Equivariant Convolution Neural Networks

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Abstract

Convolutional Neural Networks are known to work the best for spatially dependent data such as images. While they are translationally invariant they aren't rotationally invariant. What it means is that if we were to build an object classifier and pass the model the images of all upright trees during training but test on a fallen tree it will not be able to predict it with high accuracy. In the case of trees, we knew the correct orientation. But in the case of gravitational lensing, we cannot for certain provide a fixed orientation. Thus, the need for rotationally equivariant convolutional neural networks arises.

As a part of this project, I would like to propose two possible projects.

1. Transfer Learning Model - build a transfer learning model that is $P_4 / P_4 m$ equivariant from the paper Group Equivariant Convolutional Networks.
2. Implement an SE3 and SO3 equivariant model from the paper Spherical CNN.

Motivation

Why do you want to participate in GSoC?

I always have been mesmerized by technology and its application in computing. The amount of data that can be processed and interpreted is humungous. The power we possess in processing images, text, and curating videos can be done using our phones. This inspired me to work in the growing field of deep learning.

I am currently enrolled in a research program in computer science where I primarily work on machine learning and deep learning methods. I have several projects in the relevant field and won a couple of hackathons using AI. I want to dive deeper into this field and get my hands dirty with more complex tasks. I feel that GSoC provides me the opportunity to bridge the gap, get acquainted with working on more real-world projects and pick up crucial skills.

Why this year?

The GSoC program is during my third-year summer break. I feel I have built a good foundation in the past three years where I have explored a lot in machine learning and have had a few coded projects on it. My research is also in AI, and having a real-life task would give me enough experience to complete my honors project. I would also have a lot of free time during the summer break to dedicate to this project.

Why ML4SCI?

I am pursuing a dual degree at the International Institute of Information Technology, Hyderabad. I will be receiving a degree of bachelor's and masters in computer science. My research involves the application of deep learning in drug design and discovery. I have worked on using graph neural networks for classifying binding poses of protein-ligand complexes. We achieved results close to the state-of-the-art methods. We wanted to explore the are of SO(3) equivariant networks for point clouds to improve our results but was out of the scope of the project.

I want to apply to ML4SCI since it stands for my interests. I want to work on solving scientific problems using computational techniques. Machine Learning models learn features at a rate that standard algorithms take days to determine, providing us really good accuracies while taking a fraction of the time. My future plans also include pursuing research in computational methods in science and feel that this will be a stepping stone in the right direction.

Why the Equivariant Convolutional Network Project?

During the course of my binding-pose prediction project, we faced a bottleneck. In order to include angular information of point clouds, we required the model to be SO(3) equivariant. The problem otherwise is that it learns information from that particular data point but not the overall chemistry associated with it. I know firsthand the importance and advantages of equivariance in neural networks and their advantages. I would like an opportunity to work on equivariance.

Some of the groups involved in equivariance in convolutional neural networks are P_4, P_4m, P_6, P_6m, C_8, etc. I have tried out and witnessed the improvement that equivariance has over conventional methods such as data augmentation. I would like to work on this project in specific and haven't applied to any others since I am passionate about the topic, know its importance, and would like to pursue research in it.

Project Details

I would like to propose two possible projects, implementing a transfer learning-based equivariant CNN model or implementing SE(3) and SO(3) equivariant CNNs.

The transfer learning-based model will be P_4 / P_4m equivariant and will be pre-trained on several physics-related images or any other type of data provided. It can be fine-tuned on any data provided. Conventional methods of training involve a few layers being trained and freezing their weights while some layers are not trained at all. Fine-tuning on the data involves training the un-trained layers while utilizing the information learned from the frozen layers on all the data the model has seen.

The other possible project is to implement a CNN that is SE(3) and SO(3) equivariant from the paper - Spherical CNN.

Project Proposal 1: Transfer Learning using Equivariant CNNs

Project Proposal 2: Implement SE(3) and SO(3) equivariant CNNs.

Commitments During GSoC

I am completely available during the summer and would dedicate 40 hours a week to GSoC. I do not have any prior commitments and if something were to come up I will not make any decisions without discussing it with my mentors.

About Me

I am a third-year undergraduate student pursuing a dual degree at the International Institute of Information Technology, Hyderabad. I am pursuing a bachelor's in computer science and master's in computational natural sciences. My hobbies include playing the piano, composing and producing music, photography, videography, trekking, cycling, and playing football.

Some relevant projects I have undertaken are:

1. Binding-Pose Prediction: I used multiple graph-based up roaches such as graph convolutions, graph attention, message passing networks, and graph-based multi-task learning on classifying binding poses.
2. Amai Masuku - a system built using YOLOV4 and OpenCV that detects whether a person is wearing a mask, tracks them throughout the video and provides real-time statistics.
3. Minerva - A discord bot that identifies depressive behavior and actively intervenes by engaging with the user in a voice conversation, driven by a Deep Neural Network performing sentimental analysis on the messages with an accuracy of 85%.

Link to my CV.

Tasks Completed

Link to the GitHub repository.

1. Multiclass classification of gravitational lensing images - Applied a transfer learning model - Resnet18 and achieved a test AUC score of 0.984 on a 75-25 split between train and test and a validation AUC of 0.958. The train time of the model is around twenty-thirty minutes on a 2080ti GPU.

Challenges faced and overcome - the dataset was really large and did not fit into the RAM. Had to write a custom data loader and optimize it for speed of computation.

2. Equivariant CNN - Implemented a P_4 equivariant CNN from ‘Group Equivariant Convolutional Networks' - T. Cohen and M. Welling that performs binary classification of gravitational lensing images. Achieved a test AUC score of 1.0 on an 80-20 split between train and test. Also, achieve an AUC of 1.0 on rotated images belonging to the test set.

   Challenges faced and overcome - the model wasn’t learning anything in my initial attempts at using equivariant CNNs. Tackled it by implementing a flexible P_4 equivariant CNN and preprocessing the image appropriately.