Evaluation of natural language processing embeddings in protein function prediction for bacteria

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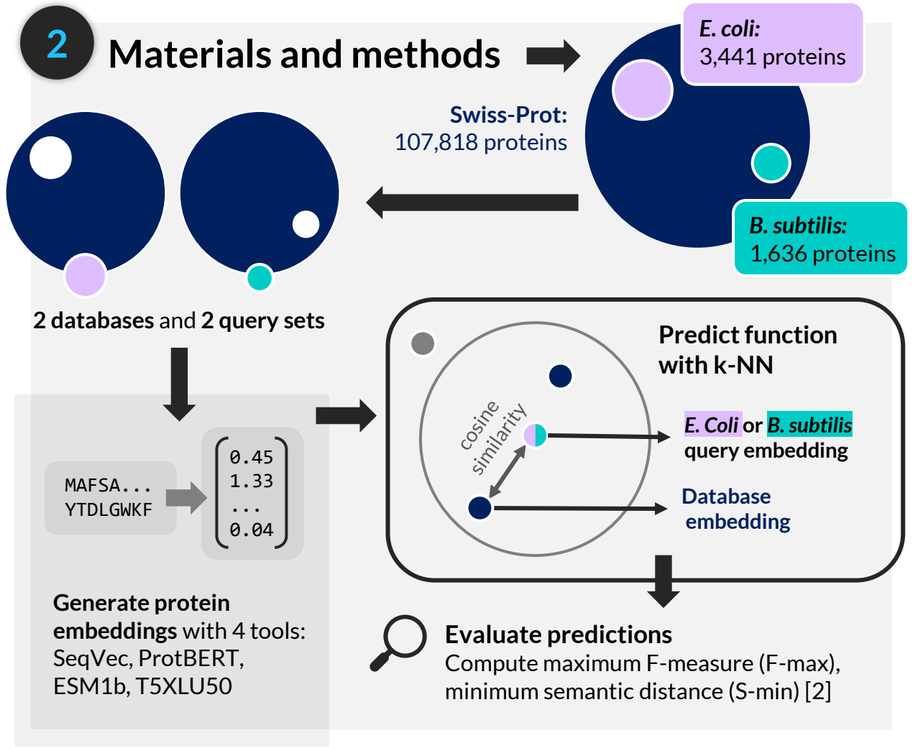
1 Introduction

- Protein function prediction is the association of a protein with its role in an organism.
- Automated function prediction is a multi-label classification task with more than 45,000 labels from the Gene Ontology (GO) hierarchy [1]. GO has 3 sub-hierarchies: molecular function, biological process, and cellular component.
- Protein sequences can be represented as real-valued vectors using ideas from natural language processing embeddings.

How do unsupervised embeddings models perform in automated protein function prediction for bacteria?

2 Materials and methods



3 Results and discussion

The k-NN predictors based on embedding similarity outperformed BLAST sequence-based annotations (see Fig. 1). The model using ESM1b embeddings performed better than goPredSim [3] in all categories, and surpassed DeepGOPlus [4] for molecular function and biological process prediction.

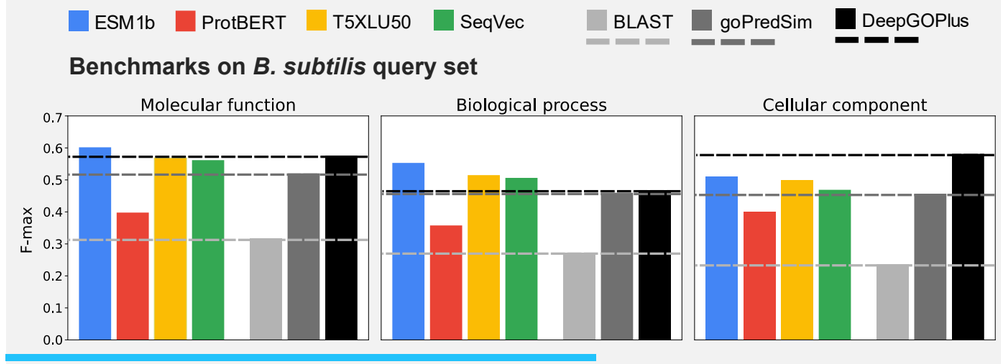


Fig. 1. The maximum F-measure (F-max) of the predictors, on the *B. subtilis* query set. Predictions from ESM1b, SeqVec, ProtBERT and T5XLU50 embeddings were made using our k-NN approach.

Previous results are reinforced by model rankings with regard to the minimum semantic distance (see Fig. 2). However, **all predictions had low recall**, which corresponds to a high rate of false negatives (see Fig. 3). This was particularly the case for *E. coli* proteins, which had more ground-truth annotations.

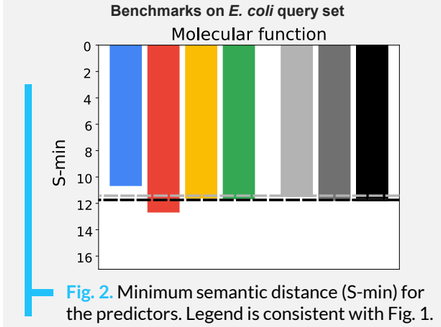


Fig. 2. Minimum semantic distance (S-min) for the predictors. Legend is consistent with Fig. 1.

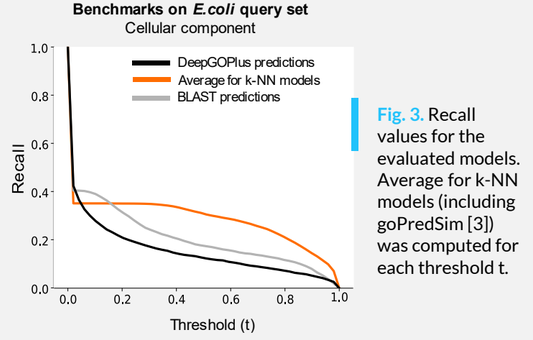


Fig. 3. Recall values for the evaluated models. Average for k-NN models (including goPredSim [3]) was computed for each threshold t.

4 Conclusion

Our k-NN models based on embedding similarity outperformed sequence-based function annotation, and their results were comparable to those from state-of-the-art predictors.

- Embeddings from deep learning can encode information about bacterial proteins beyond sequence similarity.
- The performance of all predictors was affected by high rates of false negatives.
- Complete annotation of novel bacterial protein sequences remains a prospect for future work in automated function prediction.

References

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