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)

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 resent in figure 3.
- Considering the nature of data, the results are accurate.

References


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