

An isometric representation problem in quantum multimolecular polyhedra and similarity

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Abstract Collective distances in quantum multimolecular polyhedra, which can be set as a scalar index associated to the variance vector, enhance the role of the pair density similarity matrix. This paper describes a simplified but efficient algorithm to compute triple, quadruple or higher order density similarity hypermatrices via an isometric decomposition of the pair similarity matrix. Such possibility opens the way to use these similarity elements in quantum QSAR and in the description of scalar condensed vector statistical like indices, for instance skewness and kurtosis. This might lead the way to describe the collective structure of quantum and classical multimolecular polyhedra.

Keywords Quantum molecular similarity · Quantum multimolecular polyhedra · Quantum object sets · Density functions discrete isometric representation · Collective distances · Collective similarity indices

1 The origin of the density function representation problem

A collective distance [1–5], involving the density function vertices of some quantum multimolecular polyhedron $P = \{\rho_I | I = 1, N\}$ [2,3], can be described in terms of the so-called variance function: $|\chi\rangle$ and its complete sum $\langle|\chi\rangle\rangle$ [3–5], which might be named condensed variance index. Basically, calculation of generalized collective Euclidian distances involve the quantum polyhedron set of N vertices, which are made

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by a density function set, at the same time this vertex set can be considered as forming the tag set of some quantum object set [3].

Using the involved polyhedron P vertex density functions, from them it can be easily computed a Gram matrix, which in the present particular study also becomes the similarity matrix, attached to the molecules associated to the polyhedron quantum density functions. The polyhedron similarity matrix \mathbf{Z} is defined by means of the pair density similarity integrals scalar products: $\mathbf{Z} = \{z_{IJ} = \langle \rho_I \rho_J \rangle \mid I, J = 1, N\}$. Recent research results [2–5] suggest that similarity matrices become a relevant piece of knowledge in order to obtain the condensed variance function index: $\langle |\chi\rangle \rangle$. This index, which provides a resumed or condensed scalar information about the quantum polynomial P structure, has been recently demonstrated [3] that it can be expressed as a simple average of the trace and complete sum of the similarity matrix, using:

$$\langle |\chi\rangle \rangle = N^{-1} \left(Tr [\mathbf{Z}] - N^{-1} \langle \mathbf{Z} \rangle \right),$$

where: $Tr [\mathbf{Z}] = \sum_I z_{II}$ and $\langle \mathbf{Z} \rangle = \sum_I \sum_J z_{IJ}$.

2 Quantum molecular polyhedra isometric discrete descriptions

Whenever the pair density similarity matrix \mathbf{Z} , attached to the quantum multimolecular polyhedron P is known, and if its density functions vertices are corresponding to really different quantum objects, then P could be also associated to a set of N linearly independent N -dimensional vectors, acting as columns of some $(N \times N)$ matrix, for example: $\mathbf{A} = \{|\mathbf{a}_I\rangle \mid I = 1, N\}$. Alternatively, such discrete polyhedron might be able to generate the similarity matrix in the following way:

$$\mathbf{A}^T \mathbf{A} = \mathbf{Z} = \{z_{IJ}\} \rightarrow \forall I, J : \langle \mathbf{a}_I | \mathbf{a}_J \rangle = z_{IJ}. \quad (1)$$

Then, if Eq. (1) is solved, it is easy to see that once described the matrix \mathbf{A} , its structure will correspond to find out one of the discrete isometric representations of the quantum molecular polyhedron density function vertices.

In previous studies carried on [6–38] in the past thirty years, since the first paper on quantum molecular similarity [39], it was the similarity matrix columns which were interpreted as some representation of the connected quantum polyhedron density function vertices. This was explained and set up in terms of projecting every vertex with respect of the whole density functions vertex set. Although such a possibility could be well founded, even via the quantum mechanical expectation value concept, the procedure was not sufficiently studied in deep, as the present study pretend to do. The main objection, which could be made on this former discrete interpretation of the metric associated to the polyhedron P , could be based in the fact that the Gram matrix of the similarity matrix \mathbf{Z} columns is just: \mathbf{Z}^2 , see reference [36,40,41] for a discussion on this issue and other connected problems.

Therefore, the columns of the similarity matrix, even being related to the quantum polyhedron density functions, could not generate the same metric, as proves the role, which matrix \mathbf{A} bears within the definition in Eq. (1). Consequently, the previous

interpretation of the columns of the similarity matrix \mathbf{Z} , which was carried on within our papers about quantum similarity, even at the light of the wide range of successful attached applications as previously referenced, might be now considered as a provisional isomorphic notion, which could be easily ameliorated and substituted by the present isometric conceptual discussion.

On the other hand, Eq. (1) constitutes a well-known linear algebra problem, which has not a unique solution; see for example [42]. For instance, the decomposition in (1) even admits the Cholesky triangular decomposition [42] and other variants. In the present context, as it will become evident in the following paragraphs, it is interesting to express the scalar products, involving the columns of the matrix \mathbf{A} , in terms of inward products of the same columns, followed by the complete sum of the resultant vector [43]. That is, one can write the elements of the similarity matrix by means of the expression:

$$\forall I, J : z_{IJ} = \langle \rho_I \rho_J \rangle = \langle |\mathbf{a}_I\rangle * |\mathbf{a}_J\rangle \rangle. \quad (2)$$

After these preliminary statements, then one might say that there, as a consequence of decomposition (1) feasibility, it will be present a possible connection describing an isometric relationship between the quantum object set built by the density functions, which also form the quantum molecular polyhedron $P = \{\rho_I | I = 1, N\}$, and the finite N -dimensional polyhedron $A = \{|\mathbf{a}_I\rangle | I = 1, N\} \subset C_N$, made by the columns of the postulated $(N \times N)$ matrix $\mathbf{A} = \{|\mathbf{a}_I\rangle | I = 1, N\}$, via the decomposition (1).

That is, knowing some form of the matrix \mathbf{A} , in front of the evidence that both sets $\{\rho_I\}$ and $\{|\mathbf{a}_I\rangle\}$ subtend the same metric matrix \mathbf{Z} , then it could be written an isomorphism:

$$\forall I = 1, N : \rho_I \leftrightarrow |\mathbf{a}_I\rangle,$$

which, due that both sets P and A generate the same metric matrix, maintains the distances in both generated spaces.

3 Higher order condensed statistical like indices

Higher order statistical-like vectors and their condensed indices can be then evaluated. As an example of this possibility, one can envisage the computation of the quantum molecular polyhedron skewness and kurtosis vectors and their respective scalar indices [5], obtained by the complete sum of their elements. However, to perform such calculations there are needed subsequent higher order similarity integrals involving three and four density functions respectively [44]. The triple and quadruple similarity integrals have been discussed in several instances and diverse applications proposed [45,46]. Nevertheless, such mentioned studies have been carried out in many occurrences theoretically [44–52] and in few cases practically, see for instance a recent study [47]. The reason for this kind of published papers evolution might be evidently due to the storage and computational overload, which represent such higher order similarity integral calculations. Within the present paper framework the integration problem of products, involving several density functions, might be avoided once the matrix \mathbf{A} is well-defined and chosen among the most plausible candidates.

This is so because, once known the column vector set matrix A , then the similarity integrals elements associated to triple and quadruple density functions, might be easily approximated by extending the algorithm, which implicitly appears within Eq. (2).

Indeed, it can be supposed that complicated higher order similarity integrals can be roughly written, knowing the columns of matrix A , by means of their inward matrix products and the complete sum of resultant vectors. Practically, this can be done by using the simple expressions:

$$\forall I, J, K : z_{IJK} = \langle \rho_I \rho_J \rho_K \rangle \approx \langle |a_I\rangle * |a_J\rangle * |a_K\rangle \rangle$$

and

$$\forall I, J, K, L : z_{IJKL} = \langle \rho_I \rho_J \rho_K \rho_L \rangle \approx \langle |a_I\rangle * |a_J\rangle * |a_K\rangle * |a_L\rangle \rangle$$

respectively.

Moreover, the possibility to compute approximately any similarity integral, involving an indeterminate number of density functions, R say, it is also feasible taking into account a general algorithm, which could be easily written as:

$$\forall I_S |I_S = 1, N(S = 1, R) : z_{I_1 I_2 \dots I_R} = \langle \rho_{I_1} \rho_{I_2} \dots \rho_{I_R} \rangle \approx \langle |a_{I_1}\rangle * |a_{I_2}\rangle * \dots * |a_{I_R}\rangle \rangle.$$

Then, in this way, the amount of computational work necessary to evaluate triple and quadruple, or arbitrarily higher order, density similarity hypermatrices could be reduced to a set of simple operations, just involving the column vectors of the isometric matrix A .

More explicitly and also in general, it can be written for any similarity integral of order R the practical algorithm:

$$\forall I_S |I_S = 1, N(S = 1, R) : z_{I_1 I_2 \dots I_R} \approx \sum_{J=1}^N (a_{J I_1} a_{J I_2} \dots a_{J I_R}),$$

which constitutes an approximate expression encompassing, from the pair density similarity matrix Z , where $R = 2$, up to any similarity hypermatrix or tensor of arbitrary dimension or rank, involving an arbitrary number of density functions.

4 Discussion about two plausible structures of the isometric matrix

4.1 Similarity matrix structure eigensystem

Preparation of the possible and plausible solutions of Eq. (1) in order to obtain a candidate for the isometric matrix A , could be described in the following way. One can start being aware of the fact, associated to the matrix Z , consisting about that, in practice, it corresponds to the Gram matrix of a set of linearly independent density functions forming the quantum multimolecular polynomial P and therefore can be considered a

metric matrix. Consequently, the similarity matrix can be usually considered symmetrical, nonsingular and positive definite. In some cases, though, the similarity-metric matrix can be, due to molecular superposition fluctuations, not definite [53, 54]. One must be aware of this possibility, acting accordingly and correcting such anomaly, if possible.

This discussion will only consider that the similarity-metric matrix \mathbf{Z} is positive definite. This is chosen in this manner to avoid the need of discussing many different possibilities and issues, some of them within the realm of complex algebra. The similarity matrix eigensystem can be thus written in matrix form, by means of the matrix equality:

$$\mathbf{Z}\mathbf{X} = \mathbf{X}\Theta. \quad (3)$$

where the eigenvector matrix \mathbf{X} corresponds to an orthogonal matrix, fulfilling: $\mathbf{X}^T\mathbf{X} = \mathbf{X}\mathbf{X}^T = \mathbf{I}$ and the eigenvalue matrix might be described via a positive definite diagonal matrix:

$$\Theta = \text{Diag}(\theta_I | I = 1, N).$$

4.2 Isometric matrix structure from the canonical decomposition of the similarity matrix

From Eq. (3) and the characteristics of its elements it is immediately deduced the canonical decomposition of the matrix \mathbf{Z} , which can be written by means of the triple matrix product:

$$\mathbf{Z} = \mathbf{X}\Theta\mathbf{X}^T. \quad (4)$$

Now, the square root of the diagonal eigenvalue matrix can be easily expressed:

$$\Theta^{\frac{1}{2}} = \text{Diag}(\sqrt{\theta_I} | I = 1, N), \quad (5)$$

Permitting to define one of the sought isometric matrices fulfilling Eq. (1) by means of the matrix product:

$$\mathbf{A} = \Theta^{\frac{1}{2}}\mathbf{X}^T, \quad (6)$$

which has been constructed taking into account that one can write:

$$\Theta = \Theta^{\frac{1}{2}}\Theta^{\frac{1}{2}},$$

then it is obvious that the matrix \mathbf{A} as defined in Eq. (6), fulfills the decomposition (1), via satisfying the canonical decomposition (4) at the same time.

Thus, the problem of constructing the matrix isometric to the quantum molecular polyhedron vertices might be solved in this particular way, by means of a non-symmetric matrix construction as shown in Eq. (6).

4.3 Isometric matrix structure from the square root matrix of the similarity matrix

A related alternative symmetric option to the asymmetric isometric matrix (6), constructed as discussed above, might correspond to the choice of the square root of the similarity matrix as an isometric column candidate, which will be now symbolized as \mathbf{A}_1 . Such a matrix can be computed without effort using the square root of its eigenvalues as shown in Eq. (5) and computing the symmetric square root matrix via the Löwdin algorithm [40,55]:

$$\mathbf{Z}^{\frac{1}{2}} = \mathbf{X}\Theta^{\frac{1}{2}}\mathbf{X}^T.$$

Of course, it can be now accepted that:

$$\mathbf{A}_1 = \mathbf{Z}^{\frac{1}{2}}$$

because then:

$$\mathbf{A}_1^T = \left(\mathbf{Z}^{\frac{1}{2}}\right)^T = \left(\mathbf{X}\Theta^{\frac{1}{2}}\mathbf{X}^T\right)^T = \left(\mathbf{X}^T\right)^T \left(\Theta^{\frac{1}{2}}\right)^T \mathbf{X}^T = \mathbf{X}\Theta^{\frac{1}{2}}\mathbf{X}^T = \mathbf{A}_1$$

and thus:

$$\mathbf{A}_1^T \mathbf{A}_1 = (\mathbf{A}_1)^2 = \mathbf{Z}^{\frac{1}{2}} \mathbf{Z}^{\frac{1}{2}} = \left(\mathbf{Z}^{\frac{1}{2}}\right)^2 = \mathbf{Z}. \quad (7)$$

However, one must be aware that this result is somehow equivalent to the previous asymmetric choice of the isometric matrix as described in Eq. (6). This is so, because the matrix product in Eq. (7) involving \mathbf{A}_1 and yielding the similarity-metric matrix, is equivalent to the asymmetric product of the matrix \mathbf{A} , as defined in Eq. (6). This property is due to the orthogonal structure of the eigenvector matrix, as can be straightforwardly shown by writing:

$$\mathbf{A}_1^T \mathbf{A}_1 = \left(\mathbf{X}\Theta^{\frac{1}{2}}\mathbf{X}^T\right)^T \mathbf{X}\Theta^{\frac{1}{2}}\mathbf{X}^T = \mathbf{X}\Theta^{\frac{1}{2}}\mathbf{X}^T \mathbf{X}\Theta^{\frac{1}{2}}\mathbf{X}^T = \mathbf{X}\Theta^{\frac{1}{2}}\Theta^{\frac{1}{2}}\mathbf{X}^T = \mathbf{A}^T \mathbf{A} = \mathbf{Z}.$$

Therefore, the asymmetric isometric matrix choice in Eq. (6) appears sufficient for the purposes of obtaining a decomposition of the similarity matrix as described in Eq. (1).

4.4 Final remark

All the procedures, leading to an isometric matrix, described here, can be also used within classical multimolecular polyhedra, where each molecule is represented by a discrete vector made by an arbitrary number of descriptors. That is, the development of an isometric matrix as described here can be employed whenever each one of the N classical molecular polyhedral vertices can be considered as some M -dimensional vector describing a molecule. Then, in this case, it is only necessary to construct the

associated polyhedron Gram matrix, and use it as the similarity matrix \mathbf{Z} has been used in this paper.

5 Conclusions

A quite simple reasoning, based on the concept of collective distance defined within a quantum multimolecular polyhedron, which enhances the role of the pair density similarity-metric matrix \mathbf{Z} , permits to construct a new matrix \mathbf{A} , whose columns might be considered isometric to the quantum polyhedron density functions vertices. Such isometric set of discrete columns also permits to obtain approximate higher order similarity integrals and the attached similarity hypermatrices, involving an arbitrary number of density functions. In this way, higher order statistical-like vectors and condensed indices can be easily constructed, permitting in this manner to numerically describe any quantum polyhedron.

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Conflict of interest The author declare that they have no conflict of interest.

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