PROPOSAL

Vision Transformers for Dark Matter Morphology

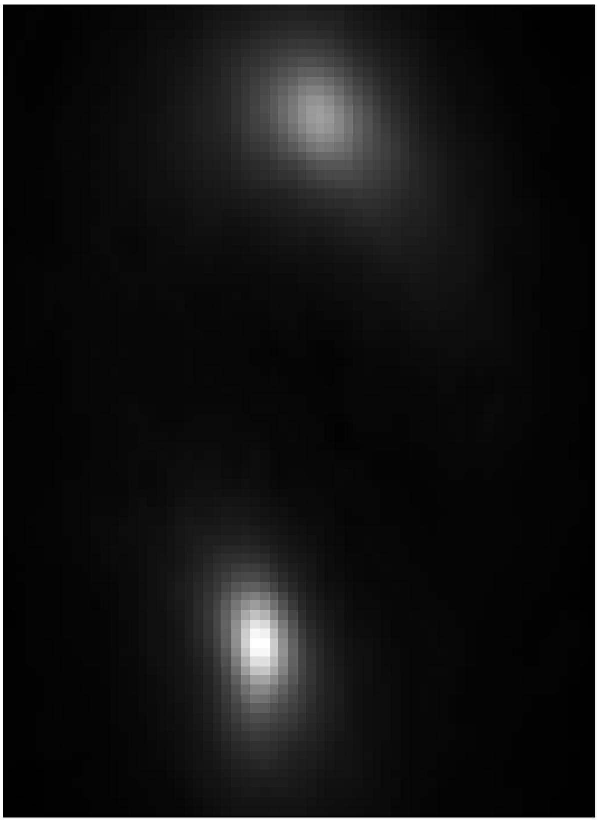
ML4SCI

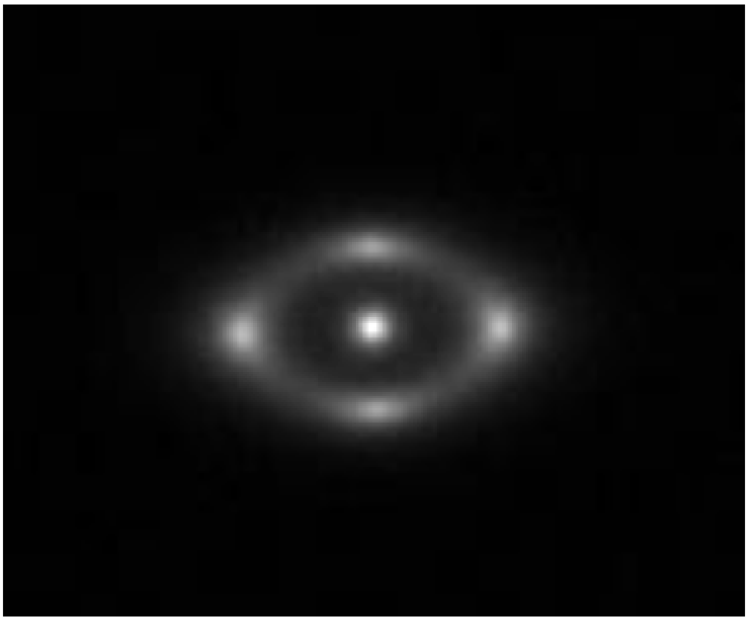
GOOGLE SOC 2023

- **Name**: Lucas José Velôso de Souza
- **Email**: lucas.jose.veloso.de.souza@gmail.com
- **Country & timezone**: Paris,France, UTC+2
- **Project Github**:https://github.com/SVJLucas/ViT-for-Dark-Matter-Morphology
- **School Name**: École CentraleSupélec - (Université Paris-Saclay)
- **Field of Study**: Data Science and Machine Learning

1. SYNOPSIS

Transformer is a neural network architecture that brought as key innovation its self-attention mechanism, which allows the model to balance the value of various sections of the input sequence while producing predictions. As a result, the Transformer design has shown to be very successful for a wide range of NLP applications, leading to its widespread acceptance in the field. In recent years, there has been growing interest in using Transformers for a variety of other applications beyond NLP, including computer vision





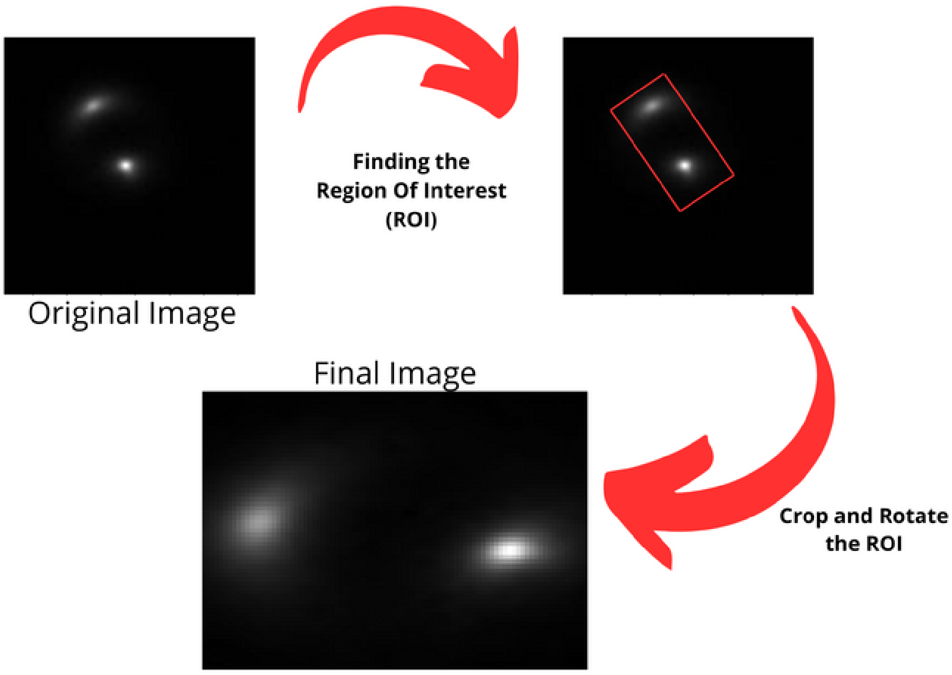
At the same time, the use of deep learning techniques in the field of science has become common, with the introduction of Physics-informed neural networks (PINNs). In this context, the purpose of this project is to use both techniques together to find Dark Matter substructures in observations, such as the images on the page, when using Transformers and extracting features of physical meaning from the image and concatenating them in the neural network

2. PROJECT DETAILS

Prerequisites

To compete for this project, ML4SCI required us to implement a transformer for computer vision. The next sections discussed my development of the test and of the proposed challenge in relation to Transformers and the detection of dark matter morphology.

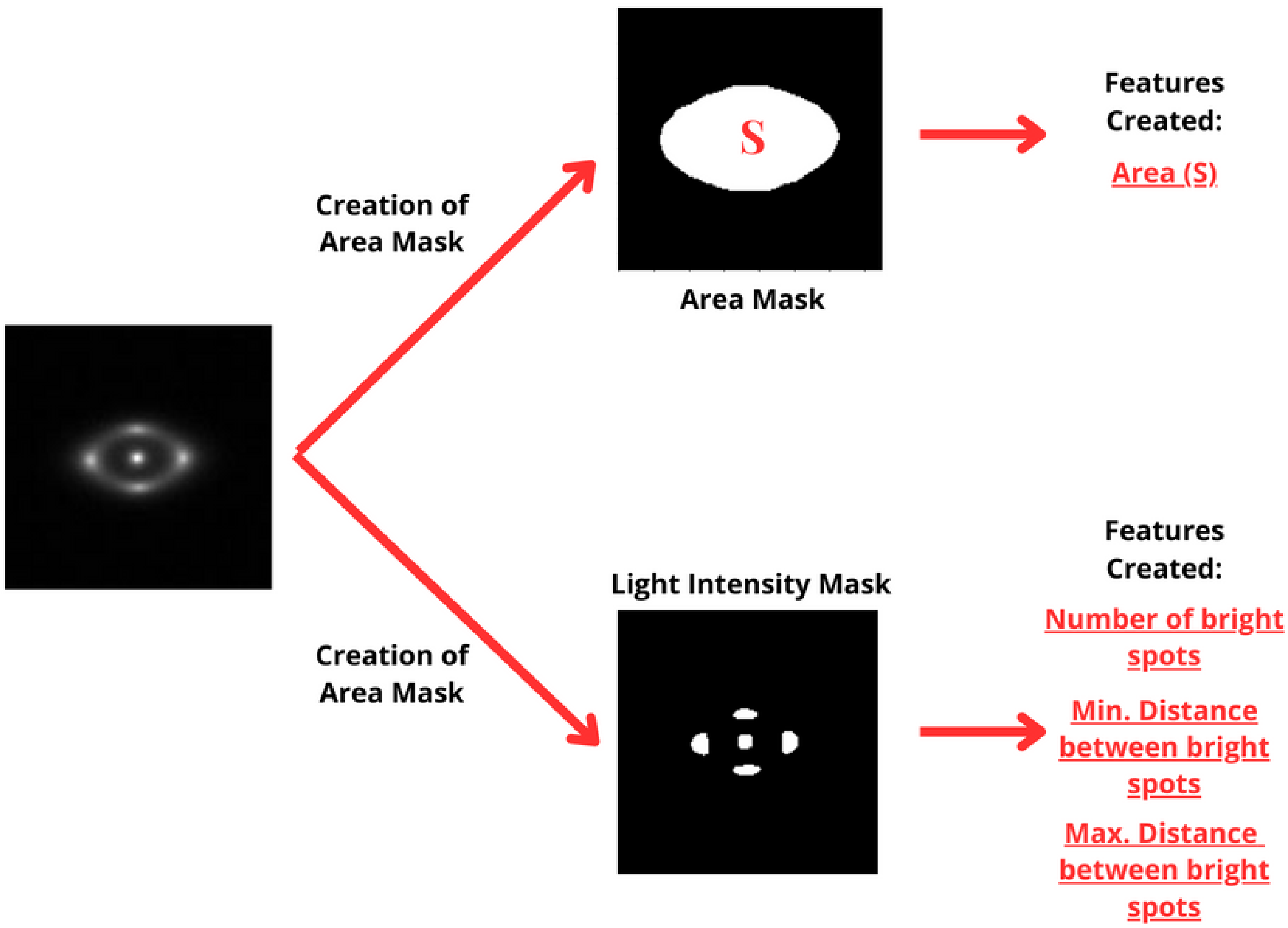
Image processing



To accomplish this feat, we need to process incoming images. By finding the region of interest (and then the possible observation of dark matter interaction), we can crop out the most important part of the image. When performing a rotation, we also decrease the space of symmetries (since we minimize the rotational symmetry), which turns rotated images into similar images and facilitates model learning.

2. PROJECT DETAILS

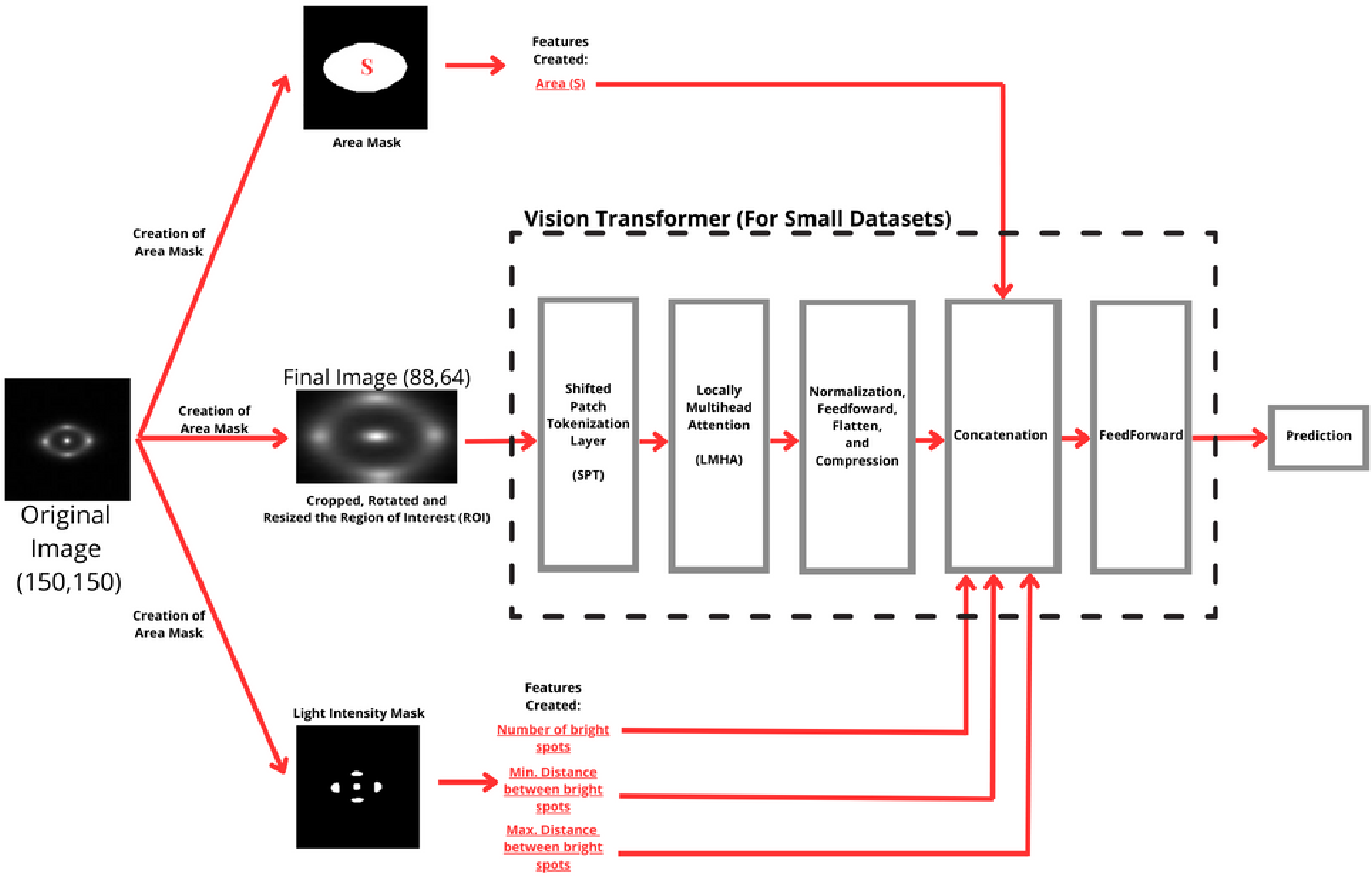
Feature Creation



Next, we will remove some features induced by physical knowledge of the problem. The area occupied in the observation of the Dark Matter substructure is a characteristic of this substructure, as well as the number of points of greater luminosity. These features have value for model prediction and will be added to the neural network.

2. PROJECT DETAILS

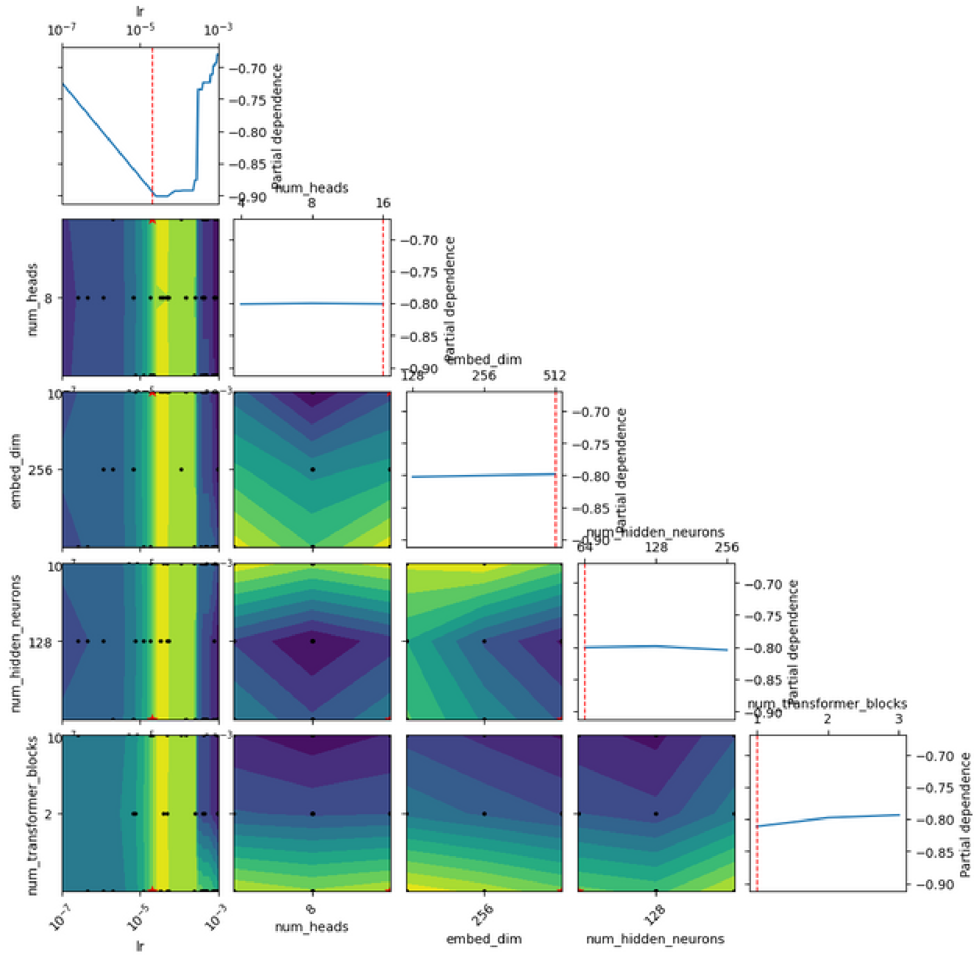
Model Architecture



The final architecture is inspired by the Transformers for Small Datasets paper, using innovations proposed in the Vision Transformers (ViT) for Small Datasets paper such as the Shifted Patch Tokenization (SPT) layer and Locally Multihead Attention (LMHA), which facilitate the learning of the ViT.

2. PROJECT DETAILS

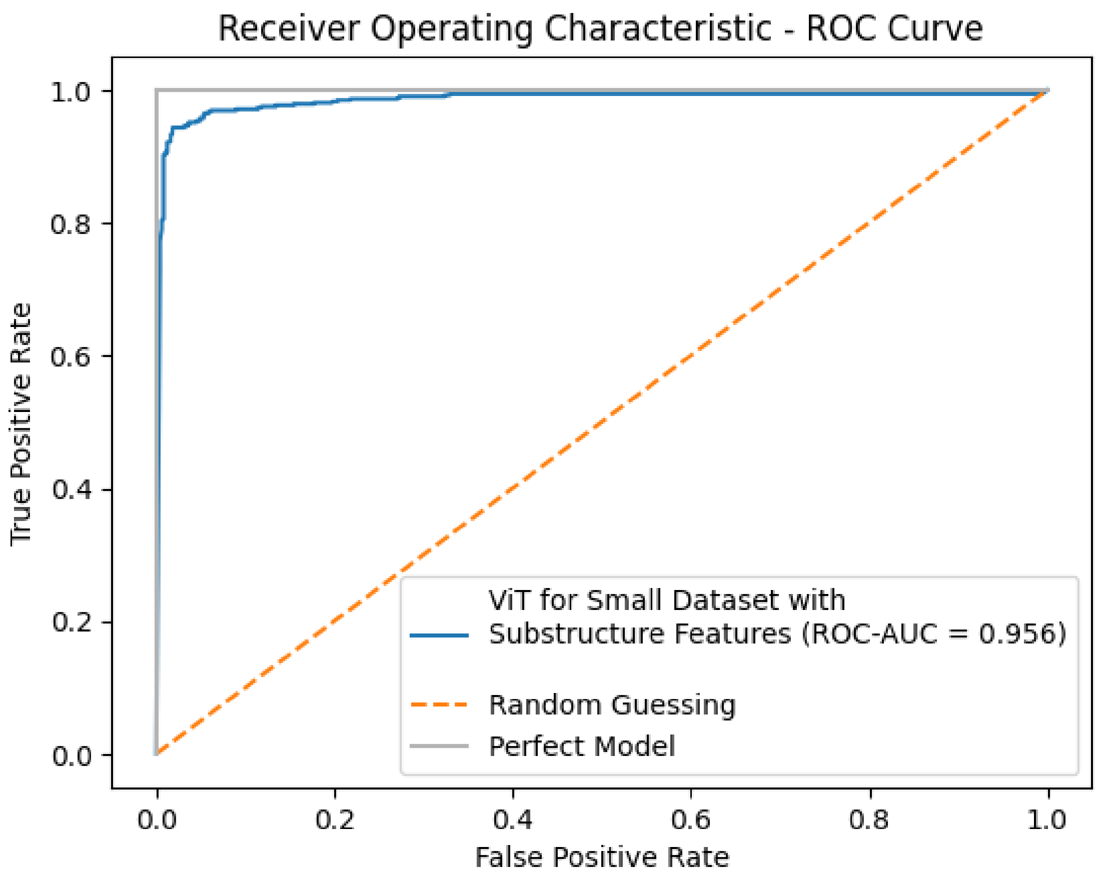
Bayesian Optimization



Since visual transformers are sensitive to some of their hyperparameters, Baysian optimization was performed on some of them. For the proposed transformer in question, the learning rate proved to be of very important optimization, since the transformer could not train if it was not in the range of 1e-4 and 1e-6, as can be seen in the graph at the top. The default choice of learning rate 1e-3 led to suboptimal results. The optimization was efficient and made it possible to find good hyerparameters for the Transformer and raised the model's ROC-AUC by 0.06.

2. PROJECT DETAILS

Model Performance



After the final training, the Transformer performed with a ROC-AUC of 0.956, a high value, showing the good performance of the technique used, approaching the ideal ROC curve, as can be seen in the graph.

WHAT I DO AS MY GSOC PROJECT

In this sense, after implementing the entire pipeline used, using Pytorch, OpenCV, and other Python libraries (in particular, the entire transformer was implemented in pytorch without using other libraries, using the paper Vision Transformers for Small Datasets as a basis), the great contribution to the project is to make all these features available to the scientific community. So, as my main task, I must re-implement all the code so that it is accessible to the user and within MP4SCI standards and norms, thus implementing image transformations, feature removals, the transformer and Baysian optimization (so that the user call is simple). You can look at a possible schedule on the next page.

GROUNDWORK

Since in order to apply for the project, it was necessary to solve a good part of the problem, I can say that we have already done a lot. The real difficulty will be refactoring the code within the standards and the MP4SCI ecosystem, in addition to debugging. So, **I believe it is a medium-sized project (175h).**

PROJECT SCHEDULE

Below is the schedule I propose for the execution of the project.

Before the Project	Better understand the needs of the ML4SCI community, both in terms of application and also in terms of development methodology. In addition to better understanding the physics of the problem. As well as aligning expectations with the mentor regarding what will be implemented.
1° Week	Try to find and extract relevant features from possible dark matter structures.
2° Week	Compare the different selected features, either by model performance and, therefore, which ones present the best results, or by statistical techniques, such as correlation with the target variable.
3° Week	Implement the innovations proposed by the Transformers For Small Datasets paper: both Shift Patch Token (SPT) and Locally Self-Attention, using the ML4SCI standards and directives.
4° Week	Finish implementing the presented transformer structure, allowing the final model to include or not the extracted features. Again, within ML4SCI guidelines.
5° Week	Start implementing Baysian optimization that searches for the best hyperparameters within the conditions informed by the user.

PROJECT SCHEDULE

6° Week	Finish implementing Baysian Optimization.
7° Week	Perform the final evaluation of the implemented model using the test dataset (allowing the user to be able to perform training and/or testing efficiently.
8° Week	Find potential coding issues and failure cases based on tested performance.
9° Week	Correct possible errors found and try to improve the performance of the model based on the feedback received from the test.
10° Week	Perform the final cleanup of the code and open the Pull Request in ML4SCI.
11° Week	Change according to user comments and other discussions pertinent to the project.
12° Week	Merge and write a documentation of the new Vision Transformer.

EXPERIENCE AND AVAILABILITY

Availability: My university vacation starts at the beginning of June, so I don't think I would have any problems with schedules.

Experience and final remarks: I've worked remotely before and have a lot of experience in machine learning, computer vision and artificial intelligence (you can look at the project's github that the entire transformers model was implemented from scratch). In addition, I have already won some data science competitions, showing my passion for the field. Finally, I would really like to participate in this project, because I believe that when better developed during the Google SoC, it could become a paper, and that, after working the last two weeks with the subject, I would really like to participate in the development of the scientific article.

Thanks for the opportunity,

Lucas José.