Weekly Report(Up until 31st October, 2015)

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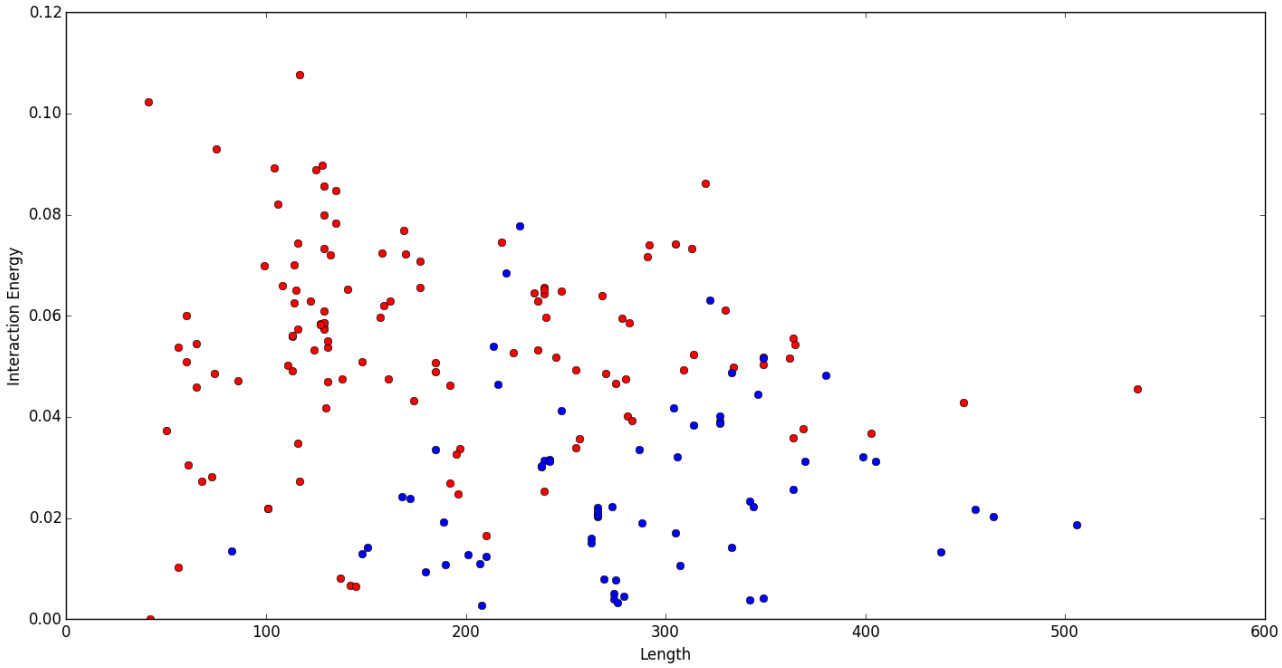
Work Done

- Previously I plotted graphs for comparison of interaction energy with length. This time, I plotted a graph with interaction energy and radius of gyration and a 3-D graph with length, radius of gyration and interaction energy on the three axes.

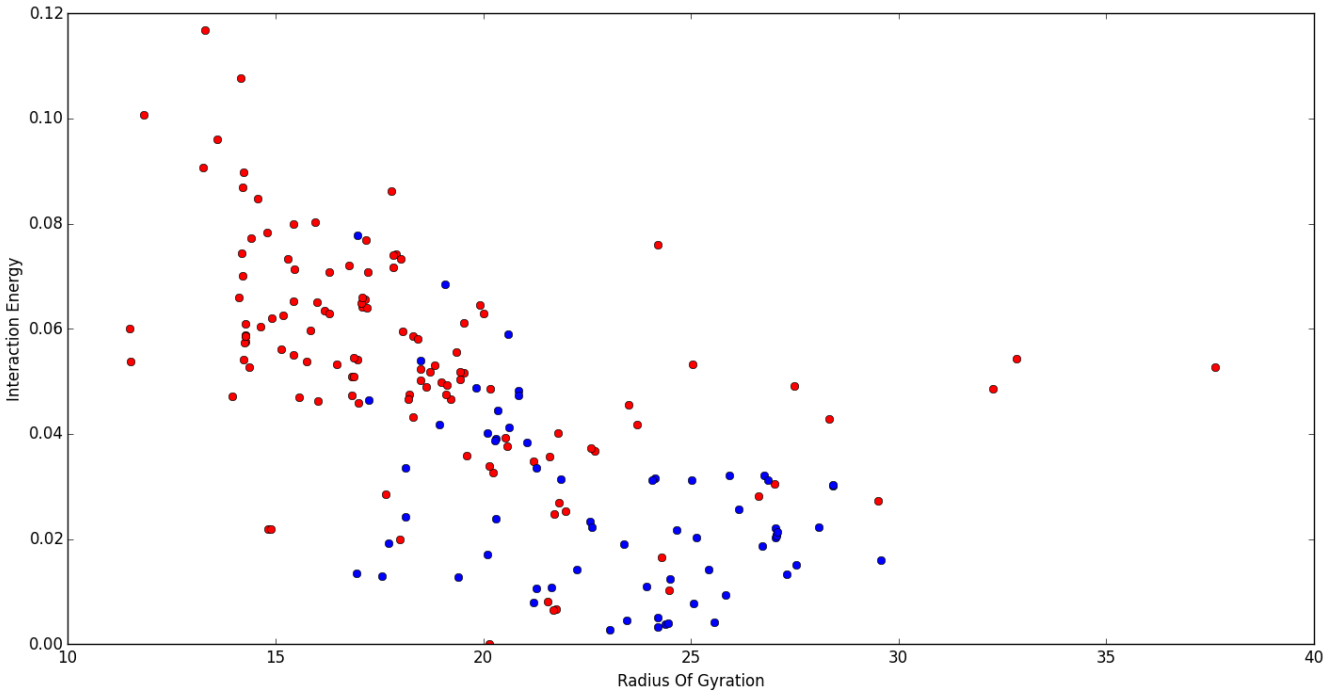
- Wrote a script to extract the Class(as per CATH) of each and every domain in my data set. I did this for both contiguous and non-contiguous proteins.

Results

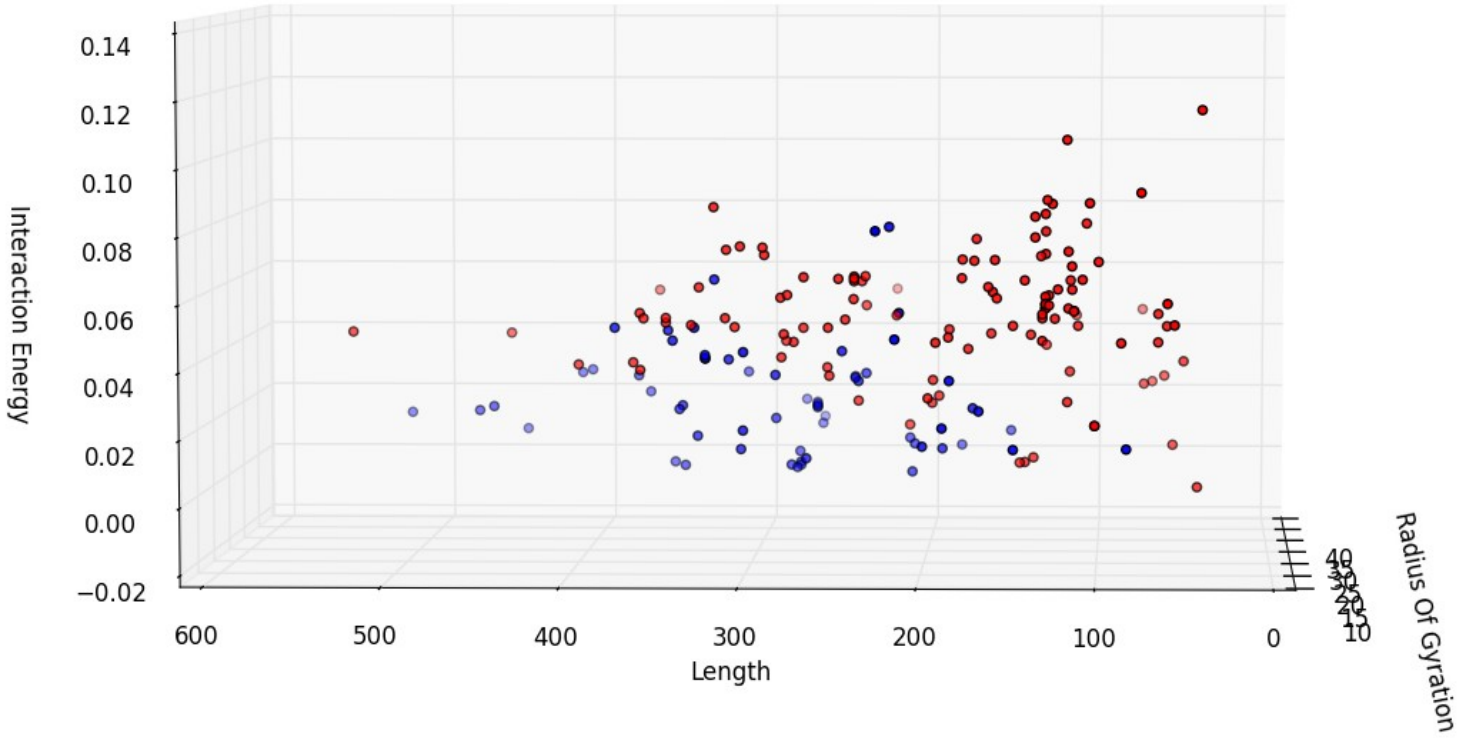
- **Interaction Energy vs Length**

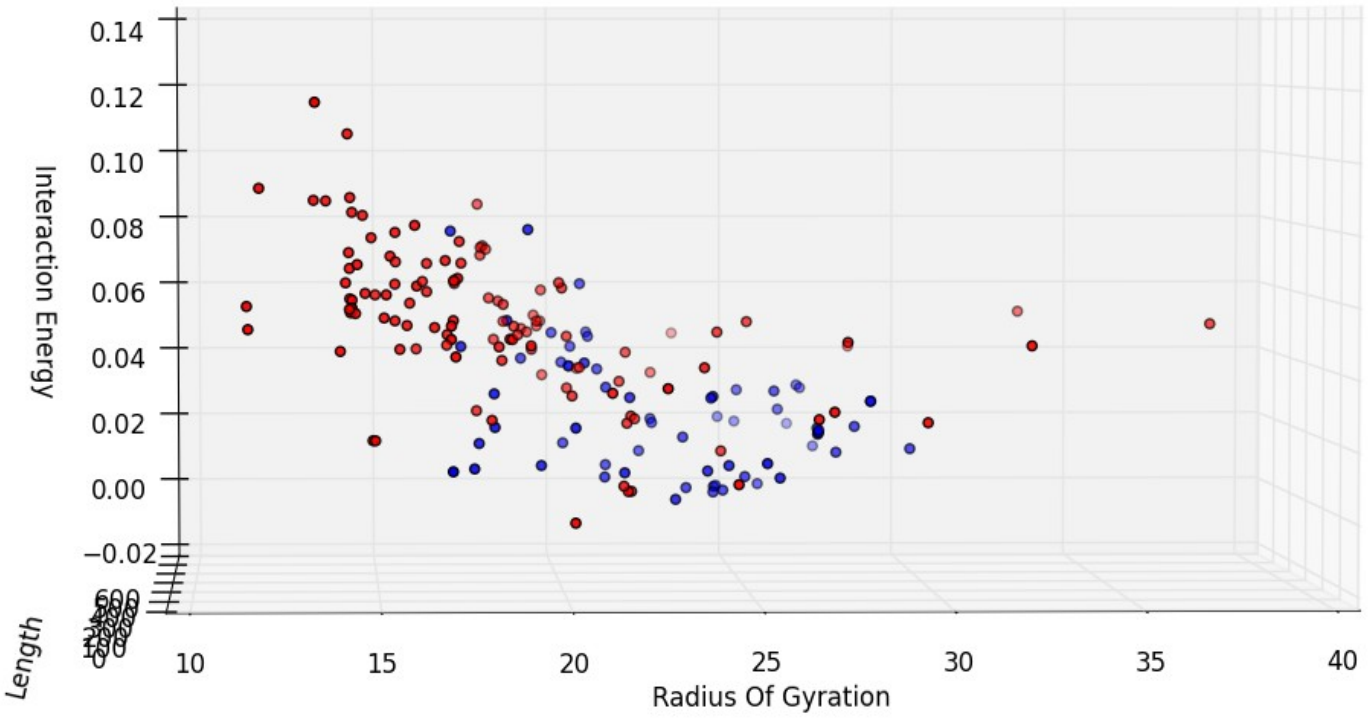


- **Interaction Energy vs Radius of Gyration**



- **Following 2 plots show the 3-D graph of Interaction energy vs Length vs Radius of Gyration**





Next Tasks

- Do a quantitative analysis of above comparison to see which which of the above attributes(length, radius of gyration or interaction energy) works best to classify single domains protein from 2 domain proteins.
- Create a data set which has contiguous and non-contiguous domains of different class and run k-means on it to see how it performs on different classes of proteins.
- Compare results of k-means with SCOP also. Also, obtain the class information of domains from SCOP.