Comvi - Comparative Visualization of Molecular Surfaces using Similarity-based Clustering

Wilhelm Buchmüller, Shoma Kaiser, Damir Ravilija, Enis ...

Abstract— The goal of this paper is to show the reader the abstract methods and concrete applications that were used to extract and compare features and rank the similarity of the molecular protein maps. Further we present a new method of how the won data can be visualized on high resolution and large displays with a The paper describes the process and the approaches that were taken to solve this task.

Index Terms—Clustering, Similarity, feature extraction, Visualization, high-resolution display, Powerwall,MegaMol, VISUS

1 Introduction

Over the span of 6 months we, the authors of this paper, have researched and implemented a comparative clustering of molecular maps. The task consisted of several challenges Over the cours of the next few pages you will learn how we tackled these challenges and how we solved them.

2 Related Work

TODO: cite kolesar for clustering

2.1 Initial Challenges and encountered problems

It is clear that the task required from us that we learn how to compare the images, measure the distances between the images, and cluster these images. The given task required that

We could chose to find similarities and cluster the proteins in the `.pdb` format or given as bitmap image generated by **TODO:** cite megamol protein image

2.2 Approaches to the Clustering-Problem

Right of the start we had several ideas of how we could approach this problem. With the recent trend in machine learning we had a couple of ideas of how we could determine a similarity metric between two images or classify an image into a more usable vector of data.

We ended up using a higher dimensional feature vector ... to determine the similarirty between two protein maps because we didnt manage to train a custom model in the given timeframe, due to .

But our initial results with a pretrained Imagenet **TODO:** cite imagenet **TODO:** cite darknet publication model let us to believe that it shoud be definetly possible for this specified task to find a machine learning solution.

2.3 Approaches to the Visualization-Task

Our aproaches to visualizing the given clusters were the following, the reader is reminded that we are not just visualizing the clusters on a ”normal machine” but rather the POWERWALL, a projected display with effectively 6-24 times the resolution of a consumer grade display. Details on the POWERWALL can be found **TODO:** cite powerwall publicatoin here if available.

Wilhelm Buchmller
buch.willi@googlemail.com
Enis .. .
example@example.com

Shoma Kaiser
example@example.com
Damir Rwilja
example@example.com

Manuscript received 31 March 2011; accepted 1 August 2011; posted online 23 October 2011; mailed on 14 October 2011.
For information on obtaining reprints of this article, please send email to: tvcg@computer.org.

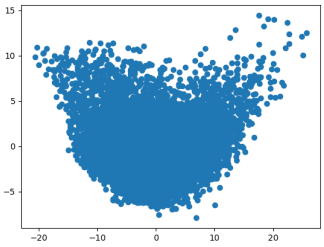

Figure 1: Early test with the Oxford flower dataset **TODO:** cite oxford flower dataset

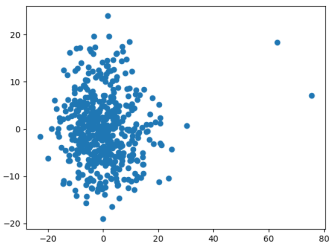

Figure 2: Early test with the bmw car dataset **TODO:** cite stanford car dataset

2.3.1 Approaches to the Interaction with the Powerwall **TODO:** cite correct pub and use correct name

2.4 Finding a feature vector to cluster the images

2.5 Finding the best performing similarity measure

2.6 Finding the best performing clustering algorithm

2.7 Testing the feature vector with other datasets

2.8 Finding the

2.9 Discussion of results

2.9.1 Dolor

Acknowledgments

We would like to thank our supervisors Michael Krone and Florian Fries as well as our project examiner Prof. Ertl . We are grateful for

Table 1: lorem ipsum tabulated

dataset	full performance (fps)	half performance (ms)
balls	1,243	0.1
buckets	23	23
bolts	23,312,134.3	22.1

the experience and knowledge that working on this project has given us. This work was partially funded by cake and cookies.