SummerSOC 2025

Crete, Greece

Uncertainty-Aware Machine Learning for Astronomical Data Analysis

Gregory Tsagkatakis

Institute of Computer Science, FORTH
Computer Science Department, University of Crete

Funded by the European Union

SPL at a glance

2006

4 Researchers/Academics (permanent)
1 Postdoctoral Researchers
12 Postgraduate Students
2 Research Engineers

> 10M€ (PI/co-PI in EU & national projects)

FORTH

ICS + 8 Institutes

SPL + 7 Labs

Research Institutes

Electronic Structure & Laser
Molecular Biology & Biotechnology
Computer Science
Applied and Computational Mathematics
Mediterranean Studies
Chemical Engineering Sciences
Astrophysics
Geoenegy
Biomedical Research

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FORTH INSTITUTE OF COMPUTER SCIENCE
Signal Processing Laboratory
CosmoStat
cea
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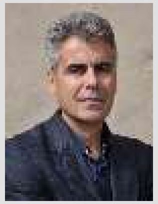
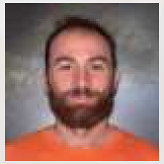
Collaborators & Funding

Panos Tsakalides
Signal Processing lab
FORTH



Jean-Luc Starck
CosmoStat lab
CEA, France

Mahta Moghaddam
MiXIL lab
USC

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ARTIFICIAL INTELLIGENCE
IN ASTROPHYSICS

RESEARCH EXECUTIVE AGENCY

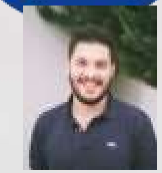
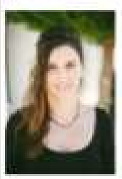
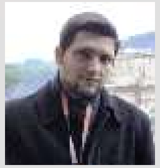
CALCHAS
Computational Intelligence for Multi-Source Remote Sensing Data Analytics

MARIE CURIE ACTIONS
European Commission | Horizon 2020 European Union funding for Research & Innovation

esa

NASA

H.F.R.I.
Hellenic Foundation for Research & Innovation

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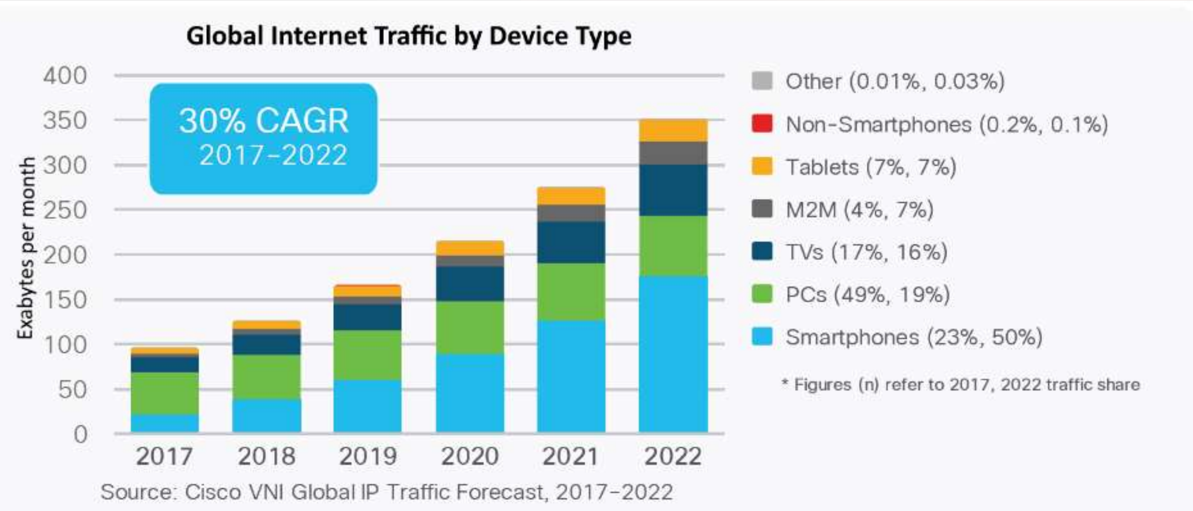
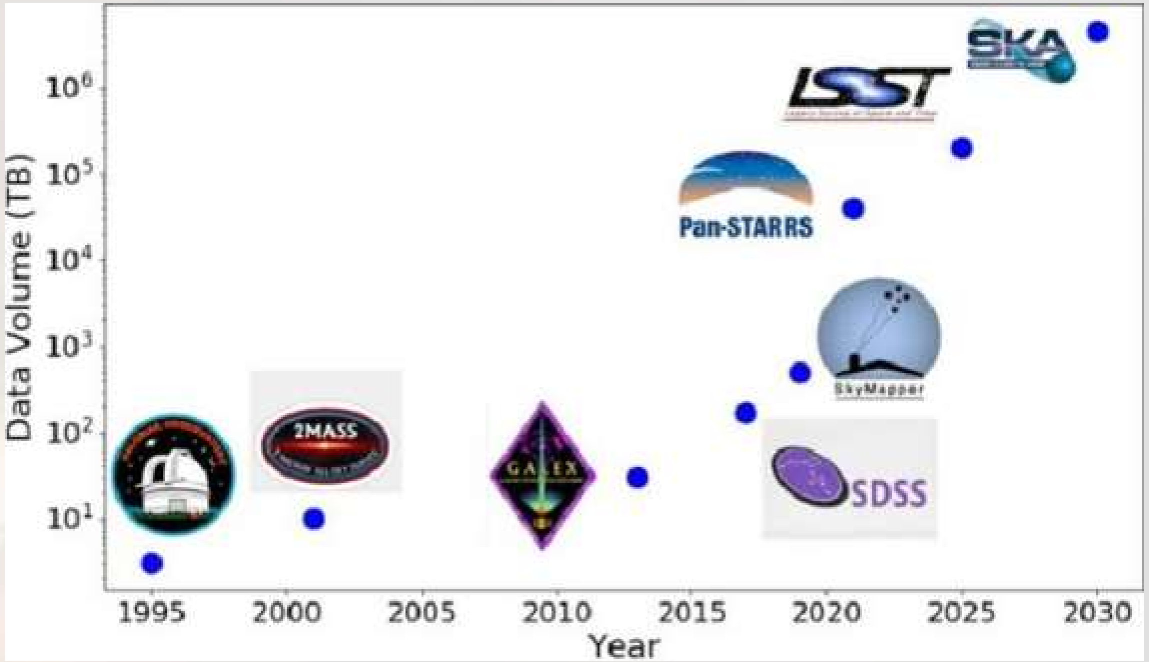
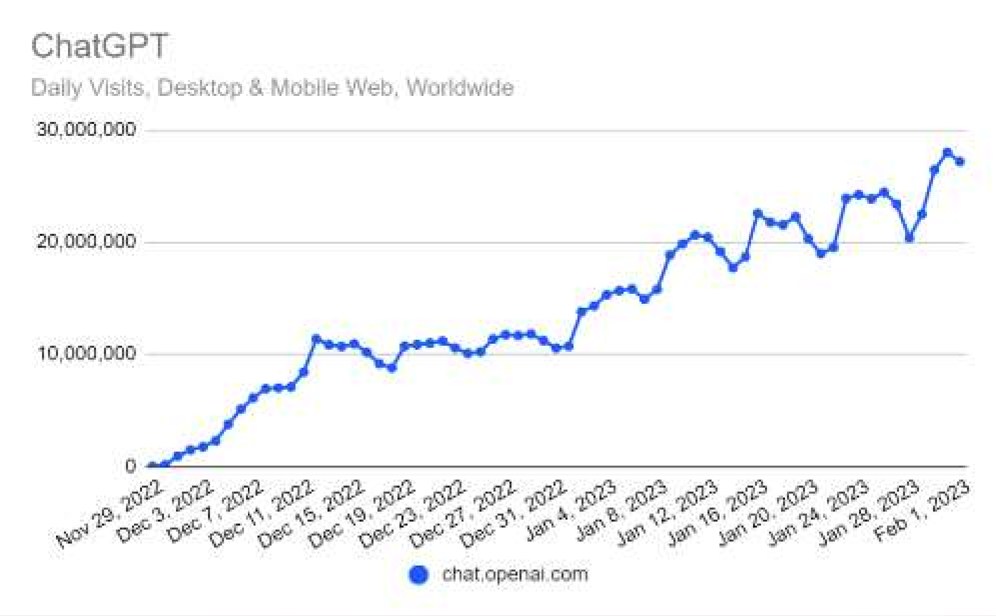
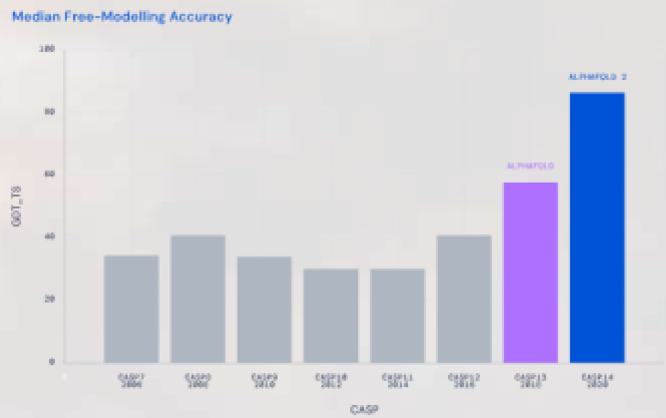
The Big Data Revolution





The AI Revolution





Jumper, John, et al. "Highly accurate protein structure prediction with AlphaFold." *Nature.* 2021.

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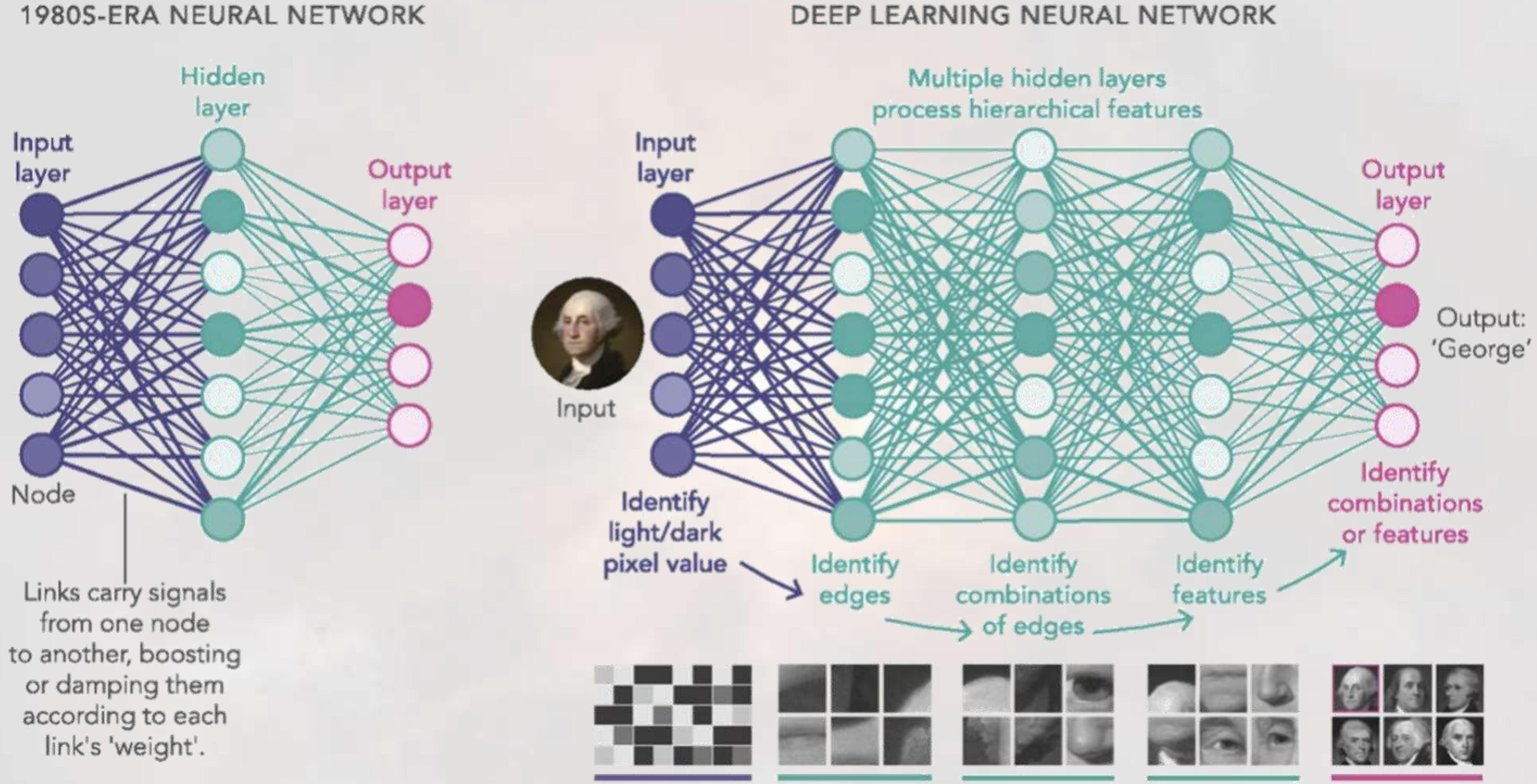
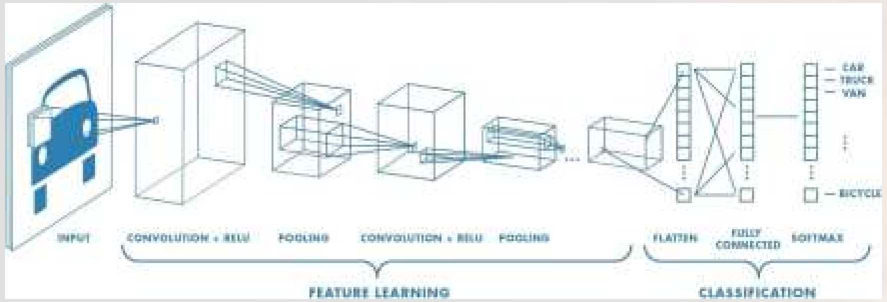
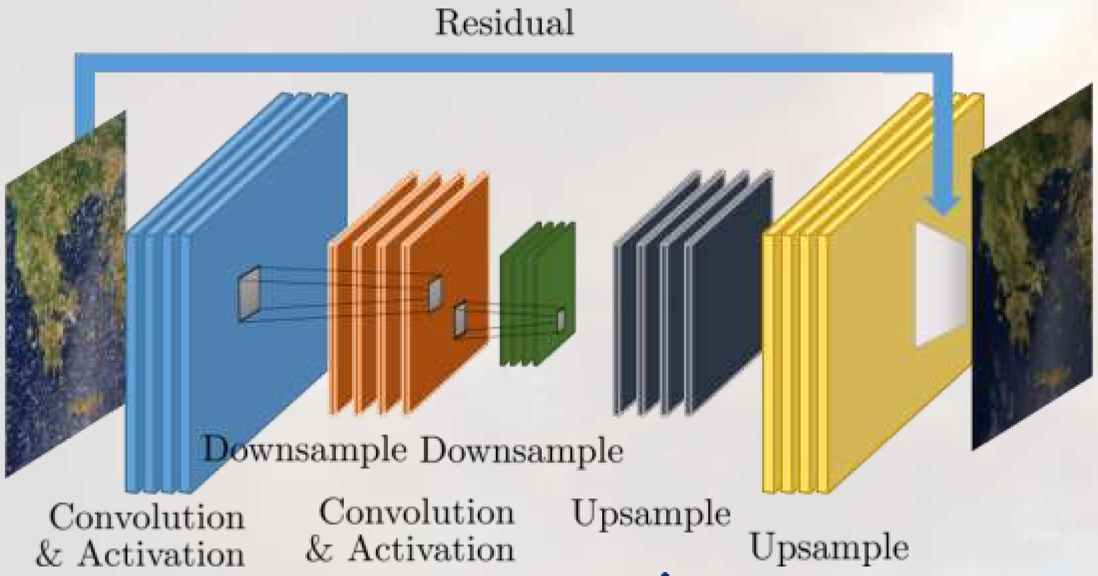
Deep Learning



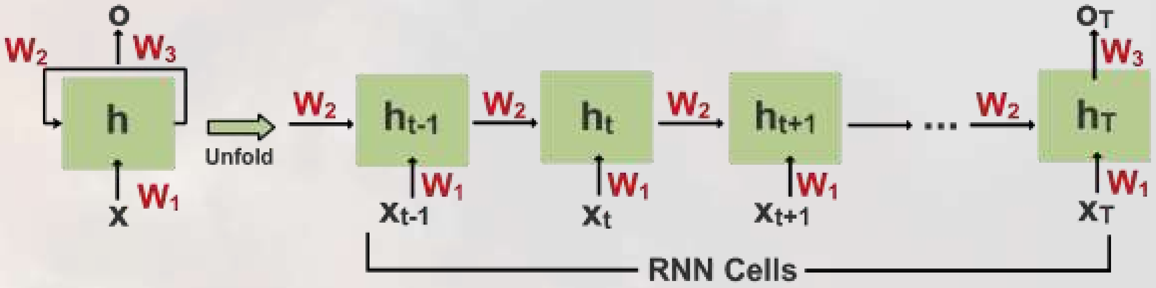
State-of-the-art in DL

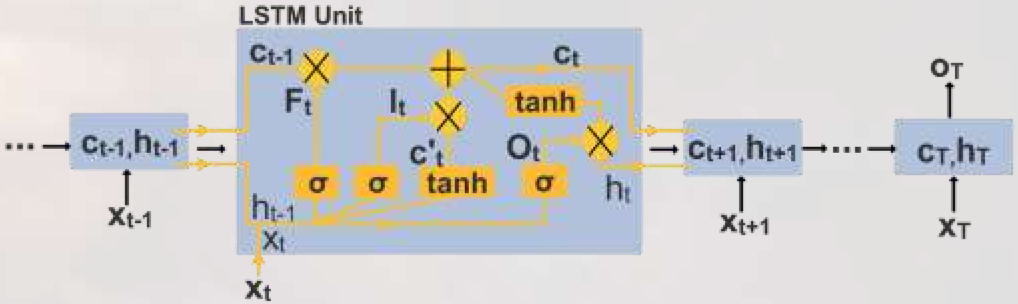
CNNs





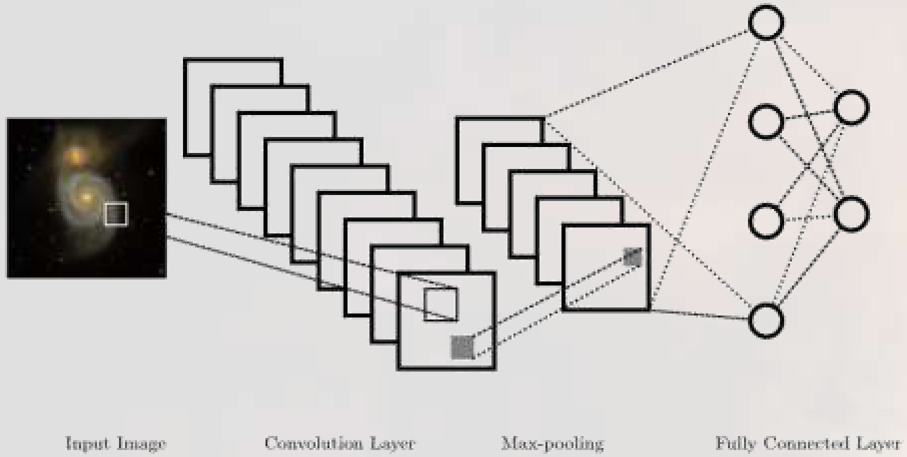
RNN/LSTMs

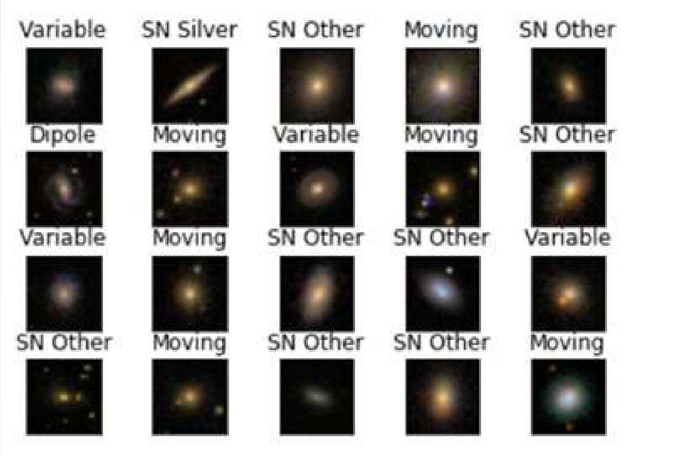


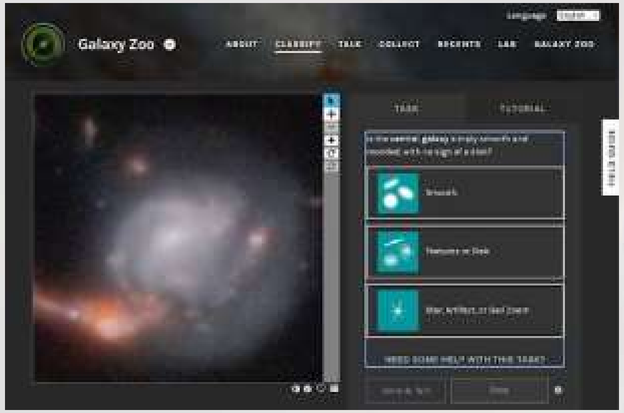


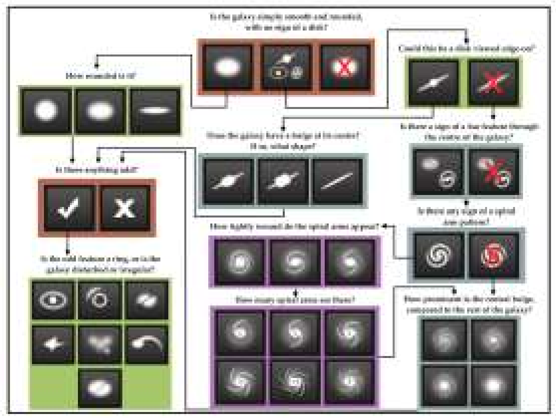
Transformers

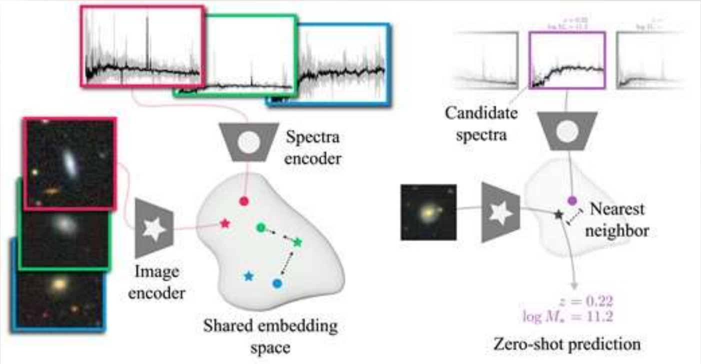
Deep Learning in Astronomy











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Uncertainty (model)

alaskan malamute

siberian husky

siberian husky

Epistemic Uncertainty:

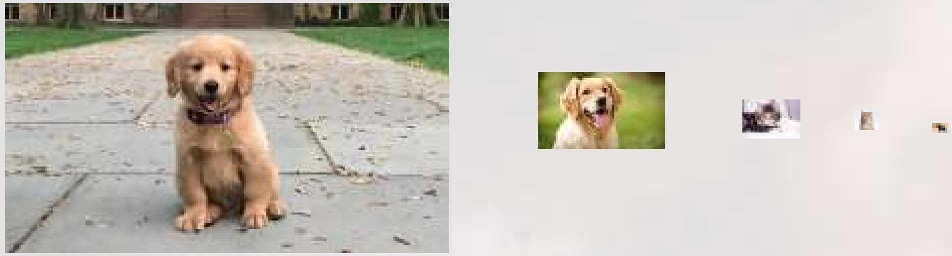
- ➢ Due to lack of knowledge about a system or process.
- ➢ Can be reduced as more knowledge is gained.

Uncertainty (data)




cat

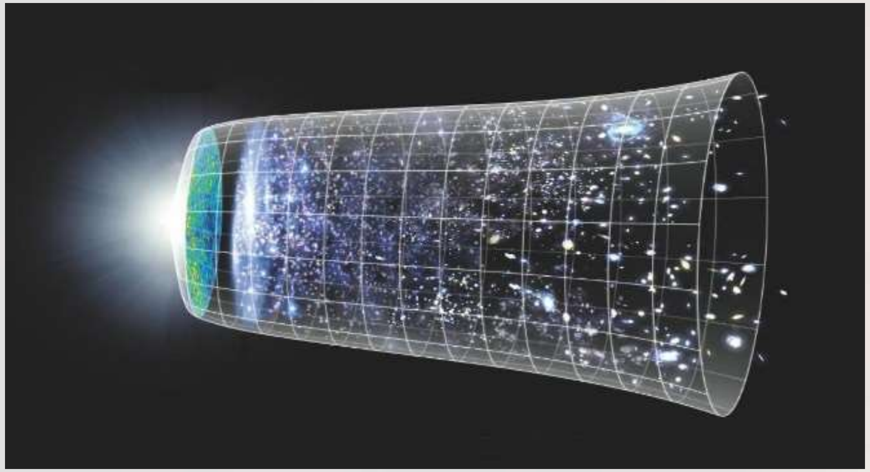
dog

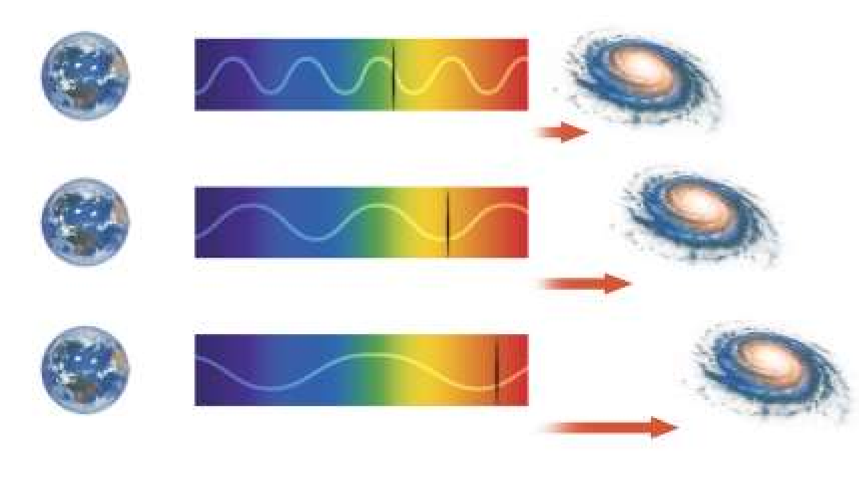


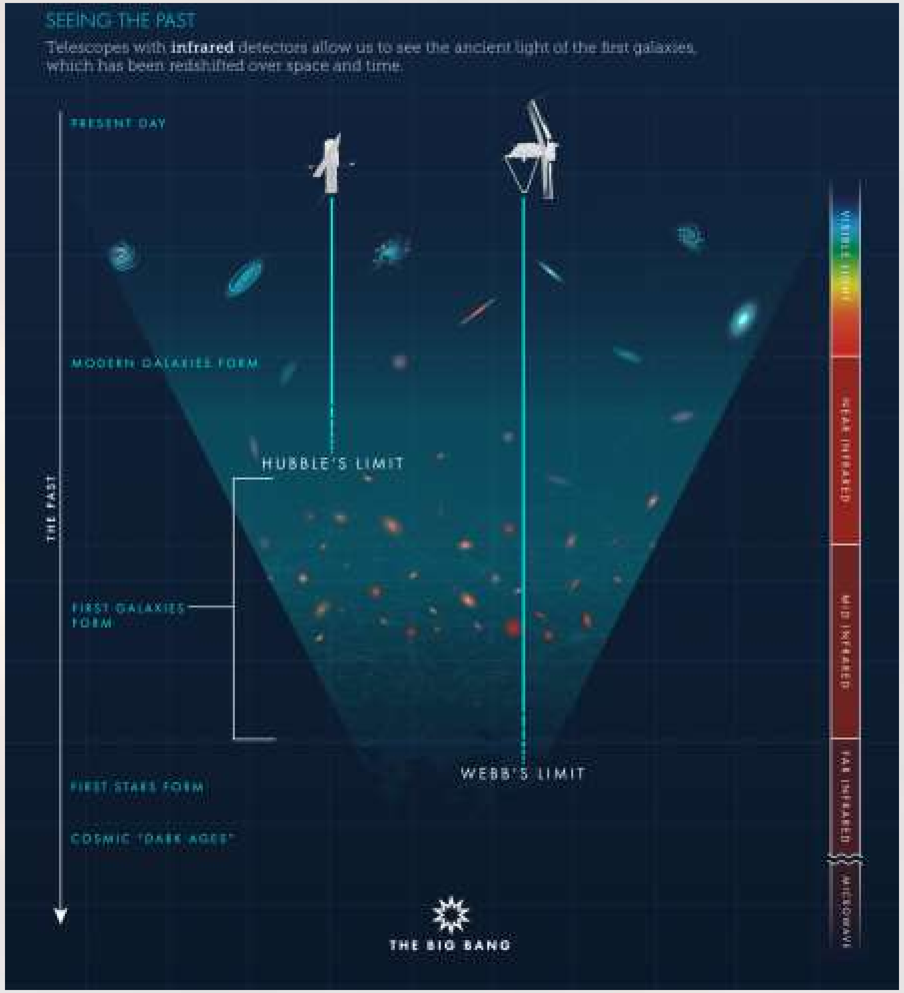
Aleatoric Uncertainty:

- inherent randomness in a system or process (flipping a coin
- cannot be reduced with more information or knowledge about the system.

Redshift estimation







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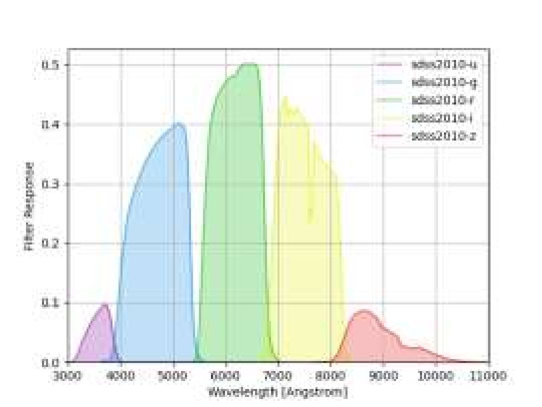
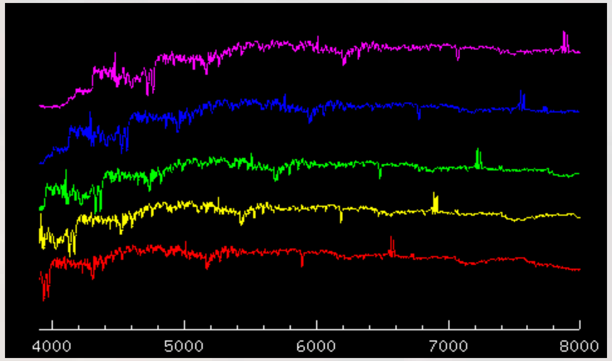
Observations for Redshift estimation





Photometric

- 3-4 broad bands
- Cheap
- Inaccurate

Spectroscopic

- Extended spectral range
- Expensive
- Accurate

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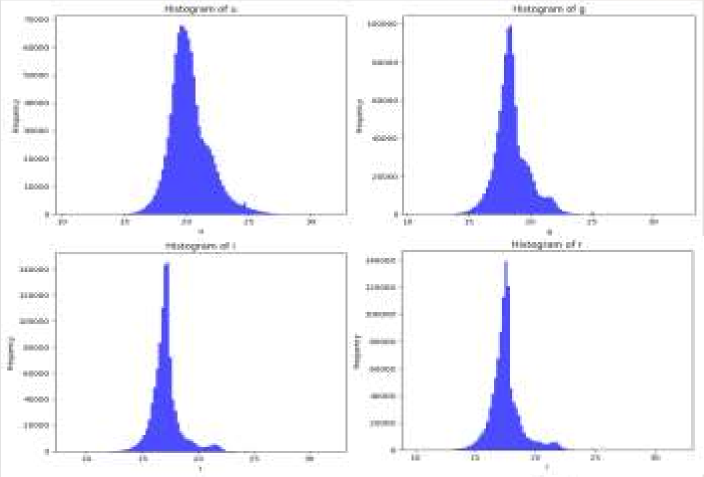
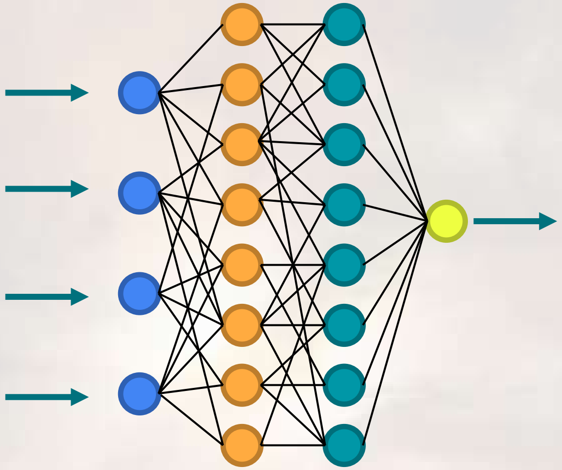
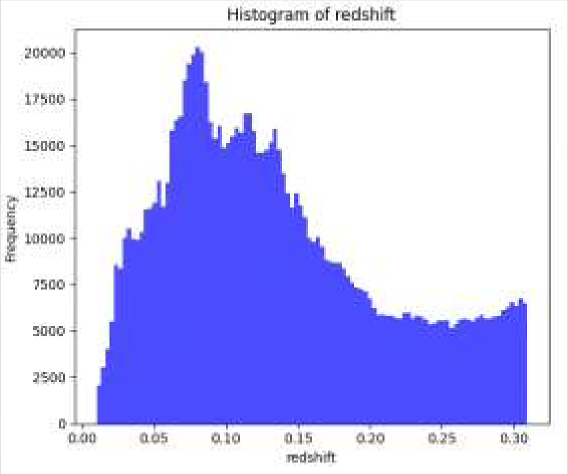
ANNs for Photometric Redshift Estimation







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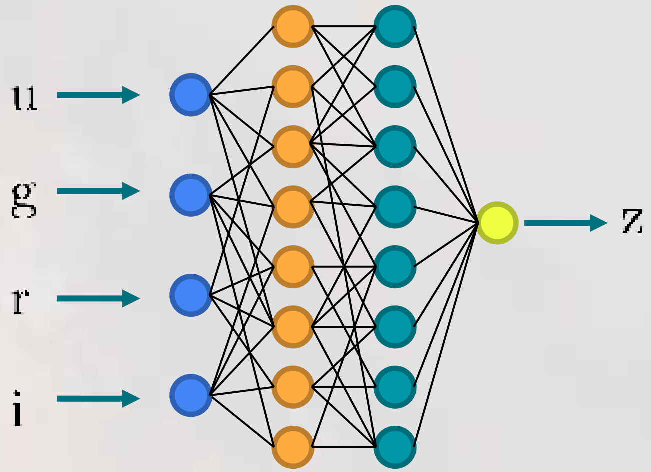
ANN - Regression

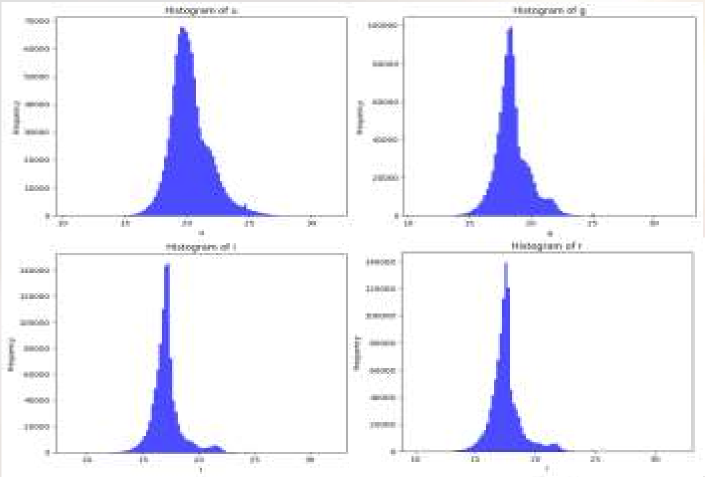
Baseline regression model $\hat{y}_i = f(x_i; \mathbf{w})$ where:

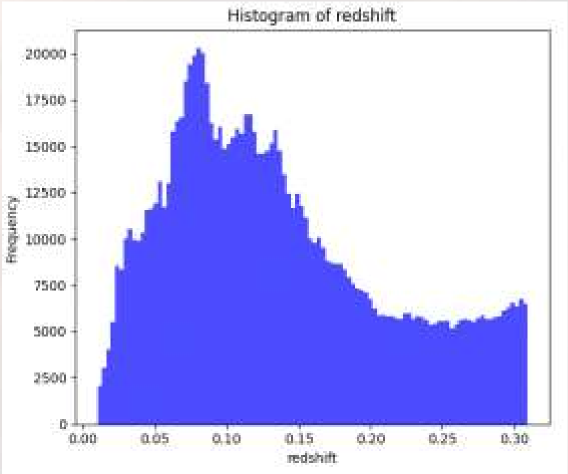
- $f(x_i; \mathbf{w})$ is the prediction for the i-th observation,
- y_i is the actual value for the i-th observation

Loss function: $\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(f(x_i; \mathbf{w}) - y_i)^2$



Dataset

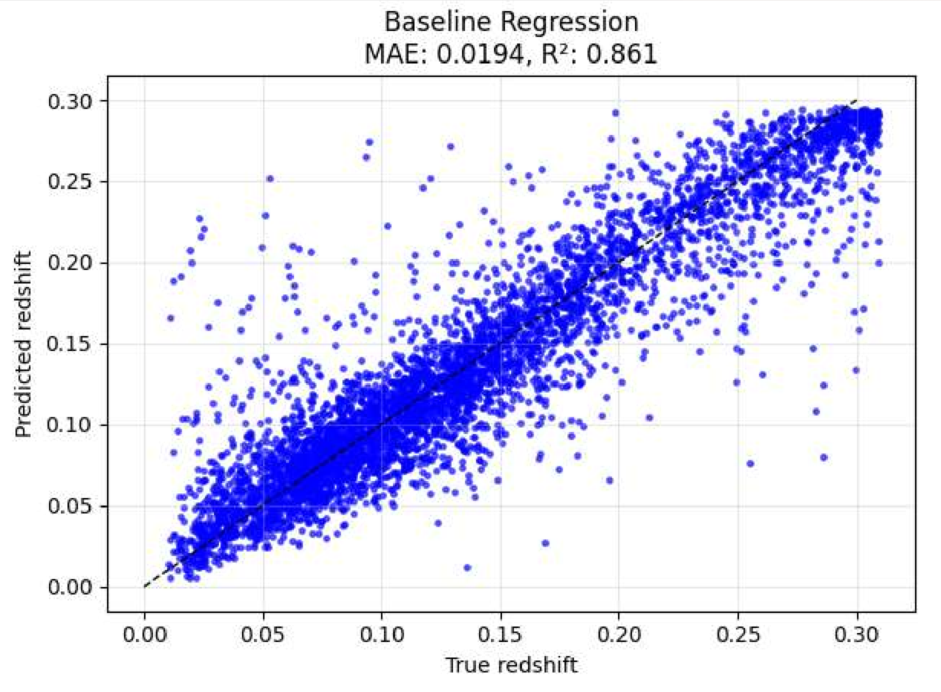


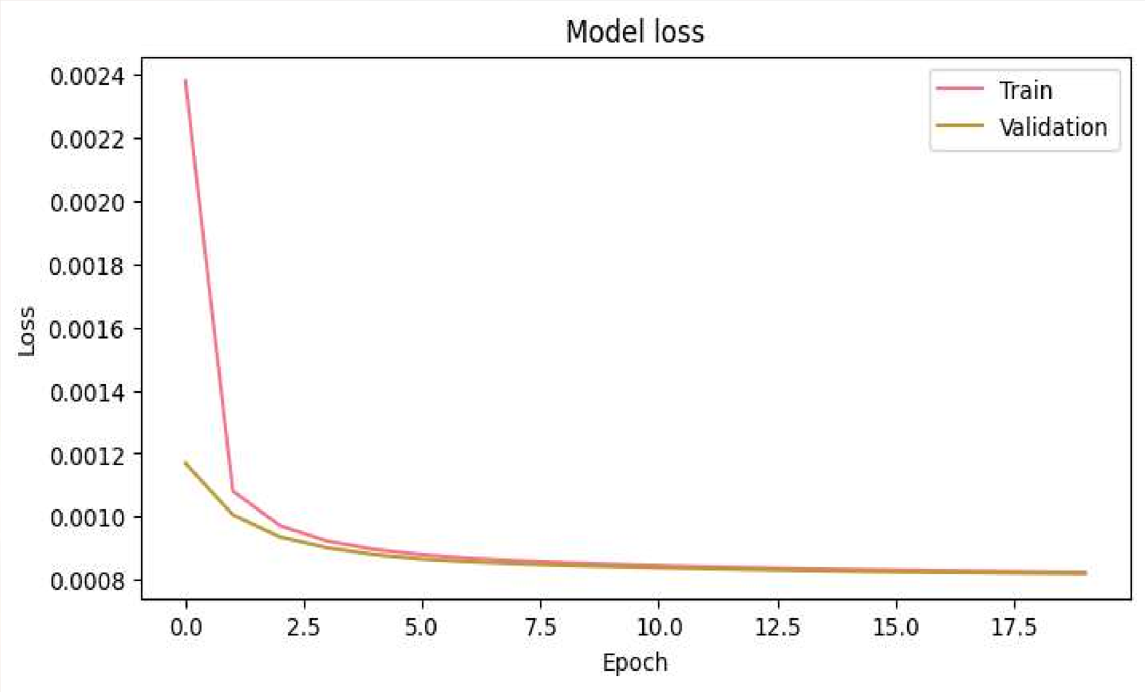


Training: 800K

Testing: 200K

Baseline model & Data





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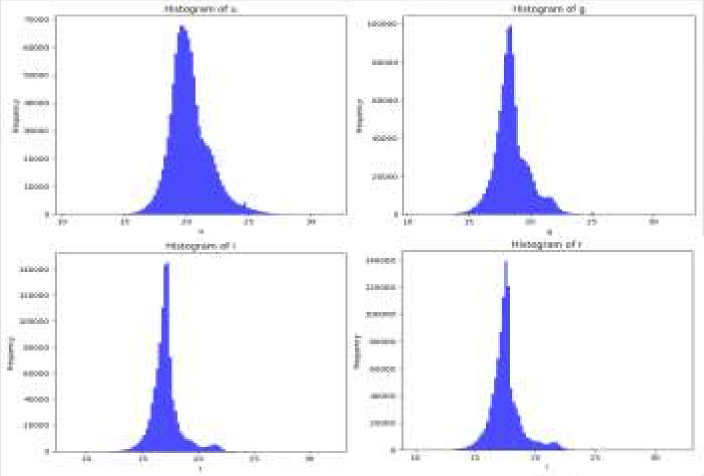
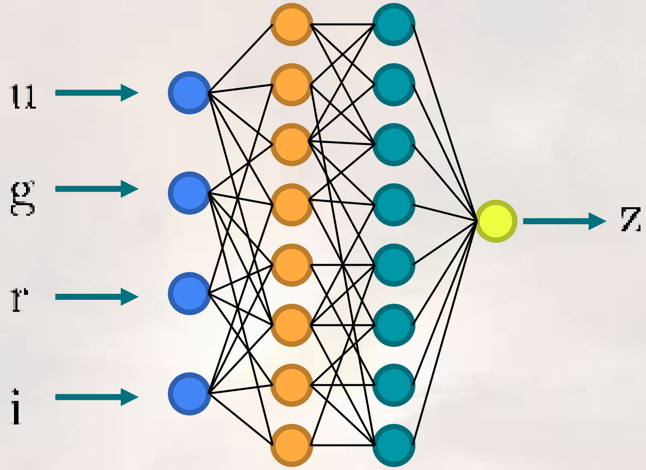
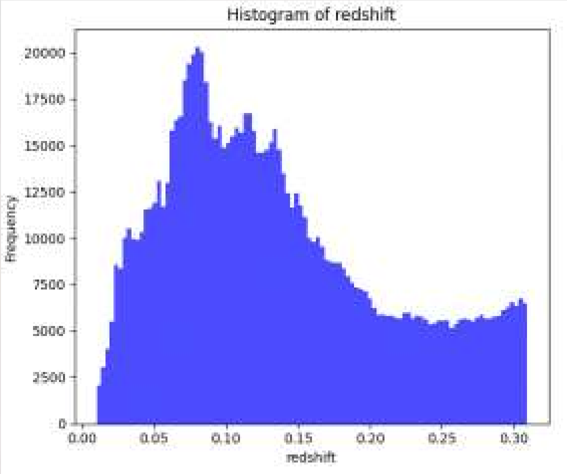
Uncertainties







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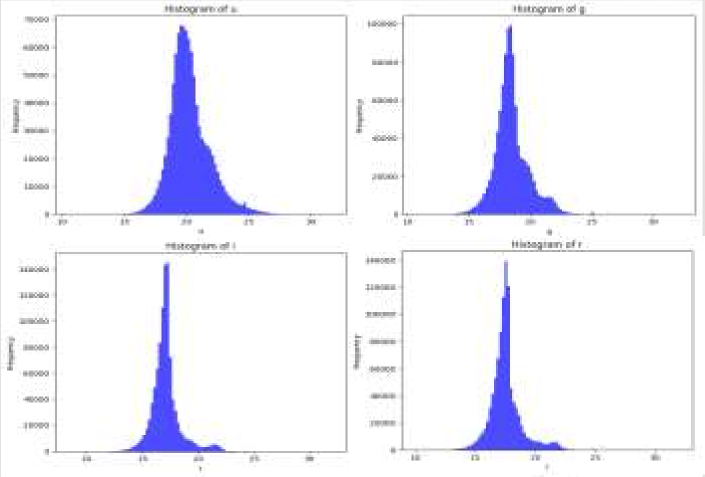
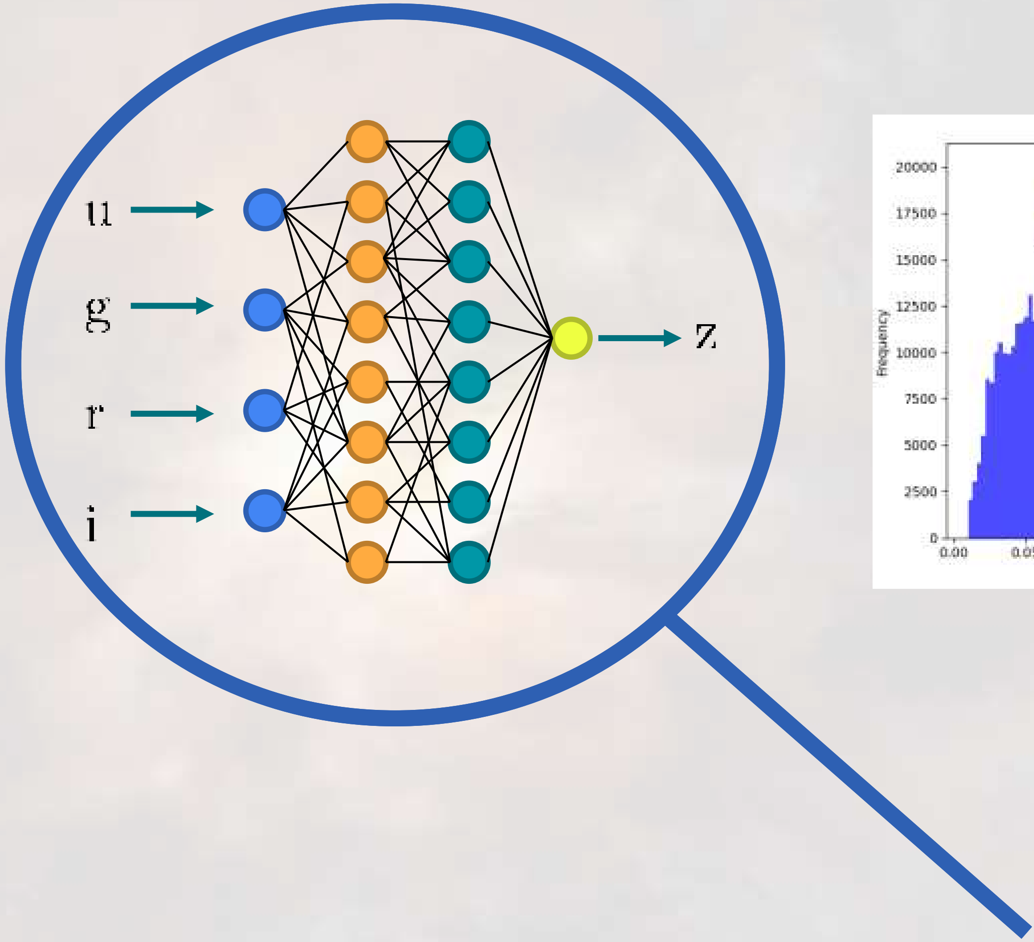
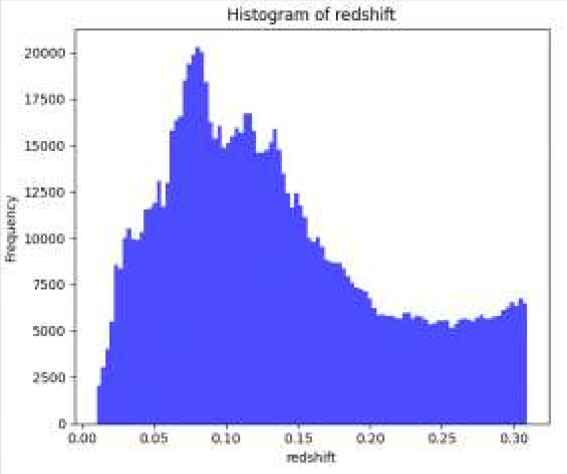
Uncertainties (model)







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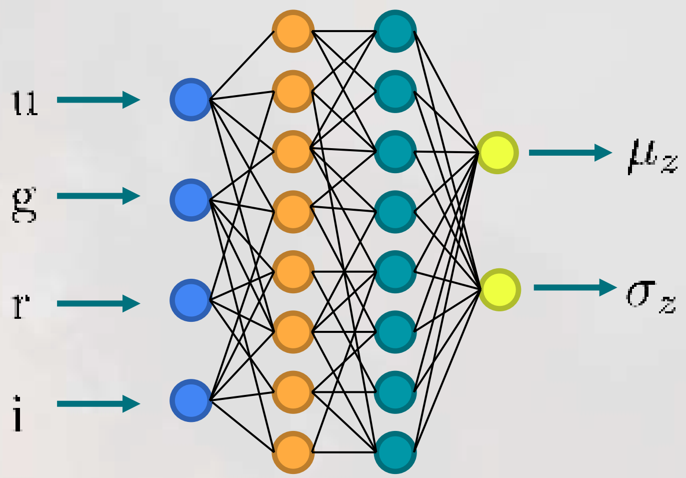
Gaussian Regression via ANN

- The target variable $y_i \sim \mathcal{N}(f(x_i; \mathbf{w}), \sigma^2)$
- The likelihood for each observation is:

$$p(y_i \mid x_i, \mathbf{w}) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - f(x_i; \mathbf{w}))^2}{2\sigma^2}\right)$$



Loss: Negative Log-Likelihood (NLL) for N observations is:

$$\mathcal{L}(\mathbf{w}) = -\sum_{i=1}^{N} \log p(y_i \mid x_i; \mathbf{w})$$

$$= \frac{N}{2} \log(2\pi\sigma^2) + \frac{1}{2\sigma^2} \sum_{i=1}^{N} (y_i - f(x_i; \mathbf{w}))^2$$

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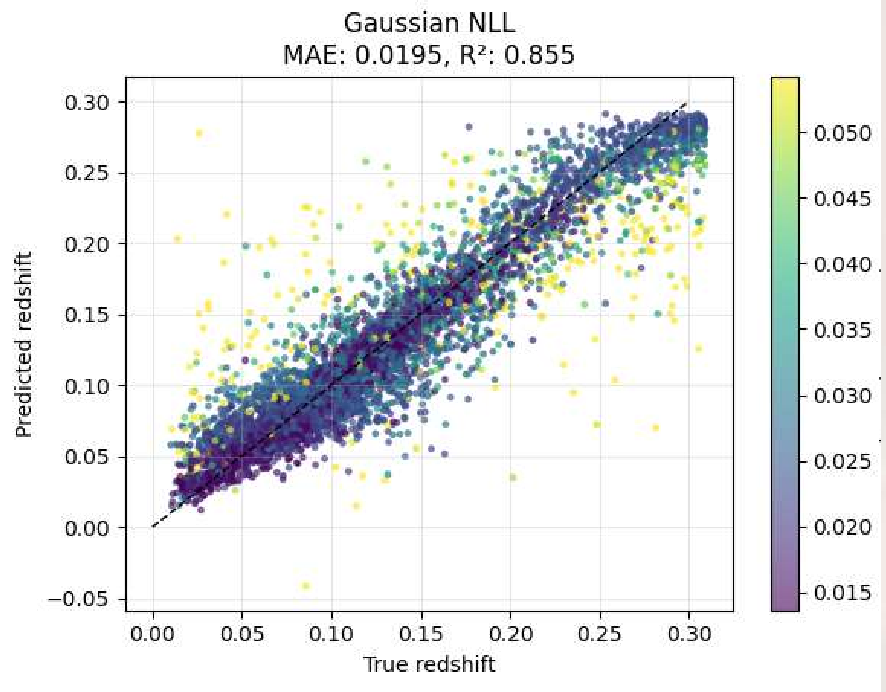
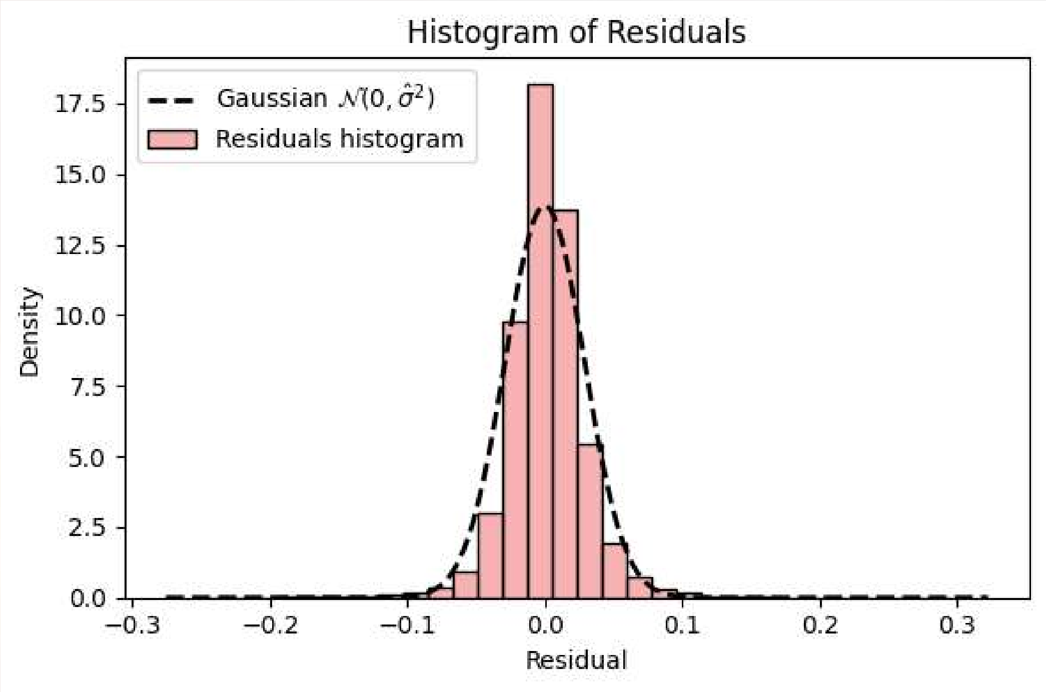
Gaussian Regression via ANN





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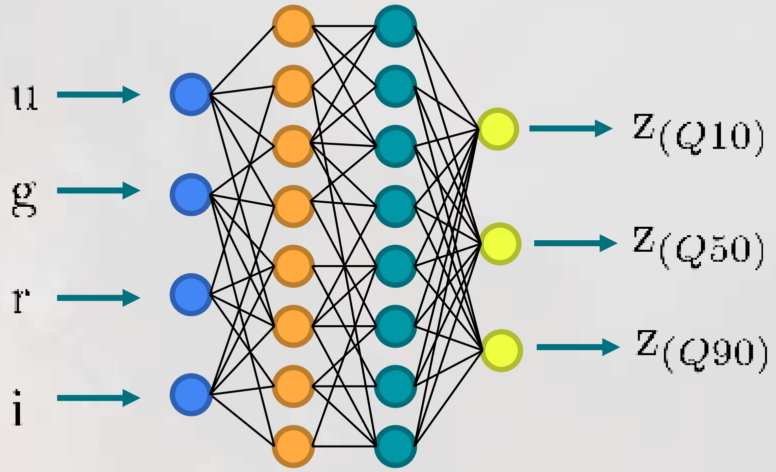
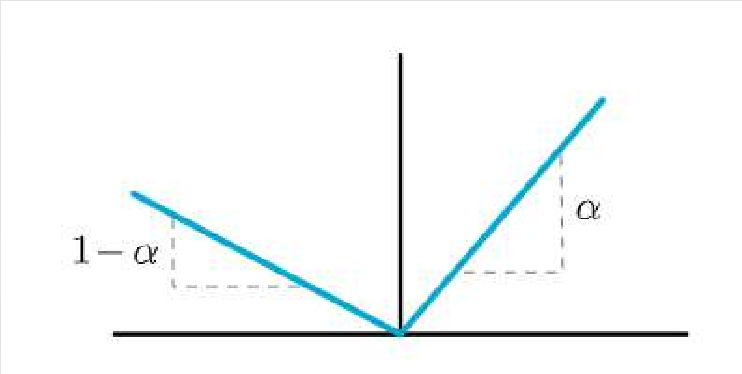
Quantile Regression

- Assume a set of target quantiles $\{\alpha_k\}_{k=1}^{K}$.
- $\hat{\mathbf{y}}_i = f(x_i; \mathbf{w}) = \left(\hat{y}_{i,\alpha_1}, \hat{y}_{i,\alpha_2}, \ldots, \hat{y}_{i,\alpha_K}\right)$

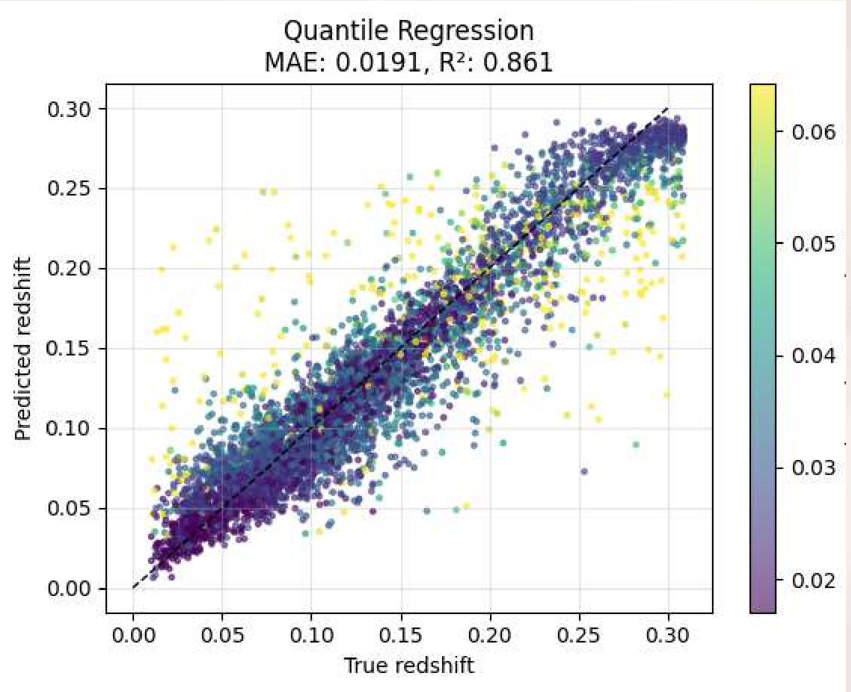


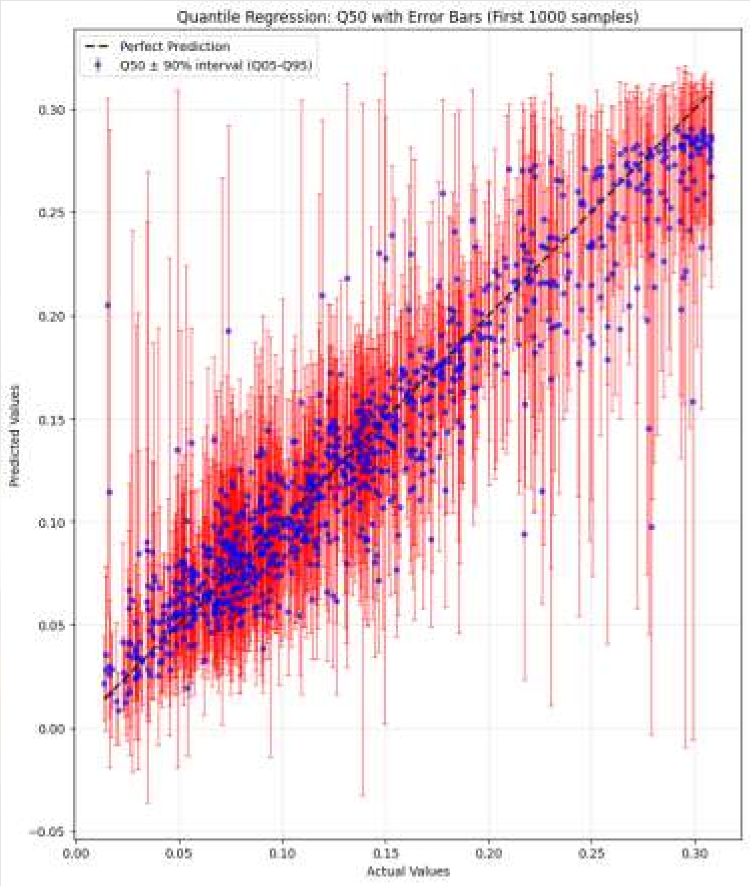
- *Mean pinball loss* (n samples, K quantiles):

$$L_\alpha\left(y, f(x)\right) = \begin{cases} \alpha\,|y - f(x)|, & y \geq f(x), \\ (1-\alpha)\,|y - f(x)|, & y < f(x). \end{cases}$$



Quantile Regression





90% Coverage: 0.922

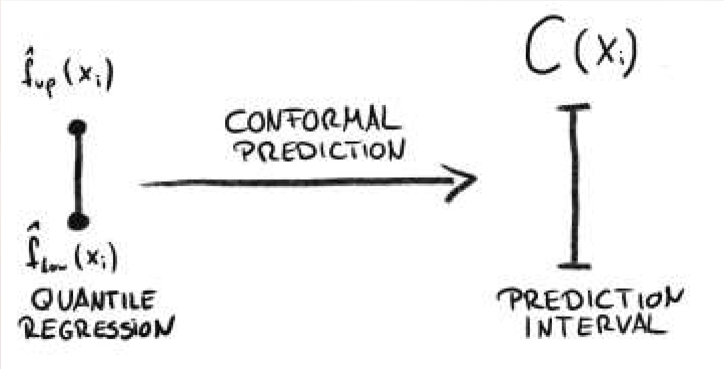
IQR $[Q_{075}(z)-Q_{0.25}(z)]$: 0.0319

Conformal Prediction

Regression task: age estimation

Model prediction: 24

MAPIE prediction interval: [20, 29]
(with 90% confidence)



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Conformal Prediction

1. Split training data to *proper training* set and *calibration*
2. Train lower and upper-quantile regressors $\widehat{Q}^{\alpha/2}$, $\widehat{Q}^{1-\alpha/2}$
3. On the calibration set, compute

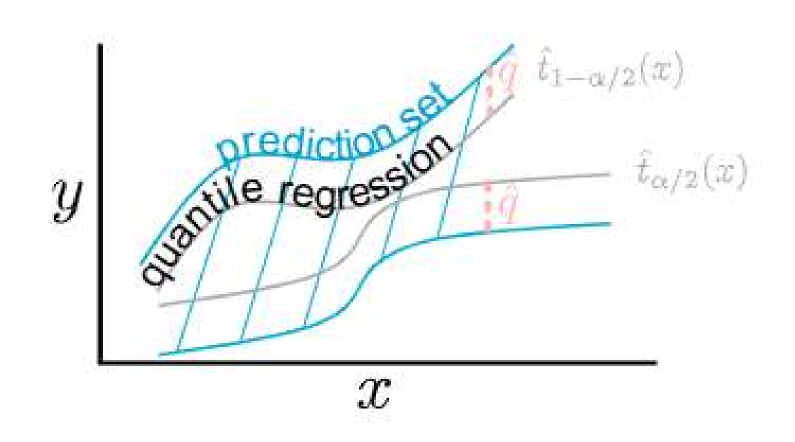
$$s_i^{\text{CQR}} = \max\left\{y_i^c - \widehat{Q}^{1-\alpha/2}(x_i^c),\ \widehat{Q}^{\alpha/2}(x_i^c) - y_i^c\right\}.$$

4. Compute the empirical $(1-\alpha)$-th quantile of the scores:

$$\widehat{q}^{\text{CQR}} = \begin{cases} s^{\text{CQR}}_{\lceil (1-\alpha)(n^c+1)\rceil}, & \text{if } \alpha \geq \dfrac{1}{n^c+1}, \\ \infty, & \text{otherwise.} \end{cases}$$

5. Output the coverage interval:

$$\mathcal{C}^{\text{CQR}}(x) = \left[\widehat{Q}^{\alpha/2}(x) - \widehat{q}^{\text{CQR}},\ \widehat{Q}^{1-\alpha/2}(x) + \widehat{q}^{\text{CQR}}\right]$$



Romano, Y., Patterson, E., & Candes, E. Conformalized quantile regression. *NeurIPS 2029*.

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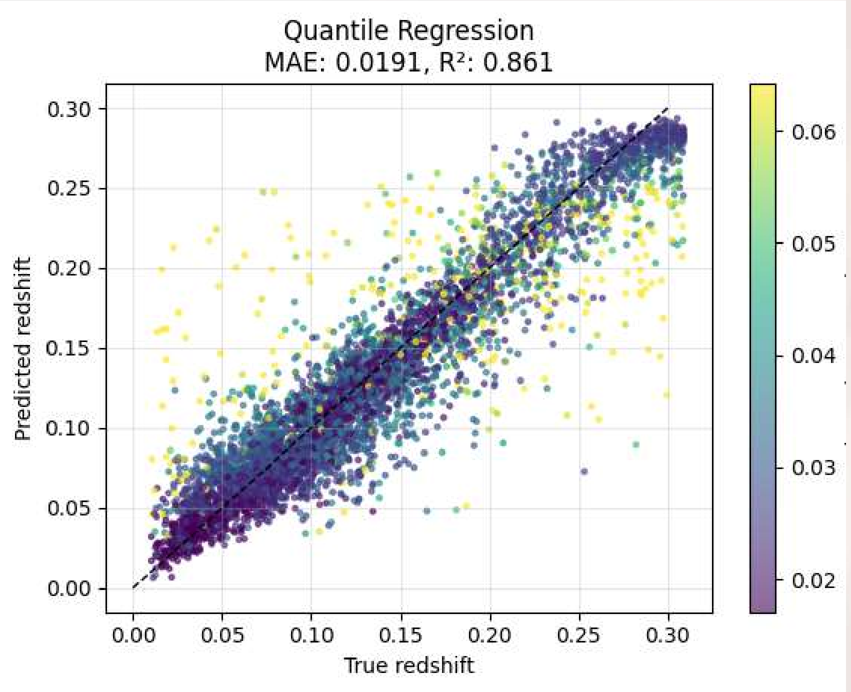
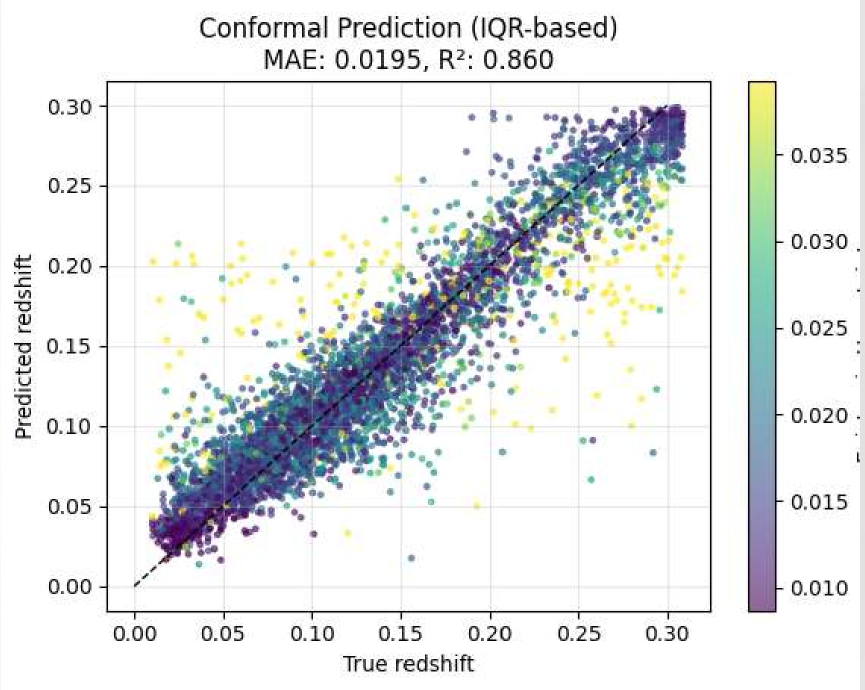
Conformal Prediction





90% Coverage: 0.922
IQR: 0.0319

90% Coverage: 0.900
IQR: 0.0184

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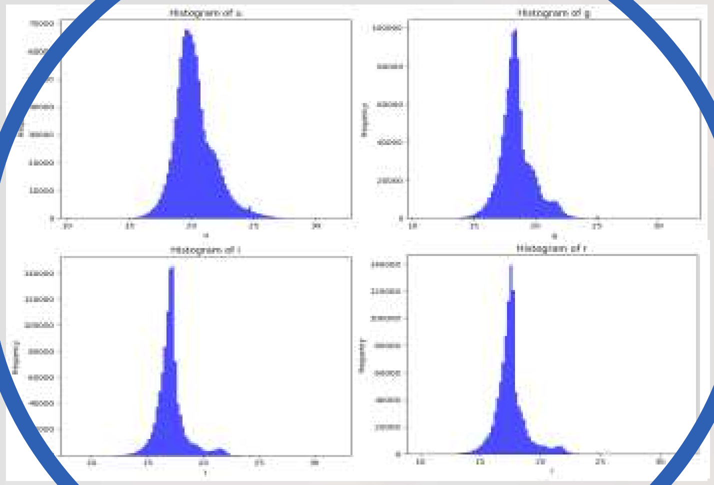
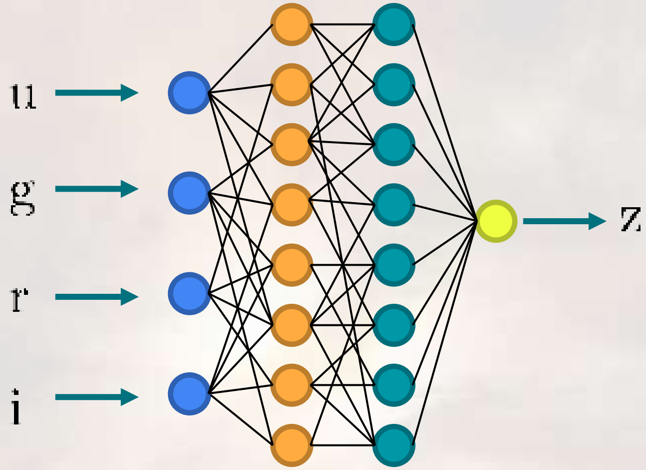
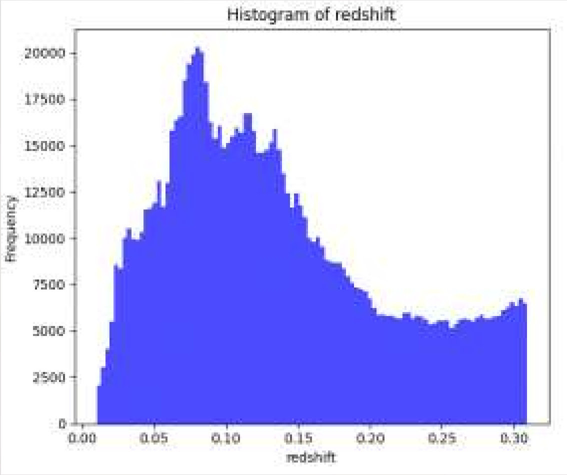
Uncertainties (data)







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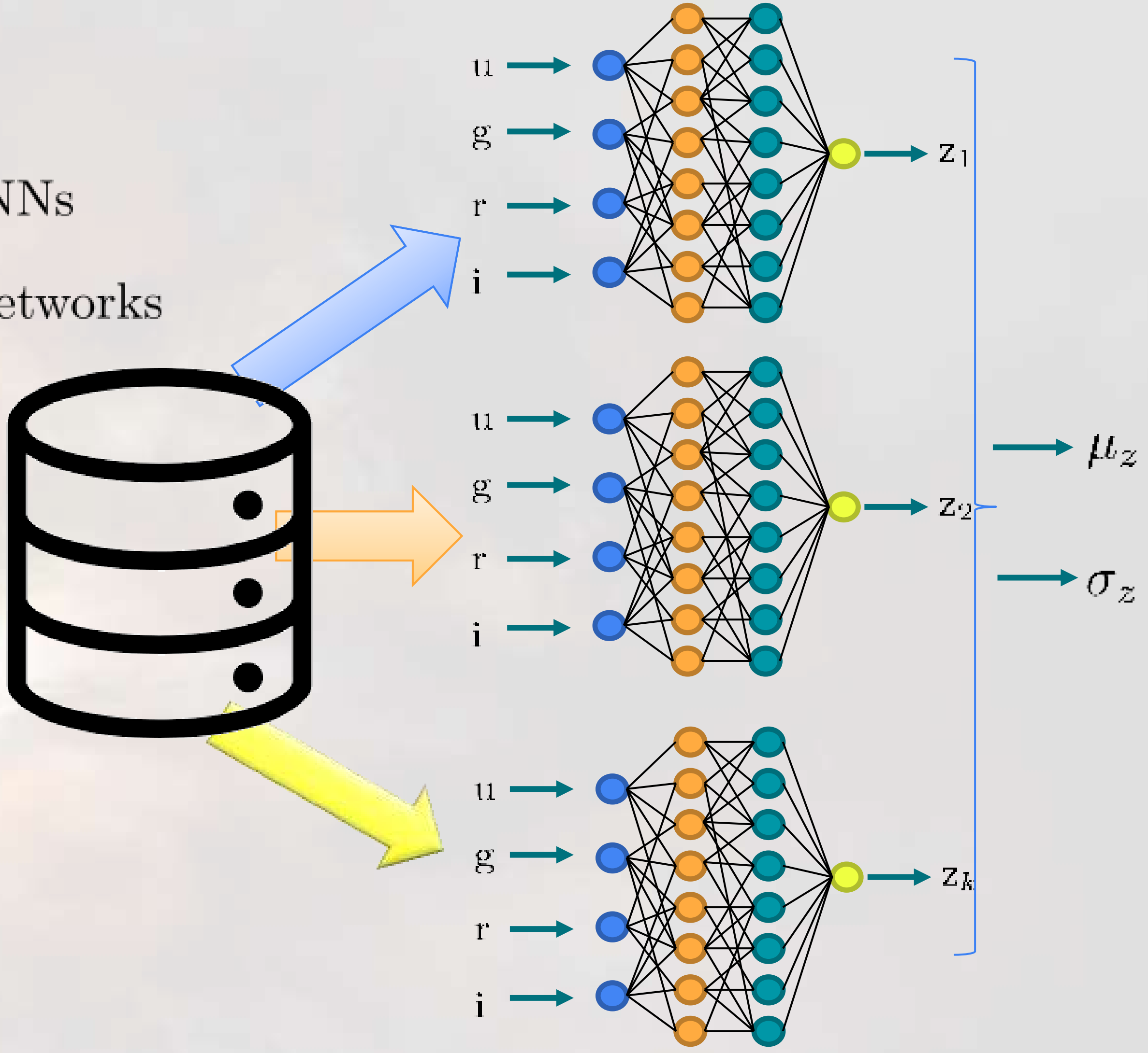
Ensembles

- Let $f^{(m)}(\cdot\,;\mathbf{w}^{(m)})$ be M independently trained ANNs
- During inference, forward-propagate through all networks

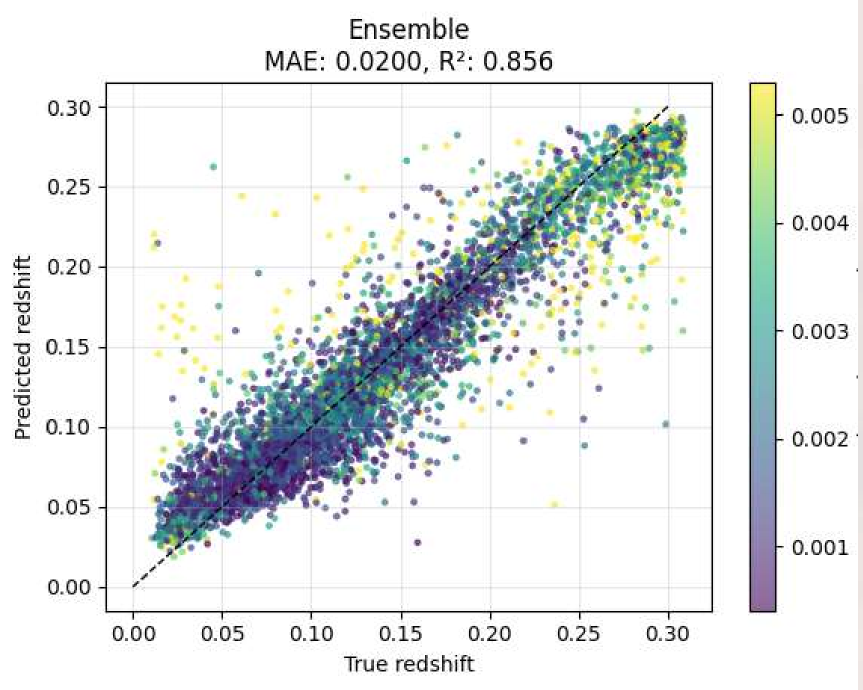
$$\mathbb{E}[y \mid x] \approx \bar{y}(x) = \frac{1}{M}\sum_{m=1}^{M} \hat{y}^{(m)}$$

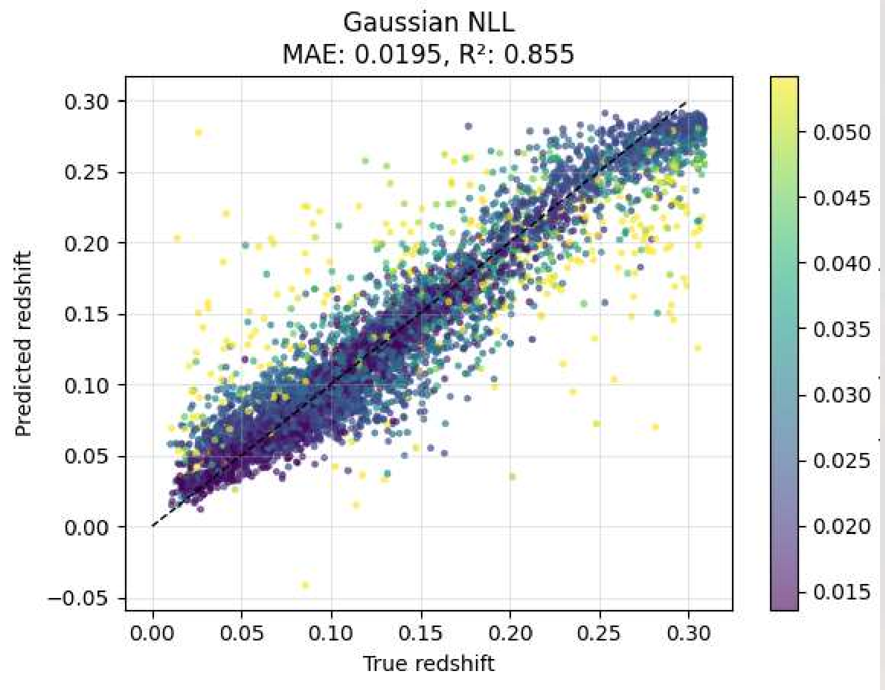
$$\mathrm{Var}[y \mid x] \approx \frac{1}{M}\sum_{m=1}^{M} \left(\hat{y}^{(m)}\right)^2 - \bar{y}(x)^2.$$



Ensemble approach

5 Models





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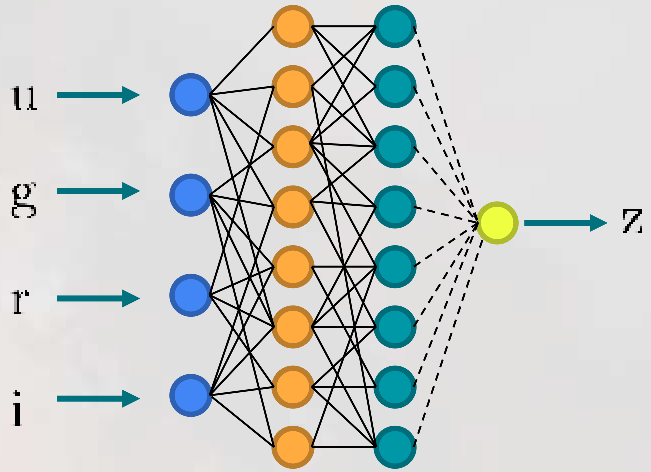
MCDropout



Apply *dropout* to forward pass

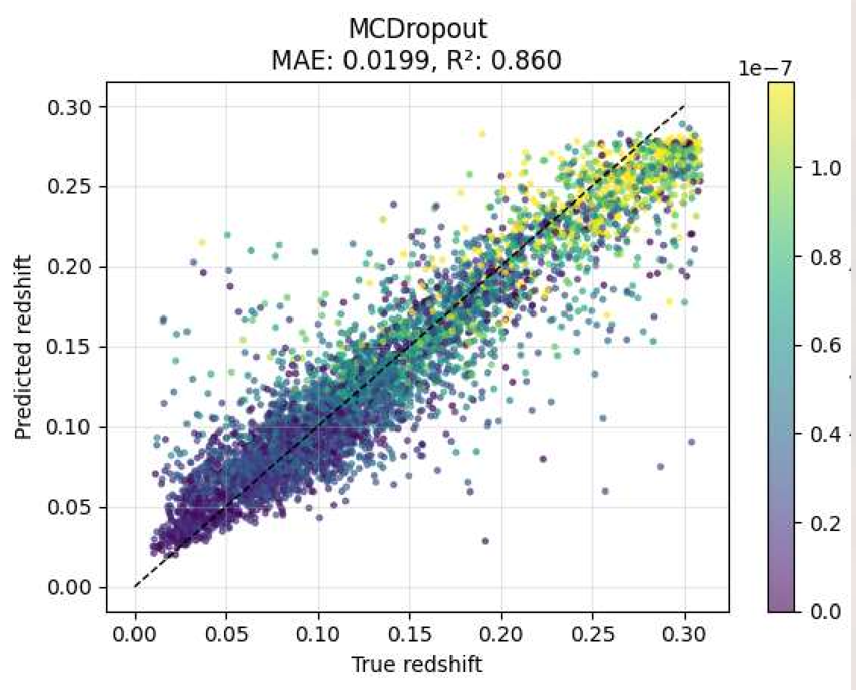
$$\hat{y}_i = f\big(x_i; \mathbf{w} \odot \mathbf{z}_i\big), \qquad \mathbf{z}_i \sim \mathrm{Bernoulli}(p),$$

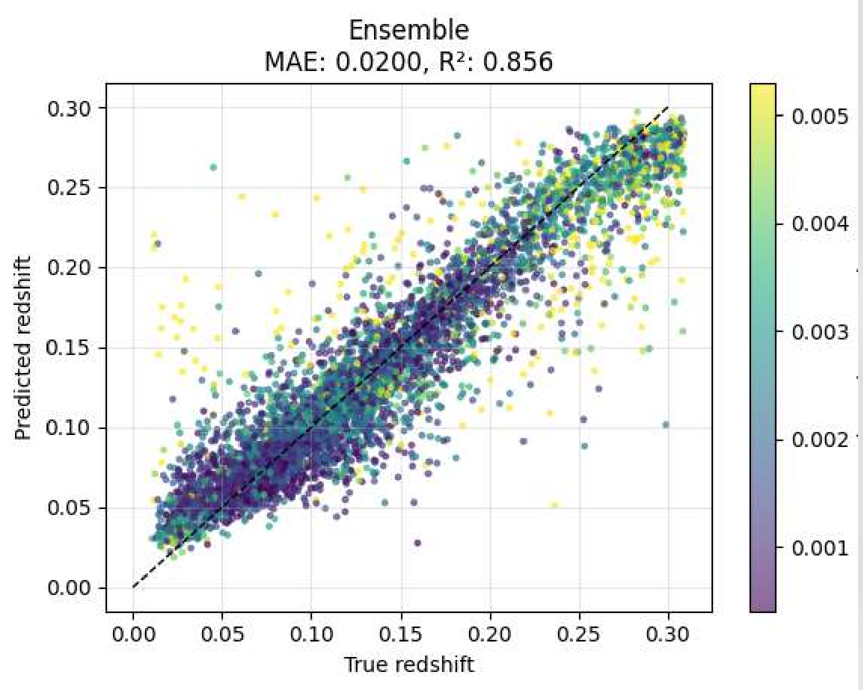
Predictive mean and variance

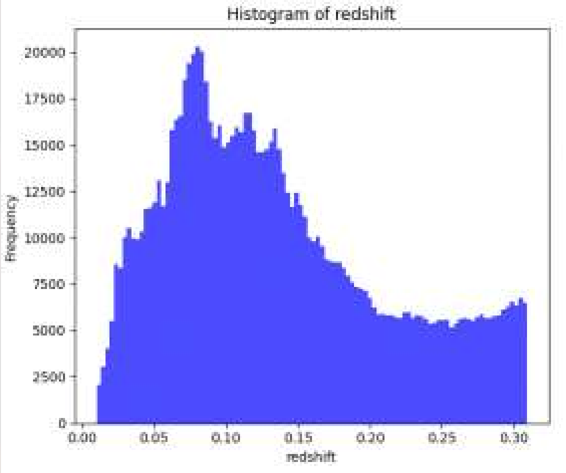
At test time keep dropout *on* and run S stochastic forward passes $\hat{y}^{(s)} = f\big(x; \mathbf{w} \odot \mathbf{z}^{(s)}\big)$, $s = 1, \dots, S$. The predictive posterior moments are approximated by

$$\mathbb{E}[y \mid x] \approx \bar{y} = \frac{1}{S}\sum_{s=1}^{S} \hat{y}^{(s)}, \quad \mathrm{Var}[y \mid x] \approx \frac{1}{S}\sum_{s=1}^{S}\big(\hat{y}^{(s)}\big)^2 - \bar{y}^{\,2} + \tau^{-1}.$$

MCDropout







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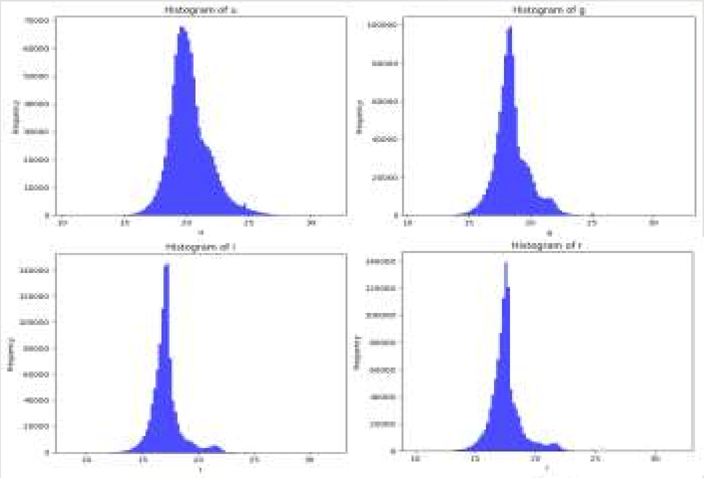
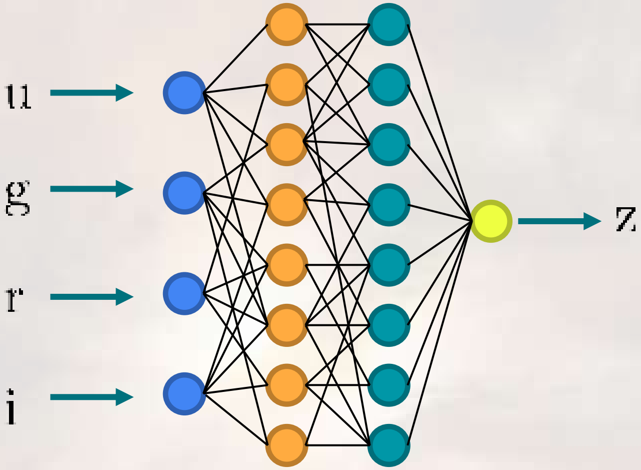
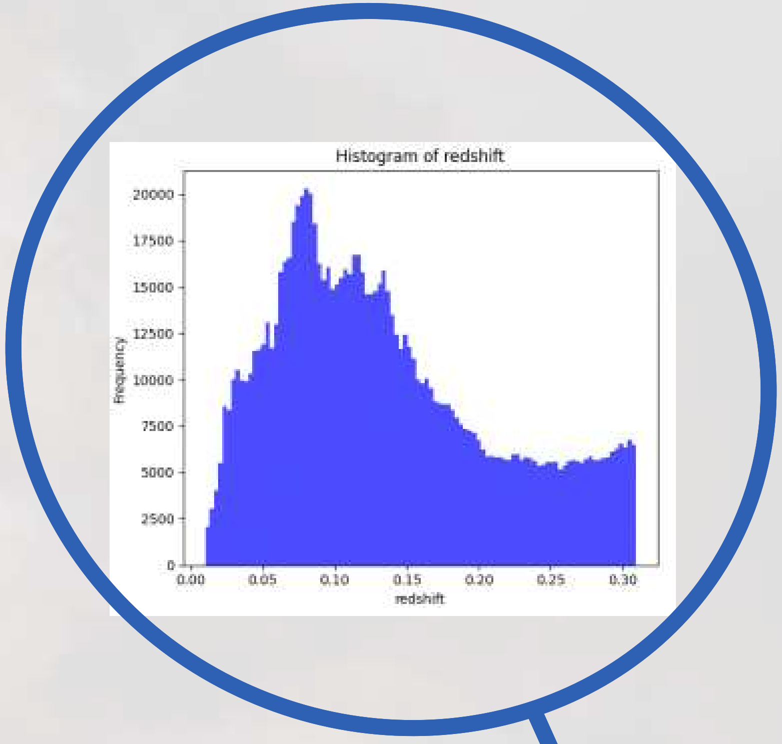
Uncertainties (labels)







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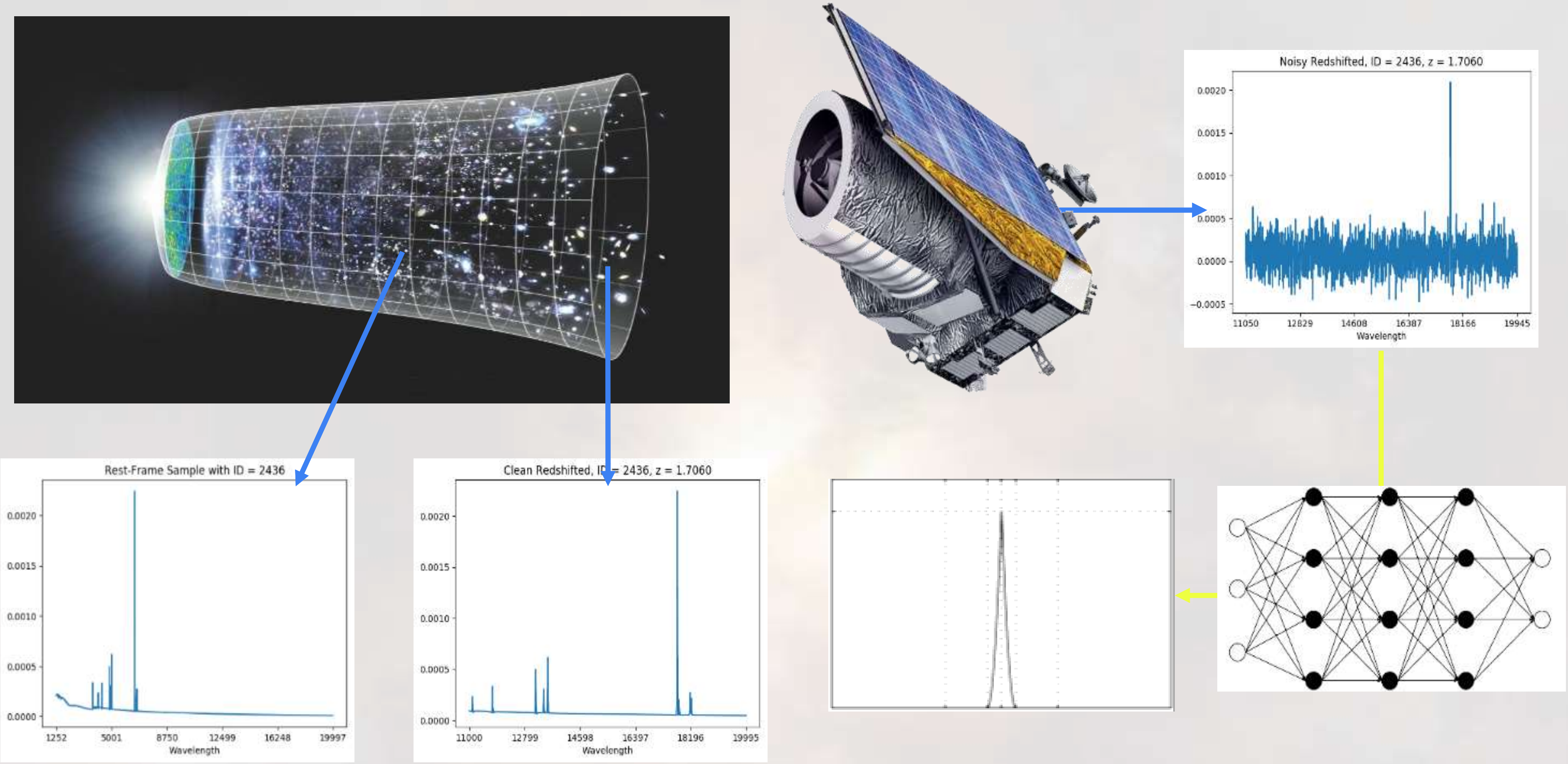
Spectroscopic Red-Shift Estimation



Predictive model

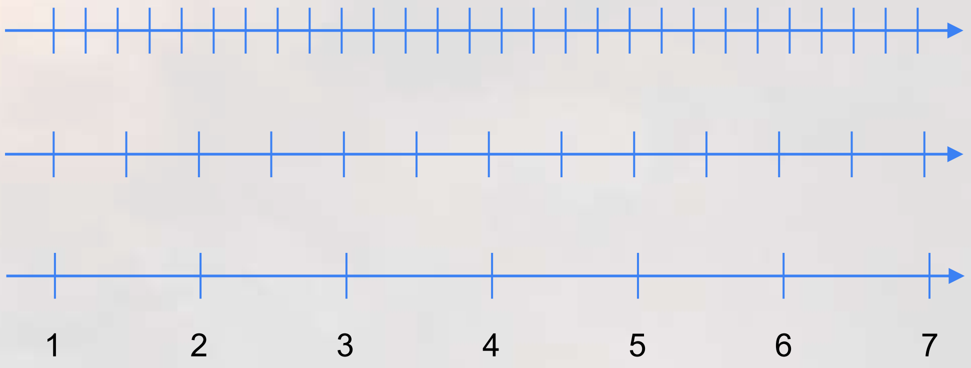
Redshift Estimation

Real-valued, non-negative number (z)

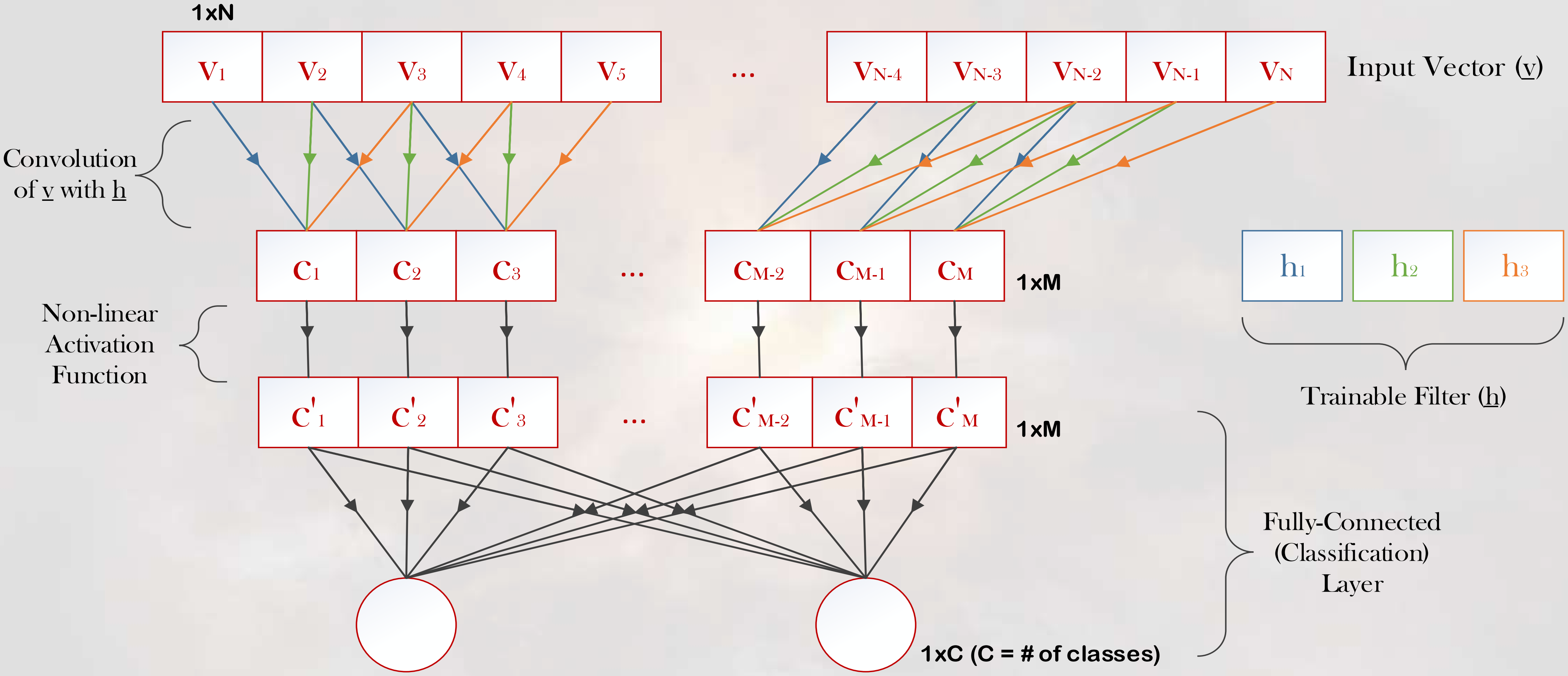
→ **Regression Analysis**

Split the examined redshift interval into ordinal classes, based on Euclid's characteristic resolution

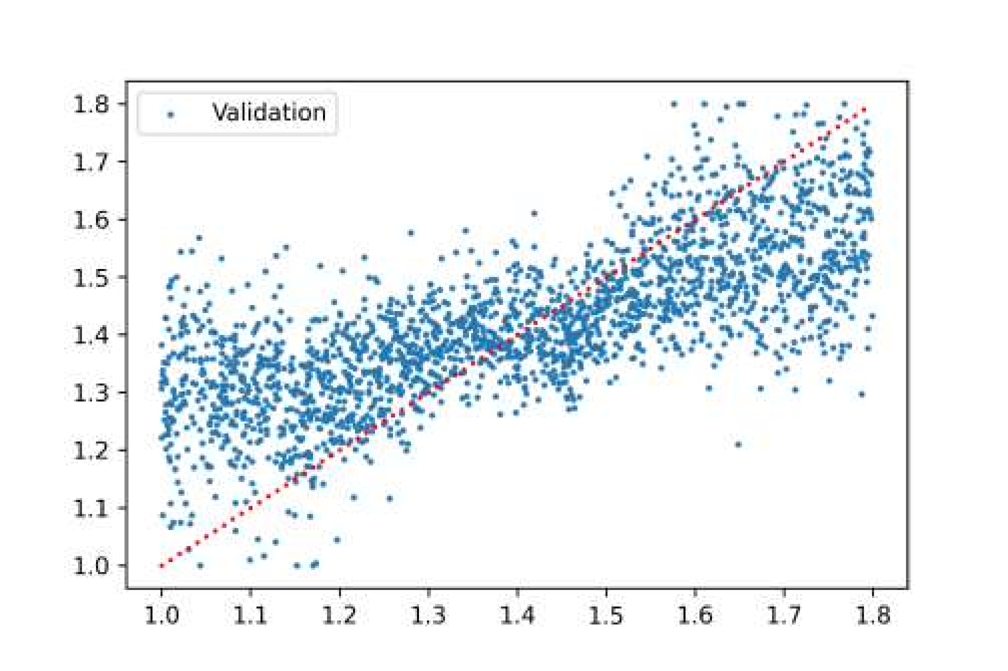
→ **Classification Problem**



1-Dimensional CNN - Classification

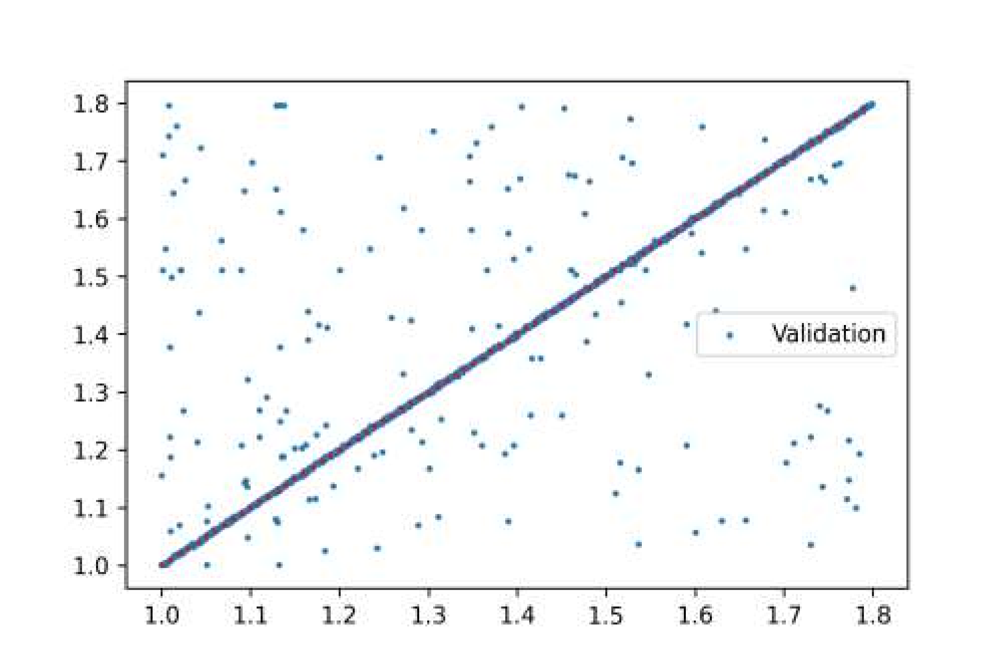


Regression



MSE 0.03811
MAE 0.16469
R^2 0.28188

Classification (800 classes)



MSE 0.00791
MAE 0.02325
R^2 0.85082

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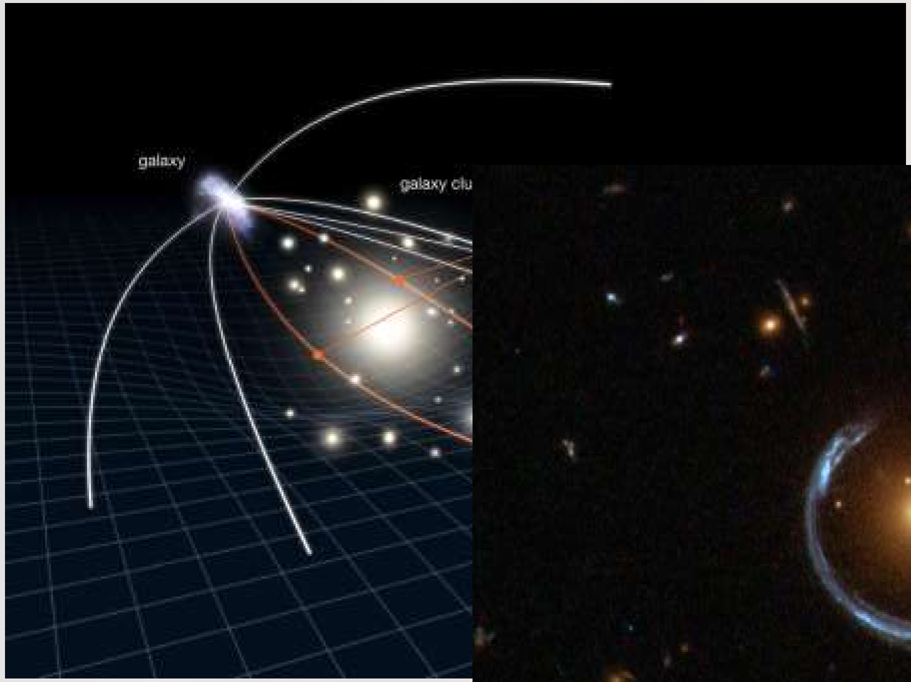
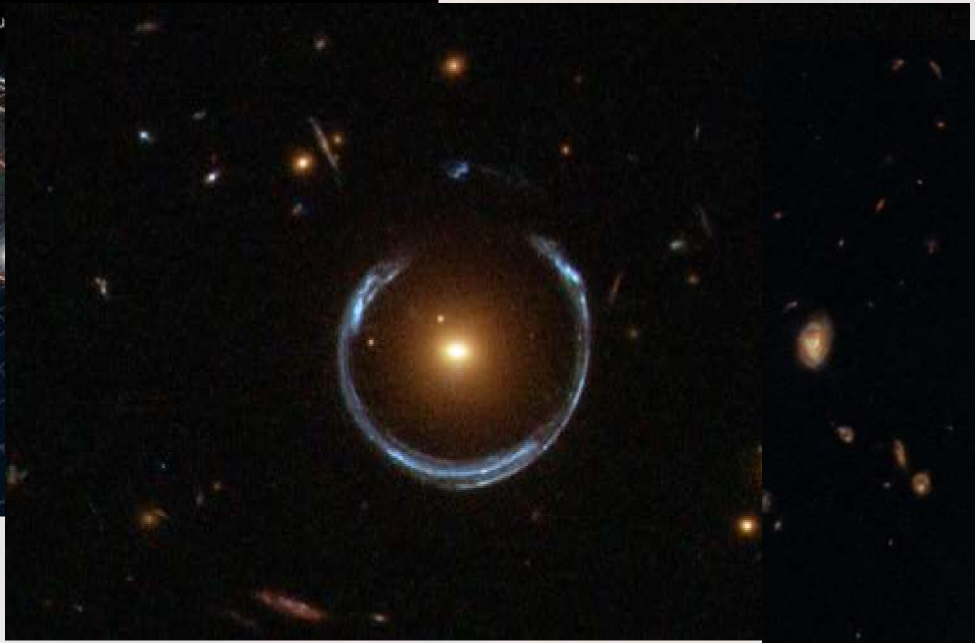
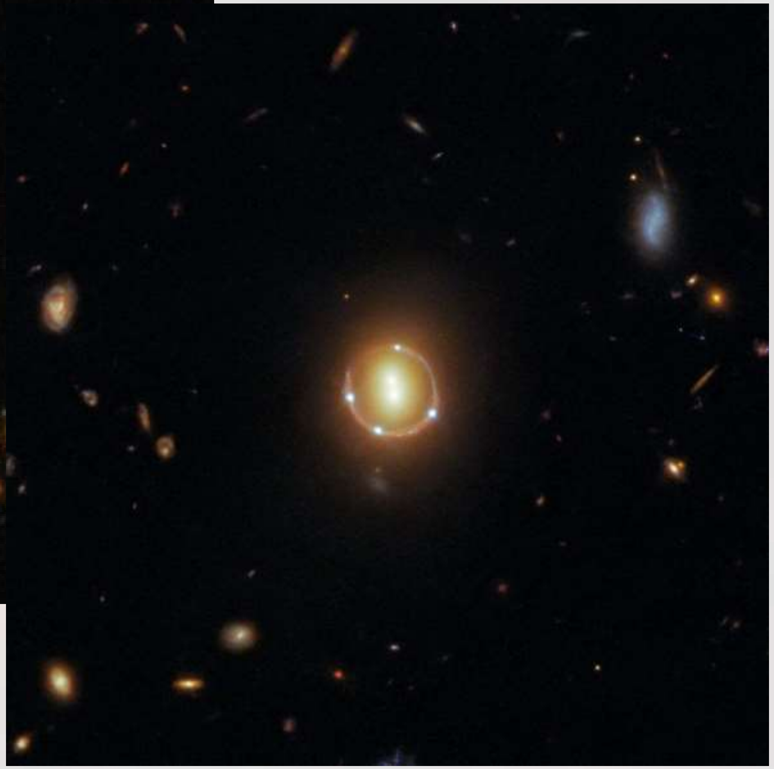
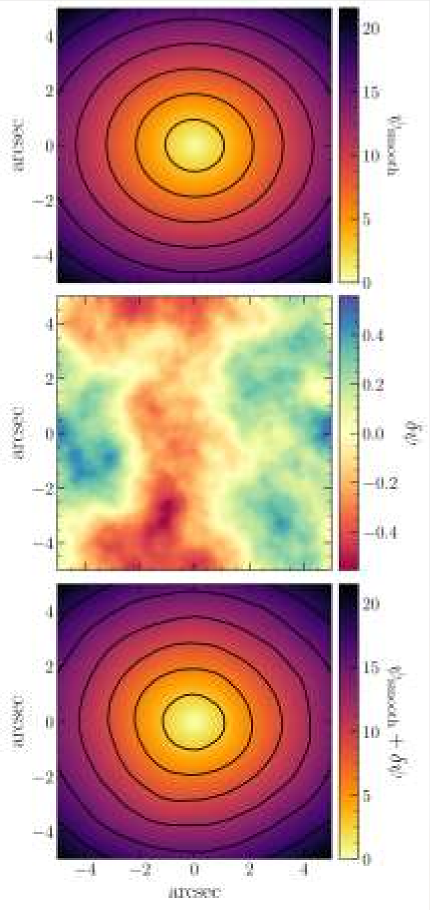
Gravitational Lensing







Modeling with uncertain labels



Singular Isothermal Ellipsoid parametric model

Realization of Gaussian Random Field perturbations

Perturbed lens potential

G. Vernardos, G. Tsagkatakis, and Y. Pantazis. "Quantifying the structure of strong gravitational lens potentials with uncertainty-aware deep neural networks." MNRAS. 2020.

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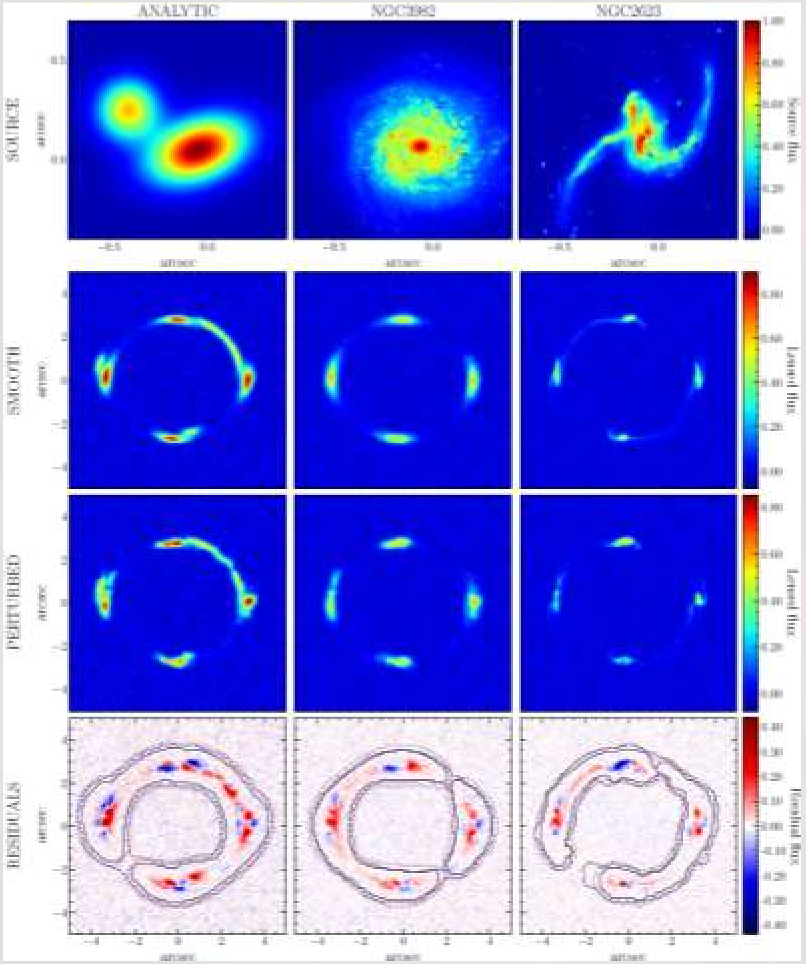
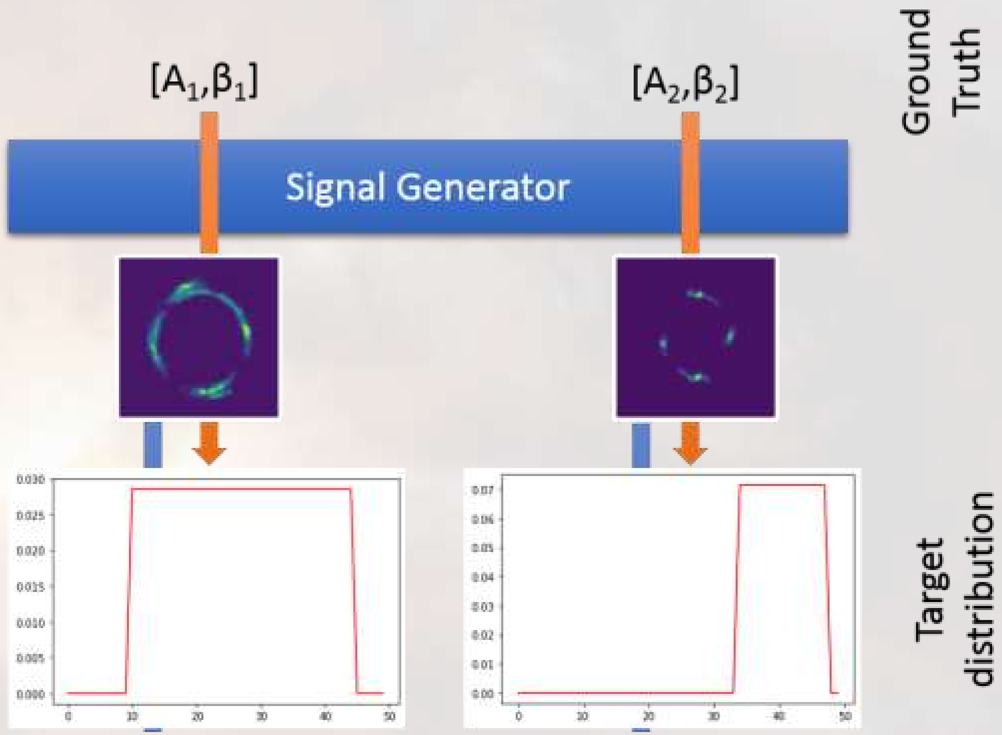
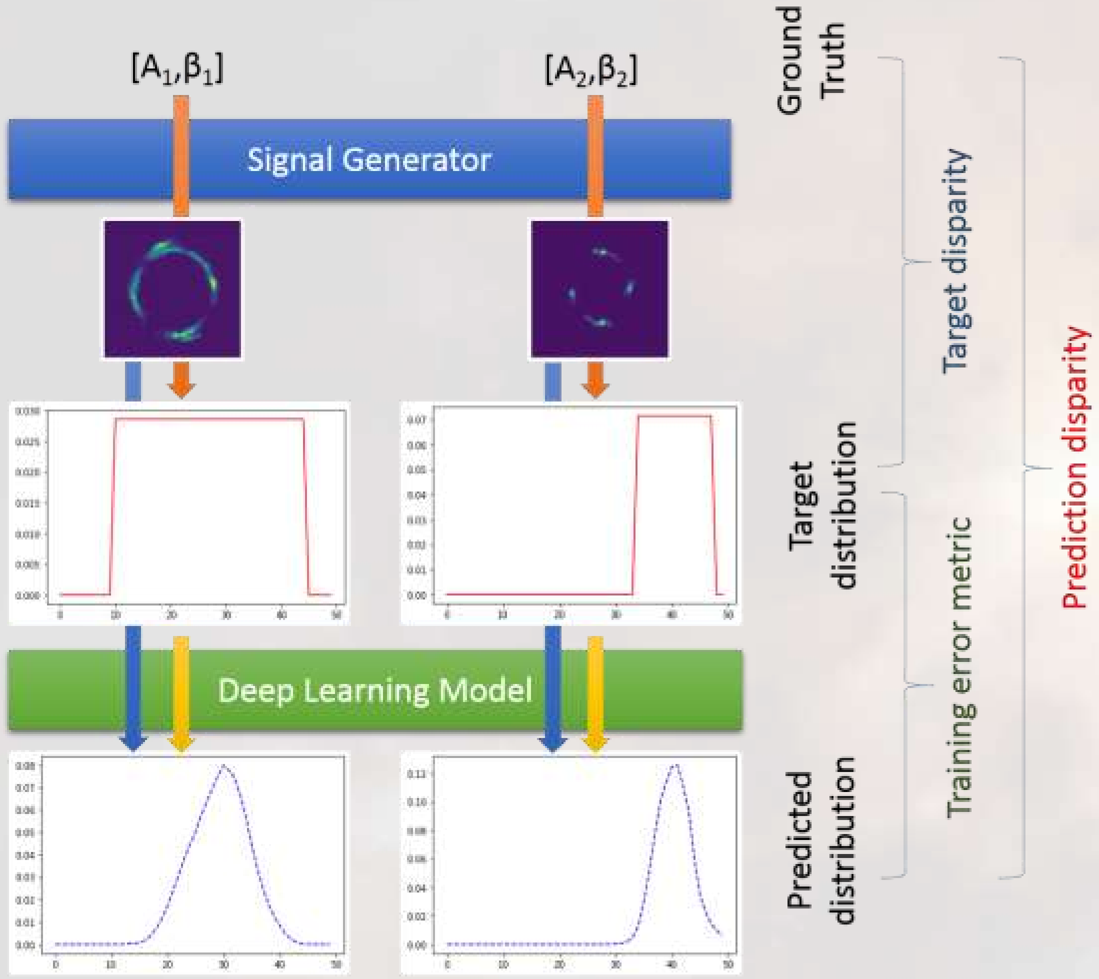
Label uncertainty





Modeling with uncertain labels



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Modeling with uncertain labels

Given the predicted distribution P and the target distribution Q, the Jensen-Shannon divergence is defined by:

$$JS(Q,P) = \frac{1}{2}KL(P\|M) + \frac{1}{2}KL(Q\|M), M = \frac{1}{2}(P+Q)$$

Formally, the entropy of the predicted distribution $H(P)$ is given by:

$$H(P) = -\sum_{x\in\mathcal{X}} P(x)\log(P(x)).$$

Entropy-regularized version of the JS divergence and is given by:

$$\mathcal{L}(P,Q) = \lambda_1 JS(P,Q) + \lambda_2 H(P),$$

where λ_1 and λ_2 control the impact of the two terms.

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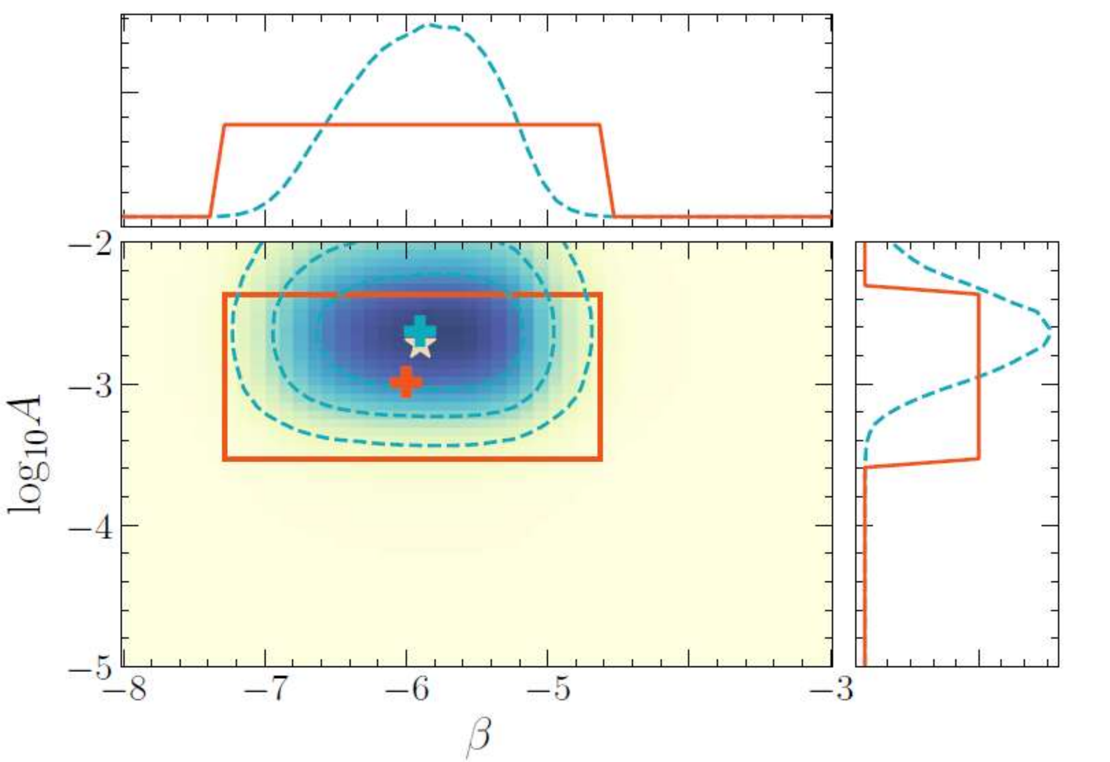
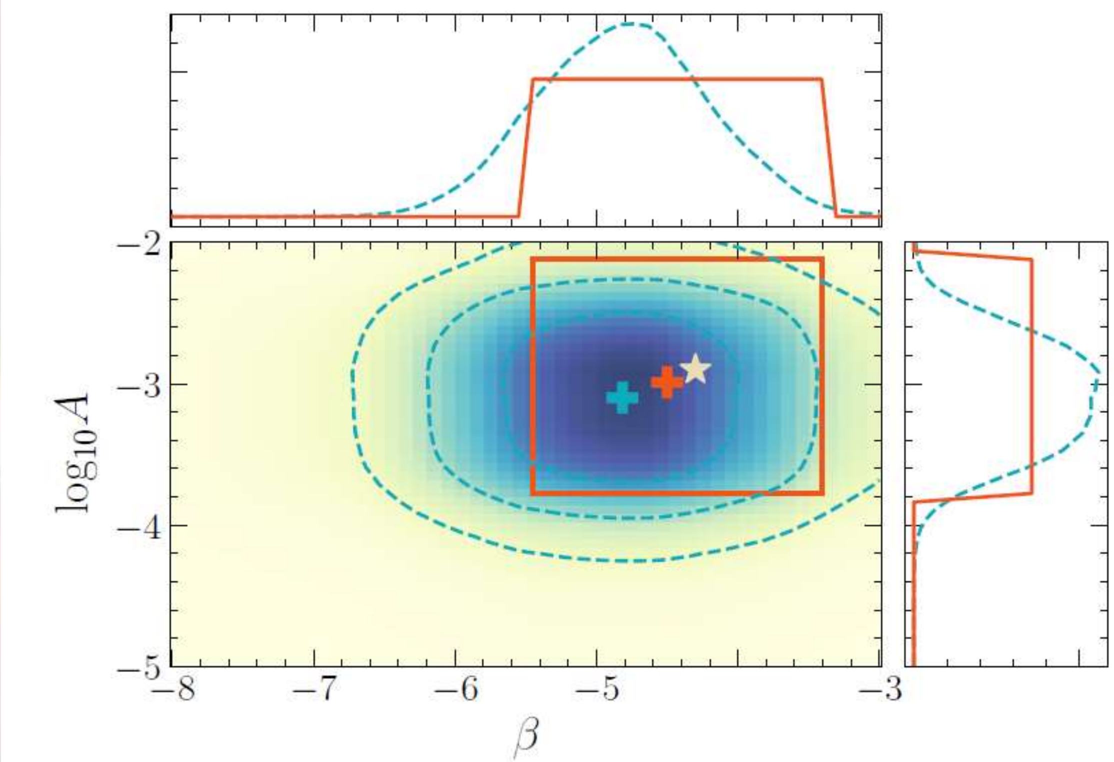
“Label-super-resolution”





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Take-home messages

- Many flavors of uncertainty (decoupling, Bayesian, ordinal regression)
- “Limited” investigation in scientific data analysis
- The case of time-domain astronomy
- The case of spatially resolved observations
- The promise of multi-modality

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Dates: 24-26 September 2025

Location: FORTH, Crete

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