Effect of missing data on multitask prediction performance

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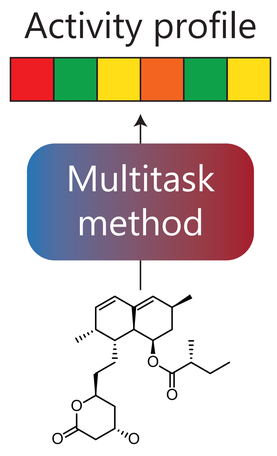
Introduction

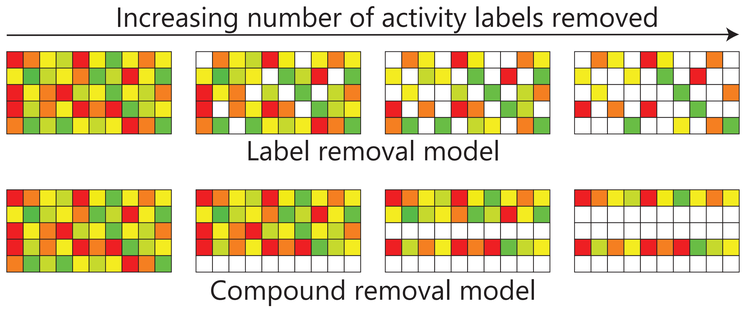
Multitask machine learning techniques are able to predict with a single model an activity profile, e.g.: a set of activity values against different kinases. They have become popular in chemoinformatics because of the rising interest in deep neural networks.[1] These techniques are frequently trained on sparse data sets, where not all compounds have been tested across all assays. The effect of the sparsity of the data on the performance of multitask prediction performance has seen little research.



Our main goal with this study was to test how performance changes as increasingly large amounts of training data are removed

Datasets

Two complete datasets were assembled: PKIS[2], a kinase profiling data set (regression task, 367 cpds, 454 assays); and HTSFP, a set of PubChem assays based on a previous publication[3] (classification task, 49 713 cpds, 5 assays). The data was randomly split into training and test data with a 3:1 ratio. Sparse training sets were generated by removing increasing numbers of activity labels from the complete training data. Two removal models were compared: removing individual labels (label removal model) or whole compounds (compound removal model).

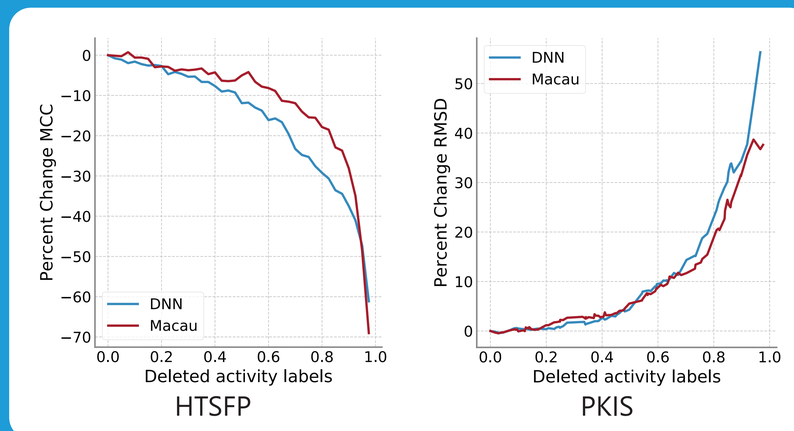


Methods

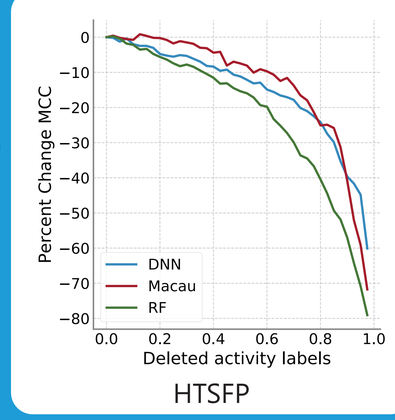
Three different multitask methods were tested: deep neural networks (DNNs), Random Forest (RF, partial comparison) and Macau[4]. Ten sets of hyperparameters were chosen for each method based on random searches of parameter space. Performance was measured as median RMSD and median MCC across all assays for regression and classification data, respectively. Performance values were scaled relative to the performance on the complete data set.

Results

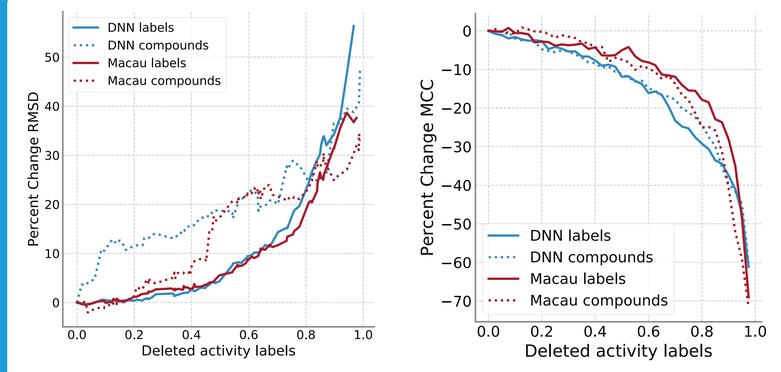
The performance progression of DNN and Macau is very similar. The decrease in performance is at first slow but accelerates after 80% of the training data is removed.



Random Forest could only be compared on data that is not sparse (compound removal model). There, it behaves similarly to the other two methods.



The performance deteriorates more rapidly for the compound removal model on the PKIS data set, while it performs similarly for HTSFP.



Conclusion

Multitask prediction methods are very promising in chemoinformatics. The removal of up to 60% of the training data decreased performance only by 10%. Macau and DNN had very similar performance progression as training data was removed. Random Forest showed similar behavior to the other methods.

Repository

All data sets, code and results are available at the following repository:
https://github.com/SheffieldChemoinformatics/missing-data-multitask-methods

References

1) LeCun et al. Nature 521, 436-444, 2015
2) https://www.ebi.ac.uk/chembldb/extra/PKIS
3) Helal et al. JCIM 56, 390-398, 2016
4) Simm et al. arXiv 1509.04610, 2015

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