

Hack presentations

Friday Sep 6 10-12

Each group 10 minutes presentation + 5 min Q&A

You may decide as a group how you structure your presentation (how many speakers, etc)

Please clearly lay out the motivation for your problem. Why is your problem interesting?

Please keep the A-H slides as demarcation markers.

A

Hack 9: A generative model for spectra

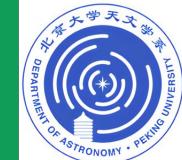
Group A : Akhil Uniyal, Jongin Park, Lei haipeng, Takuma Moriyama,
Yiming Huang, and Ziming Wang



李改道研究所
TSUNG-DAO LEE INSTITUTE



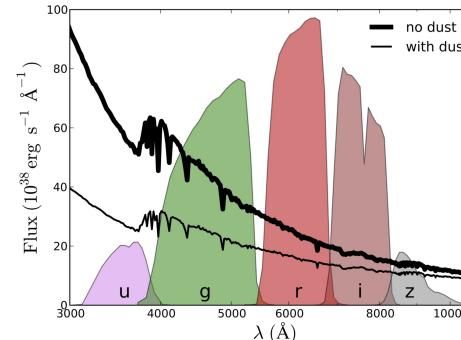
復旦大學
Fudan University



01. What is our Mission?

Generating the Synthetic Galaxy Spectra

- Testing data processing and analysis pipeline for spectra
- The amount of observation spectra is limited
 - Realistic simulations of the anticipated data can be used
 - Perform learning with any generative model! (GAN, VAE, ...)
- Our Goal is generating **synthetic galaxy spectra**, by learning from measured **Sloan Digital Sky Survey** data

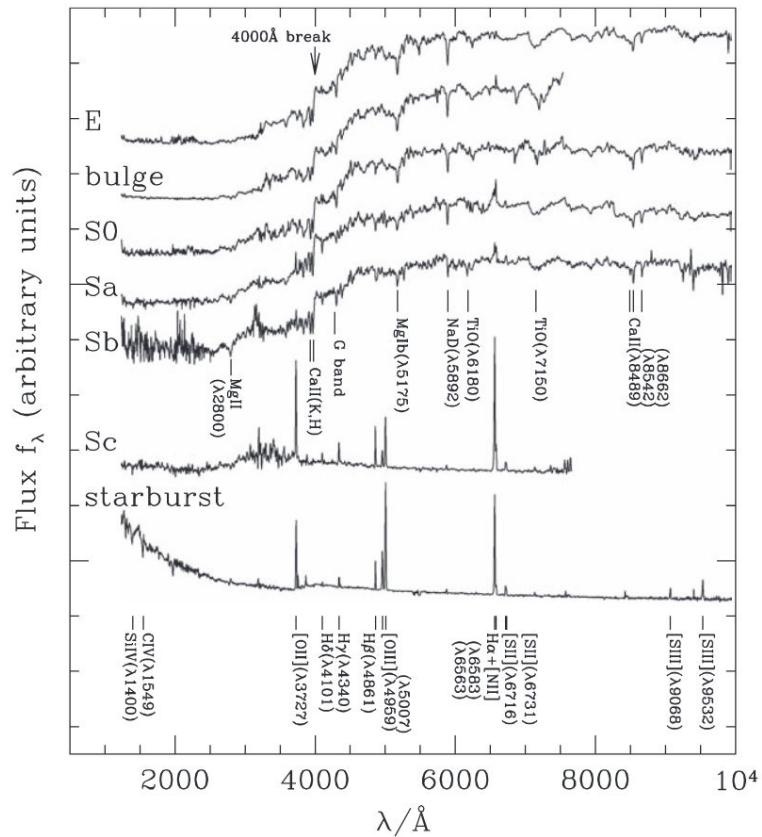


<https://tao.asvo.org.au/tao/static/documentation/Technical-Spectral-Energy-Distribution-Module.html>

02. Backgrounds

The Noticeable Feature of Galaxy Spectra

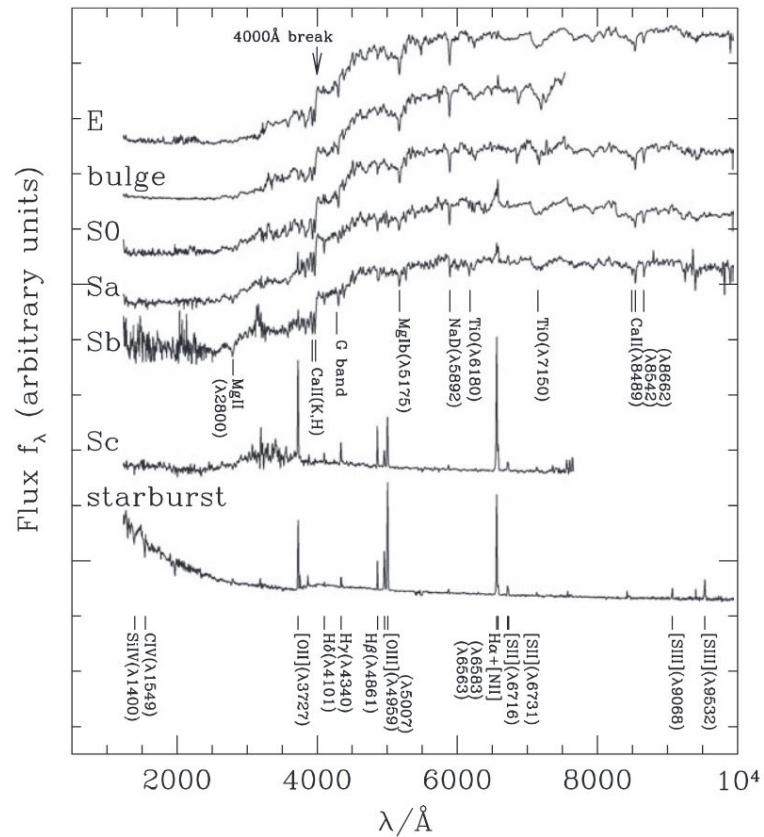
- **4000 Angstrom break:**
 - Sudden discontinuity in the spectra around 4000Å
 - This is due to sudden change in the opacity of low mass stars
 - This feature is predominantly in galaxies with stellar population ages greater than 0.1Gyr.



From Hojun Mo et al. "Galaxy Formation and Evolution"

The Noticeable Feature of Galaxy Spectra

- **Emission Line:**
 - Late type, starburst galaxies produce light in the blue and near ultraviolet from young stars
 - ISM get ionized given rise to emission line
- **Absorption line:**
 - Early type galaxies are lack of young stars, most of light emerges at the longest wavelengths.
 - Cold stars giving rise to absorption lines.

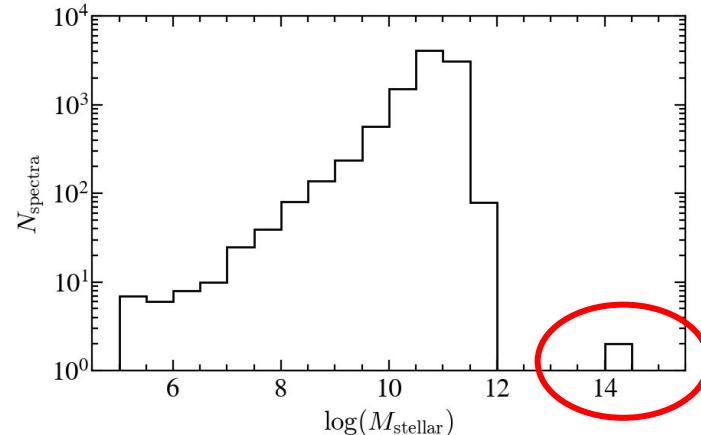
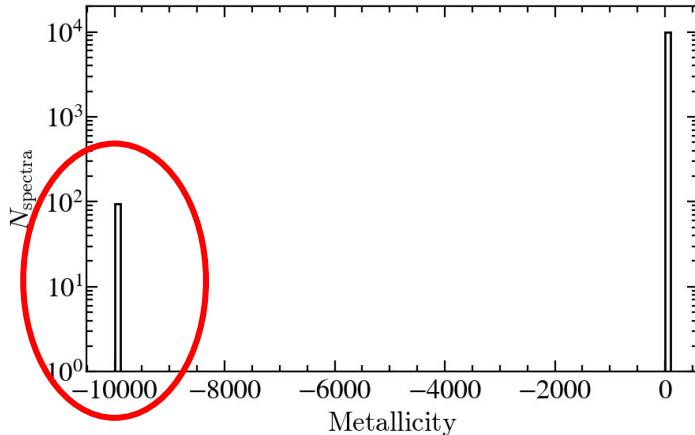


From Hojun Mo et al. "Galaxy Formation and Evolution"

03. Data Preprocess

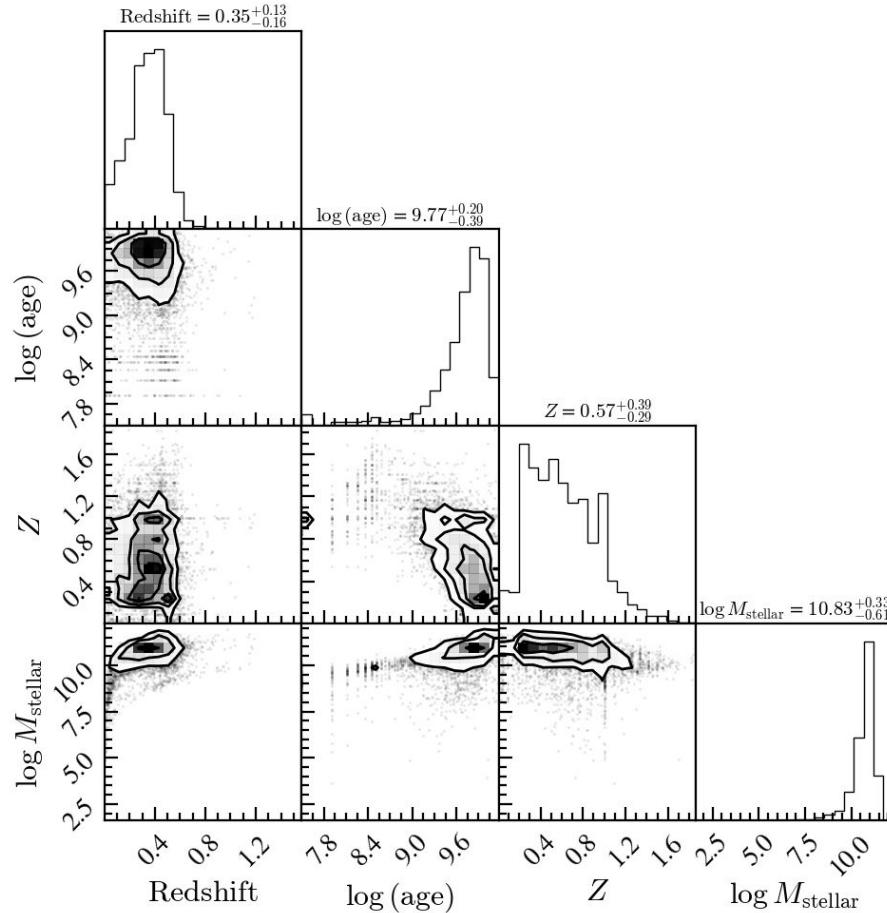
Noticeable Issues on Datasets

- Some spectra showed strange value in given physical parameters (**age, metallicity, smass**)
some spectra showed...
 - negative redshift (5 spectras)
 - negative age, metallicity, smass (95 spectras)
 - smass massive than $10^{13} M_{\odot}$ (5 spectras)



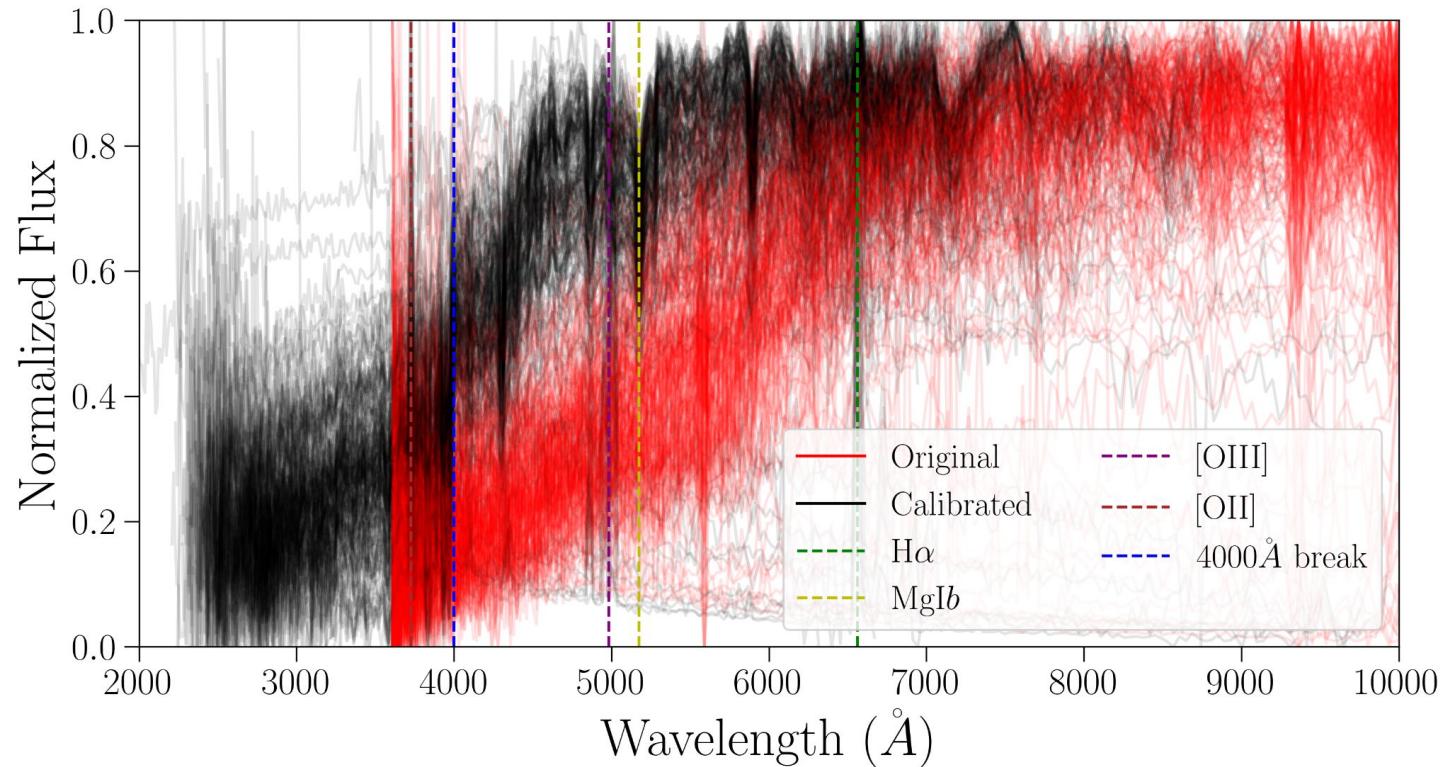
⇒ We removed unreasonable measurements from our datasets

Distribution of the Parameters after Removal

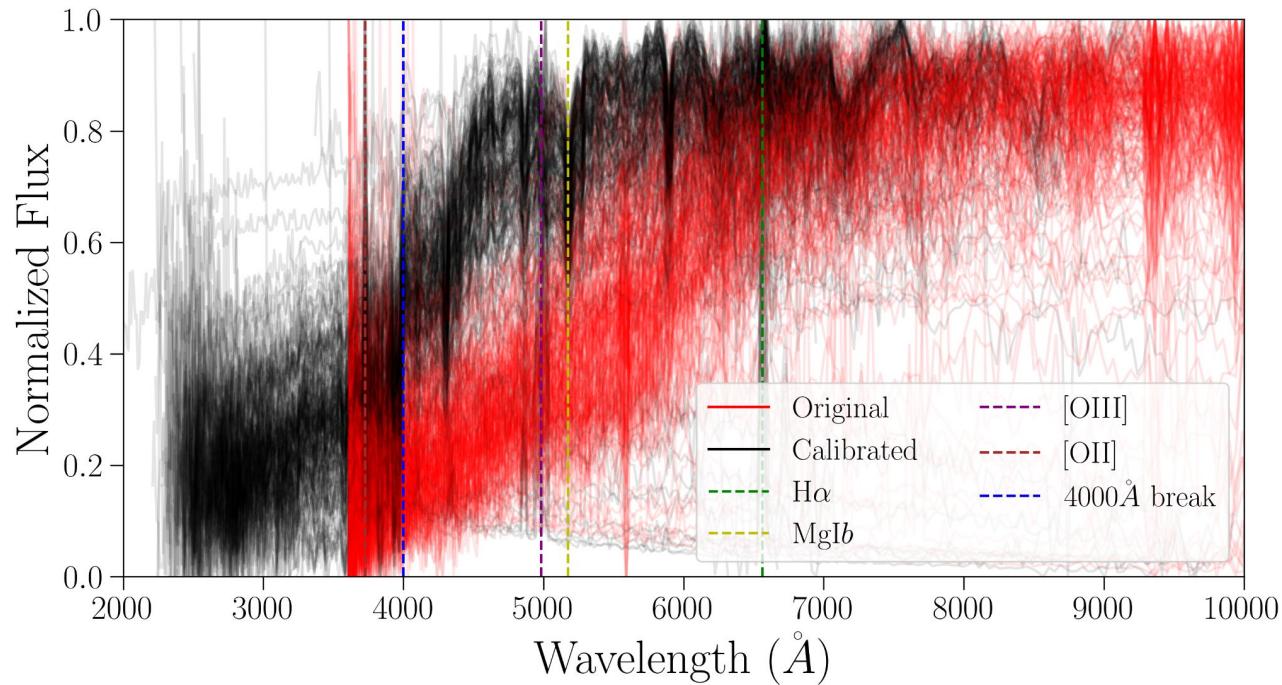


Spectra Wavelength Calibration

- The original spectra (observer frame)
→ Shift to **rest frame** based on redshift measurements



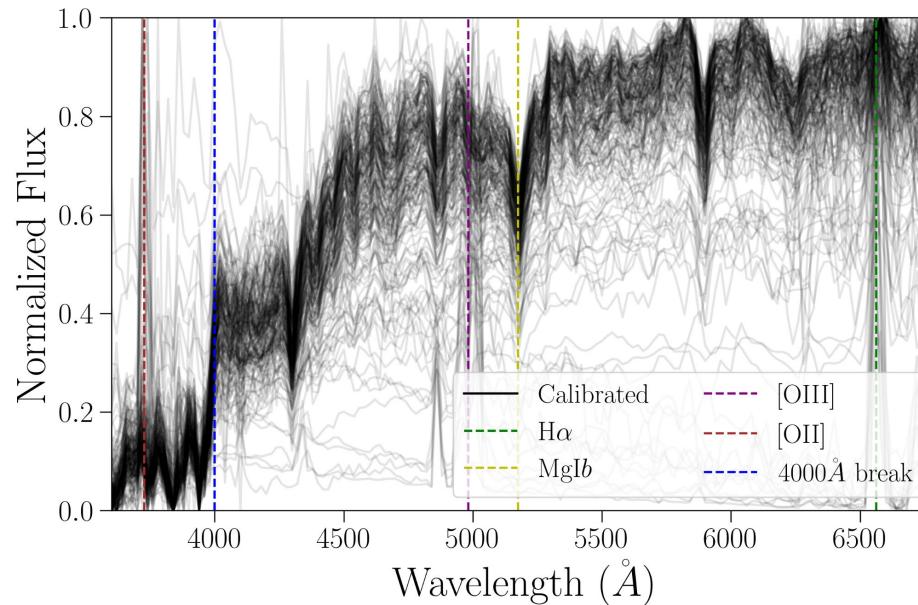
After Spectra Wavelength Calibration



- **Goods:**
 - Smaller scatter
 - Similar emission/absorption lines
- **Bads:**
 - Different wavelength range
 - Misaligned wavelength sampling points

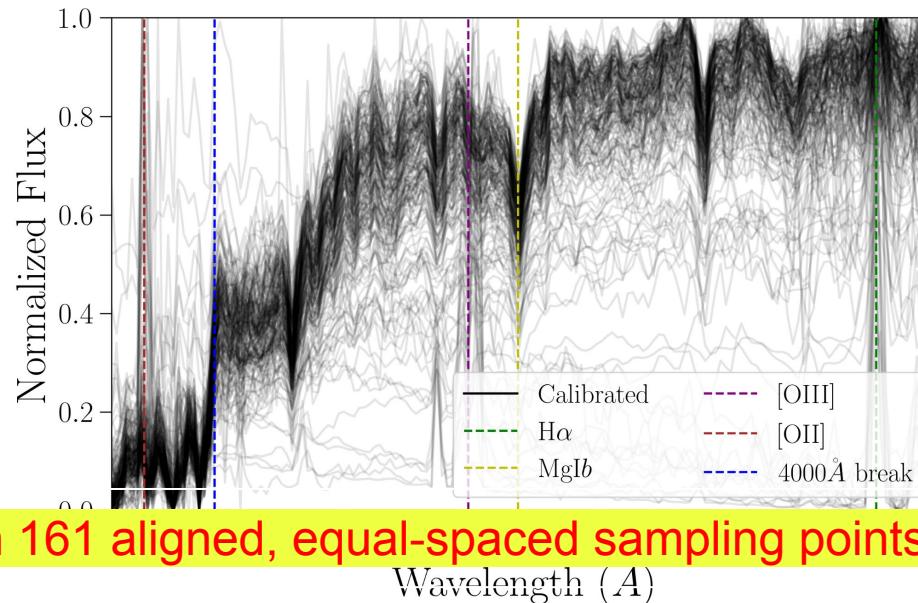
Alignment of Sampling Points in Spectra

- Different wavelength range problem
 - Extract the **overlapping parts** in different spectra
- Misaligned wavelength sampling points problem
 - Resample by **interpolating** within the overlapping range



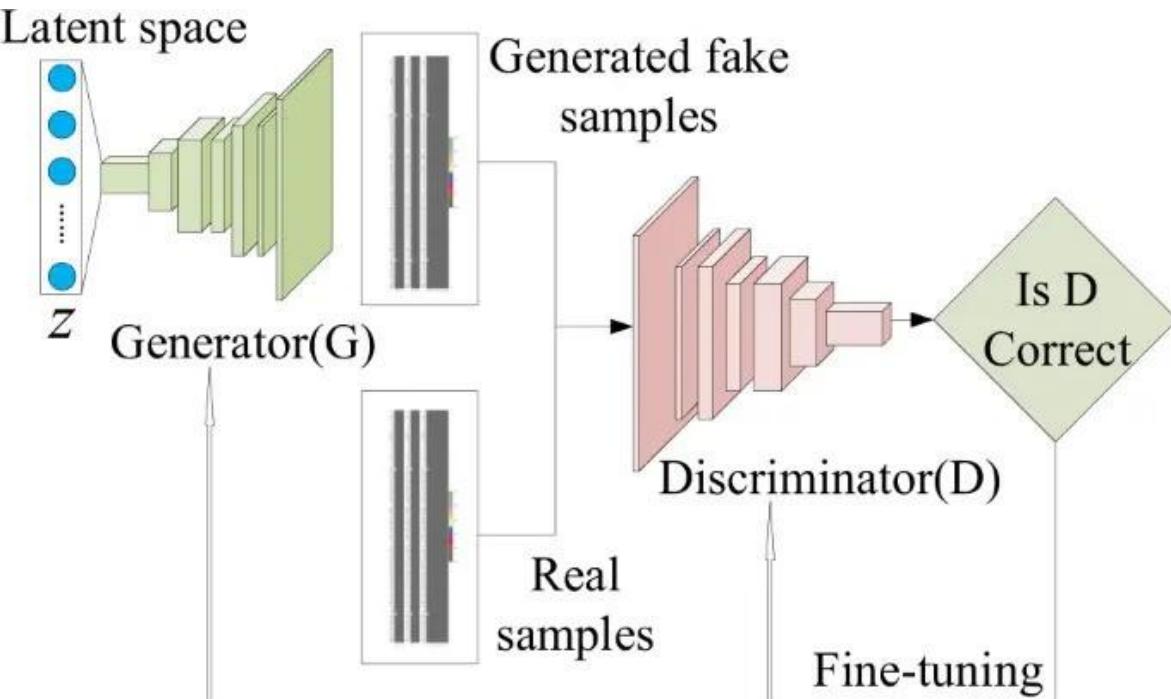
Alignment of Sampling Points in Spectra

- Different wavelength range problem
 - Extract the **overlapping parts** in different spectra
- Misaligned wavelength sampling points problem
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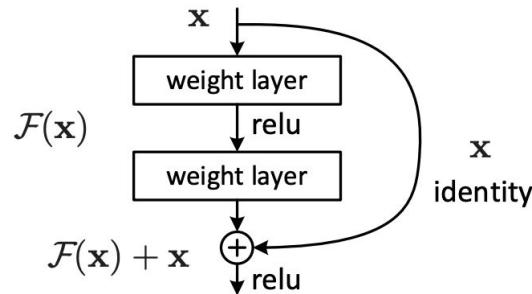
04. Semi-supervised GAN

Generative Adversarial Networks (GAN)



Fighting , finally balance

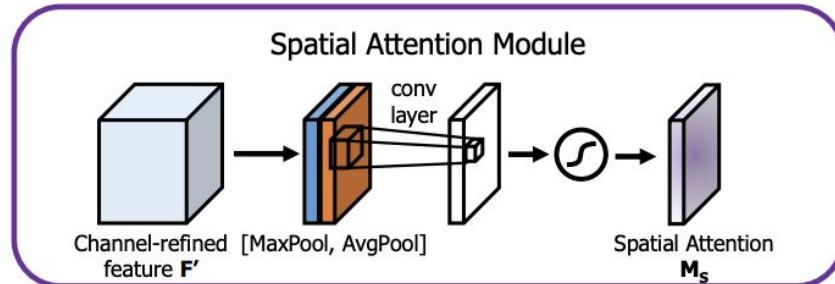
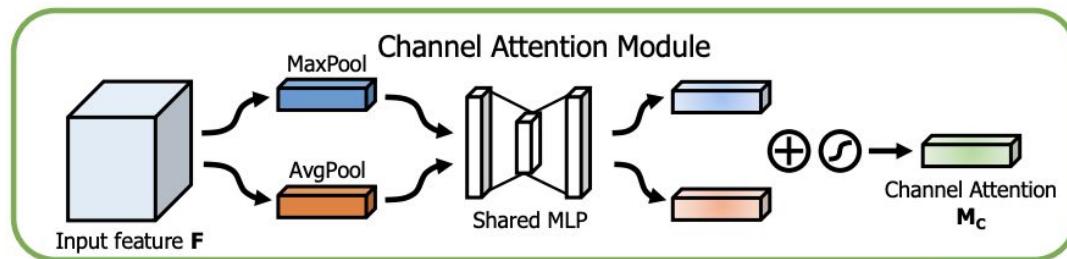
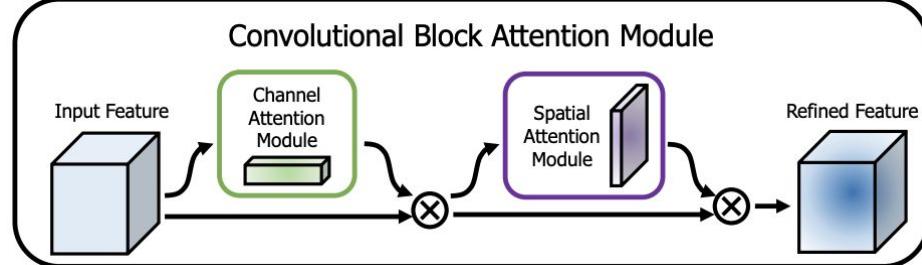
ResNet CBAM



Residual block

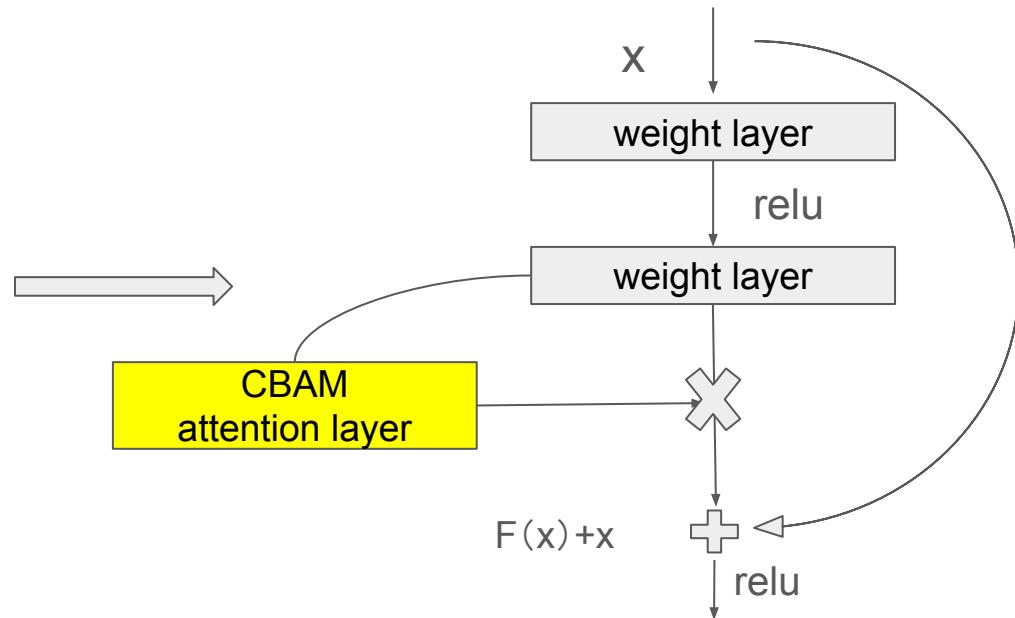
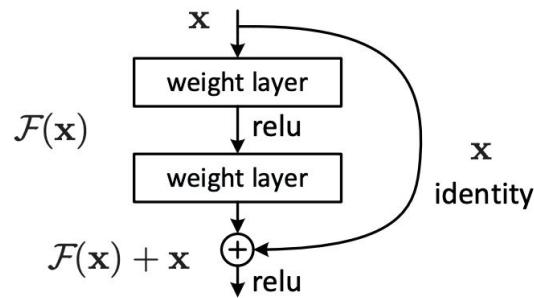
[Kaiming He , et al 2015](#)

CBAM: Convolutional Block Attention Module



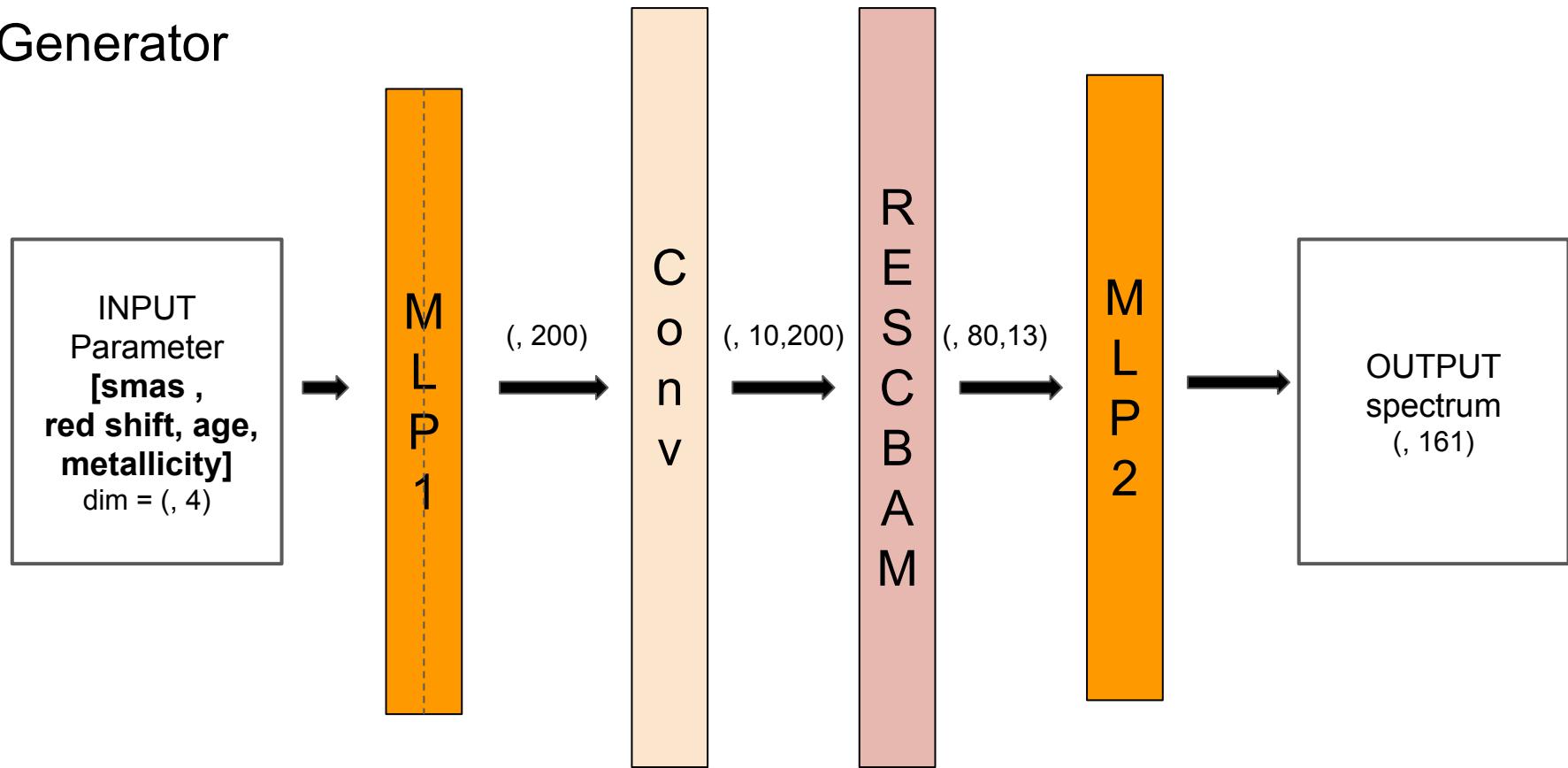
ResNet CBAM

Residual + CBAM block



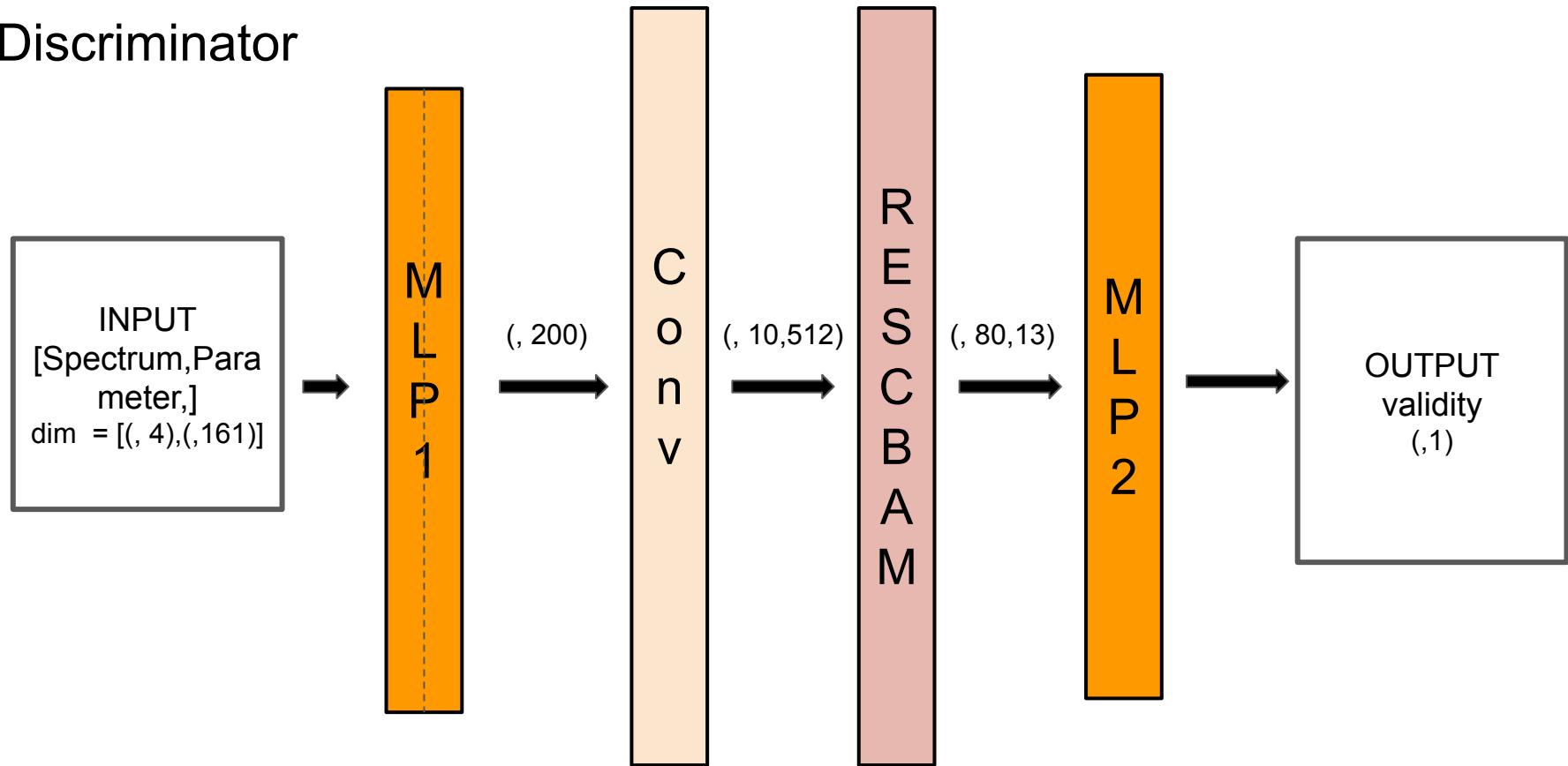
Architecture

Generator



Architecture

Discriminator



Training

Loss Function :

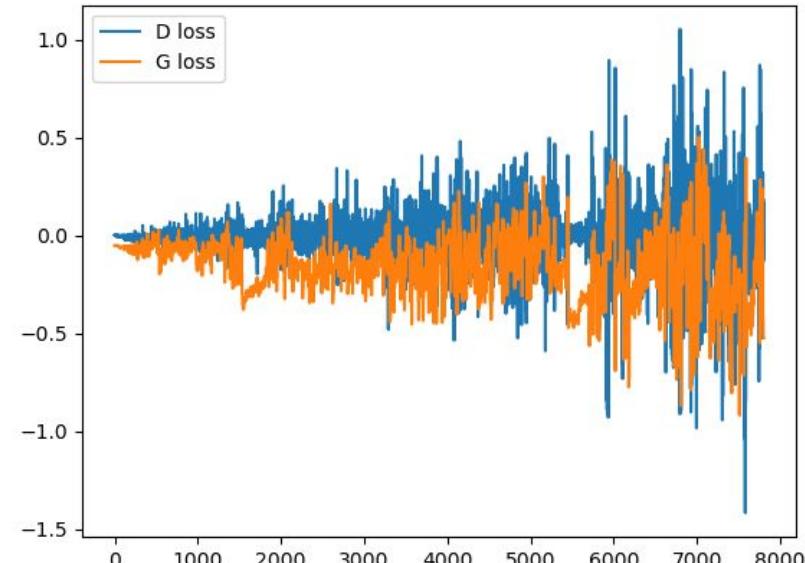
Wasserstein Lodd

Loss of discriminator :

-`torch.mean(dis(real))+torch.mean(dis(fake))`

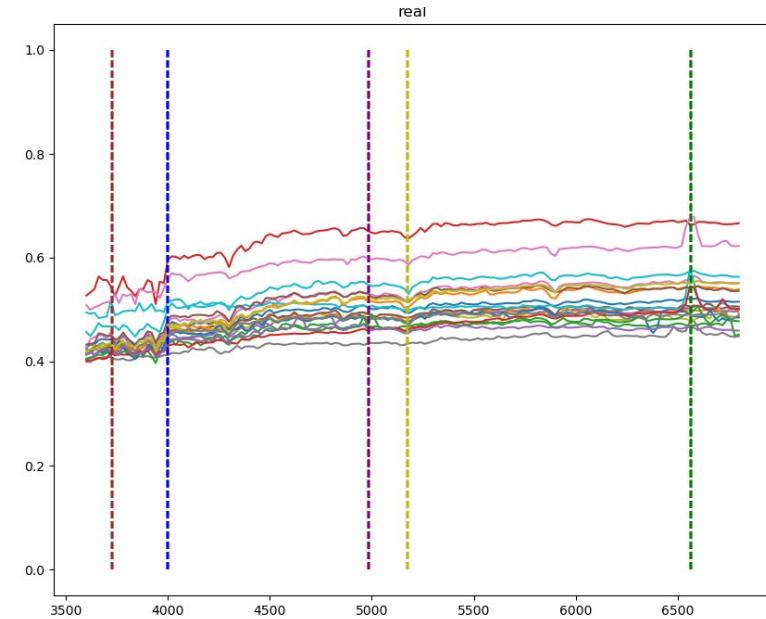
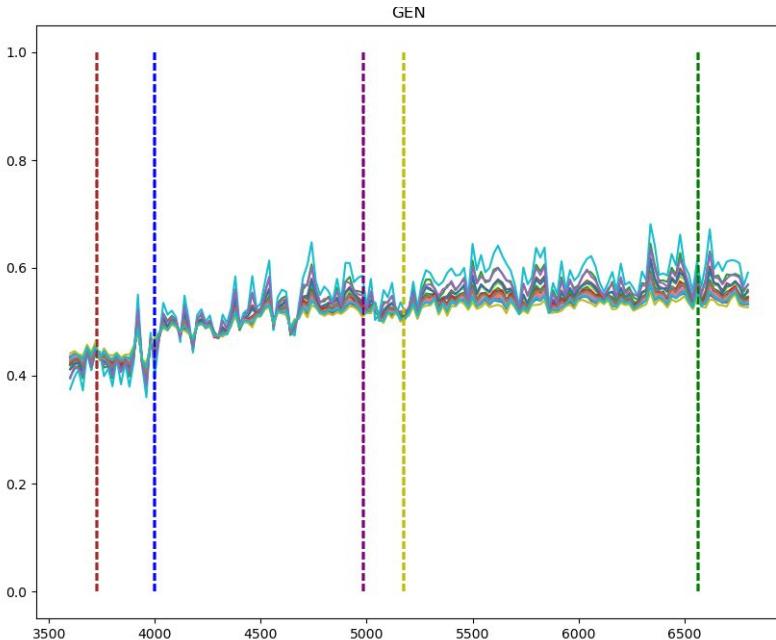
Loss of Generator :

-`torch.mean(dis(fake))`



Predict

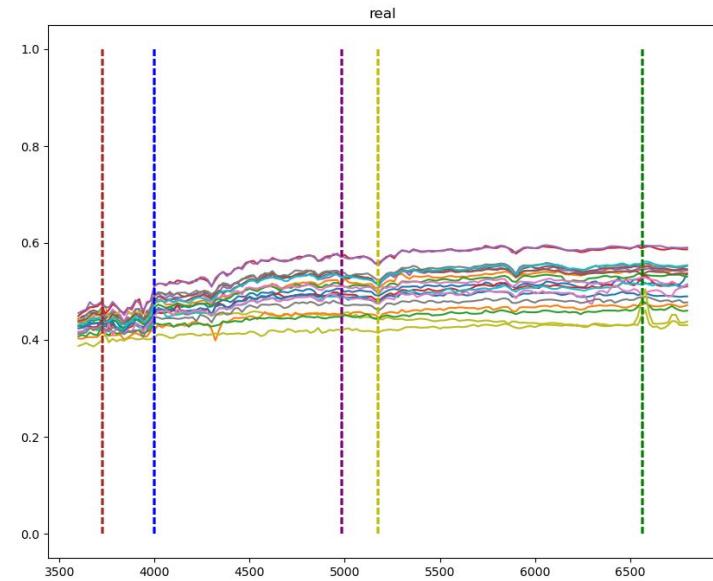
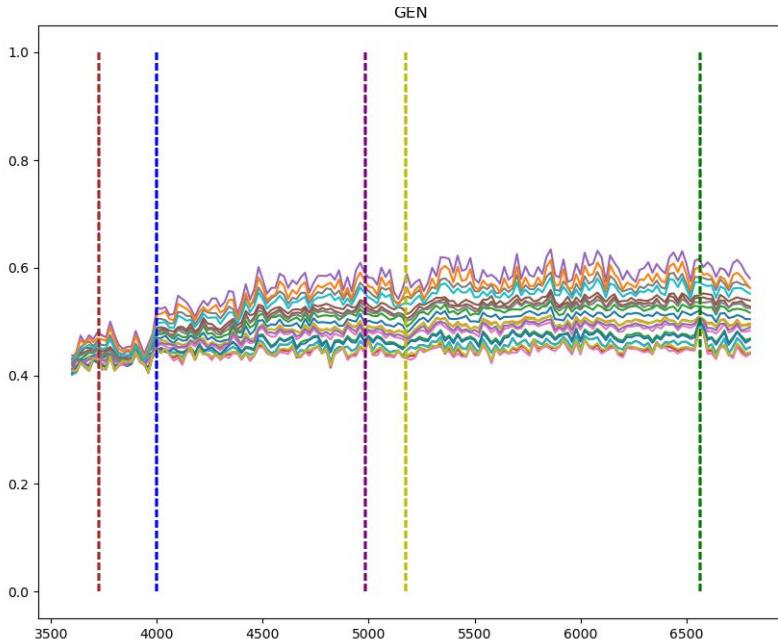
EPOCH = 20 , BATCH SIZE = 20, Clipper boundary (-0.03,0.03)



Random sample 10 group parameters

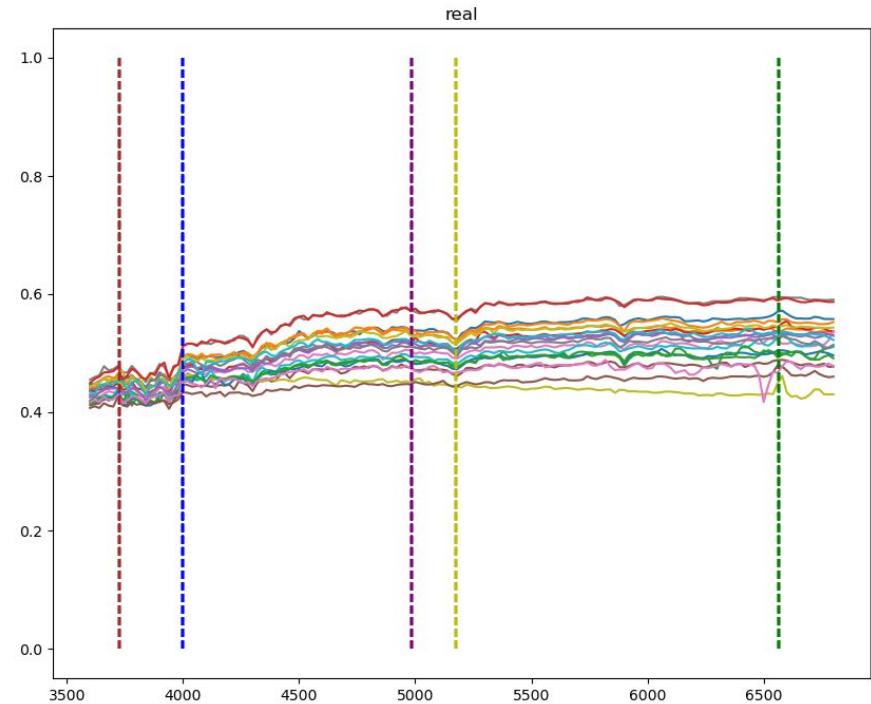
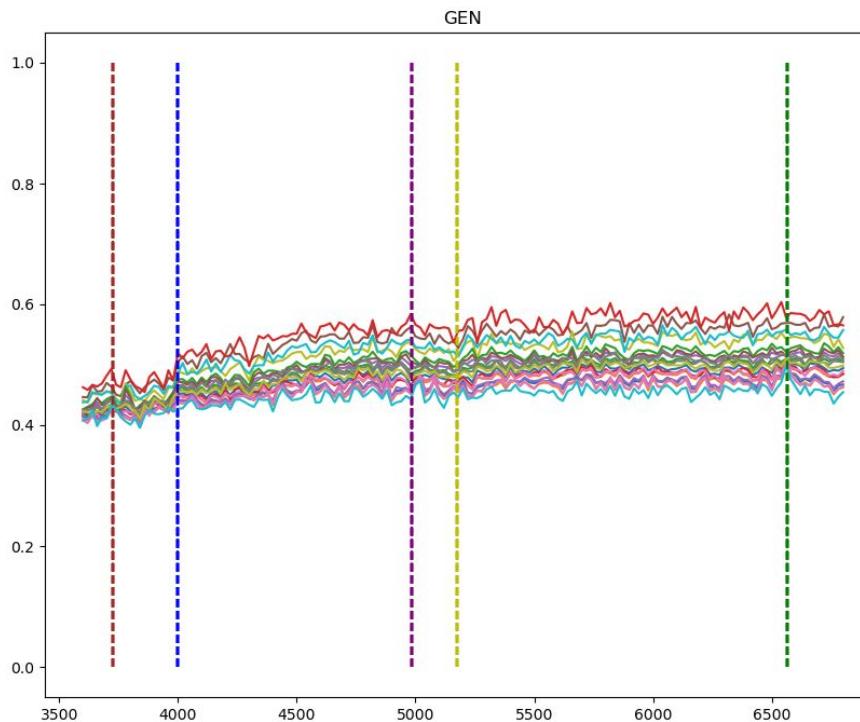
Predict

EPOCH = 50 , BATCH SIZE = 50, Clipper boundary (-0.03,0.03)



Random sample 10 group parameters

Predict



Random sample 10 group parameters

Usage

Model is available on Github :

<https://github.com/Astroyimin/WCGAN-for-Galaxy-Spectrum.git>

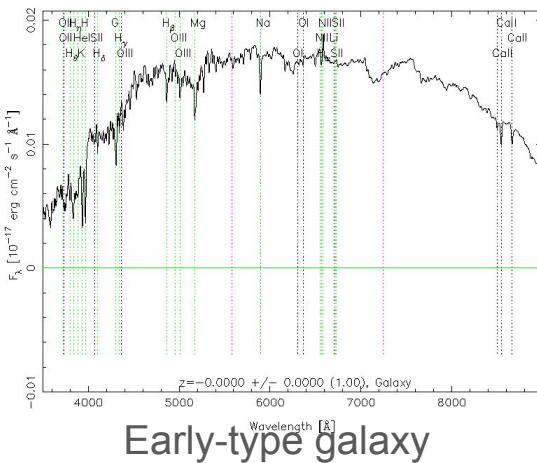
The structure and training
need more improvement

xrayspectroscopy2024 model		116d94e · 2 minutes ago	16 Commits
 Moedel	model		2 minutes ago
 __pycache__	Add files via upload		14 minutes ago
 result	WGAN		12 minutes ago
 .DS_Store	model		2 minutes ago
 Model.ipynb	Add files via upload		2 days ago
 Model.py	111		17 hours ago
 PLOT.py	111		17 hours ago
 README.md	Update README.md		18 minutes ago
 ResNet.py	111		17 hours ago
 Train.py	111		17 hours ago
 argparseinfo.py	111		17 hours ago
 hack.ipynb	111		17 hours ago
 load_data.py	111		17 hours ago

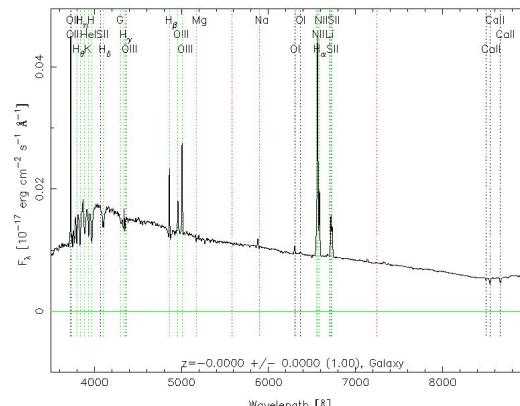
05. Validation Plan

SDSS Spectral Correlation Templates

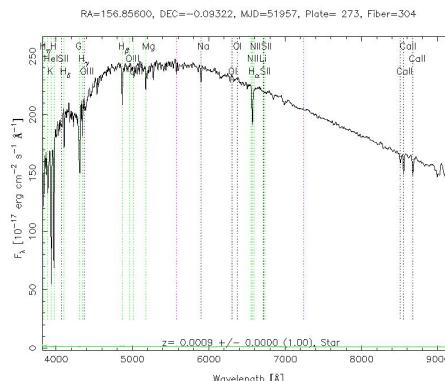
- Spectral templates for redshift measurement using cross-correlation (<https://classic.sdss.org/dr5/algorithms/spectemplates/>)
 - Standard form of spectra (33 types)
 - Containing 6 types of galaxy spectra
⇒ We can check our spectra shape is **similar to galaxy spectra**



Early-type galaxy



Late-type galaxy

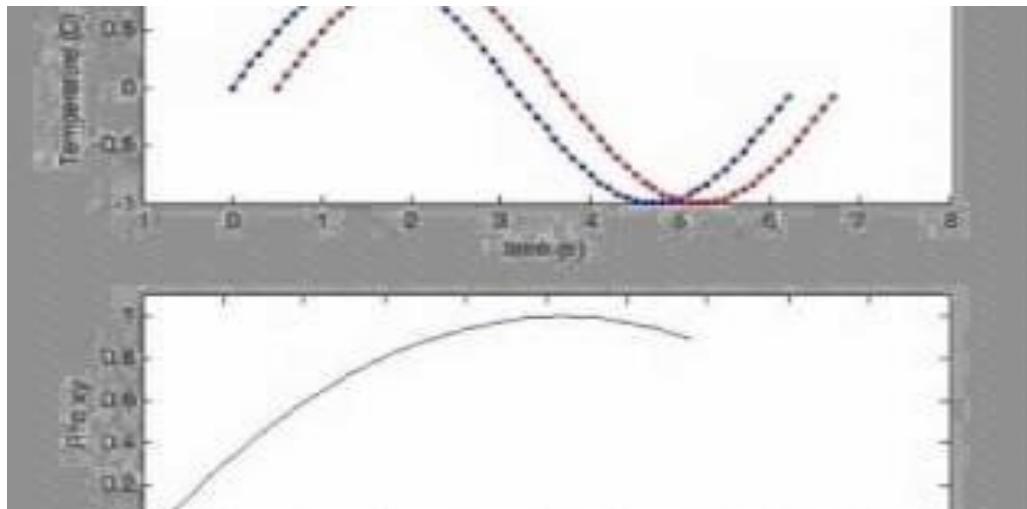


G-star

Cross-Correlation

- A way to measure **how similar two signals** are to each other
 - It checks the similarity after **shifting** one of the series
 - Find the **best-matching** shift and **template**
 - redshift measurement

$$(f \star g)(\tau) \triangleq \int_{-\infty}^{\infty} \overline{f(t - \tau)} g(t) dt$$



Cross-Correlation Tools : RVSNUpy

- Python packages to obtain redshift of spectra using cross-correlation (developed by Taewan Kim, SNU, 2024 in prep.)
 - Provide redshift, best-matching template
 - Provide r-value (cross-correlation coefficient, **how similar signal is?**)
- We can test our GAN model result to answer following questions
 - “Is the model’s output similar to the galaxy’s spectra?”
 - “Is it more similar than the real SDSS spectra (input data)?”
 - “How similar is it quantitatively?”

Q & A

B

Hack presentation:

(4) Interpretation of GAN's latent space/ Improvement of GAN's performance based the latent space configuration

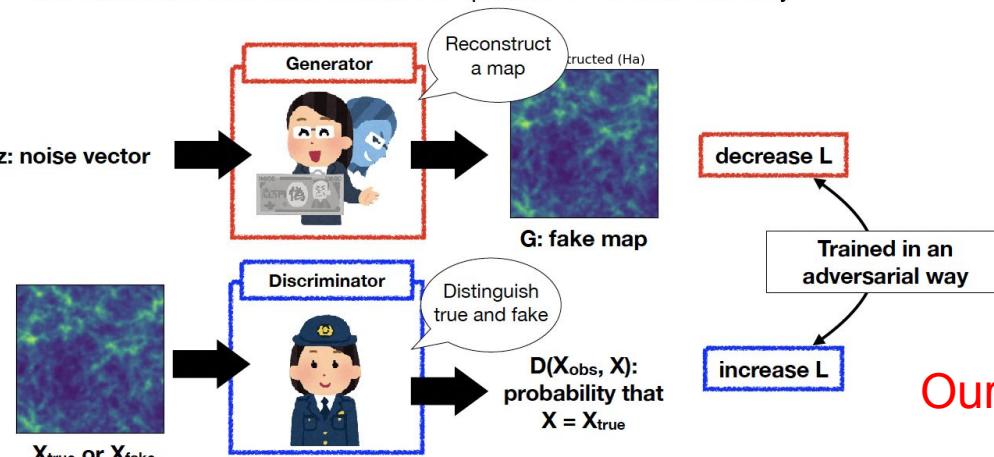
Group B

Our goals

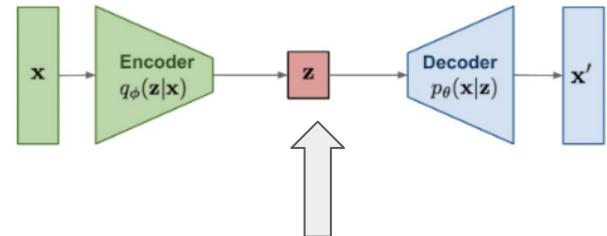
- To interpret GAN's latent space
- To gain a deeper understanding of the latent space of GANs

Generative Adversarial Network (GAN)

- GAN: Generator and Discriminator are updated in an adversarial way.

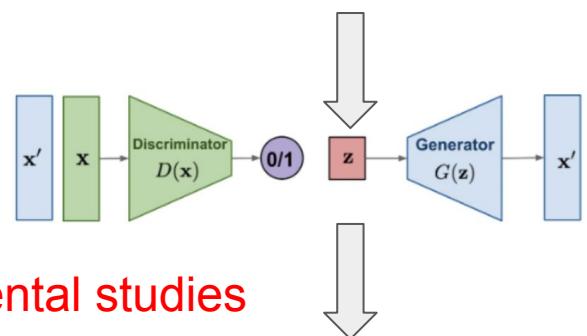


VAE: maximize
variational lower bound



Latent Space

GAN: Adversarial
training



Our experimental studies

Physical parameters
Noise + Physical parameters
Noise

From Moriwaki-san's slides

Tasks

Obtaining a model with good performance:

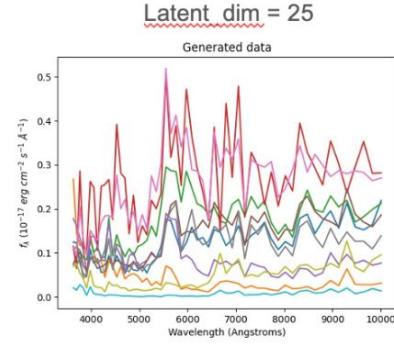
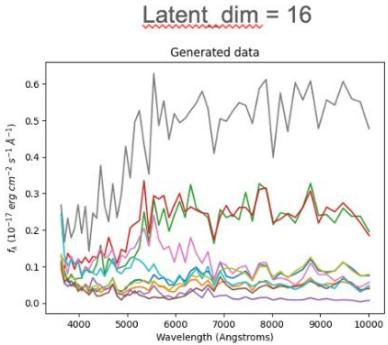
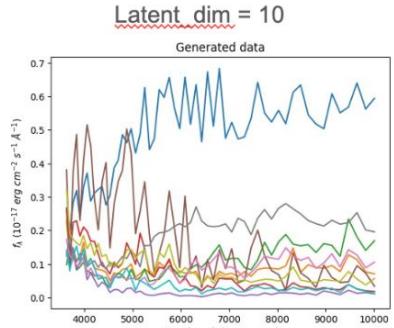
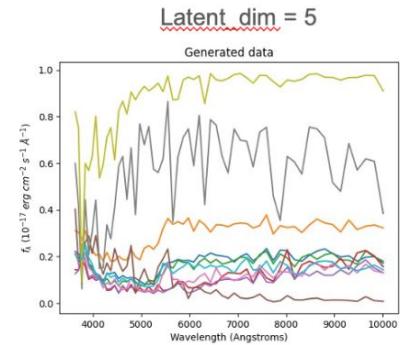
- Experimenting different setups for GAN

Configuring latent space:

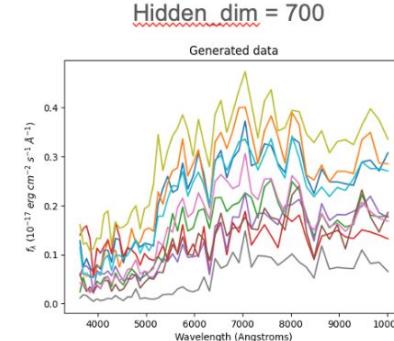
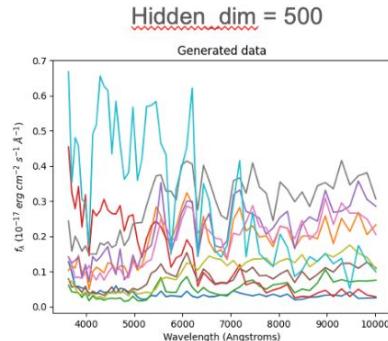
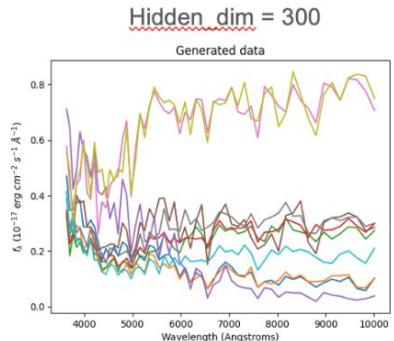
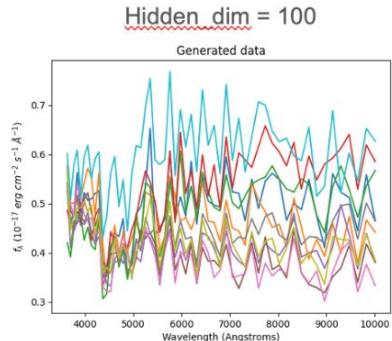
- Experimenting different setups for latent space

Experimenting different setups for GAN: latent_dim, hidden_dim

1. hidden_dim = 512



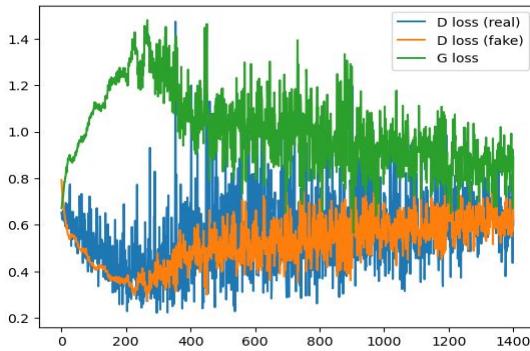
2. latent_dim = 16



Methods to setting up GAN's latent space

- (1) Brute-force approach
 - Interpolated noises between two random noises for the latent space
 - Changing input noise type
- (2) Conditional modelling approach
 - Physical parameter as the latent space
 - Integrating physical parameters with noise parameters for the latent space

Gaussian noise vs Uniform noise

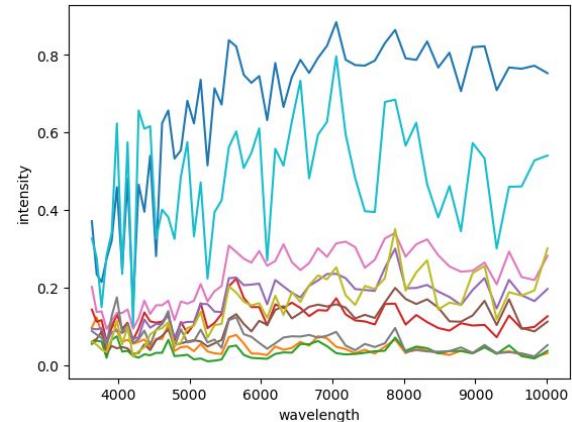
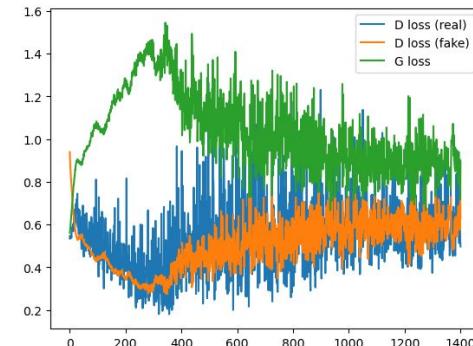
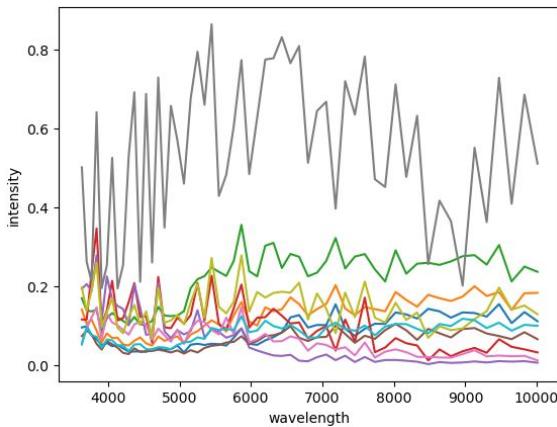


Latent_dim = 16

Hidden_dim = 512

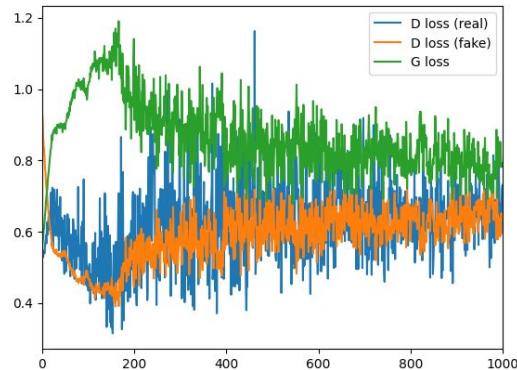
Epochs = 5

Qualitatively not
much difference to
be seen.

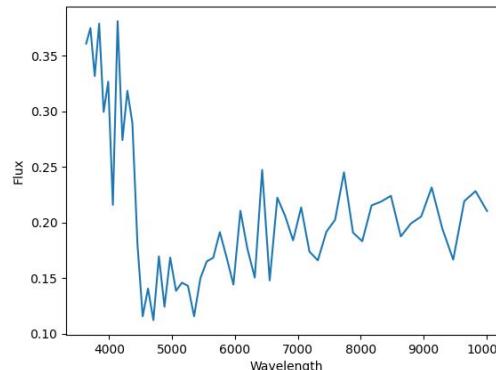
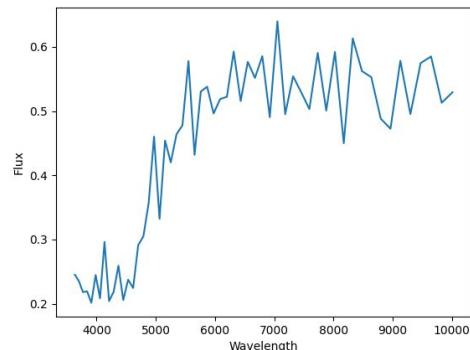
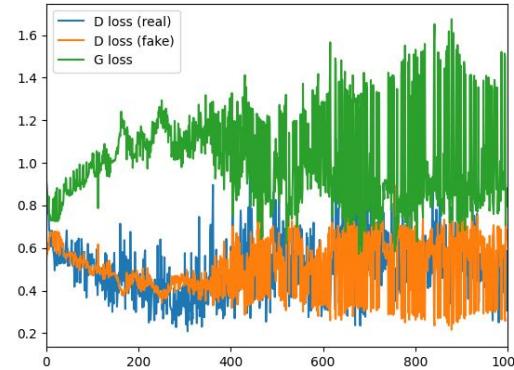


Physical parameters as the latent space (latent_dim=4)

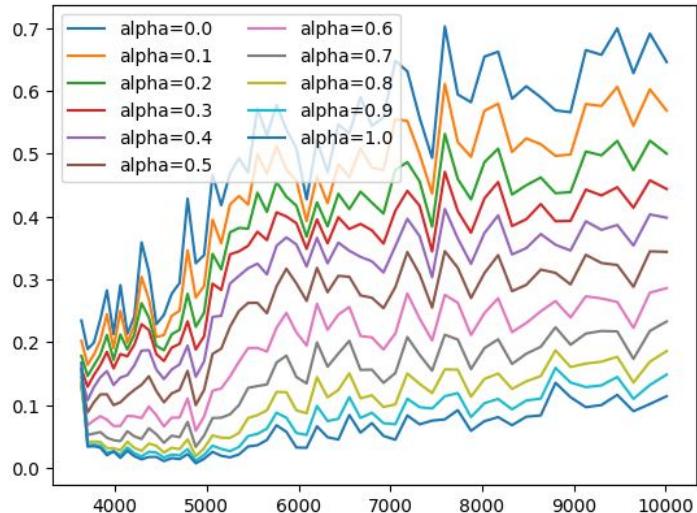
Noise case



Physical parameter



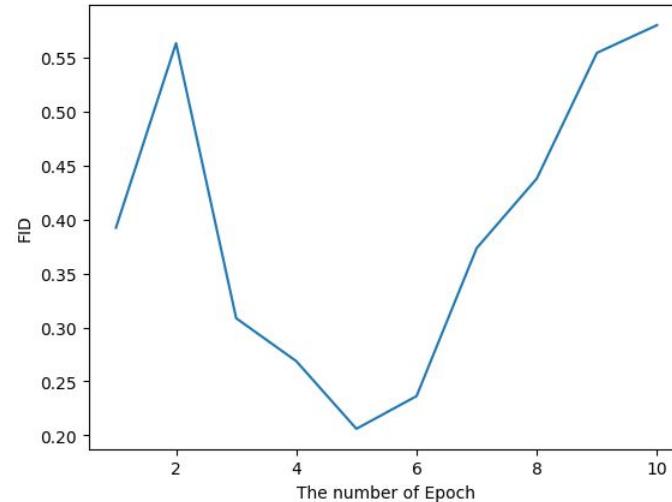
1. Brute-force



```
noise_interp = (1 - alpha) * noise1  
+ alpha * noise2
```

Fréchet Inception Distance(FID)

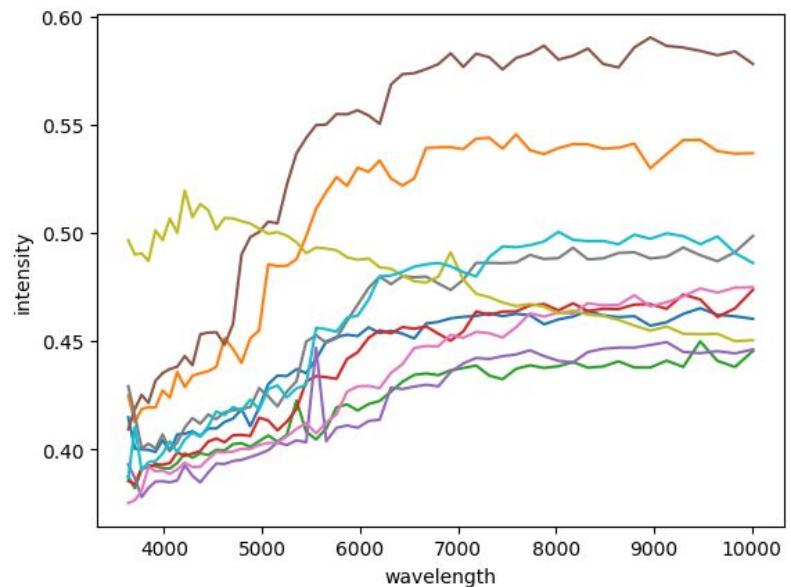
: a metric for evaluating the quality of generated images and specifically developed to evaluate the performance of GAN.



→ **5 is good:)**

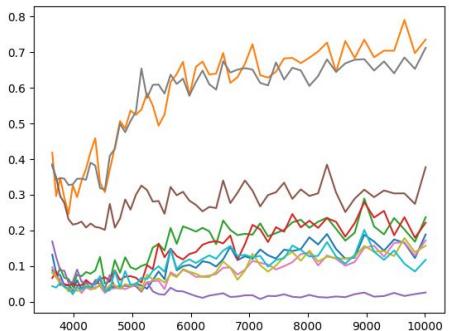
2. Conditional modelling: Parameter space as the latent space

Samples from **True** data



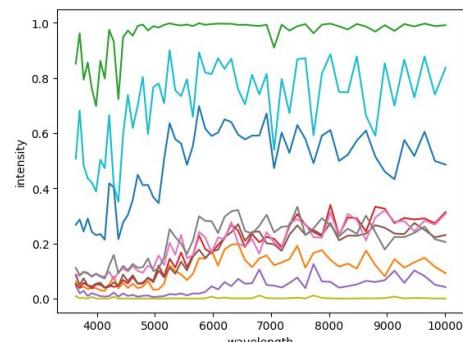
4 latent params:

- 4 random noise



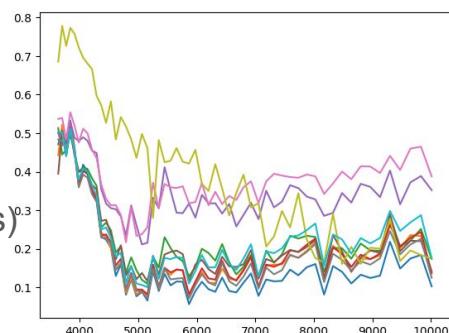
4 latent params:

- 2 random noise
- 2 physical param (z, age)



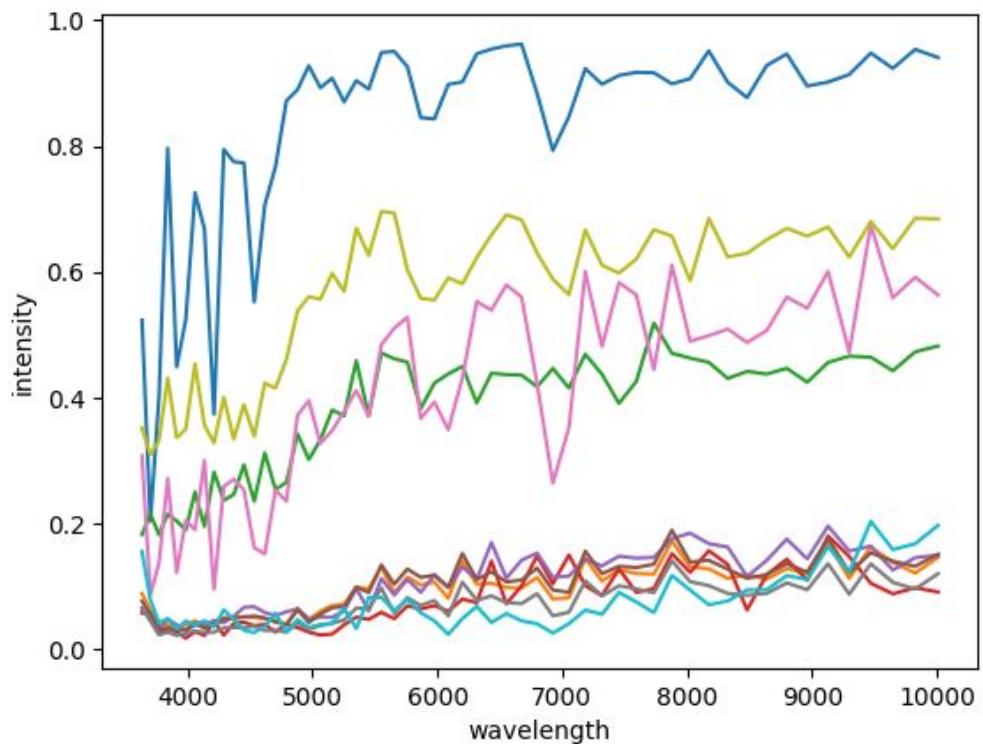
4 latent params:

- 4 physical params (z, age, metallicity, smass)



8 latent params:

- 4 noise
- 4 physical params
(z, age, metallicity, smass)



Summary

- We have experimented different setups of GAN model to generate SDSS spectra
- Using physical parameters in the latent space (conditional GAN) did not show any better results

The motivation of this task was to find a way to interpret the latent space of a GAN. Can we find a way to make better choices for choosing the latent space of a GAN?

In conclusion, we can qualitatively see that the latent space is important but it will require much more detailed study to make quantitative statements.

C

Predicting Galaxy redshifts with ML

Member

**DONG Shihao, FUJIWARA Tatsuki, JEON Mingyu, KISHIKAWA Ryo,
MANZONI Giorgio, NISHIMOTO Shimpei, and TAKAKURA Satoru**

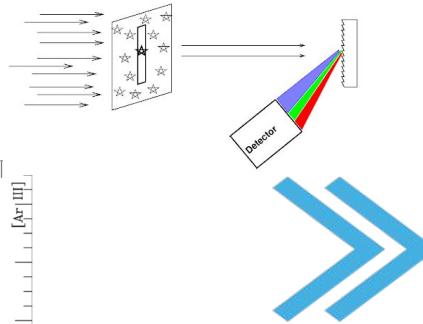
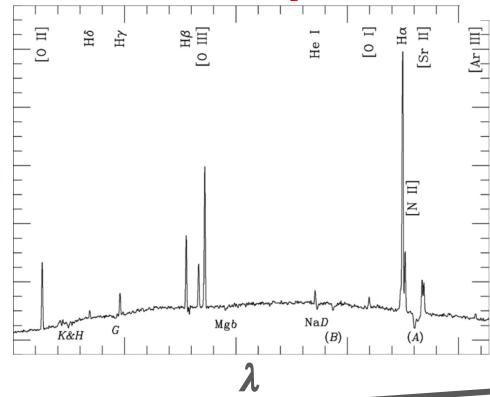
Thanks: Michelle Ntampaka & Claire Murray

Agenda

- **Introduction and aim of this work**
 - Show Skelton et al. 2014 as previous work
- **Results**
 - **Show results of ML models**
 - Gradient-Boosted Tree
 - Random Forest
 - Multi-Layer Perceptron Regressor
 - Support Vector Regression
 - **Importance of Feature Engineering**
- **Conclusion**

Introduction and aim of this work

Spectroscopic
redshift (spec-z)



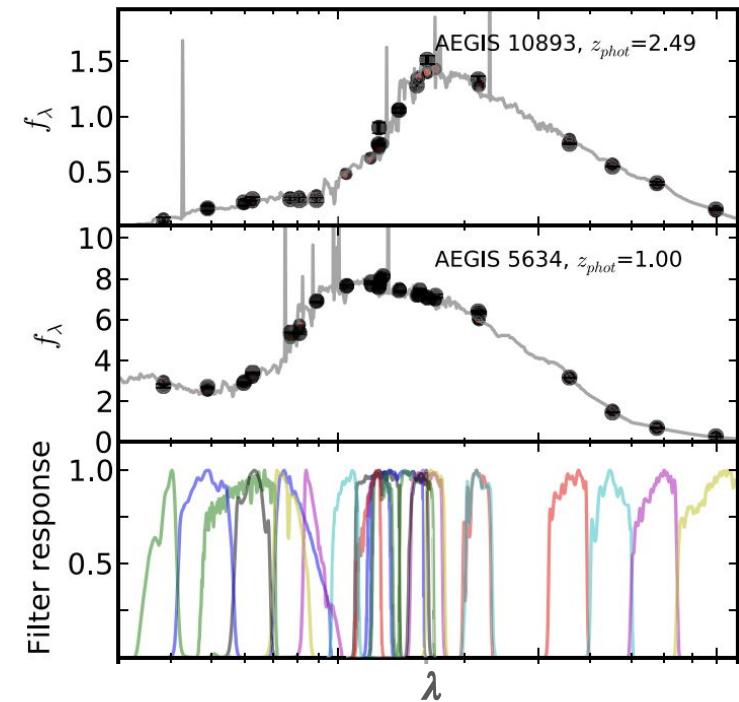
Photometric
redshift (photo-z)



Observing
Time (money)

Traditionally to estimate galaxy redshifts from photometric bands we rely on **SED fitting**

Introduction and aim of this work



The disadvantage of SED fitting

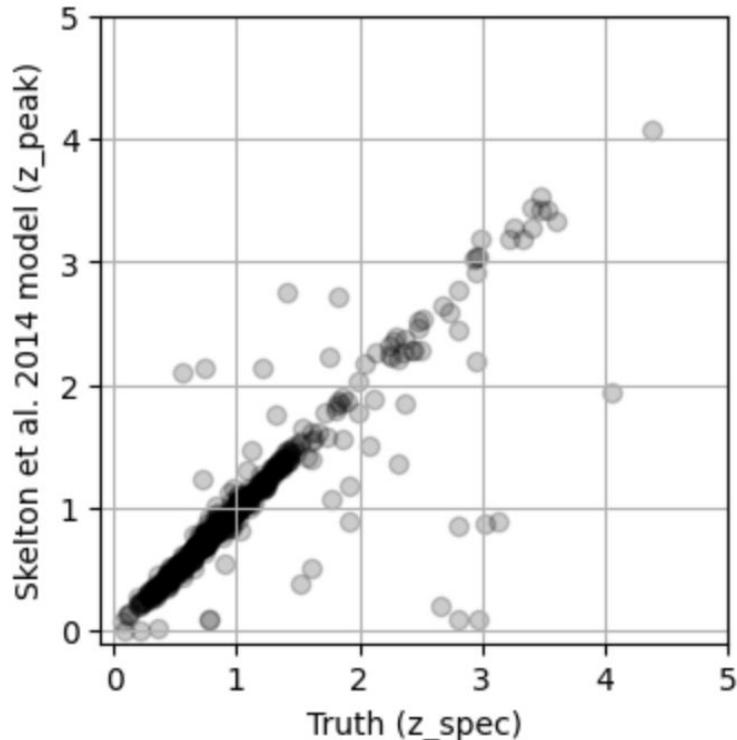
- 1 Need for the library of theoretical models
- 2 Depends on the assumption on star formation history of the galaxy

The more filter we have
the better the SED is constrained

AIM

CAN ML DO BETTER?

The Data (Skelton et al. 2014)



- 1 CANDLES+3D HST (HST) collected both **photo-z** and **spec-z** over **900 arcmin²**
- 2 Using **9 HST filter**
- 3 They apply EAZY photo-z code
(traditional template based photo-z)

AIM

CAN ML DO BETTER?

Machine learning models we tested

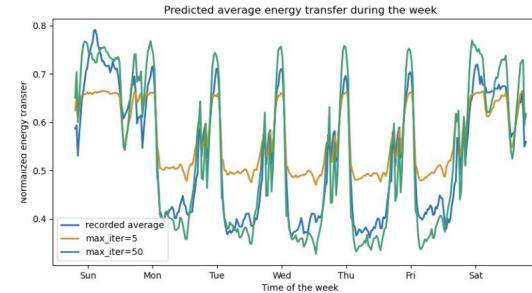
- Random Forest
- Gradient-Boosted Tree
- Multi-Layer Perceptron Regressor
- Support Vector Regression
- ...

Regression

Predicting a continuous-valued attribute associated with an object.

Applications: Drug response, stock prices.

Algorithms: [Gradient boosting](#), [nearest neighbors](#), [random forest](#), [ridge](#), and [more...](#)

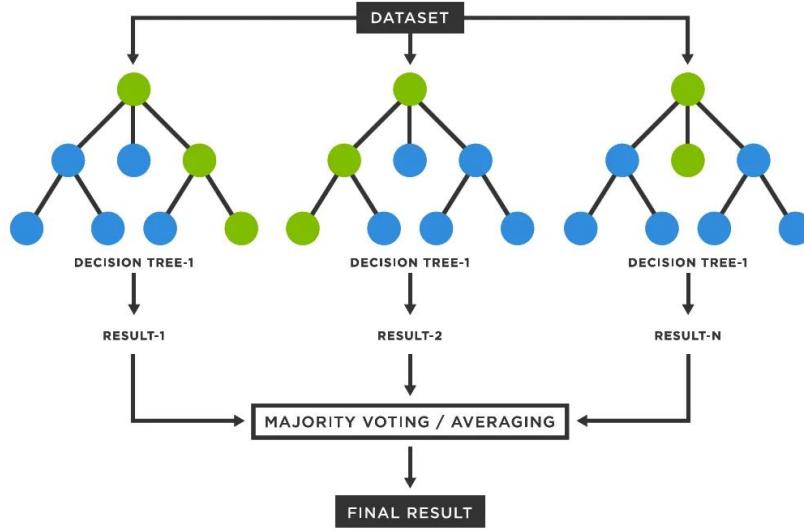


Glossary

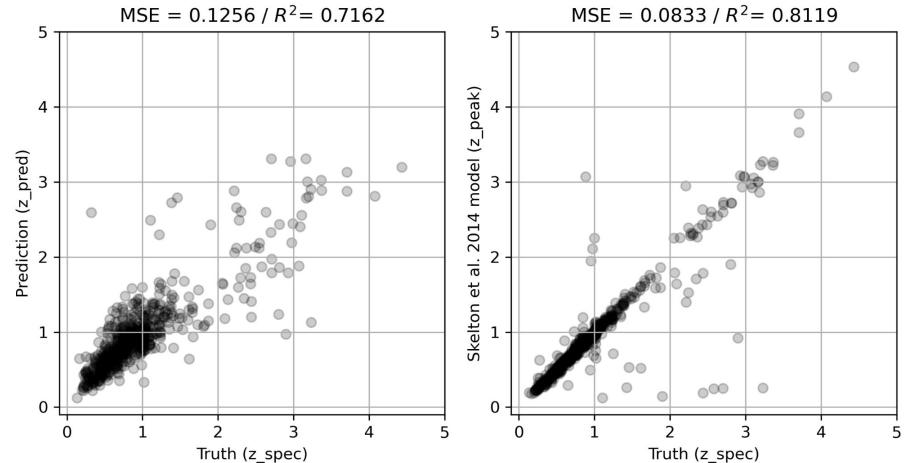
MSE

MSE is a common metric used to evaluate the performance of regression models. It measures the average of the squares of the differences between predicted and actual values. We compare mse of each model.

Random Forest

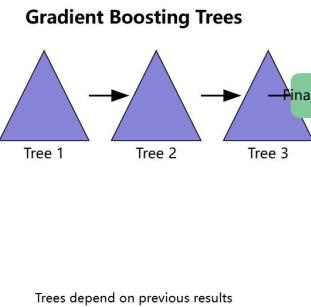
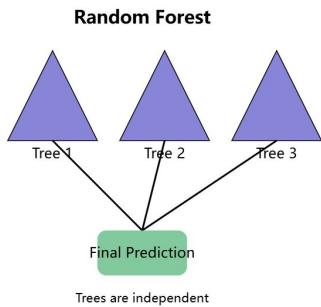


Random Forest vs. Skelton et al. 2014



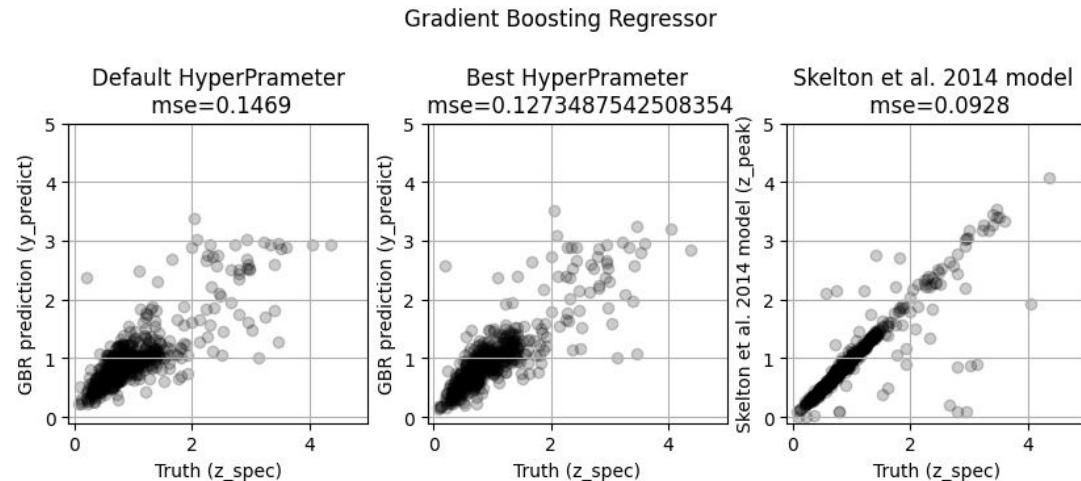
GBT(Gradient-boosted Tree)

GBT vs. skelton et.al.2014



GBT

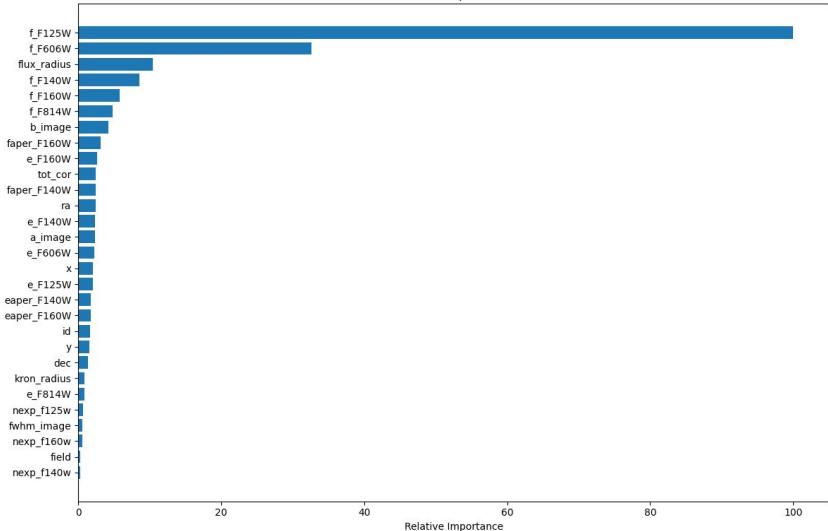
- sensitive to parameter settings
- requires careful tuning
- Time consuming...



We searched hyperparameters at 500 times using bayesian optimization, and picked up the hyperparameter pattern when MSE became the lowest

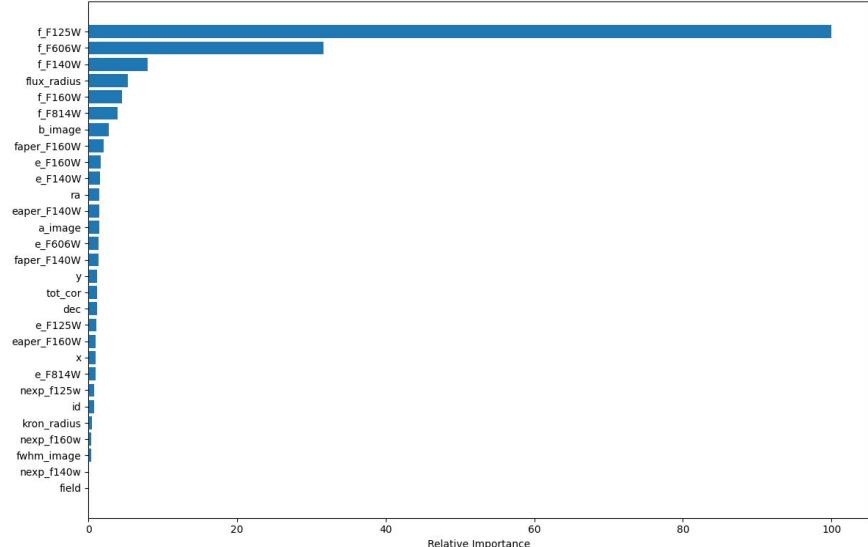
GBT vs Random Forest

Feature Importance



Feature importance in GBT

Variable Importance in Random Forest Regression

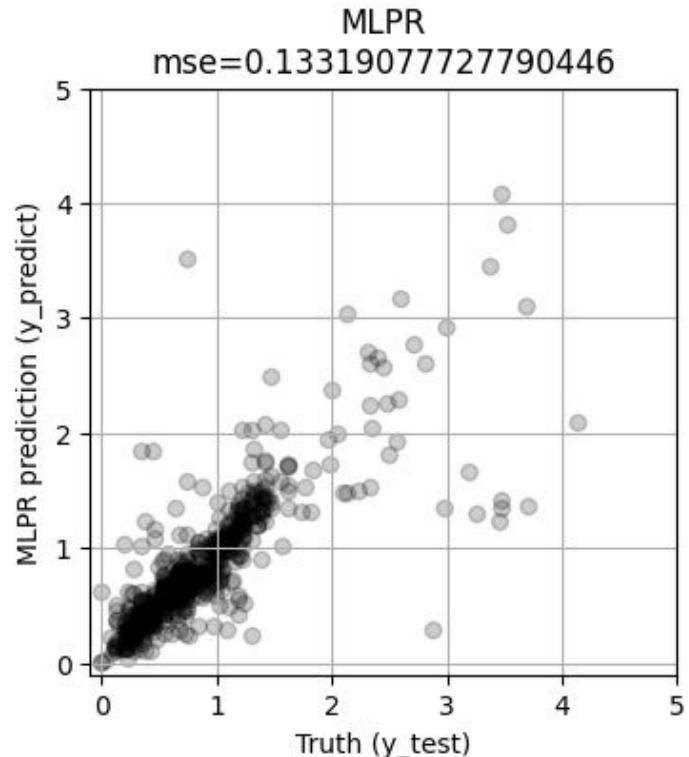
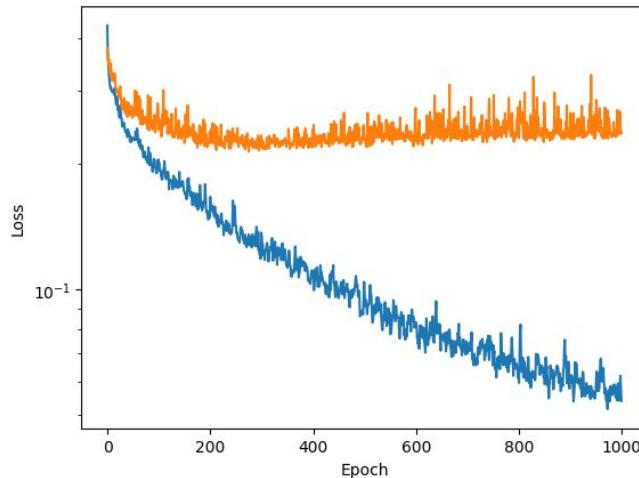


Feature importance in RF

MLP regressor

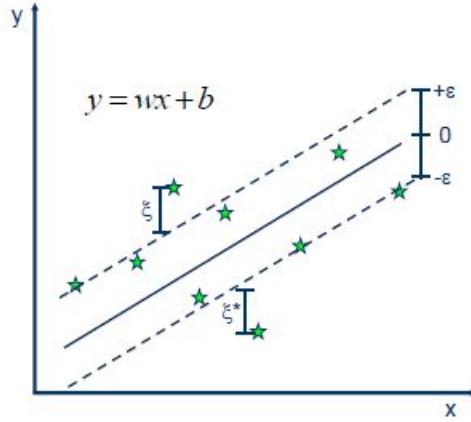
Hidden layers: (256, 256, 256)

Loss: L1Loss



[notebook](#)

Support Vector Regression



- Minimize:

$$\frac{1}{2} \|w\|^2 + C \sum_{i=1}^N (\xi_i + \xi_i^*)$$

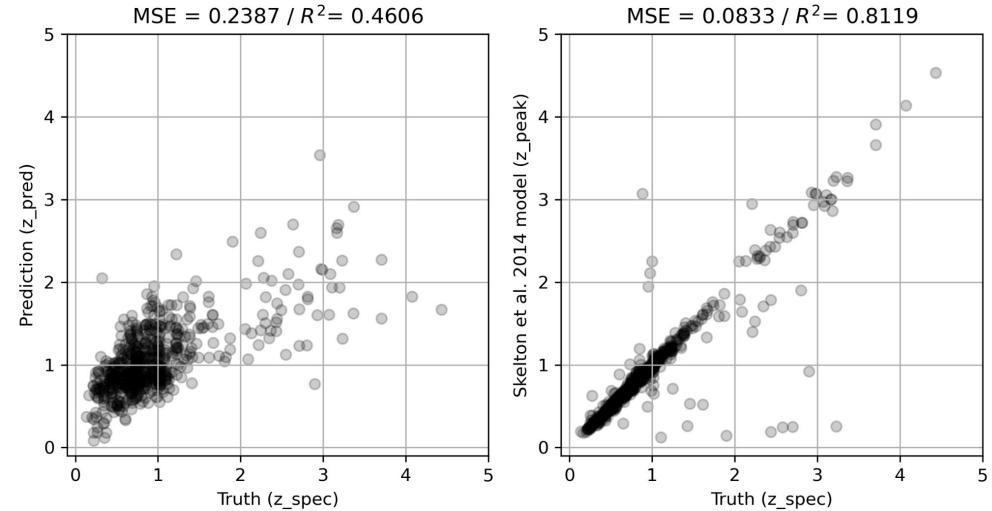
- Constraints:

$$y_i - wx_i - b \leq \varepsilon + \xi_i$$

$$wx_i + b - y_i \leq \varepsilon + \xi_i^*$$

$$\xi_i, \xi_i^* \geq 0$$

Support Vector Regression vs. Skelton et al. 2014



Regression experiment using PyCaret

	Model	MAE	MSE	RMSE	R2	RMSLE	MAPE
rf	Random Forest Regressor	0.2238	0.1337	0.3632	0.7124	0.1448	0.2432
lightgbm	Light Gradient Boosting Machine	0.2261	0.1364	0.3679	0.7061	0.1459	0.2478
et	Extra Trees Regressor	0.2410	0.1463	0.3812	0.6839	0.1518	0.2649
gbr	Gradient Boosting Regressor	0.2448	0.1472	0.3824	0.6821	0.1541	0.2775
dt	Decision Tree Regressor	0.2983	0.2440	0.4894	0.4790	0.1943	0.3187
lr	Linear Regression	0.3652	0.2676	0.5166	0.4188	0.2156	0.4513
br	Bayesian Ridge	0.3644	0.2677	0.5167	0.4188	0.2146	0.4483
ridge	Ridge Regression	0.3693	0.2859	0.5343	0.3800	0.2164	0.4496
ada	AdaBoost Regressor	0.4370	0.3005	0.5478	0.3425	0.2463	0.6345
en	Elastic Net	0.4030	0.3662	0.6040	0.2117	0.2437	0.5309
lasso	Lasso Regression	0.4194	0.4001	0.6315	0.1382	0.2570	0.5683
llar	Lasso Least Angle Regression	0.4194	0.4001	0.6315	0.1382	0.2570	0.5683
omp	Orthogonal Matching Pursuit	0.4591	0.4582	0.6757	0.0137	0.2838	0.6489
dummy	Dummy Regressor	0.4618	0.4665	0.6818	-0.0039	0.2868	0.6572
knn	K Neighbors Regressor	0.4838	0.4846	0.6955	-0.0506	0.2937	0.6450
huber	Huber Regressor	0.4544	0.4959	0.7006	-0.0610	0.2860	0.6099
par	Passive Aggressive Regressor	0.9365	1.9822	1.2151	-3.1235	0.4592	1.3608
lar	Least Angle Regression	0.8460	4.7030	1.2703	-10.2415	0.3619	1.4869

Random Forest is best

Random Forest for photometric redshift estimation

Monthly Notices
of the
ROYAL ASTRONOMICAL SOCIETY

MNRAS **505**, 4847–4856 (2021)
Advance Access publication 2021 May 29



<https://doi.org/10.1093/mnras/stab1513>

Benchmarking and scalability of machine-learning methods for photometric redshift estimation

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ABSTRACT

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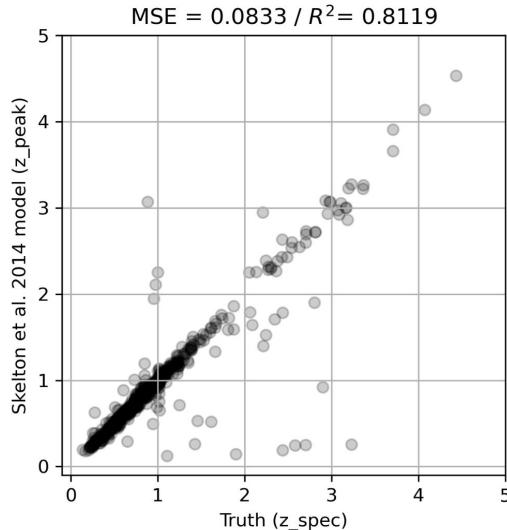
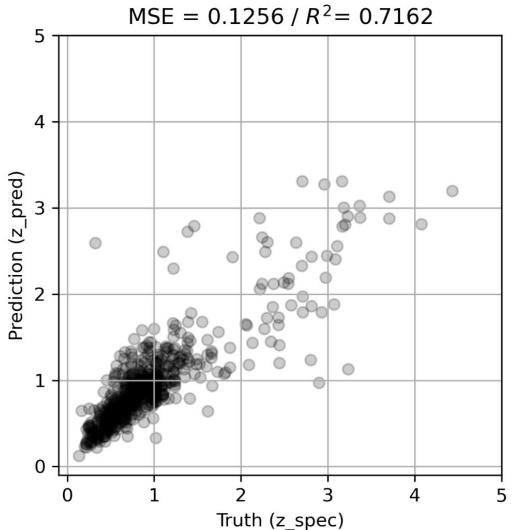
Obtaining accurate photometric redshift (photo- z) estimations is an important aspect of cosmology, remaining a prerequisite of many analyses. In creating novel methods to produce photo- z estimations, there has been a shift towards using machine-learning techniques. However, there has not been as much of a focus on how well different machine-learning methods scale or perform with the ever-increasing amounts of data being produced. Here, we introduce a benchmark designed to analyse the performance and scalability of different supervised machine-learning methods for photo- z estimation. Making use of the Sloan Digital Sky Survey (SDSS – DR12) data set, we analysed a variety of the most used machine-learning algorithms. By scaling the number of galaxies used to train and test the algorithms up to one million, we obtained several metrics demonstrating the algorithms' performance and scalability for this task. Furthermore, by introducing a new optimization method, time-considered optimization, we were able to demonstrate how a small concession of error can allow for a great improvement in efficiency. From the algorithms tested, we found that the Random Forest performed best with a mean squared error, $\text{MSE} = 0.0042$; however, as other algorithms such as Boosted Decision Trees and k -Nearest Neighbours performed very similarly, we used our benchmarks to demonstrate how different algorithms could be superior in different scenarios. We believe that benchmarks like this will become essential with upcoming surveys, such as the Vera C. Rubin Observatory's Legacy Survey of Space and Time (LSST), which will capture billions of galaxies requiring photometric redshifts.

Key words: methods: data analysis – galaxies: distances and redshifts – cosmology: observations.

Importance of Feature Engineering

When using almost all 29 features

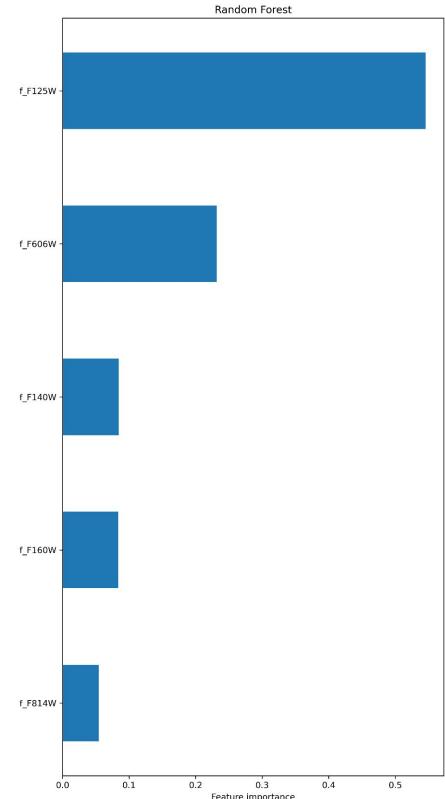
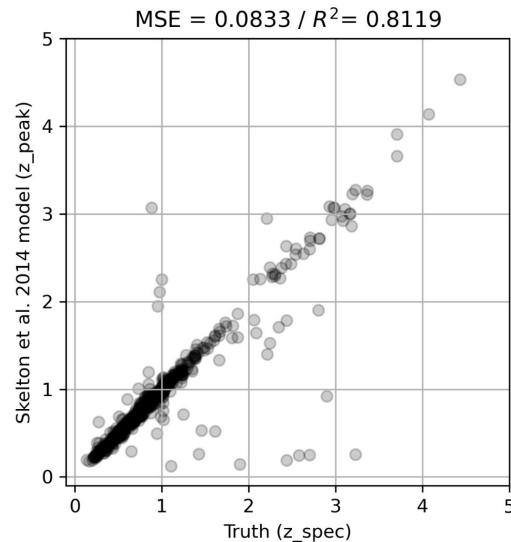
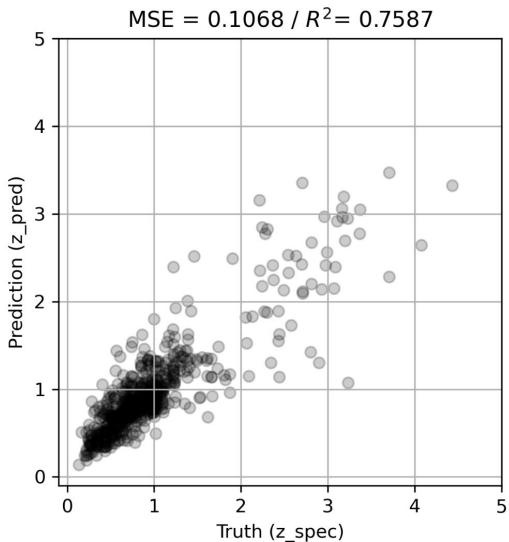
Random Forest vs. Skelton et al. 2014



Importance of Feature Engineering

When using only 5 photometric bands

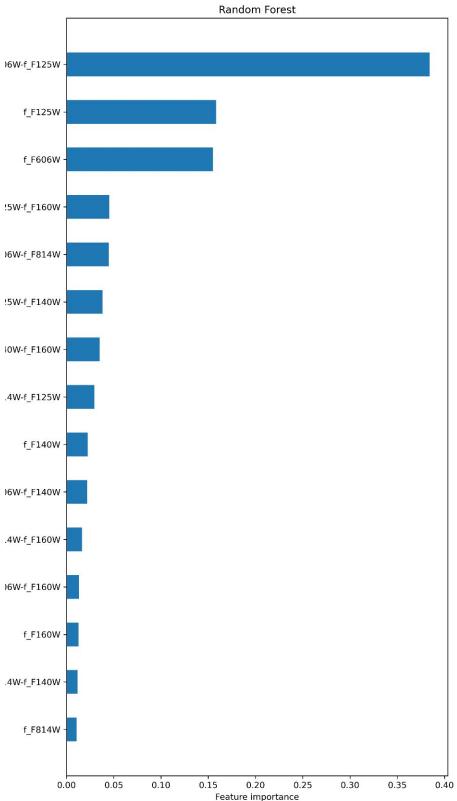
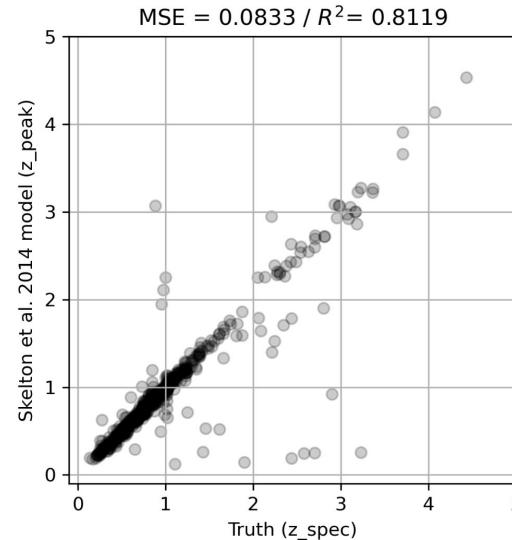
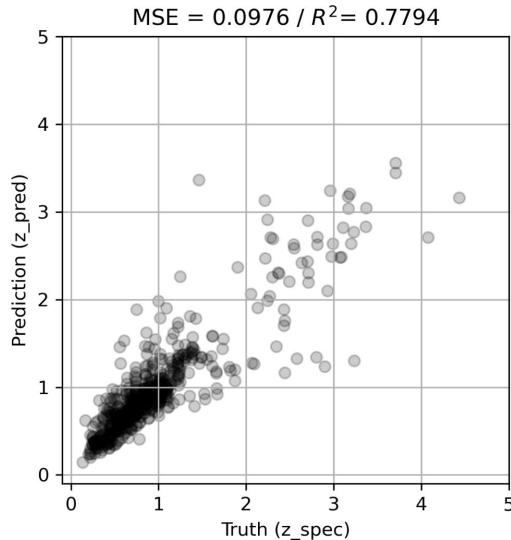
Random Forest vs. Skelton et al. 2014



Importance of Feature Engineering

When using only 5 photometric bands
+ all the possible combinations of colors

Random Forest vs. Skelton et al. 2014



Conclusion

We predict photometric redshifts using machine learning models and compare their performance with the traditional method.

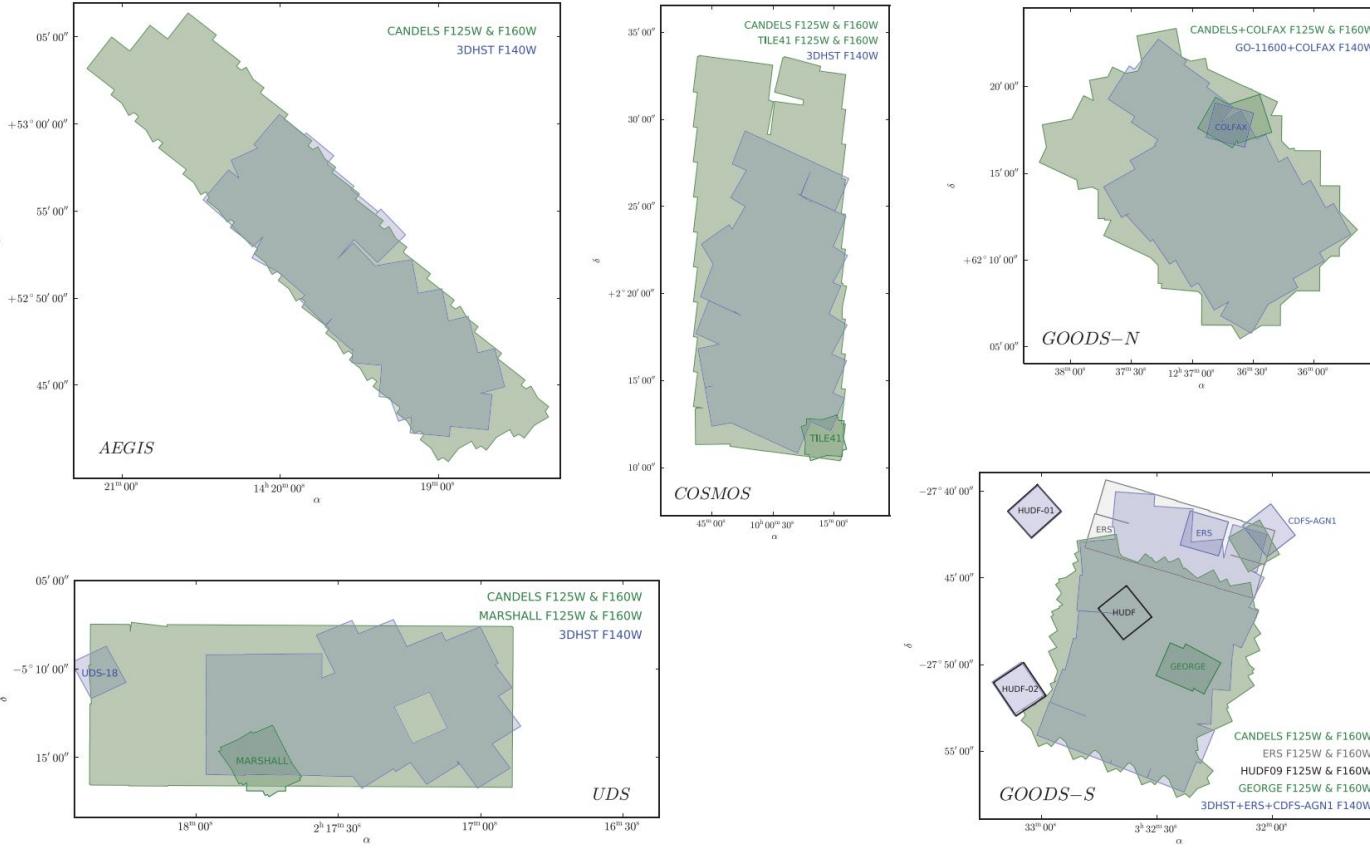
The best machine learning model (random forest) does not outperform the traditional method.

We observe that including irrelevant features can degrade the performance of ML models, while creating physically important features improves their accuracy.

This shows the critical role of feature engineering in machine learning.

Additional slides for discussion

The fields covered by Skelton et al. 2014

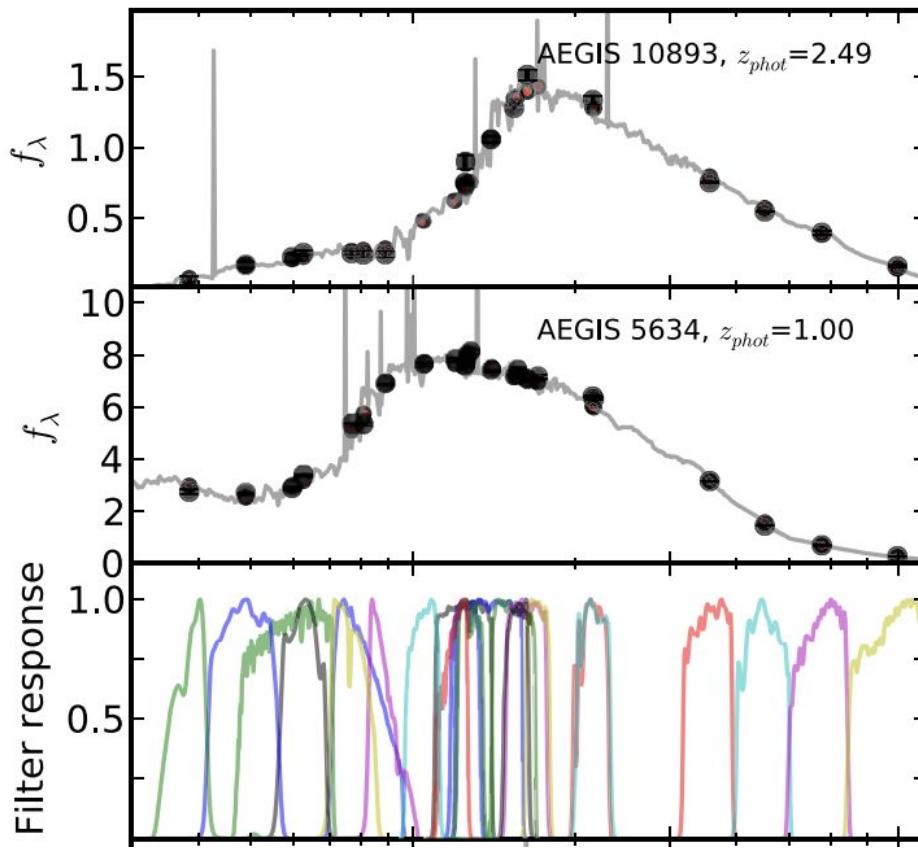


The fields covered by Skelton et al. 2014

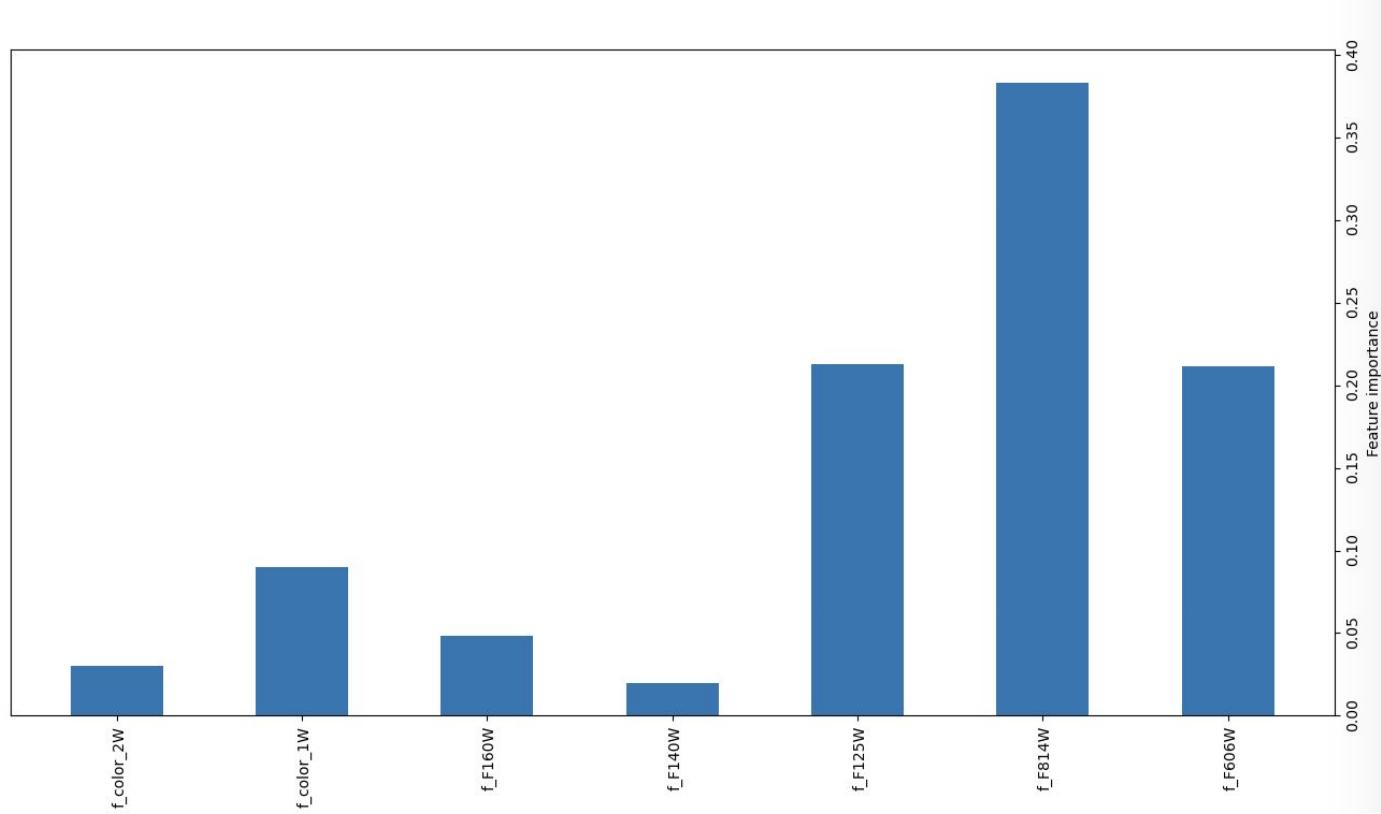
Table 1
3D-HST Fields

Field	R.A. (h m s)	Decl. (d m s)	Total Area (arcmin ²)	Science Area (arcmin ²)
AEGIS	14 18 36.00	+52 39 0.00	201	192.4
COSMOS	10 00 31.00	+02 24 0.00	199	183.9
GOODS-North	12 35 54.98	+62 11 51.3	164	157.8
GOODS-South	03 32 30.00	-27 47 19.00	177	171.0
UDS	02 17 49.00	-05 12 2.00	201	191.2

Examples of photometric points for two example galaxies



Including stellar masses above 10^9 Msun



Data preprocessing is important and could change the important features

D

Galaxy Cluster Masses with CNNs

Group-D: Mingyuan Zhang, Jing Dou, Xufan Hu, Yanchi Liu, Satsuki Sekiguchi, Kosei Matsumoto, Haosong Wang

Sep. 6, 2024 @Osaka University



中國科学院
CHINESE ACADEMY OF SCIENCES



李政道研究所
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TOHO UNIVERSITY
NATURE LIFE MAN
GHENT UNIVERSITY

南京大學
NANJING UNIVERSITY



Estimation of Galaxy Cluster Masses with CNNs

Goal: use a CNN to estimate the mass of a galaxy cluster from x-ray mock observations.

Assignments:

- (1. Reproduce the paper's results.
- (2. Apply a rotationally invariant CNN,
and see if that approach improves the results!

Hot media in Galaxy clusters emit X-ray radiation primarily through bremsstrahlung

→ this emission may tell us information of the inside of galaxy clusters



Composite image of the Perseus galaxy cluster. Image credit: NASA / CXO / Fabian et al / Gendron-Marsolais et al / NRAO / AUI / NSF / SDSS.

[1] picture

<https://www.sci.news/astronomy/x-ray-signal-perseus-galaxy-cluster-dark-matter-05556.html>

Why machine learning?

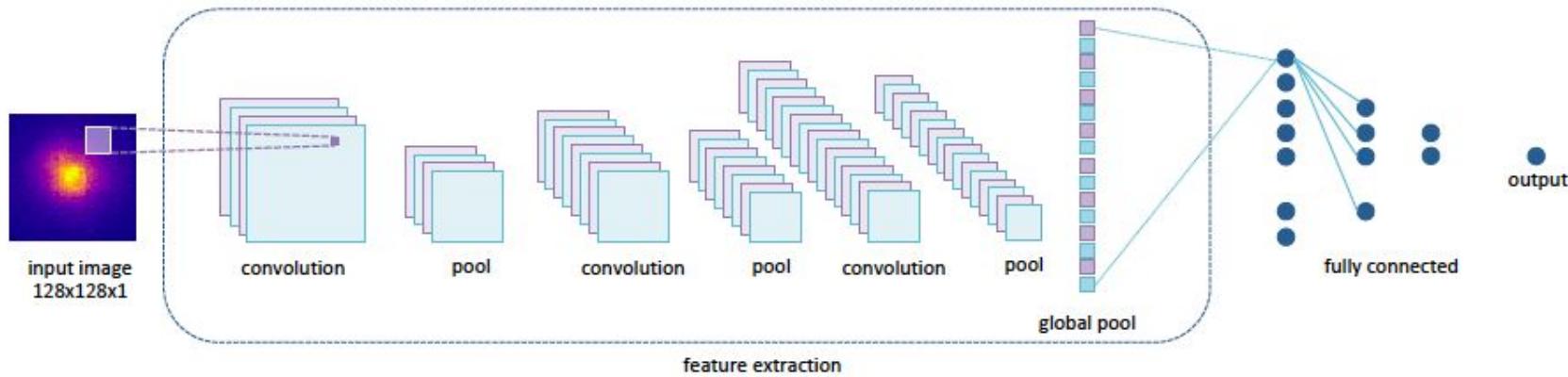
Traditional ways to estimate the cluster mass: X-ray luminosity, temperature...

Uncertainties: physical processes (e.g., gas cooling, cluster mergers) are not properly reflected in these methods... more complex...

→ Machine learning can help us!

Method: based on X-ray mock images of the [IllustrisTNG simulation](#), we can develop a CNN model to accurately estimate cluster masses

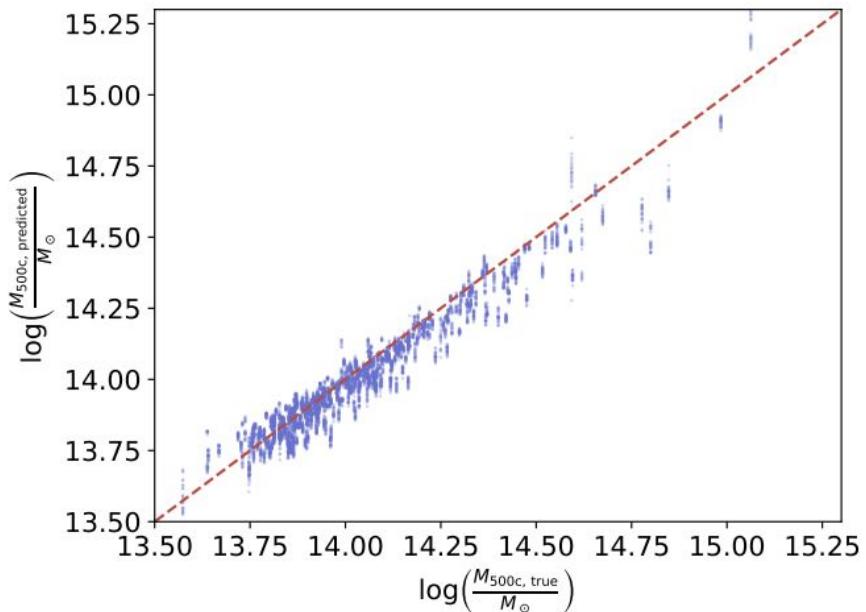
Architecture of the convolutional neural network



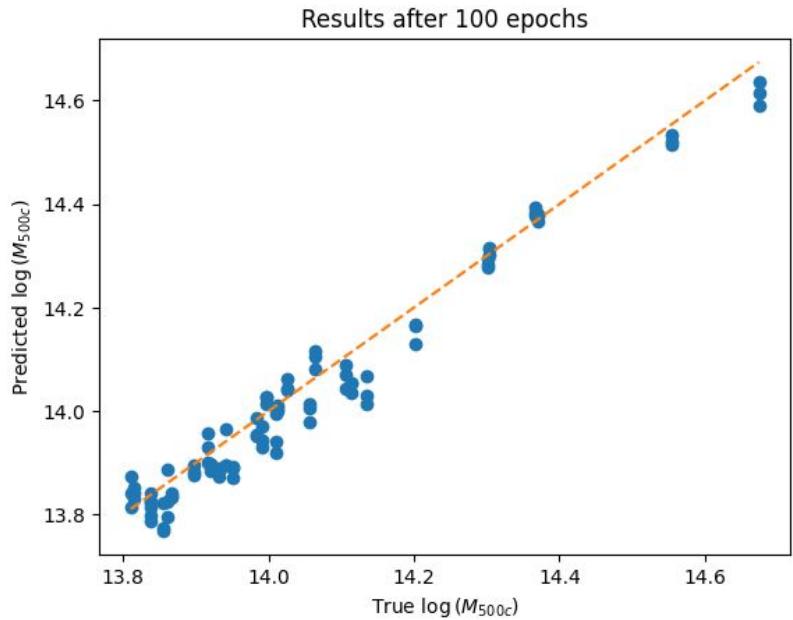
(1. Recreation of the results

Predicted mass with CNN vs true mass

(Ntampaka,et.al.2019)



Predicted mass with CNN vs true mass (Our work)



→ We reproduced the original result successfully.
but can we improve the accuracy for the estimation of the cluster mass?

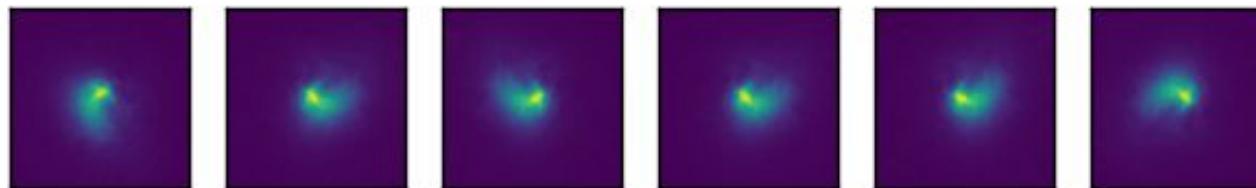
(2. Can we improve the original results?

Problems: the number of the galaxy cluster samples (986) may be too small.
there is not so many variations of the galaxy clusters.

Method: the estimation of the cluster masses is rotationally invariant to the images.
we can increase the variations and number of the galaxy clusters by rotation.

- (1) Data augmentation: rotate the galaxy cluster images
- (2) Rotate the filters in CNN
- (3) Change the architecture of the network

Data augmentation: rotated images



Results

- Image augmentation and one more layer
- Image augmentation and new CNN
- Rotation filters

Method :Image augmentation and one more layer

- Image Augmentation
 - `ImageDataGenerator(rotation_range=360, horizontal_flip=True, vertical_flip=True)`
 - 10 times amount of data
- CNN structure
 - Add a new convolution layer with 128 filters

```
input_shape = (image_size, image_size, 1)
model = Sequential()
model.add(Conv2D(16, kernel_size=(3, 3), input_shape=input_shape, activation='relu'))
model.add(MaxPooling2D(pool_size=(2, 2)))

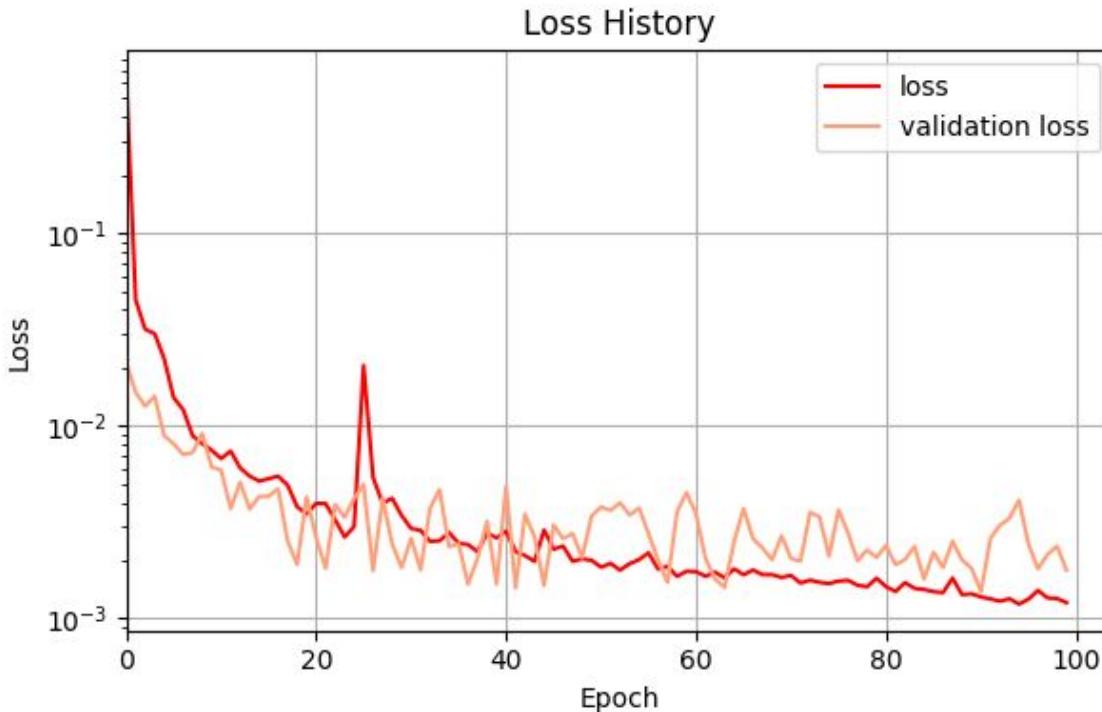
model.add(Conv2D(32, kernel_size=(3, 3), activation='relu'))
model.add(MaxPooling2D(pool_size=(2, 2)))

model.add(Conv2D(64, kernel_size=(3, 3), activation='relu'))
model.add(MaxPooling2D(pool_size=(2, 2)))#use AveragePooling2D

model.add(Conv2D(128, kernel_size=(3, 3), activation='relu'))
model.add(MaxPooling2D(pool_size=(2, 2)))#use AveragePooling2D
```



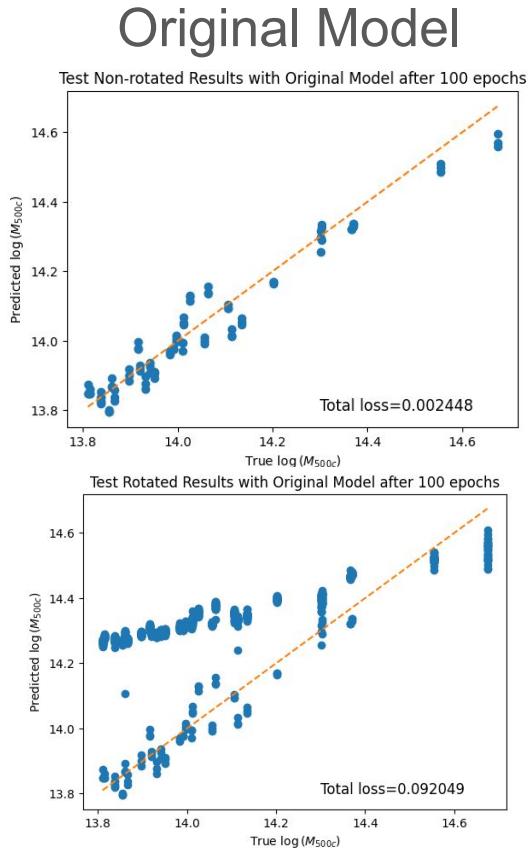
Training 1:Image augmentation and one more layer



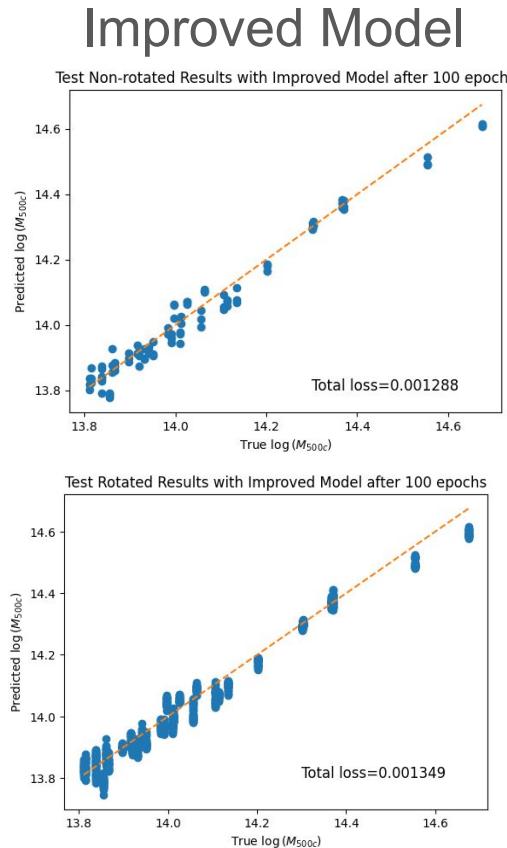
- setup
 - epochs=100
 - batchsize=16
- cost
 - platform: RTX 3090Ti
 - ~22GB
 - ~100s

Result 1: Image augmentation and one more layer

Non-rotate
d test set



Rotated
test set



- Non-rotated test set
- 0.002488/0.0012
88~1.93
- Rotated test set
- 0.092049/0.0013
49~73.70

Method 2: Image augmentation and new CNN

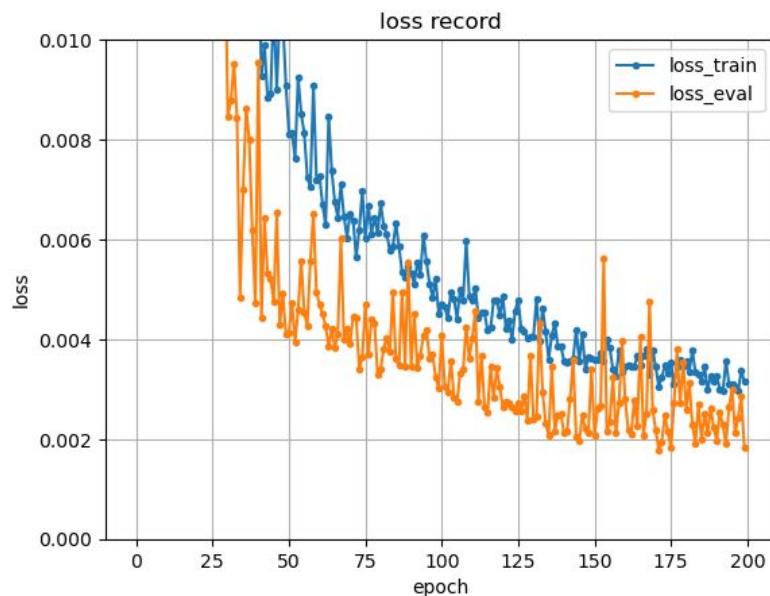
- **Data Augmentation**
 - `ImageDataGenerator(rotation_range=180, horizontal_flip=True, vertical_flip=True)`
 - 12 times amount of data for **train**, **validation**, and **test** dataset.

- **New CNN structure**
 - Add more convolution layers
 & Increase filters of convolution layers
 $(16, 32, 64 \Rightarrow 32, 32, 64, 64, 128, 128)$
 - Use **AveragePooling** to replace MaxPooling at the end
 - Change filters of Dense layers

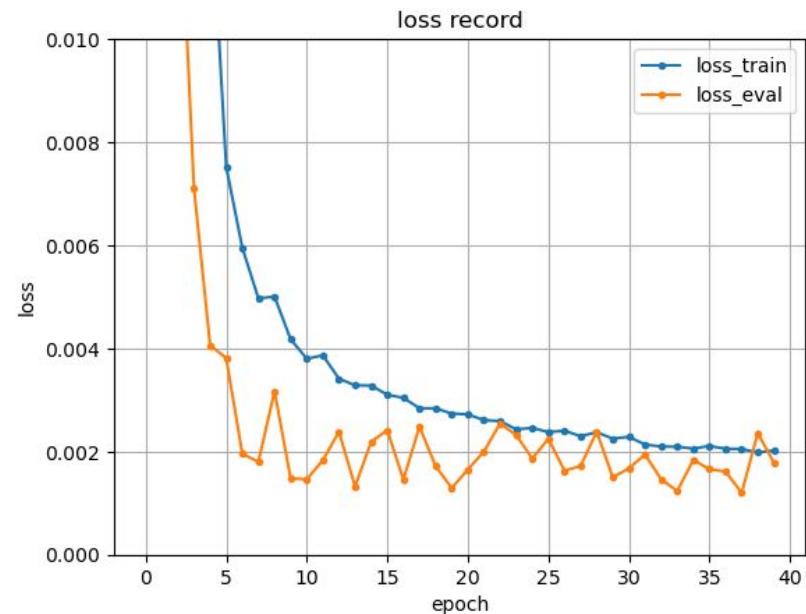
```
1 input_shape = (image_size, image_size, 1)
2 model = Sequential()
3 model.add(Conv2D(32, kernel_size=(3, 3), strides=1, padding="valid", input_shape=input_shape, activation='relu'))
4 model.add(Conv2D(32, kernel_size=(3, 3), strides=1, padding="valid", activation='relu'))
5 model.add(MaxPooling2D(pool_size=(2, 2), strides=2))
6 model.add(Conv2D(64, kernel_size=(3, 3), strides=1, padding="valid", activation='relu'))
7 model.add(Conv2D(64, kernel_size=(3, 3), strides=1, padding="valid", activation='relu'))
8 model.add(MaxPooling2D(pool_size=(2, 2), strides=2))
9 model.add(Conv2D(128, kernel_size=(3, 3), strides=1, padding="valid", activation='relu'))
10 model.add(Conv2D(128, kernel_size=(3, 3), strides=1, padding="valid", activation='relu'))
11 #28*28*128
12 model.add(AveragePooling2D(pool_size=(4, 4), strides=4)) # 使用平均池化代替最大池化，可以追踪tail特征
13 #7*7*128
14 model.add(GlobalAveragePooling2D())
15 #128
16 model.add(Dropout(0.2))
17 model.add(Dense(128, activation='relu'))
18 model.add(Dropout(0.2))
19 model.add(Dense(64, activation='relu'))
20 model.add(Dense(32, activation='relu'))
21 model.add(Dense(1, activation='linear'))
```

The structure of improved model

Training 2: Image augmentation and new CNN



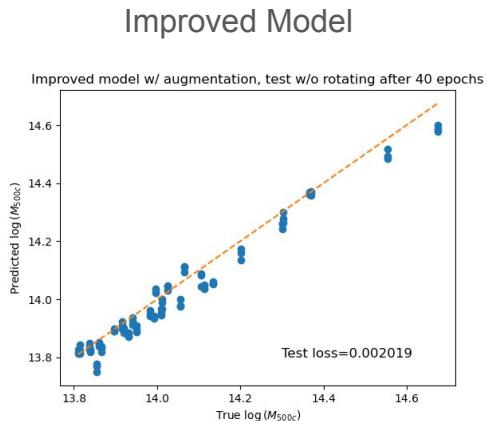
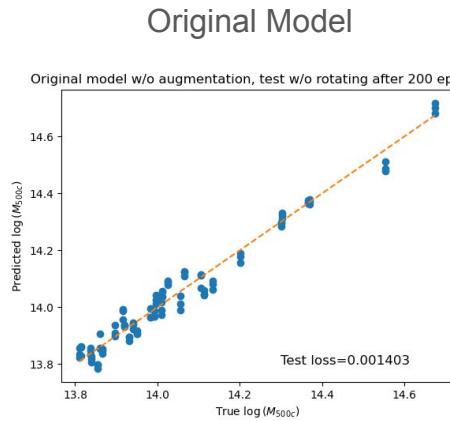
Loss of original model (epochs = 200)



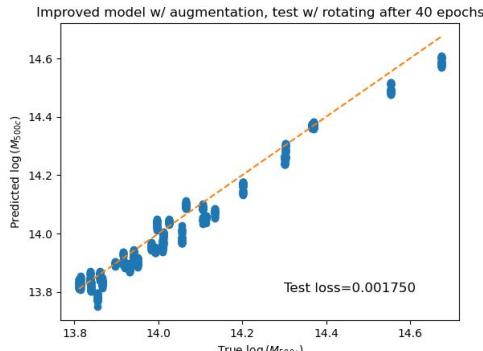
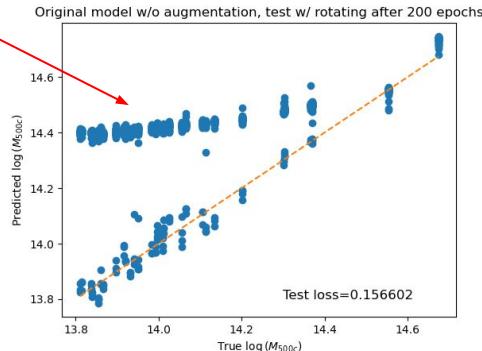
Loss of improved model (epochs = 40)

Result 2: Image augmentation and new CNN

Non-rotated
test dataset



Rotated
test dataset



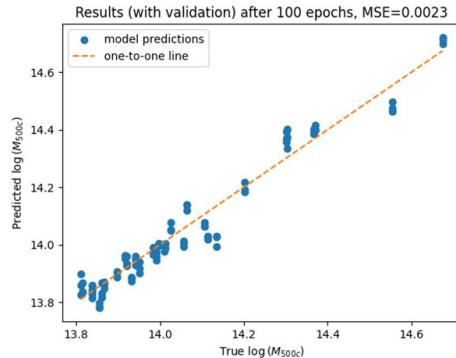
- **Similar loss of both models, evaluated through non-rotated test dataset**
- **Original model fails to distinguish the rotated images** X
- **Improved model can!** ✓

Method 3: Model augmentation with rotation filters

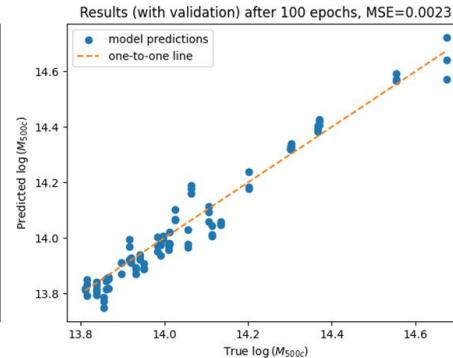
- With the class of `keras.layers.RandomRotation`, we add an extra rotational layer into the CNN, attempting to achieve a **Rotational invariant CNN**.
- The `RandomRotation` class contains 5 parameters, here are 2 important ones:
 - `factor`: it controls the rotation degree of the filter, if `factor = 0.2`, we are going to rotate the filter in a random degree between $(-0.2 \cdot 2\pi, 0.2 \cdot 2\pi)$.
 - `fill_mode`: it controls how we fill the missing pixels, 'nearest' is usually a good choice.

Result 3: Model augmentation with rotation filters

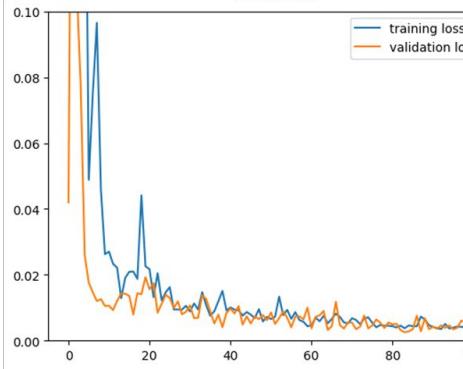
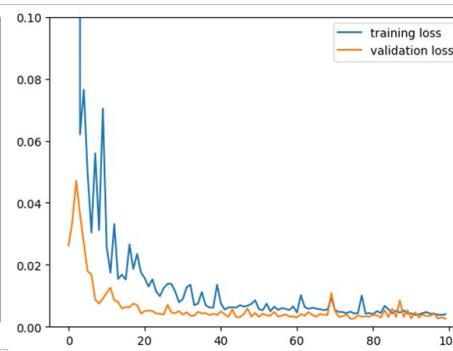
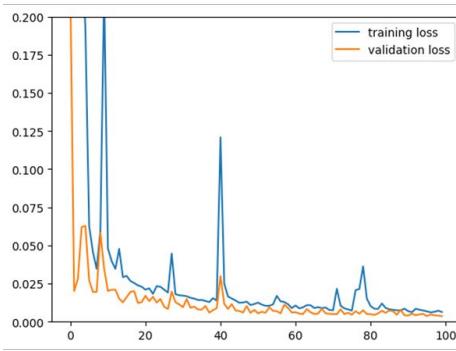
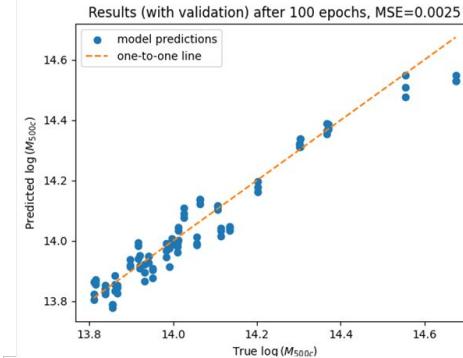
1 rotational layer, factor = 0.01



1 rotational layer, factor = 0.1

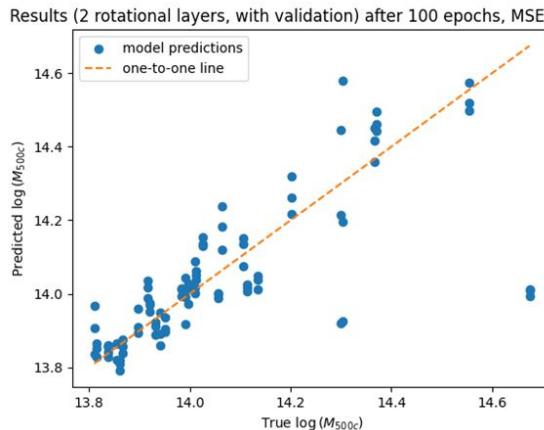


1 rotational layer, factor = 0.2

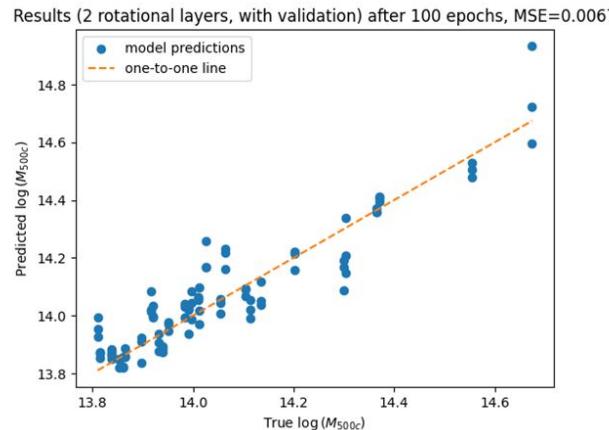


Result 3: Model augmentation with rotation filters

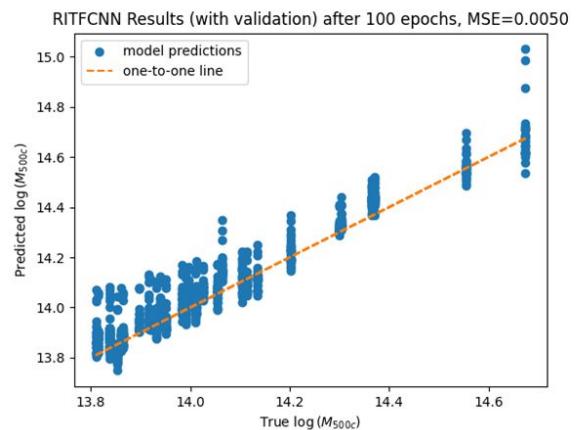
2 rotational layers, factor=0.1



3 rotational layers, factor=0.1



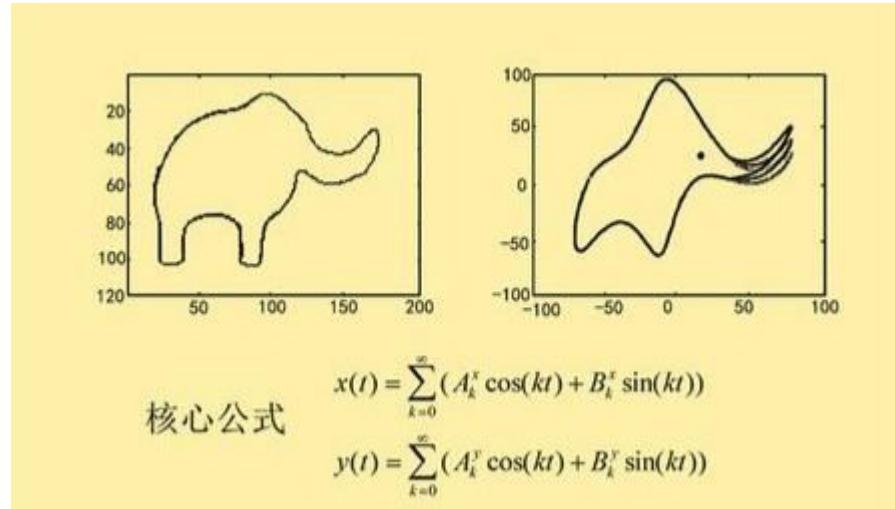
1 rotational layer,
1 transition layer,
1 flip layer
Max Ultra Plus version



Run 10 training and the result is not good at all.

Discussion

- (1) Interpret result?
- (2) other CNNs
- (3) risks of more layers



Conclusion

- We tried to improve the estimation the cluster mass from X-ray mock images with **ROTATION**.
- The smaller the rotation degrees are, the better result we get, but not that good.
- Extra layers of reflection and SO2 symmetry are not helpful, for they may mess up the image size and pixels thus resulting in more problems.

Methods	the ratio “original loss / our loss”
data augmentation	not improved
data augmentation + adding Conv. layer	1.93
data augmentation + adding Conv. layer + increasing filters	1.44
model augmentation with rotation filters	about 1.50, but not stable

Reference:

- [1] <https://www.sci.news/astronomy/x-ray-signal-perseus-galaxy-cluster-dark-matter-05556.html>
- [2] M. Ntampaka, J. Zuhone, D. Einstein, et al., (2019), arXiv:1810.07703v2

E

Using CNNs to infer the fundamental parameters of the Universe

Presenter: Zhao ZHANG, Tao JI, Nobuyuki SAKAI

Code: Zhao ZHANG (CNN), Zitao HU, Xiaoyue CAO(ResNet18), Tao JI(Keras)

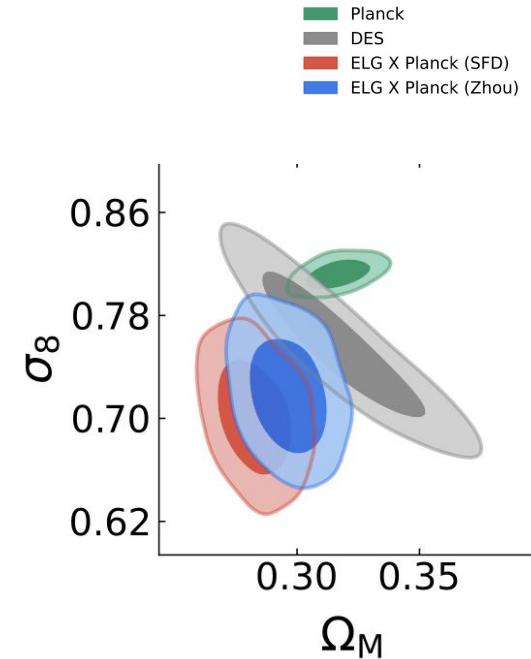
PPT slides: Tao JI, Zhao ZHANG, Yushan XIE, Xiaoyue CAO

Discuss: Nobuyuki SAKAI, Seo-eun LEE

Thanks: Leander Thiele & Michelle Ntampaka

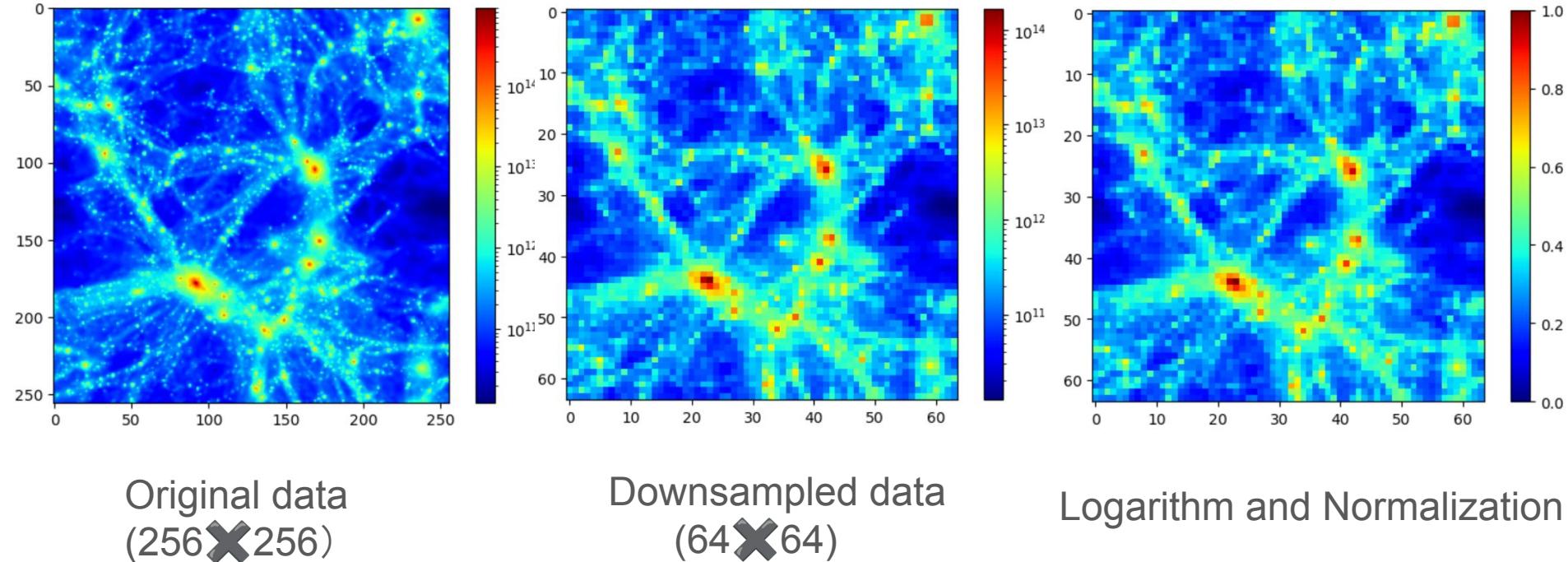
Why interesting?

- Challenge: precise estimation of cosmological parameters validating cosmological models and unlocking the puzzles of the Universe such as Hubble and S8 tensions
- Inferring cosmological parameters from highly non-linear structures is challenging for classical methods based on explicit physical models.
- Constrain the feedback process of the Universe like Active galactic nucleus (AGN) and Stellar feedback (SN, SN wind).
- For current simulation, we unable to return the starting point (nonlinear disturbance)
- For us, CNN is new thing.



Karim+24

Data preprocessing



Original data
(256×256)

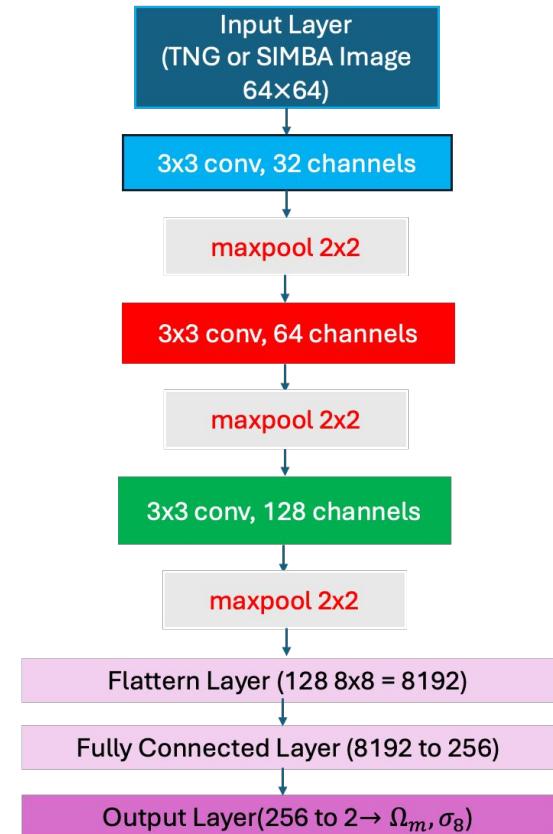
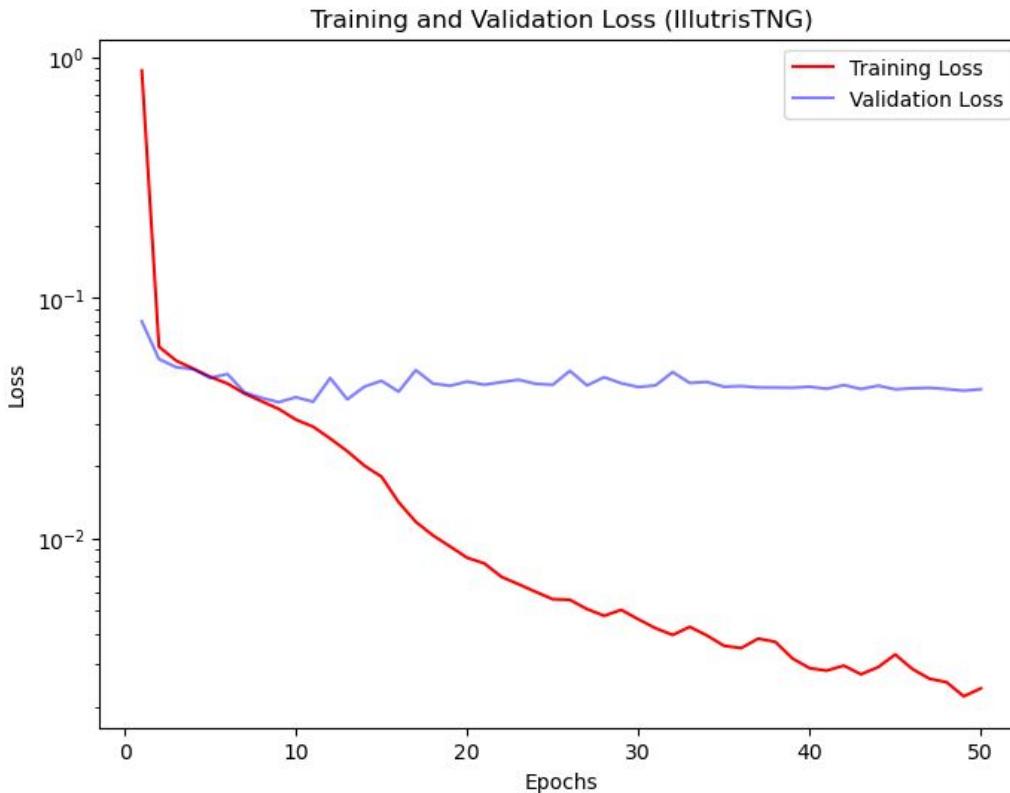
Downsampled data
(64×64)

Logarithm and Normalization

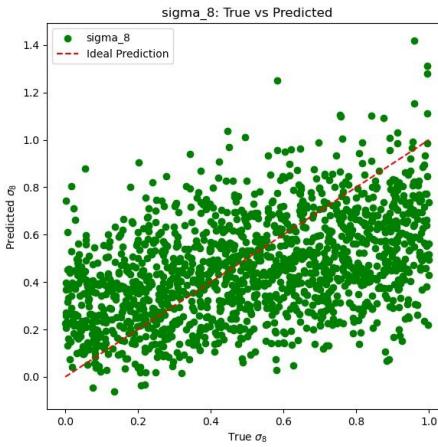
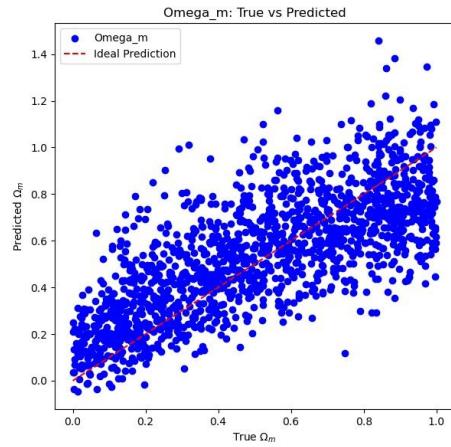
We have 1000 (simulations) × 15 (field of view) pictures
with 2 observables (Mtot and P,
and 6 parameters Ω_m , σ_8 , SN1, AGN1, SN2, AGN2)
in IllustrisTNG or SIMBA simulation

Traditional CNN Model Architecture (Pytorch)

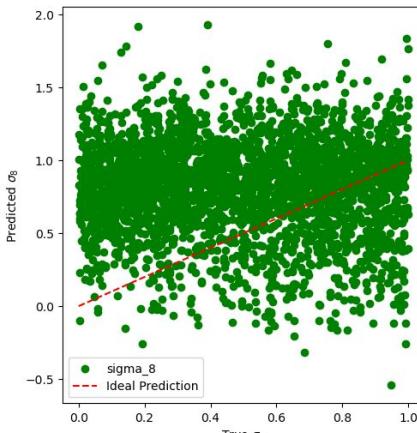
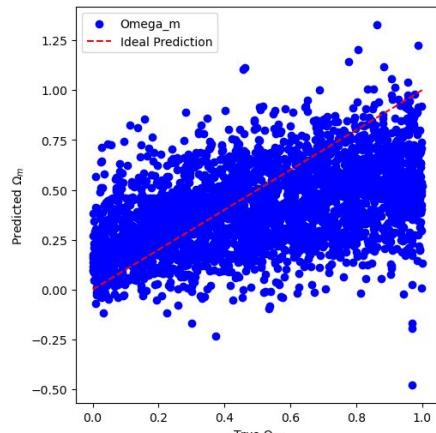
train and test using IllustrisTNG data (7:2:1 train:validation:test)



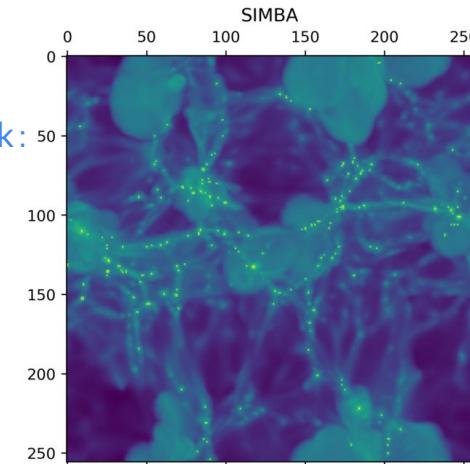
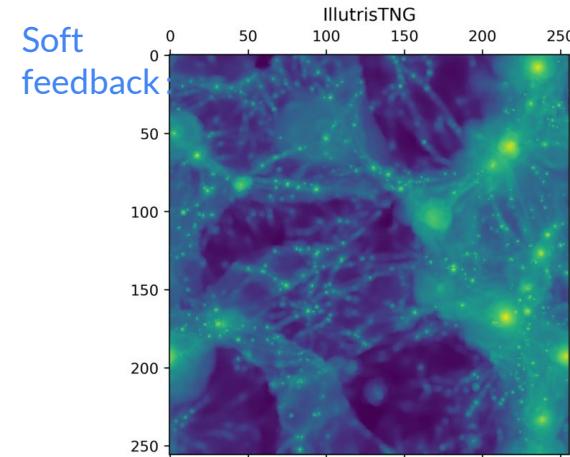
Train using IllustrisTNG data (7:2:1 train:validation:test) and test on both



IllustrisTNG train set

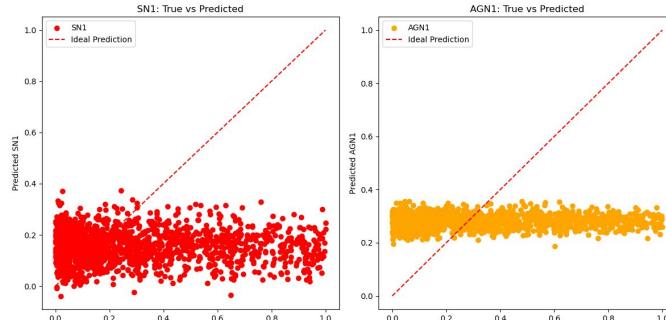
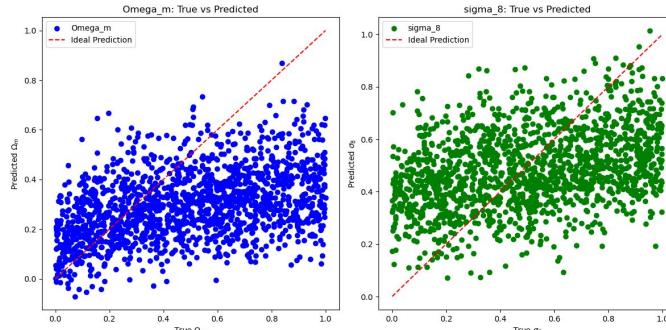


SIMBA prediction by TNG-trained model

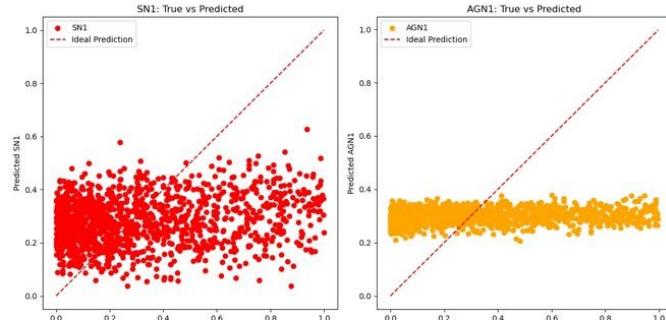
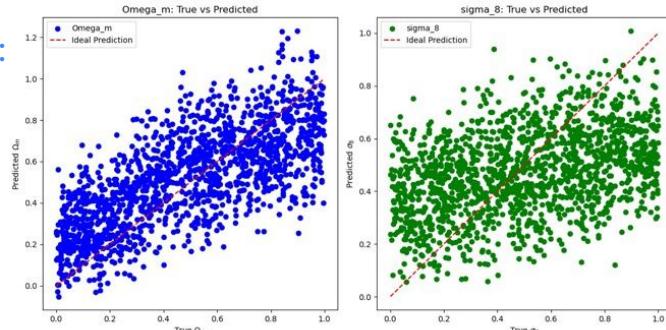


6 parameters comparison between IllustrisTNG and SIMBA

Illustris TNG:

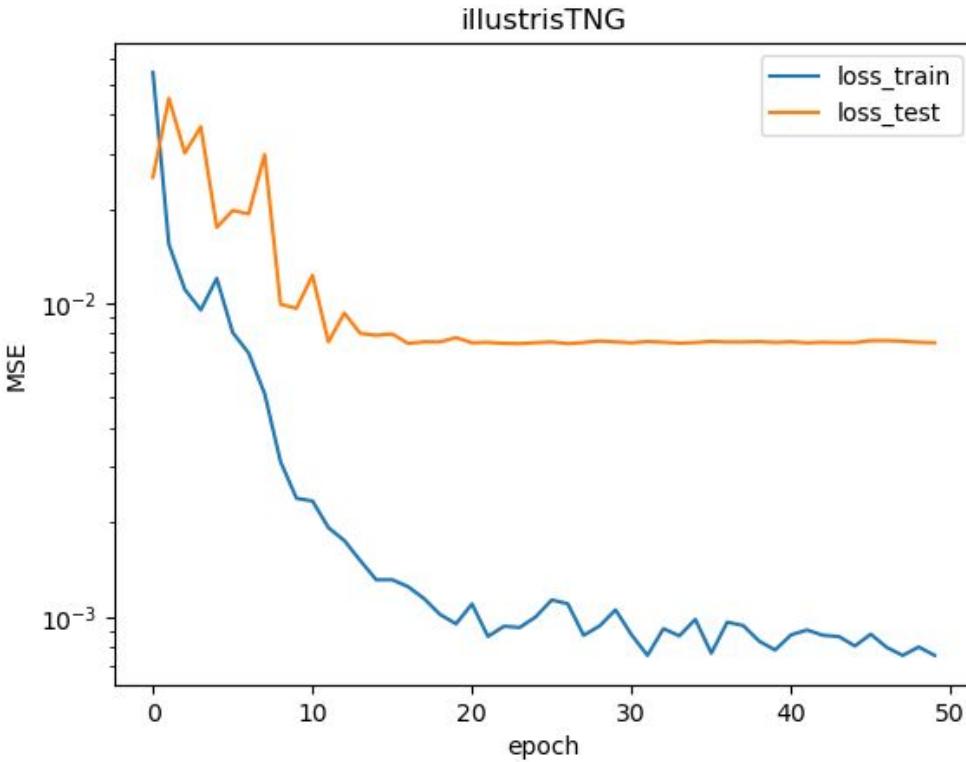


SIMBA:



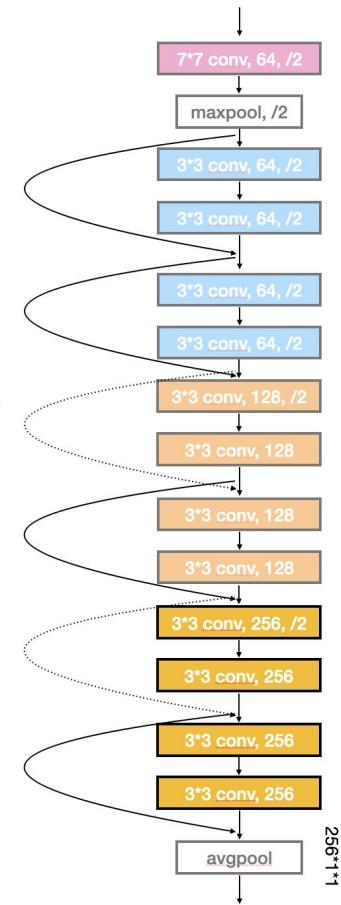
ResNet18 Model Architecture (Pytorch)

train and test using IllustrisTNG data (6:2:2 train:validation:test)



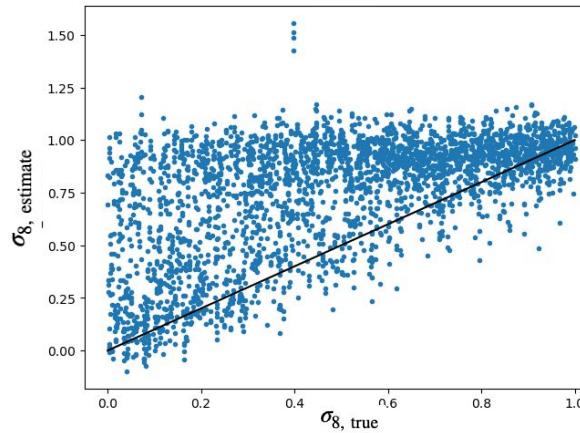
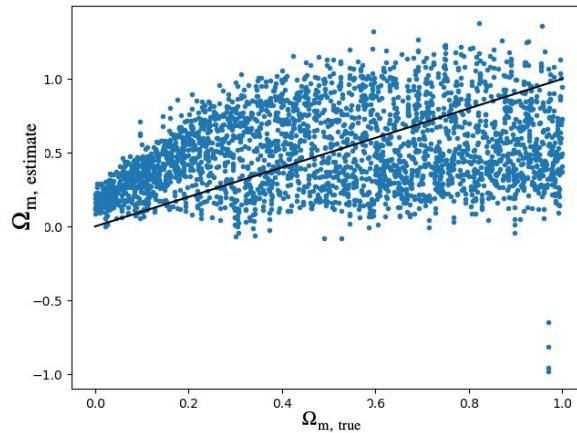
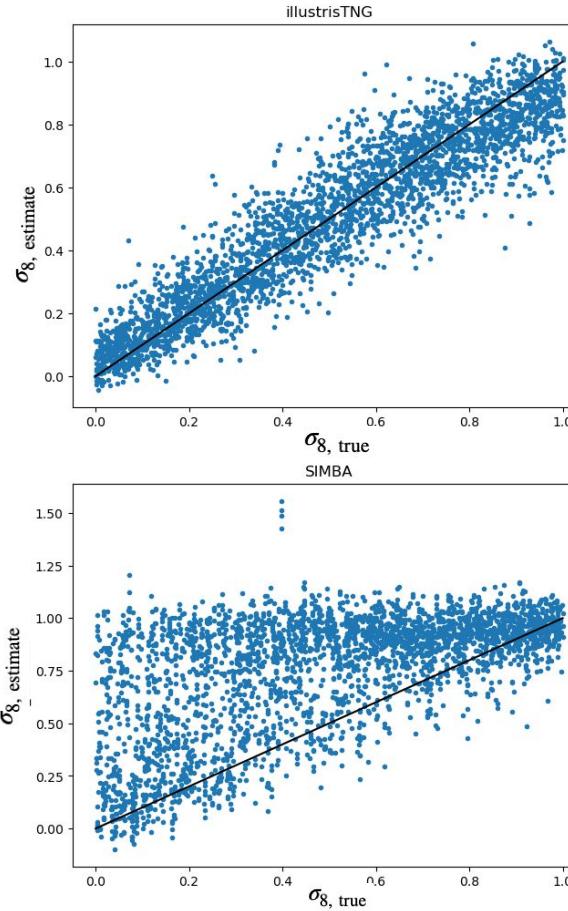
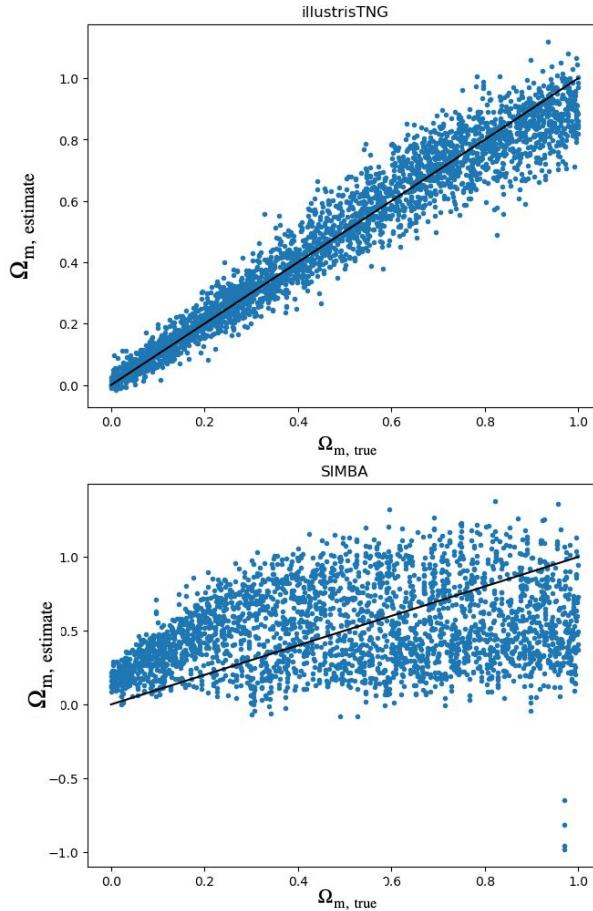
Classical
ResNet18
structure

We remove three
layers to reduce
computational
overhead



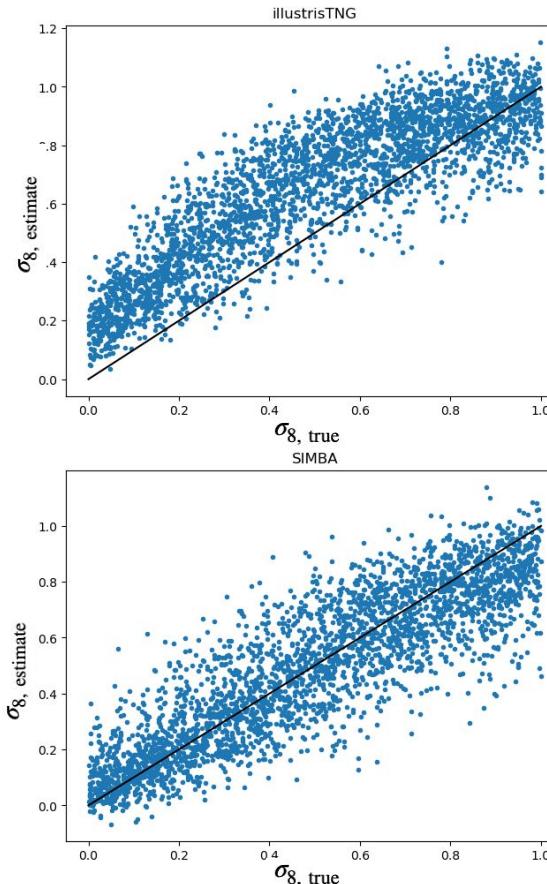
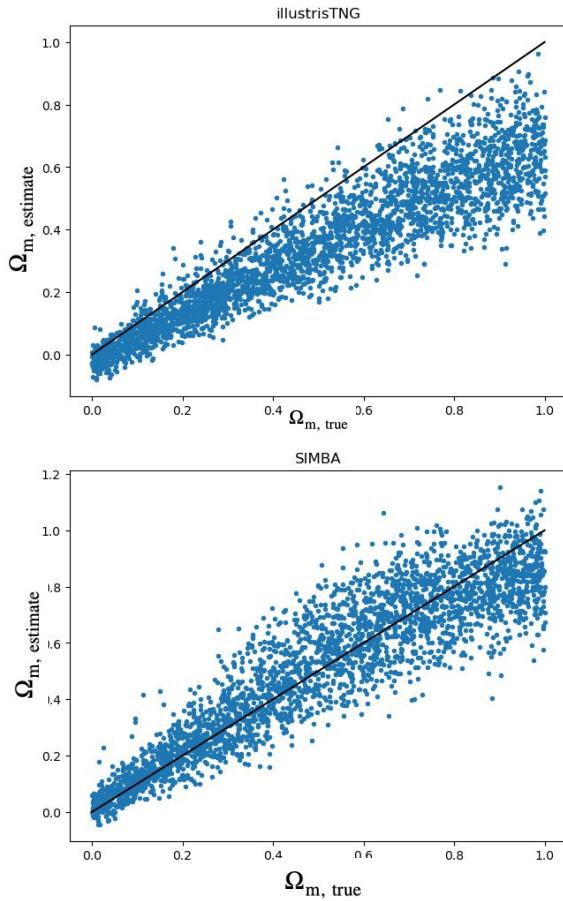
ResNet18

train using IllustrisTNG data (6:2:2 train:validation:test) and test on both

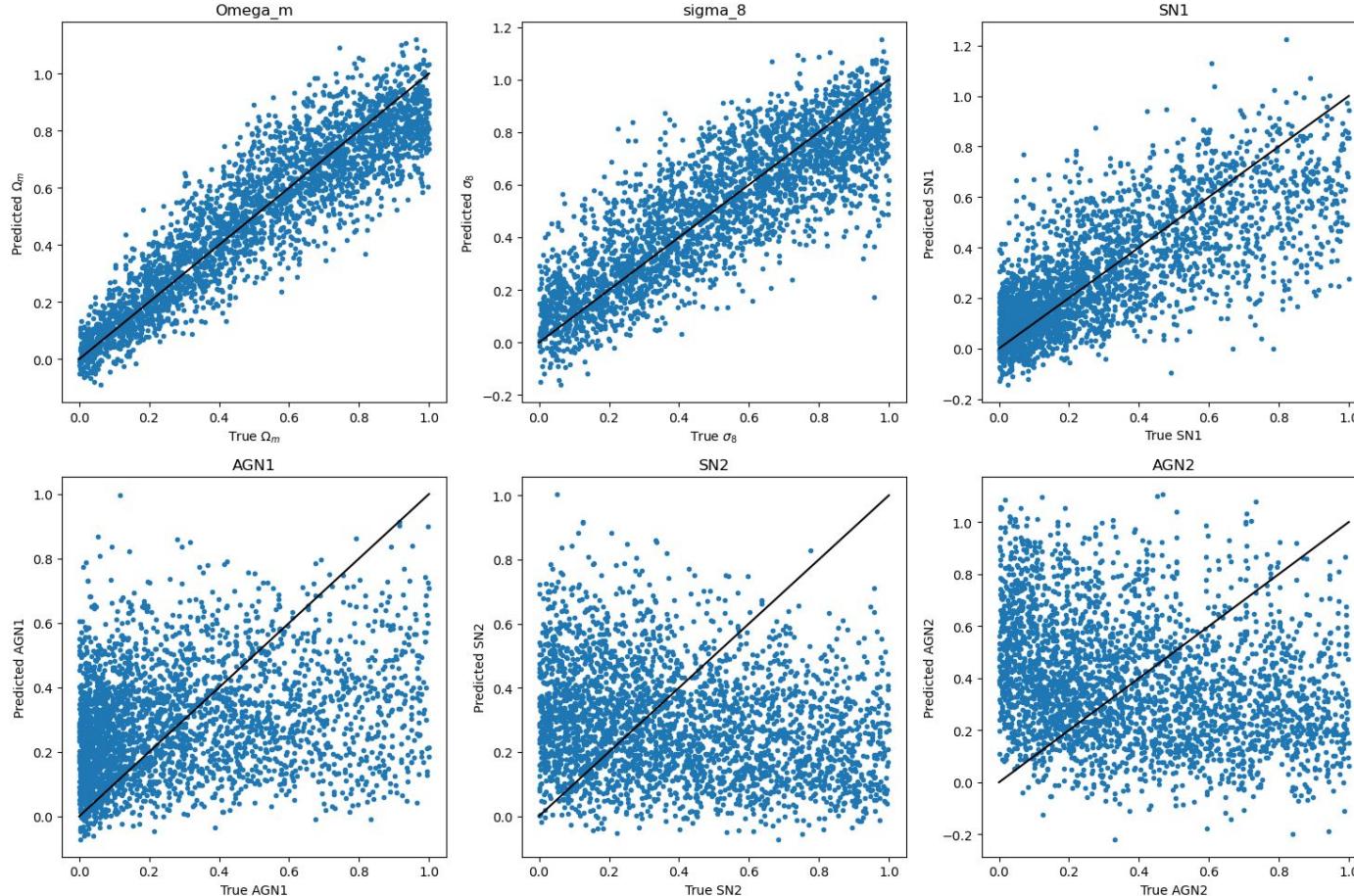


ResNet18

train using SIMBA data (6:2:2 train:validation:test) and test on both



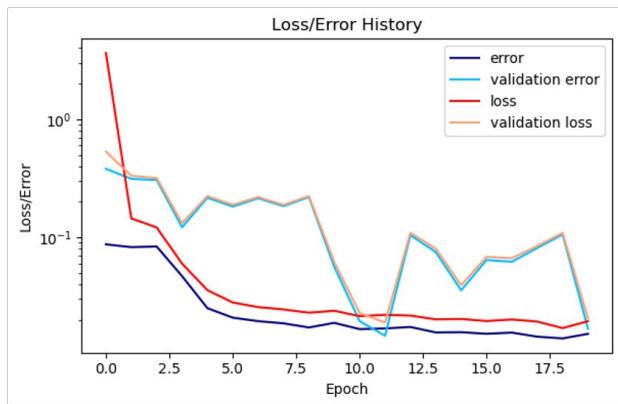
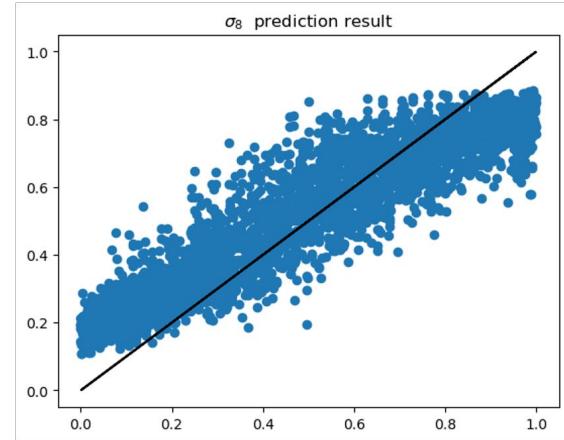
Constraining all 6 parameters of SIMBA:



Keras

train and test on IllustrisTNG (7:3:1 train:validation:test)

Layer (type)	Output Shape	Param #
input_layer (InputLayer)	(None, 64, 64, 2)	0
conv2d (Conv2D)	(None, 64, 64, 8)	408
batch_normalization (BatchNormalization)	(None, 64, 64, 8)	32
max_pooling2d (MaxPooling2D)	(None, 32, 32, 8)	0
dropout (Dropout)	(None, 32, 32, 8)	0
conv2d_1 (Conv2D)	(None, 32, 32, 32)	2,336
batch_normalization_1 (BatchNormalization)	(None, 32, 32, 32)	128
max_pooling2d_1 (MaxPooling2D)	(None, 16, 16, 32)	0
dropout_1 (Dropout)	(None, 16, 16, 32)	0
conv2d_2 (Conv2D)	(None, 16, 16, 64)	18,496
batch_normalization_2 (BatchNormalization)	(None, 16, 16, 64)	256
max_pooling2d_2 (MaxPooling2D)	(None, 8, 8, 64)	0
dropout_2 (Dropout)	(None, 8, 8, 64)	0
flatten (Flatten)	(None, 4096)	0
dense (Dense)	(None, 1024)	4,195,328
dense_1 (Dense)	(None, 32)	32,800
dense_2 (Dense)	(None, 1)	33



Discussion

Data reprocessing: downsample and normalization

Model building: Hyperparameter setting + layer number

Labels of IllustrisTNG: Ω_m , σ_8 ; Labels of SIMBA: Ω_m , σ_8 , SN1

The more, the better?

Evaluate the results

How to understand?

THANK YOU

F

A³ Net

Group F Presents: Illuminating the Future of AI with Image Mastery

Exploring Image Classification, Regression, and Generation with AI



Starring:

Hongxuan
Imkwang
Shijiao
Temurbek
Chen
Kenji

Our Challenge

Neutrino Telescopes:

Neutrino telescopes have been crucial in forming our current understanding of astrophysics.

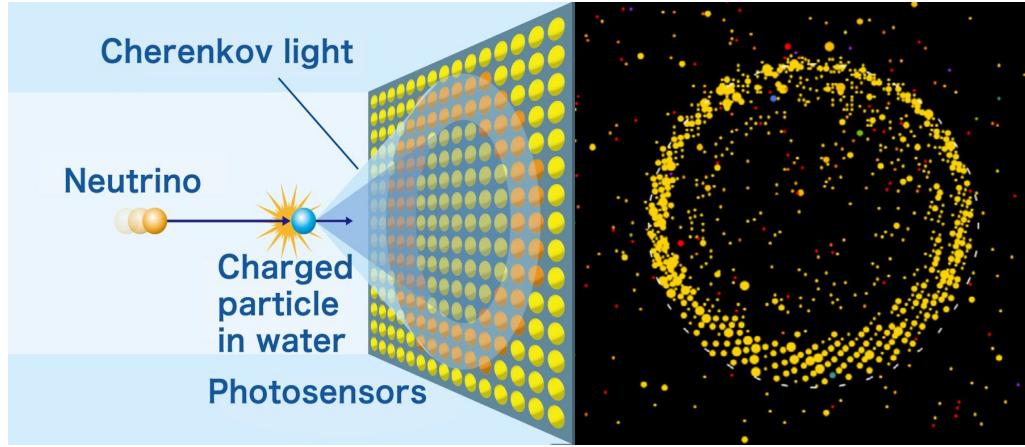
Cherenkov Light:

To detect neutrino phenomena, Cherenkov light is ideal due to its distinct and predictable patterns.

Our Mission:

Analyze Cherenkov light from neutrino detectors using AI techniques, focusing on

- (i) classification,
- (ii) image generation,
- (iii) and regression.



NRings Classifier

10000 of (28 pixels)² images

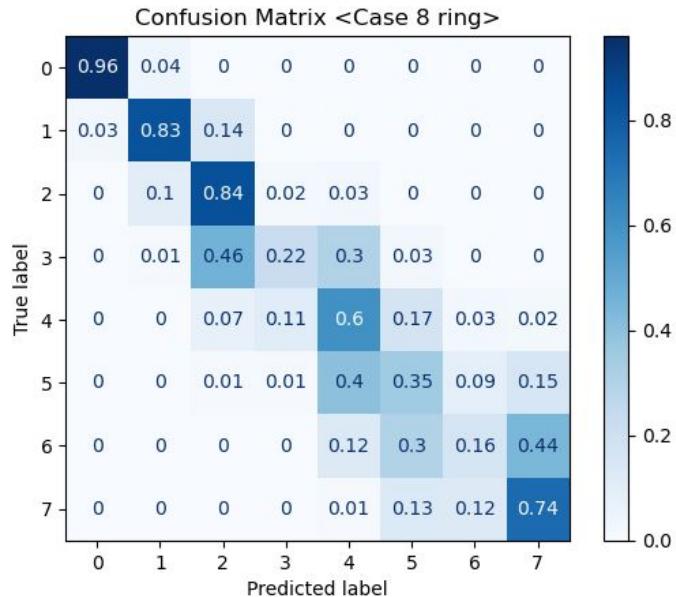
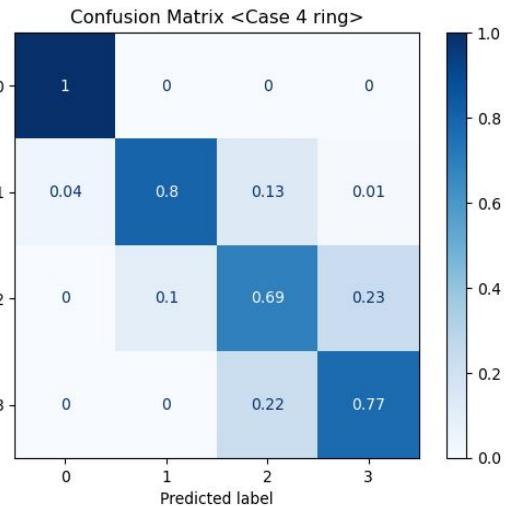
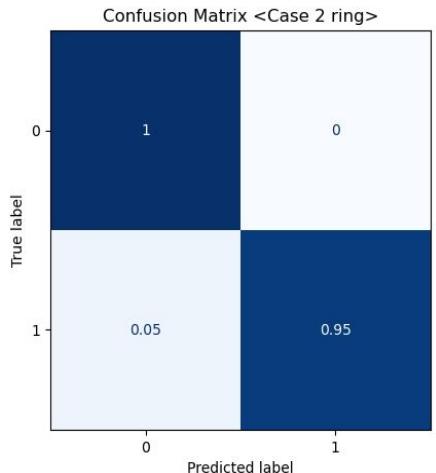
CNN: 3 convolution layers

+2 Fully connected layers

Data : Training: 7000 / Testing: 3000

Training Epoch: 5

Q: How do the performances change versus max number?

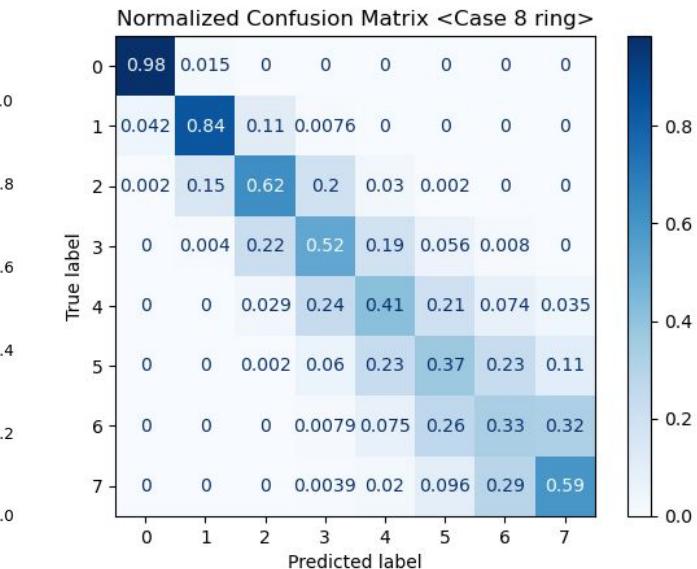
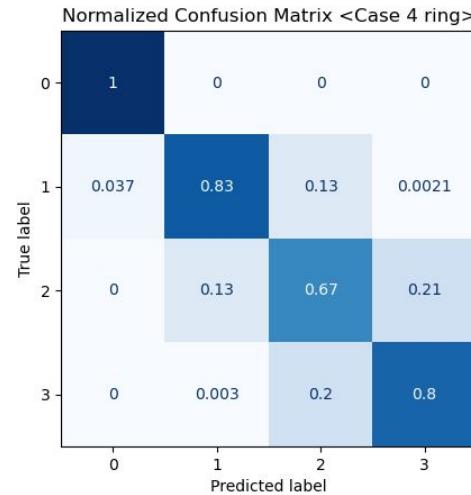
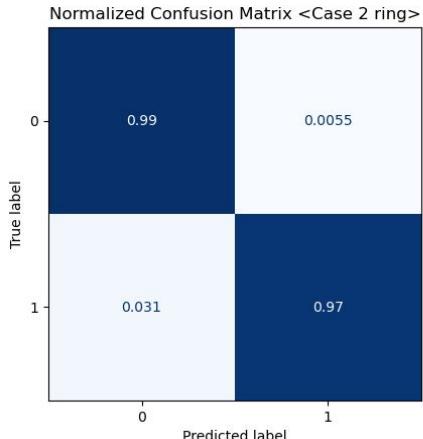


Q: Can you use a non Neural-Network-based technique to do this classification?

Principal Component Analysis (PCA): Extract important latent vectors from all images.
We used top 50 principal components.

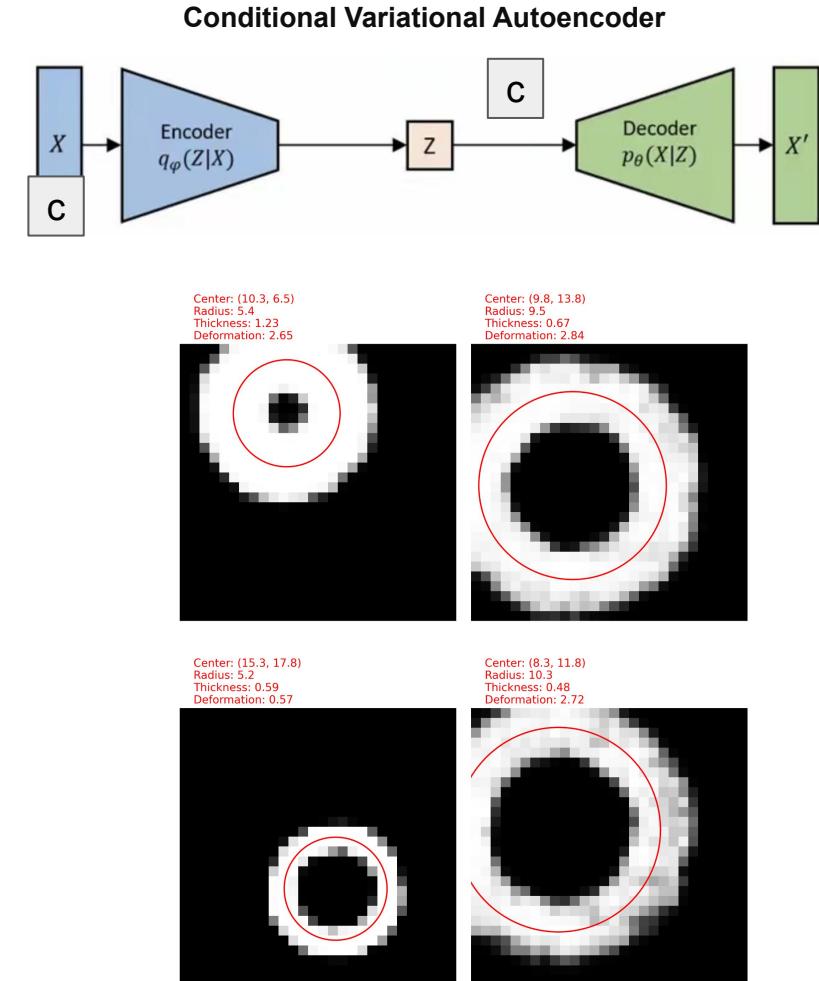
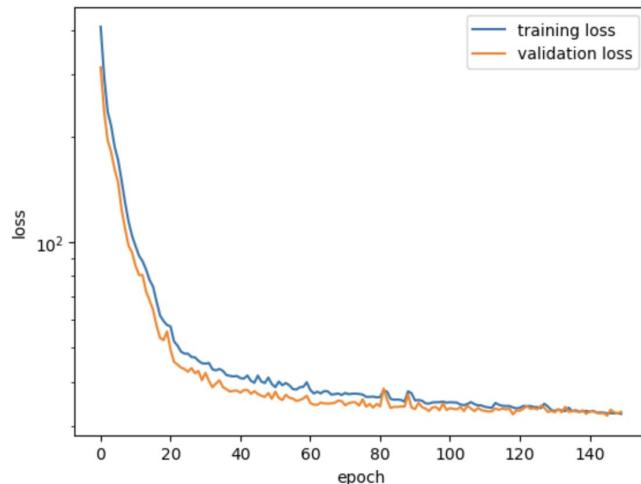
Support Vector Machine (SVM):

Separate the data into different numbers of rings using a 49-dimensional hyperplane.



Generating simulated images

- > Use conditional-VAE model
- > Fiducial: Training: 4000; Validation: 1000
- > Training epoch ~ 150

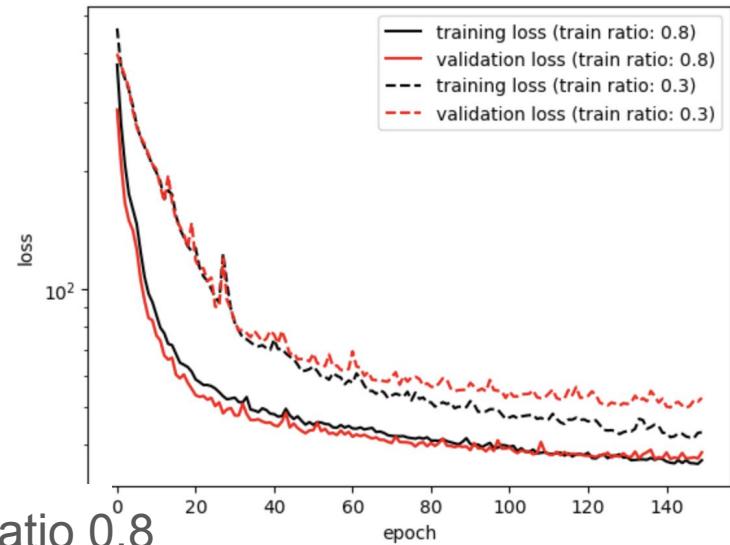


Generating simulated images

Q: How do the performances change with training set?

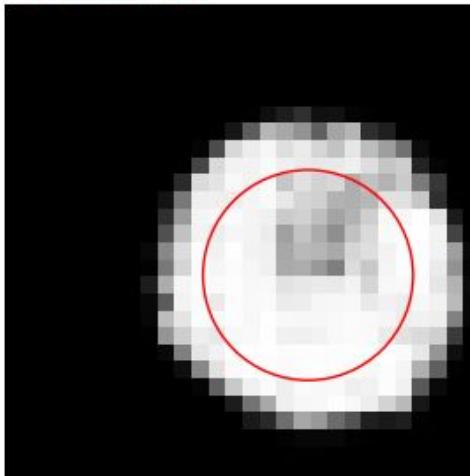
-> Use conditional-VAE model

-> Different ratios between training and validation samples make different loss rates.



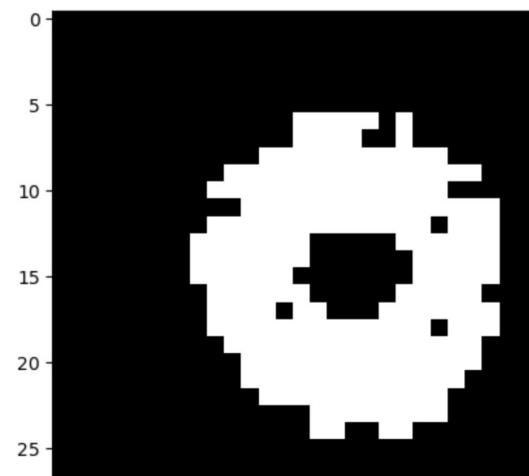
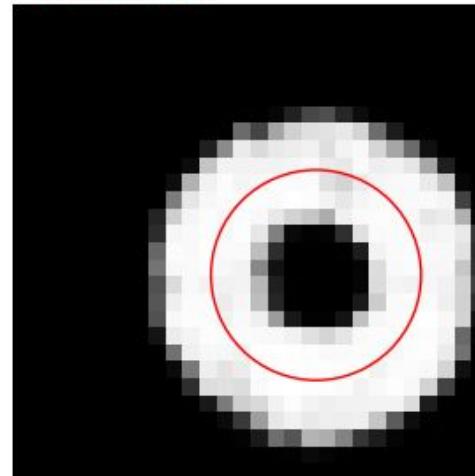
Center: (17.4, 15.4)
Radius: 6.2
Thickness: 0.42
Deformation: 2.70

train ratio 0.3

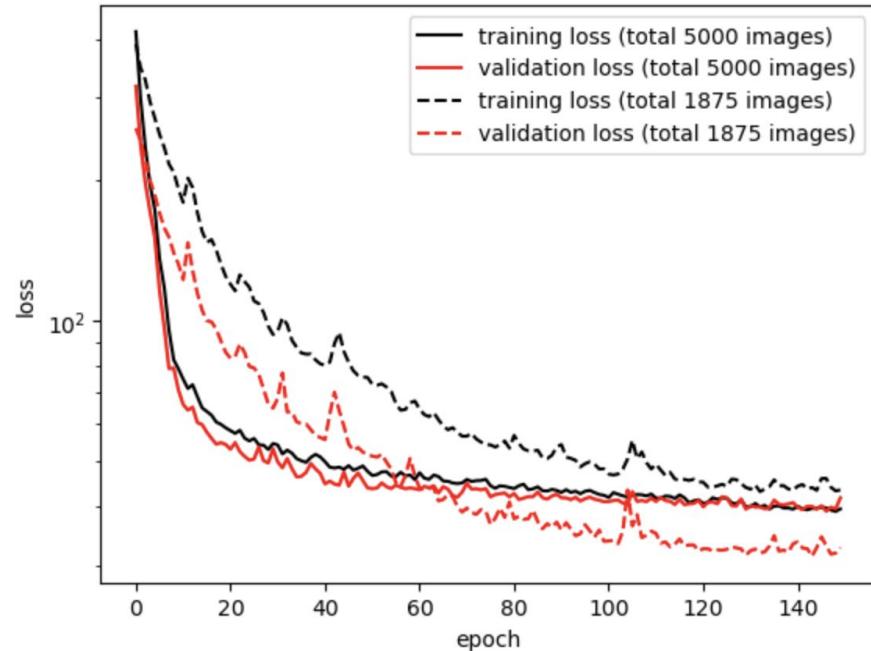
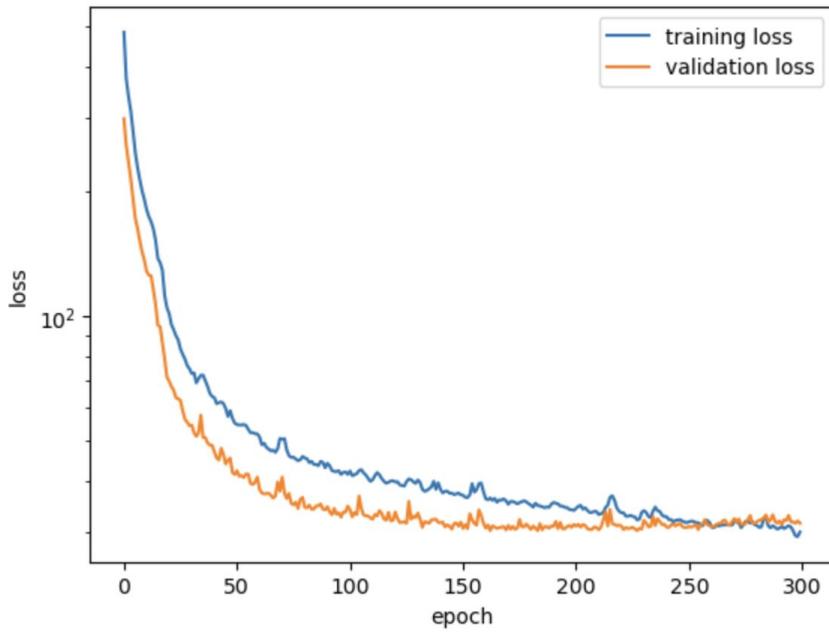


Center: (17.4, 15.4)
Radius: 6.2
Thickness: 0.42
Deformation: 2.70

train ratio 0.8



Reduce total number of the dataset with the same training ratio



Ring Regressor

Q. Can you write some algorithm to perform regression?

CNN: 2 convolution layers+2 Fully connected layers

Data: Training: 8000 / Testing: 2000

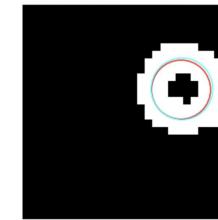
Training Epoch: 8

Fully Connected Network: 4 Fully connected layers

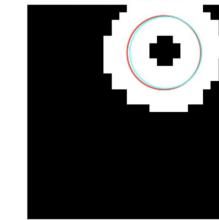
Data : Training: 8000 / Testing: 2000

Training Epoch: 8

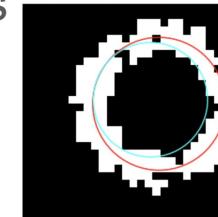
True (Red) | Predicted (Cyan)
Center: (20.2, 10.6) | (20.4, 10.5)
Radius: 3.9 | 4.0
Thickness: 0.74 | 0.96
Deformation: 1.32 | 1.27



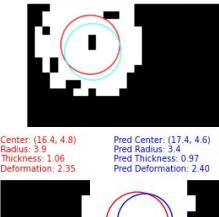
True (Red) | Predicted (Cyan)
Center: (17.4, 5.8) | (17.6, 5.8)
Radius: 4.8 | 4.7
Thickness: 1.31 | 0.95
Deformation: 1.96 | 2.16



True (Red) | Predicted (Cyan)
Center: (17.4, 12.5) | (16.2, 12.0)
Radius: 8.7 | 7.5
Thickness: 0.31 | 0.34
Deformation: 2.02 | 1.87

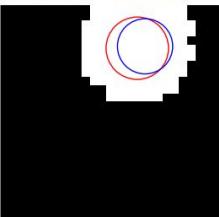


True (Red) | Predicted (Cyan)
Center: (7.7, 4.8) | (8.1, 5.7)
Radius: 3.9 | 3.7
Thickness: 0.38 | 0.32
Deformation: 2.75 | 2.59

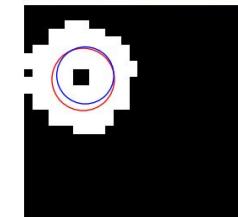


Center: (16.4, 4.8)
Radius: 8.7
Thickness: 1.06
Deformation: 2.35

Pred Center: (17.4, 4.6)
Pred Radius: 8.7
Pred Thickness: 0.97
Pred Deformation: 2.40

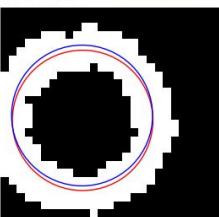


Center: (6.8, 8.7)
Radius: 3.9
Thickness: 0.72
Deformation: 2.18

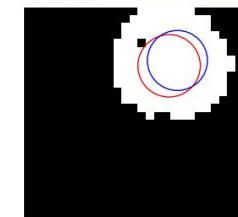


Center: (9.6, 13.5)
Radius: 8.7
Thickness: 1.37
Deformation: 1.46

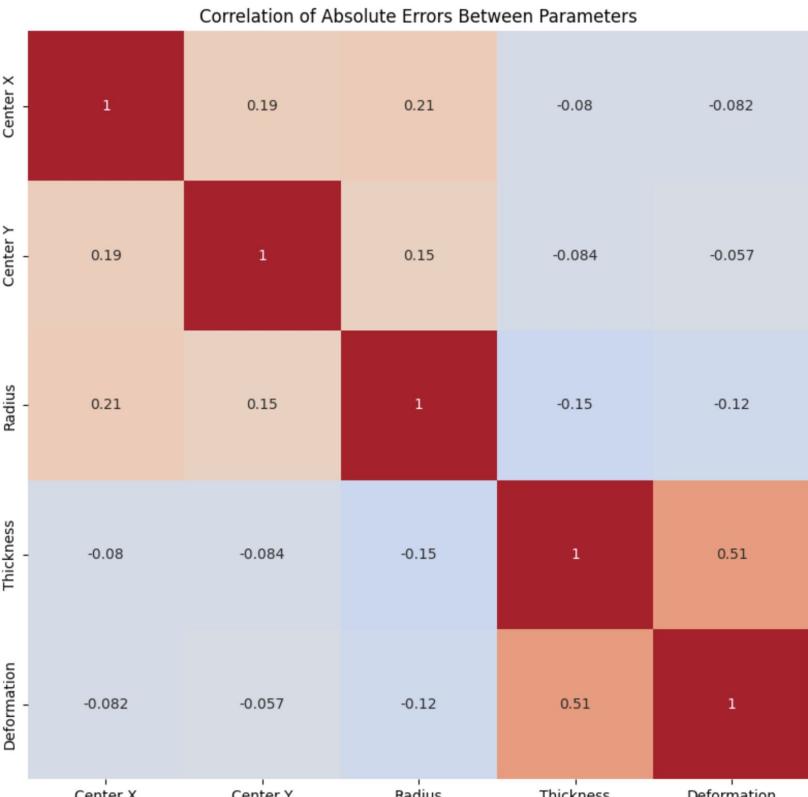
Pred Center: (9.6, 12.9)
Pred Radius: 8.7
Pred Thickness: 1.03
Pred Deformation: 1.73



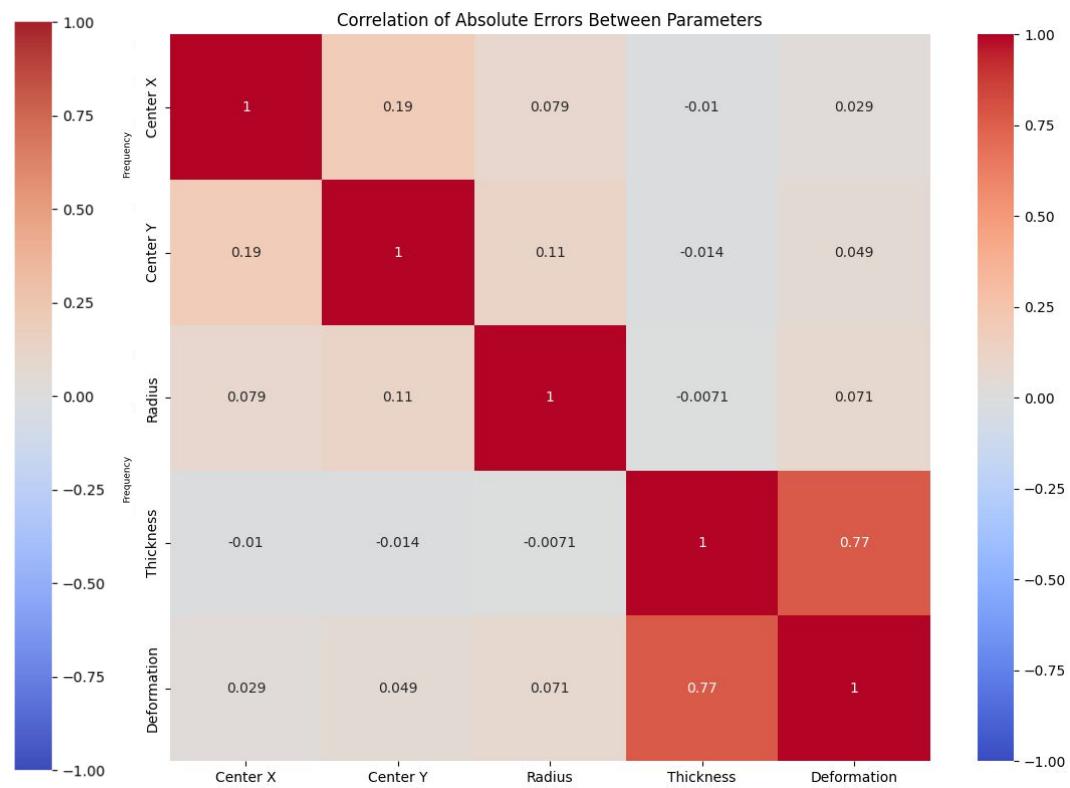
Center: (17.4, 6.8)
Radius: 3.9
Thickness: 0.53
Deformation: 2.93



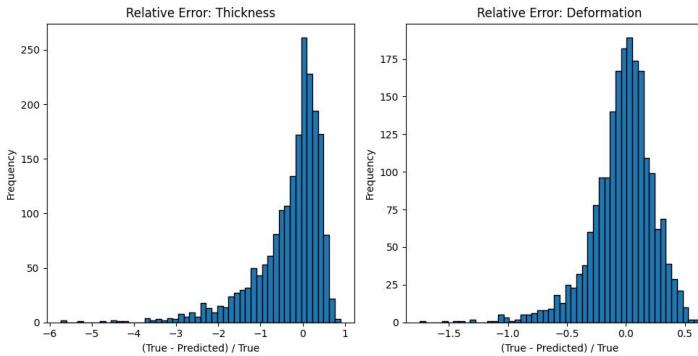
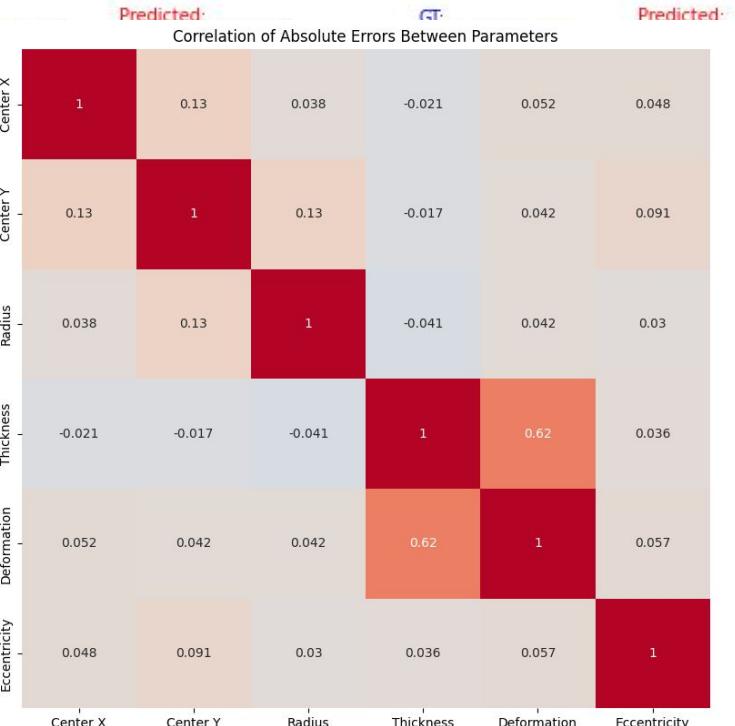
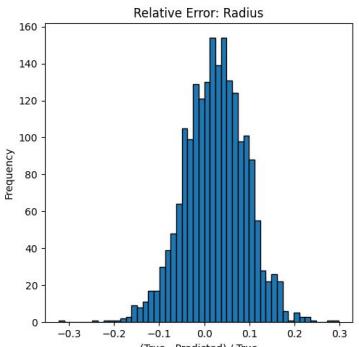
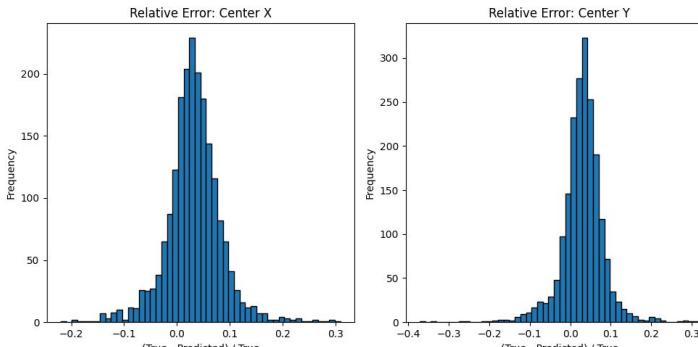
CNN



Fully Connected



Ellipse Regressor



| Linear: 2-7

774

Total params: 566,918
Trainable params: 566,918
Non-trainable params: 0

Conclusion and Applications

AI Success:

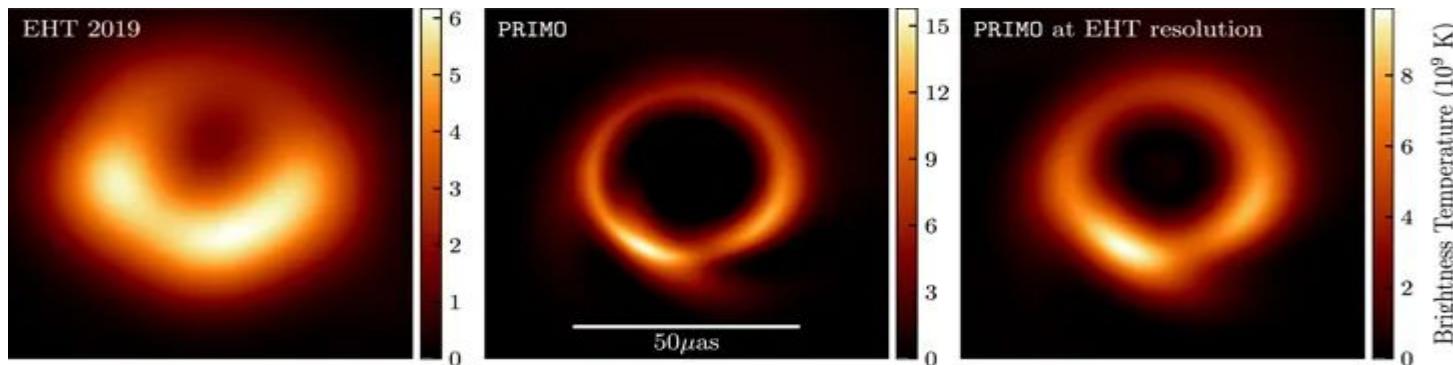
- We used AI to effectively analyze Cherenkov light, key for understanding neutrinos.

Enhanced Precision:

- By applying classification, image generation, and regression, we made data interpretation in neutrino detection more precise and versatile.

Broader Applications:

- These AI methods can also help tackle other astrophysical challenges, like analyzing black hole images from the EHT.



G

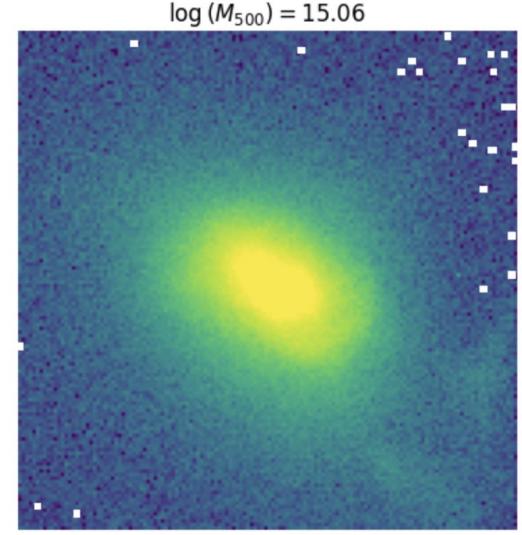
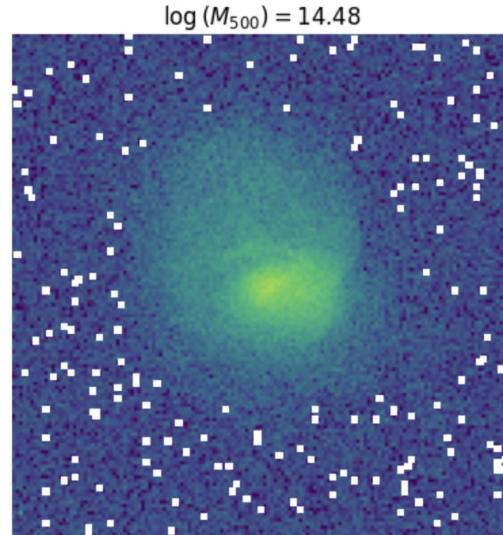
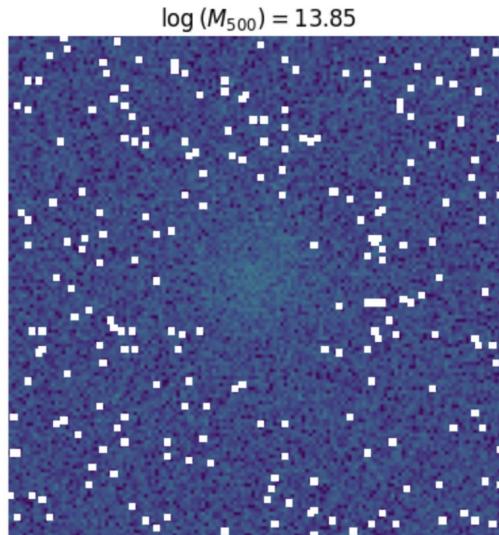
Project 2. Galaxy Cluster Masses with CNNs

Group G

Syeon Hwang, Duho Kim, Xinru Li, Tomomi Sunayama,
Shota Takahashi, Jiashuo Zhang, Zhenghao Zhu

A3Net Summer School 2024

Images of galaxy clusters from TNG

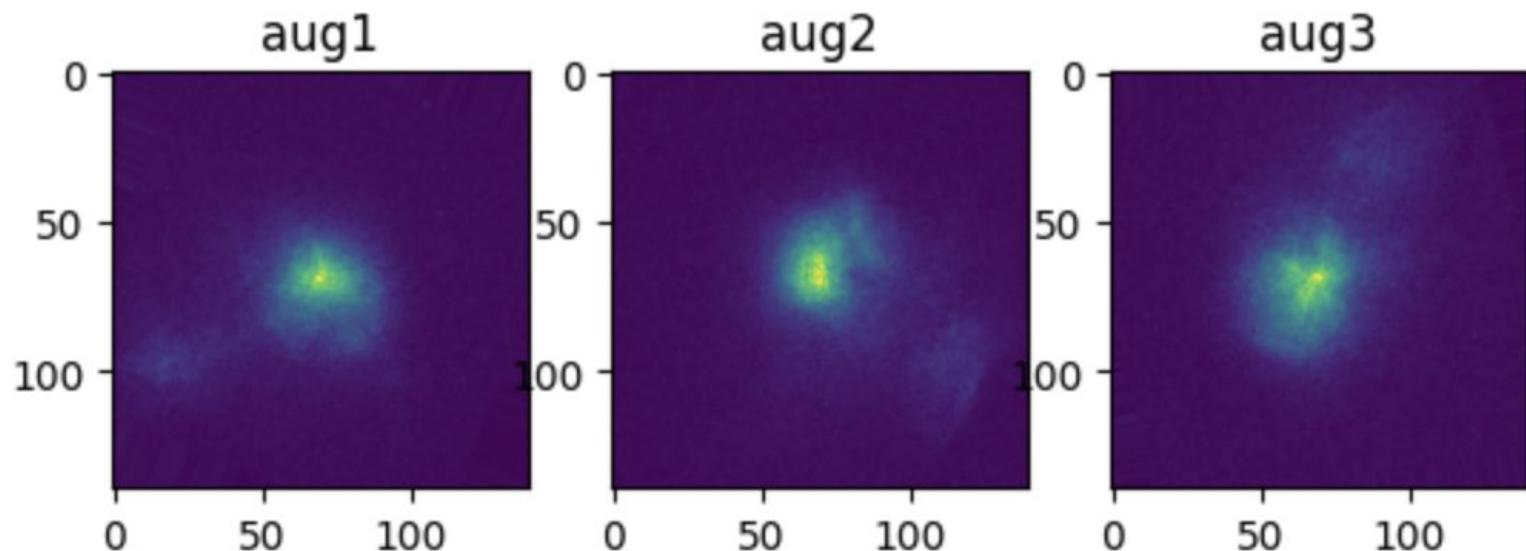


low-mass



high-mass

Augmented Data (rotating 90 degree)

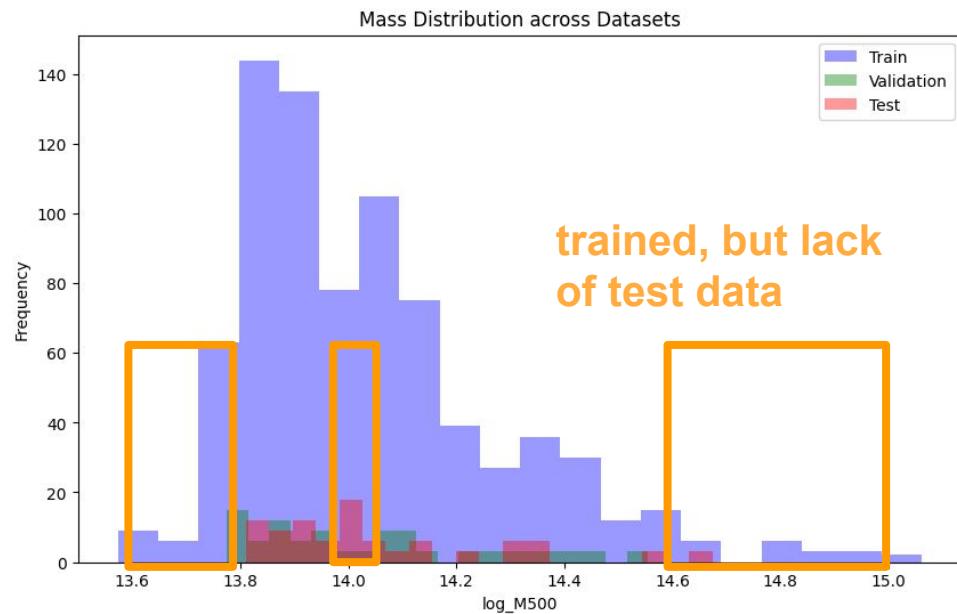


Datasets with Different Mass Distribution

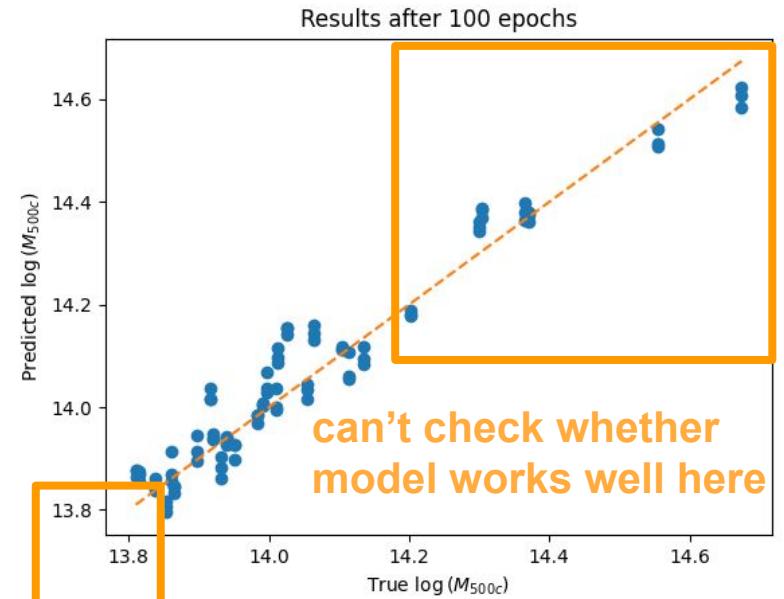
Dataset & Mass Distribution Bias?

Original Dataset: train : val : test = 794 : 99 : 93

Mass Distribution:



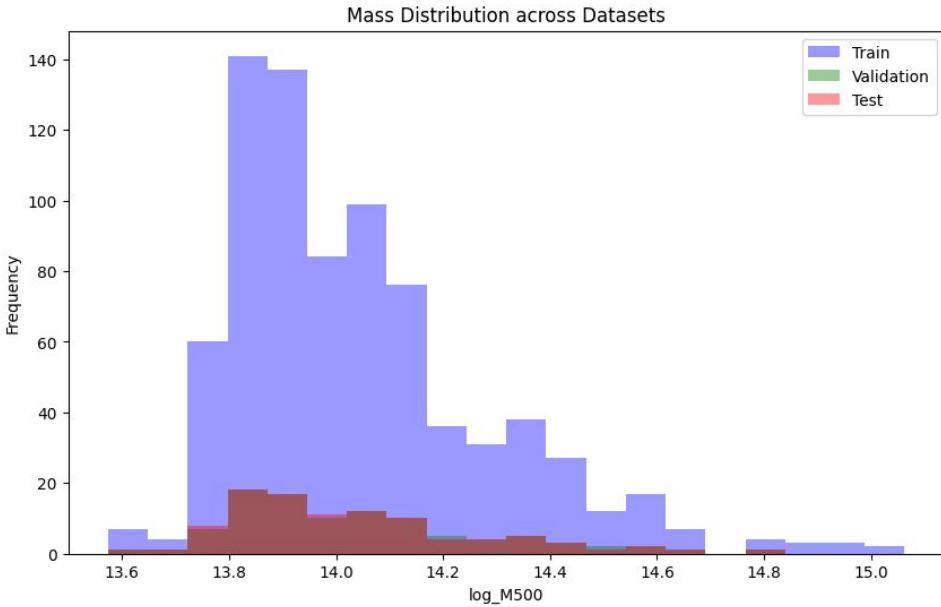
Result: Mean Squared Error = 0.00265



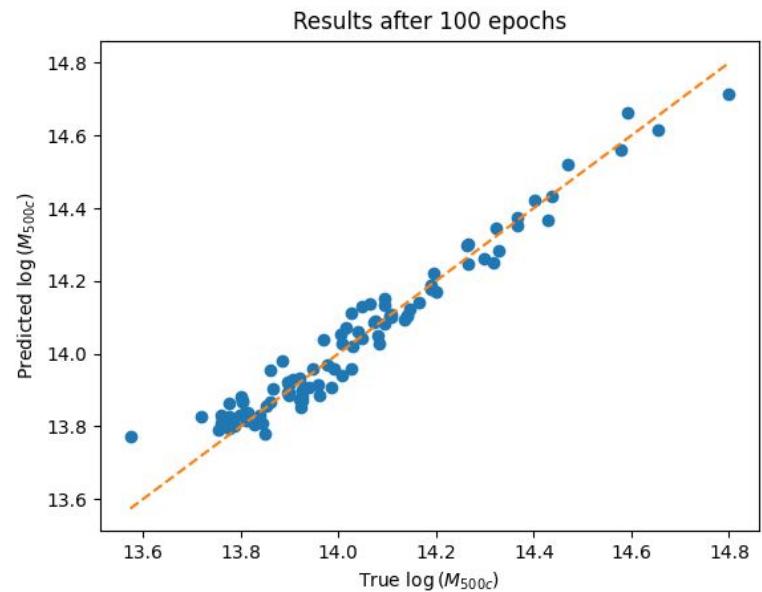
Shuffled Dataset: train : val : test = 788 : 99 : 99

use **Stratified Shuffle Split** to ensure train, val, test have similar mass distribution.

Mass Distribution:

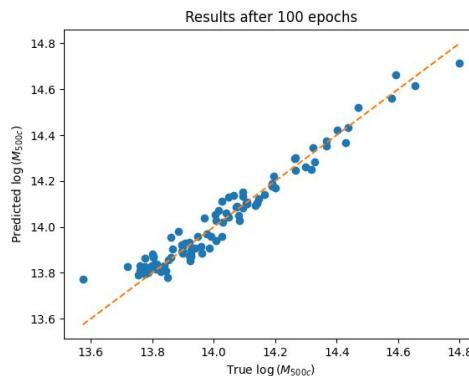
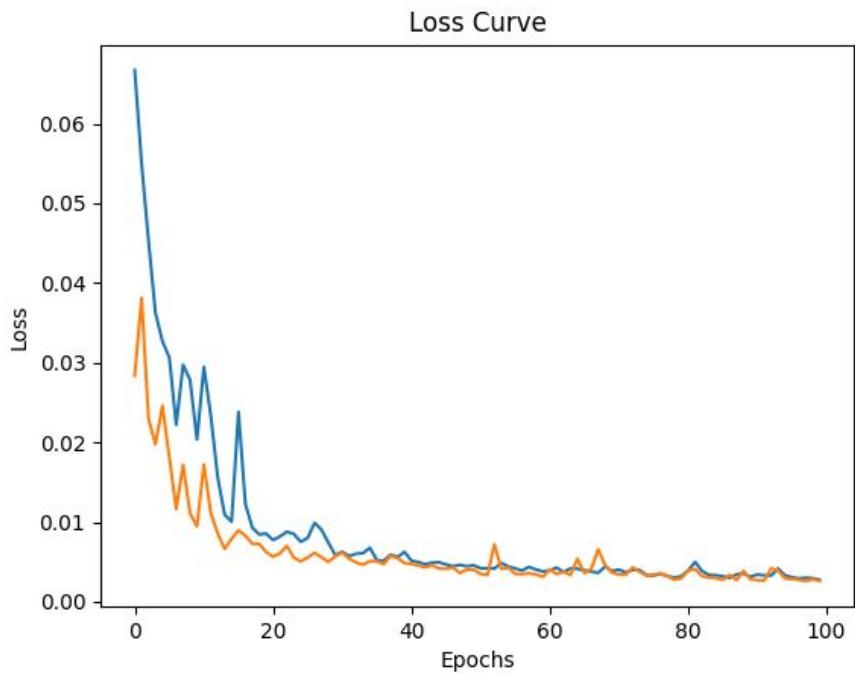


Result:

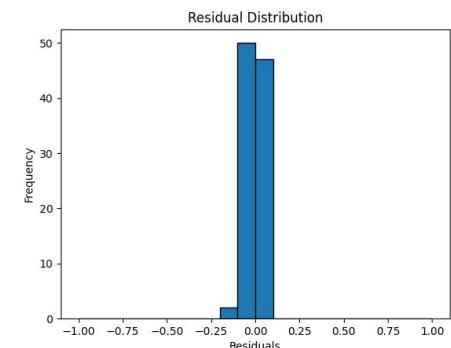


Shuffled Dataset: train : val : test = 788 : 99 : 99

Result:



residuals = test Y - prediction

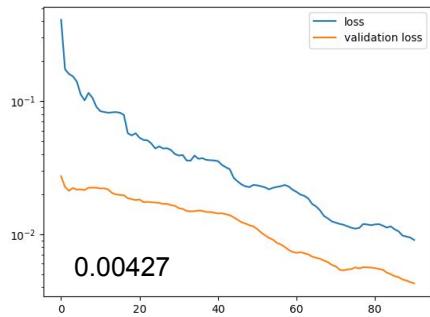
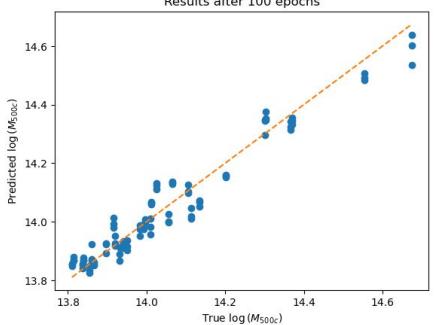
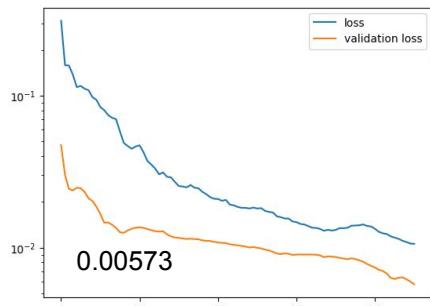
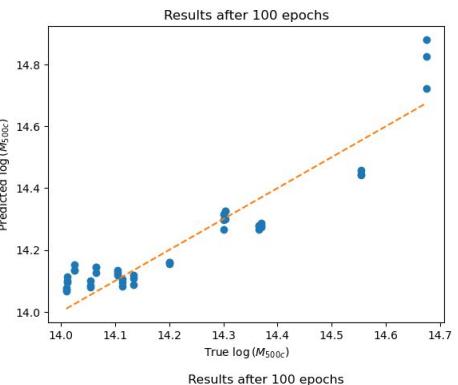
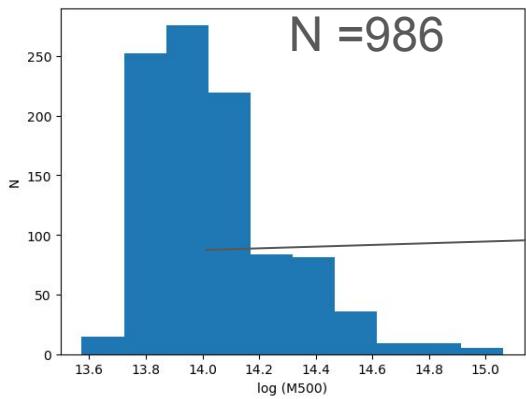
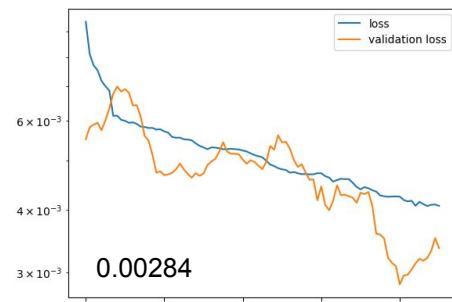
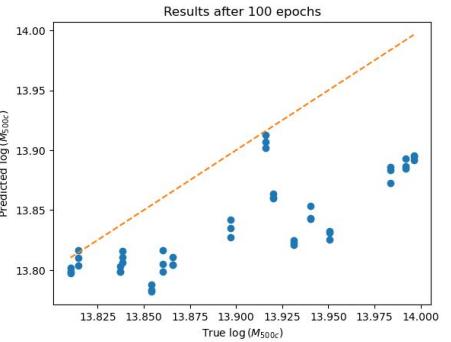
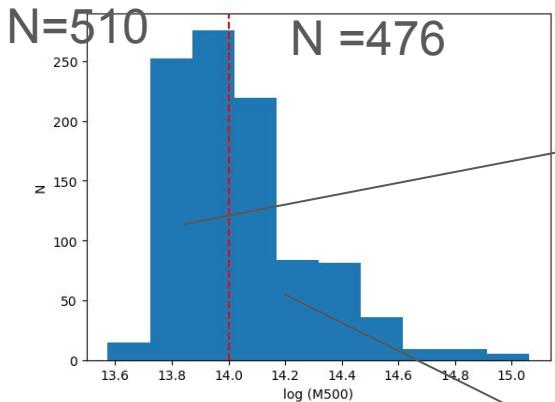


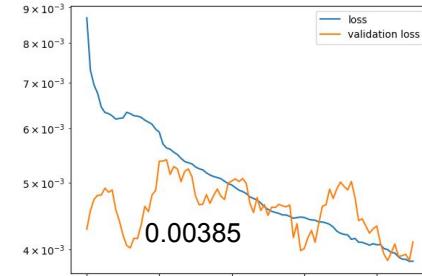
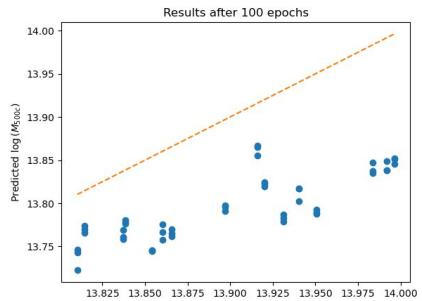
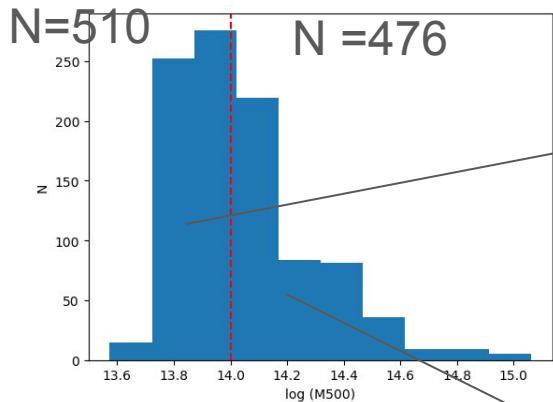
test loss: 0.0027

validation loss: 0.0026

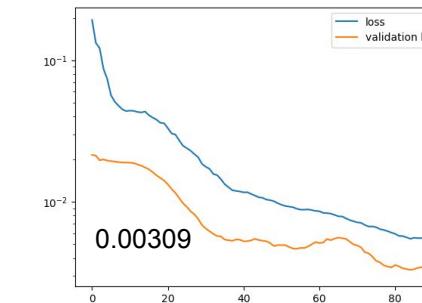
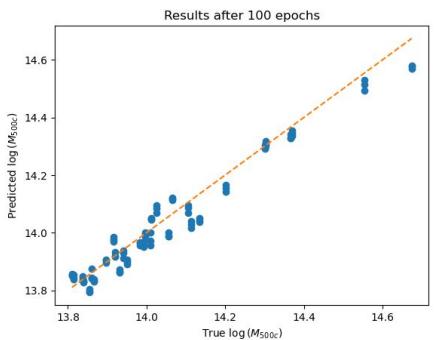
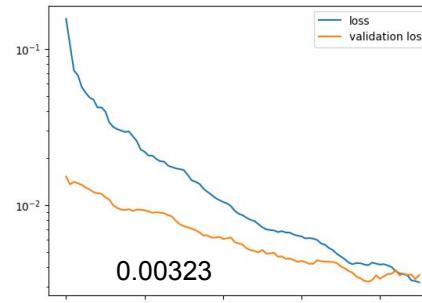
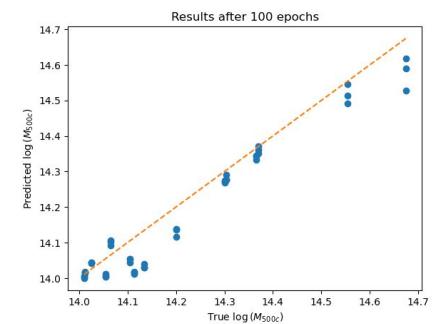
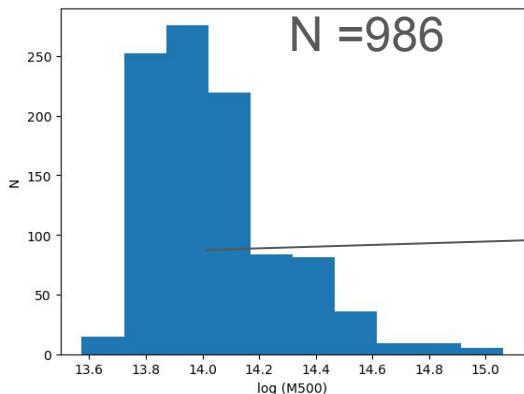
Training completed in: 303.88 seconds

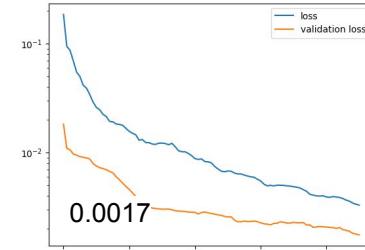
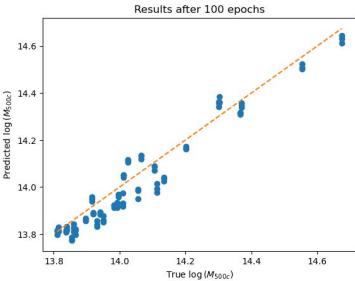
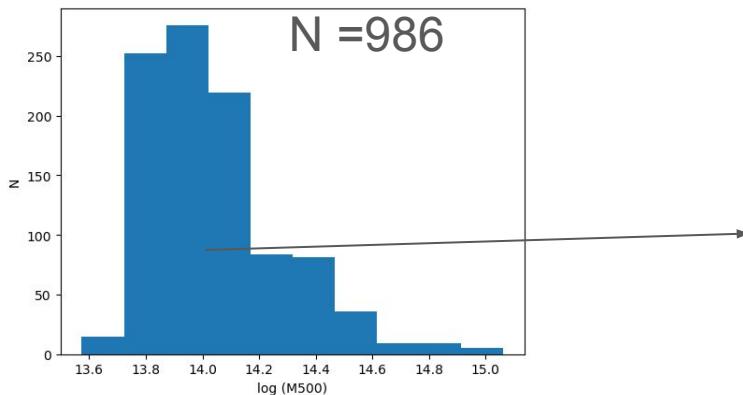
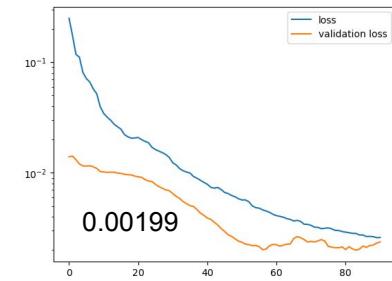
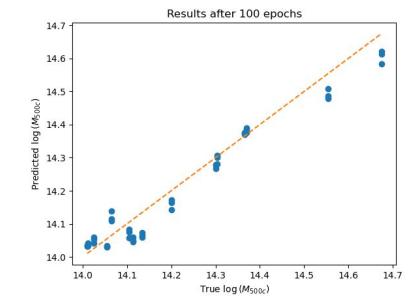
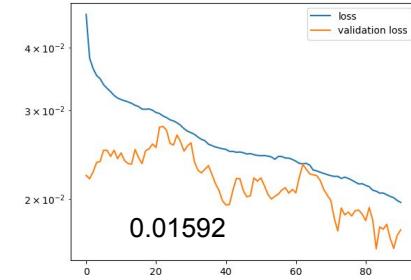
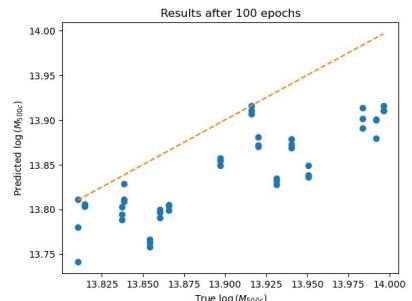
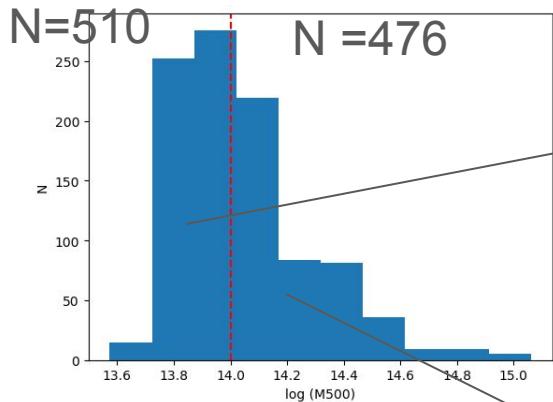
Mean Squared Error = 0.00242 < 0.00265 of original





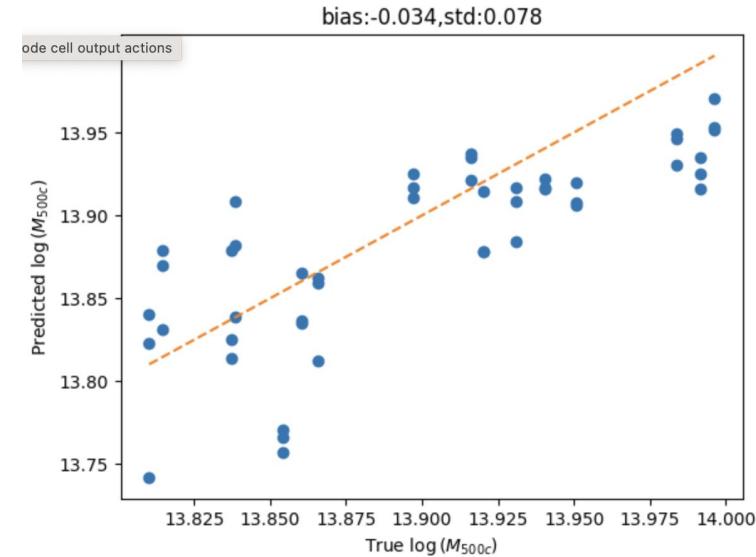
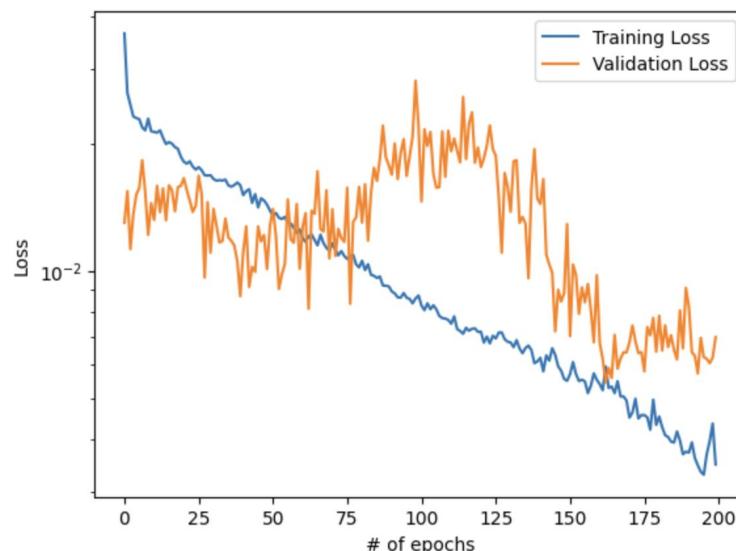
After augmenting training sample number to 1000 for all





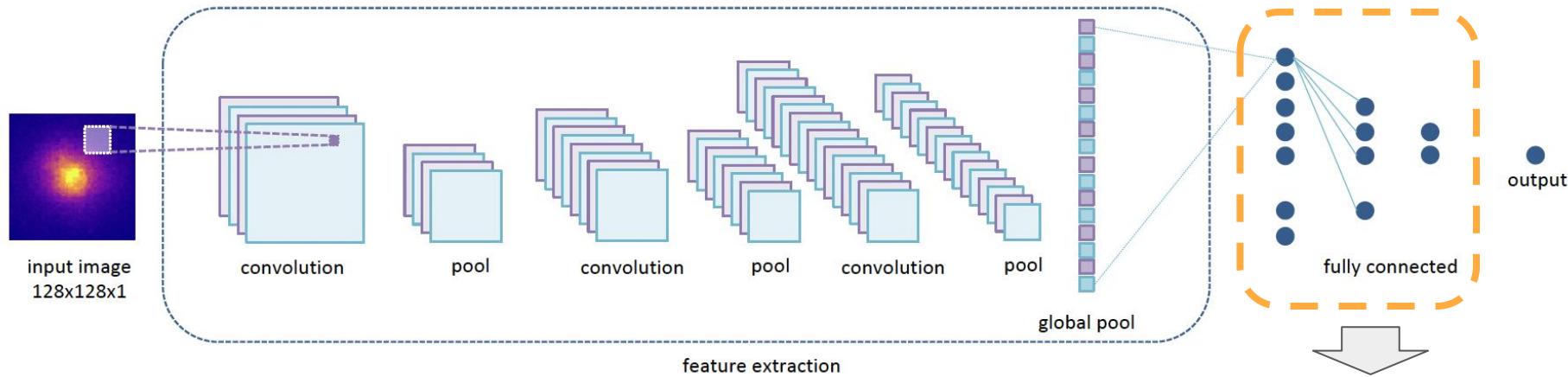
Tried with epoch=200 instead of epoch=100...

Tried with **all** the low-mass cluster sample: the subsample requires **more number of epochs** to converge and it gives a better result. However, the high-mass tail is still biased...



CNN Architecture

Varying Hyperparameters

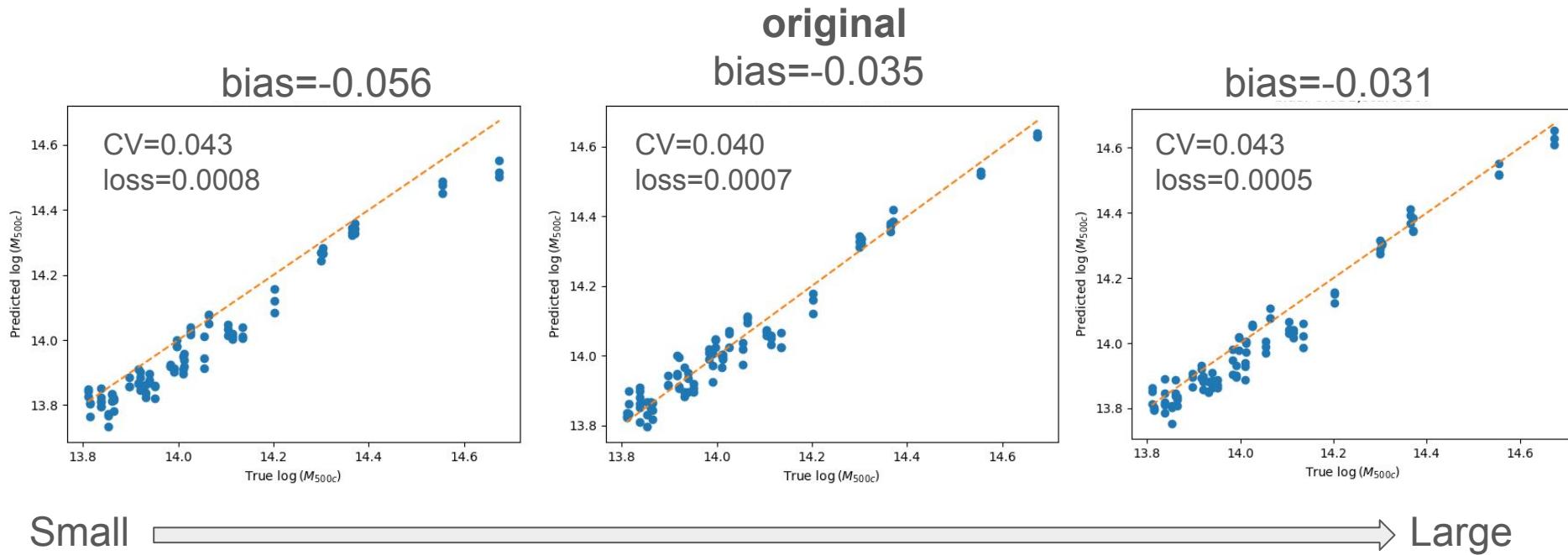


Double/half the number
of fully-connected layers

Problem: Variations in the results are large enough to make conclusions because of small sample size (~ 1000) → use k-fold cross-validation

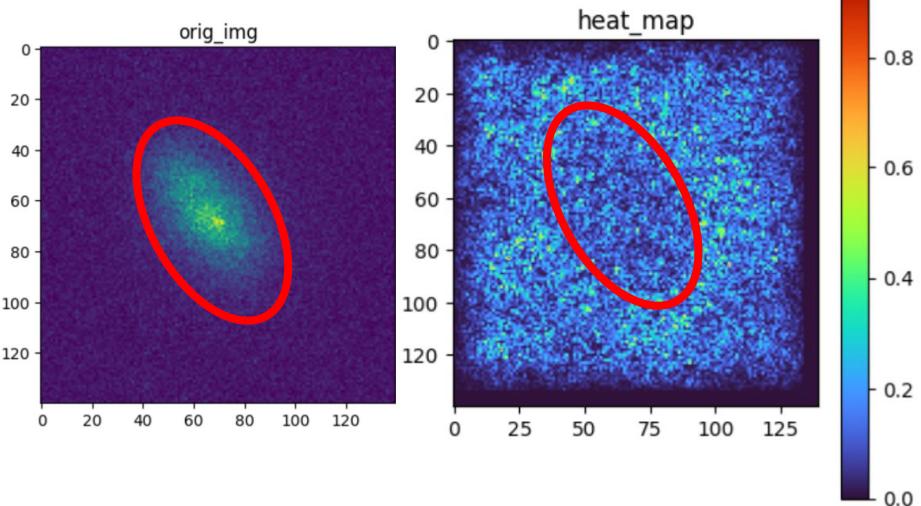
Varying Hyperparameters

By increasing the number of layers, the bias in the mass prediction becomes smaller (i.e., more accurate prediction).

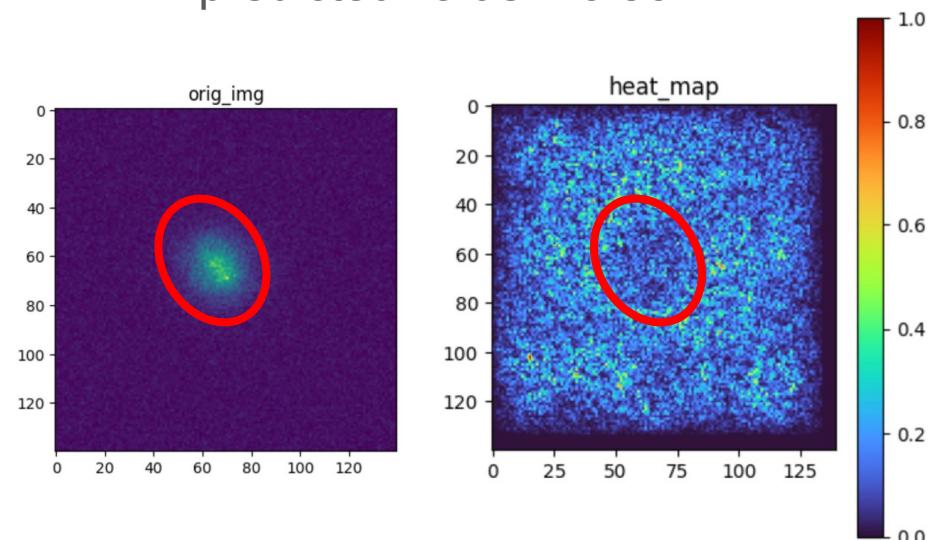


Saliency maps

predicted value = 0.74

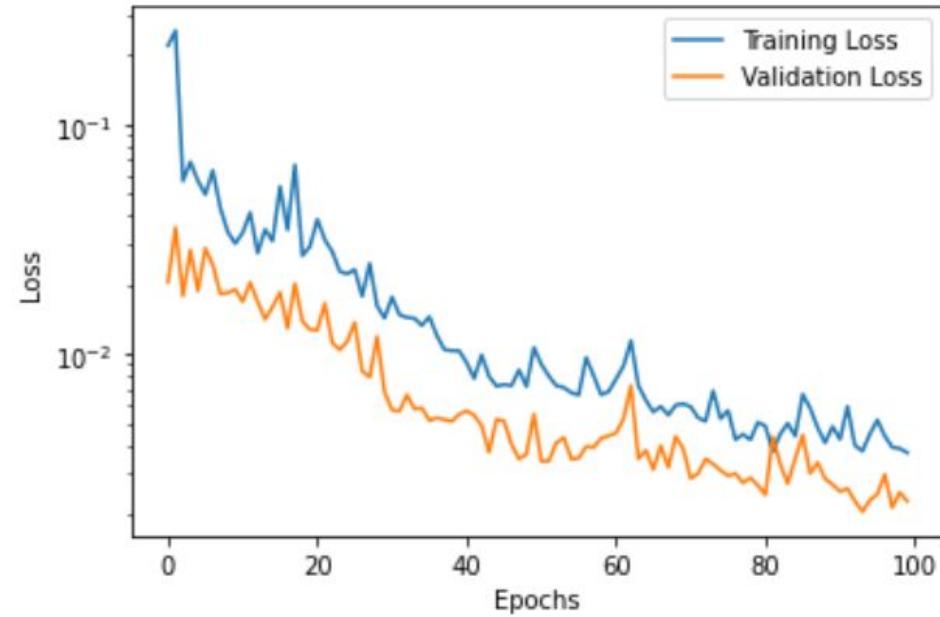


predicted value = 0.56

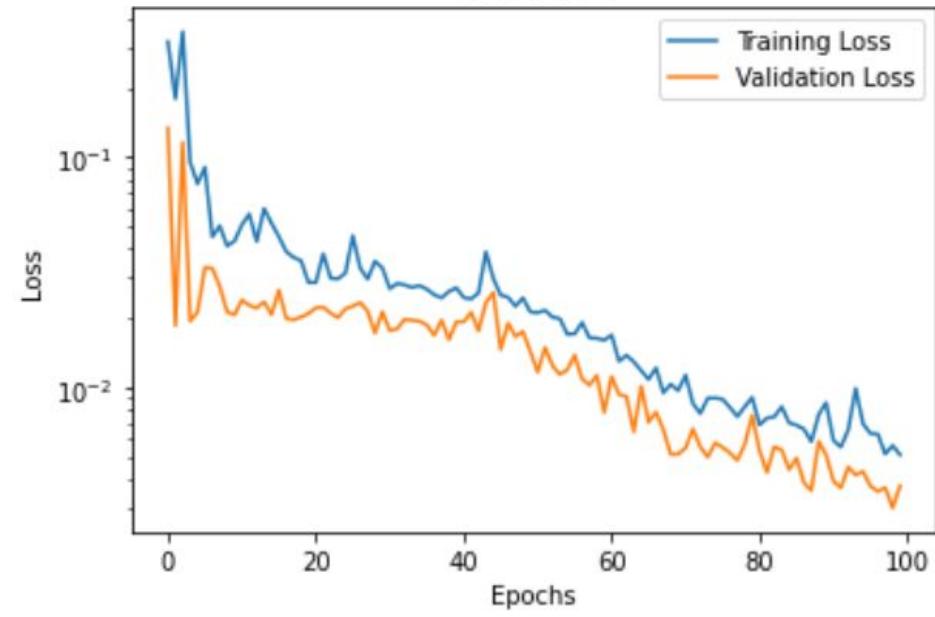


Rotational Invariance

Loss Curve



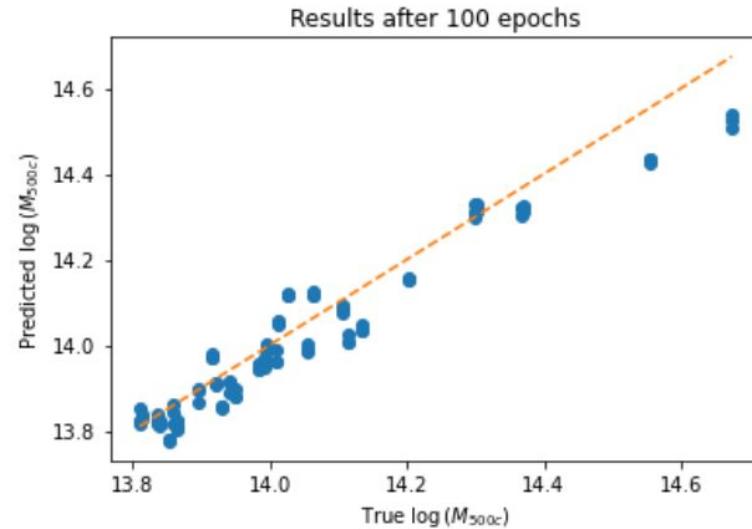
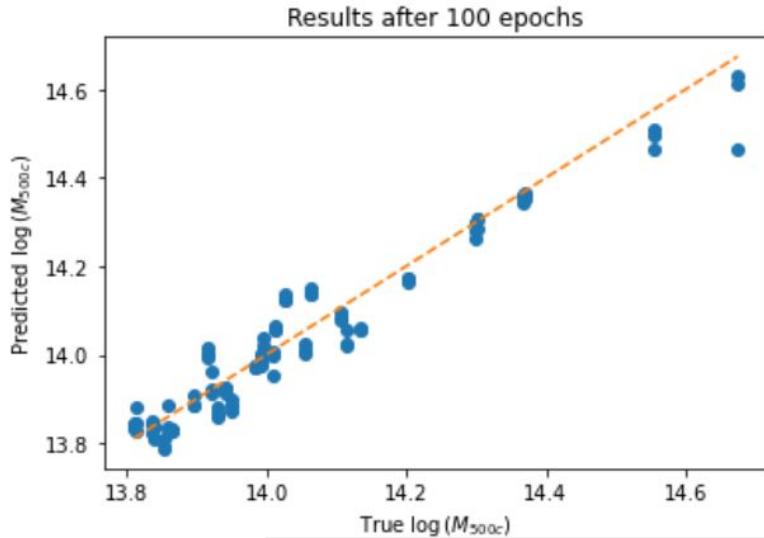
Loss Curve



Left : Original model and original dataset

Right : apply random rotation to all training, validation, and test data set

BOTH with same hyperparameters 100 epoch



As long as we start from a ‘rotational invariant’ sample, the CNN trained is ‘rotational invariant’.

Left : Original model and original dataset

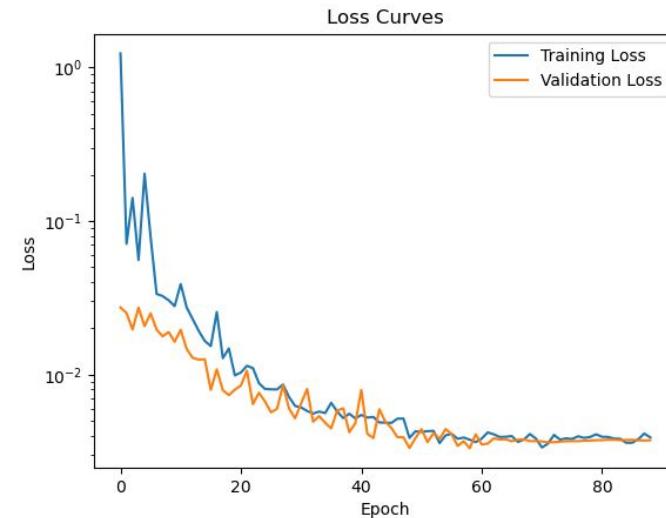
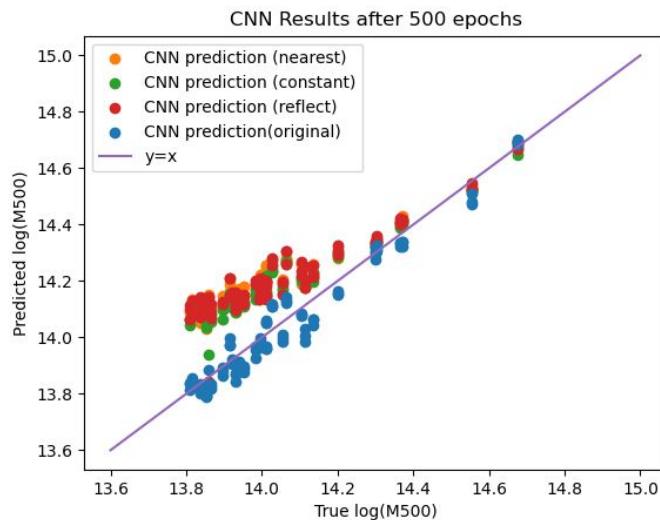
Right : apply random rotation to all training, validation, and test data set

BOTH with same hyperparameters 100 epoch

Testing rotation performance on original CNN

loss on the original test data: ~ 0.002

loss on the **rotated** test data: 0.03-0.04



Rotation invariant network: gCNN model design

gCNN: Group Equivariant CNN (e2cnn package employed)

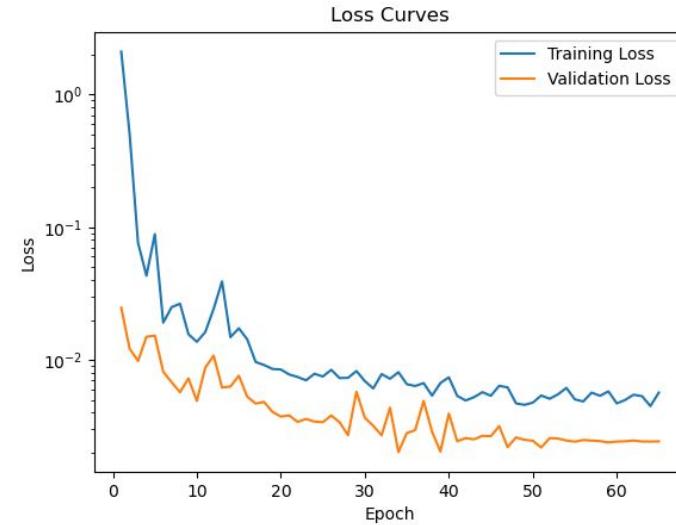
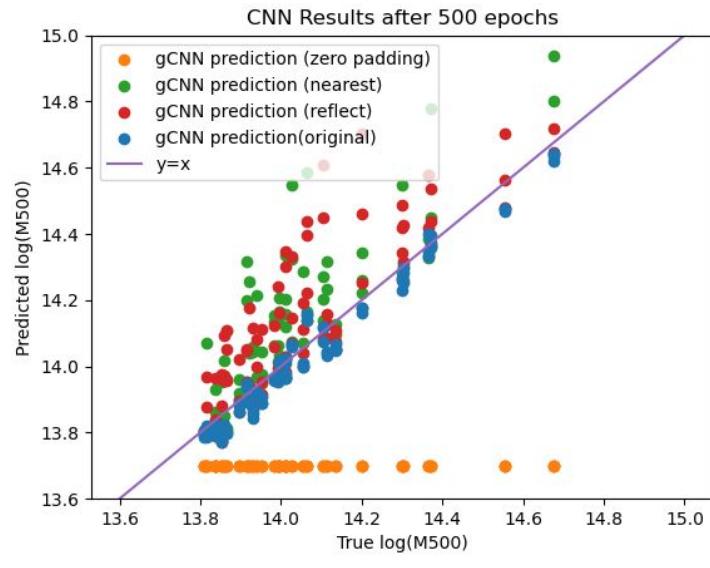
- 3 convolution layers followed by 3 pooling layers
- Group pooling layer
- mulit scale pooling
- fully conneted layer
- Dropout and Dense
- Kernel designed on Rotation Group (Num_rotation=32)
- Multi scale feature extraction

A very large model! (1.8G in size)

gCNN model result

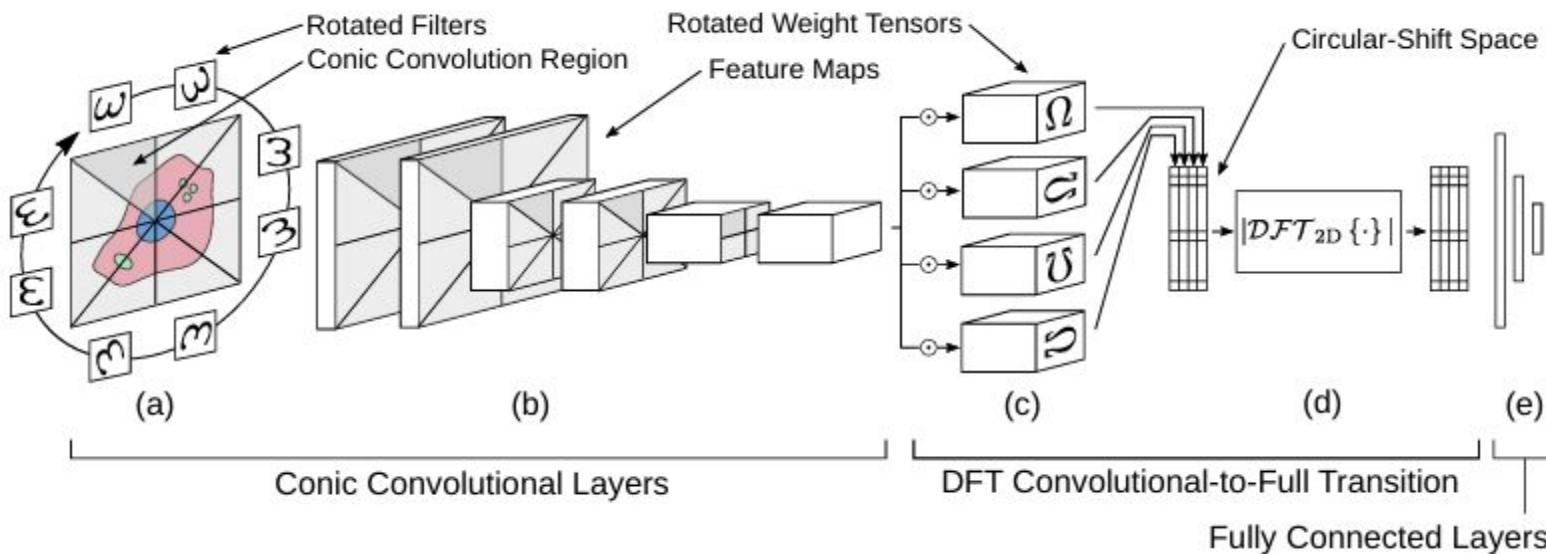
loss on original test data (blue) ~0.002

loss on **rotated** test data: 0.1(zero padding) 0.1(reflect) 0.06(nearest)



padding for the rotation? larger data set? better loss than MSE ?

RICNN



Summary

- Biased training data set could generate biased model (?), as seen in mass distribution and low-mass.
- The size of the dataset is crucial when exploring optimal architecture for CNN (i.e., data augmentation and k-fold cross-validation)
- ML considered the surrounding areas more important than the center of the cluster.
- To achieve rotational invariance in CNN, rotation needs to be applied somewhere. Either on original data-set or on the convolution kernels.

APPENDIX

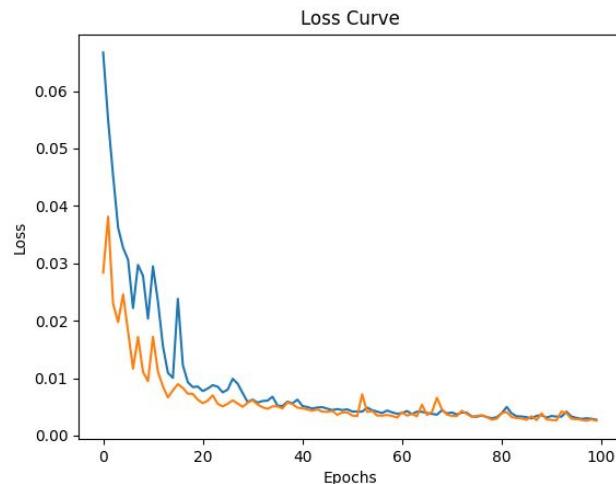
Model: "sequential_4", CNNs

Layer (type)	Output Shape	Param #
=====		
conv2d_12 (Conv2D(32, (3,3), relu))	(None, 138, 138, 32)	320
max_pooling2d_12 (MaxPooling2D(2,2))	(None, 69, 69, 32)	0
conv2d_13 (Conv2D(64, (3,3), relu))	(None, 67, 67, 64)	18496
max_pooling2d_13 (MaxPooling2D(2,2))	(None, 33, 33, 64)	0
conv2d_14 (Conv2D(64, (3,3), relu))	(None, 31, 31, 64)	36928
max_pooling2d_14 (MaxPooling2D(2,2))	(None, 15, 15, 64)	0
global_average_pooling2d_4 (GlobalAveragePooling2D)	(None, 64)	0
dropout_8 (Dropout(0.1))	(None, 64)	0
dense_16 (Dense(200, relu))	(None, 200)	13000
dropout_9 (Dropout(0.1))	(None, 200)	0
dense_17 (Dense(100, relu))	(None, 100)	20100
dense_18 (Dense(20, relu))	(None, 20)	2020
dense_19 (Dense(1,softplus))	(None, 1)	21
=====		

Total params: 90,885

Trainable params: 90,885

Non-trainable params: 0



H

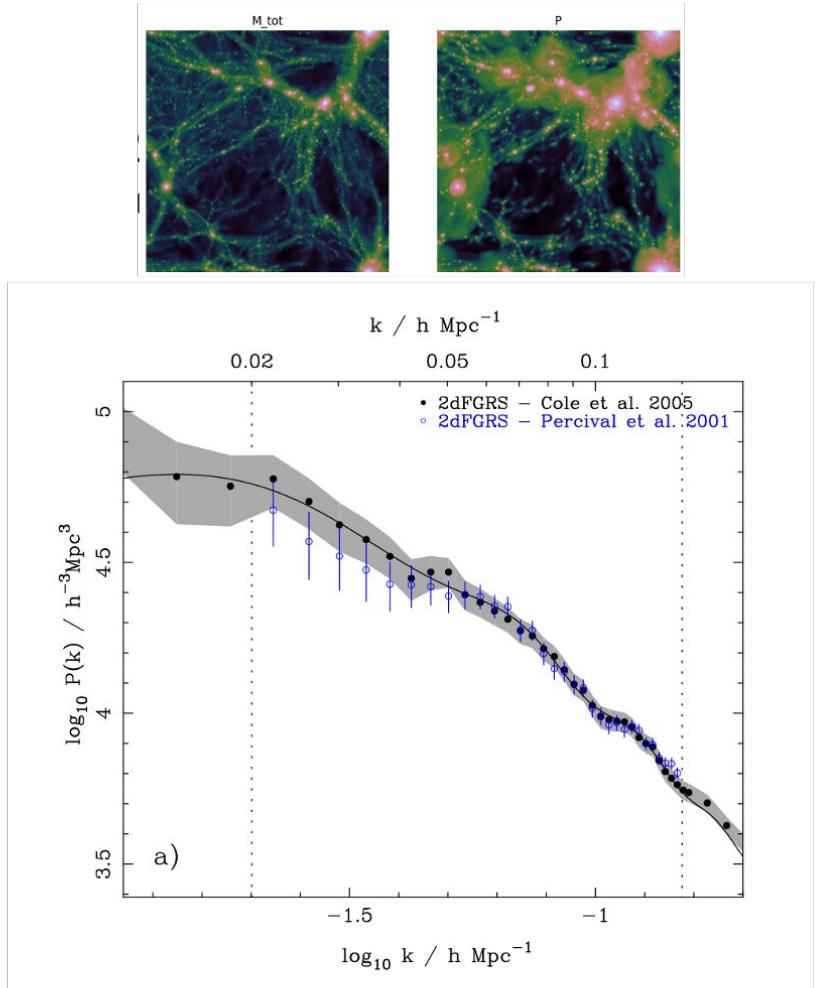
Group H

(8) Using **CNNs** to infer the fundamental **parameters** of the Universe

Chenze Dong / Jiacheng Ding / Mingyeong Yang / Shinsei Eyama
/ Xinyue Chen / YoungPyo Hong / Yiming Dong

Motivation

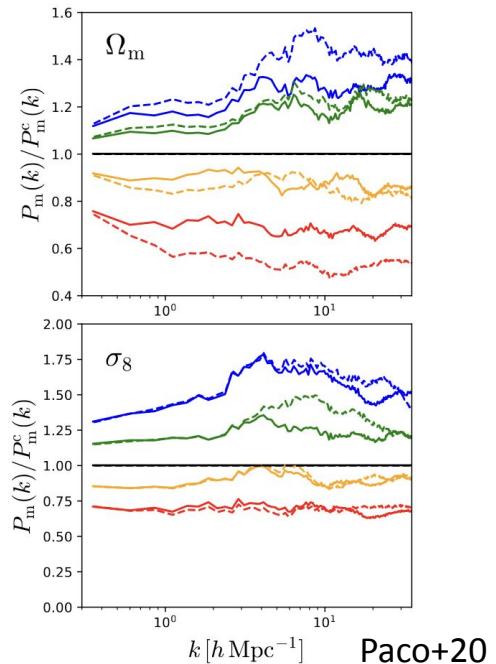
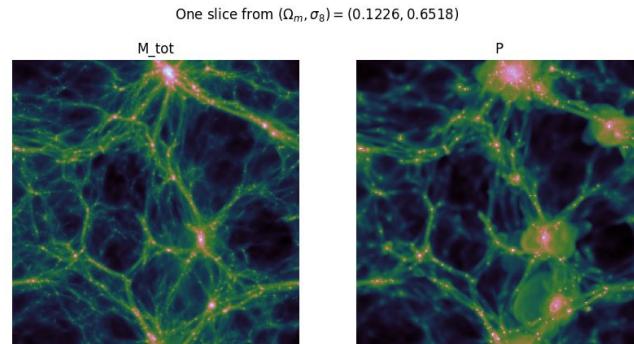
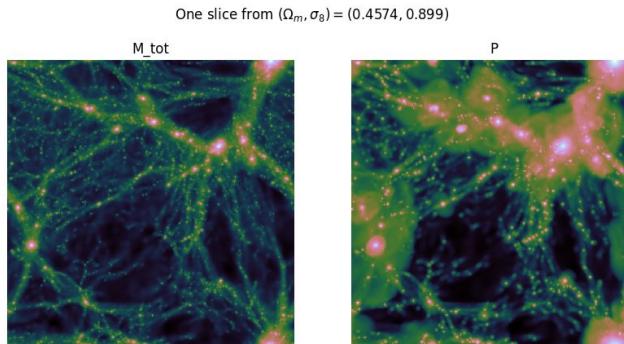
- How to determine Ω_m and σ_8 from large scale survey?
 - The main point is to **compare** observations with theoretical calculations or simulations
 - But, we have no idea how to compare 2 dimensional figure directly
 - A possible method or compromise is **data dimension reduction**, such as with power spectrum, which may cause information loss



2dFGRS Collaboration, 2005

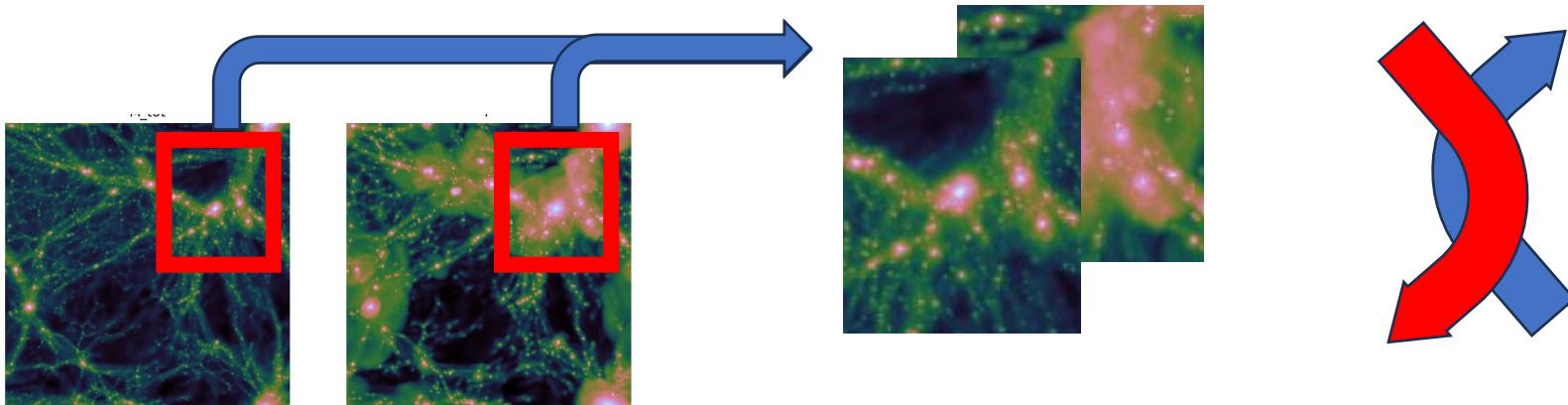
Our “raw” dataset (from TNG)

- **2D image** of M_{tot} (total mass) & P (electron pressure)
- **1000 sets** of cosmological / astrophysical **parameters** from LH sampling
 - Cosmological param. (Ω_m , σ_8)
- 15 slices x 1000 settings = **15000 images**
 - with size (2,256,256)



Preprocessing

- Strategies:
 - **Combine** the two maps together as two channels of one image
 - Work with **log-image & normalization** to $[0, 1]$
 - Crop the image to a **smaller** size
 - **Shuffle** images so different cosmologies can enter the training set



Simple model

- ***Simple CNN model***

- Taking input of $(*, 2, 64, 64)$ image
- 3 layers of Convolution + MaxPooling
- Layer normalization for each layer
- 2 fully connected layers
- Giving output two cosmo. param. $(*, 2)$
- Training for 300 epochs

Layer (type)	Output Shape	Param #
Conv2d-1	$[-1, 16, 64, 64]$	304
ReLU-2	$[-1, 16, 64, 64]$	0
LayerNorm-3	$[-1, 16, 64, 64]$	131,072
MaxPool2d-4	$[-1, 16, 32, 32]$	0
Conv2d-5	$[-1, 32, 32, 32]$	4,640
ReLU-6	$[-1, 32, 32, 32]$	0
LayerNorm-7	$[-1, 32, 32, 32]$	65,536
MaxPool2d-8	$[-1, 32, 16, 16]$	0
Conv2d-9	$[-1, 64, 16, 16]$	18,496
ReLU-10	$[-1, 64, 16, 16]$	0
LayerNorm-11	$[-1, 64, 16, 16]$	32,768
MaxPool2d-12	$[-1, 64, 8, 8]$	0
Linear-13	$[-1, 1024]$	4,195,328
ReLU-14	$[-1, 1024]$	0
Linear-15	$[-1, 2]$	2,050

Total params: 4,450,194

Trainable params: 4,450,194

Non-trainable params: 0

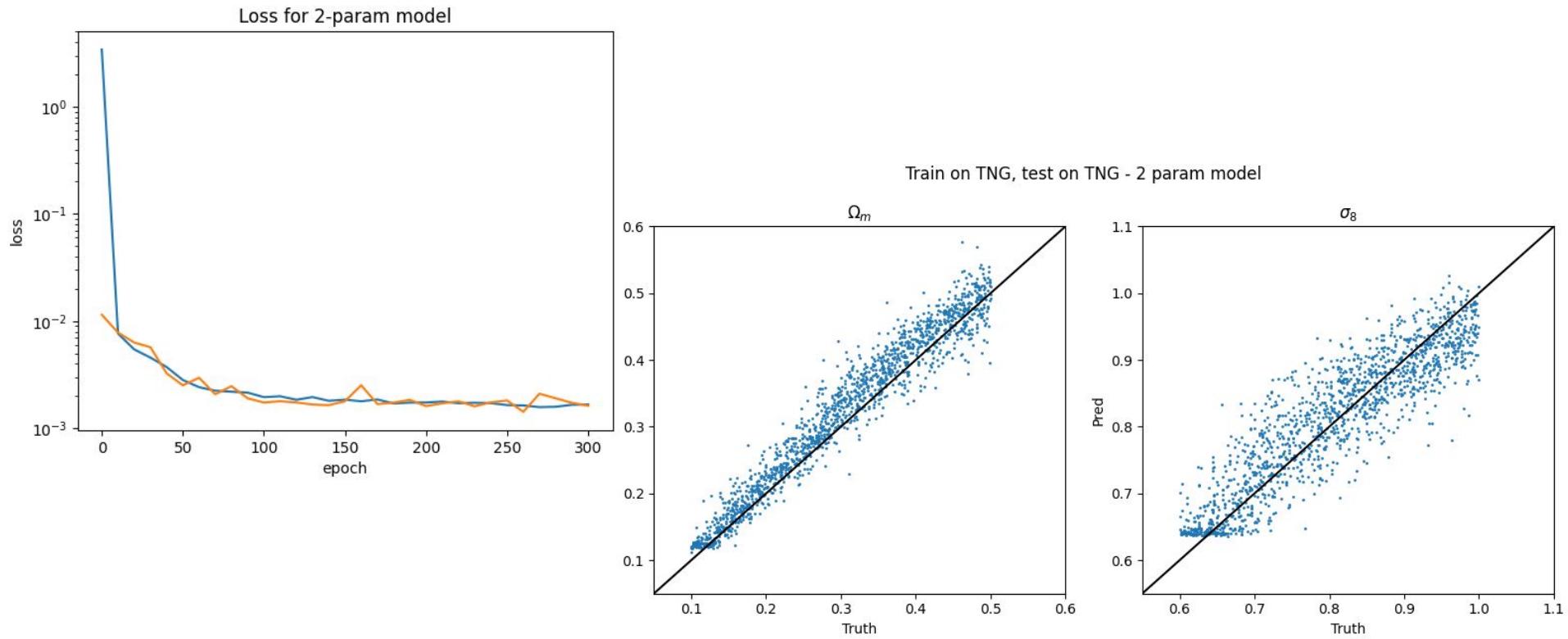
Input size (MB): 0.03

Forward/backward pass size (MB): 2.86

Params size (MB): 16.98

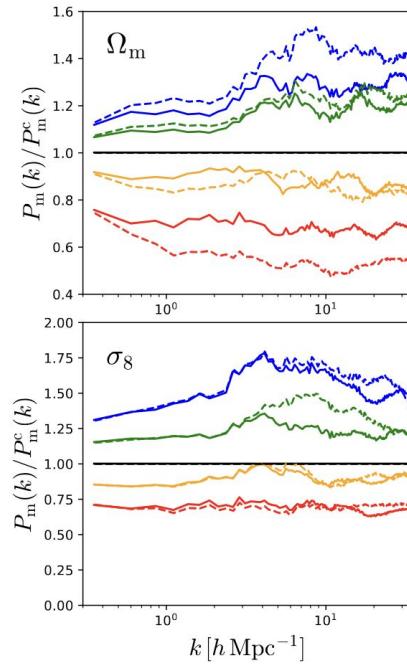
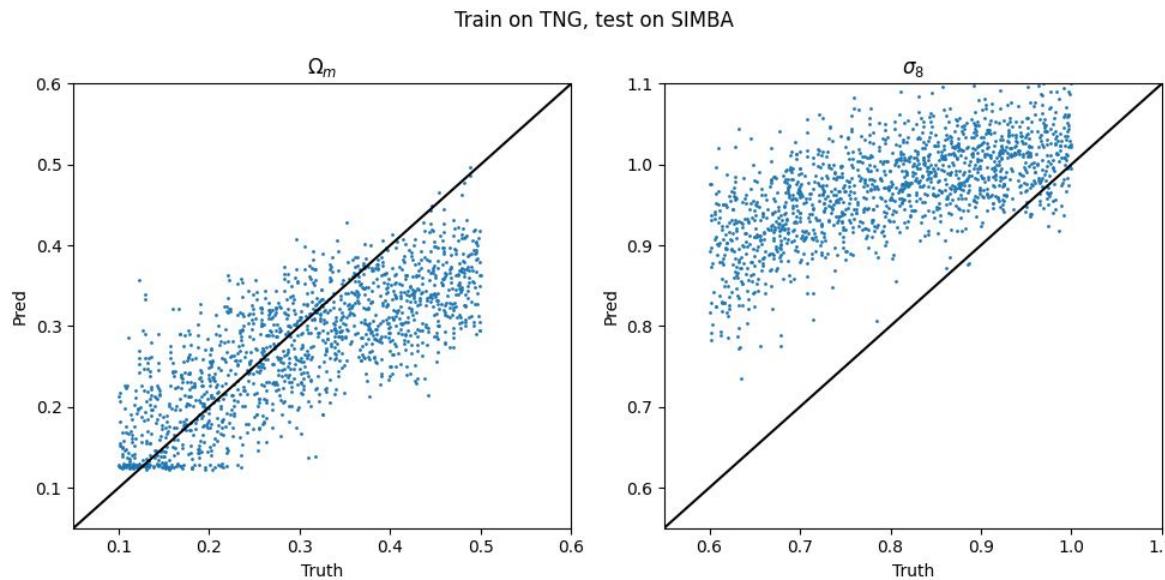
Estimated Total Size (MB): 19.87

Simple model, good performance



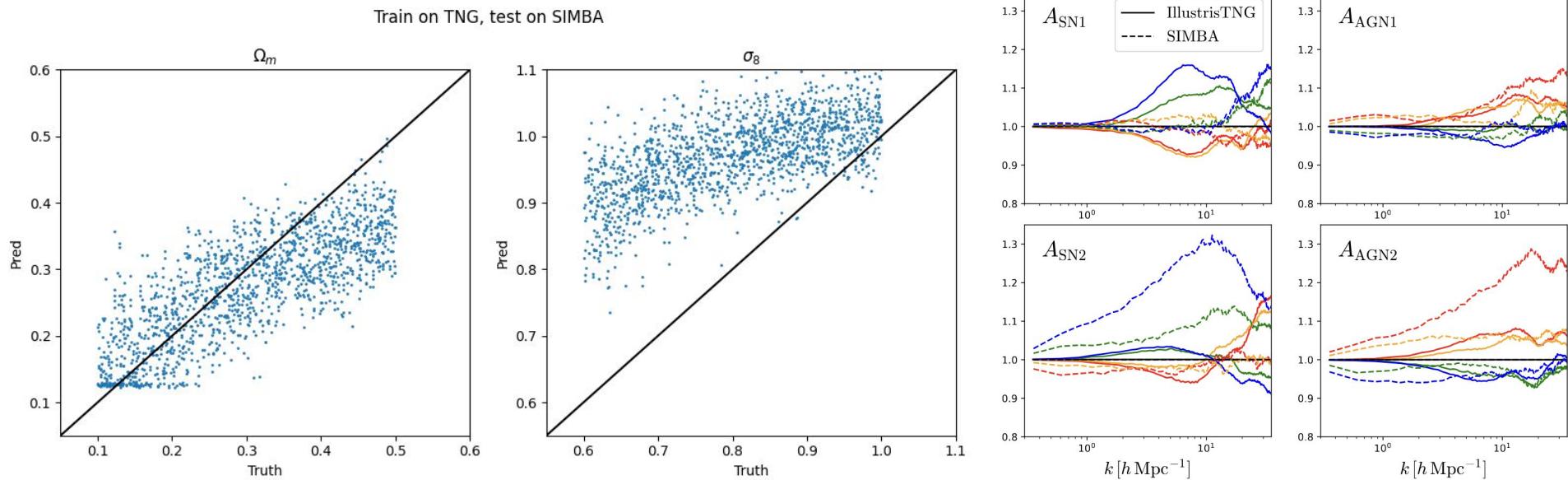
Does the model generalize?

- Not that bad on Ω_m , overestimated for σ_8



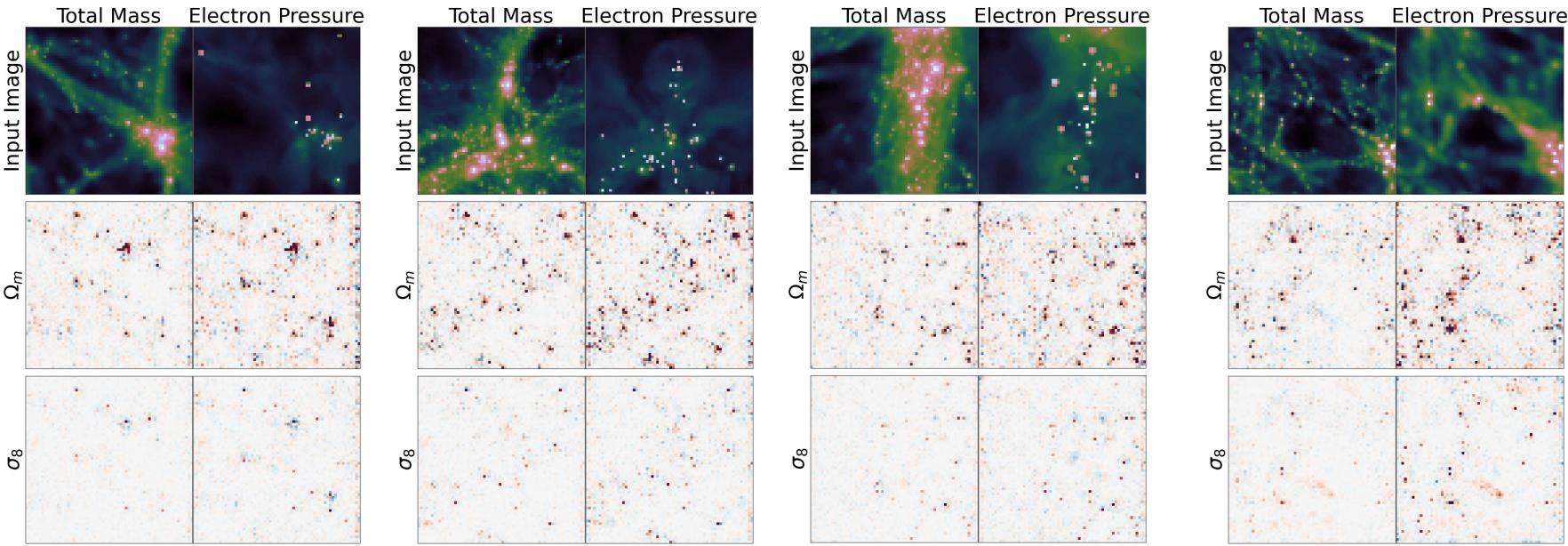
Does the model generalize?

- Not that bad on Ω_m , overestimated for σ_8



Interpret this CNN

- The network is **NOT** telling cosmology from **massive halos**
- It seemingly uses the information from value peaks in **filaments**



Layer (type)	Output Shape	Param #
Conv2d-1	[-1, 16, 64, 64]	304
ReLU-2	[-1, 16, 64, 64]	0
LayerNorm-3	[-1, 16, 64, 64]	131,072
MaxPool2d-4	[-1, 16, 32, 32]	0
Conv2d-5	[-1, 32, 32, 32]	4,640
ReLU-6	[-1, 32, 32, 32]	0
LayerNorm-7	[-1, 32, 32, 32]	65,536
MaxPool2d-8	[-1, 32, 16, 16]	0
Conv2d-9	[-1, 64, 16, 16]	18,496
ReLU-10	[-1, 64, 16, 16]	0
LayerNorm-11	[-1, 64, 16, 16]	32,768
MaxPool2d-12	[-1, 64, 8, 8]	0
Linear-13	[-1, 4096]	16,781,312
ReLU-14	[-1, 4096]	0
Linear-15	[-1, 6]	24,582

Total params: 17,058,710

Trainable params: 17,058,710

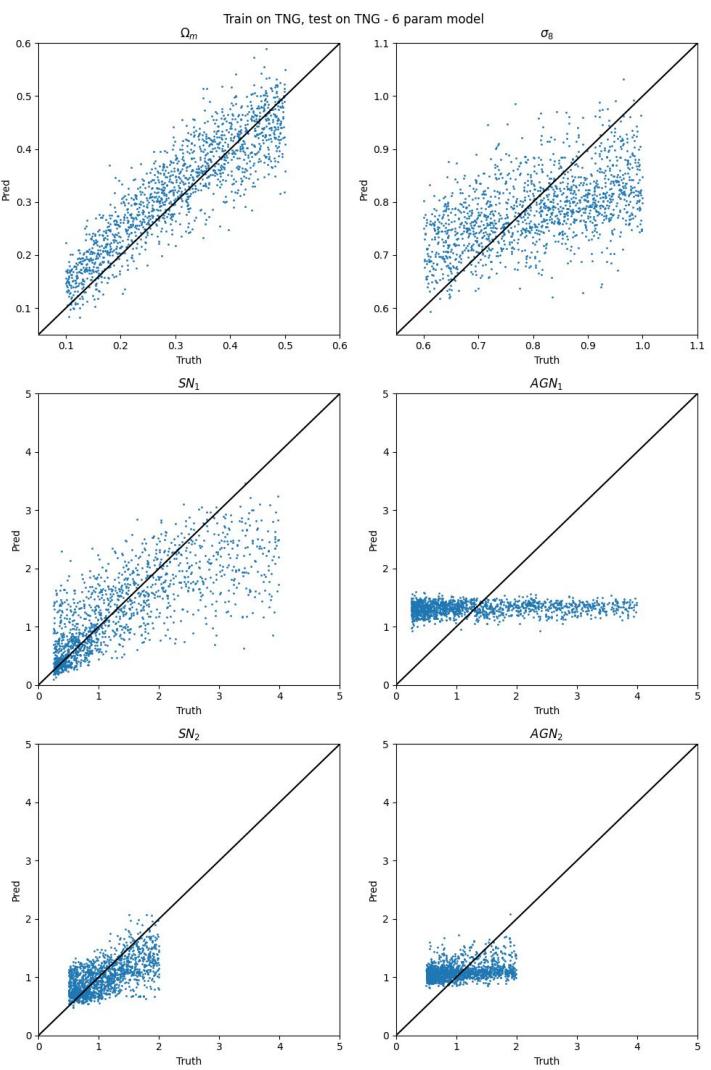
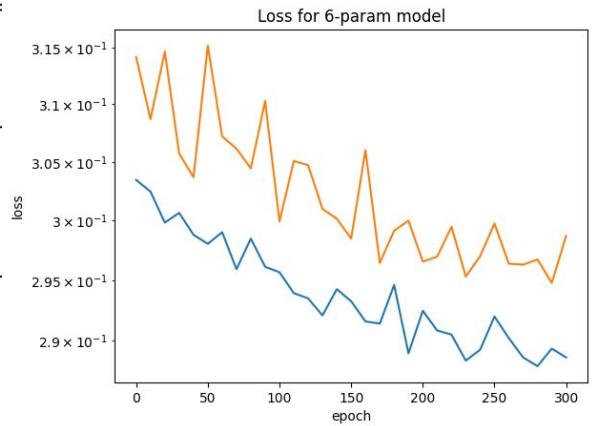
Non-trainable params: 0

Input size (MB): 0.03

Forward/backward pass size (MB): 2.91

Params size (MB): 65.07

Estimated Total Size (MB): 68.01



Can you infer 6 parameters? No:(

Summary

- We constructed a simple, **3-layer CNN** to infer (Ω_m, σ_8) from (M_{tot}, P) slices of **TNG** suites in **CAMELS** simulation.
- The **Result** is actually **good** given the simple architecture; when testing with **SIMBA** data, the model more or less **generalizes** for Ω_m , but usually **overestimate** σ_8 .
- By inspecting the saliency map, we find the **model** is likely extracting **information** from **halos** in filaments rather than **cosmic web nodes**.
- We also attempt to train a **similar model** to predict **all the 6 simulation parameters**. After 300 epoches' training, the model learns almost **nothing** about **AGN feedback**, suggesting a **minor impact** of AGN feedback on the **two input** quantities.