

Worksheet III

1 The second Vassiliev measure of SARS and SARS-CoV-2

We will use the second Vassiliev measure to detect local knots in SARS and SARS-CoV-2.

To do this, we calculate the second Vassiliev measure with specific step sizes and a window sliding approach. Namely:

- Create a double nested loop, one for the scanning length size and one for the starting point along the chain
- Use scanning lengths varying from 100 to 600 with a stepsize of 100
- Start from the first atom and slide the window in steps of 1, until the full length of the protein (minus the scanning length).
- At each step, calculate the second Vassiliev measure and put it in a list (or array).
- Create one list for each scanning size

Next:

- Download the files 6zge (SARS-CoV-2) and 6acd (SARS) from the PDB.
- Calculate the scanning Vassiliev measure lists for the two proteins
- Identify the maximum (in absolute value) values of the second Vassiliev measure and the part of the protein they correspond to.