Title

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1 Introduction

2 Related Work

3 Methods

In this section we describe the pipeline used to analyze the embeddings. As shown in Table 1, the input length is different between the models as well as the output produced. We want to address the following problems: 1) compare different methods to join togheter the amminoacid-specific contextual representations in order to have a representation for the whole chunk; 2) compare different methods to join togheter the representations of the chunks in order to have a representation for the whole protein; 3) find out if these representations reflect known properties of the proteins.

3.1 Single amminoacid contextual representation

We tried four methods to join togheter the amminoacid embeddings in order to produce a fixed size embedding for the chunk: average, maximum, sum and principal component analysis (PCA). Note that even if these operators are commutative, the overall process do takes into account the order of the amminoacids precisely because the embeddings are contextual.

The same operator used to combine the amminoacid embeddings is also used to combine the embeddings of the chunks of the sequence.

Name	input length (chunk)	embedding dimension
embedding reproduction (rep)[5]	64	64 per chunk
dnabert [2]	512	768 per chunk
prose [1]	512	100 per amino acid
alphafold [3]	1024	384 per ammino acid
evolutionary scale modeling (esm2) [4]	1024	1280 per ammino acid

Table 1: Embedders used in the experiments, their maximum imput length and the dimension of the embedding produced.

4 Results

References

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[5] Kevin K Yang, Zachary Wu, Claire N Bedbrook, and Frances H Arnold. Learned protein embeddings for machine learning. *Bioinformatics*, 34(15):2642–2648, 2018.