1 Understanding groundstate and Stiffness

1) Use cgDNAweb+ to visualise the two groundstates. To understand the location of the zero entries in the corresponding stiffness matrices use spy with a tolerance (you can use script `spy(abs(stiffness matrix)>tolerance))`) in matlab. Fig. (1) shows the sparsity pattern for AAAA. Also, for TTTT you observe sparsity pattern same as AAAA.

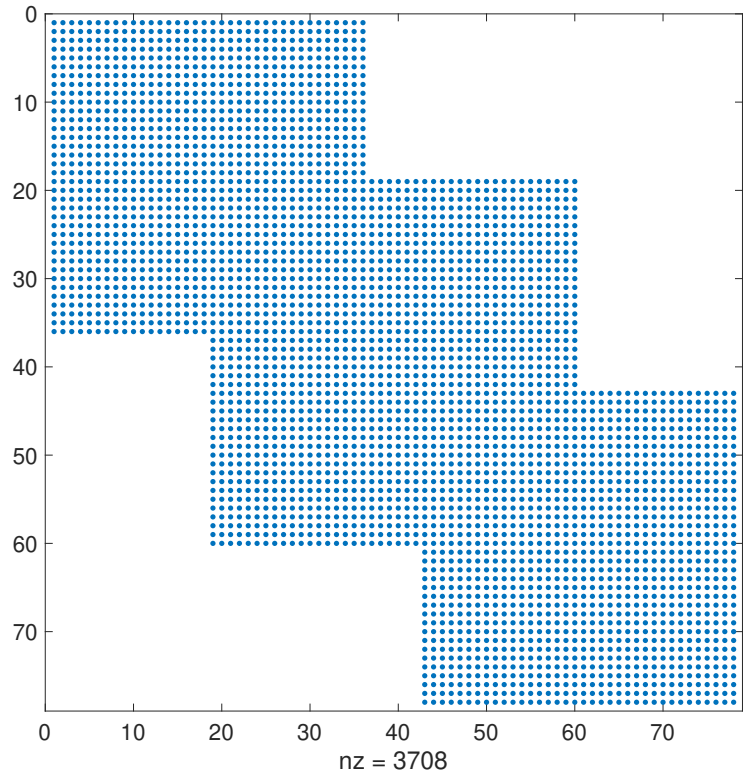

Figure 1: Using spy with tolerance 10^{-10} for AAAA.

2) Fig. (2) shows the sparsity pattern for the palindromic tetramer AATT and one can observe the set of zero entries (total 16 zeros).

3) Use cgDNAweb+ for sequences (A_{20}, G_{20}) and observe in 2D Plots that groundstate are not uniform at each end (even though sequences are uniform). However as you move 4-5 base pairs from each end then you will observe the uniformity. Then use sequence $A_{10}G_{10}$ and notice the nonlocal disruption to the groundstate at the interior boundary between the polyA and polyG segments.

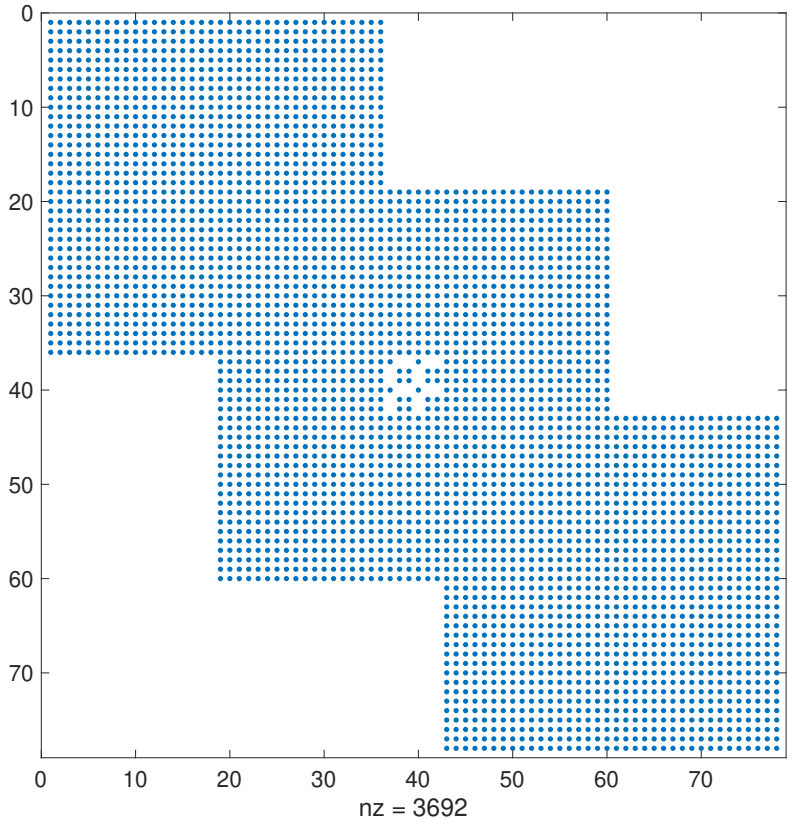

Figure 2: Using spy with tolerance 10^{-10} for AATT.

2 Effect of a point mutation on the Shape and on the Stiffness

For questions 1-4 it is useful to compute the difference $dx = x_1 - x_2$, where x_i is the groundstate of sequence S_i. In Fig. (3) we show the values of the helical parameters of dx. And in Fig. (4) we show the values of the phosphate coordinates of dx. In Fig. (5) we show, using the command `spy`, the difference $dK = K_1 - K_2$, where K_i is the stiffness matrix for sequence S_i. As already done in session 6 exercise 1.1.2, a point mutation leads to a local change in stiffness.

3 Using cgDNAweb with interesting sequences

No solution is provided for this exercise. Use cgDNAweb+ and report anything unclear.

4 cgDNA+ reconstruction of the 6 distinct poly–dinucleotide

i) We recall that the entries of the groundstate vector represent the phosphate coordinate, intra and inter relative rotations and orientations and small changes in the relative coordinates could lead to important differences in the 3D reconstruction. However we invite to check the 3D reconstructions of the six distinct poly–dinucleotides and observe that the 3D reconstructions are all super-helical. We stress also on the fact that the six poly–dinucleotides have relevant

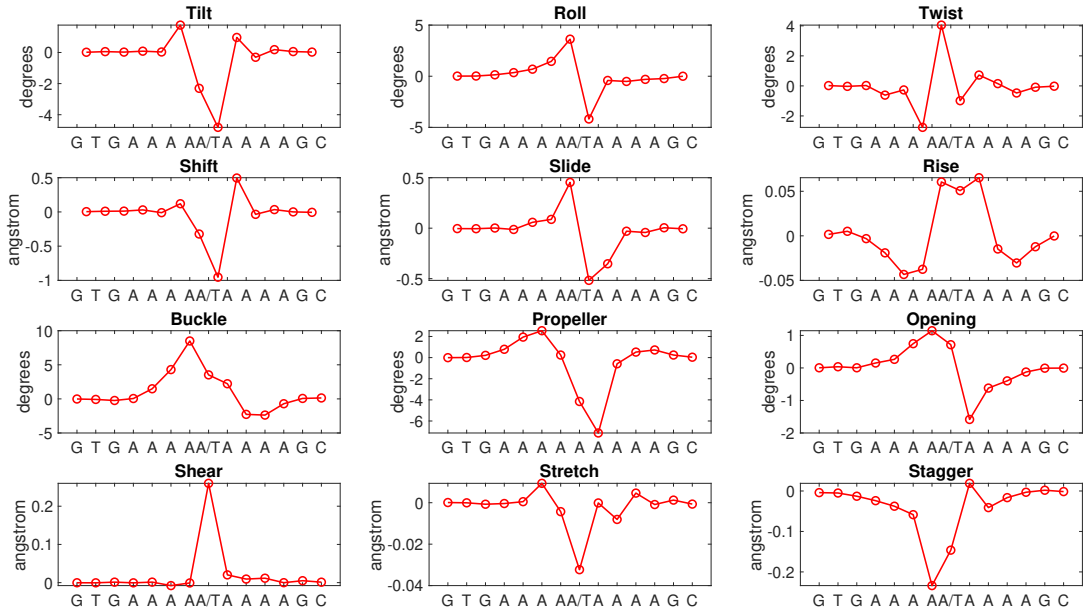

Figure 3: Values of the differences in the helical parameters between groundstate of S_1 and groundstate of S_2.

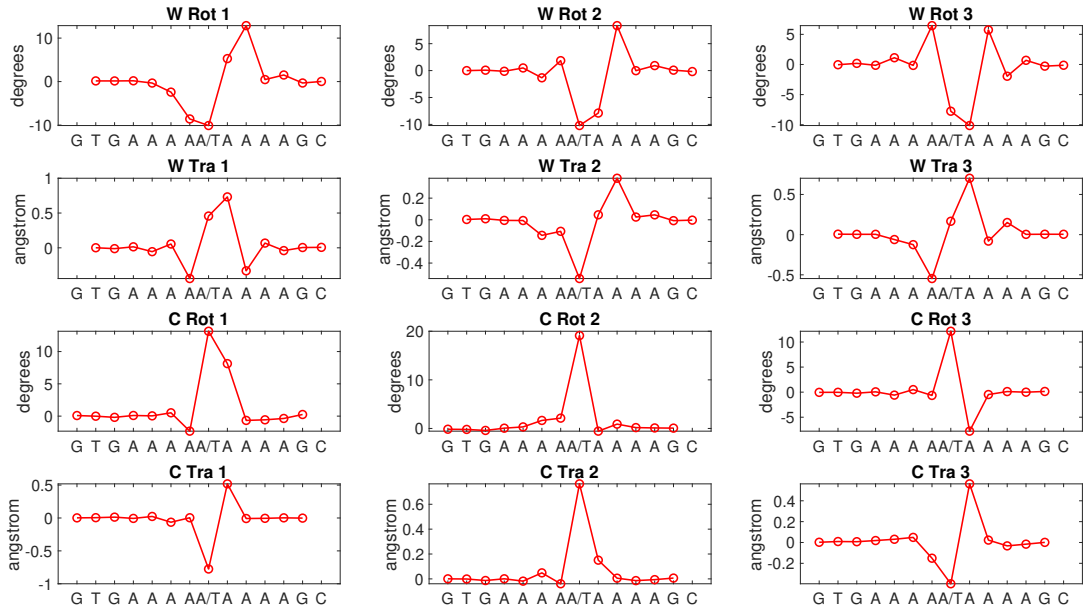

Figure 4: Values of the differences in the phosphate coordinates between groundstate of S_1 and groundstate of S_2.

differences in the shape. For example we have reconstructed the six oligomers and in Fig. (6) we show selected 30 entries (intra, phosphate, inter, phosphate, intra). Notice that intra vary considerably between the six sequences.

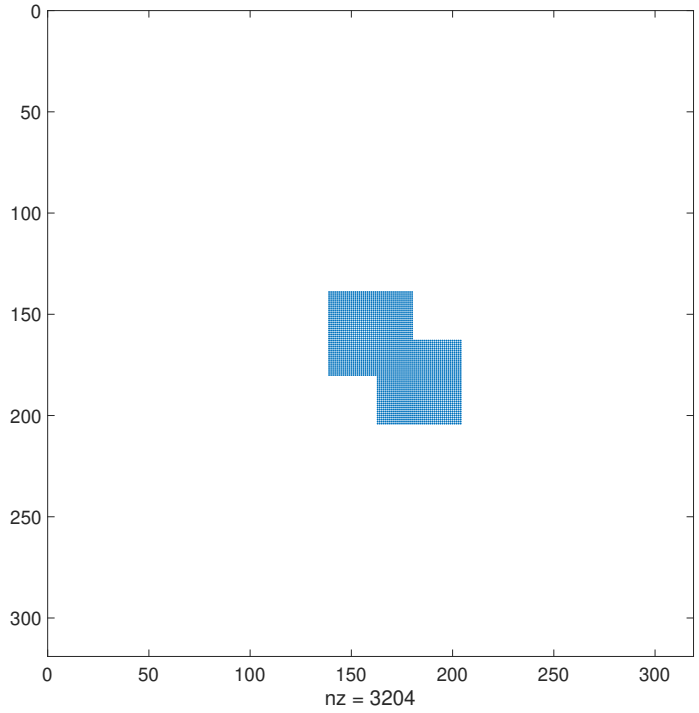

Figure 5: Difference between stiffnesses for S_1 and S_2 (spy of dK).

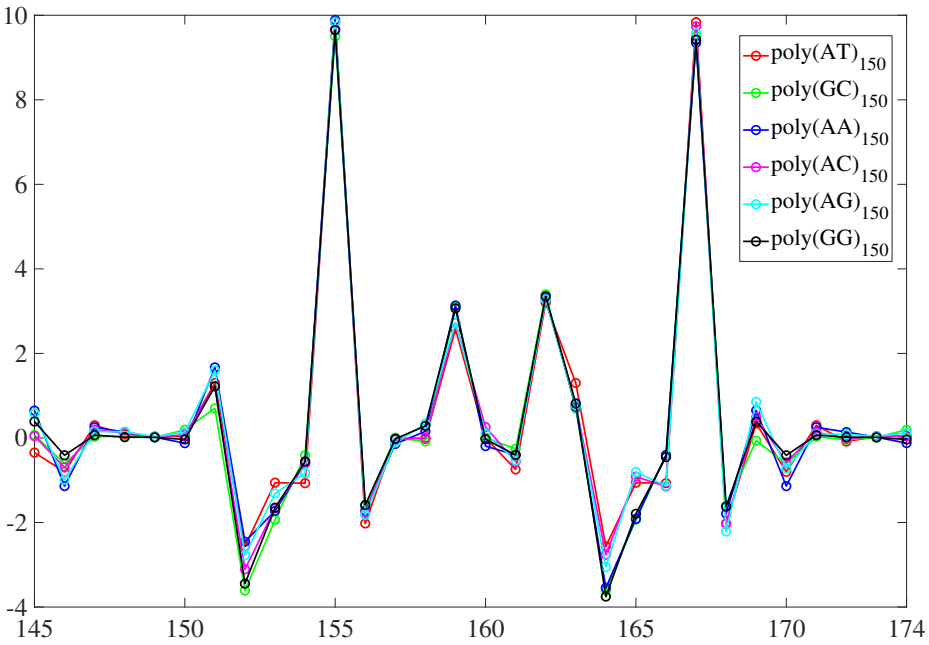

Figure 6: Comparison of 30 entries (intra, phosphate, inter, phosphate, intra) of the groundstates of the six poly($\alpha\beta$).

ii) As briefly said in the previous part, the six groundstates are different but all six present a super-helical structure (use cgDNAweb+ for better visualisation). In Fig. (7) for each poly–dinucleotide we plot the xyz position of each base-pair. The obtained helices have a different radius and a different pitch. These two features will become important for the tangent–tangent correlation, that we will see in next exercise.

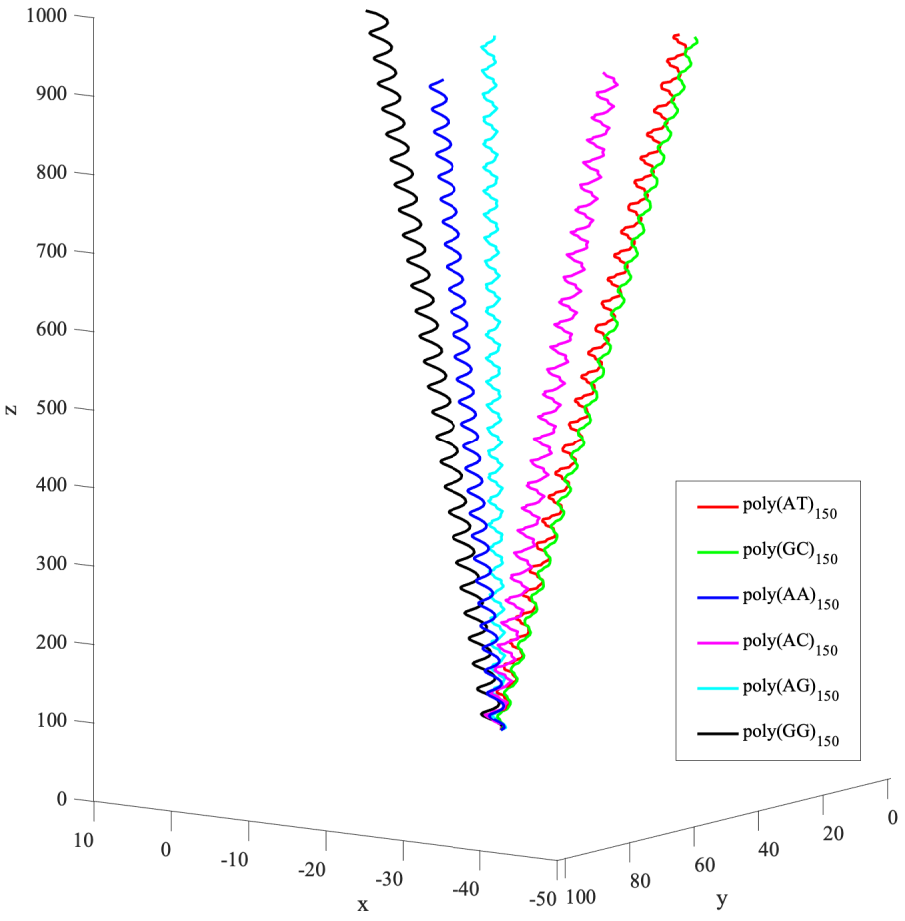

Figure 7: xyz position of each base–pair for all the six poly-dinucleotides.