# QSAR biodegradation dataset classification using neural networks

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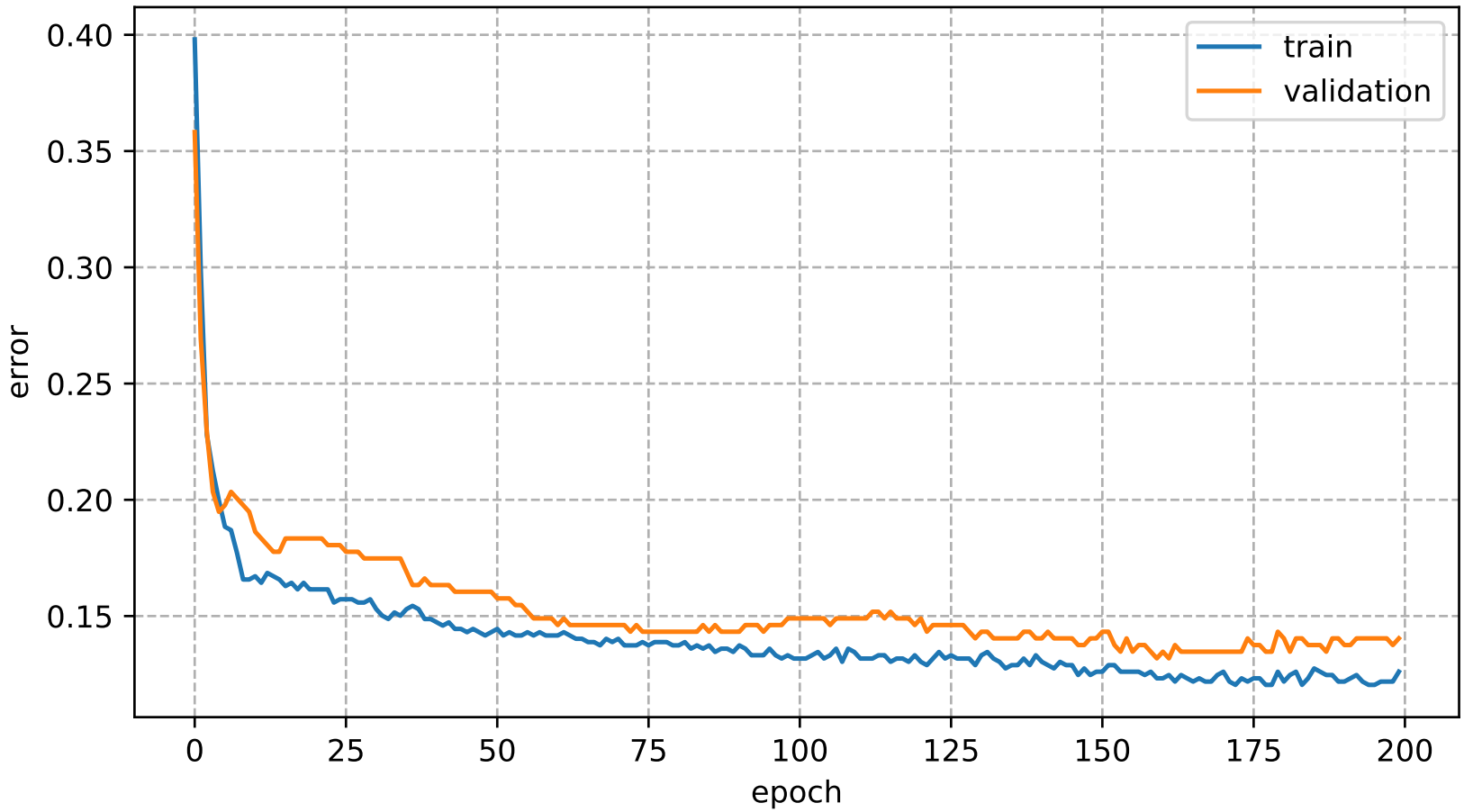
# QSAR biodegradation datasetKamel et al. (2013)

- 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

# Outline

- 3D environment simulators
- base algorithm
- our method
- experiments
- conclusions & future work

# Single layer network training



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.