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ABSTRACT

FACULTY OF PHYSICAL SCIENCES AND ENGINEERING
ELECTRONICS AND COMPUTER SCIENCE

Doctor of Philosophy

Applying Saliency Map Analysis to CNNs on Protein Secondary Structure Prediction

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The relatively new field of deep learning is slowly being transferred to the biology field and pushing its state-of-the-art achievements. However, improvements in performance come with the drawback of opaqueness, as what deep learning machines learn cannot be fully understood. Although a few authors have already started applying deep network interpretability techniques on biological problems to overcome this issue, none of them has been applied yet to the problem of protein secondary-structure prediction.

The aim of this work is to develop interpretability techniques for state-of-the-art deep networks that have been trained to solve the secondary-structure prediction problem. For doing so, a way to apply and aggregate saliency maps has been construed and applied to a near-state-of-the-art convolutional network, showing some further insights of the relationship between the inputs and the outputs. These results could be of double value: on one side, it may help biologists to get a better understanding on the underlying structural protein processes; on the other, machine learning researchers can understand better their machines and spot their flaws more easily.

Chapter 1

Results & Discussion

1.1 Network performance analysis

Refer to **??**.

1.2 Feature visualization

1.2.1 First layer filters

1.2.2 Saliency maps on layers?

1.3 Saliency maps on inputs

Talk about dimensions: saliency value, class, sequences, positions, window, amino-acids, aa/pssm (7 dimensions). From now on, individual saliency maps will refer to the saliency map of one sequence-position

Options (all options could be applied either to aa or to pssm, 6 dimensions left)

1.3.1 Saliency maps on single sample sequences

analyse per-class single sequence (sample-based) (4 dimensions left): aa-aggregated (3 dimensions) and added in the sequence position, either respecting each position (3 dimensions) or aggregating them in a heat map (2 dimensions)

1.3.2 Sheer addition

aggregate all individual saliency maps sheer addition (4 dimensions left): class-aggregated (3 dimensions), aa-aggregated (3 dimensions), or class+aa-aggregated (2 dimensions)

1.3.2.1 Per-aminoacid and class aggregations

1.3.2.2 Per-class aggregations

First thing to notice: pssm is way more relevant than one-hot encoded aas. No wonder, it learns faster.

1.3.2.3 Per-aminoacid aggregations

1.3.3 Clustering techniques

aggregate all individual saliency maps clustering (5 dimensions left) Using the per-class window-aggregated version of individual saliency maps (4 dimensions left) Cosine distance metric. Show either all profiles per-cluster (3 dimensions), or aggregated profiles (2 dimensions)

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