Sparse Modeling of Chemical Compounds

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Introduction

➢QSAR model predicts the activity/properties of the compounds based on their description.

➢Our method that will result in Neural Networks-based models in QSAR of PPAR-α ligands.

➢We introduce a new judicial selection of ensembles of trained Neural Networks to contribute to the final model.

Method

➢Too few exemplars = Difficulty in generalizing

70 Exemplars << 1000-3000 Exemplars

➢Our method is based on Regularization.

It requires smoothness.

➢Randomly setting aside compounds ➔ several sub data sets ➔ Several models (Figure 1)

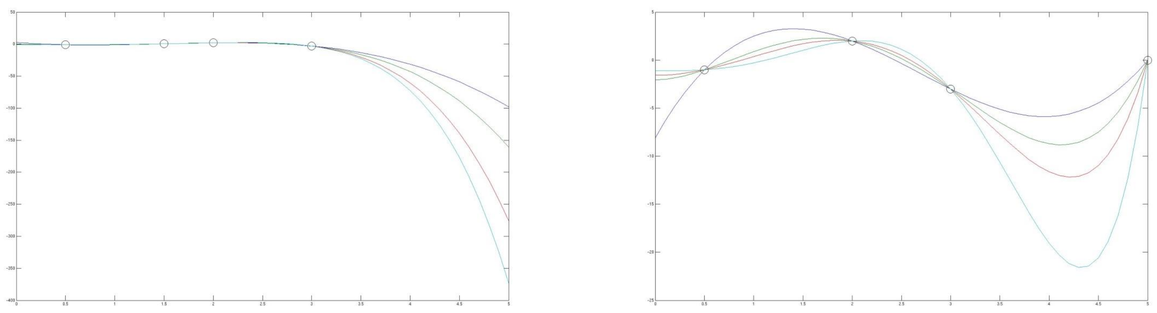

Figure 1: Different sub data sets lead to different submodels

➢Through perturbation only the NN that respond smoothly are kept.

In the last step self consistent models are chosen (Figure 2).

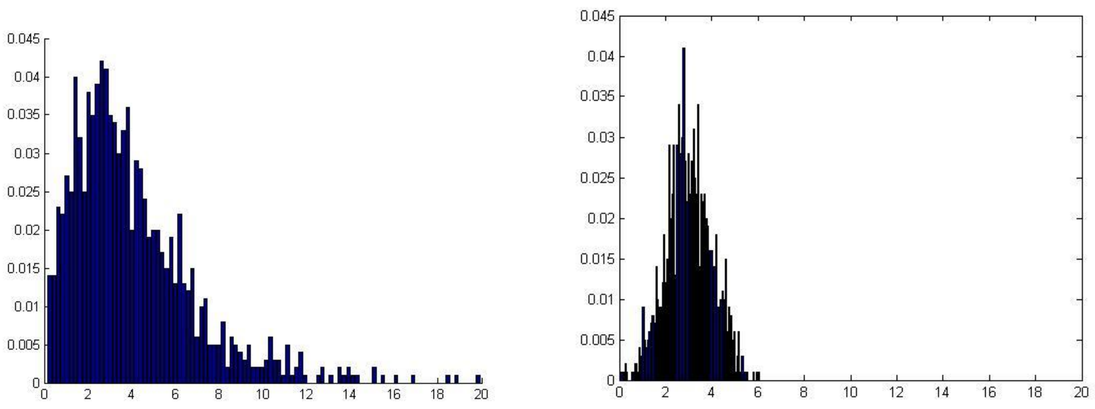

Figure 2: The result of choosing self consistent models: Before (left) and after (right)

Results and Conclusion

➢Two sets of chemical compounds [1] [2] were examined.

70 compound in data set and 23 compounds in set for alpha and for gamma.

➢The results are resented in figure 3.

➢Considering the nature of data, the results are accurate.

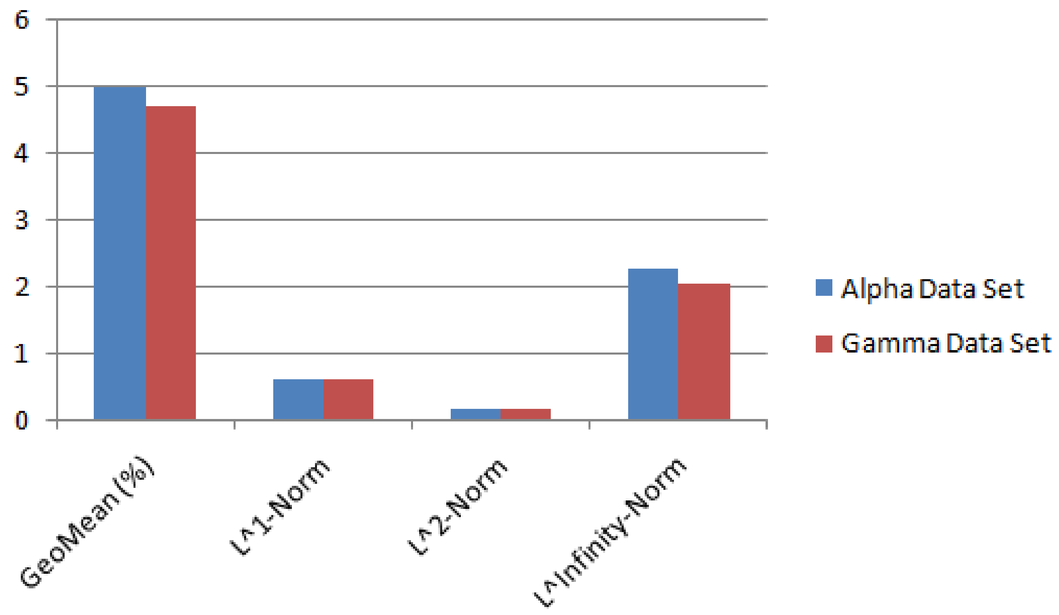

Figure 3: Prediction Results for Alpha and Gamma data sets

References

1- T.Vallianatou, B. Hedayati, N. Dimopoulos, A. Tsantili-Kakoulidou "Neural Networks-based models in QSAR of PPAR-α ligands. Comparison with linear PLS models" VIII Joint Meeting on Medicinal Chemistry, Lublin Poland, July 2013

2- T.Vallianatou, B. Hedayati, N. Dimopoulos, A. Tsantili-Kakoulidou "Comparison of the performance of Neural Network and PLS models in the prediction of PPAR-α and –γ agonism" 5th BBBB International Conference, Athens, September 2013.

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