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Chemical algebra.
V: G-weighted distance extensions and metrics

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The first formulation of the definition equation of completely-G-invariant distance extensions from the action of a compact group G onto a metric space (E, d) is reminded. A more general equation ($\mathbb{E}$) is then consistently associated to a group G mapped by a numerical function m and acting on a metric space (E, d) mapped by another continuous numerical function. A solution of ($\mathbb{E}$) is called a "G-weighted distance extension of d". A differential form of the equation is derived in order to provide a definition of a "G-weighted metric" $ds^2 = (d\sigma/\gamma)^2$ from a non-uniform map of an Euclidean space: $\gamma = \#G$ when G is a finite group, but ds^2 is also defined by continuity when G is an infinite compact group ($\gamma = \infty$).

1. Introduction

Starting from an algebraic analysis of chemical pairing equilibria $2\,MN \rightleftarrows MM + NN$, a mathematical model has been devised to show that, under specified circumstances, the constant

$$K = \frac{[MM]\cdot[NN]}{[MN]^2}$$

is always greater than 1 and equals 1 if and only if the chemical moieties M and N are identical [1]. In the model, M and N are represented by vectors of a space E whose dimension equals the number of atomic sites in the common skeleton of M and N. A somewhat abstract derivation has given rise to intriguing results related to the theory of completely G-invariant distances, where G is a compact group acting on an Euclidean space (the very first meaning of this action resides in the symmetry of the molecular skeleton of M and N): a general equation has been proposed to define a completely G-invariant extension of the Euclidean distance on E [2]. The theoretical relevance of this equation has been examined, and its differential resolution has been tackled. On the other hand, a more general equation has been constructed from non-necessarily Euclidean metric spaces: the non-Euclidean Hausdorff distance of R^n was considered in view of geometrical applications, namely the quantification of the chirality of geometrical figures [3]. In this report, a further generalization is envisaged for metric spaces and groups additionally endowed with numerical maps.

2. Reminder: definition of *completely G-invariant* distance extensions

Given a metric space (E, d) endowed with an isometric action of a compact group G, a general equation ($\mathbb{E}$) defining a completely-G-invariant distance extension D_p of d from a "discriminating pairing product K_p" [4] has been devised [2]. The definition equation has been constructed in order to meet the following requirements:

(i) G-invariance requirements
(a) D_p is completely G-invariant, i.e. the functional equation linking K_p and D_p preserves the complete G-invariance of K_p.
(b) $\forall \mathbf{u} \in E, \forall g \in G, D_p(\mathbf{u}, g\mathbf{u}) = 0$.

(ii) Extension requirements
(a) D_p is an extension of the metric distance d: if u_0 is invariant to all the operations of G, then: $\forall \mathbf{u} \in E, \forall g \in G, D_p(\mathbf{u}, \mathbf{u}_0) = d(g\mathbf{u}, \mathbf{u}_0) = d(\mathbf{u}, \mathbf{u}_0)$.
(b) When $p \to \infty, D_p$ tends to the standard completely G-invariant distance D_∞ [5].
(c) When $p \to 0$, D_p tends to the "smooth" completely G-invariant distance D_0 [6].

(iii) Distance properties on E/G
(a) $\forall (\mathbf{u}, \mathbf{v}) \in E^2, 0 \leqslant D_p(\mathbf{u}, \mathbf{v})$.
(b) $\forall (\mathbf{u}, \mathbf{v}) \in E^2, D_p(\mathbf{u}, \mathbf{v}) = 0 \Rightarrow \exists h \in G, \mathbf{v} = g\mathbf{u}$ (converse of (ib)).
(c) $\forall (\mathbf{u}, \mathbf{v}, \mathbf{w}) \in E^3, D_p(\mathbf{u}, \mathbf{w}) \leqslant D_p(\mathbf{u}, \mathbf{v}) + D_p(\mathbf{v}, \mathbf{w})$.

Two propositions are now recalled.

THEOREM 1

Let G be a finite or compact group acting on a metric space (E, d) and preserving the distance $(\forall (\mathbf{u}, \mathbf{v}) \in E^2, \forall g \in G, d(g\mathbf{u}, g\mathbf{v}) = d(\mathbf{u}, \mathbf{v}))$. For $p > 0$, let K_p be a discriminating pairing product on $(E, d; G)$ (i.e. $K_p \geqslant 1$, and $K_p(\mathbf{u}, \mathbf{v}) = 1$ if and only if $\mathbf{v} = g\mathbf{u}$ for some operation g of G). If E is an Euclidean vector space, consider the equation of an unknown function D_p: $E \times E \to R_+$:

$$\Phi_{\mathbf{u},\mathbf{v}}(D_p(\mathbf{u}, \mathbf{v})) = [K_p(\mathbf{u}, \mathbf{v})]^p \qquad (\mathbb{E})$$

with

$$\Phi_{\mathbf{u},\mathbf{v}}(x) = \iiiint\limits_{G^4} \exp\left[\frac{p}{2}\frac{(g\mathbf{u}-h\mathbf{v}|k\mathbf{u}-l\mathbf{v})}{\|g\mathbf{u}-h\mathbf{v}\|\cdot\|k\mathbf{u}-l\mathbf{v}\|}x^2\right] dg\,dh\,dk\,dl\,,$$

$$K_p^p(\mathbf{u},\mathbf{v}) = \frac{\int_G \exp\left[-\frac{p}{2}(g\mathbf{u}|\mathbf{u})\right] dg \cdot \int_G \exp\left[-\frac{p}{2}(g\mathbf{v}|\mathbf{v})\right] dg}{\left(\int_G \exp\left[-\frac{p}{2}(g\mathbf{u}|\mathbf{v})\right] dg\right)^2}\,.$$

Then, eq. ($\mathbb{E}$) has a single solution D_p. Furthermore, D_p fulfills the aforementioned consistency requirements (i), (ii) and (iii), except, perhaps, the triangular inequality (iiic).

This formulation has been generalized for any metric space [3].

THEOREM 2

Let G be a finite or compact group acting on a metric space (E, d) and preserving the distance. For $p > 0$, let K_p be a discriminating pairing product on $(E, d; G)$, consider the equation of an unknown function D_p: $E \times E \to R_+$:

$$\Phi_{\mathbf{u},\mathbf{v}}(D_p(\mathbf{u},\mathbf{v})) = [K_p(\mathbf{u},\mathbf{v})]^p \qquad (\mathbb{E})$$

with

$$K_p^p(\mathbf{u},\mathbf{v}) = \frac{\int_G \exp\left[-\frac{p}{2}\, d^2(g\mathbf{u},\mathbf{u})\right] dg \cdot \int_G \exp\left[-\frac{p}{2}\, d^2(g\mathbf{v},\mathbf{v})\right] dg}{\left(\int_G \exp\left[-\frac{p}{2}\, d^2(g\mathbf{u},\mathbf{v})\right] dg\right)^2}\,,$$

$$\Phi_{\mathbf{u},\mathbf{v}}(x) = \iiint\limits_{G^3} \exp\left[p\,\frac{C_{g,h,k}(\mathbf{u},\mathbf{v})}{C_{\mathbf{m}}(\mathbf{u},\mathbf{v})^{f(p)}}x^2\right] dg\,dh\,dk\,,$$

where

- $C_{g,h,k}(\mathbf{u},\mathbf{v}) = \dfrac{d^2(g\mathbf{u},\mathbf{v}) + d^2(k\mathbf{u},h\mathbf{v}) - d^2(g\mathbf{u},k\mathbf{u}) - d^2(\mathbf{v},h\mathbf{v})}{2d(g\mathbf{u},h\mathbf{v})\cdot d(k\mathbf{u},\mathbf{v})}\,,$
- $C_{\mathbf{m}}(\mathbf{u},\mathbf{v}) = \max\{C_{g,h,k}(\mathbf{u},\mathbf{v});(g,h,k)\in G^3\}(\geqslant 1)\,,$
- $f(p)$ is some regular function eventually depending on $(\mathbf{u},\mathbf{v})$ satisfying $f(0) = 0$ and $f(\infty) = 1$ (e.g. $f(p) = [p/(p-p_0)]^2, p_0 \neq 0$).

Then, ($\mathbb{E}$) has a single solution D_p which fulfils the aforementioned requirements, except, perhaps, the triangular inequality (iv). If (E, d) is an Euclidean vector space, then

$$C_{g,h,k}(\mathbf{u},\mathbf{v}) = \frac{(g\mathbf{u} - h\mathbf{v}|k\mathbf{u} - \mathbf{v})}{\|g\mathbf{u} - h\mathbf{v}\|\cdot\|k\mathbf{u} - \mathbf{v}\|} = \cos(g\mathbf{u} - h\mathbf{v}, k\mathbf{u} - \mathbf{v}) \leqslant C_{\mathbf{m}}(\mathbf{u},\mathbf{v}) = 1\,.$$

In this case, the definition of D_p does not require the full dermination of $f(p)$.

3. A more general formulation: definition of G-weighted distance extensions

A definition equation ($\mathbb{E}$) of a distance on E/G is associated to any given metric space E endowed with an operation of some compact group G. However, a more general equation can be naturally associated to any continuous numerical function defined on $E^2 \times G$, even if it is not uniform on E. This extension boils down to weigh the integrands taking place in ($\mathbb{E}$) in the following way:

$$\Phi_{\mathbf{u},\mathbf{v}}(D_p(\mathbf{u},\mathbf{v})) = [K_p(\mathbf{u},\mathbf{v})]^p \qquad (\mathbb{E})$$

with

$$K_p^p(\mathbf{u},\mathbf{v}) = \frac{\int_G \mu_{\mathbf{u},\mathbf{v}}(g)\exp\left[-\frac{p}{2}\,d^2(g\mathbf{u},\mathbf{u})\right]dg \cdot \int_G \mu_{\mathbf{u},\mathbf{v}}(g)\exp\left[-\frac{p}{2}\,d^2(g\mathbf{v},\mathbf{v})\right]dg}{\int_G \mu_{\mathbf{u},\mathbf{v}}(g)\exp\left[-\frac{p}{2}\,d^2(g\mathbf{u},\mathbf{v})\right]dg \cdot \int_G \mu_{\mathbf{u},\mathbf{v}}(g)\exp\left[-\frac{p}{2}\,d^2(g\mathbf{v},\mathbf{u})\right]dg}\,,$$

$$\Phi_{\mathbf{u},\mathbf{v}}(x) = \frac{\displaystyle\iiiint_{G^4} \mu_{\mathbf{u},\mathbf{v}}(g)\mu_{\mathbf{u},\mathbf{v}}(h)\mu_{\mathbf{u},\mathbf{v}}(k)\mu_{\mathbf{u},\mathbf{v}}(l)\exp\left[p\,\frac{C_{g,h,k,l}(\mathbf{u},\mathbf{v})}{C_{\mathbf{m}}(\mathbf{u},\mathbf{v})^{f(p)}}\,x^2\right]dg\,dh\,dk\,dl}{\left[\displaystyle\int_{G^4} \mu_{\mathbf{u},\mathbf{v}}(g)\,dg\right]^4}\,,$$

where $(\mathbf{u},\mathbf{v};g) \to \mu_{\mathbf{u},\mathbf{v}}(g)$ is a continuous numerical function on $E^2 \times G$ such that

$$\mu_{\mathbf{u},\mathbf{v}} = \mu_{\mathbf{v},\mathbf{u}}\,.$$

Remark 1

When $\mathbf{u} = \mathbf{v}$, the extended equation ($\mathbb{E}$) is trivially verified for $D_p(\mathbf{u},\mathbf{u}) = 0$.

Remark 2

The latter symmetry condition in $\mathbf{u}$ and $\mathbf{v}$ garantees the symmetry of the solution, i.e.: $D_p(\mathbf{u},\mathbf{v}) = D_p(\mathbf{v},\mathbf{u})$. The denominator of $K_p^p(\mathbf{u},\mathbf{v})$ is no longer a squared integral: indeed, K_p must be symmetric ($K_p(\mathbf{u},\mathbf{v}) = K_p(\mathbf{v},\mathbf{u})$). However, if $\mu_{\mathbf{u},\mathbf{v}}(g) = \mu_{\mathbf{u},\mathbf{v}}(g^{-1})$ for any $g \in G$, then the denominator is a squared integral.

Remark 3

The early formulation assumes that the integrals occurring in K_p and $\Phi_{\mathbf{u},\mathbf{v}}(x)$ stretch over the whole group G. Nevertheless, for any points $\mathbf{u}$ and $\mathbf{v}$ of E, these integrals might be naturally restricted to any fuzzy subset $\underline{A}$ of G, and $\mu_{\mathbf{u},\mathbf{v}}$ can be interpreted as the membership function of $\underline{A}$, whereas $g \to \exp[-pd(g\mathbf{u},\mathbf{u})/\sqrt{2}]$ and $g \to \exp[-pd(g\mathbf{u},\mathbf{v})/\sqrt{2}]$ were interpreted as characteristic functions of fuzzy subgroups and conjugacy links respectively [7].

Remark 4: Form of the weighting function $\mu_{\mathbf{u},\mathbf{v}}$

The group G is supposed to occur only through its action on E. It is therefore suggested that $\mu_{\mathbf{u},\mathbf{v}}$ is actually a function μ of the two arguments $g\mathbf{u}$ and $g\mathbf{v}$, time a function m of the sole operation $g \in G$, i.e.: $\mu_{\mathbf{u},\mathbf{v}}(g) = \mu(g\mathbf{u}, g\mathbf{v}) \cdot m(g)$.

Basically, eq. ($\mathbb{E}$) aims at proposing a quantitative (metric) significance to the qualitative connection exerted by G between points of E. Apart from this equation and the starting distance d, any two points of E are not supposed to be otherwise connected. Thus, $\mu_{\mathbf{u},\mathbf{v}}$ has not to represent any coupling between $\mathbf{u}$ and $\mathbf{v}$. In other words, the symmetric map $\mu(\mathbf{x},\mathbf{y})$ of $E \times E$ is a function of independent arguments $\pi(\mathbf{x})$ and $\pi(\mathbf{y})$, where π is a numerical map of E. The simplest symmetric form is henceforth retained:

$$\mu_{\mathbf{u},\mathbf{v}}(g) = \mu(g\mathbf{u}, g\mathbf{v}) \cdot m(g) = \pi(g\mathbf{u})\pi(g\mathbf{v}) \cdot m(g) .$$

In conclusion, *an equation* ($\mathbb{E}$) *is consistently constructed from a given metric space E mapped by a continuous numerical function π and endowed by the action of a given group G idependently mapped by a function m.*

Within the framework of the local interpretation of ($\mathbb{E}$), i.e. for $\mathbf{v} = \mathbf{u} + d\mathbf{u}$, most of the integrand factors $\mu_{\mathbf{u},\mathbf{v}}(g) = \mu_{\mathbf{u},\mathbf{u}+d\mathbf{u}}(g)$ can be simply replaced in ($\mathbb{E}$) by $\mu_{\mathbf{u},\mathbf{u}}(g) = \pi^2(g\mathbf{u}) \cdot m(g)$, where we have put: $d\mathbf{u} = \mathbf{0}$. The corresponding solution is expected to define a metric, and is still denoted $D_p^2(\mathbf{u}, \mathbf{u} + d\mathbf{u}) = d\sigma^2$. However, *not all* the factors $\mu_{\mathbf{u},\mathbf{u}+d\mathbf{u}}(g)$ can be consistently replaced by $\mu_{\mathbf{u},\mathbf{u}}(g)$: this point is detailed in the last section, where an improved formulation of the local equation ($\mathbb{E}$) is derived.

Example

The real axis R is considered as an Euclidean vector space. The orthogonal group reduces to $G = \{e, \sigma\}$. It is supposed that the operations of G occur with equal weights, namely: $m(g) = 1$. In order to define μ, a single free parameter, denoted a, is needed:

$$e^{-a} = \frac{\mu(\sigma x, \sigma y)}{\mu(x,y)} = \frac{\pi(\sigma x)\pi(\sigma y)}{\pi(x)\pi(y)} .$$

When μ is constant, a comprehensive study has been carried out [2,8]. An analogous technical calculation, leads to

$$\Phi_{x,y}(D_p(x,y)) = \frac{1}{(1+e^{-a})^2}\{(1+e^{-2a})\exp[pD_p^2(x,y)] + 2e^{-a}\exp[-pD_p(x,y)]\}$$

$$K_p(x,y) = \frac{\cosh(px^2+a/2)\cosh(py^2+a/2)}{\cosh^2(pxy+a/2)}\,.$$

The resolution of the associated equation ($\mathbb{E}$) gives

$$D_p(x,y) = \sqrt{\frac{1}{p}\ln\left[\frac{\cosh^2(a/2)K_p^p + \sqrt{\cosh^4(a/2)K_p^{2p} - \cosh a}}{\cosh a}\right.}\,.$$

When $a = 0$, the result of ref. [2] is reproduced. Notice that if $a = 0$, then $D_p(x,0) = |x|$, but if $a \neq 0$, then $D_p(x,0) \neq |x|$.

The differential form of ($\mathbb{E}$) corresponds to the case $y = x + dx$, and gives

$$\Phi_{x,x+dx}(d\sigma^2) = 1 + p\tanh^2\left(\frac{a}{2}\right)d\sigma^2$$

$$K_p(x,x+dx) = 1 + p\left\{\tanh\left(px^2+\frac{a}{2}\right) + \frac{px^2}{\cosh^2\left(px^2+\frac{a}{2}\right)}\right\}dx^2\,,$$

where a is now defined for $dx = 0$, by

$$e^{-a} = \frac{\mu(\sigma x,\sigma x)}{\mu(x,x)} = \frac{\pi^2(\sigma x)}{\pi^2(x)}\,.$$

Thus,

$$d\sigma^2 = \frac{1}{\tanh^2\left(\frac{a}{2}\right)}\left\{\tanh\left(px^2+\frac{a}{2}\right) + \frac{px^2}{\cosh^2\left(px^2+\frac{a}{2}\right)}\right\}dx^2\,.$$

For $a = 0$, $d\sigma^2$ is not defined by this process. This has been previously outlined, but a formal expression for $d\sigma^4$ could be derived [8].

In an attempt to regard $d\sigma^2$ as a linear element of a curve "$y = y_a(x)$" in R^2, we seek for a function y_a such that $d\sigma = ds_x = \sqrt{1 + y_a'(x)}\,dx$, i.e.:

$$y_a'(x) = \sqrt{\frac{1}{\tanh^2\left(\frac{a}{2}\right)}\left\{\tanh\left(px^2+\frac{a}{2}\right) + \frac{px^2}{\cosh^2\left(px^2+\frac{a}{2}\right)}\right\} - 1}\,.$$

The equation of the curve passing by zero is thus:

$$y_a(x) = \int_0^x \sqrt{\frac{1}{\tanh^2\left(\frac{a}{2}\right)} \left\{ \tanh\left(pt^2 + \frac{a}{2}\right) + \frac{pt^2}{\cosh^2\left(pt^2 + \frac{a}{2}\right)} \right\} - 1}\, dt\,.$$

It should be emphasized that the scalar "a" may depend on x (and on t in the integral).

4. Discussion

In a speculative interpretation, the function π can be regarded as a characteristic of the symmetry of a space endowed with a "topography", whereas the exponential integrand factors (membership functions of fuzzy subgroups or conjugacy links of G) [7] characterize the symmetry of a reference coordinate space (e.g. $E = R^n$) qualitatively endowed with a set of "allowed motions" (represented by G). The coordinate space just maps the "topographical space" with a distorted geometry (e.g. a Riemanian manifold V_n). In view of such a representation, further studies will focus on Euclidean spaces where $C_{\mathbf{m}}(\mathbf{u}, \mathbf{v}) = 1$ ($f(p)$ has not to be determined).

5. Precision on the differential form of ($\mathbb{E}$) for infinite compact group G

The left-hand term of ($\mathbb{E}$) has been first defined as an integral over G^4. However, one now carefully analyzes the case of an infinite compact group G. Let Γ be the subset of G^4 collecting the operations (g, h, k, l) such that $C_{g,h,k,l}(\mathbf{u}, \mathbf{u})$ is *a priori* defined (i.e. $C_{g,h,k,l}(\mathbf{u}, \mathbf{u}) \neq$ "$\frac{0}{0}$"). Since G^4-Γ is negligeable in G^4, the differential form can be written down (for an Euclidean space E: $C_{\mathbf{m}}(\mathbf{u}, \mathbf{v}) = 1$):

$$\Phi_{\mathbf{u},\mathbf{u}+d\mathbf{u}}(d\sigma) \approx \left[\iiiint_{G^4} \mu_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(h)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)[1 + pC_{g,h,k,l}(\mathbf{u}, \mathbf{u})d\sigma^2 + p^2 C^2_{g,h,k,l}(\mathbf{u}, \mathbf{u})d\sigma^4/2 + \ldots]\, dg\, dh\, dk\, dl \right] \Big/ \left[\iiiint_{G^4} \mu_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(h)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)\, dg\, dh\, dk\, dl \right]$$

$$\approx 1 + pA(\mathbf{u})d\sigma^2 + \ldots d\sigma^4 + \ldots\,,$$

where

$$A(\mathbf{u}) = \frac{\displaystyle\iiiint\limits_{G^4} \mu_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(h)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)\frac{(g\mathbf{u}-h\mathbf{u}\,|\,k\mathbf{u}-l\mathbf{u})}{\|g\mathbf{u}-h\mathbf{u}\|\cdot\|k\mathbf{u}-l\mathbf{u}\|}\,dg\,dh\,dk\,dl}{\displaystyle\iiiint\limits_{G^4} \mu_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(h)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)\,dg\,dh\,dk\,dl}\,.$$

The coefficient $pA(\mathbf{u})$ of $d\sigma^2$ vanishes (given any value of the integrand, the permutation of g and h simply results in the change of the sign of the integrand). Therefore, no definition of $d\sigma^2$ is furnished. Instead, we get a formal definition of $d\sigma^4$, and this state of affairs has been partially discussed in the case $\mu_{\mathbf{u},\mathbf{u}} \equiv 1$. In order to get a relevant definition of a linear element ds^2 related to $d\sigma^2$, the above formal derivation is not corrected on the basis the analysis of the finite case.

Let us consider the case of a finite group G, with a cardinality $\gamma = \#(G)$, acting isometrically on an Euclidean space.

For $g \neq k$ and $k \neq l$, the coefficient $C_{g,h,k,l}(\mathbf{u},\mathbf{u})$ is *a priori* different from "$\frac{0}{0}$", and it can be identified with the corresponding term $C_{g,h,k,l}(\mathbf{u},\mathbf{u}+d\mathbf{u})$ in the upper integral of $\Phi_{\mathbf{u},\mathbf{u}+d\mathbf{u}}(d\sigma)$. This situation is refered to as the case "0":

"0" – when $g \neq k$ and $k \neq l(\gamma^4 - 2\gamma^3 - \gamma^2$ terms among the γ^4 terms in $G^4)$.

On the other hand, there are three cases in which $C_{g,h,k,l}(\mathbf{u},\mathbf{u})$ is *a priori* not defined (i.e. $C_{g,h,k,l}(\mathbf{u},\mathbf{u}) =$"$\frac{0}{0}$"):

"1" – when $g = h$ and $k \neq l(\gamma^3$ terms among the γ^4 terms in $G^4)$,

"2" – when $g \neq h$ and $k = l(\gamma^3$ terms among the γ^4 terms in $G^4)$,

"3" – when $g = h$ and $k = l(\gamma^2$ terms among the γ^4 terms in $G^4)$.

In these cases, it is necessary to consider $d\mathbf{u} \neq \mathbf{0}$ and turn back to the complete expression $C_{g,h,k,l}(\mathbf{u},\mathbf{u}+d\mathbf{u}) \neq C_{g,h,k,l}(\mathbf{u},\mathbf{u})$.

Each situation 0, 1, 2 or 3 corresponds to a set of four-fold operations (g,h,k,l) respectively denoted G_0, G_1, G_2 and G_3.

Since G is finite, the upper or the lower integral occurring in $\Phi_{\mathbf{u},\mathbf{u}+d\mathbf{u}}(d\sigma)$ is actually an arithmetic mean and can be replaced by a sum over G^4: this sum is split into four sums over the G_i's, each of them being in turn expressed as mean integrals:

$$\frac{1}{\gamma^4}\sum_{G^4}\cdots = \frac{1}{\gamma^4}\left\{\sum_{G_0}\cdots+\sum_{G_1}\cdots+\sum_{G_2}\cdots+\sum_{G_3}\cdots\right\}$$
$$= \frac{1}{\gamma^4}\left\{\#(G_0)\int\limits_{G_0}\cdots+\#(G_1)\int\limits_{G_1}\cdots+\#(G_2)\int\limits_{G_2}\cdots+\#(G_3)\int\limits_{G_3}\cdots\right\}$$

$$= \frac{1}{\gamma^4}\left\{(\gamma^4 - 2\gamma^3 - \gamma^2)\int_{G_0}\dots + \gamma^3\int_{G_1}\dots + \gamma^3\int_{G_2}\dots + \gamma^2\int_{G_3}\dots\right\}$$

$$= \left(1 - \frac{2}{\gamma} - \frac{1}{\gamma^2}\right)\int_{G_0}\dots + \frac{1}{\gamma}\int_{G_1}\dots + \frac{1}{\gamma}\int_{G_2}\dots + \frac{1}{\gamma^2}\int_{G_3}\dots .$$

Therefore, the left-hand side of eq. ($\mathbb{E}$) reads

$$\Phi_{\mathbf{u},\mathbf{u}+d\mathbf{u}}(d\sigma)$$

$$\approx \frac{\int_{G_4} \mu_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(h)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)\exp[pC_{g,h,k,l}(\mathbf{u},\mathbf{u}+d\mathbf{u})d\sigma^2]\,d(g,h,k,l)}{\left[\int_G \mu_{\mathbf{u},\mathbf{u}}(g)\,dg\right]^4}$$

$$\approx \frac{\int_{G_4} \mu_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(h)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)[1 + pC_{g,h,k,l}(\mathbf{u},\mathbf{u}+d\mathbf{u})d\sigma^2]\,d(g,h,k,l)}{\left[\int_G \mu_{\mathbf{u},\mathbf{u}}(g)dg\right]^4}$$

$$\approx 1 + p\frac{\left(1 - \frac{2}{\gamma} - \frac{1}{\gamma^2}\right)\int_{G_0} dN_0 + \frac{1}{\gamma}\int_{G_1} dN_1 + \frac{1}{\gamma}\int_{G_2} dN_2 + \frac{1}{\gamma^2}\int_{G_3} dN_3}{\left[\int_G \mu_{\mathbf{u},\mathbf{u}}(g)\,dg\right]^4} d\sigma^2 ,$$

where

* $dN_0 = \mu_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(h)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)C_{g,h,k,l}(\mathbf{u},\underline{\mathbf{u}})\,dg\,dh\,dk\,dl\ (g \neq h, k \neq l)$,
* $dN_1 = \mu^2_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)C_{g,g,k,l}(\mathbf{u},\underline{\mathbf{u}+d\mathbf{u}})\,dg\,dk\,dl$ ($g = h$, $k \neq l$: formally, dg here represents a measure "induced" by the "diagonal measure dg^2" of G^2 onto G_1).
* $dN_2 = \mu_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(h)\mu^2_{\mathbf{u},\mathbf{u}}(k)C_{g,h,k,k}(\mathbf{u},\underline{\mathbf{u}+d\mathbf{u}})\,dg\,dh\,dk$ ($g \neq h$; $k = l$; formally, dk here represents a measure "induced" by the diagonal measure dk^2 of G^2 onto G_2).
* $dN_3 = \mu^2_{\mathbf{u},\mathbf{u}}(g)\mu^2_{\mathbf{u},\mathbf{u}}(k)C_{g,g,k,k}(\mathbf{u},\underline{\mathbf{u}+d\mathbf{u}})\,dg\,dk$ ($g = h$; $k = l$; dg and dk are formally defined as in dN_1 and dN_2).

All but one of the four upper integrals vanish. Indeed,

* $$\int_{G_0} dN_0 = \iiiint_{G^4,\,g\neq h,k\neq l} \mu_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(h)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)\frac{(g\mathbf{u}-h\mathbf{u}|k\mathbf{u}-l\mathbf{u})}{\|g\mathbf{u}-h\mathbf{u}\|\cdot\|k\mathbf{u}-l\mathbf{u}\|}\,dg\,dh\,dk\,dl = 0 ,$$

for the exchange of k and l (or g and h) in any value of the integrand affords the opposite value of the integrand.

- $$\int_{G_1} dN_1 = \iiint_{G_3} \mu^2_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)\frac{(g\mathbf{u}-g(\mathbf{u}+d\mathbf{u})|k\mathbf{u}-l\mathbf{u})}{\|g\mathbf{u}-g(\mathbf{u}+d\mathbf{u})\|\cdot\|k\mathbf{u}-l\mathbf{u}\|}\,dg\,dk\,dl = 0\,,$$

$$= \iiint_{G_3} \mu^2_{\mathbf{u},\mathbf{u}}(g)\mu_{\mathbf{u},\mathbf{u}}(k)\mu_{\mathbf{u},\mathbf{u}}(l)\frac{(gd\mathbf{u}|k\mathbf{u}-l\mathbf{u})}{\|d\mathbf{u}\|\cdot\|k\mathbf{u}-l\mathbf{u}\|}\,dg^2\,dk\,dl = 0$$

for the exchange of k and l in any value of the integrand affords the opposite value of the integrand. Likewise, $\int_{G_1} dN_2 = 0$.

- $$\int_{G_3} dN_3 = \iint_{G_2} \mu^2_{\mathbf{u},\mathbf{u}}(g)\mu^2_{\mathbf{u},\mathbf{u}}(k)\frac{(g\mathbf{u}-g(\mathbf{u}+d\mathbf{u})|k\mathbf{u}-k(\mathbf{u}+d\mathbf{u}))}{\|g\mathbf{u}-g(\mathbf{u}+d\mathbf{u})\|\cdot\|k\mathbf{u}-k(\mathbf{u}+d\mathbf{u})\|}\,dg\,dk$$

$$= \iint_{G_2} \mu^2_{\mathbf{u},\mathbf{u}}(g)\mu^2_{\mathbf{u},\mathbf{u}}(k)\frac{(gd\mathbf{u}|kd\mathbf{u})}{\|d\mathbf{u}\|^2}\,dg\,dk = \frac{\|d\mathbf{U}\|^2}{\|d\mathbf{u}\|^2} \geqslant 0\,,$$

where

$$d\mathbf{U} = \int_G \mu^2_{\mathbf{u},\mathbf{u}}(g)(gd\mathbf{u})\,dg\,.$$

In conclusion, *if G is a finite group* ($1 \leqslant \gamma < \infty$ and $dg = 1/\gamma$):

$$\Phi_{\mathbf{u},\mathbf{u}+d\mathbf{u}}(d\sigma) \approx 1 + p\frac{\frac{1}{\gamma^2}\int_{G_3} dN_3}{\left[\int_G \mu_{\mathbf{u},\mathbf{u}}(g)\,dg\right]^4}d\sigma^2 \approx 1 + pB^2(\mathbf{u},d\mathbf{u})\left[\frac{d\sigma}{\gamma}\right]^2,$$

where

$$B^2(\mathbf{u},d\mathbf{u}) = \frac{1}{\left[\int_G \mu_{\mathbf{u},\mathbf{u}}(g)\,dg\right]^4}\,\frac{\|d\mathbf{U}\|^2}{\|d\mathbf{u}\|^2}\,.$$

As it has already been underlined [8], it is clear that when $\gamma = \infty$, this derivation does not afford a definition of $d\sigma^2$. Nevertheless, it still defines the quantity: $ds = d\sigma/\gamma$, and the definition reads

$$\Phi_{\mathbf{u},\mathbf{u}+d\mathbf{u}}(\gamma ds) \approx 1 + pB^2(\mathbf{u},d\mathbf{u})\,ds^2\,.$$

Under this form (with $\Phi_{\mathbf{u},\mathbf{u}+d\mathbf{u}}(\gamma ds) = K_p(\mathbf{u},\mathbf{u}+d\mathbf{u})$), it furnishes a definition of ds^2 whatever is the finite or infinite group G considered.

The following definition of d_p and ds are therefore suggested:

$$\gamma d_p(\mathbf{u}, \mathbf{v}) = D_p(\mathbf{u}, \mathbf{v}),$$

$$\gamma ds = d\sigma = D_p(\mathbf{u}, \mathbf{u} + d\mathbf{u}),$$

where $\gamma = \#G$.

When G is a finite group, the results hitherto established for D_p and $d\sigma$ can be easily written down in terms of ds and d_p, which become distance extensions of the starting distance d/γ instead of the equivalent distance d. This definition also brings a rigorous formulation of the singularity of $d\sigma^2$ on the unit representation space V_1 contained in a larger representation space $V = V_1 \oplus V_2$ of the group $\mathcal{S}_2 \approx \{e, \sigma\}$ (where: $\forall \mathbf{u} \in V_2, e\mathbf{u} = \mathbf{u}, \sigma\mathbf{u} = -\mathbf{u}$).

When G is an infinite group, ($\mathbb{E}$) is still a definition of ds^2. However, D_p can still be finite (e.g. if G is compact) and no definition of d_p is furnished.

If $\mu^2_{\mathbf{u},\mathbf{u}}(g) = 1$ for any operation g, then $\mathbf{U} = \int_G (gd\mathbf{u})\, dg$: if there exists some operation g_0 such that $g_0 d\mathbf{u} = -d\mathbf{u}$, then $d\mathbf{U} = 0$, and no definition of ds^2 is available. The situation formerly discussed for the infinite group $G = \mathcal{C}_\infty$ in R^2 fulfills the latter condition and thus, a formal calculation of $d\sigma^4$ only remains possible [8].

If $B(\mathbf{u}, d\mathbf{u})$ does not vary with $d\mathbf{u}$, and if $B(\mathbf{u}, d\mathbf{u}) \neq 0$, then the equation provides a definition of a metric ds^2 in the classical sense of Riemannian manifolds. This problem will be discussed later.

6. Conclusion

The framework of the definition of completely G-invariant distance extensions is now generalized to the more general definition of G-weighted distance extensions. The formulation of the local version affording a definition of G-weighted metrics has been clarified. In particular, the borderline case of infinite compact groups is rigorously treated by the introduction of the related metric $ds^2 = d\sigma^2/\gamma^2$, where $\gamma = \#G$. Everything seems to be at our disposal to search (at least formally) for an eventual connection with tools of physical mathematics. This challenge will come under a speculative interpretation of the wheighting symmetry function $\mu_{\mathbf{u},\mathbf{v}}$ which is to be determined. This is undertaken in the next paper.

References and notes

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[2] R. Chauvin, Paper III of this series, J. Math. Chem. 16 (1994) 269.
[3] R. Chauvin, Entropy in dissimilarity and chirality measures, submitted for publication.
[4] R. Chauvin, Paper II of this series, J. Math. Chem. 16 (1994) 257.

[5] D_∞ is defined by: $\forall(\mathbf{u},\mathbf{v})\in E^2$, $D_\infty(\mathbf{u},\mathbf{v}) = \mathrm{Inf}_{g\in G,h\in G} d(g\mathbf{u}, h\mathbf{v})$.
[6] D_0 is defined by: $\forall(\mathbf{u},\mathbf{v})\in E^2$, $D_0(\mathbf{u},\mathbf{v}) = 1/[\int_G dg/d(g\mathbf{u},\mathbf{v})]$.
[7] R. Chauvin, Paper I of this series, J. Math. Chem. 16 (1994) 245.
[8] R. Chauvin, Paper IV of this series, J. Math. Chem. 16 (1994) 285.