QSAR biodegradation dataset classification using neural networks

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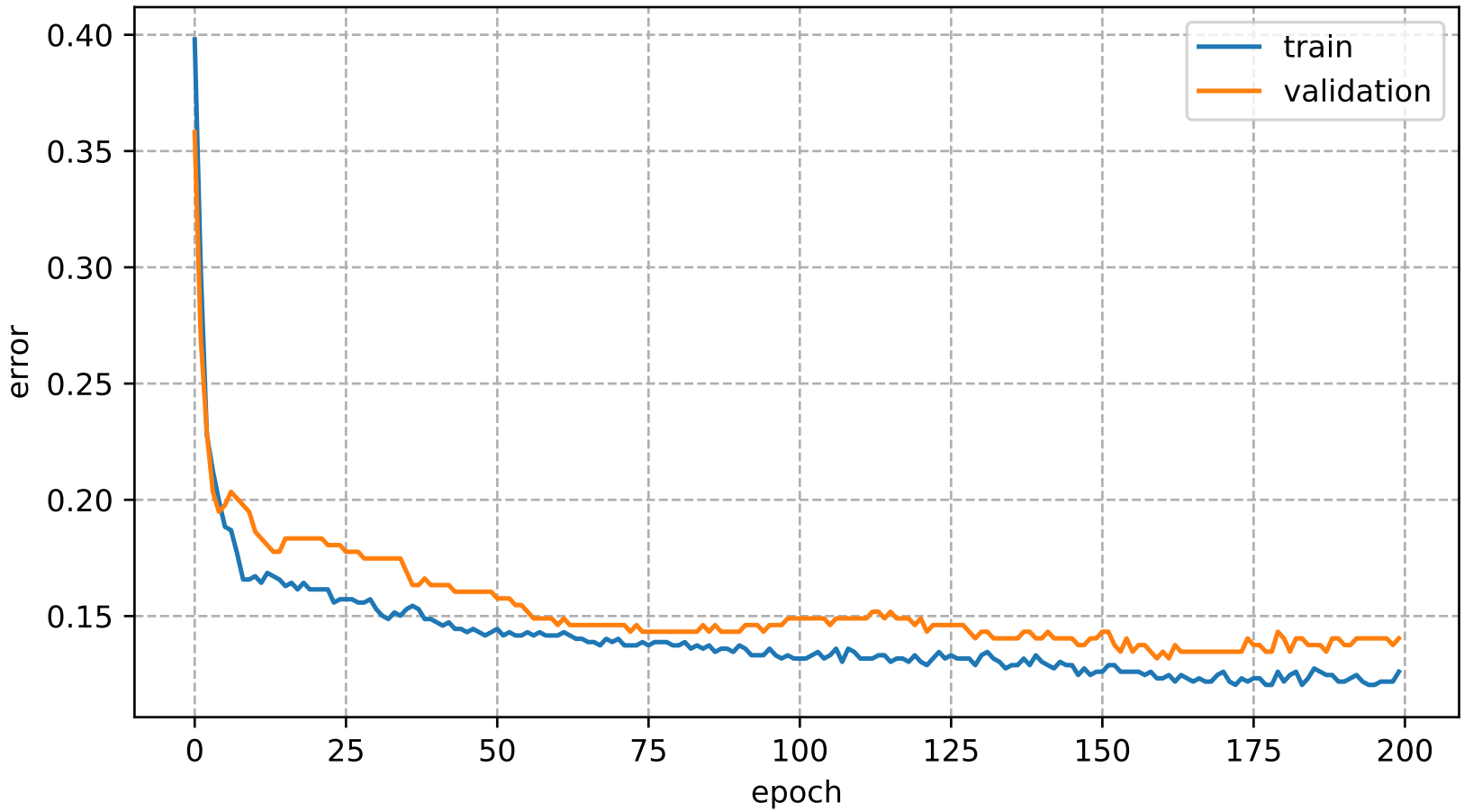
QSAR biodegradation dataset Kamel et al. (2013)

- Dataset from OpenML: qsar-biodeg
- Classification dataset where the task is to predict whether a protein is bio-degradable based on its chemical properties
- Published by Milano Chemometrics and QSAR Research Group
- 41 attributes in total, some real valued, other integer valued
- Number of proteins in the dataset is 1055
- Class 0 is bio-degradable

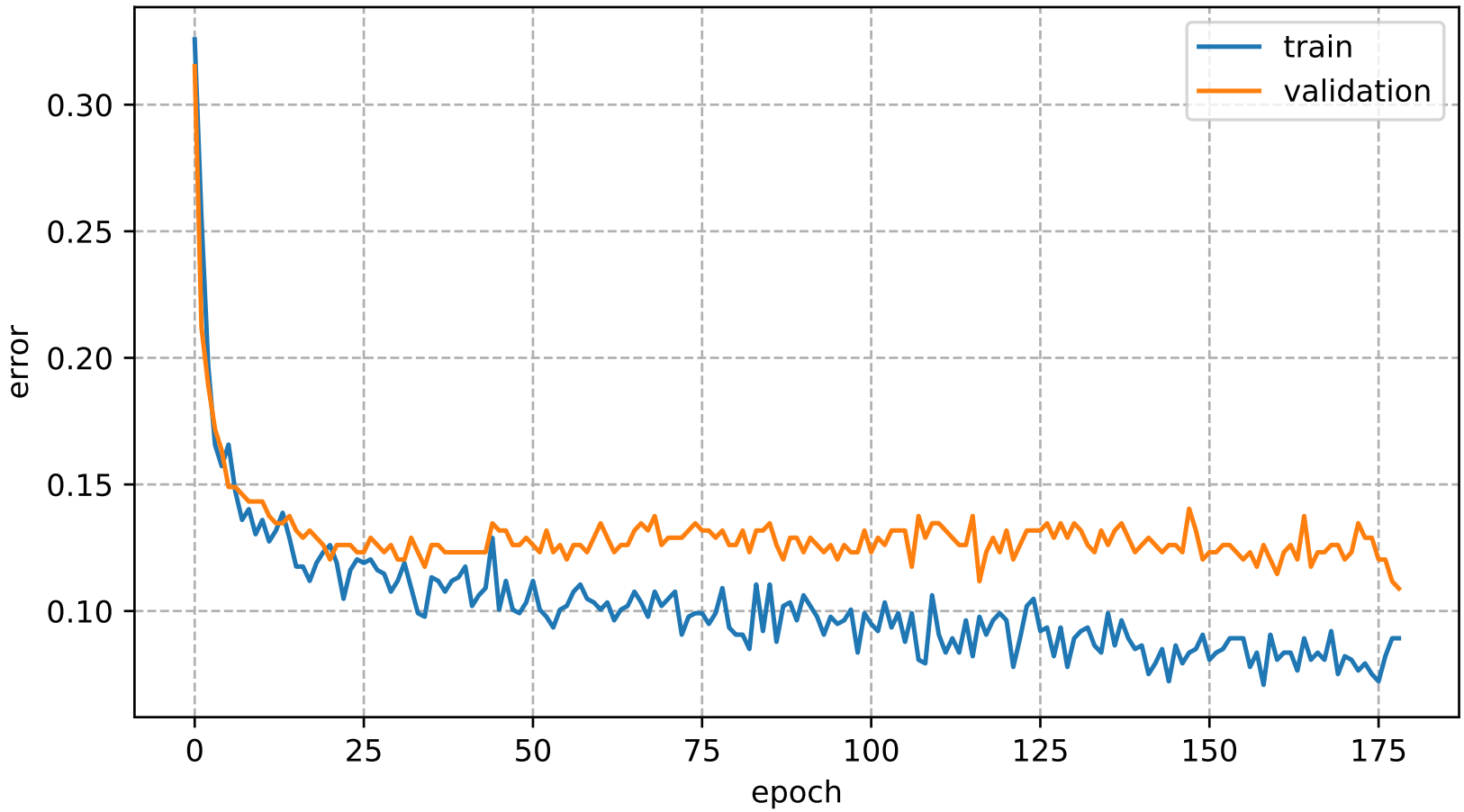
Method

- Multi Layered Perceptron (2 layers)
- 40 neurons in the hidden layer
- ReLU activation function
- trained as logistic regression with NLL loss and sigmoid activation function
- optimized using Adam Kingma and Ba (2014)
- experimented with dropout (0.5) Srivastava et al. (2014)
- weight decay (0.0045) for regularization
- trained for 120 epochs
- evaluated using cross validation (10 splits)

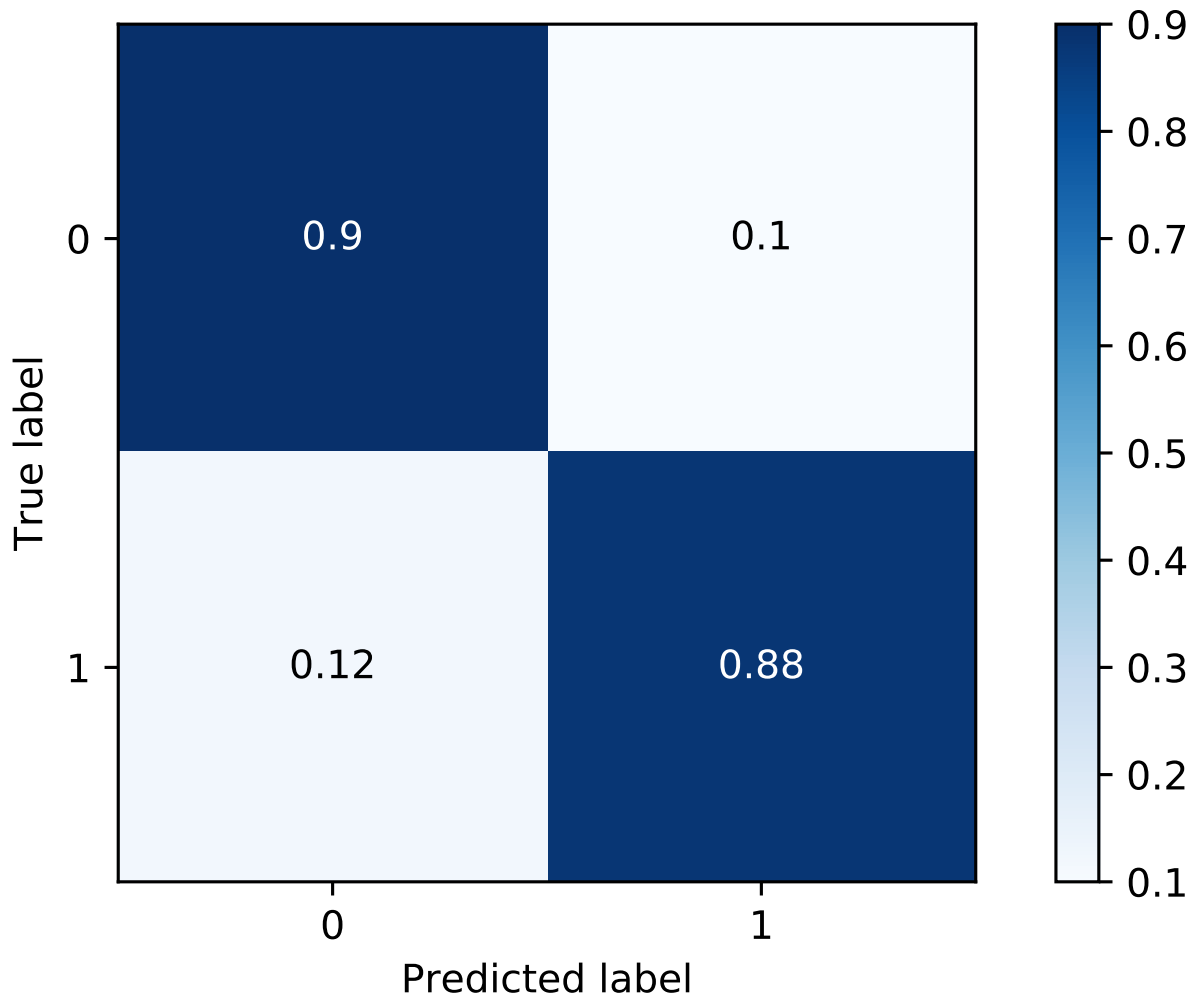
Single layer network training



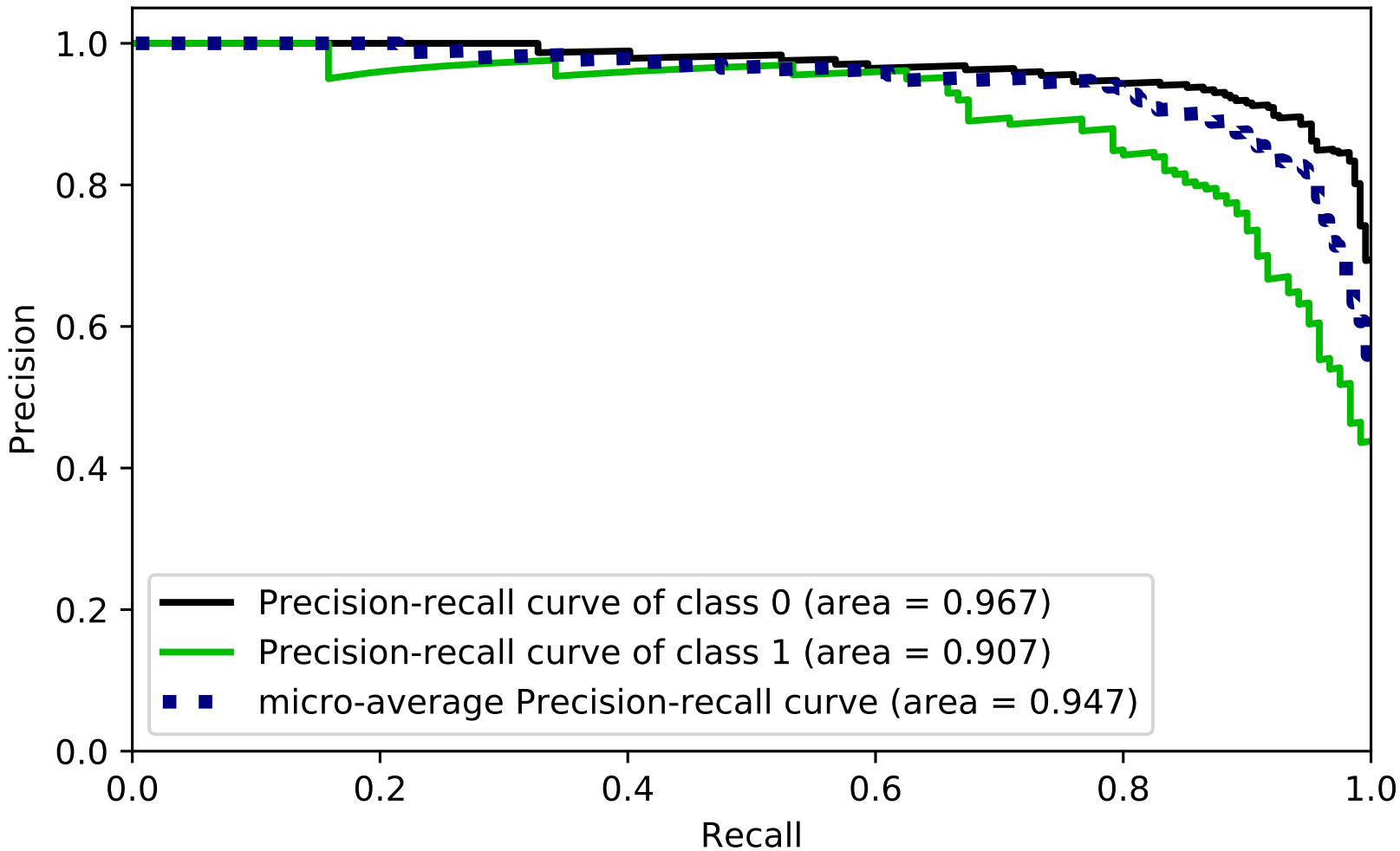
Two layers network training



Confusion matrix



Precision recall



Our results and comparisons

Method	**Predictive accuracy**
`svm.classes.SVC`	89.19%
Ours - 2 layers	**87.76%**
`xgboost`	87.68%
`weka.RandomForest`	86.67%
Ours - 1 layer	**85.12%**
`weka.VotedPerceptron`	79.43%
`weka.NaiveBayes`	75.64%
`neural_network.MLPClassifier`	66.26%

Mansouri Kamel, Tine Ringsted, Davide Ballabio, Roberto Todeschini, and Viviana Consonni. Quantitative structure-activity relationship models for ready biodegradability of chemicals. *Journal of chemical information and modeling*, 53: 867–878, 03 2013. doi: 10.1021/ci4000213.

Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization, 2014. URL http://arxiv.org/abs/1412.6980. cite arxiv:1412.6980Comment: Published as a conference paper at the 3rd International Conference for Learning Representations, San Diego, 2015.

Nitish Srivastava, Geoffrey E Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Dropout: a simple way to prevent neural networks from overfitting. *Journal of machine learning research*, 15(1):1929–1958, 2014. URL http://www.cs.toronto.edu/~rsalakhu/papers/srivastava14a.pdf.