of mathematical perspective.

Accordingly, the present work is organized as a set of twelve definitions, which cover the whole set of interests associated to quantum similarity. Some of these definitions contain more than a unique statement and if needed some subsidiary items are also defined. In order to help the understanding of every subject, in addition to every definition there have been added several notes and examples given, in order to clarify the various problems and applications associated to the included definitions.

1.1 Definitions and notes

In the following conceptual progress, several definitions will be given at each step, related with the basic mathematical structure associated to quantum similarity [4, 5, 11, 12, 16, 24, 25], which will constitute in turn the backbone of the present contribution. These definitions comprise from the concept of vector semispace [13, 14], the definition of generalized scalar products and cosines [14, 22] of vector sets, and continue up to the tensorial representation of molecular structures. This description development provides with a sufficient stable and well-defined background the practical applications, which are planned ahead from the computational point of view, in order to continue the series of works on quantum QSPR [21, 23, 24, 29–34] and several new aspects of quantum similarity [35–37]. Every definition will have several notes attached, which will serve as particular application examples or to shed light to the definition itself.

Definition 1 Vector semispaces: A vector semispace $V(\mathbf{R}^+)$ is a vector space where the vectors are defined over the positive (semi-)definite real field: \mathbf{R}^+ . In vector semispaces the additive group is a semigroup. A semigroup is a group without reciprocal elements.

- Here and in the following Dirac's notation for vectors will be employed. Thus one can write, for instance: $|\mathbf{u}\rangle, |\mathbf{v}\rangle \in V(\mathbf{R}^+)$. The dual will be noted as: $\langle \mathbf{u}|, \langle \mathbf{v}| \in V^*(\mathbf{R}^+)$.

Definition 2 Inward vector products: Given a vector space $V(\mathbf{K})$, an *inward vector product* is defined as producing as a result another vector of the same space: $\forall |\mathbf{u}\rangle, |\mathbf{v}\rangle \in V(\mathbf{K}) : |\mathbf{u}\rangle * |\mathbf{v}\rangle \in V(\mathbf{K})$. Inward vector products are distributive with respect the vector sum and define a multiplicative abelian semigroup over the vector space $V(\mathbf{K})$.

- This definition applies to any vector space. For instance in Hilbert spaces one can define the inward product as:

$$|\mathbf{u}\rangle, |\mathbf{v}\rangle \in V(\mathbf{C}) \wedge \langle \mathbf{u}| = (|\mathbf{u}\rangle)^* \rightarrow |\mathbf{u}\rangle * |\mathbf{v}\rangle \equiv \langle \mathbf{u}| * |\mathbf{v}\rangle \in V(\mathbf{C})$$

- The neutral element with respect the inward vector product is the *unity* vector, which is defined in such a manner that:

$$\exists |\mathbf{1}\rangle \in V(\mathbf{K}) \rightarrow \forall |\mathbf{u}\rangle \in V(\mathbf{K}) : |\mathbf{1}\rangle * |\mathbf{u}\rangle = |\mathbf{u}\rangle * |\mathbf{1}\rangle = |\mathbf{u}\rangle .$$

- *Reciprocal elements* exist for some vectors, but inward product inverses have not a general existence. That is: some vectors do not possess an inward inverse. For example, the vector zero in general or more specifically in matrix vector spaces, matrices with one or several null elements do not possess an inward product reciprocal element.

Definition 3 Vector semispace generators: A vector space of dimension D : $V_D(\mathbf{K})$ defined over an arbitrary field \mathbf{K} , can be used as a *generator of a vector semispace*: $V_D(\mathbf{R}^+)$, provided that $\mathbf{R}^+ \subseteq \mathbf{K}$. The dimension of the generated vector semispace

is coincident with the dimension of $V_D(\mathbf{K})$. The generation of the vector semispace $V_D(\mathbf{R}^+)$ is made as follows:

$$\forall |\mathbf{x}\rangle \in V_D(\mathbf{R}^+) \rightarrow \exists |\mathbf{v}\rangle \in V_D(\mathbf{K}) : |\mathbf{x}\rangle = |\mathbf{v}\rangle * |\mathbf{v}\rangle .$$

- In Hilbert spaces associated to quantum mechanics this generation procedure can produce *density functions*, as elements of the generated Hilbert semispace:

$$\forall |\mathbf{u}\rangle \in V(\mathbf{C}) \wedge \langle \mathbf{u} | = (|\mathbf{u}\rangle)^* \rightarrow |\mathbf{u}\rangle * |\mathbf{u}\rangle \equiv ||\mathbf{u}\rangle|^2 = \langle \mathbf{u} | * |\mathbf{u}\rangle \in V(\mathbf{R}^+)$$

Definition 4 Point clouds: A P -point cloud $B_P(\mathbf{R}^+) = \{|\mathbf{x}_I\rangle | I = 1, P\}$ defined in a vector semispace $V_D(\mathbf{R}^+)$ is a linearly independent vector set of $V_D(\mathbf{R}^+)$ with cardinality: $\# [B_P(\mathbf{R}^+)] = P \leq D$. Thus, $B_P(\mathbf{R}^+)$ can be considered as a basis set of some subsemispace: $V_P(\mathbf{R}^+) \subseteq V_D(\mathbf{R}^+)$, which is a vector semispace itself.

- A molecular P -point cloud or briefly: *molecular point cloud* (MPC) is a point cloud as defined before, but constructed by discrete or continuous vector representations of molecular structures.
- In classical QSPR procedures the vectors gathered to form the MPC are finite dimensional column (or row) vectors made of arbitrarily chosen parameters. However, within quantum similarity field the molecular description is made with density functions or alternatively by their discrete representations, like vectors or tensors, as elements of some vector semispace [13, 14].
- Usually, classical QSPR MPC are statistically manipulated in such a way that a dimensionality paradox appears [33].
- A quantum MPC (QMPC) corresponds to a P -point cloud, whose elements are quantum molecular density functions or their discrete representations.
- MPC can be also thought as related to tagged sets [8].
- A *tagged set* W is the Cartesian product composition of two sets: the *object set* O and the *tag set* T , in such a way that:

$$W = O \times T \rightarrow \forall w \in W : w = (o; t) \wedge o \in O; t \in T.$$

- In fact, according to this, any MPC can be considered as the tag set of a tagged set where the object set is made of molecular structures.

Definition 5 Complete sum of a vector: A *complete sum* of a vector, which will be noted: $\forall |\mathbf{u}\rangle \in V(\mathbf{K}) : \langle |\mathbf{u}\rangle \rangle \in \mathbf{K}$, corresponds to the sum of the vector elements in case of discrete vector spaces and to an integral in case of functional spaces.

- $\forall |\mathbf{u}\rangle = \{u_I\} \in V_N(\mathbf{K}) : \langle |\mathbf{u}\rangle \rangle = \sum_{I=1}^N u_I \in \mathbf{K}$
- $\forall |\mathbf{f}\rangle = f(\mathbf{x}) \in V_\infty(\mathbf{K}) : \langle |\mathbf{f}\rangle \rangle = \int_D f(\mathbf{x}) d\mathbf{x} \in \mathbf{K}$
- A complete sum of a vector acts as a linear operator over vector spaces:

$$\forall \alpha, \beta \in \mathbf{K} \wedge \forall |\mathbf{u}\rangle, |\mathbf{v}\rangle \in V(\mathbf{K}) : \langle \alpha |\mathbf{u}\rangle + \beta |\mathbf{v}\rangle \rangle = \alpha \langle |\mathbf{u}\rangle \rangle + \beta \langle |\mathbf{v}\rangle \rangle .$$

Definition 6a Shells of normed vector semispaces: If $V_D(\mathbf{R}^+)$ is normed, a λ -shell: $S_D^{(\lambda)}(\mathbf{R}^+)$ is defined as the set of all vectors with norm: λ . That is:

$$\forall |\mathbf{r}\rangle \in S_D^{(\lambda)}(\mathbf{R}^+) \subset V_D(\mathbf{R}^+) : \|\mathbf{r}\| = \lambda.$$

Definition 6b Unit shell of normed vector semispaces: The *unit shell* $S_D^{(1)}(\mathbf{R}^+)$ of a normed vector semispace $V_D(\mathbf{R}^+)$ collects all vectors such that: $\forall |\mathbf{s}\rangle \in S_D^{(1)}(\mathbf{R}^+) \subset V_D(\mathbf{R}^+) : \|\mathbf{s}\| = 1$. Conversely, the unit shell of a normed vector semispace can generate any other element of it, that is:

$$\forall |\mathbf{v}\rangle \in V_D(\mathbf{R}^+) \wedge \|\mathbf{v}\| = v \in \mathbf{R}^+ \rightarrow \exists |\mathbf{s}\rangle \in S_D^{(1)}(\mathbf{R}^+) : |\mathbf{v}\rangle = v |\mathbf{s}\rangle.$$

Some properties can be easily deduced, complementing earlier studies [13–15, 19, 22, 27] on this subject:

- In normed vector semispaces an associated *Minkowski norm* corresponds to the complete sum of a vector:

$$\forall |\mathbf{v}\rangle \in V_D(\mathbf{R}^+) : \|\mathbf{v}\| = \langle |\mathbf{v}\rangle \rangle = v \in \mathbf{R}^+$$

- *Unit shells as probability distribution sets.* The unit shell of a normed vector semispace $V_D(\mathbf{R}^+)$ contains all the probability distributions, which can be constructed within $V_D(\mathbf{R}^+)$.
- *Unit shells as holograms:* Knowing the unit shell $S_D^{(1)}(\mathbf{R}^+)$ of a given normed vector semispace $V_D(\mathbf{R}^+)$, then any vector, P -point cloud, subset or λ -shell of $V_D(\mathbf{R}^+)$, can be obtained from an element or set of $S_D^{(1)}(\mathbf{R}^+)$ by simple homothetic scaling. Therefore, all the information about $V_D(\mathbf{R}^+)$ is contained in $S_D^{(1)}(\mathbf{R}^+)$.
- Thus, unit shells can be considered as *holograms* of normed vector semispaces.
- A quantum mechanical molecular unit shell can be made of *shape functions*, that is: molecular density functions Minkowski normalized by the number of electrons, see for example [15].

Definition 7 Generalized scalar products in vector semispaces: A *generalized scalar product* of a P -point cloud in a vector semispace is defined as the complete sum of the inward vector product of the P -point cloud elements. Suppose the P -point cloud: $B_P(\mathbf{R}^+) = \{|\mathbf{x}_I\rangle | I = 1, P\}$; then, the generalized scalar product of its elements is defined as: $\left\langle \begin{matrix} P \\ * \\ I=1 \end{matrix} |\mathbf{x}_I\rangle \right\rangle = \langle |\mathbf{x}_1\rangle * |\mathbf{x}_2\rangle * \dots * |\mathbf{x}_P\rangle \rangle \in \mathbf{R}^+$.

- The usual scalar product can be retrieved as a particular case of this general definition with $P = 2$:

$$\forall |\mathbf{u}\rangle, |\mathbf{v}\rangle \in V(\mathbf{K}) : \langle \mathbf{u}|\mathbf{v}\rangle \equiv \langle |\mathbf{u}\rangle * |\mathbf{v}\rangle \rangle \in \mathbf{K}$$

Definition 8 *P*-norm of a vector element in semispaces: Such a norm is defined as a generalized scalar product affecting a unique vector, as follows:

$$\forall |\mathbf{u}\rangle \in V(\mathbf{R}^+) : ||\mathbf{u}\rangle|_P = \langle |\mathbf{u}\rangle * |\mathbf{u}\rangle * \dots * |\mathbf{u}\rangle \rangle = \left\langle \begin{matrix} P \\ * \\ I=1 \end{matrix} |\mathbf{u}\rangle \right\rangle$$

- The well-known Euclidian norm is just a 2– norm:

$$\forall |\mathbf{u}\rangle \in V(\mathbf{R}^+) : ||\mathbf{u}\rangle|_2 = \langle |\mathbf{u}\rangle * |\mathbf{u}\rangle \rangle = \langle \mathbf{u}|\mathbf{u}\rangle$$

- A Minkowski norm in a vector semispace is defined as a 1-norm:

$$\forall |\mathbf{u}\rangle \in V(\mathbf{R}^+) : ||\mathbf{u}\rangle|_1 = \langle |\mathbf{u}\rangle \rangle.$$

Definition 9 Cosine of the angle of a *P*-point cloud: The cosine of the angle ‘subtended’ by a *P*-point cloud: $B_P(\mathbf{R}^+) = \{|\mathbf{x}_I\rangle | I = 1, P\}$ can be calculated by means of:

$$\cos(\alpha)_{(P)} = \langle |\mathbf{v}_1\rangle * |\mathbf{v}_2\rangle * \dots * |\mathbf{v}_P\rangle \rangle \left(\prod_{I=1}^P ||\mathbf{v}_I\rangle|_P \right)^{-\frac{1}{P}} = \left\langle \begin{matrix} P \\ * \\ I=1 \end{matrix} |\mathbf{v}_I\rangle \right\rangle \left(\prod_{I=1}^P ||\mathbf{v}_I\rangle|_P \right)^{-\frac{1}{P}}.$$

However, constructing a scaled *P*-point cloud as follows:

$$Z_P(\mathbf{R}^+) = \left\{ |\mathbf{z}_I\rangle = ||\mathbf{v}_I\rangle|_P^{-\frac{1}{P}} |\mathbf{v}_I\rangle | I = 1, P \right\},$$

then, one can also have the equivalent general cosine definition over the scaled *P*-point cloud:

$$\cos(\alpha)_{(P)} = \langle |\mathbf{z}_1\rangle * |\mathbf{z}_2\rangle * \dots * |\mathbf{z}_P\rangle \rangle = \left\langle \begin{matrix} P \\ * \\ I=1 \end{matrix} |\mathbf{z}_I\rangle \right\rangle$$

- The following property will hold in any circumstance:

$$\forall |\mathbf{z}\rangle \in Z_P(\mathbf{R}^+) : \langle |\mathbf{z}\rangle * |\mathbf{z}\rangle * \dots * |\mathbf{z}\rangle \rangle = 1.$$

Proof

$$\langle |\mathbf{z}\rangle * |\mathbf{z}\rangle * \dots \rangle = ||\mathbf{v}\rangle|_P^{-1} \langle |\mathbf{v}\rangle * |\mathbf{v}\rangle \dots \rangle = \langle |\mathbf{v}\rangle * |\mathbf{v}\rangle \dots \rangle^{-1} \langle |\mathbf{v}\rangle * |\mathbf{v}\rangle \dots \rangle = 1.$$

- The so-called Carbó index [1,5] is just a particular case of this general definition when *P* = 2. That is:

$$\begin{aligned} \cos(\alpha)_{(2)} &= (||\mathbf{v}_1\rangle|_2 ||\mathbf{v}_2\rangle|_2)^{-\frac{1}{2}} \langle |\mathbf{v}_1\rangle * |\mathbf{v}_2\rangle \rangle \\ &= (\langle \mathbf{v}_1|\mathbf{v}_1\rangle \langle \mathbf{v}_2|\mathbf{v}_2\rangle)^{-\frac{1}{2}} \langle \mathbf{v}_1|\mathbf{v}_2\rangle \end{aligned}$$

Definition 10 Point cloud huts (PCH): A P -point cloud hut $H_P(\mathbf{R}^+)$ is a P -point cloud redefined in the unit shell of a vector semispace.

$$B_P(\mathbf{R}^+) = \{|\mathbf{v}_I| \mid I = 1, P\} \subset V_D(\mathbf{R}^+) \rightarrow$$

$$H_P(\mathbf{R}^+) = \left\{ |\mathbf{c}_I\rangle = \langle |\mathbf{v}_I\rangle \rangle^{-1} |\mathbf{v}_I\rangle \mid I = 1, P \right\} \subset S_D^{(1)}(\mathbf{R}^+)$$

- The cosine of a point cloud is *invariant*, when computed over a related PCH. To prove this, it is sufficient to write the cosine of a PCH and substitute it by the Minkowski normalized points of the original P -point cloud:

$$\begin{aligned} \cos(\alpha)_{(P)} &= \langle |\mathbf{c}_1\rangle * |\mathbf{c}_2\rangle * \cdots * |\mathbf{c}_P\rangle \rangle \left(\prod_{I=1}^P \|\mathbf{c}_I\| \right)_P^{-\frac{1}{P}} \\ &= \left(\prod_{I=1}^P \langle |\mathbf{v}_I\rangle \rangle \right)^{-1} \langle |\mathbf{v}_1\rangle * |\mathbf{v}_2\rangle * \cdots * |\mathbf{v}_P\rangle \rangle \left(\prod_{I=1}^P \left[\langle |\mathbf{v}_I\rangle \rangle^{-P} \|\mathbf{v}_I\| \right]_P \right)^{-\frac{1}{P}} \\ &= \langle |\mathbf{v}_1\rangle * |\mathbf{v}_2\rangle * \cdots * |\mathbf{v}_P\rangle \rangle \left(\prod_{I=1}^P \|\mathbf{v}_I\| \right)_P^{-\frac{1}{P}} \end{aligned}$$

- A P -ball is a sphere of unit radius and dimension P .
- In a P -PCH every element is contained on the surface of a P -ball. In such a way that every P -PCH vector can be considered possessing the same origin at the center of the P -ball, while the other end lying at the P -ball surface.
- Therefore every P -PCH is circumscribed into a corresponding P -ball.
- A molecular set described by a P -PCH can be termed as a MPCH.
- A quantum MPCH (QMPCH) is a MPCH whose vector elements are shape functions.
- Any P -point cloud hut is coincident to a set of probability distributions possessing cardinality P .
- Comparing the elements of a MPCH is equivalent to compare probability distributions.
- Consistently with the fact that the P -PCH elements are lying in the $P - 1$ dimensional surface of a P -ball, any P -PCH can be considered as a polytope in a subsemispace of dimension $P - 1$. In this way 3-PCH generate a 2-dimensional triangle, 4-PCH generate a 3-dimensional pyramid, and so on.
- Such last property contains a holographic structure.

Definition 11 Similarity tensors: Knowing a P -point cloud of some vector semispace, defined as: $B_P(\mathbf{R}^+) = \{|\mathbf{v}_I| \mid I = 1, P\} \subset V_D(\mathbf{R}^+)$ a similarity tensor of order Q : $\mathbf{Z}^{(Q)} = \{z_{i_1 i_2 \dots i_Q} \equiv z(\mathbf{i})\}$ can be constructed as a covariant tensor, whose elements are obtained by the generalized scalar products of Q vectors of the point cloud:

$$\forall k = 1, Q \wedge \forall i_k = 1, P : z_{i_1 i_2 \dots i_Q} = \left\langle \prod_{k=1}^{k=Q} * | \mathbf{v}_{i_k} \right\rangle.$$

- In practical computations, quantum similarity procedures have usually employed second order tensors:

$$\mathbf{Z}^{(2)} = \{ z_{ij} = \langle | \mathbf{v}_i \rangle * | \mathbf{v}_j \rangle \mid i, j = 1, P \}$$

which have been customarily called *similarity matrices* and correspond to symmetric ($P \times P$) matrices [4, 16, 29]. They match the metric matrices of the P -dimensional subsemispace, generated by the linearly independent P -point cloud elements.

- When dealing with quantum MPC, the associated tensor family $\mathbf{Z} = \{ \mathbf{Z}^{(Q)} \}$ is constructed by means of a set of density or shape functions acting as MPC elements.
- When looking at a MPC, the P tensor components of order $Q - 1$ of every *similarity tensor* of order Q present in the tensor collection: \mathbf{Z} , can be associated to a discrete *tensorial* representation of the molecules included in the MPC.
- That is, suppose the tensor: $\mathbf{Z}^{(Q)} \in \mathbf{Z}$. Such tensor can be considered as a vector whose components are tensors of order: $Q - 1$. That is: $\mathbf{Z}^{(Q)} = \{ \mathbf{Z}_I^{(Q-1)} \mid I = 1, P \}$.
- Therefore, such a tensorial representation of a MPC can be considered at the same time as elements of a discrete MPC, belonging to the corresponding vector semispaces and simultaneously also behaving as tag sets of some molecular tagged set.
- A *similarity tensor* belongs to the P^Q - dimensional semispace generated by the elements of the tensorial products of the associated P -point cloud elements: $\forall K_I \in \{ 1, \dots, P \} : \left\{ \bigotimes_{I=1}^Q | \mathbf{v}_{K_I} \right\}$.
- Similarity components of any quantum similarity tensor can be easily transformed into unit shell elements of the corresponding semispace. Suppose the decomposition $\mathbf{Z}^{(Q)} = \{ \mathbf{Z}_I^{(Q-1)} \mid I = 1, P \}$ of some similarity tensor; then, using *stochastic scaling* one can define a new set of tensors:

$$\forall I : \Theta_I^{(Q-1)} = \left\langle \mathbf{Z}_I^{(Q-1)} \right\rangle^{-1} \mathbf{Z}_I^{(Q-1)}.$$

The resultant scaled tensor: $\Theta^{(Q)} = \{ \Theta_I^{(Q-1)} \mid I = 1, P \}$ has components belonging to the unit shell, because their complete sums are unit:

$$\forall I : \left\langle \Theta_I^{(Q-1)} \right\rangle = \left\langle \mathbf{Z}_I^{(Q-1)} \right\rangle^{-1} \left\langle \mathbf{Z}_I^{(Q-1)} \right\rangle = 1.$$

- Thus, the scaled similarity tensor $\Theta^{(Q)} = \{ \Theta_I^{(Q-1)} \mid I = 1, P \}$ components constitute a P -PCH.

2 Final remarks

Besides the precise statements associated to quantum similarity and providing the basic definitions related to the concept of vector semispace, here have been put forward several new aspects of the mathematical background of this discipline. The holographic character of the unit shell in normed vector semispaces has been described for the first time. The connection between vector semispace subsets and tagged sets has been evidenced also in a first instance. The generalization of scalar products and norms in vector spaces has been unambiguously structured to be applied in further developments. New concepts, such as the point cloud hut one, have been developed. The invariance of the generalized cosine between vector semispace shells of a P -point cloud set of vectors has been shown. The generation feasibility of tensorial descriptions of a molecular set has been discussed and constructed, as a trivial consequence of the theoretical framework, which originates within the structure of vector semispaces and ends with the concept of generalized scalar products. In general, one can say that a solid succinct basis of the mathematical backbone of quantum similarity and beyond has been described.

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