

Subject Section

This is a title

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Abstract

Motivation:  
Results:  
Availability:  
Contact: name@bio.com  
Supplementary information: Supplementary data are available at *Bioinformatics* online.

1 Abstract

The accurate prediction of enzyme commission numbers (EC numbers) is not only crucial for the classification and understanding of newly discovered enzymes but also for completing the annotation of already known enzymes. Therefore, developing a reliable method for predicting EC numbers is of great importance.

However, due to insufficient data, enzyme function prediction using machine learning is an ongoing challenge. In this paper, we propose several methods for predicting enzymes in three different problem categories (Table 1). Throughout the developing of our models, we used a variety of different input features and machine learning algorithms, of which the best will be thoroughly reviewed in this paper.

2 Introduction

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3 Approach

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Table 1. Description of subproblem categories

Level	Description	Best performing method	F1 score
0	Binary classification	Random Forest	score
1	Main class classification	Feedforward neuronal network	score
2	Subclass classification	Feedforward neuronal network	score

4 Methods

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5 Discussion

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6 Conclusion

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7 Supplementary Information

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7.1 K-nearest neighbors algorithm using ncd vectors

An less popular approach of transforming string like input features into numerical values is the normalized compression distance (ncd) algorithm. The ncd algorithm is based on the idea that the similarity of two strings can be measured by the amount of information needed to describe one string given the other string. The ncd of two strings  $x$  and  $y$  is defined as follows:

$$ncd(x,y) = \frac{C(xy) - \min(C(x),C(y))}{\max(C(x),C(y))}$$
 (1)

where  $C(x)$  is the length of the compressed string  $x$  and  $C(xy)$  is the length of the concatenated string  $xy$ .

We implemented this algorithm in python and used it to transform  $n$  input sequences into  $n$ -dimensional numerical vectors by calculating the ncd of each sequence with every other sequence. These vectors were then used as input for the k-nearest neighbors algorithm. The results of this approach are shown in figure 1. The model outperformed the baseline model on the validation set with a F1 score of 0.73 TODO: Redo gzip knn and make a plot where we can see performance on validation set and test set the performance on the test dataset is significantly worse. This has two reasons. First, as TODO: find source on gzip algorithm shows, the ncd algorithm is not suited for biological sequences. Second, the test dataset is highly imbalanced, which makes it hard to beat the baseline model, since the baseline model predicts the labels based on the lable distribution of the training dataset, which was also highly imbalanced. TODO: Yet it is interesting to see that the ncd algorithm is able to achieve a comparable performance on the validation dataset, which is balanced,

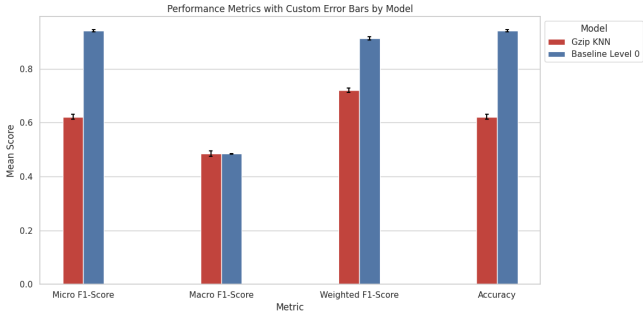


Fig. 1. Performance on test dataset compared to baseline

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