Algebraic Forms

If a (protein or peptide), hereafter protein, representation consists of *n* atoms (*vector of* $\Re^n$), then the k^{th} *total (global) two-linear* indices are calculated as *2-linear algebraic maps* (forms) in $\mathbb{R}^n$, in a canonical basis set. Specifically, the k^{th} *bilinear* $b^k(\bar{x},\bar{y})$, *quadratic* $q^k(\bar{x},\bar{y})$ and *linear* $f^k(\bar{x},\bar{y})$ indices for a protein are calculated from the k^{th} *two-tuple multimetric-(dis)similarity matrix*, $[M^k]$, as shown in Eqs. **1-3**:

$$b^k(\bar{x},\bar{y}) = \sum_{i=1}^{n}\sum_{j=1}^{n} m_{ij}^k x^i y^j = [X]^T \mathrm{M}^k [Y] \quad (\mathbf{1})$$

$$q^k(\bar{x},\bar{y}) = \sum_{i=1}^{n}\sum_{j=1}^{n} m_{ij}^k x^i y^j = [X]^T \mathrm{M}^k [Y] \quad (\mathbf{2})$$

$$f^k(\bar{x},\bar{y}) = \sum_{i=1}^{n}\sum_{j=1}^{n} m_{ij}^k x^i y^j = [X]^T \mathrm{M}^k [Y] \quad (\mathbf{3})$$

where, *n* is the number of atoms in a protein, m_{ij}^k are the coefficients of the matrix M^k,and $x^1,\ldots,x^n$, $y^1,\ldots,y^n$ are the coordinates (components) of the macromolecular vectors $\bar{x}$, $\bar{y}$ in a system of canonical ('natural') basis vectors of $\mathbb{R}^n$. As can be noticed, these macromolecular vectors are weighted with different amino acid side-chain and atomic properties (labels) and thus several combinations are obtained. In this way, in the MuLiMs software are employed the algebraic forms shown in the Table 1.

Table 1. Two-linear algebraic forms implemented in the MuLiMs program.

1. Two-linear [$m^k(\bar{x},\bar{y})$]	Used symbols
- Linear (X=1, Y) - Bilinear (X<>Y) - Quadratic (X=Y)	1: Using the unitary vector <>: Using different properties =: Using equal properties