Work review : summer 2016
Varun Naganathan
201464022

1.GRAPH CONSTRUCTION:
Learnt how to parse a protein pdb file and construct the protein contact network.Implemented the construction in a python program.Primaily 2 types of interactions mmonitored – The ones with the C-alpha atoms as the nodes and their interactions and the one with C-beta atoms as nodes and the interactions between them.Since C-beta atoms reside on the amino acid side chains which are the major source of non covalent ineractions amongst amino acids,the C-beta network more effectively captures the interactions.Apart from that, they also take into aspect the orientation aspect of the interaction of the two interacting atoms.

2.BASIC NETWORK PROPERTIES:
Implemented the basic properties of the network like average degree, clustering coefficient, shortest path between all pairs of nodes etc to get a brief idea of the topology of the network.

3.NON COVALENT INTERACTIONS:
Studied about the various non covalent intearctions that exist amongst proteins like electrostatic interaction, dipolar interactions, H-bonds and hydrophobic interactions.Found out the threshold distances for all of these interactions and related to the threshold set for the protein contact network. Calculated the vanderwaal radii of all the amino acids to get an idea of the max distance at which these amino acids can interact in the network.

4.CENTRALITY ANALYSIS:
Went deeper into the study of the spectral properties of the network by implementing the calculation of properties like :
1.degree distribution
2.clustering coefficient distribution
3.Closeness centrality of the nodes
4.betweenness centrality of the nodes.
All of these give us an idea of which nodes are kind of “hubs” or the busy nodes in the network which are important to the network based on the properties we define as important.Also nodes having similar properties may be categorized as having “similar neighbourhoods” thus in the long

run which would help us in clustering of the network.

5.RANDOM GRAPH CONSTRUCTION:
Also learnt and implemented how to construct a random graph from a existing protein contact network with the ERDOS RENYI model which keeps the edge count constant and also alalternative method which keeps both the edge count ads well as the degree distribution constant.This helps us in comparing the properties of a protein graph to a random graph thus establishing its “small world network” property.

6.EIGEN SPECTRA ANALYSIS:
Also implemented the calculation of the largest eigen value and the corresoinding eigen vector of the adjacency matrix of the contact network.Since the components of the eigen vector give us an idea of ehich node is of highest degree and also has nodes of high degree surounding it, this analysis also gives us an idea of which nodes are important ones and should be monitored to check the effect of various binding that may take place in the protein.

7.ALLOSTERIC REGULATION:
Read a paper on allostric regulation and the various methods through which allosteric control is exhibited in the protein.It portrayed as to how binding of an allostric inhibitor or activator can affect the active site of a protein without even being in direct contact with it.

8.GPCR PROTEINS:
Finally, I implemented the knowledge gained by the network analysis till now on GPCR proteins(chosen as a lot of annotated data available on them).This analysis is curently going on.We have taken pairs of GPCR pdb files in their bounded and unbounded state and studying the effects of bindng of allostric controllers on the network be it on certain “busy nodes” or the network as a whole using the previously implemented properties like closeness, clustering coefficient, betweenness centrality , eigen spectral analysis etc.Since a lot of annotated data is available,we compare our findings with them and once we obtain a pattern , we apply these concepts to various unknown classes of proteins to get an effective insight of allostric regulation on them.