Uncertainty Quantification for Generative Models in Astrophysics

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Co-funded by the European Union

Uncertainty Quantification in Gen Models

Novel Generative Models are vital because of **increasing**

- Data Volume
- Data Complexity

We need to understand how the Model behaves if we are to use it for

- Modeling the Prior Distribution
- Approximate the Posterior Distribution

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It is imperative that we ensure our generative models are well calibrated

    - Small modeling errors can lead to vastly different results when doing inference!

Specifically, it is crucial to verify that these generative models accurately represent the **full distribution of their training data**

Published as a conference paper at ICLR 2025

PQMass: Probabilistic Assessment of the Quality of Generative Models using Probability Mass Estimation

Pablo Lemos, Sammy Sharief, Nikolay Malkin, Salma Salhi,
Connor Stone, Laurence Perreault-Levasseur, Yashar Hezaveh

PQMass: Probabilistic Assessment of the Quality of Generative Models using Probability Mass Estimation

Given two set of independent and identically distributed (i.i.d) samples

$$(x_i)_{i=1}^m,\ x_i \sim p$$

$$(y_i)_{i=1}^n,\ y_i \sim q$$

Our aim is to test the hypothesis of

$$p = q$$

We use the fact that p and q are equal if they assign the same probability mass to all measurable sets

$$p(R) = q(R) \quad \forall R \subseteq X,\ R$$

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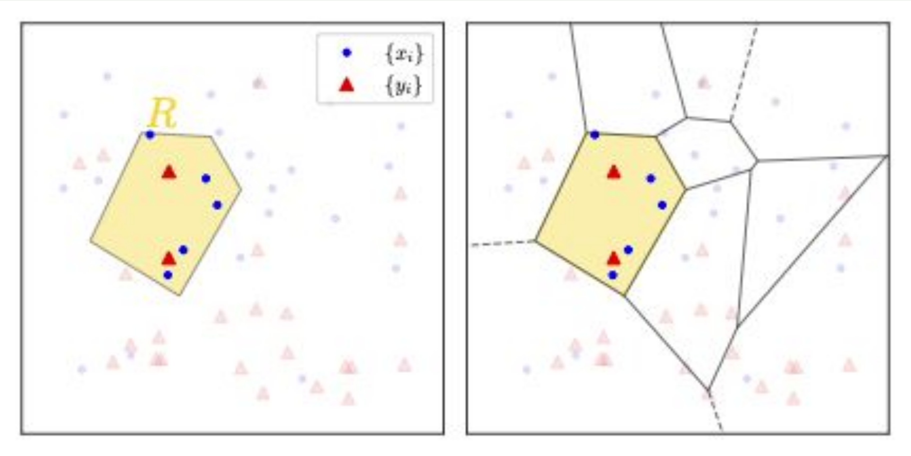
We define our measurable set **R** as a fixed partition of the space

- Each Region is <u>measurable</u> and <u>non-overlapping</u>

$$\mathbb{R}^d = R_1 \sqcup R_2 \sqcup \ldots \sqcup R_{n_R}$$

We partition our space using **<u>Voronoi Cells</u>**



The probability distribution describing the number of samples in the regions is given by a **multinomial distribution**

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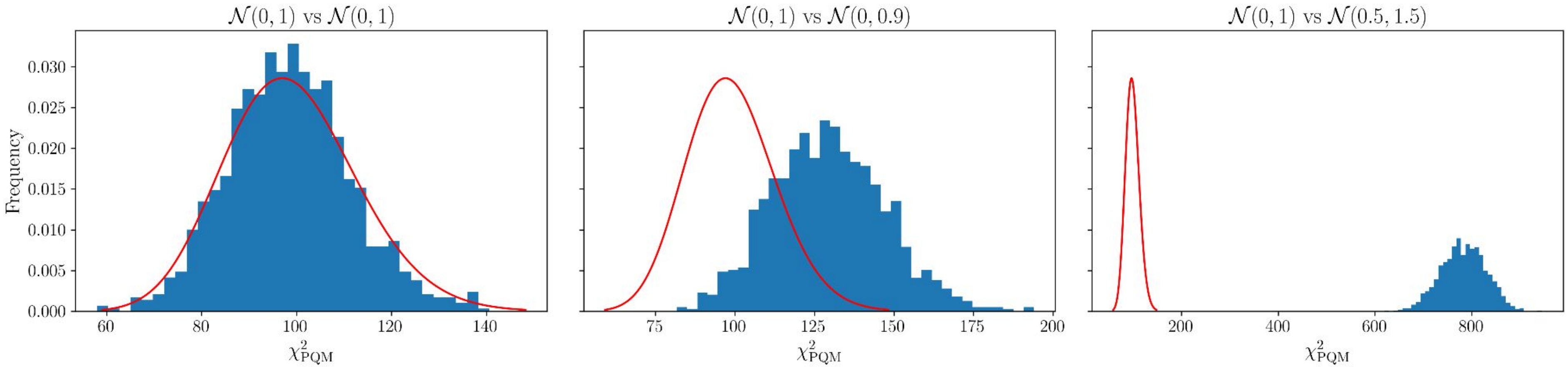

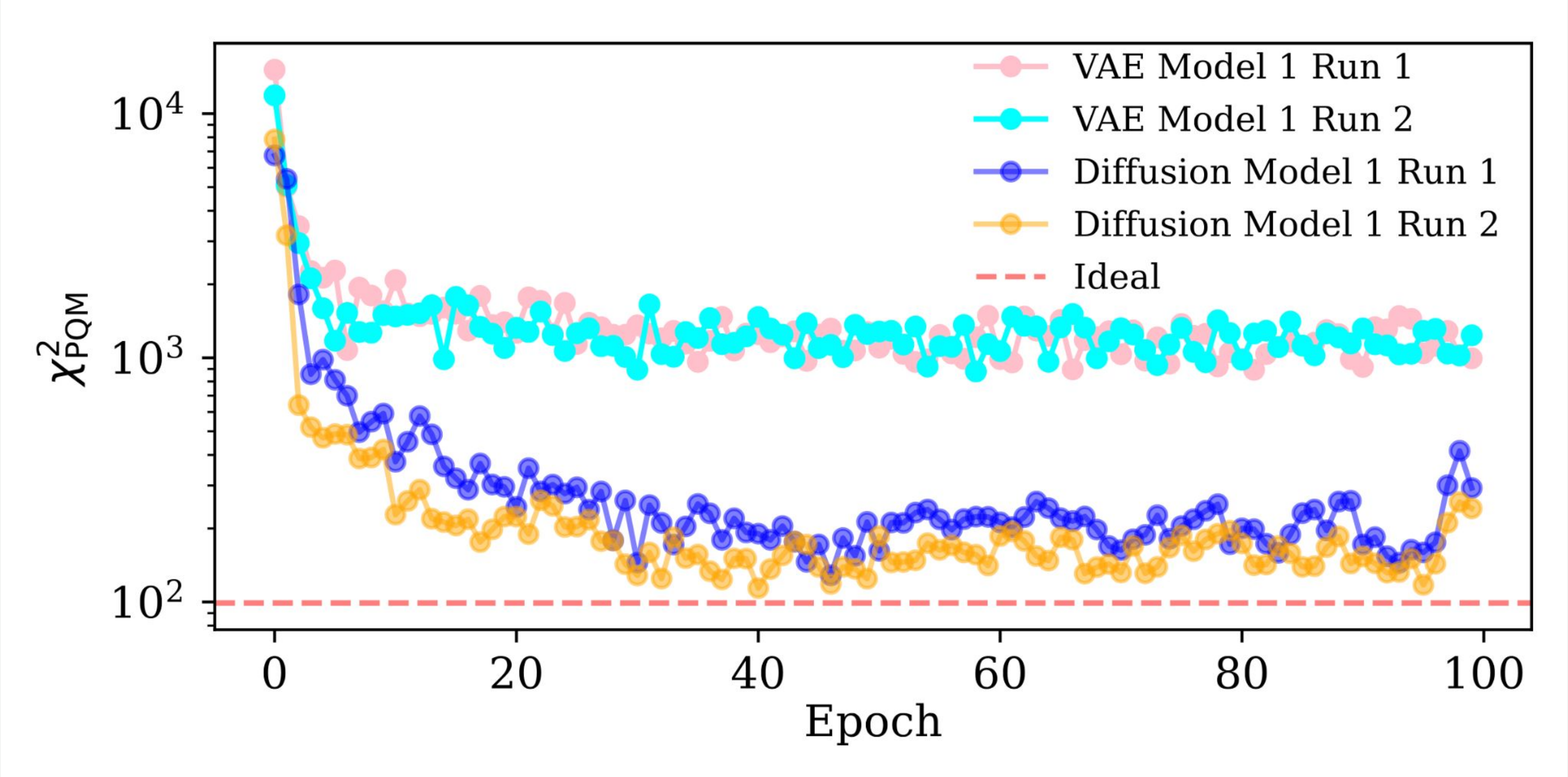
VAE Model 1 Run 1
VAE Model 1 Run 2
Diffusion Model 1 Run 1
Diffusion Model 1 Run 2
Ideal
10^4
10^3
10^2
χ^2_{PQM}
0
20
40
60
80
100
Epoch

Limitation of PQMass

When performing Inference, having methods that

1. Assess the calibration of the *posterior*
2. Methods that perform model comparison

are extremely powerful and important

PQMass is designed to check if a model has learned the training data but cannot evaluate the **conditional distribution** p(y|x) for all observations x

- Inference typically provides only a **single ground-truth realization** (y^*) for any given observation but PQMass requires multiple i.i.d. samples from both distributions

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We need alternative methods for **Uncertainty Quantification (UQ)** of posteriors.

MIRA: A Score for Conditional Distribution Accuracy and Model Comparison

Sammy Sharief, Justine Zeghal, Gabriel Missael Barco, Pablo Lemos,
Yashar Hezaveh, Laurence Perreault-Levasseur

MIRA: Mass in Random Area

We define our true unknown conditional distribution

$$p(y|x^*, M^*)$$

We define our proposed conditional distribution

$$p(y|x^*, M)$$

The main questions we want to answer is

$$p(y|x^*, M) = p(y|x^*, M^*)$$

MIRA: Mass in Random Area

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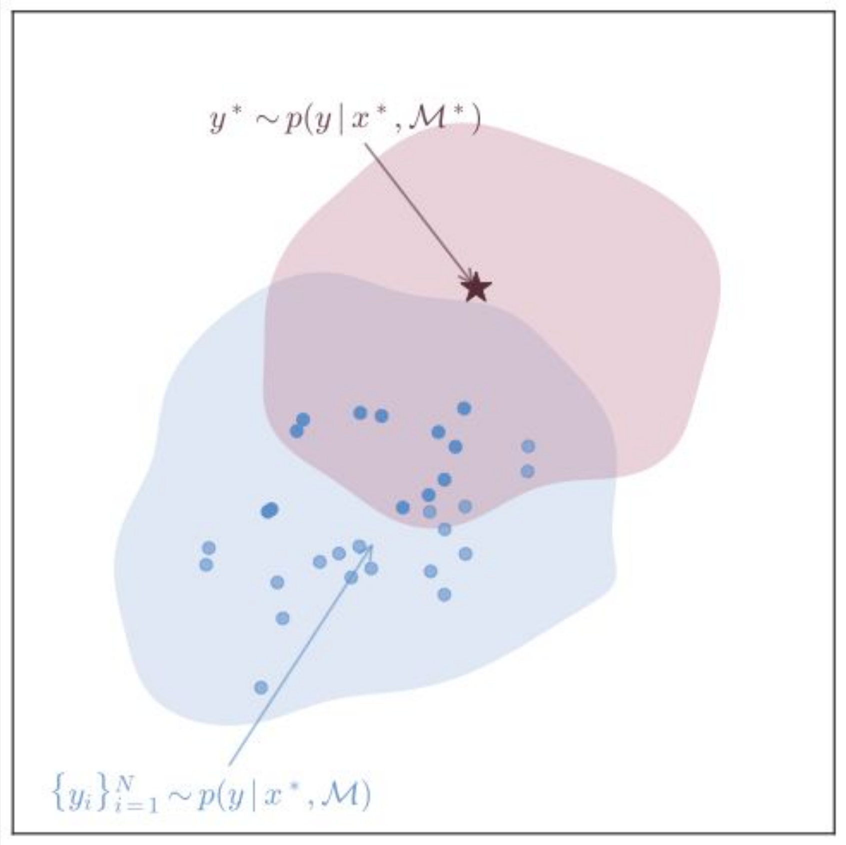
$p(y|x, M) = p(y|x, M^*)$



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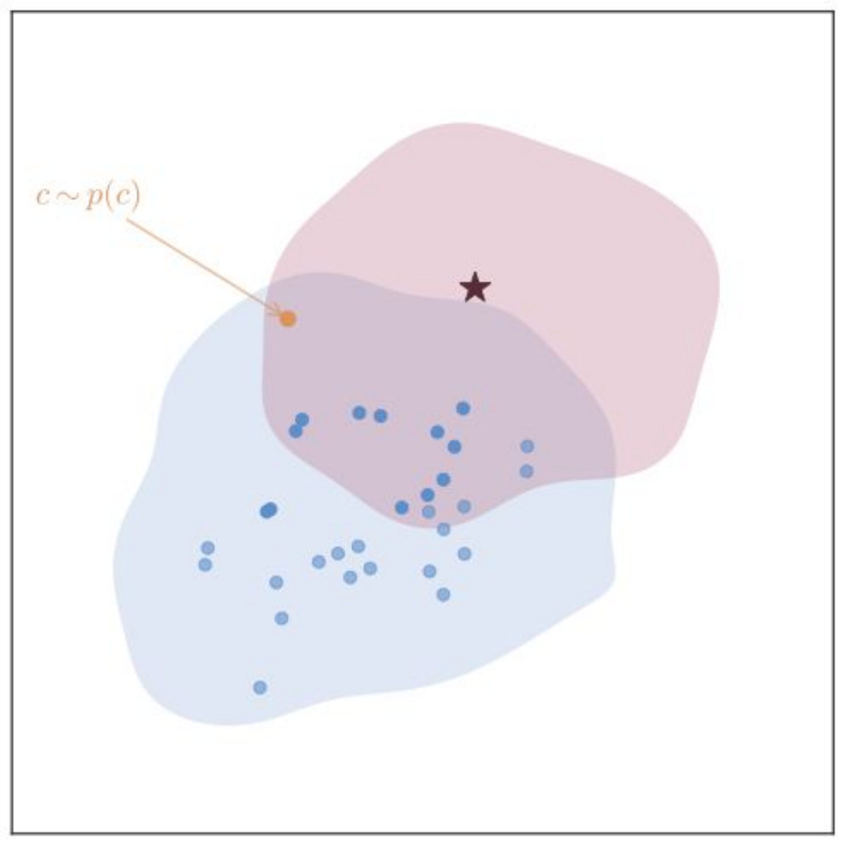

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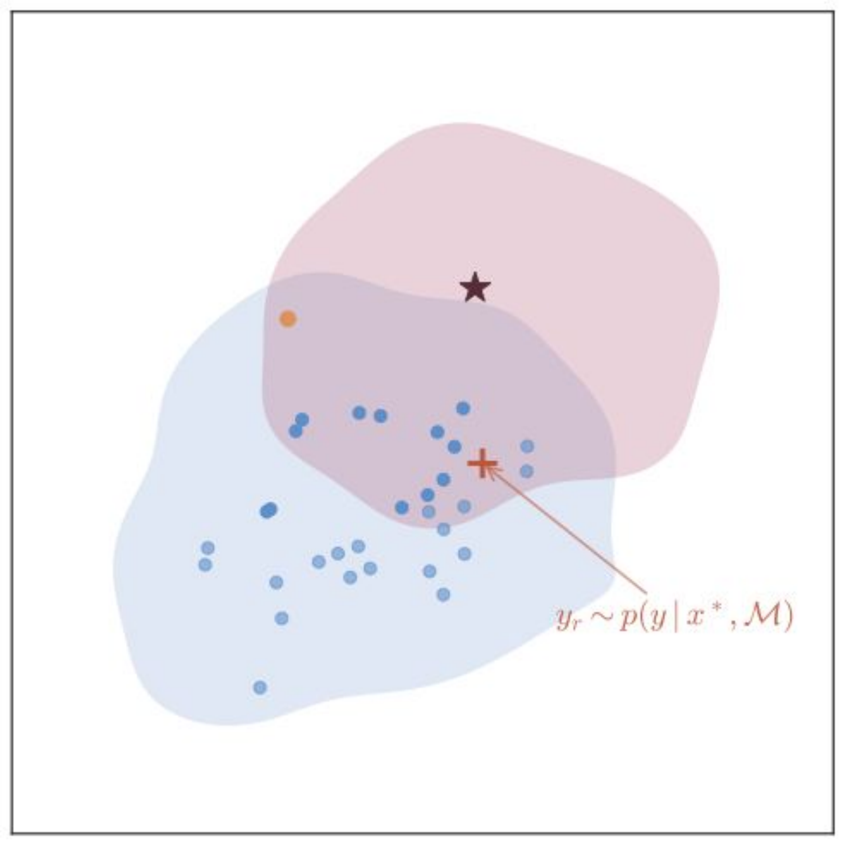

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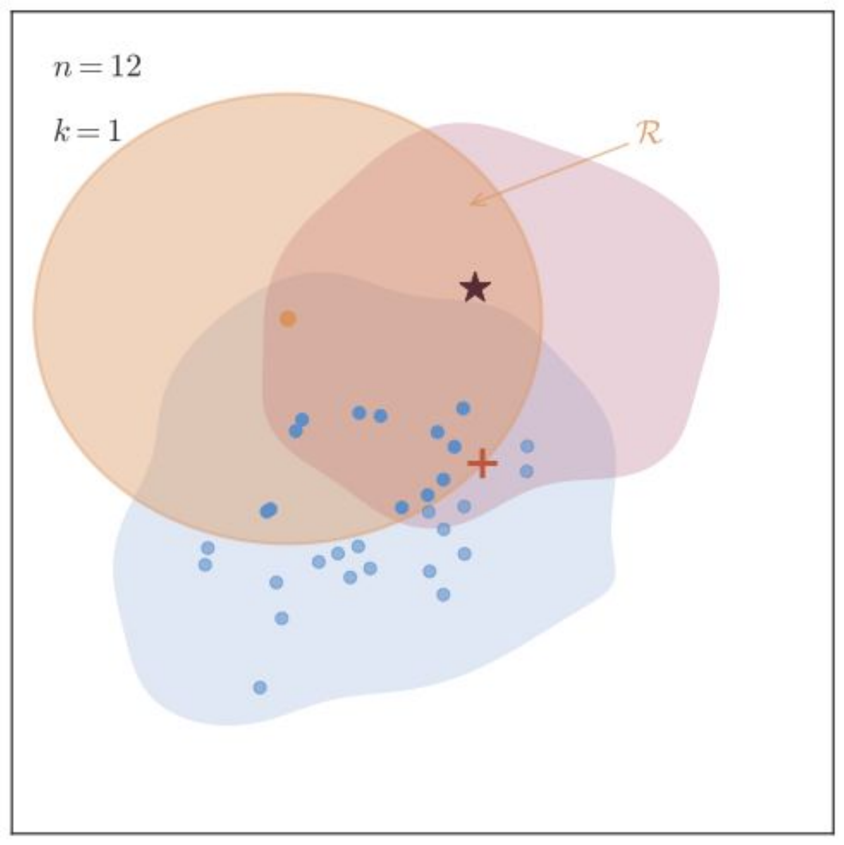

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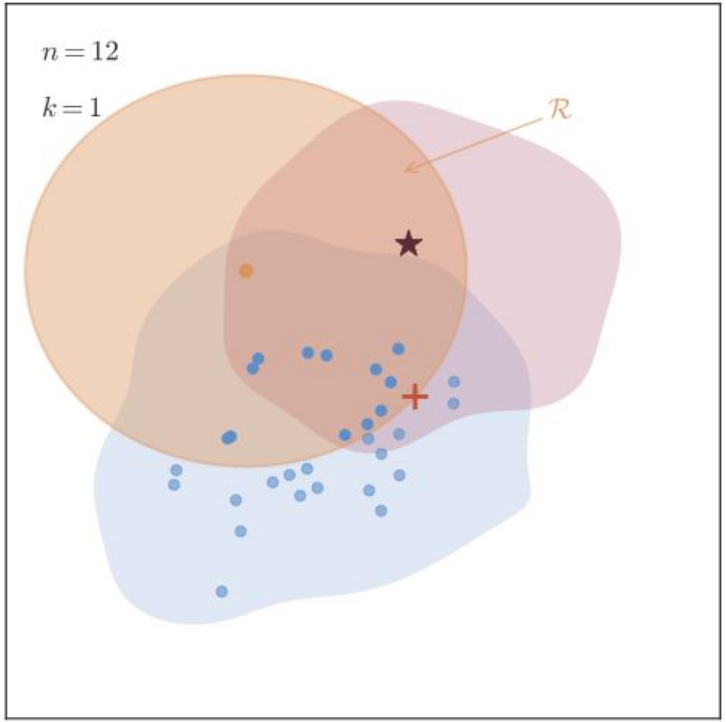
The main questions we want to answer is

$$p(y|x, M) = p(y|x, M^*)$$

MIRA statistic for a single realization

$$p\big(k \mid n\big) = \frac{n+1}{N+2}\mathbb{1}(k=1) + \frac{N-n+1}{N+2}\mathbb{1}(k=0)$$



MIRA: Mass in Random Area

After marginalizing over all sources of Randomness Z to get the MIRA Score

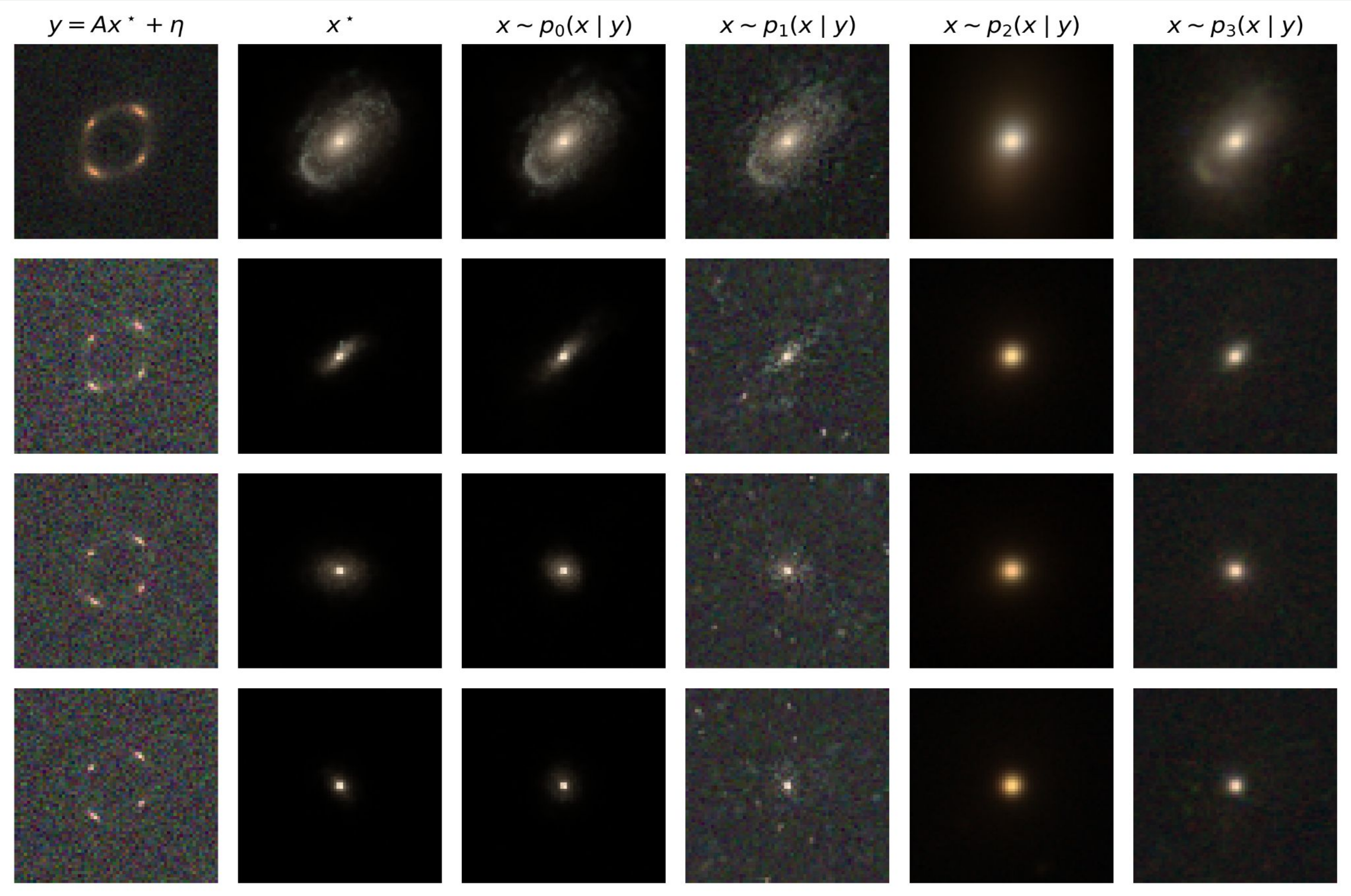
$$\mu_{\text{Mira}}(\mathcal{M}) = \mathbb{E}_{p(Z)}\left[\mathbb{E}_{p(k,n|Z)}\left[p(k \mid n)\right]\right]$$

In the limit of $N \to \infty$, given that the $p(y|x, M) = p(y|x, M^*)$, then the mean and variance will converge to

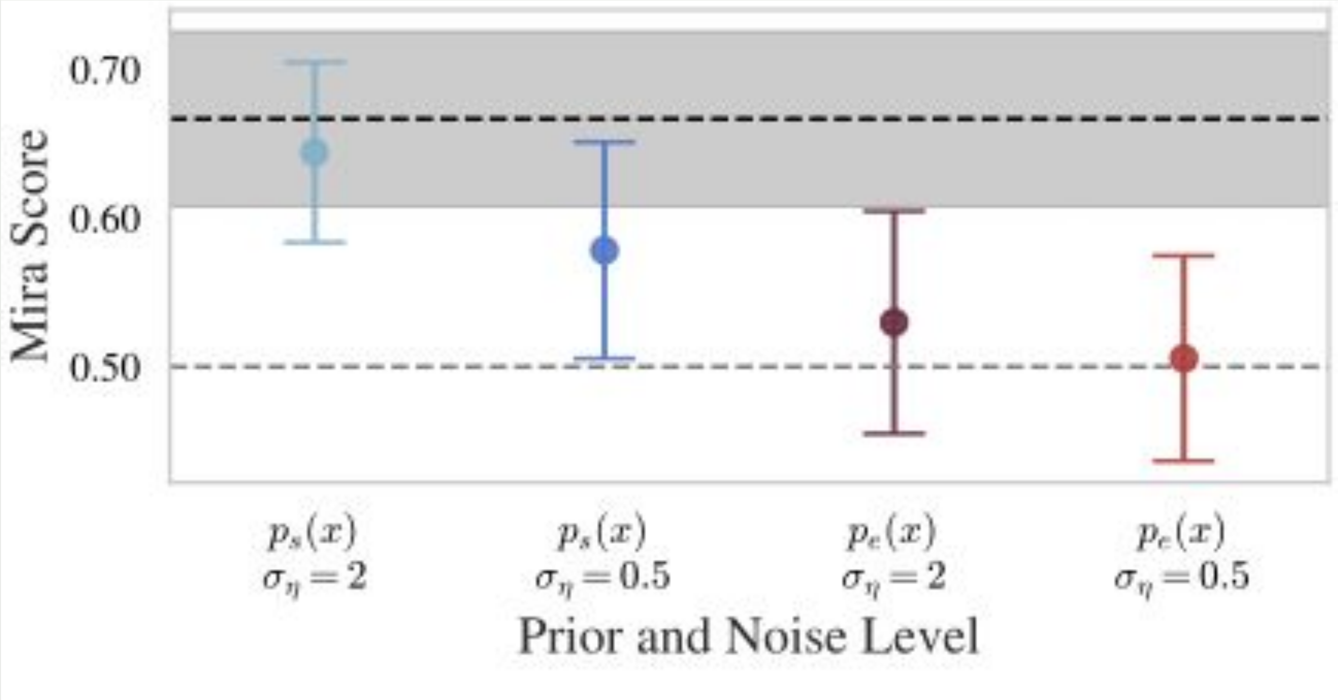
$$\mathbb{E}_{p(k,n)}\left[P_N\right] \to \frac{2}{3} \quad as\ N \to \infty$$
$$Var_{p(k,n)}\left[P_N\right] \to \frac{1}{18} \quad as\ N \to \infty$$

In the limit of $N \to \infty$, given that the $p(y|x, M) \perp\!\!\!\perp p(y|x, M^*)$, the Mira score is

$$\mu_{\text{Mira}}(\mathcal{M}) = \frac{1}{2}$$



$y = Ax^\star + \eta$
$x^\star$
$x \sim p_0(x \mid y)$
$x \sim p_1(x \mid y)$
$x \sim p_2(x \mid y)$
$x \sim p_3(x \mid y)$



0.70
0.60
0.50
Mira Score
$p_s(x)$ $\sigma_\eta = 2$
$p_s(x)$ $\sigma_\eta = 0.5$
$p_e(x)$ $\sigma_\eta = 2$
$p_e(x)$ $\sigma_\eta = 0.5$
Prior and Noise Level

Conclusion

Performing Uncertainty Quantification is vital when working in Scientific Domains such as Astrophysics!

PQMass can be used to determine the quality of the model to learn the training data distribution

ArXiv: Github Repo:

MIRA can be used to determine the quality of the conditional distribution

- Paper & code, will be public soon!

Thank You!