**10.5 Weekly Report**

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**What you have done in the past week:**

1. Based on last week's session, this week I first continued my understanding of the mCSM -PPI2 [1] dataset.
   1. I reviewed the modeling approach of the original mCSM [2] project and supplemental files of mCSM-PPI2, which are both predecessors of the target project, and specifically understood the idea of "Graph-based structural signatures" construction relied on in these projects.
   2. Then I focused back to the mCSM-PPI2 paper, to understand the six features presented in “Modelling effects of mutation” section. With previous understanding of mCSM-PPI2 data, I found the graph modeling ideas of above-mentioned projects are invariant, all of them represent atoms as nodes and their interactions as edges, and use pharmacological features to illustrate the effects of physicochemical changes caused by point mutations. Regarding the six newly proposed features in mCSM-PPI2, they are different effects on single point mutations, and are used to combine with their well-established graph-based signatures for regression and classification.
2. I discussed the investigated dataset with Yan in our meeting, and we found, although this project uses a graph-based structure, its most dominant predictive model is still a traditional machine learning algorithm, where there may not much guidance on our GNN-based framework. So we still need to spend some time doing some literature review in the next weeks.
3. Yan has sent me three papers she found on related work, of which I am following one to understand how to generate the graph [3].
4. I was also preparing a short report for presentation in this week's meeting.

**What are major challenges/issues you need to discuss in the meeting:**

1. There is not much concern so far, since I’m still in progress of accumulating knowledge of relevant works.

**What you want to accomplish in the next week/weeks:**

1. Continue studying the papers Yan sent me, while I can also find one or two similar projects that may give me some inspirations.
2. Based on the ideas that have been accumulated so far and the proposal I received at the very beginning, I’m going to write a draft for the formal proposal I need to submit two weeks later.

**Reference**

[1] Rodrigues, C. H. M., Myung, Y., Pires, D. E. V., & Ascher, D. B. (2019). mCSM-PPI2: Predicting the effects of mutations on protein–protein interactions. *Nucleic Acids Research*, *47*(W1), W338–W344. <https://doi.org/10.1093/nar/gkz383>

[2] Pires, Ascher, D. B., & Blundell, T. L. (2014). mCSM: predicting the effects of mutations in proteins using graph-based signatures. Bioinformatics, 30(3), 335–342. <https://doi.org/10.1093/bioinformatics/btt691>

[3] Liu, Luo, Y., Li, P., Song, S., & Peng, J. (2021). Deep geometric representations for modeling effects of mutations on protein-protein binding affinity. *PLoS Computational Biology*, *17*(8), e1009284–. <https://doi.org/10.1371/journal.pcbi.1009284>