

# Computation of the Writhe of a protein

## 1 The writhe of a protein

A measure for the degree of intertwining of the chain around itself is the Writhe, which is defined by taking the Gauss linking integral over one curve (instead of two)

(Writhe). For a curve  $\ell$  with arc-length parameterization  $\gamma(t)$  is the double integral over  $l$ :

$$Wr(l) = \frac{1}{4\pi} \int_{[0,1]} \int_{[0,1]} \frac{(\dot{\gamma}(t), \dot{\gamma}(s), \gamma(t) - \gamma(s))}{\|\gamma(t) - \gamma(s)\|^3} dt ds. \quad (1)$$

The Writhe is a continuous function of the chain coordinates for both open and closed chains.

By taking the absolute value of the integrand, we obtain the Average Crossing Number, ACN. This is another informative measure which shows how many crossings we see in a random projection of the protein.

## 2 Python script for the writhe of a protein

### 2.1 Computations of the Writhe

Consider one polygonal curve:

$$l_1 = ((0, 0, 0), (1, 0, 0), (1, 0.9, 0.1), (0.1, 0.8, -0.1), (0.17, 0.22, 0.31))$$

In other words,  $l_1$  is formed by 4 edges:

$$e_1 = ((0, 0, 0), (1, 0, 0)), e_2 = ((1, 0, 0), (1, 0.9, 0.1)), e_3 = ((1, 0.9, 0.1), (0.1, 0.8, -0.1)) \text{ and } e_4 = ((0.1, 0.8, -0.1), (0.17, 0.22, 0.31)).$$

Create a python function that takes as input  $l_1$

1. For each pair of edges in  $l_1$ ,  $(e_i, e_j)$ , such that  $j > i + 1$ , computes the  $\text{gausslk}(e_i, e_j)$  (use python function provided by email last week)
2. Compute the sum of all  $\text{lk}(e_i, e_j)$
3. Return the writhe of  $l_1$ ,  $Wr(l_1) = \sum_{1 \leq i < j \leq 4, j > i+1} \text{lk}(e_i, e_j)$ .

(Note: the Writhe was also contained in last week's python script)

### 2.2 Computation of the writhe of a protein

1. Download the PDB file of the SARS-Cov-2 (COVID19) Spike protein, 6zge from the Protein Data Bank.
2. Create a script that reads the CA Atoms of the Spike protein and appends them in a list, called *protein*
3. Compute the writhe of the protein using the code of the previous section.