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ORIGINAL PAPER

Geometry of n-dimensional Euclidean space Gaussian enfoldments

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Abstract In this study the geometric features and relationships of the points contained into a Gaussian enfoldment of n-dimensional Euclidean space are analyzed. Euclidean distances and angles are described by means of a simple formulation, which demonstrates the topological change underwent by n-dimensional Euclidean spaces upon Gaussian enfoldment, transforming the Euclidean points into *enfoldment points* lying in a closed sphere of unit radius. This property relates Gaussian enfoldments with the holographic electronic density theorem.

Keywords Gaussian enfoldment of n-dimensional Euclidean spaces · Geometry of Gaussian enfoldment · Multivariate Gaussian functions · Enfoldment points · Generalized distances and angles in Gaussian enfoldments · Holographic electronic density theorem (HEDT)

1 Introduction

The concept of an n-dimensional Euclidean space Gaussian enfoldment has been recently described [1]. The idea basic about any enfoldment mathematical construct is simple enough and easy to describe. In fact, an enfoldment is the same as to consider that at every n-dimensional Euclidean point, there is located a vector or vectors belonging to some ∞-dimensional function space.[1]

[1] In fact, at every n-dimensional Euclidian point one can also consider the possibility that there lies a whole 8-dimensional Hilbert or functional space of any kind, whose elements are centered at the enfoldment point.

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A basic enfoldment of this sort has been constructed as an example, by centering at every Euclidean space point a function, which has been chosen to be, for the sake of simplicity, a zeroth order Gaussian one. Therefore, following this preceding naïve framework, the geometry of a case study enfoldment has been chosen as essentially based on the description of a spherical Gaussian function, depending of a pair of arbitrary n-dimensional Euclidean vectors, acting as Gaussian function variables $\{\mathbf{r}\}$ and centering positions $\{\mathbf{R}\}$:

$$\gamma_0\left(\mathbf{r}-\mathbf{R}\left|\alpha\right.\right)=\exp\left(-\alpha\left|\mathbf{r}-\mathbf{R}\right|^2\right). \quad (1)$$

Within the Gaussian enfoldment general structure, variables and center position vectors are interchangeable and independent of the fact that, as it is suggested in reference [1], there can be employed for enfolding Euclidean space higher order Gaussian functions or higher rank tensorial Gaussians instead of scalar zeroth order functions.

In order to have more information about this space saturation with functions, the simplest Gaussian function of type (1) has been proved quite sufficient to study the structure and properties of the n-dimensional Euclidean space enfoldment, as it has been done in the previous study of reference [1].

Therefore, this paper will be organized in the following fashion: first, normalized Gaussian enfoldments will be described and then Gaussian enfoldment points will be defined; next, Euclidian distances and subtended angles involving two enfoldment points will be set up, followed by the description of homothetic enfoldments and enfoldment point neighborhoods, with these concepts this study will end.

2 Normalized Gaussian enfoldments

Euclidean normalization of the enfoldment is also simply obtained in two possible manners yielding the same result as:

$$\begin{aligned}\forall\mathbf{r},\mathbf{R}:\left\langle\left|\gamma_0\right|^2\right\rangle_{\mathbf{r}}&=\int_{-\infty}^{+\infty}\gamma_0\left(\mathbf{r}-\mathbf{R}\left|2\alpha\right.\right)d\mathbf{r}=\left(\frac{\pi}{2\alpha}\right)^{\frac{n}{2}}\\&=\int_{-\infty}^{+\infty}\gamma_0\left(\mathbf{r}-\mathbf{R}\left|2\alpha\right.\right)d\mathbf{R}=\left\langle\left|\gamma_0\right|^2\right\rangle_{\mathbf{R}}.\end{aligned} \quad (2)$$

So, nothing opposes that every Gaussian function, present in the enfoldment can be considered normalized. This can be done scaling the functions of type (1) by the normalization factor:

$$N_n\left(\alpha\right)=\left(\frac{2\alpha}{\pi}\right)^{\frac{n}{4}} \quad (3)$$

which provides the normalized enfoldment:

$$\gamma_{N;0}\left(\mathbf{r}-\mathbf{R}\left|\alpha\right.\right)=N_n\left(\alpha\right)\gamma_0\left(\mathbf{r}-\mathbf{R}\left|\alpha\right.\right)\rightarrow\forall\mathbf{R}:\left\langle\left|\gamma_{N;0}\right|^2\right\rangle_{\mathbf{r}}=1. \quad (4)$$

With such easy notions in mind, there becomes also a straightforward matter to establish some geometric features, which can be associated to normalized Gaussian enfoldments.

3 Gaussian enfoldment points

Described any Gaussian enfoldment using normalized zeroth order Gaussian functions, there it is also easy to assign to every Euclidean n-dimensional enfoldment center $\{\mathbf{R}\}$ a new object category, which can be named as an: *enfoldment point*, described by the normalized Gaussian function itself:

$$\gamma_{N;0}(\mathbf{R}) = \gamma_{N;0}(\mathbf{r}-\mathbf{R}\,|\alpha\,) = \left(\frac{2\alpha}{\pi}\right)^{\frac{n}{4}} \exp\left(-\alpha\,|\mathbf{r}-\mathbf{R}|^2\right),$$

as such, a scalar function acts as a point belonging to some ∞-dimensional space. Two enfoldment points: $\left\{\gamma_{N;0}(\mathbf{R}_a)\,;\,\gamma_{N;0}(\mathbf{R}_b)\right\}$can be considered distinct, whenever the squared Euclidean distance between both position centers is different from cero; that is, when:$|\mathbf{R}_a-\mathbf{R}_b|^2>0$.

4 Euclidean distances and subtended angles

Then, it is extremely easy to define the form Euclidean distances between two enfoldment points can have; as one can write the square of such a distance as the integral:

$$\begin{aligned} D_{ab}^2 &= \left\langle \left|\gamma_{N;0}(\mathbf{R}_a)-\gamma_{N;0}(\mathbf{R}_b)\right|^2\right\rangle \\ &= N_n^2\int_{-\infty}^{+\infty}\left|\exp\left(-\alpha\,|\mathbf{r}-\mathbf{R}_a|^2\right)-\exp\left(-\alpha\,|\mathbf{r}-\mathbf{R}_b|^2\right)\right|^2 d\mathbf{r}; \end{aligned} \tag{5}$$

owing to the normalized nature of the enfoldment points, the above expression 5 can be immediately transformed into a simple Gaussian expression, which contains the Euclidean squared distance between the implied n-dimensional Euclidean coordinates of the enfoldment points position centers, that is:

$$D_{ab}^2 = 2\left(1-\exp\left(-\frac{\alpha}{2}\,|\mathbf{R}_a-\mathbf{R}_b|^2\right)\right), \tag{6}$$

due to the fact that every norm is unit and the scalar product between both enfoldment points can be finally written as:

$$\left\langle\gamma_{N;0}(\mathbf{R}_a)\,\gamma_{N;0}(\mathbf{R}_b)\right\rangle = \exp\left(-\frac{\alpha}{2}\,|\mathbf{R}_a-\mathbf{R}_b|^2\right). \tag{7}$$

In this case of normalized Gaussian enfolding, the scalar product (7) also acts as a positive definite cosine of the subtended angle between the pair of enfoldment points, because due to the normalization of both enfoldment points one can immediately write the mentioned cosine as:

$$\cos(\phi_{ab}) = \left\langle \gamma_{N;0}(\mathbf{R}_a)\, \gamma_{N;0}(\mathbf{R}_b) \right\rangle. \tag{8}$$

As a trigonometric function resulting from the integral of two positive definite functions, the above defined cosine in Eq. (8) cannot allow values outside of the interval $[0, 1]$, a condition easily met, as the squared distance term in Eq. (7): $|\mathbf{R}_a - \mathbf{R}_b|^2$ can vary in turn within the interval:$[0, +\infty]$. A situation quite similar to quantum similarity measures results within its working pattern, see for example a recent series of papers on the subject [2–4].

Therefore, one can write the squared Euclidean distance scaled by the factor 2 as:

$$\frac{1}{2} D_{ab}^2 = 1 - \cos(\phi_{ab}) \tag{9}$$

Showing that in this case scaled distances and cosines of the subtended angle of the two enfolding points are just complementary elements varying with shifted intervals:

$$\left(\frac{1}{2} D_{ab}^2 \right) \in [0, 1] \leftrightarrow \cos(\phi_{ab}) \in [1, 0],$$

but certainly corresponding to complementary properties, that is: the intrinsic variation of the scaled Euclidean distance or subtended angle between two enfoldment points.

Such a geometrical element provides the picture of the ∞-dimensional enfoldment points, as a point set bounded by a closed sphere of unit radius.

Furthermore, one can say that by the presence of a normalized Gaussian enfoldment, the whole n-dimensional Euclidean space becomes projected into a closed sphere of unit radius. A related qualitative construct was employed by Mezey to express the holographic electronic density theorem (HEDT) [5]. HEDT connections and extensions have been recently discussed by the present authors in three different ways: (a) in relationship with quantum similarity [2], (b) afterwards and more precisely within the problem of Gaussian functions holographic properties [6] and finally, (c) related to the Taylor series expansion of electronic density functions [7].

The normalized Gaussian enfolding becomes in this way related to the HEDT, as a consequence of the holographic properties of Gaussian functions.

5 Homothetic enfoldments

The previous discussion about normalized Gaussian enfoldments can also be easily observed from a broad point of view. For instance, by using homothetic transformations of the Gaussian enfoldment as expressed by Eq. (1). That is, simply defining the enfoldment points with the straightforward scaling:

$$\gamma_{K;0}(\mathbf{R}) = \gamma_{K;0}(\mathbf{r} - \mathbf{R}\,|\alpha) = K \exp\left(-\alpha\, |\mathbf{r} - \mathbf{R}|^2 \right),$$

where $K \in \mathbf{R}^{+}$ is just an arbitrary constant, which can include the normalization factor of the enfoldment points. Then, the scaled squared Euclidean distance between two enfoldment points can be written as:

$$d_{ab}^{2} = L^{-2} D_{ab}^{2} = 1 - \exp\left(-\frac{\alpha}{2} \left|\mathbf{R}_{a} - \mathbf{R}_{b}\right|^{2}\right) \tag{10}$$

with the constant L including a factor with the square root of two, the homothetic constant K and the Euclidean norms of the Gaussian enfolding. Therefore, whatever has been described within the normalized Gaussian enfoldments can be easily extended to any homothetic ones.

A general picture emerges from this result, indicating the intrinsic connection between scaled distances and subtended angles of the enfoldment points. Moreover: the same holographic property can be associated to any homothetic enfoldment.

In fact, Eqs. (9) and (10), are simplified structures of the more complicated general Euclidean distance pattern recently analyzed [8]. But of course, they equally result into the fact that scaled distances correspond to general dissimilarity indices, with the appearance of just a reciprocal behavior from the cosine of the subtended vector angle, which can be considered as a similarity index.

6 Neighborhood of an enfoldment point

Equation (10) can be also employed to express how the neighborhood of an enfoldment point can be like. For that purpose one can try first on Eq. (10) any enfoldment point like: $\mathbf{R}_{a} = \mathbf{R}$ and for the second point a neighborhood point of the first: $\mathbf{R}_{b} = \mathbf{R} + \delta\mathbf{R}$; thus, one can write taking this into account:

$$\delta d^{2}(\mathbf{R}) = 1 - \exp\left(-\frac{\alpha}{2} \left|\delta\mathbf{R}\right|^{2}\right),$$

yielding an expression, which allows the determination of the surrounding geometry of any enfoldment point, which can be associated to any n-dimensional Euclidean center point arbitrarily chosen. This consists of a result, which appears to be once more in accordance of the holographic nature of Gaussian functions, showing in this way the relationship of Gaussian enfoldments with HEDT.

In fact, this outcome proves that, as any arbitrarily chosen point in n-dimensional Euclidean space has the same features as any other point in the same space; then, the corresponding Gaussian enfolding point has the same features as any other enfolding point, attached to the corresponding arbitrary Euclidean point.

7 Conclusions

n-dimensional Euclidean space Gaussian enfoldment constitutes an interesting mathematical tool to transform points of the Euclidean space into enfoldment points; that is: into Gaussian functions acting as ∞-dimensional vectors. Euclidean distances or subtended angles between pairs of associated normalized enfoldment points, makes them to appear as corresponding to a set of points lying within a closed unit sphere. Consequently, Gaussian enfoldments possess holographic properties, which Gaussian functions contain and in this way are related to HEDT.

References

1. E. Besalú, R. Carbó-Dorca, J. Math. Chem. doi:10.1007/s10910-011-9882-8
2. R. Carbó-Dorca, E. Besalú, J. Comp. Chem. **31**, 2452 (2010)
3. R. Carbó-Dorca, L.D. Mercado, J. Comp. Chem. **31**, 2195 (2010)
4. R. Carbó-Dorca, E. Besalú, L.D. Mercado, J. Comp. Chem. **32**, 582 (2011)
5. P.G. Mezey, Mol. Phys. **96**, 169 (1999)
6. R. Carbó-Dorca, E. Besalú, J. Math. Chem. **48**, 914 (2010)
7. R. Carbó-Dorca, E. Besalú, J. Math. Chem. **49**, 836 (2011)
8. R. Carbó-Dorca, *Scaled Euclidean Distances: A General Dissimilarity Index with a Sound Geometrical Foundation*. IQC Technical report TR-2011-4