

Shell partition and metric semispaces: Minkowski norms, root scalar products, distances and cosines of arbitrary order

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Vector semispaces are studied from a realistic way with the intention to define a natural metric, adapted to their peculiar structure, which reside on the essential positive definiteness of their elements. From this point of view, *Minkowski norms* allow classifying semispaces in *shells*, that is: subsets where all the vector elements possess the same norm values. Shell structure appears to be a possible disjoint *partition* of any semispace and so shells become *equivalence classes*. Then, the *unit shell* appears to be the core of the semispace homothetic construction as well as the origin of the semispace metrics. *Minkowski or root scalar products* permit to connect two or more semispace elements and conduct towards generalized definitions of *Pth order root distances and cosines*. Finally, the unit shell of a given semispace, in company of both Boolean tagged sets, inward matrix products and with the aid of the matrix signatures as well, it is seen as the seed to construct any arbitrary element of the semispace connected vector space. Finite and infinite dimensional vector spaces application examples are provided along the work discussion.

KEY WORDS: vector semispaces, Minkowski norms, semispace shells, homothetic structures, unit shell, root scalar products, root distances, root cosine, tagged sets, Boolean tagged sets, inward matrix products, matrix signature, matrix nullity, vector space generation, density functions

1. Introduction

1.1. Vector semispaces

Vector semispaces, $V(\mathbf{R}^+)$, have been described several years ago [1] within a framework, where the main objective has taken a double path. First, in semispace study was followed the direction providing with adequate mathematical tools the framework of *quantum similarity* (QS) and, at the same time, the second research track was also chosen for the sake to find out how to properly describe the associated background of *quantum density functions* sets. The main basic original idea was to construct sets, related to parent vector spaces defined over the real field¹, $V(\mathbf{R})$, but with all elements

¹ Parent vector spaces defined over the *complex field* can be also studied within the same context. However, such alternative and general framework would complicate the basic notions which will be developed here and, thus, only the simpler real field case will be taken into account.

being positive definite. In this fashion, semispaces can describe a vector set whose elements are made of measures, like the collections of QS measures, forming matrix arrays, and can end up into the sets of discrete or continuous probability distributions.

In order to achieve this goal, semispaces are made as usual vector spaces, but are restrictedly defined over the positive definite real field \mathbf{R}^+ only. The main axiomatic characteristic of semispaces consists into that the vector addition is constructed with an Abelian *semigroup* structure [2]², instead of the usual Abelian additive group associated to vector spaces.

Moreover, if time can be associated to some structure, as a recent study points out [3], then the time structure elements will definitively belong to a semispace construct.

1.2. Tagged and quantum object sets

Several discussion studies have been performed on vector semispaces and their connection with QS *measures* and *matrices* [4,5]. Of the two mentioned concepts, the last one is obviously linked with vector semispace features, as QS matrices are symmetric and bearing positive definite elements, according to the fact that such elements are the result of QS measures, usually computed between pairs of *quantum object* descriptors defined in turn by computationally connecting the appropriate quantum state density functions.

Besides all of these considerations, vector semispace subset elements are perfect candidates to naturally become the *tag set* part of *tagged sets* [5,6] constructions. Such tagged sets are defined as the Cartesian product: $Z = Q \times T$ of a set of object entities or *object set*, Ω , which can be formed by any collection of arbitrary elements, and another set, the *tag set*, T , whose elements contain known information about the objects. Tags are usually chosen as, or can alternatively be transformed into, bit strings, constituting *Boolean tagged sets* [6]. Tags can be also formed by positive definite N -tuples or functions. Then, in any of these cases the ordered pairs: $(\omega; t) \in Z$, with $\omega \in \Omega \wedge t \in T$, constitute the generic elements of any tagged set.

Quantum object sets are a convenient and useful example of tagged sets, as they are defined as being formed by submicroscopic quantum systems chosen as object entities, which possess attached, by quantum mechanical postulate construction, *quantum density state functions* [7]. Such probability functions, which depend on the quantum object particle coordinates, act in this case as positive definite tags and, thus, form the tag set part [6,8] of the quantum object set. *Discrete quantum object sets* are constructed as a mathematical elaboration of quantum object sets [3,9,10], as the object entities are the

² Semigroups are groups without reciprocal elements. Additive semigroups like the ones employed in order to construct semispaces, lack of negative elements and, thus, differences, negative vectors and scalars are not present.

same as in the former quantum object set definition, but tags become the columns of a QS matrix or a manipulation of their positive definite elements in form of QS indices.

Despite of all this developed work, *metric vector semispaces* structure and tools have not been deeply discussed so far, though. Thus, it seems worthwhile at this moment of the theoretical development of QS to present and to discuss the possible way to describe an *ad hoc* metric in semispaces. This will be the main purpose of the present study.

2. Vector spaces as Boolean tagged sets

2.1. Signatures and vector spaces as Boolean tagged sets

The elements of a given N -dimensional vector semispace can be employed not only as tags in a tagged set assembly, as discussed in the introduction above, but they can be also contemplated as object entities, in order to construct any element associated to a parent N -dimensional vector space.

Indeed, in the case where supposedly the vector space is considered defined over the real set, one can use the semispace elements as the object set part, while as the tag set part one can employ the possible 2^N vector *signatures* [11], Σ_N , made of N -dimensional vectors using the combinations with repetition of the binary elements in the set: $\{-1; +1\}$. Equivalently a bit source: $\{0, 1\}$, can be envisaged for signature build up, but in this bit-like case one has to admit the adequate relationship between bits and equivalent sign conventions.

Thus, vectors can be associated to the following construction rule as tagged set elements:

$$\forall \mathbf{x} \in V_N(\mathbf{R}): \exists \mathbf{z} \in V_N(\mathbf{R}^+) \wedge \exists \sigma \in \Sigma_N \rightarrow \mathbf{x} = (\mathbf{z}; \sigma).$$

So, this is equivalent to consider that one can construct vector spaces from vector semispaces by using the Cartesian product of such sets with the signature set: $V_N(\mathbf{R}) = V_N(\mathbf{R}^+) \times \Sigma_N$ [12].

2.2. Inward matrix products and sign reversal

Keeping in mind vector spaces can be assembled from vector semispaces, as collections of tagged set elements, then it can be also said that any N -dimensional vector space element can be alternatively built up just by using the *inward matrix product* [11–13] of a N -dimensional semispace element by the corresponding signature vector. The semispace elements themselves can be considered bearing unity signature, a vector whose elements are made by the unity vector: $\mathbf{1} = \{1_I = 1\}^3$.

However, one must keep in mind that even if 2^N signature elements can be made from the bit-like form of signature sets, in practice half of the possible signatures are

³ See appendix A, for more details on inward products.

symmetrical to the other half, simply *reversing or exchanging* one of the needed signs by the other. For example, to the unity signature above the sign reversal provides the signature: $-\mathbf{1} = \{-1_I = -1\}$.

2.3. Vector signature and nullity

Constructed in this manner, that is: employing semispace elements as object entities and signatures as tags, vector spaces can be considered sets bearing a Boolean tagged set structure. Generalization of this construction to matrix or hypermatrix spaces is straightforward [11,13]. The interesting consequence of this construct is resumed taking into account the importance which acquires the semispace structure, being the core of classical vector spaces building.

However, such simple structure rules will not take care of the possible existence of vectors with null elements. This is so, in the case that semispaces are made of strictly positive definite elements, involving \mathbf{R}^+ without taking into account the zero, the neutral element in addition. The construction of canonical basis sets will not be possible without considering the possibility of null elements within space vectors, although it is preferable to do not include this feature in semispaces. As a consequence of the zero exclusion, the vector space elements, made as discussed of semispace vectors and signatures do not reproduce all the possible vectors or coordinates.

The procedure to overcome this problem does not substantially change the previous tagged set structure of vector spaces. Indeed, there is only necessary to modify the signature tags by choosing one of two alternative but equivalent ways.

2.4. Ternary vector tags

Within the first choice, one can consider to enlarge the structure of the signature form and make signature vectors bearing three signs instead of two: $\{-1, 0, +1\}$. In this way one must accept the rule, consisting in the fact that, the presence of a zero as a signature component will produce a zero element at the final vector in the same position. Also this feature may indicate that in the semispace originating vector the value of the corresponding component could be arbitrarily adopted. The problem will consist here in the fact that signatures will be made of *trits* instead of bits, and this could be a practical nuisance in present time binary driven computers⁴. Also, the number of signature elements will be no longer 2^N , but will be increased up to 3^N .

2.5. Quaternary vector tags

The second construction choice will produce a binary tagged set formalism but associated to a degenerate pattern. In this case, the signature tags shall be accompanied by another tag, which for each vector can be made over the $\{0, 1\}$ set, and which could

⁴ However, this ternary possibility of organizing computation has been contemplated by Knuth [14] several years ago.

be called the *nullity tag set*. The final tags, leading to the total vector space, including vectors with null elements, will be made by the Cartesian product of two N -dimensional binary strings, in the following way:

$$\begin{aligned}\Sigma &= \{\sigma \mid \sigma = \{s_I\} \wedge s_I \in \{-1, +1\}\}, \\ \mathbf{N} &= \{\nu \mid \nu = \{n_I\} \wedge n_I \in \{0, 1\}\}, \\ \Theta &= \Sigma \times \mathbf{N} = \{\theta \mid \theta = (\sigma, \nu): \sigma \in \Sigma \wedge \nu \in \mathbf{N}\}, \\ V(\mathbf{R}) &= V(\mathbf{R}^+) \times \Theta.\end{aligned}$$

An equivalent, but more practical result from the computational point of view, can be obtained by using the inward matrix product involving elements of the signature tag set, Σ , the nullity tag set, \mathbf{N} , and the original vector semispace, $V(\mathbf{R}^+)$. In this built in picture, the number of distinct tag set possible classes will increase up to: 4^N , or 2^{2N} . The interesting situation to note is that the tag set: $\Sigma \times \mathbf{N}$, can be visualized as the Cartesian product of the vertices of two N -dimensional hypercubes.

In addition, some situations will appear to be degenerate in this signature-nullity case, as a null component could possess two signs in this tag set structure. This has been previously noticed, when matrix signatures were studied for the first time [11] and discussed with detail. In this previous work, the vector zero, the vector space additive neutral element, was considered as an element potentially associated to the existing 2^N signature tag classes. However, in case that such degenerate description appears to be poor or inelegant to the reader, there is always present the ternary picture as a possible alternative non-degenerate solution, which can be also easily implemented by means of inward matrix products.

In any case, the most interesting consequence of this discussion can be resumed considering the fact that vector semispaces are the crucial elements in order to construct vector spaces by means of two sets made of vectors of binary origin: matrix signature and nullity.

3. Normed vector semispaces: Minkowski norm

3.1. Minkowski norm

After this previous discussion intended to make evident the basic nature of vector semispaces, it is time to start a discussion on the natural semispace metric features. A natural norm can be easily adopted in semispaces, and it seems that the most immediate rule at hand for such kind of a task becomes a *Minkowski norm*. Indeed, being vector semispace elements positive definite, a sum of their components within matrix semispaces, or the integral of the function, when dealing with infinite dimensional probability density semispaces, will produce a positive real number in any case.

As an example of such Minkowski norm definition, let us choose a matrix semispace of dimension $(m \times n)$: $M_{(m \times n)}(\mathbf{R}^+)$, supposing in addition that the basic construction algorithm holds:

$$\forall \mathbf{A} \in M_{(m \times n)}(\mathbf{R}^+) \rightarrow \mathbf{A} = \{a_{ij}\} \wedge \forall i, j: a_{ij} \in \mathbf{R}^+.$$

3.2. Matrix summation symbols

Then, a Minkowski norm in such a semispace can be simply symbolized by $\langle \mathbf{A} \rangle$ and computed by means of the algorithm:

$$\langle \mathbf{A} \rangle = \sum_i \sum_j a_{ij} \in \mathbf{R}^+.$$

The matrix elements summation symbol $\langle \mathbf{A} \rangle$ acting on arbitrary vectors or matrices, has been defined and employed some years ago [15,16] to ease the mathematical notation, as well as in order to define a mathematical symbol set, able to have an immediate translation into a high level programming language like Fortran 95, see, for example, [17]⁵. The summation symbol can be also associated to a linear operator, transforming vector semispace elements into scalars.

Also, as another example of Minkowski norm, it is worthwhile to consider the domain of Hilbert semispaces, $H(\mathbf{R}^+)$, where quantum density functions, $\rho(\mathbf{r})$, can be considered as their elements, that is: $\rho(\mathbf{r}) \in H(\mathbf{R}^+)$. There, in the present context, the Minkowski norm is immediately defined as the integral over the appropriate domain of a given function:

$$\langle \rho(\mathbf{r}) \rangle = \int_D \rho(\mathbf{r}) \, d\mathbf{r} \in \mathbf{R}^+.$$

The real positive definite result is a consequence of the real positive definite nature over the domain D , associated by construction to quantum density functions in particular. The same definition can be applied to any set of continuous statistical probability density functions.

4. Shell structure in vector semispaces

4.1. α -shells

An interesting albeit immediate application of Minkowski norms can be employed to classify vector semispaces in terms of shells. An α -shell, $S(\alpha)$, is defined as a closed

⁵ In Fortran 90 and 95 compilers, there is present an intrinsic function, which can be employed to sum up all the elements of a matrix. Such compiler facility is called within the code by the function symbol written as: SUM([Argument]), with [Argument] being any previously defined integer, real or complex array name.

subset of a vector semispace, whose elements possess the same Minkowski norm α , that is:

$$S(\alpha) \subset V(\mathbf{R}^+) \rightarrow \forall \mathbf{x} \in S(\alpha): \langle \mathbf{x} \rangle = \alpha.$$

From all the possible shells the *unit shell*, $S(1)$, is the most representative of these elements belonging to a vector semispace, as it is straightforward to demonstrate that from the elements of the unit shell any α -shell element can be constructed, or:

$$\forall \mathbf{a} \in S(\alpha) \rightarrow \exists \mathbf{x} \in S(1): \mathbf{a} = \alpha \mathbf{x},$$

and conversely:

$$\forall \mathbf{x} \in S(1) \rightarrow \exists \mathbf{a} \in S(\alpha): \mathbf{x} = \alpha^{-1} \mathbf{a}.$$

4.2. Homotheties and convex sets

Thus, any α -shell belonging to a given vector semispace is nothing else but a *homothety* of the unit shell. As it is so, and because of the possible primordial role that semispaces can take in order to construct vector spaces, as discussed above, it can be immediately deduced that the unit shell, being the core to construct any other shell in semispaces, it can be also considered the ultimate core to generate any vector space.

Moreover, the α -shells in vector semispaces are *convex sets*, see, for example, [18]. In order to see this property fulfilled for any arbitrary α -shell, it is worthwhile to define a *convex condition symbol* [5] over a set of appropriate scalars. By the symbol $K(\{w_I\})$, associated to a known set of scalars $\{w_I\}$, it will be understood the pair of features:

$$K(\{w_I\}) = \left[\forall I: w_I \in \mathbf{R}^+ \wedge \sum_I w_I = 1 \right].$$

Thus, knowing an arbitrary set of vectors belonging to a given α -shell $\{\mathbf{x}_I\} \in S(\alpha)$ and a convex condition symbol over a known scalar set $K(\{w_I\})$, then the convex linear combination

$$\mathbf{z} = \sum_I w_I \mathbf{x}_I,$$

belongs to the same α -shell as the generating vectors:

$$\langle \mathbf{z} \rangle = \sum_I w_I \langle \mathbf{x}_I \rangle = \alpha \sum_I w_I = \alpha \rightarrow \mathbf{z} \in S(\alpha).$$

4.3. Semispace partition and equivalence classes

This property indicates that any vector semispace can be considered as the union of all of its shells:

$$V_N(\mathbf{R}^+) = \bigcup_{\forall \alpha \in \mathbf{R}^+} S(\alpha).$$

Still more interesting is the property consisting into that semispace shells are disjoint sets, that is:

$$\forall S(\alpha), S(\beta) \subset V_N(\mathbf{R}^+): S(\alpha) \cap S(\beta) = \emptyset.$$

This allows saying semispaces *are partitioned by* the α -shell structure. In consequence, the α -shells themselves can be considered *equivalence classes* of the semispace [19].

4.4. Shell direct sums

A *shell sum* corresponds to another shell, with their elements possessing a Minkowski norm, which is the sum of those associated to the involved shell norm values, that is:

$$S(\alpha) + S(\beta) = \Sigma \rightarrow \Sigma \equiv S(\alpha + \beta).$$

To prove this, it is just needed to define the shell sum in the usual way:

$$\Sigma = \{s \mid s = a + b: a \in S(\alpha) \wedge b \in S(\beta)\},$$

then the elements of the shell sum possess the property:

$$\begin{aligned} s \in \Sigma \rightarrow s = a + b \rightarrow \langle s \rangle &= \langle a + b \rangle = \langle a \rangle + \langle b \rangle = \alpha + \beta \\ \Rightarrow \Sigma &= S(\alpha + \beta). \end{aligned}$$

Moreover, being the shells disjoint sets as commented above, the shell sum can be written as the *direct sum* of two or more shells, that is:

$$S(\alpha) \oplus S(\beta) = S(\alpha + \beta).$$

5. Scalar products in vector semispaces

5.1. Minkowski scalar products

In the same fashion as Minkowski norms were adopted as a natural way to choose a norm in semispaces, it seems that there could exist as well a natural way to define *scalar products* in vector semispaces. This choice has to be coherently structured in such a manner as to match the previously chosen Minkowski norms. This prospect could be initiated by means of the following symbol:

$$\forall \mathbf{x}, \mathbf{y} \in V(\mathbf{R}^+): \langle \mathbf{xy} \rangle \in \mathbf{R}^+,$$

which will be attached the following algorithm:

$$\langle \mathbf{xy} \rangle = \sum_i (x_i y_i)^{1/2}.$$

To stress the parent norm structure, the same symbol as in the Minkowski norm has been assumed, however two or, as it will be studied later on, more vectors are written within the symbol without separation signs added. This scalar product symbol has

been also chosen in this way in order to distinguish it from other possibilities already discussed [12,18] and, of course, from the *Euclidean scalar product*.

In this manner, it is immediate to see that the property below holds, connecting the scalar product, as defined in the algorithm above, with the previously described Minkowski norm:

$$\langle \mathbf{x}\mathbf{x} \rangle = \sum_i (x_i^2)^{1/2} = \sum_i x_i = \langle \mathbf{x} \rangle.$$

Such coherency characteristic found in this simple manner, tells us it is already time, that such scalar product can be named as *root*, for short, or *Minkowski scalar product*.

5.2. Inward matrix product structure and Minkowski scalar product of two vectors

The definition provided above of the root scalar product can be also interpreted in terms of an inward matrix product⁶, just one must take into account the definition of inward product:

$$\mathbf{x} * \mathbf{y} = \{x_i y_i\},$$

which shall be associated to the inward square root form:

$$\mathbf{x}^{[1/2]} = \{x_i^{1/2}\}.$$

It is obvious that, then one can write the equality:

$$\langle \mathbf{xy} \rangle = \langle \mathbf{x}^{[1/2]} * \mathbf{y}^{[1/2]} \rangle,$$

where the second bracket has to be taken as a matrix summation symbol.

5.3. Minkowski scalar product main properties

Due to the nature of vector semispaces, it is interesting to simplify the root scalar product, taking into account the shell structure of the involved vectors:

$$\mathbf{x}^{(\alpha)} \in S(\alpha) \wedge \mathbf{y}^{(\beta)} \in S(\beta) \rightarrow \langle \mathbf{x}^{(\alpha)} \mathbf{y}^{(\beta)} \rangle = (\alpha\beta)^{1/2} \langle \mathbf{x}^{(1)} \mathbf{y}^{(1)} \rangle,$$

where superscripts have been used to stress the association of each vector to a given shell. Thus, this result implies that any root scalar product within a vector semispace can be related to the root scalar product of the unit shell associated homothetic vectors, appropriately scaled by the geometric mean of the Minkowski norms of both vectors.

This kind of root scalar product produces a symmetric metric with positive definite elements on it, as the following property

$$\langle \mathbf{xy} \rangle = \langle \mathbf{yx} \rangle \wedge \langle \mathbf{xy} \rangle \in \mathbf{R}^+,$$

⁶ As defined in appendix A.

holds for any couple of vectors, according to the root scalar product above defined. However, nothing assures that, in any case, the metric is positive definite, adopting for the metric matrix the usual sense for this property, associated to *Euclidean vector spaces*. In order to discuss this issue, even if it has to be from a simple point of view, the main arguments shall be postponed until some other properties of root scalar product have been studied.

The rest of main properties of root scalar products have to be observed now, as it is not so obvious whether they are fulfilled in the same way as scalar products in Euclidean spaces. For example, multiplication by a scalar of one of the involved vectors in the root scalar product appears to possess similar properties as the usual Euclidean scalar product:

$$\lambda \in \mathbf{R}^+: \langle (\lambda \mathbf{x}) \mathbf{y} \rangle = \lambda^{1/2} \langle \mathbf{x} \mathbf{y} \rangle.$$

The next property to be handled is related to root scalar product and addition. The adequate handling of this part is most interesting in order to make root products as similar as possible to the Euclidean counterpart.

5.4. Distributive law and root scalar products involving linear combinations

A distributive law with respect vector addition has to be sought through the definition of inward matrix product subjacent structure of root scalar products. The algorithm definition of root scalar product must be adapted to vector sum, and the straightforward way to define the interaction of sum and product is:

$$\langle (\mathbf{x} + \mathbf{y}) \mathbf{z} \rangle = \sum_i (x_i^{1/2} + y_i^{1/2}) z_i^{1/2} = \langle \mathbf{x} \mathbf{z} \rangle + \langle \mathbf{y} \mathbf{z} \rangle.$$

At the same time, in order to obtain a coherent reduction to the Minkowski norm, the product of two vector sums has to be structured in form of a *Hadamard product* (see appendix A), that is, just dropping the cross terms while keeping the diagonal ones:

$$\langle (\mathbf{x} + \mathbf{y})(\mathbf{t} + \mathbf{u}) \rangle = \langle \mathbf{x} \mathbf{t} \rangle + \langle \mathbf{y} \mathbf{u} \rangle.$$

With these definitions the Minkowski norm of a sum is preserved as can be easily deduced:

$$\langle (\mathbf{x} + \mathbf{y})(\mathbf{x} + \mathbf{y}) \rangle = \langle \mathbf{x} \mathbf{x} \rangle + \langle \mathbf{y} \mathbf{y} \rangle = \langle \mathbf{x} \rangle + \langle \mathbf{y} \rangle = \langle \mathbf{x} + \mathbf{y} \rangle,$$

and the product of two linear combinations, *restricted* to possess an equal number of terms, can be handled in the following way, using again the Hadamard diagonal formalism:

$$\begin{aligned} \mathbf{x} &= \sum_i^P \alpha_i \mathbf{a}_i \wedge \mathbf{y} = \sum_i^P \beta_i \mathbf{b}_i: \\ \langle \mathbf{x} \mathbf{y} \rangle &= \sum_i^P (\alpha_i \beta_i)^{1/2} \langle \mathbf{a}_i \mathbf{b}_i \rangle = \sum_i^P \left[(\alpha_i \beta_i)^{1/2} \sum_k (a_{ki} b_{ki})^{1/2} \right]. \end{aligned}$$

A final remark should be given, before proceed with the study of the possibilities of root scalar products in semispaces. One must insist that Hadamard products were originally defined within infinite sums pairs of elements [20]. When described, as in the present case, within sums possessing a finite number of terms, then the sum upper limit shall be the same in both factors. Otherwise the product is not feasible.

6. Angles subtended by two vectors

Root scalar products and Minkowski norms can be joined together in order to construct, as in the classical Euclidean way, the cosine of the angle subtended by two semispace vectors. To grasp such a goal, it is only needed the following practical definition, based on Minkowski norms and root scalar products as defined beforehand:

$$\forall \mathbf{x}, \mathbf{y} \in V(\mathbf{R}^+) \wedge \mathbf{x} \in S(\alpha), \mathbf{y} \in S(\beta):$$

$$\cos(\phi) = \frac{\langle \mathbf{xy} \rangle}{(\langle \mathbf{x} \rangle \langle \mathbf{y} \rangle)^{1/2}} = (\alpha\beta)^{-1/2} \langle \mathbf{xy} \rangle = \langle \mathbf{x}^{(1)} \mathbf{y}^{(1)} \rangle.$$

Such a classical definition, demonstrates again the coherent result that, under the present semispace description, the angle subtended by a pair of semispace vectors, even if they belong to different shells, it can be established within the unit shell by the root scalar product of the unit shell vectors. In order to stress the different nature of the cosine defined here, from the usual Euclidean algorithm, the present cosine computation will be named *root or Minkowski cosine*.

7. Minkowski metric properties

7.1. Minkowski product fundamental property involving unit shell vectors

There is still a point to be demonstrated, which can be postulated in the following way:

$$\forall \mathbf{x}, \mathbf{y} \in S(1) \rightarrow \langle \mathbf{xy} \rangle \leq 1.$$

A straightforward demonstration of the previous inequality can be put in the following terms. Given two arbitrary vectors of the unit shell: $\mathbf{x}, \mathbf{y} \in S(1)$, then one can suppose that both unit shell elements are constructed by means of the rules⁷: $\mathbf{x} = \{u_i^2\}$ and $\mathbf{y} = \{v_j^2\}$, just to fulfill: $\langle \mathbf{x} \rangle = \langle \mathbf{y} \rangle = 1$. Using generating symbols it can be simply written: $R(\mathbf{u} \rightarrow \mathbf{x}) \wedge R(\mathbf{v} \rightarrow \mathbf{y})$, as well as the unit shell association of both generated vectors can be symbolized by the convex conditions: $K(\mathbf{x}) \wedge K(\mathbf{y})$.

⁷ Such procedure has been formally described [8,9,18] with the use of a *generating symbol*: $R(\mathbf{u} \rightarrow \mathbf{x}) = \{\mathbf{x} = \mathbf{u} * \mathbf{u}\}$, where the inward matrix product is explicitly written. This kind of symbolic form can be easily extended in order to connect Hilbert spaces and semispaces, one just has to remember the construction of density functions with squared modules of wave functions.

The sets $\{u_I\}$ and $\{v_I\}$ can always be found, being the vector components in semispaces real positive definite scalars. This also becomes the same as to consider that the generating vectors: $\mathbf{u} = \{u_I\}$ and $\mathbf{v} = \{v_I\}$, are normalized in the Euclidean space sense:

$$\mathbf{u}^T \mathbf{u} = \mathbf{v}^T \mathbf{v} = 1.$$

This can be always stated because, for example,

$$\mathbf{u}^T \mathbf{u} = \sum_I u_I^2 = \sum_I x_I = \langle \mathbf{x} \rangle = 1,$$

can be directly written and an equivalent relationship holds relating the components of the other chosen vectors \mathbf{y} and \mathbf{v} .

From here, recalling the well-known Schwartz inequality in Euclidean spaces (see, for example, [21]):

$$(\mathbf{u}^T \mathbf{v})^2 \leq (\mathbf{u}^T \mathbf{u})(\mathbf{v}^T \mathbf{v}),$$

which, in this particular case where the involved vectors are normalized, permits to finally write:

$$\mathbf{u}^T \mathbf{v} \leq 1.$$

As a consequence, the scalar product used here in this work can be written as:

$$\langle \mathbf{x}\mathbf{y} \rangle = \sum_I (x_I y_I)^{1/2} = \sum_I u_I v_I = \mathbf{u}^T \mathbf{v} \leq 1.$$

Thus, the root scalar product obtained with a pair of arbitrary vectors of the unit shell is always less or equal to one, and consequently behaves as a cosine, inducing the same behaviour into the previously defined root cosine.

7.2. A property of the elements of the unit shell vectors

It is interesting to know a general form of this cosine definition based on root scalar products, when one of the vectors involved into the root scalar product is the unity vector: $\mathbf{1} = \{1_I = 1\}$, already described. Such a vector in any N -dimensional semispace, in order that it is forced to belong to the unit shell, has to be written with a normalisation factor: N^{-1} . Then, choosing any unit shell semispace vector, defined for instance as:

$$\mathbf{z} = \{\theta_I\} \in S(1) \rightarrow \langle \mathbf{z} \rangle = \sum_I \theta_I = 1,$$

it produces the following root cosine, when confronted with the unity vector:

$$\cos(\phi) = \langle \mathbf{z}(N^{-1}\mathbf{1}) \rangle = N^{-1/2} \sum_I \theta_I^{1/2}.$$

According to the previous discussion this particular root cosine expression, as obtained above, has to be less or equal than one. From here, one can deduce that the unit

shell vector components in any N -dimensional semispace will fulfill in any case the relationship

$$\sum_I \theta_I^{1/2} \leq N^{1/2}.$$

The unity vector used twice within this argument will allow the equality to hold.

7.3. Positive definite structure of Minkowski metric matrices involving two unit shell vectors

The property $\langle \mathbf{x}\mathbf{y} \rangle \leq 1$, associated to unit shell vectors and demonstrated above, can be used to build up a particular proof of the positive definiteness of metric matrices involving two vectors of $S(1)$. Suppose known two linearly independent unit shell vectors $\mathbf{x}, \mathbf{y} \in S(1)$, the root metric matrix associated to both vectors can be written as:

$$\begin{pmatrix} 1 & \langle \mathbf{x}\mathbf{y} \rangle \\ \langle \mathbf{x}\mathbf{y} \rangle & 1 \end{pmatrix} = \begin{pmatrix} 1 & p \\ p & 1 \end{pmatrix},$$

the characteristic polynomial, and its roots, of such metric matrix is simply:

$$\text{Det} \begin{bmatrix} 1 - \lambda & p \\ p & 1 - \lambda \end{bmatrix} = (1 - \lambda)^2 - p^2 = 0 \quad \Rightarrow \quad \lambda = 1 \pm p.$$

This proves that being the root scalar product: $p < 1$, because the vectors have been chosen linearly independent, then, the two possible eigenvalues will bear the property: $\lambda > 0$. Thus, the root metric matrix associated to a couple of linearly independent unit shell vectors is positive definite.

7.4. Linear independence of unit shell vectors

Here a remark must be proposed, concerning the unit shell elements and, by extension, implying the elements of any shell. By construction, the vector pairs of a given shell are linearly independent. This can be proved by using the fact that Minkowski norms of all shell components are equal. Then, there is no scalar $\lambda \neq 1$ for which two vectors, say: $\mathbf{x}, \mathbf{y} \in S(1)$, fulfill $\mathbf{x} = \lambda\mathbf{y}$. This is so, because: $\langle \mathbf{x} \rangle = \langle \lambda\mathbf{y} \rangle = \lambda\langle \mathbf{y} \rangle \rightarrow 1 = \lambda$.

8. Positive definite nature of root metric matrices

In order to get a hint about the positive definiteness of root metric matrices of arbitrary dimension, one can also employ the argument consisting in the following reasoning. Suppose a set of M linearly independent vectors belonging to some vector space is known:

$$Z = \{\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_M\} \subset V(\mathbf{R}),$$

such that, their inward product generates another set:

$$X = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_M\} \rightarrow \forall I: \mathbf{x}_I = \mathbf{z}_I * \mathbf{z}_I = \mathbf{z}_I^{[2]}.$$

Euclidean normalization of the set Z is equivalent to Minkowski normalization of the set X , as can be easily proved:

$$\forall I: 1 = \langle \mathbf{z}_I | \mathbf{z}_I \rangle = \sum_P z_{PI}^2 = \sum_P x_{PI} = \langle \mathbf{x}_I \rangle \rightarrow \mathbf{x}_I \in S(1),$$

so, using this construction, the set $X \subseteq S(1)$. As the set Z has been chosen linearly independent, then the Gram matrix of the set Z , $\mathbf{G} = \{g_{IJ} = \langle \mathbf{z}_I | \mathbf{z}_J \rangle\}$, is positive definite: $\mathbf{G} > 0$. However, the matrix constructed with the root scalar products of the parent set X , can be manipulated in such a way that:

$$\begin{aligned} \mathbf{R} = \{r_{IJ} = \langle \mathbf{x}_I | \mathbf{x}_J \rangle\} &\rightarrow \forall I, J: r_{IJ} = \langle \mathbf{x}_I | \mathbf{x}_J \rangle = \sum_P (x_{PI} x_{PJ})^{1/2} \\ &= \sum_P (z_{PI}^2 z_{PJ}^2)^{1/2} = \sum_P z_{PI} z_{PJ} = \langle \mathbf{z}_I | \mathbf{z}_J \rangle = g_{IJ} \\ \Rightarrow \mathbf{R} = \mathbf{G} \wedge \mathbf{R} &> 0. \end{aligned}$$

Then, as a unit shell subset X can always supposed to be generated by a set like the set Z , one arrives to the conclusion that a root metric matrix over a set of unit shell elements will be positive definite, or at least that, when the generating vectors are not linearly independent, it will be nonnegative definite.

9. Root distances in vector semispaces

9.1. Root distances in semispaces

From the previous definition of the root scalar product, it is almost compulsive that an associated *root or Minkowski distance* definition could be also proposed. This can be done again by inspection of the classical Euclidean definition, while substituting the usual distance elements by the appropriate Minkowski ones. After scaling by two, the following rule can be used, despite the need of using a difference in a strictly positive definite set:

$$d(\mathbf{x}, \mathbf{y}) = \frac{1}{2}(\langle \mathbf{x} \rangle + \langle \mathbf{y} \rangle) - \langle \mathbf{xy} \rangle.$$

Now supposing that $\mathbf{x} \in S(\alpha) \wedge \mathbf{y} \in S(\beta)$, it is easily deduced the algorithm, which takes into account the shell structure in semispaces:

$$d(\mathbf{x}, \mathbf{y}) = \frac{1}{2}(\alpha + \beta) - (\alpha\beta)^{1/2} \langle \mathbf{x}^{(1)} | \mathbf{y}^{(1)} \rangle,$$

and, using the definition of the root cosine of the angle subtended by both vectors, the root distance can be also written as

$$d(\mathbf{x}, \mathbf{y}) = \frac{1}{2}(\alpha + \beta) - (\alpha\beta)^{1/2} \cos(\phi).$$

Proving that, under the proposed definition, root distances in vector semispaces can be computed over the unit shell with the *arithmetic mean shell* value as origin and the *geometrical mean shell* value as scale factor.

9.2. Root distance properties

Also, the root distance symmetry obviously holds, that is:

$$d(\mathbf{x}^{(\alpha)}, \mathbf{y}^{(\beta)}) = d(\mathbf{y}^{(\alpha)}, \mathbf{x}^{(\beta)}).$$

The following property must be also noted now, when both vectors are equal:

$$d(\mathbf{x}, \mathbf{x}) = \alpha(1 - \langle \mathbf{x}^{(1)} \mathbf{x}^{(1)} \rangle) = \alpha(1 - \langle \mathbf{x}^{(1)} \rangle) = \alpha 0 = 0,$$

as well as it must be also noted the interesting result, which appears when two homothetic vectors, related to the same unit shell vector, are considered:

$$d(\mathbf{x}^{(\alpha)}, \mathbf{x}^{(\beta)}) = \frac{1}{2}(\alpha + \beta) - (\alpha\beta)^{1/2} \langle \mathbf{x}^{(1)} \mathbf{x}^{(1)} \rangle = \frac{1}{2}(\alpha + \beta) - (\alpha\beta)^{1/2}.$$

This result may be taken as a constant, connecting any α -shell with another β -shell. One can, then, speak of a *shell root distance*, when referring to this quantity. As arithmetic means are always greater than or equal to geometric means, then this statistical property assures the positive definite nature of shell root distances.

The same root distance positive definiteness property holds as well in the general algorithm involving any pair of vectors, as the root scalar product or the equivalent root cosine within the unit shell are less than one. Then one can write, in general, that the positive definiteness of root distances is fulfilled:

$$d(\mathbf{x}^{(\alpha)}, \mathbf{y}^{(\beta)}) \in \mathbf{R}^+.$$

There, is no proof by which the *triangle inequality* (see, for example, [21]) generally holds within the root distance description. It can be easily found a counterexample, involving for instance the shell root distances of three different collinear homothetic vectors, which proves that the root distances in this case *do not* fulfill the triangle inequality. Thus, perhaps one can speak of an *ultrametric* definition in the present root distance case and in further generalizations, employing this word to represent the distance axioms when void of the triangle inequality.

10. Generalized root scalar products and distances

It is interesting to study, besides the highlights and limitations of both semispaces and their natural root operations, if such algorithmic definitions can be associated to

more than a vector couple. Such aim is unusual in Euclidean spaces, although some attempts have been done recently [18] within other ideas, just to provide with a prospect of open computational horizons the field of QS descriptors.

As has been previously described, various QS measures involving the density tags of several quantum objects can be computed [9,10,18]. One of such possible definitions is the so-called *triple density QS measures*, where three quantum object density functions are involved in the measure computation. Such measures involving multiple quantum object tags are not unique, due to possible alternative definitions of the density functions [22,23]. Because of this lack of uniqueness, several possible forms have been put forward, see, for example, [18], although the most straightforwardly defined triple density measure, associated to the integral of a triple product of first order density functions, is the one which has been employed several times [24,25].

10.1. Generalized root scalar products involving several vectors

Now, the structure of the root scalar product is such, that it can be also naturally generalized into a form, involving an arbitrary number of vectors. In order to obtain a general algorithm for a root scalar product, suppose known a set of vectors of some semispace: $X = \{\mathbf{x}_I\}(I = 1, P) \subset V(\mathbf{R}^+)$, defined in such a way as allowing each of them to belong to an arbitrary shell, that is: $\forall I: \mathbf{x}_I \in S(\alpha_I) \subset V(\mathbf{R}^+)$. A *root scalar product of order P* can be defined over the set X by means of the algorithm:

$$\langle \mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_P \rangle = \sum_I (x_{I1} x_{I2} \cdots x_{IP})^{1/P} = \sum_I \left(\prod_{J=1}^P x_{IJ} \right)^{1/P}.$$

Taking into account the above definition, the already discussed root scalar product, corresponds to a second order algorithm. In any case and up to any order, the root scalar product reverts to the Minkowski norm, when the involved vectors are the same. Also, it is trivial to see that the root scalar product bears permutational symmetry, and thus is independent of the order of the factors.

Besides, the following property:

$$\begin{aligned} \langle \mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_P \rangle &= (\alpha_1 \alpha_2 \cdots \alpha_P)^{1/P} \sum_I (x_{I1}^{(1)} x_{I2}^{(1)} \cdots x_{IP}^{(1)})^{1/P} \\ &= (\alpha_1 \alpha_2 \cdots \alpha_P)^{1/P} \langle \mathbf{x}_1^{(1)} \mathbf{x}_2^{(1)} \cdots \mathbf{x}_P^{(1)} \rangle, \end{aligned}$$

is also trivially demonstrated. Consequently the root scalar product can be referred to the homothetic unit shell vectors, while scaled by the geometric mean of their shell values.

10.2. Generalized root distances involving several vectors

It is straightforward to construct a generalized root distance. Owing to the previous discussion and the second order formalism discussed above, there can be written, the *root*

distance of order P , as:

$$d(\mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_P) = \frac{1}{P} \left(\sum_I^P \alpha_I \right) - (\alpha_1 \alpha_2 \cdots \alpha_P)^{1/P} \langle \mathbf{x}_1^{(1)} \mathbf{x}_2^{(1)} \cdots \mathbf{x}_P^{(1)} \rangle.$$

Thus, producing a computational structure with the same properties as the second order root distance previously discussed.

10.3. Proving the fundamental property of generalized scalar products involving unit shell elements

Moreover, if the following conjecture can be admitted to hold for any number of semispace unit shell vectors:

$$\langle \mathbf{x}_1^{(1)} \mathbf{x}_2^{(1)} \cdots \mathbf{x}_P^{(1)} \rangle \leq 1,$$

then, not only this will ensure the positive definiteness associated to the root distances of any order, but also will permit to define a kind of generalized root cosines of the *pseudo-angle* subtended by P semispace vectors. To illustrate this affirmation one could write, mimicking the second order result:

$$\cos(\Phi_P) = \langle \mathbf{x}_1^{(1)} \mathbf{x}_2^{(1)} \cdots \mathbf{x}_P^{(1)} \rangle.$$

In order to demonstrate the above stated conjecture, consisting in that the root scalar product of an arbitrary number of unit shell vectors is less or equal to one, suppose known a set of unit shell vectors with the superscript dropped to simplify notation: $X = \{\mathbf{x}_I\} \subset S(1)$. Then, the following equalities will be associated to the elements of the set X : $\forall \mathbf{x}_I \in X: \langle \mathbf{x}_I \rangle = 1$. Keeping this in mind, one can recall the definition of the root product involving the elements of X , supposedly associated with a cardinality P :

$$\begin{aligned} \langle \mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_P \rangle &= \sum_j (x_{j1} x_{j2} \cdots x_{jP})^{1/2} < \sum_j \left[\frac{1}{P} (x_{j1} + x_{j2} + \cdots + x_{jP}) \right] \\ &= \frac{1}{P} \left[\sum_I \sum_j x_{jI} \right] = \frac{1}{P} \sum_I \langle \mathbf{x}_I \rangle = \frac{1}{P} P = 1. \end{aligned}$$

Then, in this way the less than sign part of the conjecture is simply proved. It just has been needed the already employed argument, consisting into the well-known property, making geometric means less than arithmetic means, and this property, holding for each term in the sum, produces the global result. Such property involving the arithmetic–geometric means has an exception when all the terms are the same. In this situation equality will hold between both means, even if this is not the most interesting case. It is obvious that under this circumstance the property:

$$\forall \mathbf{x} \in S(1): \langle \mathbf{x} \mathbf{x} \cdots \mathbf{x} \rangle = \sum_j (x_j x_j \cdots x_j)^{1/P} = \sum_j (x_j^P)^{1/P} = \sum_j x_j = \langle \mathbf{x} \rangle = 1$$

will be found. Then, it has been proved that in any situation the root scalar product, involving an arbitrary number of unit shell vectors, will always be less than or equal to one.

11. Inward matrix structure of generalized root scalar products

It has been proved that the cornerstone of semispace metric can be associated to the root scalar product of an arbitrary number of vectors, belonging to arbitrary shells, which can always be associated to the product of the homothetic unit shell parent vectors. This is so because it has been proved that, when all vectors in the root scalar product are the same, then the Minkowski norm is recuperated as the result. So, the scalar product is involved in the same manner in order to describe root cosines of the subtended pseudo-angle and root distances as well. Keeping these considerations in mind, then it is straightforward to write in the same way as it was set for the second order root scalar product:

$$X = \{\mathbf{x}_I\} (I = 1, P) \subset V(\mathbf{R}^+)$$

$$\rightarrow \langle \mathbf{x}_1 \mathbf{x}_2 \cdots \mathbf{x}_P \rangle = \sum_I (x_{I1} x_{I2} \cdots x_{IP})^{1/P} \equiv \langle [\mathbf{x}_1 * \mathbf{x}_2 * \cdots * \mathbf{x}_P]^{[1/P]} \rangle,$$

where the last expression present within the matrix elements sum, corresponds to the inward matrix power of the inward matrix product involving the vectors of the set X , and is defined accordingly as

$$[\mathbf{x}_1 * \mathbf{x}_2 \cdots * \mathbf{x}_P]^{[1/P]} = \{(x_{I1} x_{I2} \cdots x_{IP})^{1/P}\}.$$

12. Hilbert semispaces and root products

All the definitions, algorithms and properties of Minkowski operations on vector semispaces can be translated to the spaces of density functions or *Hilbert semispaces*. An example of this possibility has been already described when Minkowski norms were defined in semispaces. Another application has been based on the possibility to use unit shell functions to construct, by means of convex linear combinations, other unit shell density functions.

12.1. Atomic shell approximation functions

The so-called *atomic shell approximation* (ASA) [18,26] has to be considered a practical consequence of these theoretical ideas. ASA technique constructs quite accurate approximate atomic density functions by using a convex restricted fitting of a known set, Σ , made of spherical density functions, to atomic *ab initio* densities [27]. This can be resumed by the statement:

$$\begin{aligned} K(\{w_I\}) \wedge \Sigma &= \{s_I(\mathbf{r})\} \subseteq S(1) \subseteq H(\mathbf{R}^+) \\ \rightarrow \rho(\mathbf{r}) &= \sum_I w_I s_I(\mathbf{r}) \in S(1). \end{aligned}$$

The ASA functions not only can be applied to QS measures calculation, see for a recent example on antimalarial QSAR reference [28], but appeared to be interesting for initial HF procedures in molecular structures with heavy elements [29], among other applications [30–32].

12.2. Minkowski scalar products between ASA functions

Minkowski scalar products may be employed within ASA approximation, but may produce difficult integrals when applied over exact *ab initio* density functions. Coming back to the ASA possibility in order to describe feasible computational structures, the appropriate root product involving a pair of ASA density functions may be defined as:

$$\langle \rho_A(\mathbf{r}) \rho_B(\mathbf{r}) \rangle = \int (\rho_A(\mathbf{r}) \rho_B(\mathbf{r}))^{[1/2]} \mathbf{dr} = \int (\rho_A(\mathbf{r})^{[1/2]} * \rho_B(\mathbf{r})^{[1/2]}) \mathbf{dr},$$

defining the square root of both ASA density functions as an inward power (see appendix A):

$$\rho(\mathbf{r}) = \sum_I w_I s_I(\mathbf{r}) \rightarrow \rho(\mathbf{r})^{[1/2]} = \sum_I w_I^{1/2} s_I^{1/2}(\mathbf{r}),$$

while the inward matrix product, involving both density functions can be expressed as a *Hadamard product* (see appendix A). Then one can finally write:

$$\langle \rho_A(\mathbf{r}) \rho_B(\mathbf{r}) \rangle = \sum_I w_{AI}^{1/2} w_{BI}^{1/2} \int s_{AI}^{1/2}(\mathbf{r}) s_{BI}^{1/2}(\mathbf{r}) \mathbf{dr}.$$

Such an algorithm, although unusual has been described to coherently describe the Minkowski norm, in the same way as the related property is fulfilled in finite-dimensional vector spaces:

$$\langle \rho_A(\mathbf{r}) \rho_A(\mathbf{r}) \rangle = \langle \rho_A(\mathbf{r}) \rangle.$$

From this definition cosines and distances involving two ASA density functions can be straightforwardly computed. In the same way, products of higher order than two can be so easily defined, that there is no need of supplementary description.

12.3. ASA pseudo-wave functions

The Hadamard square root of an ASA density function:

$$\rho(\mathbf{r})^{[1/2]} = \sum_I w_I^{1/2} s_I^{1/2}(\mathbf{r}) = \psi(\mathbf{r}),$$

may be employed, in the same way as semispace vectors have been used, to construct any vector space element. However, in the Hilbert semispace case one is facing continuous vectors, so as the *pseudo-wave function*, $\psi(\mathbf{r})$, is positive definite everywhere in the associated domain, as the original ASA density function is, the function signature and nullity may be structured as phase function, so one can construct in general a Hilbert space function as:

$$\Psi(\mathbf{r}) = \psi(\mathbf{r})e^{i\alpha} \in H(\mathbf{C}).$$

Then, it is quite interesting to note how the phase function acts in this case as a signature-nullity tag of the Hilbert semispace pseudo-wave function. The most similar finite-dimensional tag to the phase functions tags to be used in the pseudo-wave functions may be the ternary tags involving sign and nullity already discussed above.

13. Conclusions

Semispace structure is not only helpful in order to describe mathematical object entities related to quantum mechanics, quantum similarity and statistical probability distributions, but can be further structured with an original and rich collection of particular operative tools. These operations are also related to the usual and well-known mathematical manipulations and structure of classical Euclidean vector spaces, but in some way provide semispace structures with a great computational and generalization powers.

Minkowski norms, scalar products, cosines and distances, involving an arbitrary number of vectors, may indeed become a source of interesting parameters, which can connect positive definite molecular descriptors, as these provided by quantum similarity measures, in new unsuspected ways.

But over all these concluding considerations, the semispace root metric, as defined in this work, enhances the role of the shell structure of semispaces with the important result, consisting in that the unit shell acquires a distinctive relevant role. In this way the unit shell appears to be the core of the generation of all the elements of any vector space, by means of homothetic operations and inward matrix products with the adequate matrix signature and nullity.

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Appendix A. Inward matrix product

Inward matrix product definition

An essential piece of the toolbox related with QS theory is constituted by the matrix operation so-called *inward matrix product* (IMP) [11–13,18], which has been based on

the structure of the so-called *Hadamard product* [20]⁸. Such an operation is an internal composition law, which can be defined within a matrix (or hypermatrix) vector space $M_{(m \times n)}(\mathbf{K})$ of arbitrary dimension ($m \times n$) and defined over a field \mathbf{K} , producing a matrix whose elements are products made, in turn, by the elements of the matrices appearing in the IMP itself, according to the straightforward algorithm:

$$\begin{aligned} \forall \mathbf{A} = \{a_{ij}\}, \mathbf{B} = \{b_{ij}\} \in M(\mathbf{K}): \\ \mathbf{P} = \mathbf{A} * \mathbf{B} \rightarrow \mathbf{P} = \{p_{ij}\} \in M(\mathbf{K}) \wedge p_{ij} = a_{ij}b_{ij} \forall i, j. \end{aligned}$$

Defined in such a way, IMP and classical matrix products coincide in the subspaces made by diagonal matrices as elements. From now on, IMP and Hadamard products will be used as synonyms of an operation, which can be applied not only to matrix spaces but over a wide variety of mathematical objects. The main characteristic of such a product is the result producing another mathematical object of the same kind as the involved objects in the operation.

Inward matrix product properties

IMP is a feature included in high-level computer languages such that Fortran 95 [17], where it has been implemented in an easy manner, so the practical use of the following IMP properties and characteristics can be immediate.

IMP is commutative:

$$\mathbf{A} * \mathbf{B} = \mathbf{B} * \mathbf{A},$$

associative:

$$\mathbf{A} * (\mathbf{B} * \mathbf{C}) = (\mathbf{A} * \mathbf{B}) * \mathbf{C} = \mathbf{A} * \mathbf{B} * \mathbf{C},$$

and distributive with respect to the matrix sum:

$$\mathbf{A} * (\mathbf{B} + \mathbf{C}) = \mathbf{A} * \mathbf{B} + \mathbf{A} * \mathbf{C}.$$

Furthermore, it has a multiplicative neutral element, the *unity matrix*, which customarily has been represented by a bold real unit symbol: $\mathbf{1} = \{1_{ij} = 1\}$, that is:

$$\mathbf{A} * \mathbf{1} = \mathbf{1} * \mathbf{A} = \mathbf{A}.$$

⁸ The *Hadamard product* is related to the multiplication result of two sums and constructed by the sum of the resultant diagonal products only. In this way, the Hadamard (or inward) product of two sums can be specified by the following algorithm:

$$\left(\sum_I a_I \right) \left(\sum_I b_I \right) = \sum_I a_I b_I.$$

IMP powers, functions and inverses

IMP *powers* are defined as powers over the involved matrix elements, and are written in the usual way, but between square brackets. As an example can be chosen the following algorithm:

$$\mathbf{A} = \{a_{ij}\} \in M \wedge P \in \mathbf{R}: \mathbf{A}^{[P]} = \{a_{ij}^P\} \in M.$$

The same can be said of IMP *functions*, which can be simply defined as:

$$f[\mathbf{A}] = \{f(a_{ij})\}.$$

IMP *inverses* are defined accordingly with the algorithm:

$$\mathbf{A}^{[-1]} = \{a_{ij}^{-1}\},$$

fulfilling:

$$\mathbf{A} * \mathbf{A}^{[-1]} = \mathbf{A}^{[-1]} * \mathbf{A} = \mathbf{1},$$

obviously demanding the definition of IMP *non-singular* matrices, which can be taken as these which possess the unity matrix as nullity tag. But even this restriction can be relaxed somehow [33].

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