

Generative models in neutron star physics

Márcio Ferreira

Hadrons and Hadron Interactions in QCD

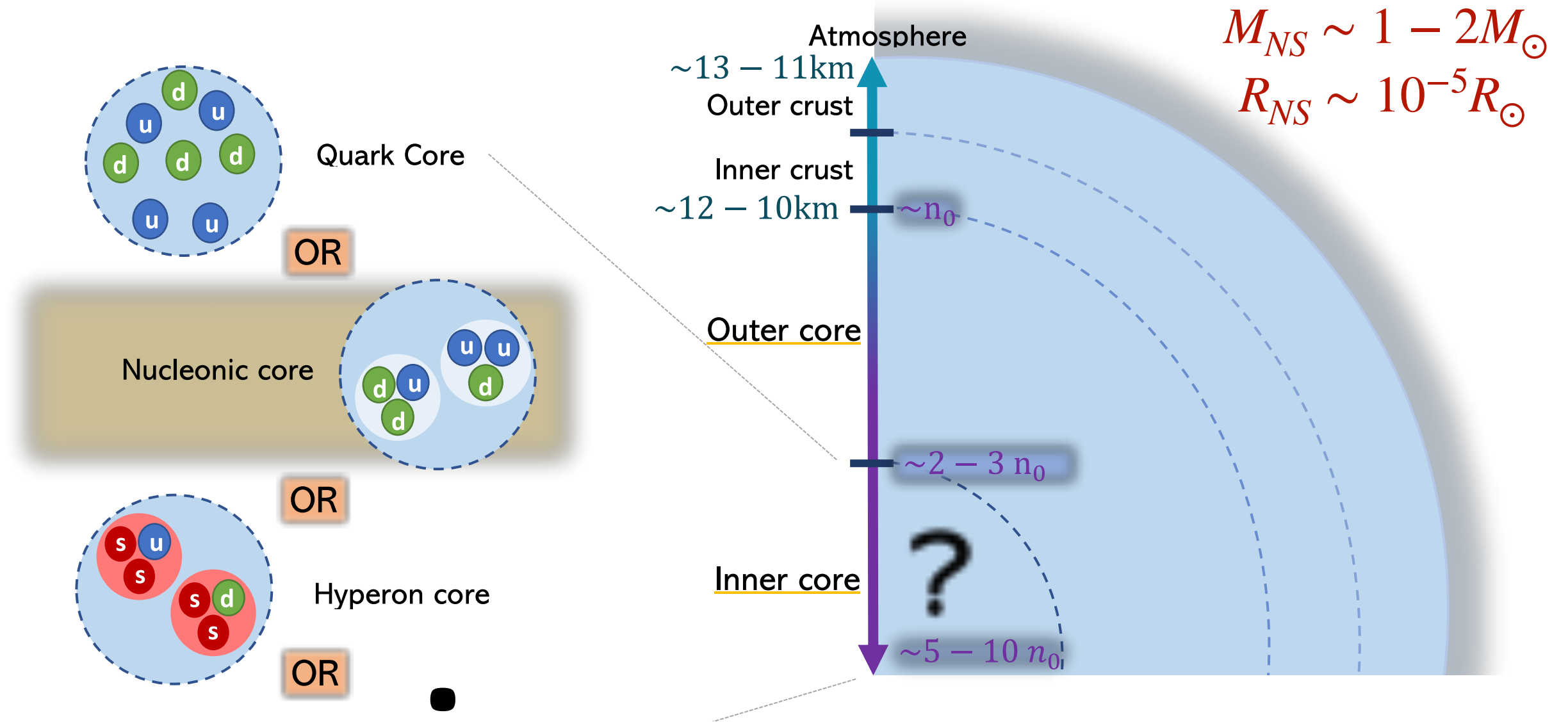
Yukawa Institute for Theoretical Physics

Kyoto University

14Oct - 15Nov (2024)



Neutron star physics

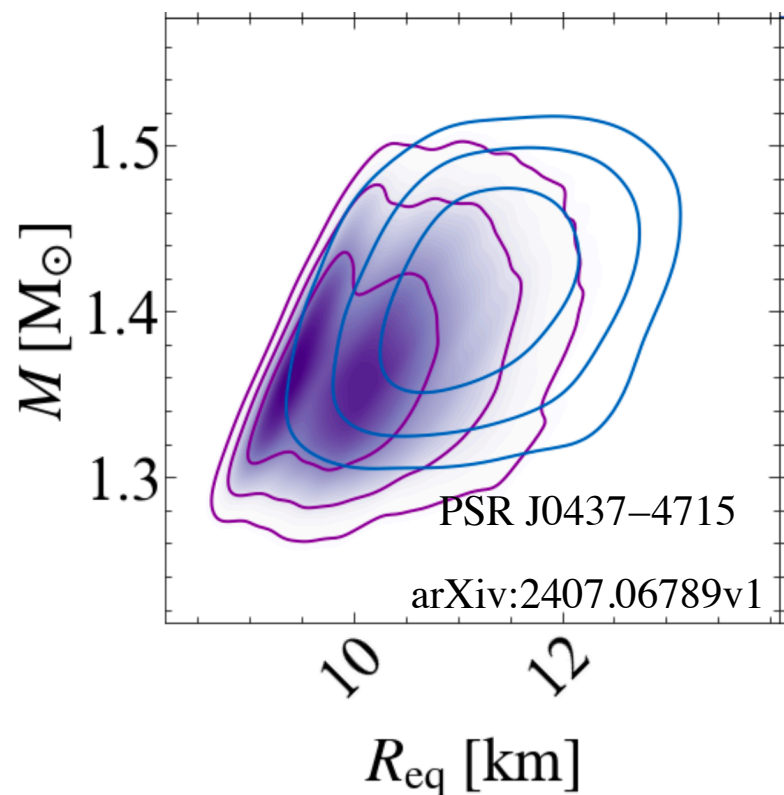


The neutron star equation of state remains unknown.

Constraining the EOS

Pulsar Observations

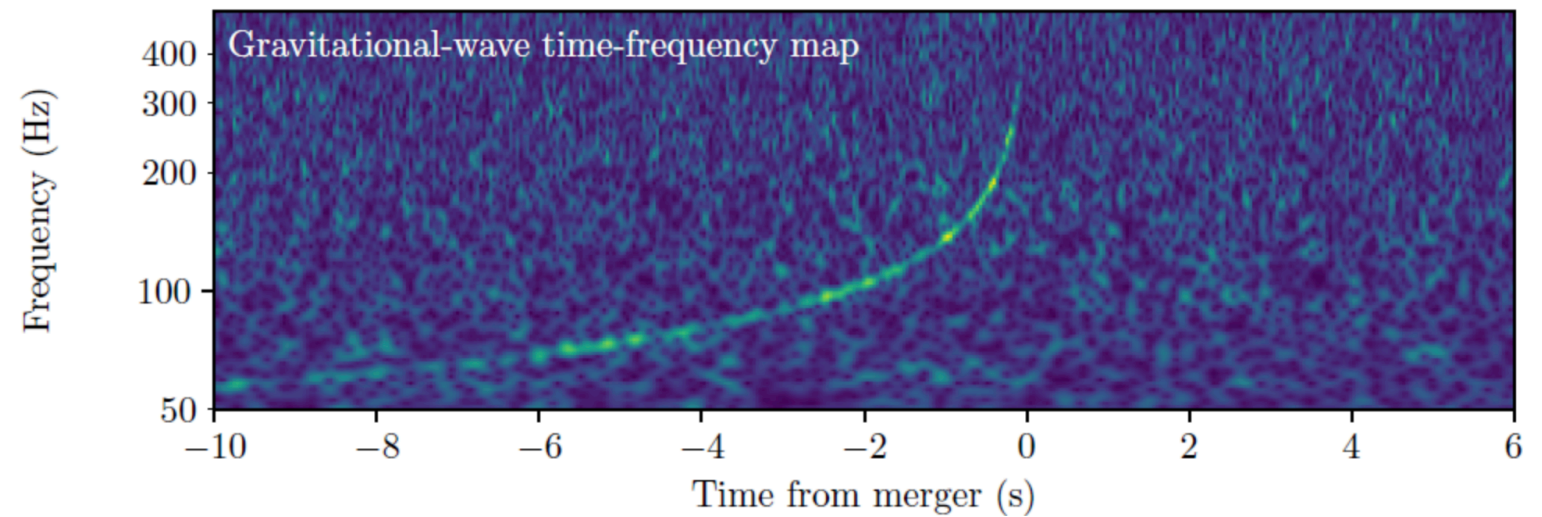
NICER and XMM-Newton
(X-ray observatories)



Gravitational Waves

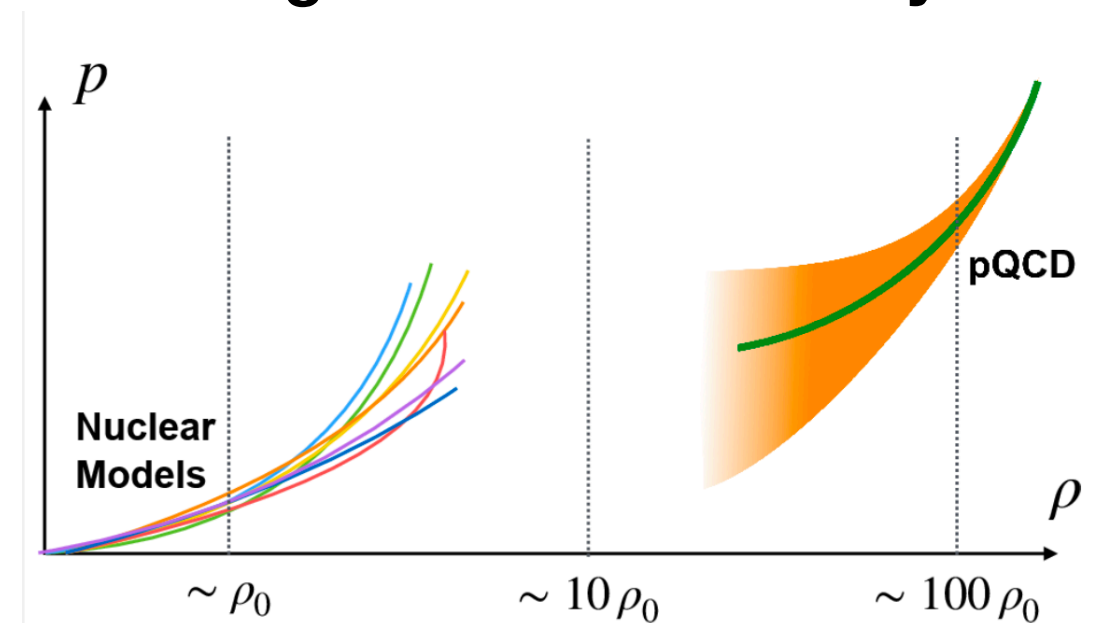
LIGO-Virgo collaboration

GW170817



Combine these data to
learn about NS physics

Strong interactions theory



Generative machine learning models in NS physics

- **Conditional variational autoencoders (cVAE):** deep conditional generative model for structured output variables using Gaussian latent variables
 - Fast prediction using stochastic feed-forward inference (efficient and flexible approach to perform Bayesian inference)

$$P(\text{EOS} | d), \quad d = [(M, R)_1, \dots, (M, R)_N]$$

MF, Michał Bejger, 2403.14266 [nucl-th]

- **Normalizing flows (NF):** define complex distributions by transforming a simple probability density through a series of invertible mappings.
 - Both sampling and density evaluation can be efficiently performed

$$P(d), \quad d = [(M, R)_1, \dots, (M, R)_N]$$

Probability of d belonging to a continuous $M(R)$ solution

(anomaly detection framework)

Valéria Carvalho, MF, et. al, PRD109 (2024) 103032

Parameter estimation using simulated-based inference

- Bayesian Inference:

$$p(\theta | d) \propto p(d | \theta) p(\theta)$$

posterior likelihood prior

- Markov Chain Monte Carlo is used to populate the posterior $\theta \sim p(\theta | d)$
 - Requires a huge number of likelihood evaluations
 - Computationally expensive (namely, high-dimensional θ)
 - Convergence issues
- **Simulated-based inference:** no likelihood evaluation needed but just samples

$$d_i \sim p(d | \theta_i)$$

Learn the posterior $q(\theta | d) \approx p(\theta | d)$ using the cVAE
(Neural posterior estimation)

(θ_i, d_i)

Simulated inference - dataset

$$p(d | \theta) \propto \exp\left(-\frac{(d^{EOS}(\theta) - d)^2}{2\sigma^2}\right) \quad \text{Likelihood}$$

- Dataset construction

$$\text{Piecewise polytropes: } p(n) = K_i n^{\Gamma_i}$$

$$\theta_i \sim p(\theta) \sim \{\Gamma_0, \Gamma_1, n_1, \Gamma_2, n_2, \Gamma_3, n_3, \Gamma_4, n_4\} \quad \text{Sample from the prior}$$

- Likelihood samples: uniformly select 5 points over the $TOV(\theta_i)$

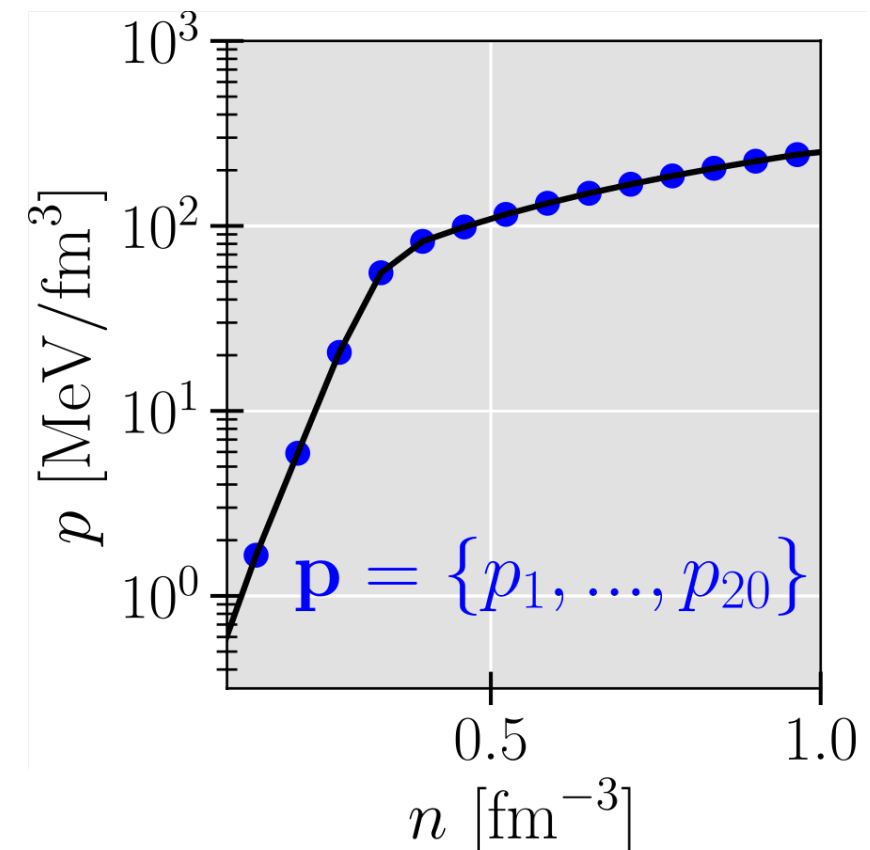
$$M_i \sim \mathcal{N}(M_i^{TOV(\theta_i)}, \sigma_M)$$

$$R_i \sim \mathcal{N}(R_i^{TOV(\theta_i)}, \sigma_R)$$

$$d_i = (M_i, R_i)$$

- Training dataset: $\{(\theta_1, d_1), (\theta_2, d_2), \dots, (\theta_5, d_5)\}$

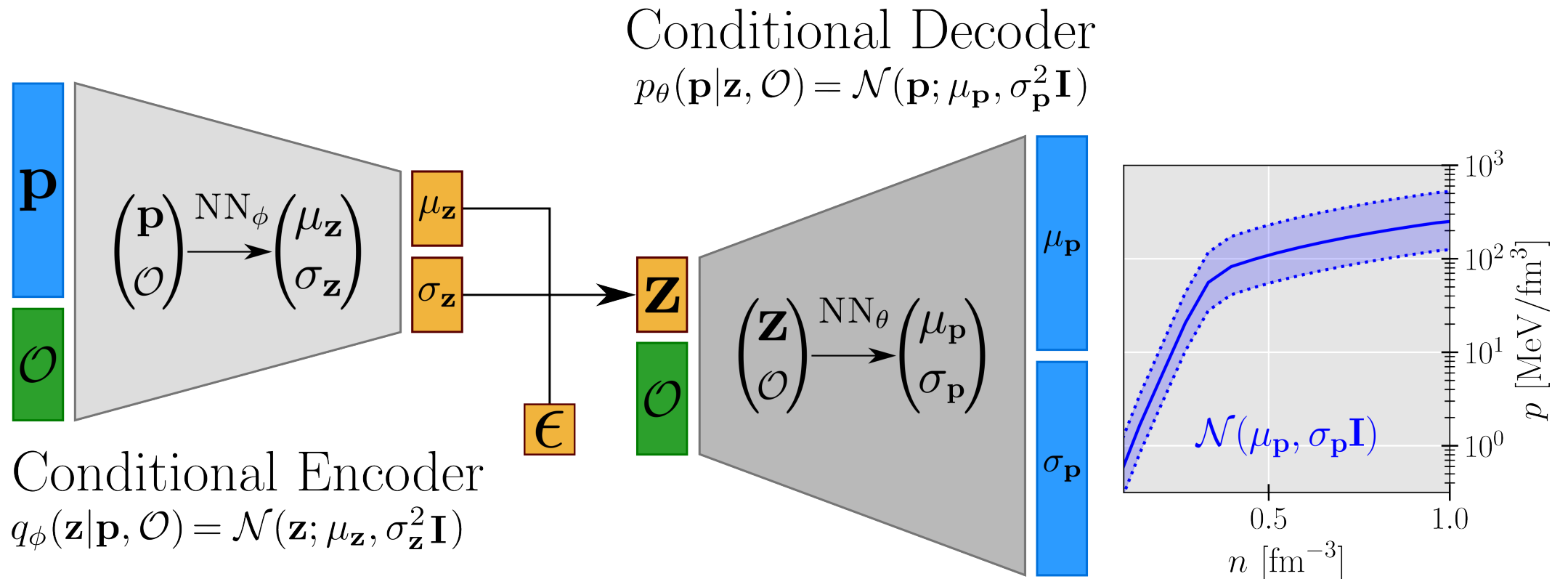
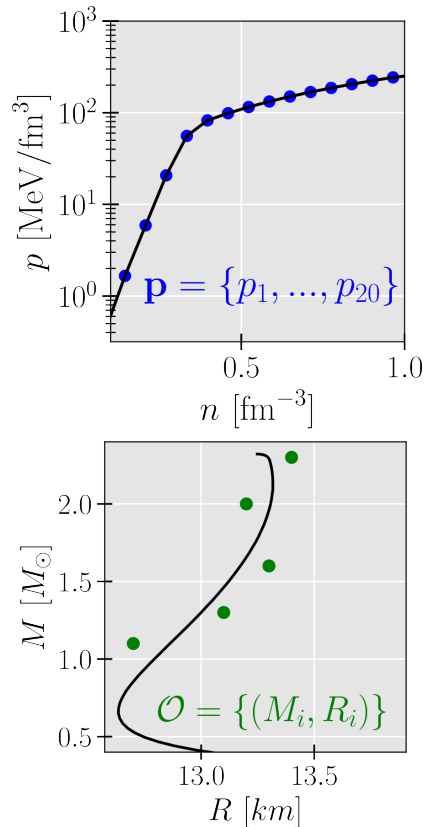
$$\{(p_1, d_1), (p_2, d_2), \dots, (p_5, d_5)\}$$



Conditional Variational Autoencoders (cVAE)

- Reconstruct the EOS given a set of noisy observations

$$x = [\mathbf{p}, \mathcal{O}] = [p_1, p_2, p_3, \dots, p_{20}, M_1, R_1, M_2, R_2, \dots, M_5, R_5]$$



Loss function:

$$\mathcal{L}_{\text{VAE}}(\theta, \phi, \mathbf{x}, \mathcal{O}) = \mathbf{E}_{\mathbf{z} \sim q_\phi(\mathbf{z}|\mathbf{x})} [\log p_\theta(\mathbf{x}|\mathbf{z}, \mathcal{O})] - D_{\text{KL}}(q_\phi(\mathbf{z}|\mathbf{x}, \mathcal{O}) || p_0(\mathbf{z}))$$

Reconstruction term

Regularizer

Kullback-Leibler divergence $D_{\text{KL}}(P || Q) = \int_{-\infty}^{\infty} p(x) \log\left(\frac{p(x)}{q(x)}\right) dx$

Forces the encoder probability to be close to $p_0(\mathbf{z}) = \mathcal{N}(0, \mathbf{1})$

Training - cVAE

- During training a single sample from the latent space is used for each EOS

$$\mathbb{E}_{\mathbf{z} \sim q_{\phi}(\mathbf{z}|\mathbf{p})} [\log p_{\theta}(\mathbf{p}|\mathbf{z}, \mathcal{O})] \approx \log p_{\theta}(\mathbf{p}|\mathbf{z}_1, \mathcal{O})$$

$$D_{\text{KL}}(q_{\phi}(\mathbf{z}|\mathbf{p}, \mathcal{O}) || p(\mathbf{z})) = q_{\phi}(\mathbf{z}_1|\mathbf{p}, \mathcal{O}) \log \left(\frac{q_{\phi}(\mathbf{z}_1|\mathbf{p}, \mathcal{O})}{p(\mathbf{z}_1)} \right)$$

The encoder/decoder PDFs are Gaussian:

$$p(\mathbf{z}_1) = \mathcal{N}(\mathbf{z}_1; \mathbf{0}, \mathbf{I})$$

$$q_{\phi}(\mathbf{z}_1|\mathbf{p}, \mathcal{O}) = \mathcal{N}(\mathbf{z}_1; \boldsymbol{\mu}_{\mathbf{z}}, \boldsymbol{\sigma}_{\mathbf{z}}^2 \mathbf{I})$$

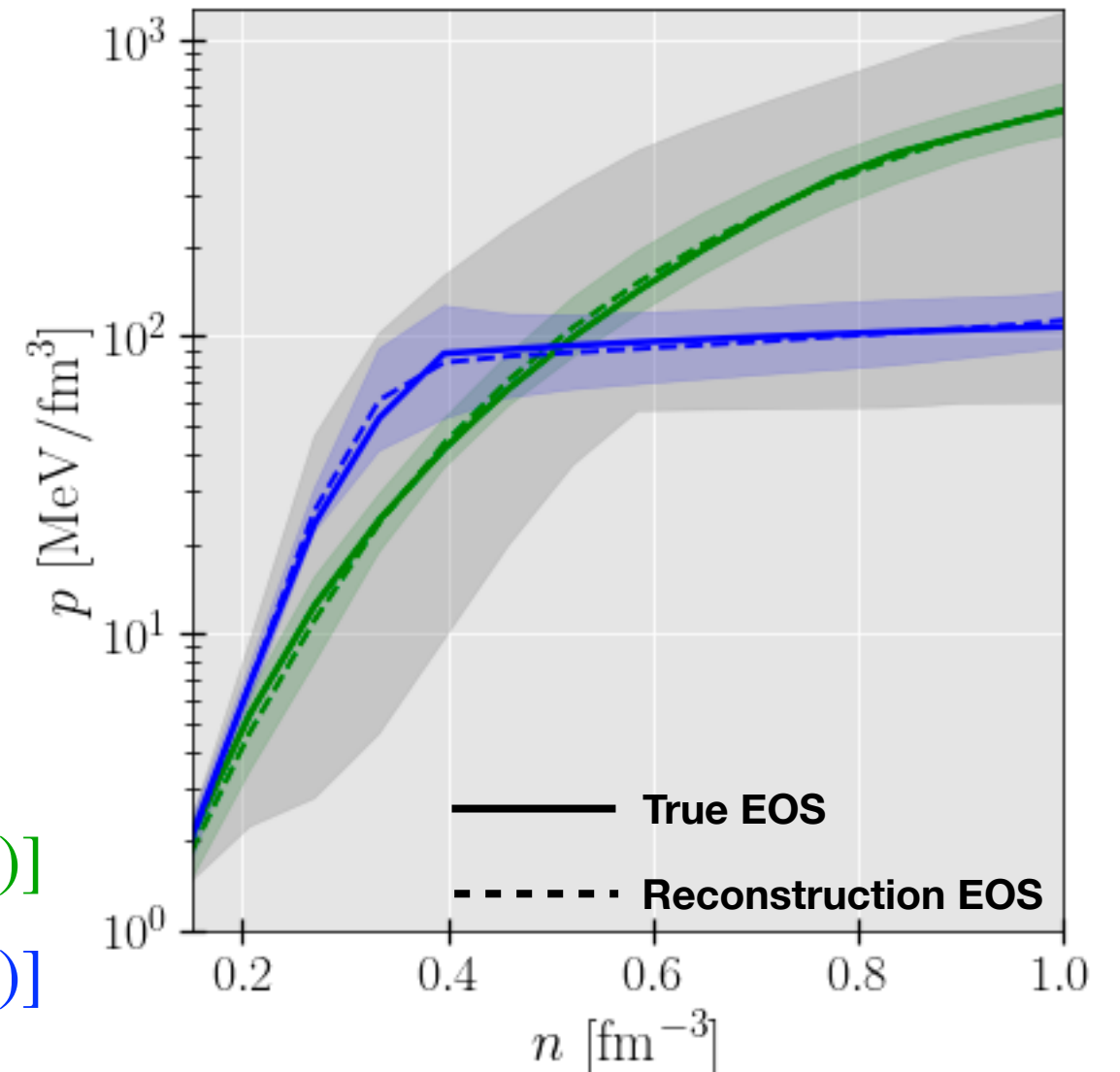
$$p_{\theta}(\mathbf{p}|\mathbf{z}_1, \mathcal{O}) = \mathcal{N}(\mathbf{p}; \mathbf{z}_1, \mathbf{z}_1^2 \mathbf{I})$$

The loss function has a closed form solution

Reconstruction of two EOS during training:

$[(p_1, p_2, p_3, \dots, p_{20}), ((M_1, R_1), (M_2, R_2), \dots, (M_5, R_5))]$

$[(p_1, p_2, p_3, \dots, p_{20}), ((M_1, R_1), (M_2, R_2), \dots, (M_5, R_5))]$

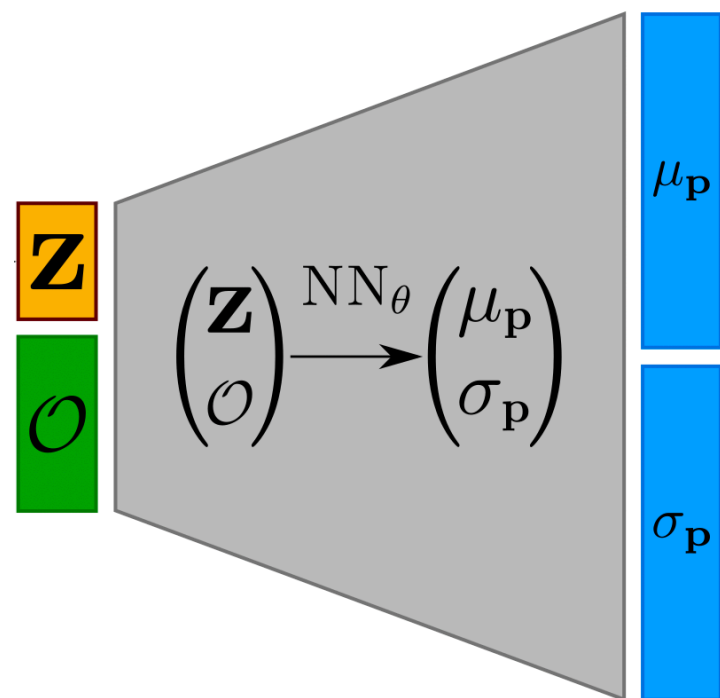


Generative block (cVAE) - Inference model

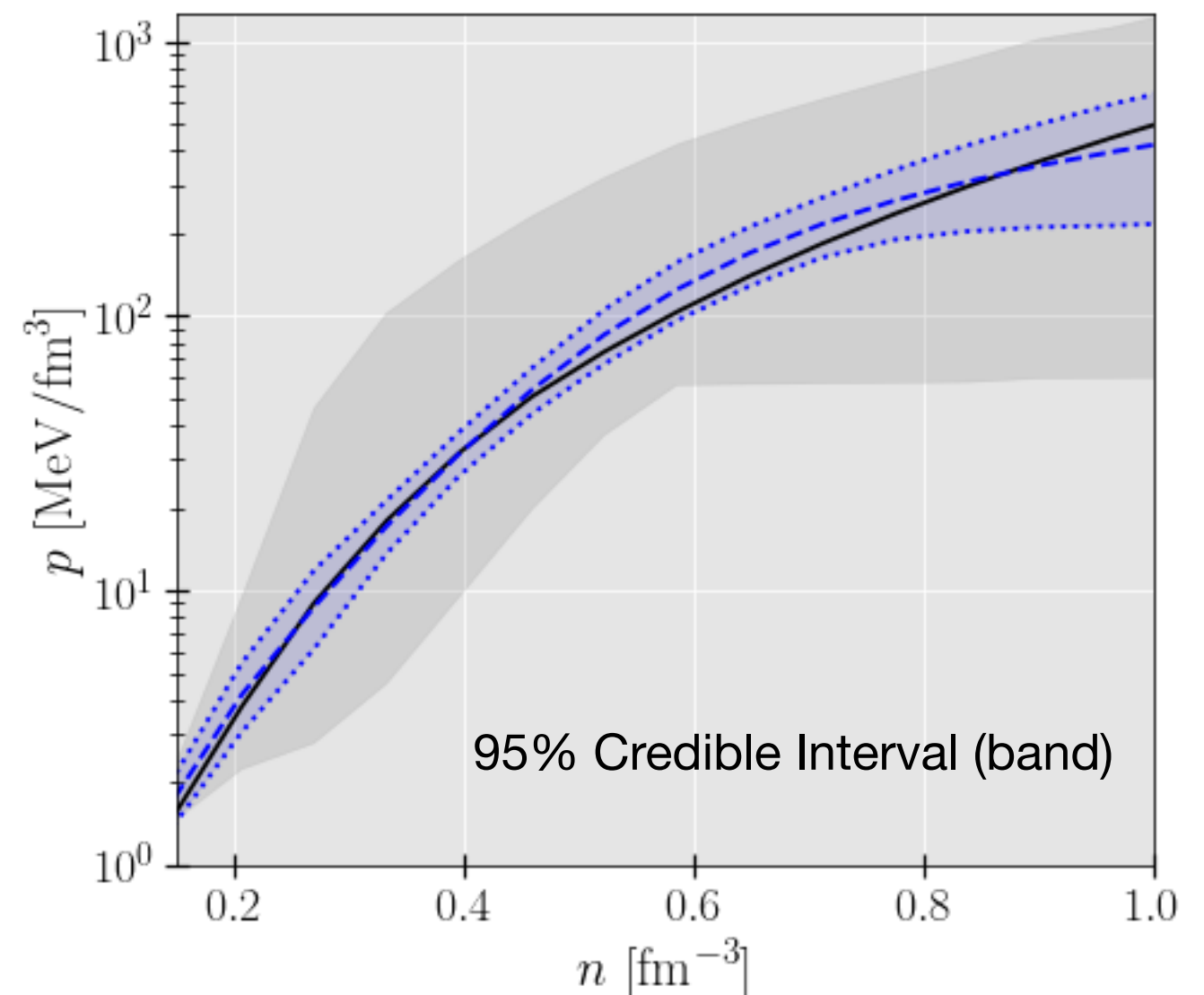
- The generative block as an inference framework: $P(\text{EOS} | \text{Observation set})$
- During inference phase, we must marginalize over the latent space

$$p_{\theta}(\mathbf{p} | \mathcal{O}) \approx \frac{1}{L} \sum_{l=1}^L \mathcal{N}_{\theta}(\mathbf{p} | \mathbf{z}^l, \mathcal{O})$$

Monte Carlo approximation
with $L=2000$



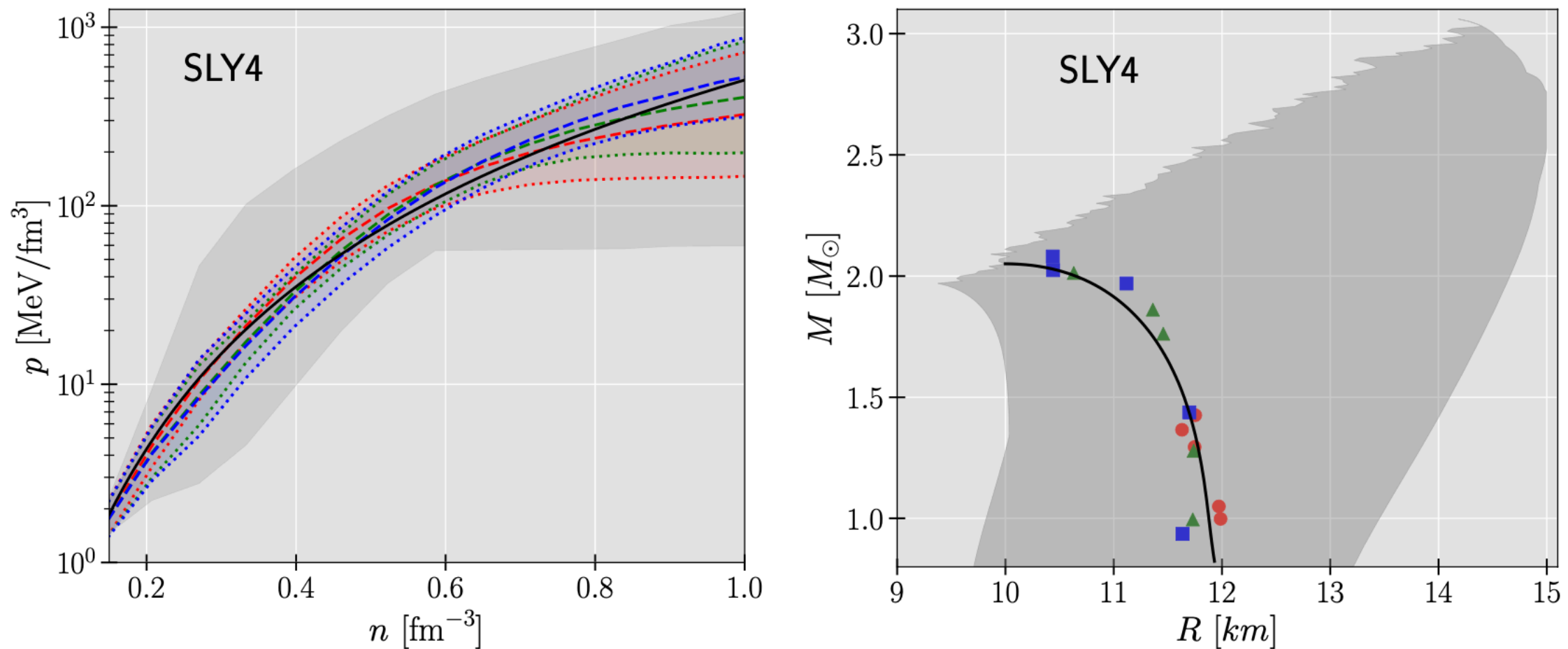
$$\mathcal{O} = [(M_1, R_1), \dots, (M_5, R_5)]$$



cVAE reconstruction of a nuclear model

- Reconstruction of SLy4 model from a set of noisy observations (5 NS)

$$\mathcal{O} = \{(M_1, R_1), \dots, (M_5, R_5)\}, \quad \mathcal{O} = \dots, \quad \mathcal{O} = \dots$$



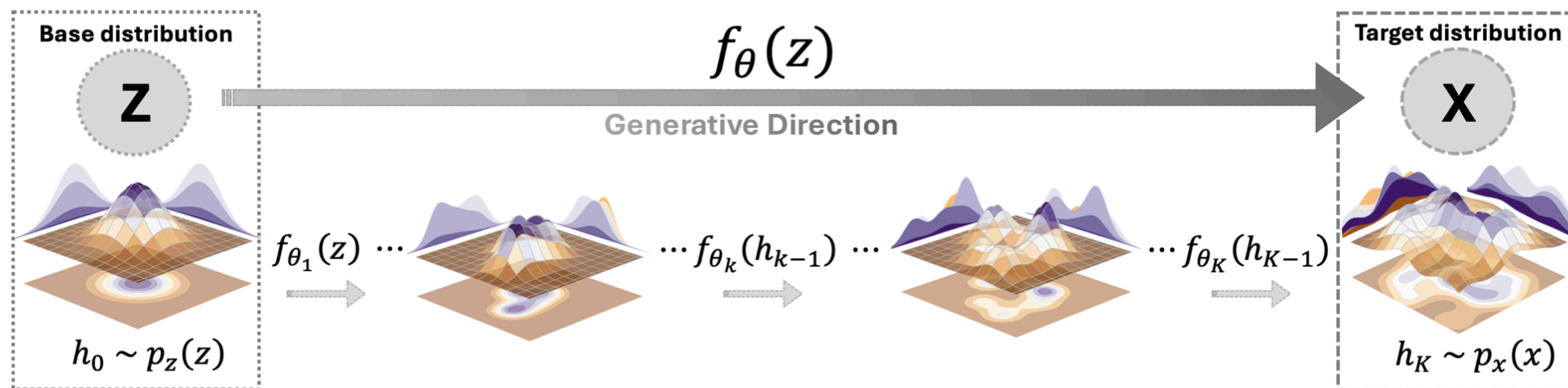
- High density region is restricted by the presence of massive NS
- Low density region more constrained for \mathcal{O} (presence of 5 light NS)
- Good reconstruction (within uncertainty bands)

Conclusions - cVAE

- New generative framework for the equation of state of NS
- Instantaneous inference for any observation set
- The posterior dimension could be easily increased
- The dimension of the conditional vector is flexible (**tidal deformability**)

Normalizing flows

- Model $p_x(x)$ from multiple **invertible and differentiable transformations** f_{θ_k} of a simple base distribution $p_z(z)$
- Capable of generating new samples $x \sim p_x(x)$ and density estimation $p_x(x)$



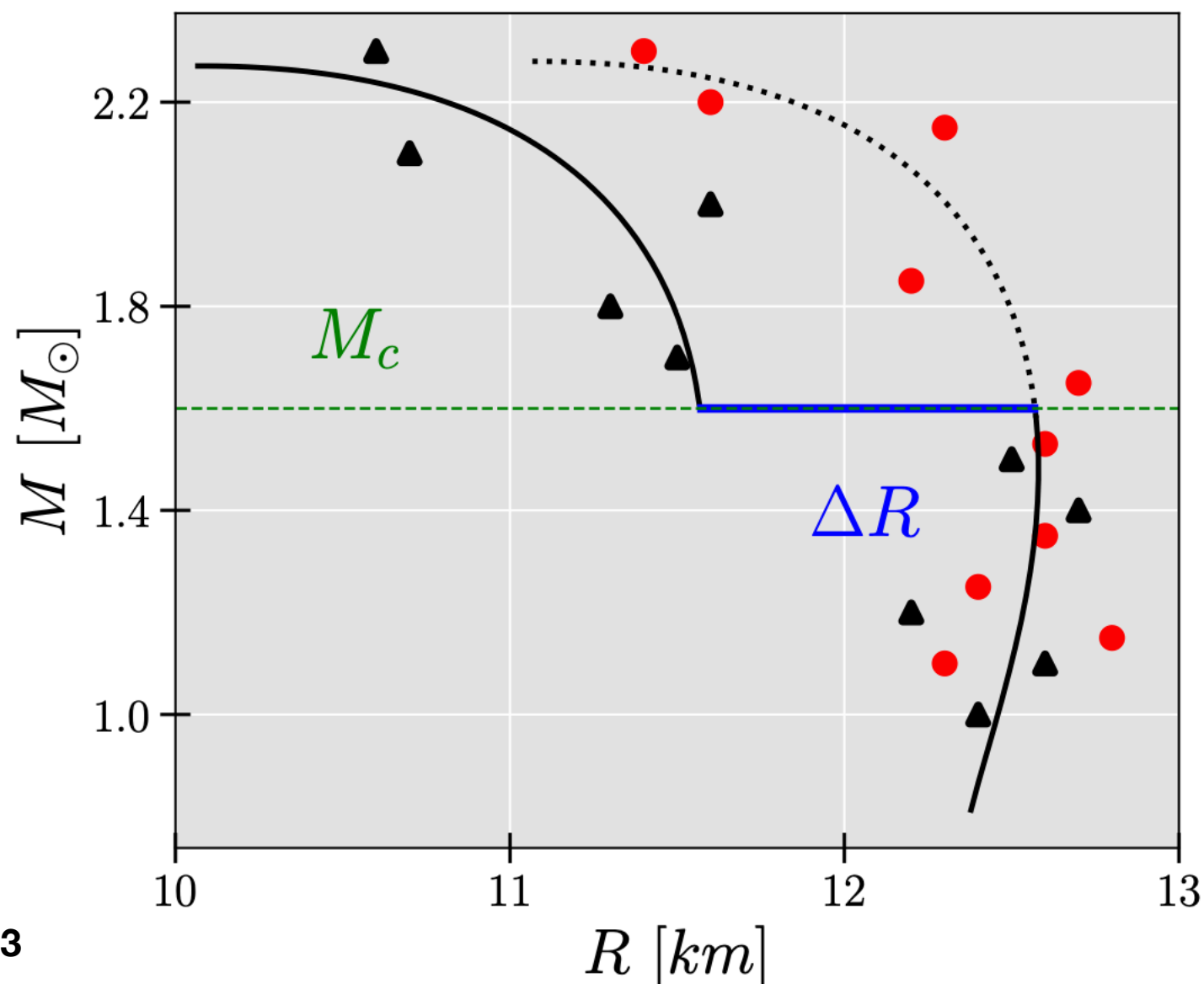
Loss function: minimizing the negative log-likelihood of the data under the NF

$$\mathcal{L}(\mathcal{D}) = -\frac{1}{|\mathcal{D}|} \sum_{\mathbf{x} \in \mathcal{D}} \log p_x(\mathbf{x})$$

$$\log p_x(\mathbf{x}) = \log p_z(\mathbf{f}_{\theta_k}^{-1}(h_{k-1})) + \sum_{k=1}^K \log \left| \det \frac{\partial \mathbf{f}_{\theta_k}^{-1}(h_{k-1})}{\partial h_{k-1}} \right|$$

Normalizing flows: detecting a phase transition

- Train on continuous $M(R)$ samples
 - **Training set:** 25287 hadronic models (RMF framework)
- Estimate the likelihood of a non-continuous solutions (two-branch solution)



- Low likelihood for any sample that deviates considerably from the train statistics

$$P(d) \ll P(d)$$

- **Test sets** are parametrized by

$$M_c \quad \Delta R$$

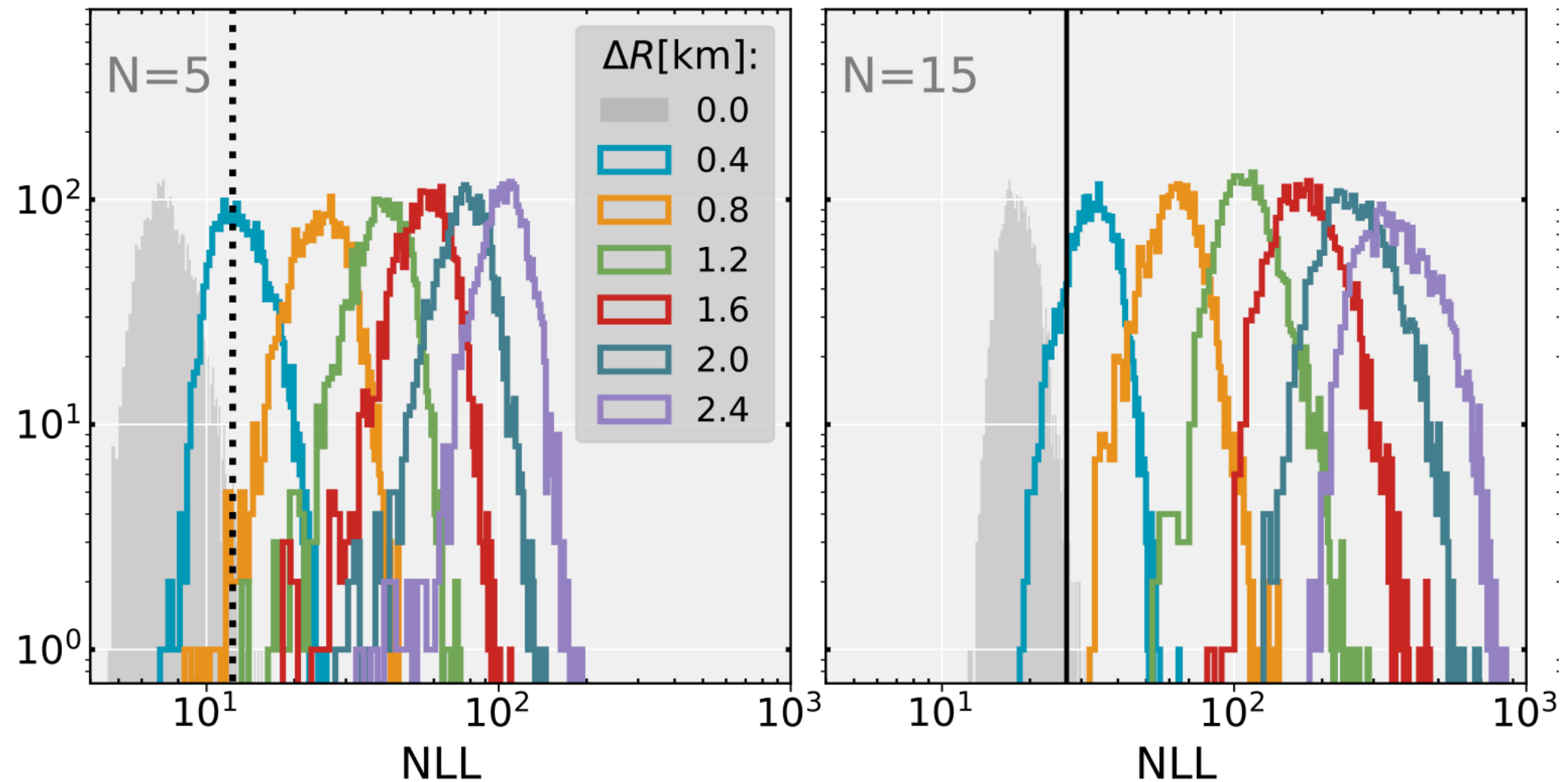
Results: two-branch detection

$$M_C = 1.5M_\odot$$

Generation parameters for each dataset.

Dataset	$\sigma_M [M_\odot]$	$\sigma_R [\text{km}]$
Set 0	0	0
Set 1	0.1	0.2
Set 2	0.136	0.626

Threshold: False Positive Rate at 1%

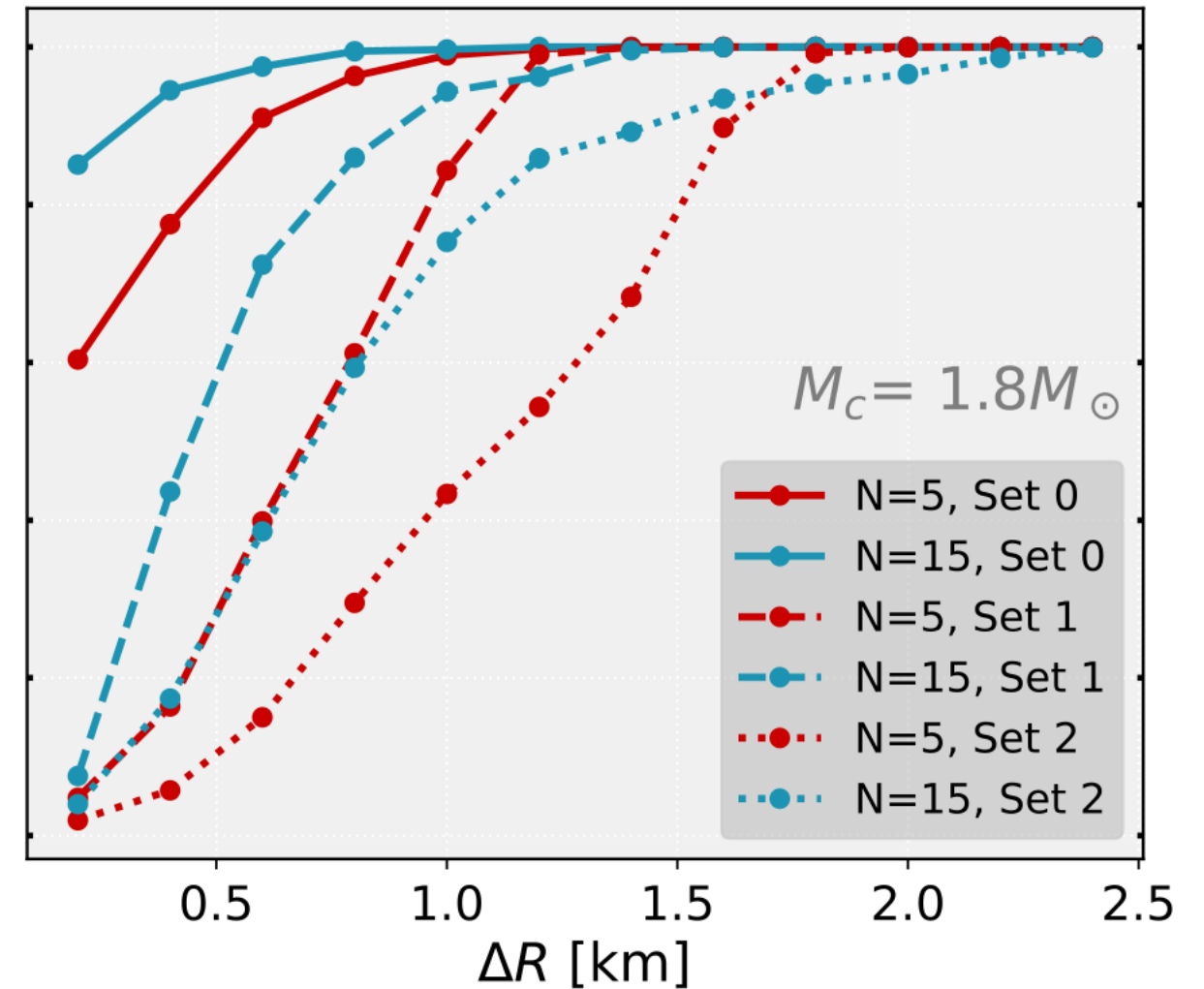
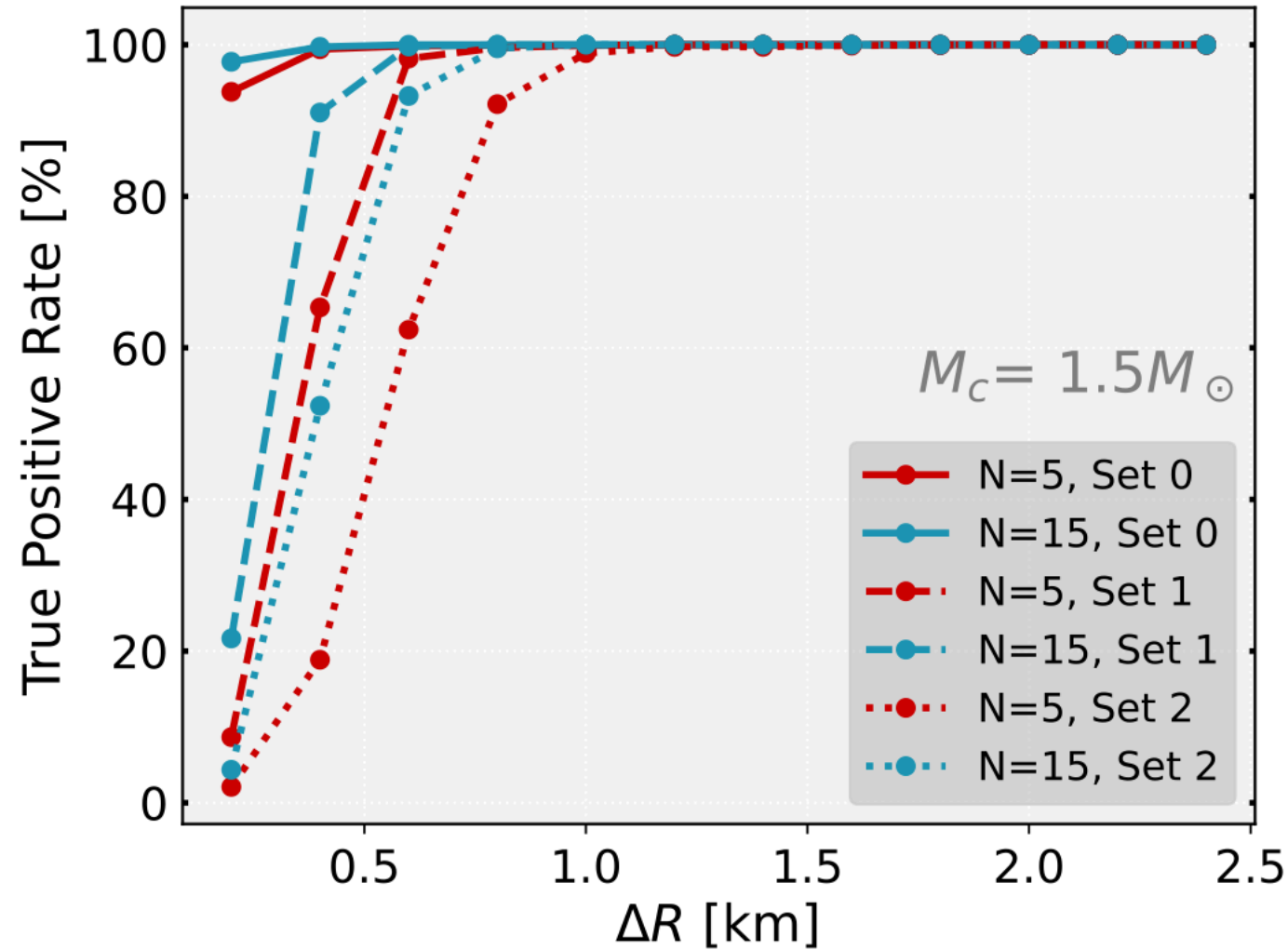


- Detection rate for a two-branch solution is 100% for N=15 stars if $\Delta R \geq 0.8$ km

Results: impact of noise level

Generation parameters for each dataset.

Dataset	$\sigma_M [M_\odot]$	$\sigma_R [\text{km}]$
Set 0	0	0
Set 1	0.1	0.2
Set 2	0.136	0.626

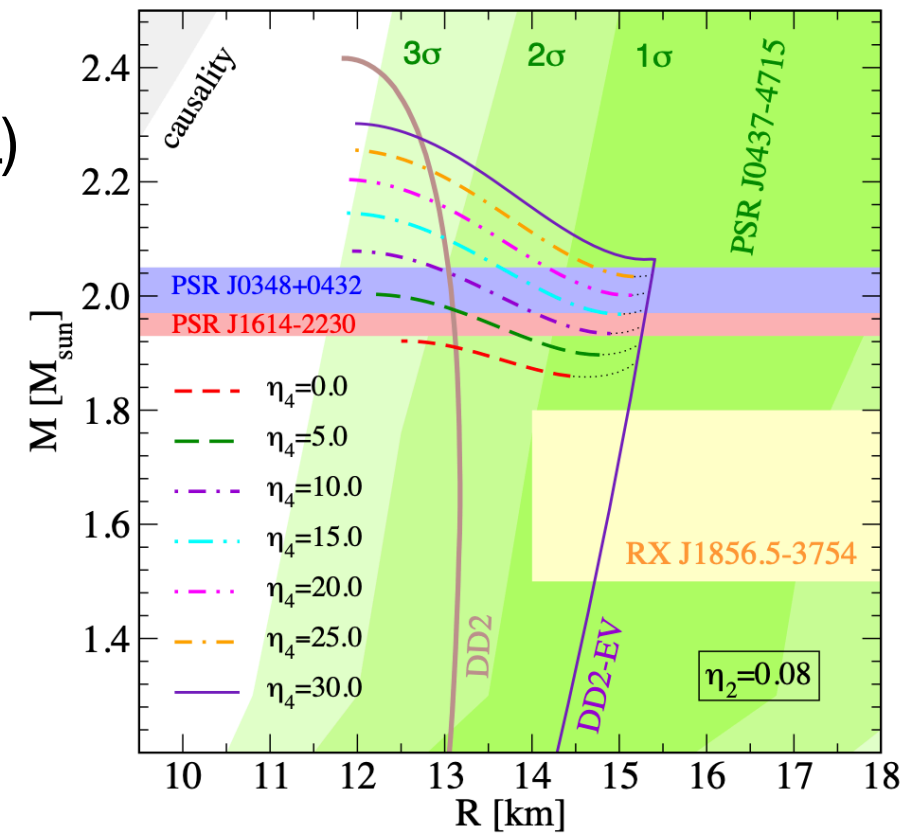
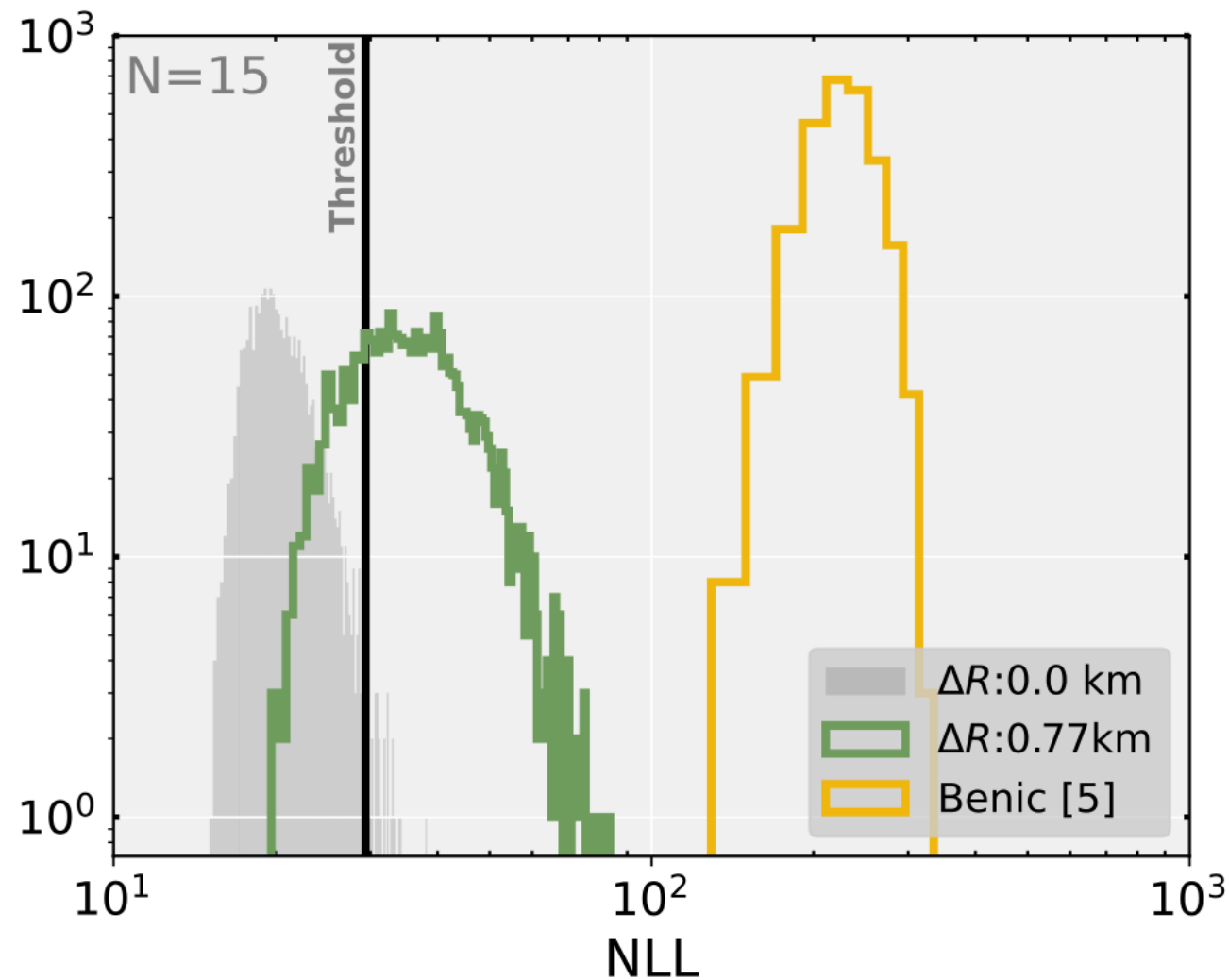


- TPR: lower for $M_c = 1.5 M_\odot$, increases with N , decreases with noise level
- 100% TRP is reached for 15 neutron stars if

$$\Delta R > 0.6 \text{ km (Set 1) and } \Delta R > 0.8 \text{ km (Set 2)}$$

Test with a microscopic two-branch solution

- Two-branch solution from microscopic models (DD2+NJL) [S. Benic, et. al., *Astron. Astrophys.* 577, A40 (2015)]
- Test set with $(M_c, \Delta R) = (1.91 M_\odot, 0.77 \text{ km})$



- Our test sets give a lower bound on the model performance

Conclusions - NF

- NF are flexible models for density estimation (and sampling)
- Differentiate the NS composition from the $M(R)$ curve
- Capable of detecting deviations (anomalies) from a continuous $M(R)$ curve
- For a given observation uncertainty σ_R , we can estimate the ΔR below which the two-branch solution has a low detection probability