



GSOC Proposal 2022

Organization: ML4SCI

Thermonuclear Supernova Classification via their Multi-Wavelength Signatures

Mentors

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Contents

1	Introduction and Student Information		
2	Abst	tract	3
3	Tech	nnical Details	4
	3.1	Supernova	4
	3.2	SNela	5
	3.3	UVOIR	5
	3.4	Evaluation Task Results	6
		3.3.1 Model Results	18
4	Prop	posed Deliverables	21
	4.1	Schedule of Deliverables	22
5	Oth	er Information	24
	5.1	Why ML4SCI?	24
	5.2	Relevant Background	25
	5.3	Past Experience	25
		5.3.1 Knowledge of Libraries and/or Technology stacks	27
	5.4	Past Interaction with the Mentors	27
	5.5	Other commitments	27
6	Refe	erences	28

1 Introduction and Student Information

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2 Abstract

White dwarfs are the remnant stars and they are the cores of big stars and stars less than the mass of the Sun. The core itself is supported against gravity by electron degeneracy pressure. If the initial star begins with less than 4 solar masses then the end white dwarf [9] is made of carbon and oxygen but if it's between four and eight solar masses as an initial star then it becomes an oxygen neon magnesium white dwarf which is much more dense and more massive. There is a maximum limit to the mass of a white dwarf called the Chandrasekhar limit [11] at 1.44 solar masses and this is because that if we keep packing masses on top of the white dwarf, it gets smaller and smaller and the electrons in it have to go faster and faster and faster and eventually they have enough amount of energy such that their their kinetic energy is almost at the speed of light. An interesting detail to note is white dwarfs do not glow because of the electron degeneracy pressure do not shine by nuclear fusion or by gravitational contraction but because the protons and helium nuclei and carbon-oxygen-neon and magnesium nuclei that are inside the white dwarf those things are still hot on they would have an equivalent temperature of almost billions of degrees inside, so it's the residual heat of those things glowing. One of the end results of a white dwarf can be a nova which is a star that suddenly flares up extraordinarily then dims back down. And it will last ten days or maybe up to a hundred days while it fades away. A white dwarf that is a part of a semi-detached binary system that can undergo several novas. Due to the gravitational pull of the dwarf star, it starts to form a stream of materials from

the other star in the binary system which is a red giant and as hydrogen can be the material so it can do thermonuclear fusion on the surface of the white dwarf rapidly and blow material. But if suppose the mass of the dwarf star exceeds the Chandrasekhar limit of 1.44 solar masses, electron degeneracy pressure would fail to balance the gravitational pull and hence it would collapse, though the temperature is not increasing and the density gets incredibly high such that the carbon and oxygen nuclei become hot enough on their own to burn and do explosive explosive detonation of nuclear fusion inside which generates the heat and then since the electron degeneracy no longer works the extra heat leads to more fusion more fusion means more heat it goes on and on and ultimately that makes a huge new supernova and fuses all the light elements in the white dwarf into iron and nickel and the white dwarf itself gets completely consumed in this explosion and forms a type 1a supernova. There's nothing left behind when this happens as the white dwarf completely explodes and is responsible for a huge amount of iron in the universe. This type of supernovae tend to get really bright and then fade away. Now, the GSOC Project idea under this topic is to understand the clues and different aspects that reveal the identity of these progenitor systems, and the physical conditions that govern their explosions. But optical evidence is insufficient due to information loss and hence the goal is to combine the UVOIR (near-UV to far-infrared) and nuclear characteristics of SNeIa (Type 1a Supernova) to gain insights into these enigmatic objects along with a classification based on a machine learning approach or anything similar. And also to understand the relation between the observable and physical parameters related to these explosions.

3 Technical Details

3.1 Supernova

Supernovae are the source of elements such as carbon [10] (3 helium atoms fusion - triple alpha process) which are the building blocks of life in the universe. They release these elements as they explode thousands of light years away along with dust particles. The residues of the explosion also spread out in the universe to form new planets or stars which might later support life, provided adequate conditions evolve.

As the quest to find the rate at which our universe is expanding remains uncertain even with the two famous theories which are as follows:

1. Distance Ladder: This method looks for stars in the nearby universe whose absolute luminosity we have knowledge about and we use how bright they appear to us to determine how far away they are. And after combining this distance information with how red-shifted (increase in the wavelength) their light is, we can find out how fast the universe is expanding with Hubble

constant.

2. Lambda CDM: This method studies the features in the cosmic microwave background radiation (electromagnetic radiation which is a remnant from an early stage of the universe) which is just a picture of the early universe.

But these two models were never in sync and hence supernova comes to the rescue where the process is to look at a multiply-lensed supernova (happens due to gravitational lensing by another galaxy) and use the time delay between their appearances to find out how fast the universe is expanding.

3.2 SNela

SNela [13] is important because of their role in the chemical evolution of galaxies and as cosmological distance indicators. They are the brightest of all supernovae and have thus been used as cosmological distance candles. But the progenitor system that gives rise to Type Ia supernovae remains unknown. Though the view presented today for this type of supernova is the result of a thermonuclear detonation of a carbon-oxygen composite white dwarf star that accreted mass from a companion (eg: red giant), finding the exact candidate for the companion star remains a doubt. The two most sought choices at present for this companion star in the binary system are either an evolved main sequence star (single degenerate model), or a second white dwarf star that merges with the previously mentioned carbon-oxygen white dwarf star (double degenerate model).

3.3 UVOIR

Light curves [3] are an important source of information about the physics of supernovae. The Thermalized Energy from the radioactive decays of 56Ni (carbon and oxygen fuse) [6] and 57Ni and their daughter nuclides power the light curves of supernovae near maximum light. Combining the ultraviolet and near-IR data with the optical data the UVOIR bolometric [12] luminosity [14] can be computed, which itself integrates the flux emitted in the U, B, V, R and I passbands. The amount of 56Ni mass ejected can be estimated using the peak luminosity. Also, initially, most of the radiation from the supernova escapes in the UV [8] [5].

Two types of radiations can be studied: [6]

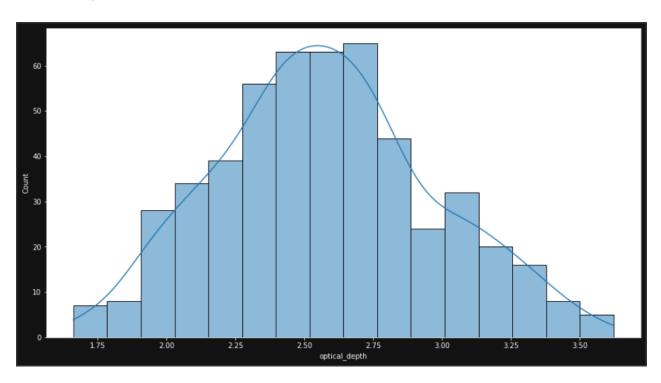
1. The shock energy that was deposited in the ejecta by the initial shock wave (mostly significant to

- Type II supernovae).
- 2. The radioactive energy produced from the decay of radioactive ⁵⁶Ni that is produced in the explosion decays first to ⁵⁶Co and ultimately to ⁵⁶Fe. This is very important in Type Ia supernovae as the main lightcurve peak is dominated by radioactivity. [1]

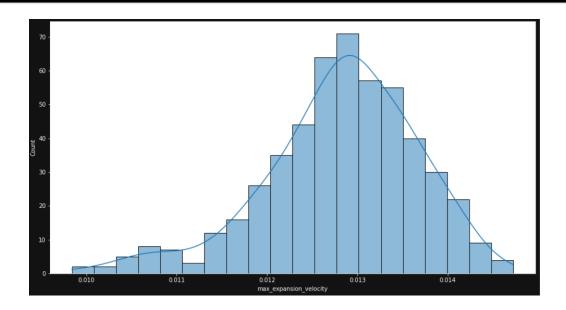
3.1 Evaluation Task Results

In the evaluation task, I looked at several metrics and graphs built using Python libraries, pandas, seaborn and matplotlib. Here are the results of Task1 and Task2 evaluations using GSOC Data DataCube.txt file as the data source:

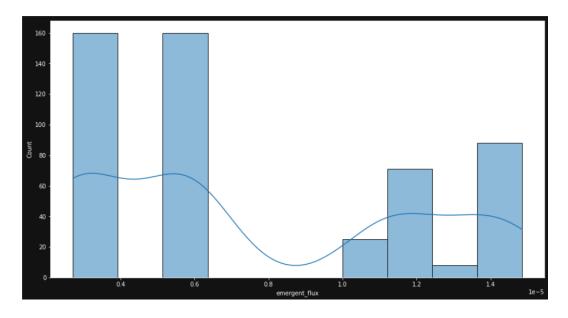
1. Below given graph shows the distribution of the observable parameter, optical depth [2] or thickness, it shows an almost normal distribution



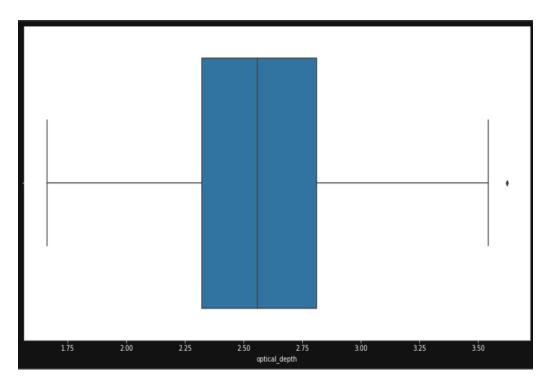
2. Below graph for the max_expansion_velocity of the ejecta shows a somewhat left skewed distribution



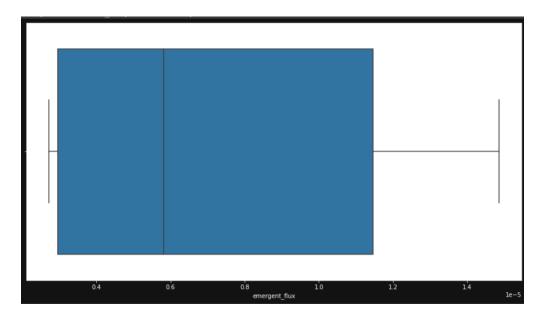
3. Below graph for emergent flux show a distinct distribution with larger frequency below $0.7~\rm X~10^{-5}$ photons cm-2 s-1



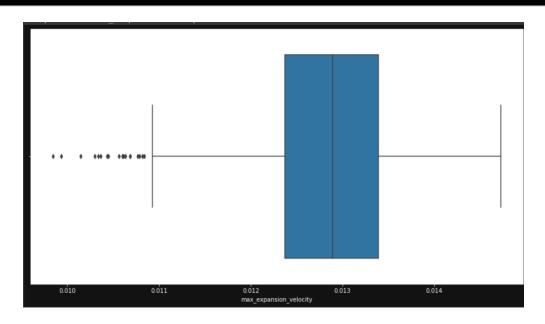
4. The below box-plot for optical depth shows that optical depth has only one outlier with a value of 3.621963.



5. Below emergent flux box plot doesn't show any visual outliers

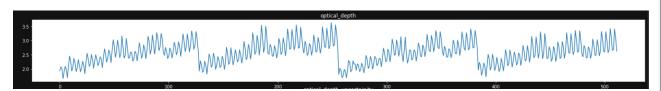


6. Below box-plot for max_expansion_velocity shows higher number of outliers towards minimum

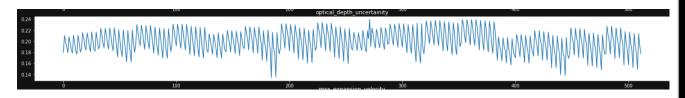


Below are the trends of the observable parameters;

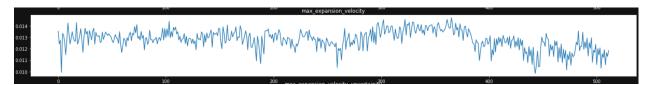
1. Optical Depth



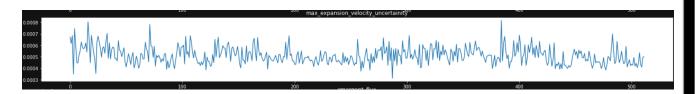
2. Optical Depth Uncertainty



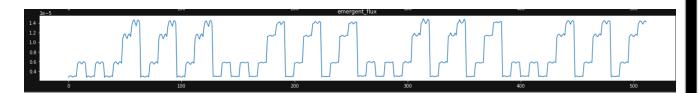
3. Maximum Expansion Velocity of the Ejecta



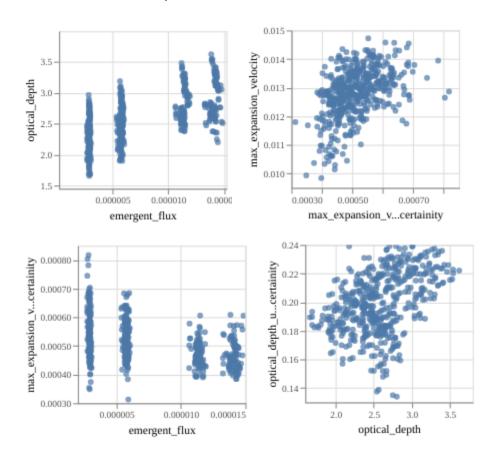
4. Maximum Expansion Velocity of the Ejecta Uncertainty

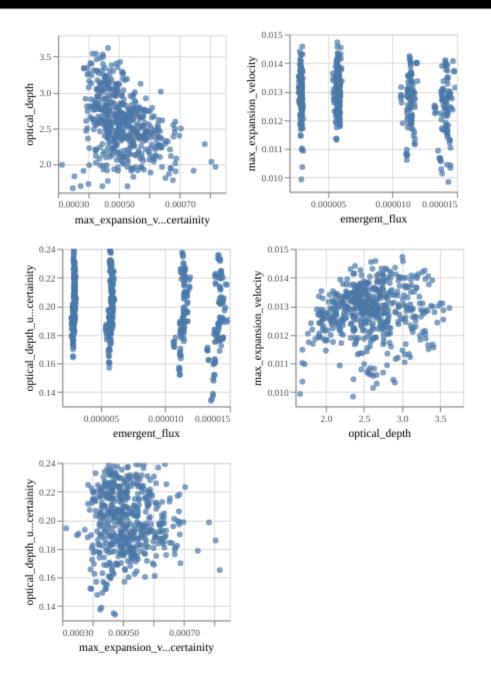


5. Emergent Flux

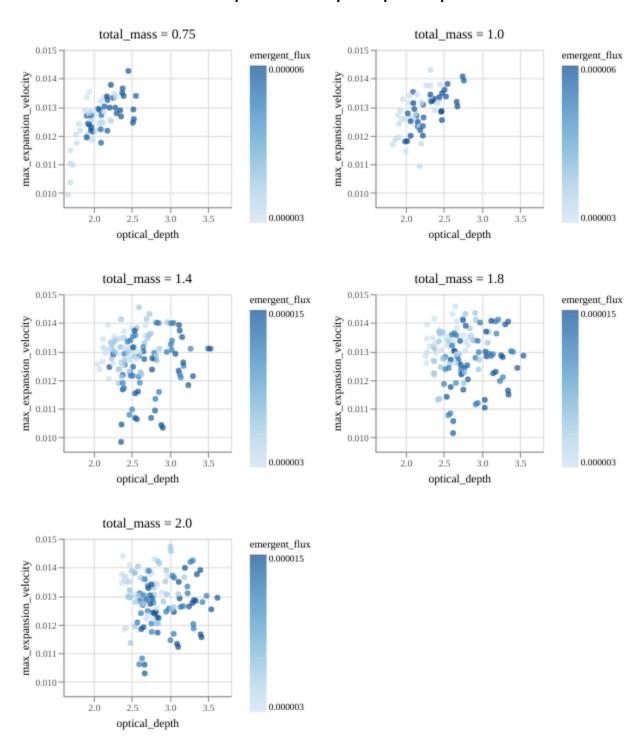


Relations between the parameters:

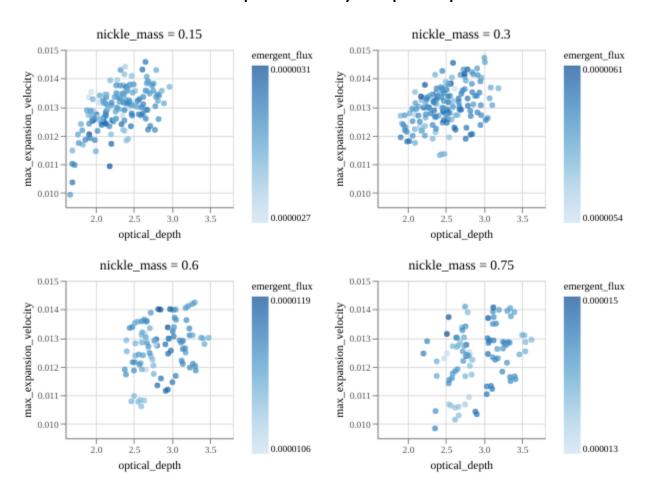




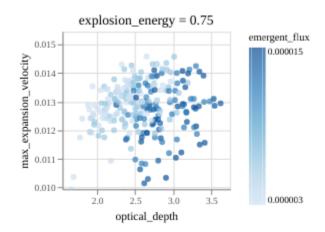
Relation of total mass with max expansion velocity and optical depth:



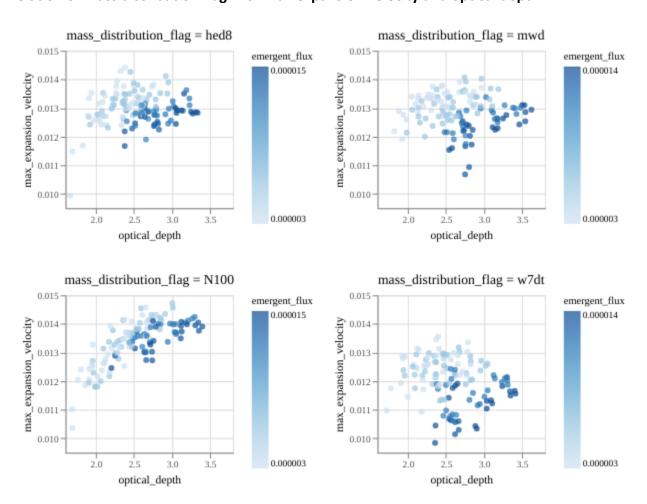
Relation of nickel mass with max expansion velocity and optical depth:



Relation of explosion energy with max expansion velocity and optical depth:



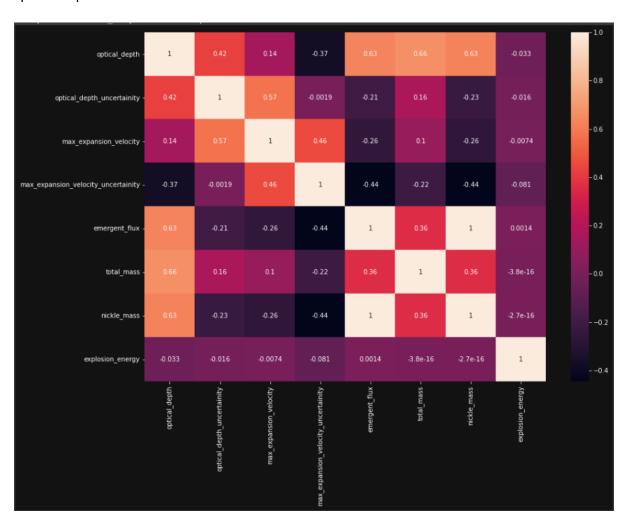
Relation of mass distribution flag with max expansion velocity and optical depth:



Correlation Matrix (Pearson method):

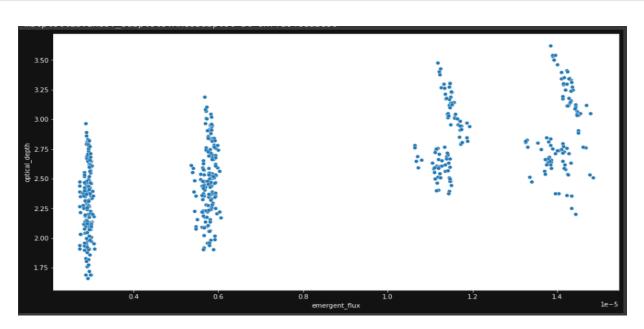
This shows a good correlation between optical depth and max expansion velocity, with a strong correlation with emergent flux with a value of 0.63.

Total mass shows a good correlation of 0.36 with emergent flux, with a 0.66 correlation with optical depth

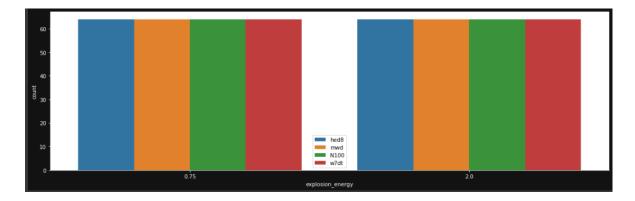


Relation among the physical and observable parameters:

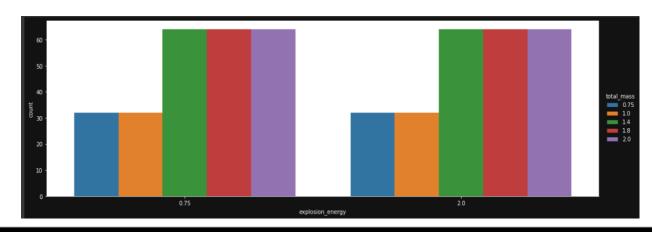
1. Emergent flux and optical depth



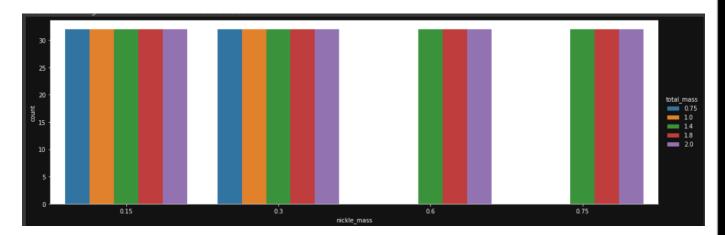
2. Explosion energy shows an equal distribution among the nickel radial distribution flag classes



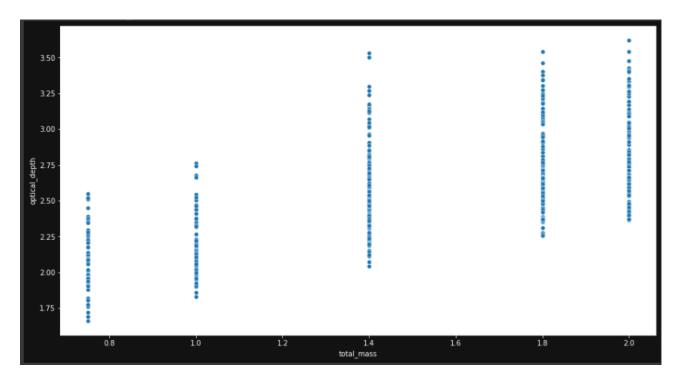
3. Total mass and explosion energy



4. Chandrasekhar Mass Models tend to produce more nickel-56 present in them, compared to sub-Chandrasekhar Mass Models [7]



5. As optical depth is the natural log of incident light and transmitted light, therefore transmitted light is inversely proportional to optical depth and from the above graph as we can see since with increasing total mass the optical depth increases, therefore the transmitted light decreases.



3.3.1 Model Results (Task-3)

- 1. The dataset from GSOC_Data_DataCube.txt was first preprocessed with scaling methods from Scikit library such as Robust Scaler, Standard Scaler, MinMax Scaler. Then confirmed if any null values are there. Then, the categorical variables, i.e., nickel radial distribution flag, mass distribution flag, were encoded using the Ordinal Encoder (maps each unique label to an integer value). Finally the dataset was divided into a set of 80:20, train and validation set.
- 2. Machine Learning [15] Algorithms: The traditional ML Algorithms didn't perform well for multi-output regression dataset, as in this case the outputs are 5, namely, Total mass, nickel mass, mass distribution flag, explosion energy and nickel radial distribution flag. Many of the Machine Learning don't support multi-output regression, such as, Adaboost, Random Forest, Gradient Boost, XGBoost, and so on.
- 3. Linear Regression was able to perform on the dataset, but the performance was too low to be considered, apart from the Decision Tree was the one who was able to perform better than other algorithms, but Decision Tree heavily overfitted on the training subset and therefore performed poorly on the validation subset.

Table 1: Model results

Sr no	ML model	Training MSE	Validation MSE
1	Keras Sequential Model	0.431	0.421
2	Multi-output regression	2.343	2.453
	model		

4. For deep learning, firstly I looked into a Keras Sequential model, with one Dense Layer, and 5 output layers as the final one. The loss was taken as mse and the optimizer was taken as Adam with a learning rate of 0.001, and it was trained for 100 epochs, a neural network with lesser dense units was selected as the dataset didn't show much complexity, otherwise the models would have overfitted. Results are below:

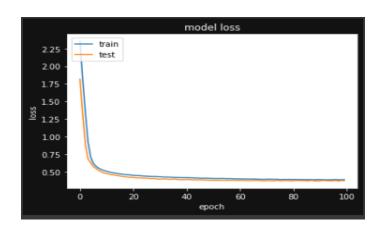


Figure 1: Model Performance

5. Finally, I built a model, based on a multi-output regression model, using Keras Functional API, with three Dense Layers and 5 output layers. The loss was taken as Sparse Categorical CrossEntropy and the optimizer was taken as Adam with a learning rate of 0.001, and it was trained for 10000 epochs. Below are the Model Results and structure:

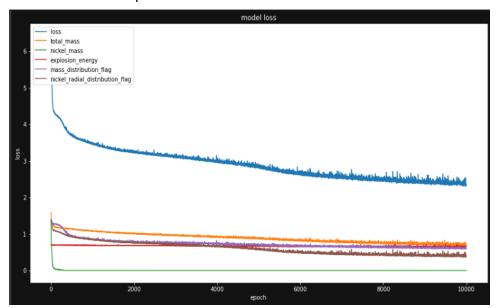


Figure 2: Model Performance

Layer (type)	Output Shape	Param #	Connected to
input_1 (InputLayer)	[(None, 3)]	 Θ	[]
flatten (Flatten)	(None, 3)		['input_1[0][0]']
dense_1 (Dense)	(None, 64)	256	['flatten[0][0]']
dense_2 (Dense)	(None, 128)	8320	['dense_1[0][0]']
total_mass_output (Dense)	(None, 5)	645	['dense_2[0][0]']
nickel_mass_output (Dense)	(None, 4)	516	['dense_2[0][0]']
$\begin{array}{l} {\sf explosion_energy_output} \ \ ({\sf Dense} \\) \end{array}$	(None, 2)	258	['dense_2[0][0]']
<pre>mass_distribution_flag_output (Dense)</pre>	(None, 4)	516	['dense_2[0][0]']
<pre>nickel_radial_distribution_fla g_output (Dense)</pre>	(None, 4)	516	['dense_2[0][0]']
Total params: 11,027 Trainable params: 11,027 Non-trainable params: 0			

Figure 3: Model Structure

Possible Challenges/Insights:

- Hyperparameter tuning with the Neural Network
 - We can vary the number of layers in the Dense network, the number of neurons in each layer and tune additional parameters like Batch Normalization, Max pooling, Dropout and analyze its implications on our final model. It's advisable to use less complex models as the dataset is not complex enough to have a larger number of layers.
- Clustering after regression
 - After the regression process to predict the physical parameters, we can go on to explore various methods of clustering to categorize the data for classes of supernovae. One of the methods can be to use autoencoders as they are designed in a way that they can be used to learn feature representation in an unsupervised manner as in this we don't know the classes yet
- More data is required to train a robust model and to get a low Mean Squared Error value for validation data.
- 6. Test results:
 - 1. Test Case 1:
 - 1. optical depth = 3.35
 - 2. maximum expansion velocity = 0.015
 - 3. emergent flux = $1.20 \times 10-5$
 - 4. Output results from the model:
 - 1. total mass = 2.35
 - 2. nickel mass = 0.40
 - 3. explosion energy =
 - 4. mass distribution flag = w7dt
 - 5. nickel radial distribution flag = w7dt

2. Test Case 2:

- 1. optical depth = 2.54
- 2. maximum expansion velocity = 0.013
- 3. emergent flux = $5.02 \times 10-6$
- 4. Output results from the model:
 - 6. total mass = 2.13
 - 7. nickel mass = 0.405
 - 8. explosion energy = 1.43
 - 9. mass distribution flag = w7dt
 - 10. nickel radial distribution flag = w7dt

3. Test Case 3:

- 1. optical depth = 2.46
- 2. maximum expansion velocity = 0.013
- 3. emergent flux = $1.03 \times 10-5$
- 4. Output results from the model:
 - 11. total mass = 2.11
 - 12. nickel mass = 0.404
 - 13. explosion energy = 1.5
 - 14. mass distribution flag = w7dt
 - 15. nickel radial distribution flag = mwd

4 Proposed Deliverables

1. Explore, analyze and compare the ideas that the progenitor system might be a single carbon-oxygen white dwarf in a tight binary with a stellar companion (eg: Red giant) or another white dwarf.

Challenges:

a. With the first idea, the challenge is, though the accretion rate or transfer rate of matter from the companion star to white dwarf might be high, which is the

accumulation of hydrogen rich envelope around the white dwarf, but there are no signatures of hydrogen features in the spectra of Type la supernovae.

- 2. Utilize the power of neural networks to predict the strength and range of the observable parameters, i.e., the initial optical depth, the maximum expansion velocity of the ejecta and the emergent flux of gamma-rays at 300 days post-explosion.
- 3. Study the various nuclear radiation that escapes just after the explosion, which might contain evidence of elements generated in the process and might uncover important information about the progenitor
- 4. Develop an algorithm predicts the physical parameters, i.e., Total mass, Mass of 56Ni, Explosion energy, Initial SNeIa mass distribution flag and Initial 56Ni radial distribution flag along with a classification of the supernova based on the input parameters
- 5. For classifying new supernova classes, the optical depth/ brightness can be used to identify the differences, the emergent flux also can give us new insights into the amount of gamma rays being spread at the beginning or during the explosion. [4]

4.1 Schedule of Deliverables

1. Community Bonding Period, 17 May - 12 June 2022:

I will get to know the community and get familiar with their code base and work style. Understanding the structure of ML4SCI, its objectives, motivation and so on. Getting familiarized with the concepts of the projects, reviewing relevant literature, which would include various articles, papers, etc. I have basic knowledge about supernovae, and will further work on understanding the core principles (theories) that guide these supernovas until now. 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 of learning, sharing and open-source contribution.

2. Week 1 - Week2, 13 June - 27 June 2022:

Literature Review on Type Ia supernovae and how they are important to our universe. Study about the coming from these supernovae which include UV light curves, and other nuclear radiation. Research on how to combine the UVOIR and nuclear characteristics of SNeIa to gain insights into these objects from the UVOIR bolometric light curves.

3. Week 3, 28 June - 11 July 2022:

Literature Review on various observable parameters, and how they affect the Type la supernovae. Use data analysis to verify their relationships along themselves, study their distribution and see how they affect the physical parameters. Identify various Machine Learning and computational techniques suitable for SNeIa classification. Literature Review of various papers and articles to find the best suitable techniques for the classification model.

4. Week 4 - Week 5, 12 July - 25 July 2022:

Work on applying ML algorithms (such as Support vector Machines, Random Forest, Decision Trees) and optimizing (hyperparameter tuning) an artificial neural network to predict the physical parameters. Also, continue to work from the evaluation task and try to use techniques like Transfer learning to attain state-of-the-art accuracies and prediction-levels. Work on developing classification algorithms for the supernova based on the various observable parameters, which can include neural networks or combination of ML algorithms or transfer learning.

Phase 1 Evaluation

5. Week 6, 26 July - 1 August 2022:

This is a buffer week for any unprecedented delays. Write and publish a blog post and prepare for Phase 1 Evaluation.

6. Week 7, 2 August - 8 August 2022:

Work on further optimizing the model if required. And analyze the important features of the model to determine what aspects of them are most important.

7. Week 8 - Week 9, 9 August - 22 August 2022:

Work on integrating all the proposed methods and test them with test cases of observable parameters. Complete documentation for newly built methods, verify results, fix bugs (if any) and write additional unit tests.

8. Week 10, 23 August - 29 August 2022:

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

Phase 2 Evaluation

Post GSoC and Future Work

After the specified 10-week timeline, I would definitely love to start adding or implementing additional relevant features in my contributions to ML4SCI even post completion of GSOC and would be honored to participate in research with the mentors on such amazing ideas.

5 Other Information

5.1 Why ML4SCI?

I believe that right now, Artificial Intelligence is driving every solution, be it Agriculture, Medicine Industry, or Human Computer Interface, from understanding simple pixel level features to implementing complex tasks with AI, it has outperformed all our hopes of its applications, the main reason being it is driven by data which is the new oil. And Python being the engine to this oil, it is a multi-disciplinary programming language in this field, which has an abundant source of libraries supporting each and every task in AI/ML. Moreover, the applications of Machine Learning in Science is increasing at an exponential rate, starting from helping to understand exoplanets, finding super habitable planets like Kepler-452 b to understanding chemical, physical and even biological properties of a celestial body to name a few. And with a background in Biology, major in Computer Science and with interest in the fields of machine learning, artificial intelligence, and astrophysics (Celestial Mechanics), I can complement well with this GSoC22 summer project. I feel with this amazing project, I will be able to help researchers and practitioners to explore new insights with the help of data analysis and Machine Learning and maybe it would simplify their work to some extent. Lastly, being a fan and devotee of open-source, it would indeed be an absolute pleasure to contribute these to such amazing meaningful projects which can help the society.

5.2 Relevant Background

5.3 Past Experience

I have a potentially good background in machine learning and astrophysics. I am an advanced Python user with 2 years 6 months of experience in working with the design of pipeline, development, and deployment of Machine learning and Deep Learning models along with experience in Image Processing. I am currently working as a Data Engineer in Al4Bharat, Chennai, India. I have previously contributed to many open source projects, namely:

- 1. Sukeesh: Jarvis (Contributed to Issue #894) (merged #900)
- 2. Sukeesh: Jarvis (Contributed to Issue #862) (merged #892)
- 3. codethesaurus: codethesaur.us (Contributed to Issue #300) (merged #452)
- 4. blobcity: autoai (Contributed to Issue #60) (merged #89)
- 5. Tenet-Coding: Hacktoberfest-Projects (Contributed to Issue #11) (merged #61)

Omdena community, open-source projects:

1. Project on Anomaly Detection On Martian Surface (Ahmedabad Local Chapter, India):

The martian surface is very uneven and hence it contains a lot of anomalies. The objective of this project was to detect the various anomalies on the Martian (MARS) surface caused by non-terrestrial artifacts like derbies of MARS lander missions, rovers, etc. Recently looking for extraterrestrials in the form of techno signatures has gained new interest. These signatures are measurable properties that provide scientific evidence of past or present extraterrestrial technology. There were a total 7 classes in the dataset used for training namely, Craters, Spiders, Impact Ejects, Dark dunes, Bright dunes, Swiss Cheese and Slope Streaks considered in the project. A YOLOv4 with pre-trained weights of ImageNet was used for training the Model. The dataset originates from Mars ODE Explorer created by NASA

2. Project on Kutch Water Quality Monitoring (Kutch Local Chapter, India):

The aim was to develop a centralized dashboard with different water quality parameters for analyzing, interpretation, and visualization in near real-time using Remote Sensing and AI for better decision making. This identifies if any water quality parameter is not within standard limits for taking up an immediate action and reinforces the abilities to monitor water quality more

effectively & efficiently.

3. Project on Improve sorting and segregation of waste using machine learning (France Local Chapter):

The biggest challenge in recycling/reusing waste is sorting and segregating different types of waste since segregation of waste aids in targeted recycling or even decomposition. As an example, segregating a dry metal can from a metal can containing organic matter eases recycling. The necessary action for proper segregation of the waste on a large scale is to identify various materials first. However, while there exist several methods to identify different materials such as visual sensors, olfactory sensors as well as spectroscopic tools, there are very few or no attempts at using artificial intelligence to specifically identify materials from the waste, which could then be applied to ease the segregation process. This project which is based on the Computer Vision model enables visual image recognition to first identify objects, in their full form or by parts in order to be used later for segregation.

I have authored two research projects:

- 1. App Based Tracking of Food Intake and Nutritional Values:
 - Through this app, an attempt to highlight the nutritional values was made . It gives a crisp detail of calories, vitamins, and other nutritional constituents along with a dashboard showing the daily consumption and the weekly/yearly consumption with a suitable data visualization after performing data analysis on the daily consumption of a person. It will also show the food ingredients that may result in allergies. It also recommends the amount of exercise depending on the consumption of the food items by the person thereby reducing the chances of any long-term diseases which if not taken care of may turn fatal in near-future.
- 2. Detection of Lung Nodules in Chest Radiographs using Wiener Filter and D-CNN Model: This paper proposes a modified wiener filter to remove the adaptive noise from the Chest X-Ray (CXR) images which has not been attempted by any researcher, further to make nodules clearer and contrasting we have enhanced the filtered CXR image by using adaptive histogram equalization (AHE). Later, classification using the simplified VGG network for Deep Convolutional Neural Network (D-CNN) model was performed to detect and classify the lung nodules from CXR images.

Currently, I am working on a project to study the variation of the orbital parameters other than eccentricity, semi-major axis, semi-minor axis and time; like inclination, true anomalies etc in

different planetary systems and carry out comparative analysis using data analysis and machine learning models.

I am confident that my skills and passion will allow me to uphold the status of the work expected by me.

5.3.1 Knowledge of Libraries and/or Technology stacks

With respect to the familiarity with various technology stacks, I have used Google developed library, Tensorflow, for deep learning projects, scikit-learn library for Machine Learning projects, pandas, numpy for data analysis and various data visualization libraries such as seaborn, matplotlib and lux. I have also enriched myself with fundamental concepts of supernova, its features, the types, concepts on white dwarfs, red-giants and the application of Machine Learning in solving this problem, as these concepts are very much relevant to the project. As all the above mentioned libraries have a support in Python, I am fluent with Python programming in general and I am ready to put in each every extra effort and work hard during the project to learn about various aspects of UVOIR and nuclear radiation data from LOX (Lunar Occultation eXplorer) (my favorite part of the project) since the project will certainly require a strong knowledge base in those areas as well.

5.4 Past Interactions with the Mentors

I had contacted my mentors, via the email ids shared in the project page. I have emailed them my results from the tasks provided in the evaluation document as well as my CV as instructed in the project page.

5.5 Other commitments

My 4th-year final exams will get over by the end of April and post-that, I will be able to spend 40-50 hours per week throughout the duration on this project. A reduction in the working hours in any particular week because of unavoidable conditions in these pandemic times might happen and will surely be compensated later in the following weeks. In such circumstances, I will communicate with my project mentors in advance to keep them in sync. For any project

meet-ups, I am available via Zoom/Google-Meet in Indian Standard Time Zone, UTC+05:30.

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