GSoC 2023 Project Proposal
Organization: ML4SCI

Transformers for Dark Matter Morphology with Strong Gravitational Lensing

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Contents

1 Student Information and Introduction

1.1 Student Information

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- More information: Curriculum Vitae
- Time Zone: IST(GMT + 5:30)

1.2 Introduction

I am a junior studying Chemical science and technology at the Indian Institute of Technology Guwahati, and I constantly seek to expand my knowledge and understanding of Machine Learning. While my interest in this field is broad, I am working to focus on a specific area within it. I am fortunate to have experience working as a research intern at multiple prestigious universities, giving me valuable insights and practical skills to apply to my current projects. Currently, I am focusing on federated learning, bayesian deep learning, and MCMC, and I am excited to see where these avenues of research will take me. I am part of the Transitional Artificial Intelligence Research Group, UNSW, and DMLSys (Distributed Machine Learning Systems) Lab, UMN. My research interests are Deep Learning, Large Deep Learning Models, Federated Learning, and Computer Optimization.

2 Description

Strong gravitational lensing is a promising probe of the substructure of dark matter to better understand its underlying nature. Deep learning methods have the potential to accurately identify images containing substructure and differentiate WIMP particle dark matter from other well-motivated models, including vortex substructure of dark matter condensates and superfluids.

This project will focus on the further development of the DeepLense pipeline that combines state-of-the-art of deep learning models with strong lensing simulations based on lenstronomy. The focus of this project is using transformers (e.g., vision transformers) to augment the performance of DeepLense algorithms (e.g., classification and regression).

3 Technical Details

3.1 Transformers

Transformers use a self-attention mechanism to directly compute a set of weighted features from the input image. This allows transformers to capture long-range dependencies between pixels and reduce the number of parameters required for the model, resulting in improved efficiency and accuracy. Recent studies have shown that transformer-based models, such as the Vision Transformer (ViT), can outperform traditional CNNs on various benchmark datasets, making them a promising approach for image classification tasks.

3.2 Lenstronomy

Lenstronomy is a Python library for modeling and simulating gravitational lenses. Gravitational lensing is a phenomenon in which the light from a distant object is bent and distorted by the gravitational field of an intervening massive object, such as a galaxy or a cluster of galaxies.

The Lenstronomy library provides a set of tools and models for simulating and analyzing gravitational lenses, including tools for modeling the mass distribution of the lensing object, fitting observed lensing data, and simulating lensed images. The library is designed to be modular and customizable, allowing users to easily construct complex lensing models and compare them to observational data. Lenstronomy has been used in a variety of applications, including studying the dark matter distribution in galaxy clusters, probing the expansion history of the universe, and testing alternative theories of gravity.

3.3 Evaluation Test and Results

3.3.1 Common Test

The dataset comprises three classes: strong lensing images with no substructure, subhalo substructure, and vortex substructure. To tackle this task, a custom model was developed, which drew inspiration from the Densenet and Convolutional Block Attention Module approaches.

Initially, Cross Entropy Loss was used as the loss function, but it was observed to cause overfitting. To address this, Label Smoothing Binary Cross-Entropy (BCE) was employed, which reduces the number of overconfident predictions that are extremely close to 1 or 0. This type of loss function acts as a regularizer.

The model was trained for three epochs using Cross Entropy Loss to build confidence before switching to Label Smoothing BCE. After experiments, it was determined that this approach yielded the best-performing model.

The achieved ROC AUC accuracy for the no substructure class was 0.96911, while for the spherical and vortex substructure classes, it was 0.93808 and 0.94485, respectively. The micro-average accuracy was 0.95389, and the macro-average accuracy was 0.95093.[Link]

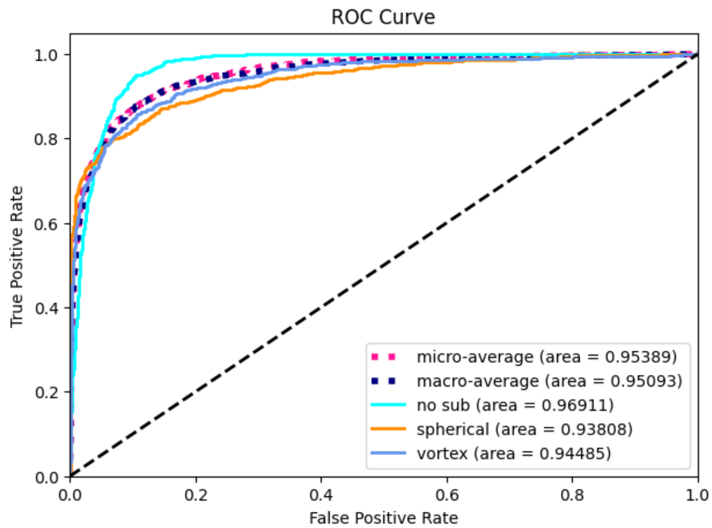

Figure 1: ROC curve for multi-class classification of test 1.

3.3.2 Exploring Transformers (Specific Test 5)

Transformer	Accuracy score	ROC-AUC score	Run time
Vision Transformer(paper)	0.994	0.9933	14.764
BEiT(paper)	0.611	0.8752	13.479
DeiT(paper)	0.985	0.9849	13.763
Swim Transformer V2(paper)	0.927	0.9276	9.6318
Efficientformer(paper)	0.927	0.9275	4.9952

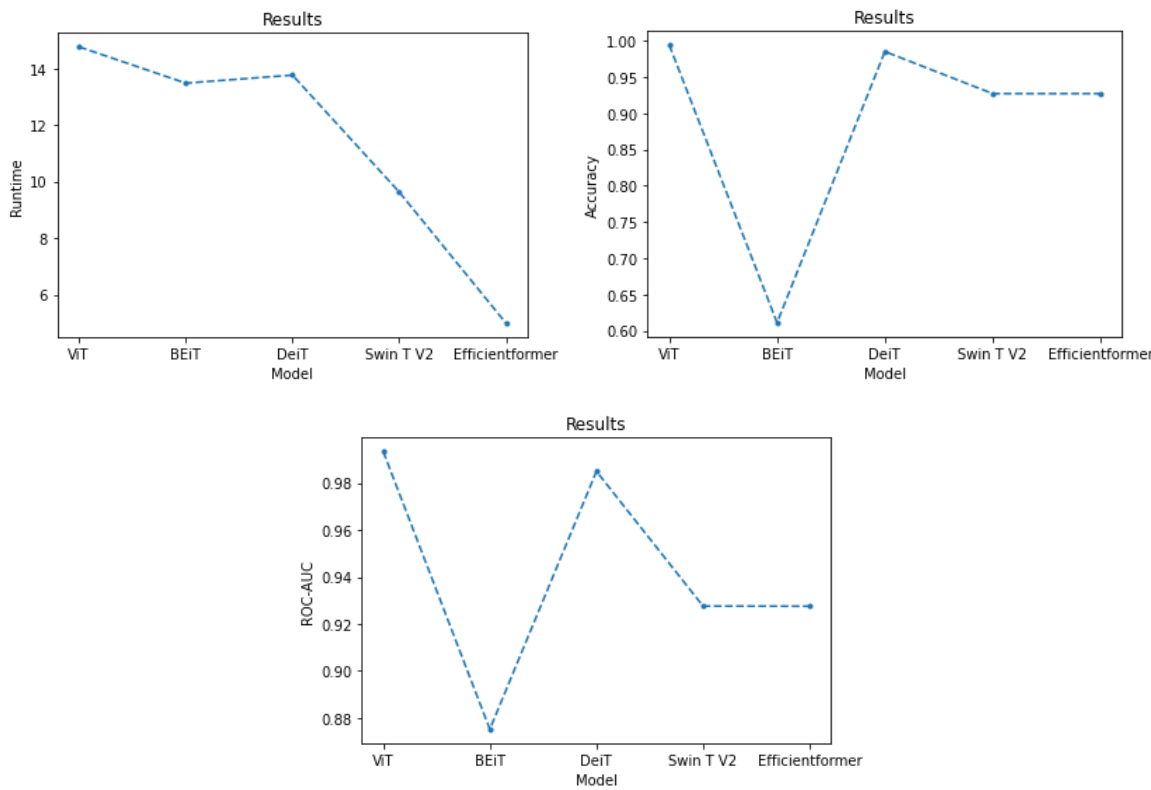

Figure 2: Analysis of results from image classification.

From the results, we can infer the following:

1. Transformer models can be applied to binary image classification tasks with high accuracy scores.
2. The best-performing model in terms of accuracy and ROC-AUC score is the Vision Transformer, with an accuracy score of 0.994 and a ROC-AUC score of 0.9933.
3. The BEiT model, which performed poorly in terms of accuracy with a score of 0.611, still managed to achieve a relatively high ROC-AUC score of 0.8752, suggesting that it is good at distinguishing between positive and negative classes.

4. The DeiT model performed well in terms of accuracy, achieving a score of 0.985 and a relatively high ROC-AUC score of 0.9849.
5. The Swim Transformer V2 and Efficientformer models achieved the same accuracy score of 0.927, with ROC-AUC scores of 0.9276 and 0.9275, respectively.
6. The Efficientformer model achieved the lowest run time, indicating that it is a faster model than the others in the set.

Overall, the results suggest that transformer models can be effective in binary image classification tasks, with the Vision Transformer being the best-performing model in this study. The results also indicate that the BEiT and DeiT models can be good alternatives for achieving high ROC-AUC scores, while the Efficientformer is a good option for those looking for faster model run times.[Link]

4 Proposed Deliverables

1. Implement multiple transformers for binary/multiclass classification.

2. Implementing NAS(neural architecture search) for the transformer models used.

3. Implement regression-based transformer models for the lens datasets. For this, metrics like mse and rmse can be used.

4.1 Schedule of Deliverables

1. **Community Bonding Period: May 4, 2023 - May 28, 2023**
   During the community bonding period, I will look into the relevant literature useful for the project and brush up on transformer and deep learning-based concepts. In the past, I have leveraged state-of-the-art deep learning models, such as ViT, BEiT, DeiT, etc, to solve various tasks. These models have demonstrated superior performance compared to other existing models and have significantly advanced the field of machine learning. I will also try as much as possible to get to know the ML4SCI developer community, interact with them, and head start a great journey.

2. **Week 1 and 2**
   Work on developing a classification model to accurately identify whether images contain lenses or not. In the evaluation task, we achieved a roc-auc score of 0.9933 while using the ViT model. Further, this will be extended to PVT (Pyramid Vision Transformer), TNT (Transformer in Transformer), Focal Transformer, CaiT (Constrained Attention Transformers), CoaT (Co-Scale Conv-Attentional Image Transformers), and Bottleneck Transformer. These will be explored using metrics like AUC, ROC, and confusion matrices.

3. **Week 3**
   Work on enhancing transformer models for image classification through the implementation of neural architecture search (NAS) techniques. By utilizing NAS, it may be possible to automatically search for and identify optimal architecture configurations and hyperparameters for transformer models in a data-driven manner. By integrating NAS into the development process, it may be possible to produce transformer models that are tailored to the specific needs of a given dataset while also minimizing the need for manual design and tuning.

4. **Week 4 and 5**
   Work on transformer-based regression models can be developed and trained on the simulated images to predict the mass density of the vortex substructure. These models can be designed to effectively capture the complex relationships between input features and output targets through the use of self-attention mechanisms. To evaluate the performance of the transformer models, metrics such as mean squared error (MSE) and root mean squared error (RMSE) can be used. In addition, the performance of various transformer models, including ViT, BEiT, DeiT, Swim Transformer V2, and Efficientformer, can be explored and compared

5. **Week 6**
   Complete all previous tasks. This is a buffer week for any unprecedented delays. Publish blog posts. Prepare for Phase 1 Evaluation.

Phase 1 evaluation

6. **Week 7 and 8**
   Work on benchmarking the four proposed methods, testing them, verifying results, and fixing bugs (if any).

7. **Week 9**
   Work on integrating the four proposed methods and testing them. Complete documentation for newly built methods, verify results, fix bugs (if any) and write additional unit tests.

8. **Week 10**
   Complete Jupyter Notebook Tutorials for all the proposed methods and modifications. Publish blog posts and prepare for Phase 2 Evaluation.

Phase 2 evaluation

9. **Future Works and Post GSoC**
   After the proposed 10-week timeline, I would love to start implementing any additional features and contribute to ML4SCI even after GSoC, and given an opportunity, I would love to pursue Ph.D. on related topics.

5 Other Information

5.1 Why ML4SCI?

As a Chemistry major with a keen interest in deep learning, ML4SCI is the perfect organization for me to participate in the GSoC program. ML4SCI's focus on applying Machine Learning techniques to fundamental sciences aligns well with my academic background and research interests. By working on ML4SCI projects, I will be able to expand my knowledge and skills in both fields and gain valuable experience working with a team of experts in the field.

Furthermore, the opportunity to work on real-world problems in collaboration with established researchers is an excellent way to gain practical experience and enhance my research abilities. Additionally, ML4SCI's focus on basic sciences research makes it an ideal organization for me to gain experience and knowledge for my future Ph.D. program. The research experience gained through GSoC can be an added advantage when applying to top universities for doctoral studies. As someone who has already worked at renowned institutions and submitted research papers.

I am excited about the opportunity to continue contributing to cutting-edge research and further advancing the frontiers of science through ML4SCI. Overall, participating in GSoC with ML4SCI will not only enhance my skills and knowledge but also provide a stepping stone for my future academic pursuits.

5.2 Relevant Background

I have over one year of experience conducting research in machine learning. During this time, I have authored four preprint publications. Additionally, I have submitted a paper on reward-based personalized federated learning to the upcoming International Conference on Machine Learning (ICML) 2023 and another paper on class imbalance and ensemble learning to the journal Neurocomputing, also set to publish in 2023.

In addition to these accomplishments, I have developed a new metaheuristic optimization algorithm based on principles from quantum physics. Furthermore, I am actively engaged in three ongoing research projects focused on personalized federated learning, Bayesian and variational deep learning, and Markov Chain Monte Carlo (MCMC). I have also applied transformer models in feature generation in the tabular dataset. To the best of my knowledge, this is the first such approach. [Link to repository]

Currently, I am further expanding my expertise through enrollment in a course on reinforcement learning, aiming to broaden my skill set and contribute to future advances in reinforcement learning.

5.3 Other commitments

Between May 12th and June 25th, I will be on summer break and able to commit up to 50 hours per week to any given task. Once my college classes resume on June 26th, I will transition to part-time work and be available for approximately 40 to 50 hours per week. My research internships are scheduled to be completed by mid-May 2023 as planned. In the event of any unforeseeable circumstances resulting in a reduction in weekly working hours, I will promptly inform my project mentor, Dr. Emanuele Usai, and make arrangements to compensate for the missed time in subsequent weeks. To ensure that I am readily available for any necessary catch-up work, I will be accessible via Skype or Zoom during Indian Standard Time Zone, GMT +5:30.