Quality prediction of proteins models with spherical convolutions on three-dimensional graphs.

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Convolutional neural networks have become very popular in recent years, and, in particular, have found widespread application in computer vision. Recently, active work has also begun on graph convolutional networks. In general, the graphs, unlike the pictures, are irregular structures, and in many tasks of learning on graphs sample objects also do not have unified topology. Therefore, the existing operations of convolution on the graphs are very much simplified, and the task of pulling on the graphs remain open in general. The purpose of this work is to study new operations of convolution on three-dimensional graphs within the framework of solving the problem of quality estimation of three-dimensional models of proteins (the problem of regression on the graph nodes).

Key words: *graph convolutional networks, spherical convlutions, three-dimensional graphs learning.*

1 Introduction

Let's consider a 3D model of a protein in space. The protein represents a chain of amino acids rolled up in space. Through dividing space around a protein into cells (for example, by the Voronoi method), we can get a 3D-graph, the vertexes of which are amino acids of protein and edges are carried out between those amino acids that are in adjacent cells. On these data we will solve a regression problem: to predict for each vertex v_i a real number - its "score"(how correctly it is placed in the given 3D-model in comparison with by the actual conformation of this protein).