Research paper reviews

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Paper 1: SHIFTX2 a significantly improved protein chemical shift prediction [1]

This paper proposes a computer program, called SHIFTX2, accurately calculating diamagnetic 1H, 13C and 15N chemical shifts from protein coordinate data. Chemical shifts plays a major role in the molecular dynamics study of proteins and other biological macromolecules. This method named SHIFTX2 combines the idea of sequence-based (SHIFTY) and structure-based (SHIFTX) approaches of predicting chemical shift

Strengths:

1. This method makes use of improved sequence and shift databases and work on the local sequence alignments instead of global. It makes a substantial improvement in the model.
2. Comparision of SHIFTX2 with many state-of-the-art methods is clearly shown in this paper. SHIFTX2 utilises advance machine learning techniques and incorprates various features which substantially improves the performance. .
3. This paper has shown that SHIFTX2 is particularly useful in assessments and validation of protein structures and adjustment of chemical shift assignments.

Weakness:

1. Considering thousands of protein structures and chemical shift data available in the data banks, this model is trained only on a small subset of the data.
2. The paper does not show how similarity of datasets with each other can be calculated.

Paper 2: Selective sampling for accelerating training of deep neural networks [2]

This paper presents a novel measurement, the minimal margin score (MMS) which measures the minimal amount of displacement an input should take until its predicted classification is switched.

Strengths:

1. A new measure for accelerating the training of deep neural networks has been proposed in this paper.
2. The proposed method is also compared for efficiency against the standard training procedures, and against commonly used selective sampling alternatives as well.
3. A substantial acceleration has been demonstrated when training commonly used deep neural network architectures for popular image classification tasks.
4. A detailed insight into training of deep neural networks has also been presented in this paper.

Weakness:

1. This paper does not consider introducing an additional gain for active learning.
2. Minimal Margin Score has been considered for calculation at the last fully connected layer whereas it should have been also considered at intermediate layers.
3. This method has made comparison with a very few other datasets.
4. Improvements are marginal as compared to that of the baseline approach.
5. The design of a novel Active Learning method has not been mentioned in this paper.

References

[1] B. Han, Y. Liu, S. W. Ginzinger, and D. S. Wishart, "Shiftx2: significantly improved protein chemical shift prediction," *Journal of biomolecular NMR*, vol. 50, no. 1, pp. 43–57, 2011.

[2] B. Weinstein, S. Fine, and Y. Hel-Or, "Selective sampling for accelerating training of deep neural networks," *arXiv preprint arXiv:1911.06996*, 2019.