

# Challenges in processing and knowledge discovery in specifications of scientific resources

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TNC2022

# What's wrong with doing science?

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## Improving Point Cloud Based Place Recognition with Ranking-based Loss and Large Batch Training

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Abstract—The paper presents a simple and effective learning-based method for computing a discriminative 3D point cloud descriptor for place recognition purposes. Recent state-of-the-art methods have relatively complex architectures such as multi-scale pyramid of point Transformers combined with a pyramid of feature aggregation modules. Our method uses a simple and efficient 3D convolutional feature extraction, based on a sparse residual representation, enhanced with channel attention blocks. We employ recent advances in image retrieval and propose a modified version of a loss function based on a differentiable average precision approximation. Such loss function requires dealing with very large baselines for the best results. This is enabled by using sophisticated backpropagation. Experimental evaluation on the popular benchmarks proves the effectiveness of our approach, with a consistent improvement over state of the art.

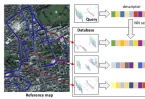


Fig. 1. Point cloud-based place recognition. The trained network computes a global descriptor of a query point cloud. Localization is performed on 3D point cloud atlases.

CVJ 2 Mar 2022

## Beyond Self-attention: External Attention using Two Linear Layers for Visual Tasks

Meng-Hao Guo, Zheng-Ning Liu, Tai-Jiang Mu, Shi-Min Hu, Senior Member, IEEE,

Abstract—Attention mechanisms, especially self-attention, have played an increasingly important role in deep feature representation for visual tasks. Self-attention updates the feature at each position by computing a weighted sum of features using pair-wise affinities across all positions to capture the long range dependency within a single sample. However, self-attention has quadratic complexity and ignores potential correlation between different samples. This paper proposes a novel attention mechanism which we call external attention, based on two external, small, learnable, shared memories, which can be implemented easily by simply using two cascaded linear layers and two normalization layers. It conveniently replaces self-attention in existing popular architectures. External attention has linear complexity and implicitly considers the correlations between all data samples. We further incorporate the multi-head mechanism into external attention to provide an all-MLP architecture, external attention MLP (EAMLP), for image classification. Extensive experiments on image classification, object detection, semantic segmentation, instance segmentation, image generation, and point cloud analysis reveal that our method provides results comparable or superior to the self-attention mechanism and some of its variants, with much lower computational and memory costs.

Index Terms—Deep Learning, Computer Vision, Attention, Transformer, Multi-Layer Perceptron.

## 4D Spatio-Temporal ConvNets: Minkowski Convolutional Neural Networks

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### Abstract

In many robotics and VR/AR applications, 3D-videos are readily-available sources of input (a continuous sequence of depth images, or LIDAR scans). However, these 3D-videos are processed frame-by-frame either through 2D convnets or 3D point cloud atlases in many cases. In this work, we



Figure 1: An example of 3D video: 3D scenes at different time steps. Best viewed on display.

proposed 4D spatio-temporal convolutional neural networks that can directly process such spatio-temporal convolutions. For this, we propose the generalized sparse convolution, which bypasses all discrete convolutional sparse convolution, and differentiation library for intensive functions for high-level networks. We create 4D neural networks using the previous 3D semantic segment-4D datasets for 3D-videos in the high-dimensional kernel, a special case of the and the trilateral-stationary forces spatio-temporal convnets space. Experimentally, our networks with only gen- per outperform 2D or 2D-3D gen. Also, we show that



Figure 2: 2D projections of hypercubes in various dimensions

more affordable and widely used for robotics applications, 3D-videos became readily-available sources of input for robotics systems or AR/VR applications.

However, there are many technical challenges in using 3D-videos for high-level perception tasks. First, 3D data requires heterogeneous representations and processing those either alienates users or makes it difficult to integrate into larger systems. Second, the performance of the 3D convolutional neural networks is worse or on-par with 2D convolutional networks. Third, there are limited number of open-source libraries for fast large-scale 3D data.

To resolve most, if not all, of the challenges in the high-dimensional perception, we adopt a sparse tensor [8, 9] for our problem and propose the generalized sparse convolu-

4D spatio-temporal convolutional neural networks are robust to noise, outperform 3D convolutional neural networks and are faster than the 3D counterpart in some cases.

# What's wrong with doing science?

## Structural bioinformatics

### Automatic recognition of ligands in electron density by machine learning

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Associate Editor: Robert Murphy  
Received on March 24, 2018; revised on June 1, 2018

#### Improving Point Cloud Based Place Recognition with Ranking-based Loss and Large Batch Training

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#### Abstract

**Motivation:** The recent identification of ligands in electron density maps is a time-consuming iterative task.



Jacek Komarowski

E. INTERVIEW

#### Beyond Self-attention: Beyond Two Linear Layers for Visual Tasks

H. Senior Member, IEEE.

#### TransLoc3D : Point Cloud based Large-scale Place Recognition using Adaptive Receptive Fields

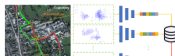
Tian-Xing Xu<sup>1</sup>, Yuan-Chen Guo<sup>1</sup>, Yu-Kun Lai<sup>2</sup> and Song-Hai Zhang<sup>1</sup>

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#### Abstract

Place recognition plays an essential role in the field of autonomous driving and robot navigation. Although a number of point cloud based methods have been proposed and achieved promising results, few of them take the size differ-



## Recognizing and validating ligands with CheckMyBlob

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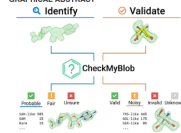
<sup>1</sup>Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, VA 22908, USA, <sup>2</sup>Institute of Computing Science, Poznan University of Technology, Poznan, 60-965, Poland, <sup>3</sup>Center for Biocrystallographic Research, Institute of Bioorganic Chemistry, Polish Academy of Sciences, Poznan, 61-704, Poland, <sup>4</sup>College of Inter-Faculty Individual Studies in Mathematics and Natural Sciences, University of Warsaw, Warsaw, 02-087, Poland and <sup>5</sup>Faculty of Chemistry, Biological and Chemical Research Center, University of Warsaw, Warsaw, 02-089, Poland

Received February 22, 2021; Revised April 04, 2021; Editorial Decision April 06, 2021; Accepted April 11, 2021

#### ABSTRACT

Structure-guided drug design depends on the correct identification of ligands in crystal structures of protein complexes. However, the interpretation of the electron density maps is challenging and often burdened with confirmation bias. Ligand identification can be aided by automatic methods such as CheckMyBlob, a machine learning algorithm that learns to generalize ligand descriptions from sets of moieties deposited in the Protein Data Bank. Here, we present the CheckMyBlob web server, a platform that can identify ligands in unmodeled fragments of electron density maps or validate ligands in existing models. The server processes PDB/mmCIF and MTZ files and returns a ranking of 10 most likely ligands for each detected electron density blob along with interactive 3D visualizations. Additionally, for each prediction/validation, a plugin script is generated that enables users to conduct a detailed analysis of the server results in Coot. The CheckMyBlob web server is available at <https://checkmyblob.bioreproducibility.org>.

#### GRAPHICAL ABSTRACT



#### INTRODUCTION

Many macromolecular crystal structures contain ligand molecules that can reveal the function of the protein or nucleic acid. Ligands are usually manually modeled by crystallographers, which requires good judgment and expertise

1D: Line 2D: Square 3D: Cube 4D: Torus  
Figure 2: 2D projections of hypercubes in various dimensions.

more affordable and widely used for robotics applications, 3D-videos became readily-available sources of input for robotics systems or AR/VR applications.

However, there are many technical challenges in using 3D-videos for high-level perception tasks. First, 3D data requires heterogeneous representations and processing these often alternates users or makes it difficult to integrate into larger systems. Second, the performance of the 3D convolutional neural networks is worse or on-par with 2D convolutional neural networks. Third, there are limited number of open-source libraries for fast large-scale 3D data.

To resolve most, if not all, of the challenges in the high-dimensional perception, we adopt a sparse tensor [1] for our problem and propose the generalized sparse convolu-

Preprints.

1) Important role in these feature representations for tasks of feature using per-pixel affinities across all and high-level task-agnostic representations for high-level networks. 2) We create 4D-representations for 3D-videos in the high-dimensional space, a special case of the 4D-representations gives spatio-temporal context. 3) We create 4D-representations for 3D-videos in the high-dimensional space, a special case of the 4D-representations gives spatio-temporal context. 4) We create 4D-representations for 3D-videos in the high-dimensional space, a special case of the 4D-representations gives spatio-temporal context.

# Why is EOSC so cool?

## European Open Science Cloud

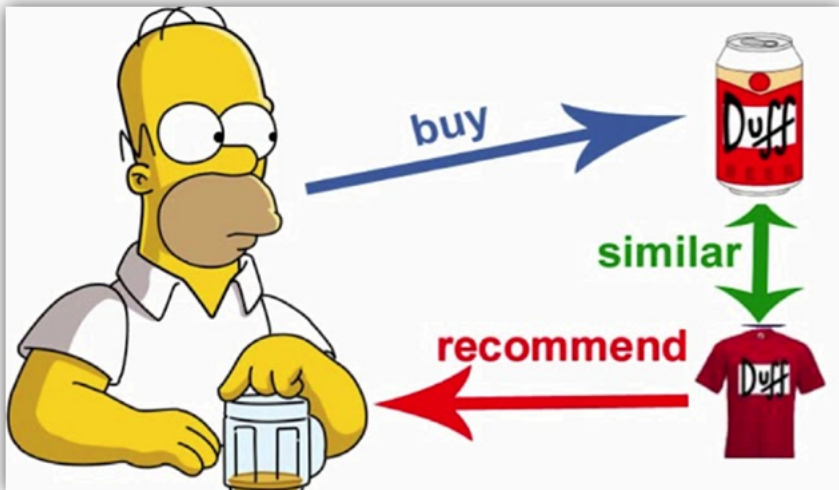
One system to rule them all, one system to find them, One system to bring them all, and in the references bind them; In the Land of Citations where the shadows lie.

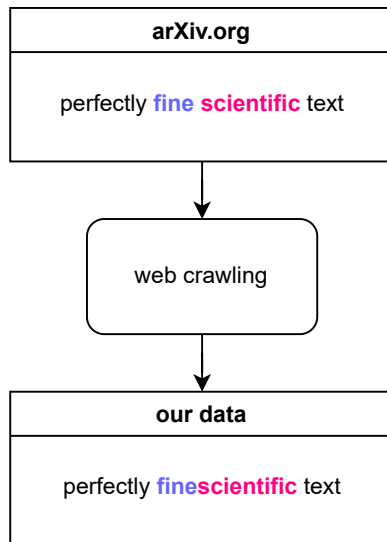


**EUROPEAN OPEN  
SCIENCE CLOUD**

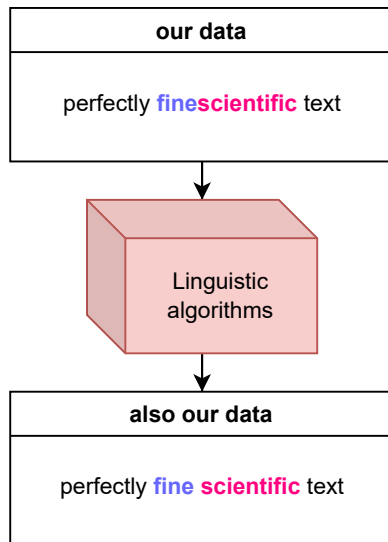
<https://eosc-portal.eu/>

# EOSC Recommender System



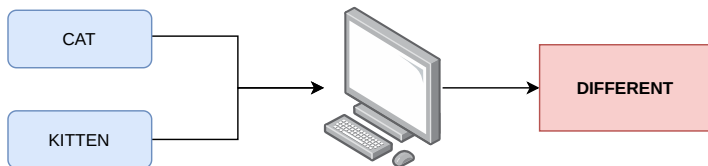


# Linguistic knowledge

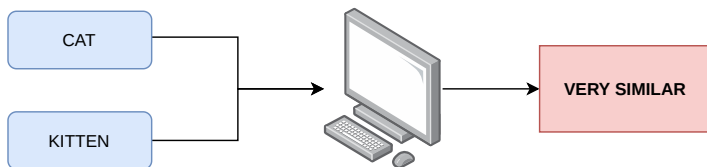




## How it looks:



## How it should look:



# Contribute to open science!

