Algebraic Forms

Three different algebraic forms can be calculated from input structures. Shortly, if a molecule consists of *n* atoms (*vector of* $\Re^n$), then the k^{th} *total (whole) two-linear, three-linear* and *four-linear* indices are calculated as *N-linear algebraic maps* (forms) in $\mathbb{R}^n$, in a canonical basis set. Specifically, the k^{th} *non-stochastic atom-based two-linear*, *three-linear* and *four-linear* indices for a molecule, $m^k(\bar{x},\bar{y})$, $tr^k(\bar{x},\bar{y},\bar{z})$ and $qu^k(\bar{x},\bar{y},\bar{z},\bar{w})$, respectively, are computed from the k^{th} *two-tuples, three-tuples* and *four-tuples spatial (dis-)similarity matrices*, [$\mathbb{G}^k$, $\mathbb{GT}^k$ and $\mathbb{GQ}^k$], as shown in Eqs. **1-3**, correspondingly:

$$m^k(\bar{x},\bar{y}) = \sum_{i=1}^{n}\sum_{j=1}^{n} g_{ij}^k x^i y^j = [X]^T\,\mathbb{G}^k[Y] \qquad (\mathbf{1})$$

$$tr^k(\bar{x},\bar{y},\bar{z}) = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{l=1}^{n} gt_{ijl}^k x^i y^j z^l = \mathbb{GT}^k \cdot \bar{x} \cdot \bar{y} \cdot \bar{z} \qquad (\mathbf{2})$$

$$qu^k(\bar{x},\bar{y},\bar{z},\bar{w}) = \sum_{i=1}^{n}\sum_{j=1}^{n}\sum_{l=1}^{n}\sum_{h=1}^{n} gq_{ijl}^k x^i y^j z^l w^h = \mathbb{GQ}^k \cdot \bar{x} \cdot \bar{y} \cdot \bar{z} \cdot \bar{w} \qquad (\mathbf{3})$$

where, *n* is the number of atoms in a molecule, g_{ij}^k, gt_{ijl}^k and gq_{ijl}^k are the coefficients of the matrices $\mathbb{G}^k$, $\mathbb{GT}^k$ and $\mathbb{GQ}^k$ respectively, and and $x^1,\ldots,x^n$, $y^1,\ldots,y^n$, $z^1,\ldots,z^n$ and $w^1,\ldots,w^n$ are the coordinates or components of the molecular vectors $\bar{x}$, $\bar{y}$, $\bar{z}$ and $\bar{w}$ in a system of canonical ('natural') basis vectors of $\mathbb{R}^n$. As can be noticed, these molecular vectors are weighted with different atomic properties and thus several combinations are obtained. In this way, in the QuBiLS software are employed the algebraic forms shown in the Table 1.

Table 1. N-linear algebraic forms implemented in the QuBiLS program.

1. Two-linear [$m^k(\overline{x},\overline{y})$]
- Linear (X, Y = 1)
- Bilinear (X <> Y)
- Quadratic (X = Y)

Used symbols
1: Using the unitary vector
<>: Using different properties
=: Using equal properties

2. Three-linear [$tr^k(\overline{x},\overline{y},\overline{z})$]
- Threelinear (X <> Y <> Z)
- Threelinear-Quadratic-Bilinear ((X = Y) <> Z)
- Threelinear-Bilinear (X <> Y, Z = 1)
- Threelinear-Linear (X, Y = 1, Z = 1)
- Threelinear-Cubic (X = Y = Z)

3. Four-linear [$qu^k(\overline{x},\overline{y},\overline{z},\overline{w})$]
- Fourlinear (X <> Y <> Z <> W)
- Fourlinear-Quadratic-Threelinear ((X = Y) <> Z <> W)
- Fourlinear-Threelinear (X = 1, Y <> Z <> W)
- Fourlinear-Cubic-Bilinear ((X = Y = Z) <> W)
- Fourlinear-Bilinear (X = Y = 1, Z <> W)
- Fourlinear-Linear (X = Y = Z = 1, W)
- Fourlinear-Quadruple (X = Y = Z = W)