**Dimensionality reduction and Algorithmic steps**

After the feature extraction step , we have feature vector of each ligand compound and it’s target protein. Different approaches have been tested to combine the feature vector of ligand and protein to produce a single combined feature vector **(This feature vector should represent the interaction of ligand with the protein).**

The best combination of feature vectors was found to be component wise product of compound’s feature vector and receptor feature vector producing a vector of n\*m size for each compound and target pair.

**Dimensionality Reduction techniques**

Partial least square method to reduce the dimension was found to be more better than the PCA .Since Partial least square find the components such that the variance w.r.t. predictor variables as well as the target variable is minimized.