Two-way (Dis)-Similarity Metrics

Metrics	Formula[a]	Range[b]	Average	Range
Minkowsky (**M1-M7**) p = 0.25, 0.5, 1, 1.5, 2, 2.5, 3, and ∞ [where, when p= 1 it is the Manhattan, city-block or taxi distance (also known as Hamming distance between binary vectors) and p = 2 is Euclidean distance)	$d_{XY} = \left(\sum_{j=1}^{h} \lvert x_j - y_j \rvert^p\right)^{\frac{1}{p}}$	$[0, \infty)$	$\bar{d} = \frac{d_{XY}}{n^{1/p}}$	$[0, \infty)$
Chebyshev/Lagrange (**M8**) (Minkowsky formula when p = ∞)	$d_{XY} = max\{\lvert x_j - y_j \rvert\}$			
Canberra (**M10**)	$d_{XY} = \sum_{j=1}^{h} \frac{\lvert x_j - y_j \rvert}{\lvert x_j \rvert + \lvert y_j \rvert}$	$[0, n]$	$\bar{d} = \frac{d_{XY}}{n}$	[0,1]
Lance - Williams/Bray-Curtis (**M11**)	$d_{XY} = \frac{\sum_{j=1}^{h} \lvert x_j - y_j \rvert}{\sum_{j=1}^{h} (\lvert x_j \rvert + \lvert y_j \rvert)}$	[0,1]	$\bar{d} = \frac{d_{XY}}{n}$	$\left[0, \frac{1}{n}\right]$
Clark/Coefficient of Divergence (**M12**)	$d_{XY} = \sqrt{\sum_{j=1}^{h} \left(\frac{x_j - y_j}{\lvert x_j \rvert + \lvert y_j \rvert}\right)^2}$	$[0, n]$	$\bar{d} = \frac{d_{XY}}{\sqrt{n}}$	$[0, \sqrt{n}]$
Soergel (**M13**)	$d_{XY} = \frac{1}{n} \sum_{j=1}^{h} \frac{\lvert x_j - y_j \rvert}{max\{x_j, y_j\}}$	[0,1]	$\bar{d} = \frac{d_{XY}}{n}$	$\left[0, \frac{1}{n}\right]$
Bhattacharyya (**M14**)	$d_{XY} = \sqrt{\sum_{j=1}^{h} \left(\sqrt{x_j} - \sqrt{y_j}\right)^2}$	$[0, \infty)$	$\bar{d} = \frac{d_{XY}}{\sqrt{n}}$	$[0, \infty)$
Wave – Edges (**M15**)	$d_{XY} = \sum_{j=1}^{h} \left(1 - \frac{min\{x_j, y_j\}}{max\{x_j, y_j\}}\right)$	$[0, n]$	$\bar{d} = \frac{d_{XY}}{n}$	[0,1]
Angular Separation/[1-Cosine (**Ochiai**)] (**M16**)	$d_{XY} = 1 - Cos_{XY}$ where, $Cos_{XY} = \frac{\boldsymbol{XY}}{\lVert \boldsymbol{X} \rVert \lVert \boldsymbol{Y} \rVert} = \frac{\sum_{j=1}^{h} x_j y_j}{\sqrt{\sum_{j=1}^{h} x_j^2 \sum_{j=1}^{h} y_j^2}}$	[0,2]		

[a]The variable $x_j(y_j)$ is the value of the coordinate j of the atom s and the atom t, corresponding to the molecule X (Y), respectively. The h value is the Cartesian coordinates (x, y, z) of an atom. The p values in Minkowsky metric are 0.25, 0.5, 1 (Manhattan), 1.5, 2 (Euclidean), 2.5 and 3 (Minkowsky). [b]"*Range*" refers to "range" and not to "rank" and is defined as $Range = max\{x_j\} - min\{x_j\}$.

Three- and Four-way (Dis)-Similarity Multi-Metrics

A) Ternary Measures *(T_{XYZ})*

Measure	Formula
Perimeter (**M19-M20**)	$T_{XYZ} = d_{xy} + d_{yz} + d_{zx}$
Triangle Area (**M21-M22**)	$T_{XYZ} = \sqrt{s(s-d_{XY})(s-d_{YZ})(s-d_{ZX})}$ $s = \frac{d_{XY}+d_{YZ}+d_{ZX}}{2}$
Summation Sides (**M25-M26**)	$T_{XYZ} = d_{XY} + d_{YZ}$
Bond angle (Angle between sides) (**M27-M28**)	A_X, A_Y, A_Z *coordenates of three atoms of a molecule* $U = A_X - A_Y, V = A_Z - A_Y$ $T_{XYZ} = \alpha = \arccos\left(\frac{U * V}{\lvert U \rvert * \lvert V \rvert}\right)$

B) Quaternary Measures *(Q_{XYZW})*

Measure	Formula
Perimeter (**M19-M20**)	$Q_{XYZW} = d_{XY} + d_{YZ} + d_{ZW} + d_{WX}$
Volume (**M23-M24**)	A_X, A_Y, A_Z, A_W *coordenates of four atoms of a molecule* $Q_{XYZW} = \frac{1}{6}\begin{pmatrix} A_{Y1}-A_{X1} & A_{Z1}-A_{X1} & A_{W1}-A_{X1} \\ A_{Y2}-A_{X2} & A_{Z2}-A_{X2} & A_{W2}-A_{X2} \\ A_{Y3}-A_{X3} & A_{Z3}-A_{X3} & A_{W3}-A_{X3} \end{pmatrix}$
Summation Sides (**M25-M26**)	$Q_{XYZW} = d_{XY} + d_{YZ} + d_{ZW}$
Dihedral Angle (**M29-M30**)	A_X, A_Y, A_Z *coordenates of three atoms of a molecule in the plane A* B_W, B_Y, B_Z *coordenates of three atoms of a molecule in the plane B* $U_A = (A_X - A_Y) \times (A_Z - A_y)$ $U_B = (B_W - A_Y) \times (B_Z - A_y)$ $Q_{XYZW} = \alpha = \arccos\left(\frac{U_A * U_B}{\lvert U_A \rvert * \lvert U_B \rvert}\right)$