

Numerical Representations Summary

For the M mapping of the genomic sequence S of length N, the following statements apply:

Voss:

$$B(x) = \begin{cases} (1,0,0,0) & \text{if } S(x)=A \\ (0,1,0,0) & \text{if } S(x)=T \\ (0,0,1,0) & \text{if } S(x)=C \\ (0,0,0,1) & \text{if } S(x)=G \end{cases}, x \in [0, N-1], \quad M = B^T$$

Tetrahedron

with $B_0^T = A_n, B_1^T = T_n, B_2^T = C_n, B_3^T = G_n$, where

$$M_r = \frac{\sqrt{2}}{3} (2T_n - C_n - G_n)$$

$$M_g = \frac{\sqrt{6}}{3} (C_n - G_n)$$

$$M_b = \frac{1}{3} (3A_n - T_n - C_n - G_n)$$

$$M(x) = (M_r, M_g, M_b)(x)$$

Chaos Game Representation (CGR)

$$P_0 = (0.5, 0.5)$$

$P_x = 0.5(P_{x-1} + M(S(x)))$, where

$$M(S(x)) = \begin{cases} (0,0) & \text{if } S(x)=A \\ (1,0) & \text{if } S(x)=T \\ (0,1) & \text{if } S(x)=C \\ (1,1) & \text{if } S(x)=G \end{cases}, x \in [1, N]$$

Integer CGR

$$P_1 = M(S(1))$$

$P_n = P_{n-1} + 2^{(n-1)} M(S(n-1))$, where $n = x + 1$, and

$$M(S(x)) = \begin{cases} (1,1) & \text{if } S(x)=A \\ (-1,1) & \text{if } S(x)=T \\ (-1,-1) & \text{if } S(x)=C \\ (1,-1) & \text{if } S(x)=G \end{cases}, x \in [1, N]$$

DNA Walk

$$P_1 = M(S(1))$$

$P_x = P_{x-1} + M(S(x))$, where

$$M(S(x)) = \begin{cases} -1 & \text{if } S(x)=A \vee S(x)=G \\ 1 & \text{if } S(x)=T \vee S(x)=C \end{cases}, x \in [1, N]$$

Paired Numeric Mapping:

$$M(x) = \begin{cases} 1 & \text{if } S(x)=A \vee S(x)=T \\ -1 & \text{if } S(x)=C \vee S(x)=G \end{cases}, x \in [0, N-1]$$

Complex:

$$M(x) = \begin{cases} 1+i & \text{if } S(x)=A \\ 1-i & \text{if } S(x)=T \\ -1+i & \text{if } S(x)=C \\ -1-i & \text{if } S(x)=G \end{cases}, x \in [0, N-1]$$

Eiip:

$$M(x) = \begin{cases} 0.1260 & \text{if } S(x)=A \\ 0.1335 & \text{if } S(x)=T \\ 0.1340 & \text{if } S(x)=C \\ 0.0806 & \text{if } S(x)=G \end{cases}, x \in [0, N-1]$$

Atomic:

$$M(x) = \begin{cases} 70 & \text{if } S(x)=A \\ 66 & \text{if } S(x)=T \\ 58 & \text{if } S(x)=C \\ 78 & \text{if } S(x)=G \end{cases}, x \in [0, N-1]$$

2-bit binary:

$$M(x) = \begin{cases} 00 & \text{if } S(x)=A \\ 01 & \text{if } S(x)=T \\ 11 & \text{if } S(x)=C \\ 10 & \text{if } S(x)=G \end{cases}, x \in [0, N-1]$$

4-bit binary:

$$M(x) = \begin{cases} 0100 & \text{if } S(x)=A \\ 1000 & \text{if } S(x)=T \\ 0001 & \text{if } S(x)=C \\ 0010 & \text{if } S(x)=G \end{cases}, x \in [0, N-1]$$

Integer:

$$M(x) = \begin{cases} 2 & \text{if } S(x)=A \\ 0 & \text{if } S(x)=T \\ 1 & \text{if } S(x)=C \\ 3 & \text{if } S(x)=G \end{cases}, x \in [0, N-1]$$

Molecular Mass:

$$M(x) = \begin{cases} 134 & \text{if } S(x)=A \\ 125 & \text{if } S(x)=T \\ 110 & \text{if } S(x)=C \\ 150 & \text{if } S(x)=G \end{cases}, x \in [0, N-1]$$

$$\begin{aligned} & \text{Real:} \\ M(x) = & \begin{cases} -1.5 & \text{if } S(x)=A \\ 1.5 & \text{if } S(x)=T \\ 0.5 & \text{if } S(x)=C \\ -0.5 & \text{if } S(x)=G \end{cases}, x \in [0, N-1] \end{aligned}$$

For the representations Z Curve (Original publication) and Liao 2D graphical representation in the sequence S of size N, whether A_n, T_n, C_n, G_n , the accumulated occurrences of nitrogenous bases A, T, C, G, respectively, up to position n .

The Z curve is defined as a set of nodes $P_0, P_1, \dots, P_n, \dots, P_N$, whose x_n, y_n, z_n coordinates are described below:

$$\begin{aligned} & \text{Z Curve} \\ \begin{cases} A_0 = T_0 = C_0 = G_n = 0 \\ x_n = (A_n + G_n) - (C_n + T_n) \\ y_n = (A_n + C_n) - (G_n + T_n) \\ z_n = (A_n + T_n) - (G_n + C_n) \end{cases}, n \in [0, N] \end{aligned}$$

The 2D graphical representation of Liao assumed two constants, defined as n and m, which in Seqreppy are assigned to the values 1/2 and 3/4, respectively. Thus, the coordinates of the method's constituent points are defined as:

$$\begin{aligned} & \text{Liao} \\ \begin{cases} x_0 = y_0 = 0 \\ x_i = A_n m + G_n \sqrt{n} + C_n \sqrt{n} + T_n m \\ y_i = -A_n \sqrt{n} - G_n m + C_n m + T_n \sqrt{n} \end{cases}, i \in [1, N] \end{aligned}$$

In Seqreppy they are simplified as follows:

$$\begin{cases} x_0 = y_0 = 0 \\ x_i = m(A_n + T_n) + \sqrt{n}(G_n + C_n) \\ y_i = \sqrt{n}(T_n - A_n) + m(C_n - G_n) \end{cases}, i \in [1, N]$$