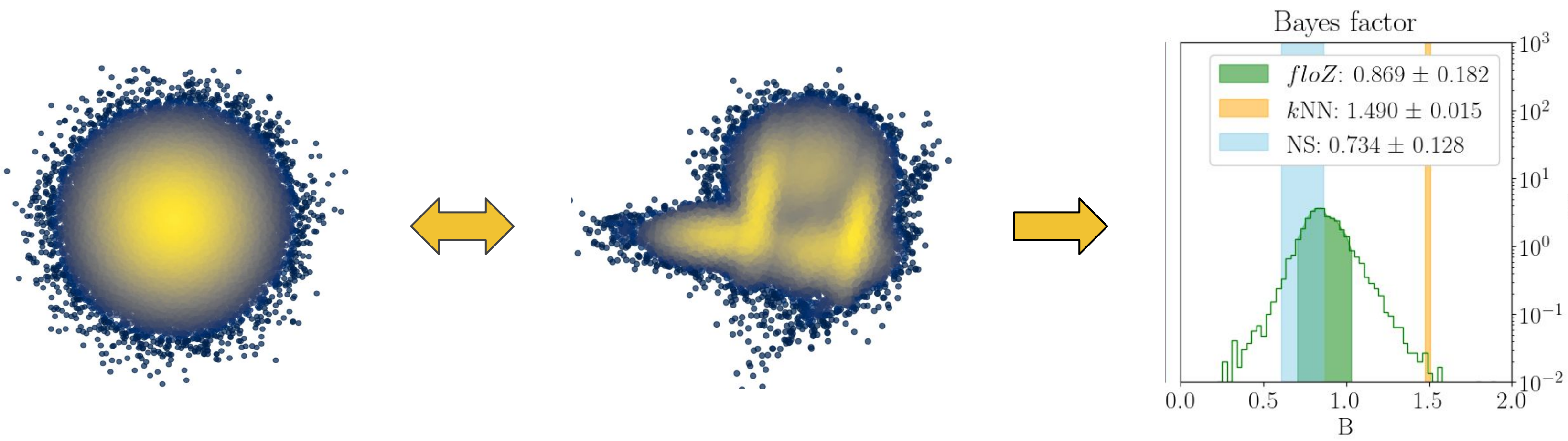
floZ

Bayes factor from normalizing flows

Rahul Srinivasan, Marco Crisostomi, Roberto Trotta, Enrico Barausse, and Matteo Breschi



1st TEONGRAV international workshop on theory of gravitational waves

arXiv:2404.12294v2; submitted to PRD
https://github.com/Rahul-Srinivasan/floZ

The Bayes Theorem

$$p(A|\mathrm{B}) = \frac{p(\mathrm{B}|\mathrm{A}) \;\; . \;\; p(A)}{p(\mathrm{B})}$$

The Bayes Theorem

$$p(A|\mathrm{B}, \mathrm{C}) = \frac{p(\mathrm{B}|\mathrm{A}, \mathrm{C}) \,.\, p(A|\mathrm{C})}{p(\mathrm{B}|\mathrm{C})}$$

The Bayes Theorem

$$p(\theta|\text{data}, M) = \frac{p(\text{data}|\theta, M)\ .\ p(\theta|M)}{p(\text{data}|M)}$$

The Bayes Theorem

$$\mathit{Posterior} = \frac{\mathit{Likelihood} \;.\; \mathit{Prior}}{\mathit{Evidence}}$$

Competing models

$$p(\theta|\text{data}, M_1) = \frac{p(\text{data}|\theta, M_1) \;\cdot\; p(\theta|M_1)}{p(\text{data}|M_1)}$$

Does the data favour M_1 or M_2?
And by how much?

$$p(\theta|\text{data}, M_2) = \frac{p(\text{data}|\theta, M_2) \;\cdot\; p(\theta|M_2)}{p(\text{data}|M_2)}$$

Competing models

$$p(\theta|\text{data}, M_1) = \frac{p(\text{data}|\theta, M_1) \quad . \quad p(\theta|M_1)}{p(\text{data}|M_1)}$$

$$p(\theta|\text{data}, M_2) = \frac{p(\text{data}|\theta, M_2) \quad . \quad p(\theta|M_2)}{p(\text{data}|M_2)}$$

The Bayes Factor

By what factor does the data favour M_1 over M_2?

$$B = \frac{p(\text{data}|M_1)}{p(\text{data}|\mathrm{M}_2)}$$

$$= \frac{Evidence_1}{Evidence_2}$$

The Evidence

$$p(\theta|\text{data},M) = \frac{p(\text{data}|\theta,M)\ .\ p(\theta|M)}{p(\text{data}|M)}$$

Probability density
i.e., normalized.

The Evidence

$$p(\theta|\text{data},M) = \frac{p(\text{data}|\theta,M)\ .\ p(\theta|M)}{p(\text{data}|M)}$$

$$p(\text{data}|M) = \int p(\text{data}|\theta,M)\ .\ p(\theta|M)\ d\theta$$

$$Evidence = \int Likelihood\ .\ Prior\ d\theta$$

Computing this integral can be quite non-trivial, and often, intractable.

State of the art and their ***shortcomings***

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Nested sampling[1]:

Evidence estimated by iteratively computing the likelihood.

- ***Computationally intensive*** likelihood *re*calculation.
- ***Slow***, CPU calculations, not parallelizable with GPUs.
- ***Scalability*** issues for high dimensions
    - Ex: 150 dimensions are computationally prohibitive

1. John Skilling "Nested Sampling," 10.1063/1.1835238.

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Other techniques:

1. k-nearest neighbours[2], Laplace approx. - ***Less expressive***: fails for large non-gaussianity.
2. Normalizing flow-based nested[3]/Gaussianized bridge[4] sampling - ***Requires likelihood re-calculation***

1. John Skilling "Nested Sampling," 10.1063/1.1835238.
2. A. Heavens, et al 2017 arXiv:1704.03472 [stat.CO]
3. Nested sampling with normalizing flows for gravitational-wave inference, 10.1103/PhysRevD.103.103006
4. Jia, He; Seljak, Uroš, 2019 10.48550/arXiv.1912.06073

State of the art and their ***shortcomings***

Nested sampling[1]:

Evidence estimated by iteratively computing the likelihood.

Likelihood evaluation can be expensive.
These are pre-computed for MCMC samples in parameter estimation pipelines.
Why not use it?

Useful to have a fast, scalable, and expressive method that does not require extra likelihood evaluations.

1. k-nearest neighbours[2], Laplace approx. - ***Less expressive***: fails for large non-gaussianity.
2. Normalizing flow-based nested[3]/Gaussianized bridge[4] sampling - ***Requires likelihood re-calculation***

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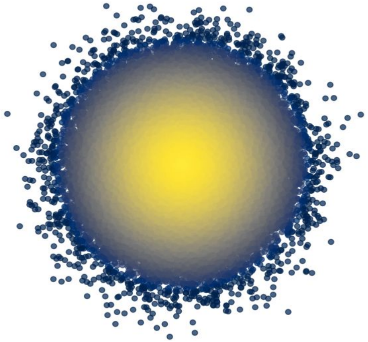
A normalizing flow

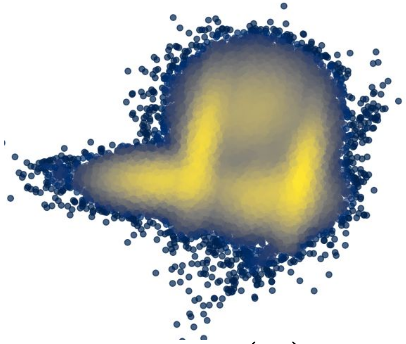
Flows solves for a bijective map b/ the *latent* Normal distribution and the *real* non-trivial distribution.

Known *latent* distribution



$$\boldsymbol{y} \sim \mathrm{n}(\boldsymbol{y})$$

Target *real* distribution



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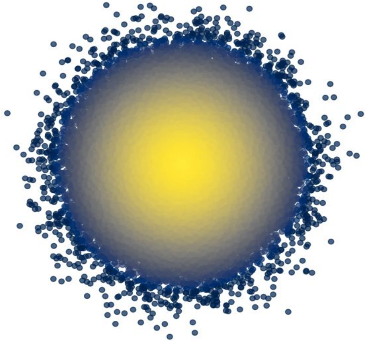
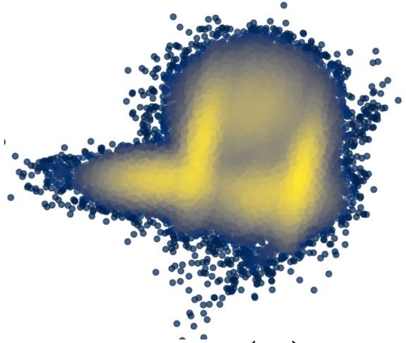


$\boldsymbol{y} \sim \mathrm{n}(\boldsymbol{y})$

$$\boldsymbol{x} = \mathbf{f}_{\boldsymbol{\phi}}(\boldsymbol{y})$$

$$\boldsymbol{y} = \mathbf{f}_{\boldsymbol{\phi}}^{-1}(\boldsymbol{x})$$

Target *real* distribution



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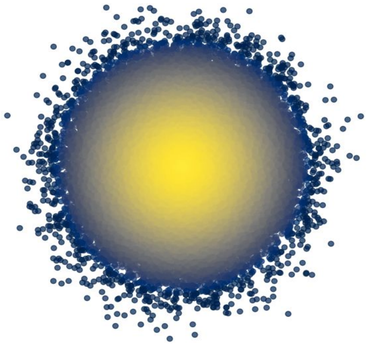

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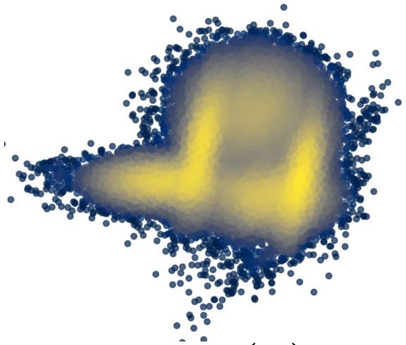

$\boldsymbol{x} \sim \mathrm{p}(\boldsymbol{x})$

$$\text{Target distribution} \quad \mathrm{p}(\boldsymbol{x}) \mapsto \mathrm{q}_{\boldsymbol{\phi}}(\boldsymbol{x}) \quad \text{Flow prediction} \quad = \mathrm{n}(\mathbf{f}_{\boldsymbol{\phi}}^{-1}(\boldsymbol{x})) \left| \det \frac{\partial \mathbf{f}_{\boldsymbol{\phi}}^{-1}}{\partial \boldsymbol{x}}(\boldsymbol{x}) \right|$$

Theory behind *floZ*

Evidence = normalization constant of likelihood x prior

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Evidence Ground Truth

$$\boxed{Z \mapsto \zeta(\boldsymbol{x}, \boldsymbol{\phi}) = \frac{\hat{\mathrm{p}}(\boldsymbol{x})}{\mathrm{q}_{\boldsymbol{\phi}}(\boldsymbol{x})}}$$

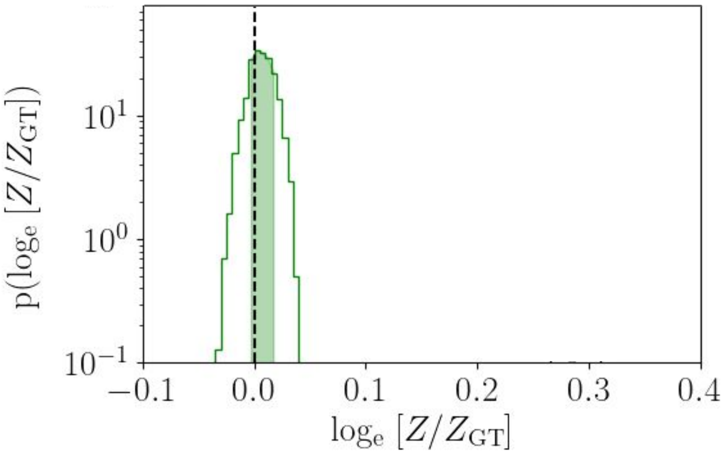
Likelihood . prior
= *Unnormalized* posterior probability

Evidence Estimation Distribution

floZ
= *Normalized* posterior probability

Expected output:

Evidence *distribution*



Ideally a delta function

Implementation:

Loss Terms

1. Normalizing flow loss:

floZ prediction

$$\mathcal{L}_1(\boldsymbol{\phi}) = -\mathrm{E}_{\mathrm{p}(\boldsymbol{x})}\left[\log(\mathrm{q}_{\boldsymbol{\phi}}(\boldsymbol{x}))\right]$$

Expectation over posterior samples

Implementation:

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2. Reducing evidence estimation error:

$$\mathcal{L}_2(\phi) \simeq \log \sigma_{\mathfrak{h}}$$

Standard deviation of evidence estimation

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3. Identity evidence ratio of all pairs of samples:

Mean evidence ratio

$$\mathcal{L}_{3a}(\phi) \ = \ |\log \mu_{\mathfrak{g}}|$$

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$$\mathcal{L}_{3a}(\phi) = |\log \mu_{\mathfrak{g}}|$$

4. Reducing evidence ratio error:

$$\mathcal{L}_{3b}(\phi) = \log \sigma_{\mathfrak{g}}$$

Standard deviation of the ratio of evidence

Implementation:

Loss Terms

1. Normalizing flow loss:

floZ prediction

$\mathcal{L}_1(\phi) =$ $\mathbf{L_1}$ $q_\phi(x))]$

Expect *rior samples*

2. Reducing evidence estimation error:

$\mathcal{L}_2(\phi) \simeq 1$ $\mathbf{L_2}$

viation
of evidence estimation

3. Identity evidence ratio of all pairs of samples:

idence ratio

$\mathcal{L}_{3a}(\phi)$ $\mathbf{L_{3a}}$

4. Reducing evidence ratio error:

$\mathcal{L}_{3b}(\phi) =$ $\mathbf{L_{3b}}$

Standard deviation of the ratio of evidence

Implementation:
Loss Scheduling

Solving the four losses simultaneously:
1) Weighted sum of losses.
2) Schedule the losses

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Loss Scheduling

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1) Weighted sum of losses.
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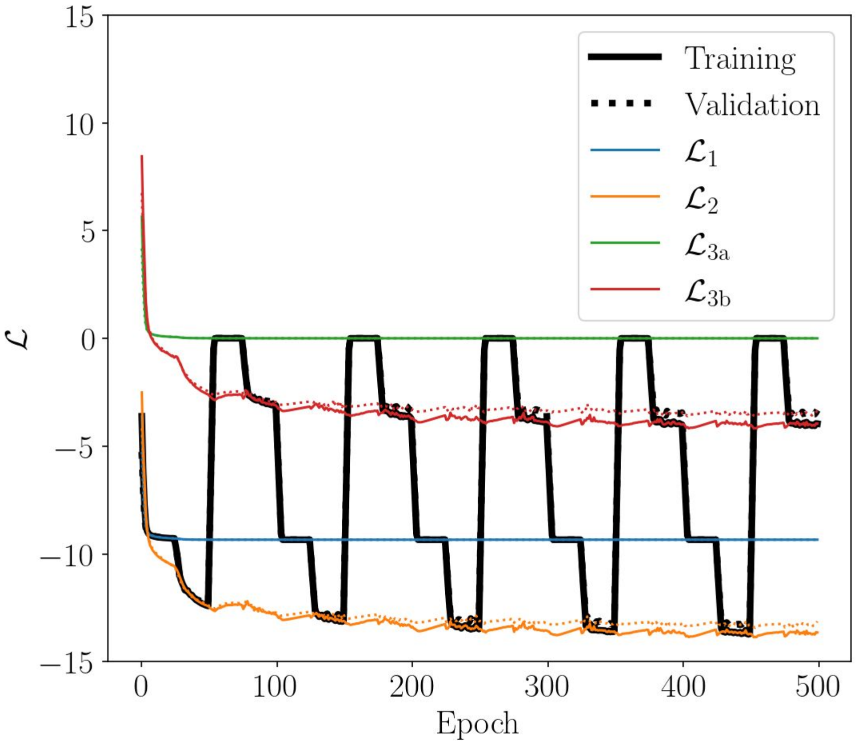
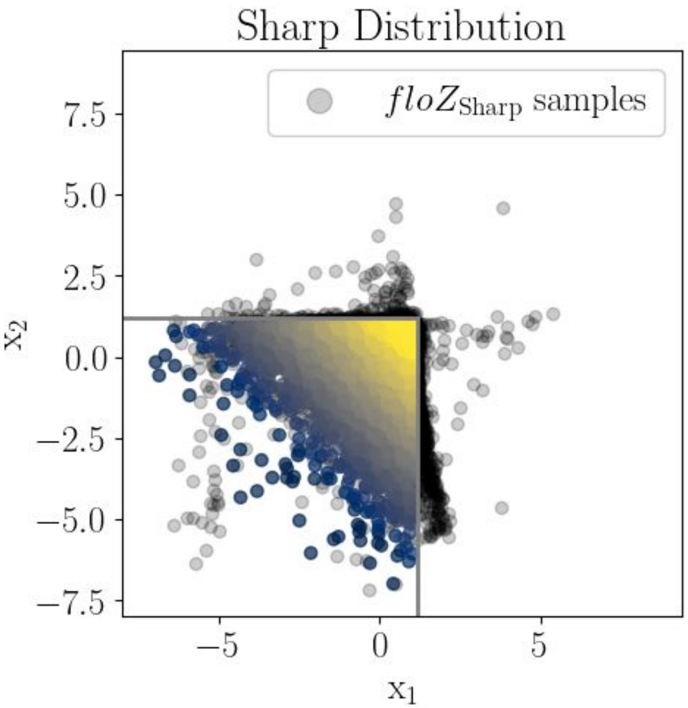
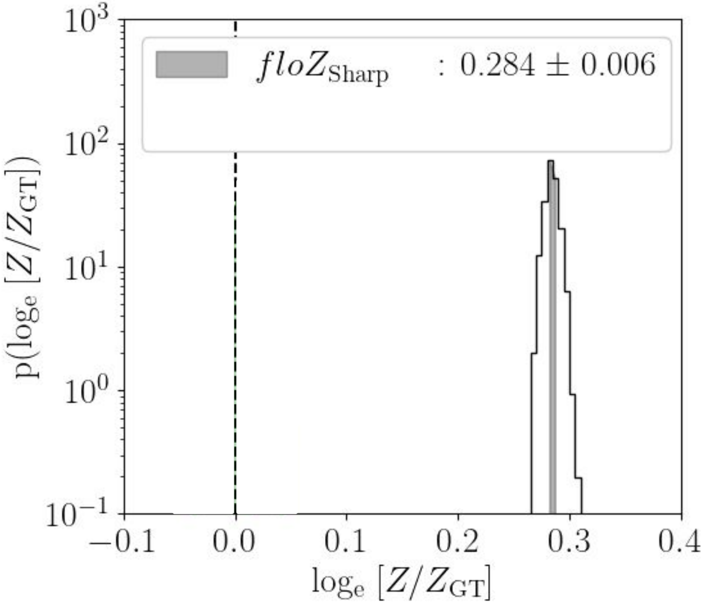


Implementation:

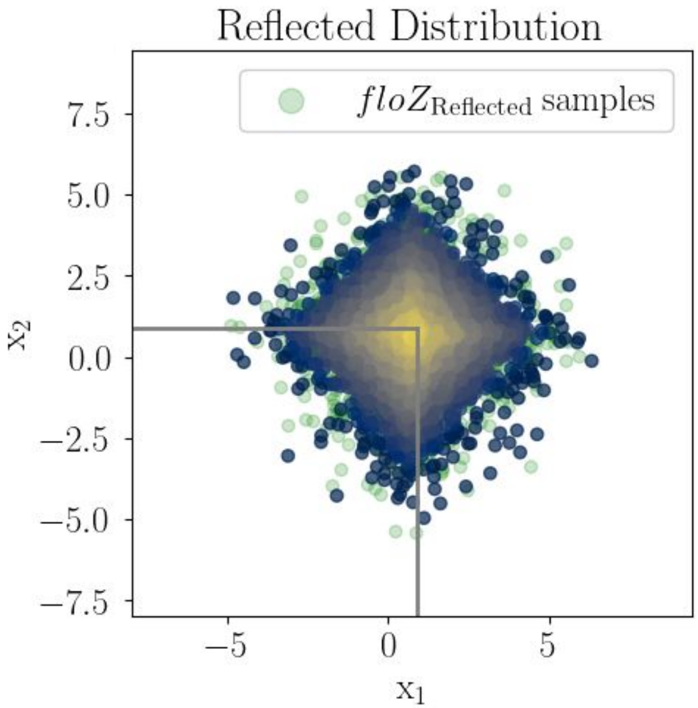
Dealing with sharp boundaries

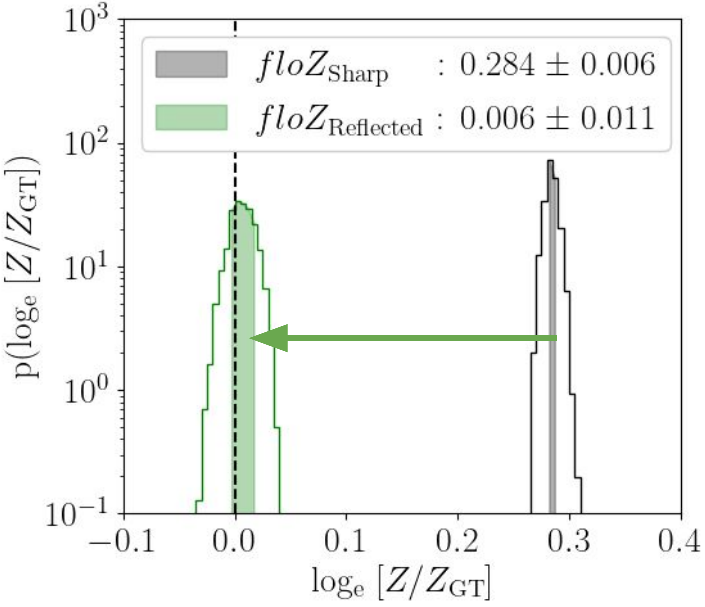




Implementation:

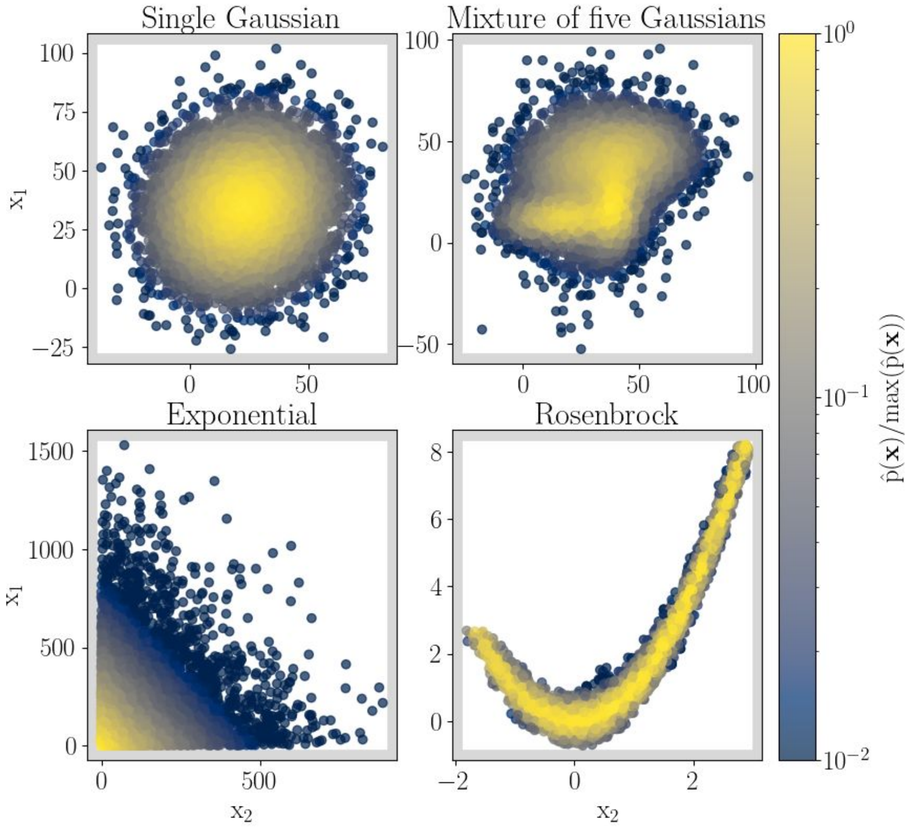
Dealing with sharp boundaries





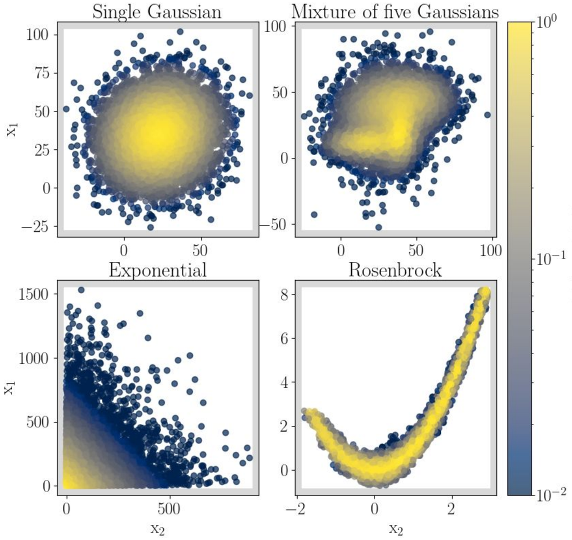
Distributions for benchmarking

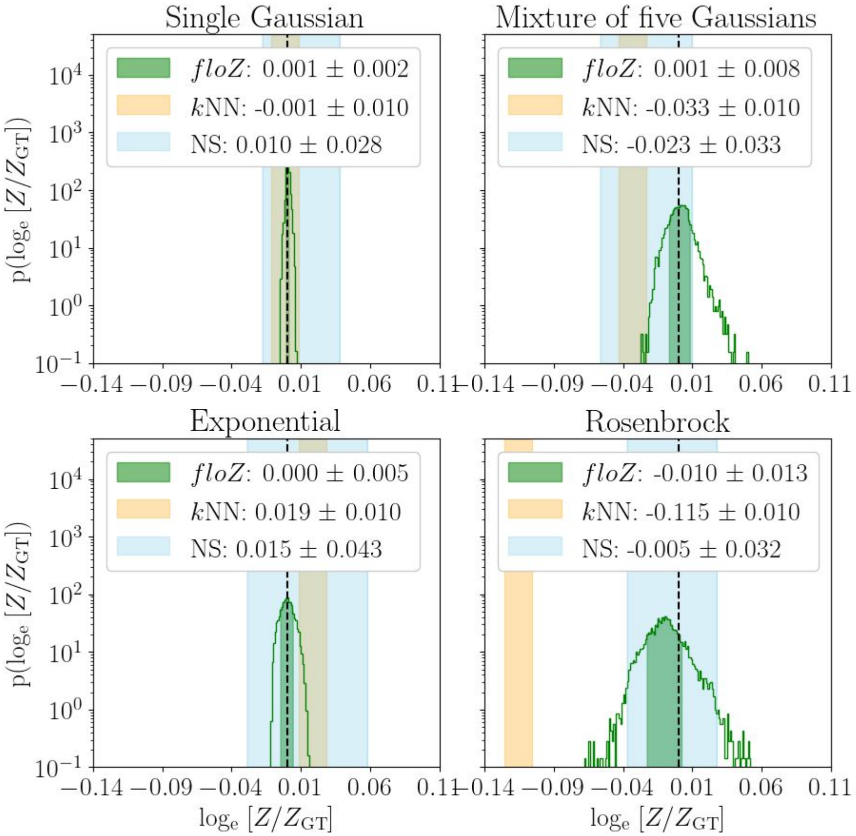
2, 10, 15 dimensions



Benchmarking w/ StateOfTheArt

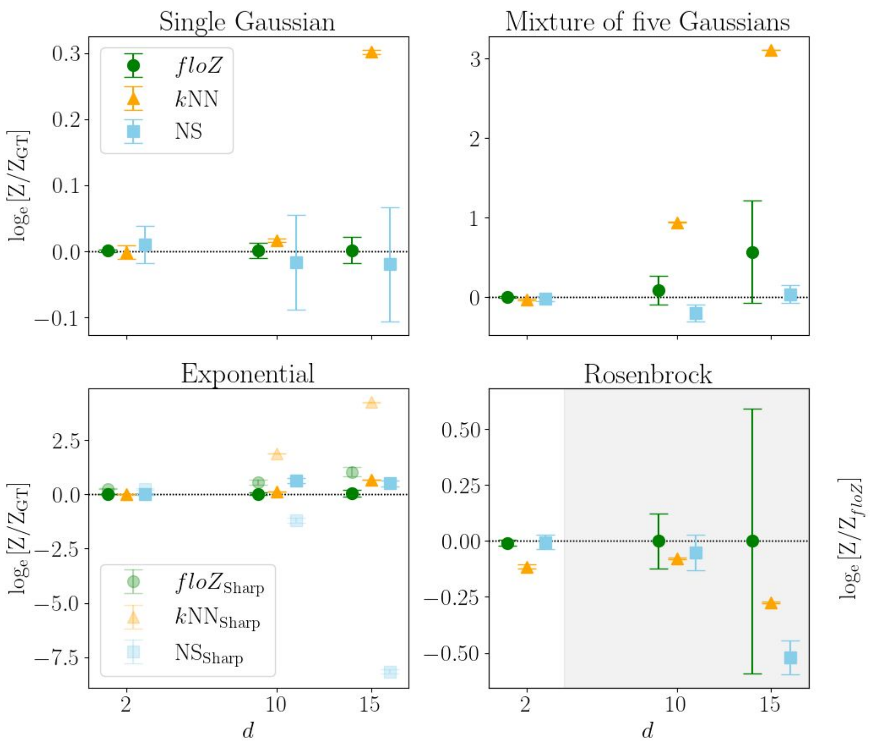
kNN: k-Nearest Neighbours
NS: Nested Sampling





Benchmarking w/ StateOfTheArt

4 Distributions x {2,10,15} Dimensions



- ***Accurate***:

  floZ and NS are in good agreement.

  Outperforms *k*NN

- ***Scalable***:

  15d require no more than 10^5 samples.

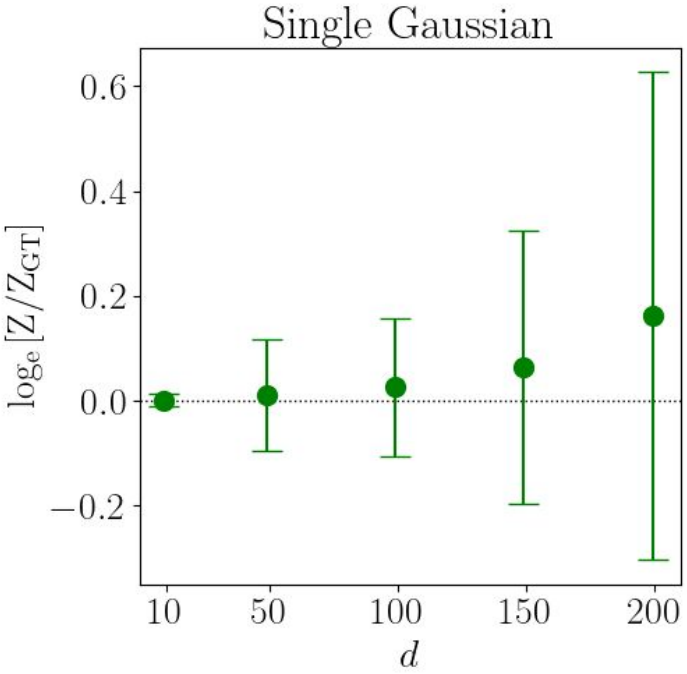
- **Rapid**

  15d results of ***floZ*** obtained in ~ 20min on an A100 GPU

High dimensional scalability

For the same number of samples (10^5) & model complexity.

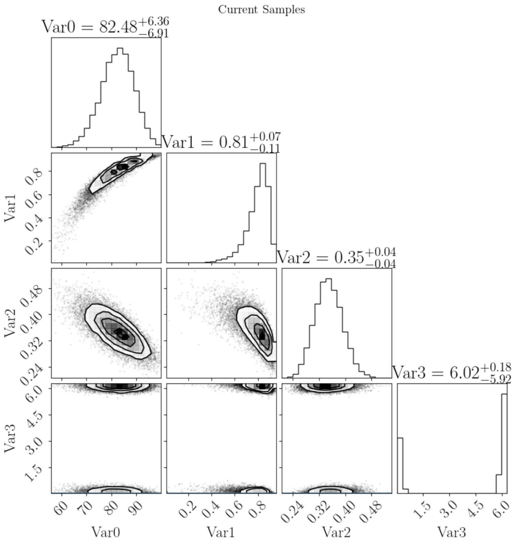
* For complex distributions, we need a combination of more samples, longer training time, and deeper networks.

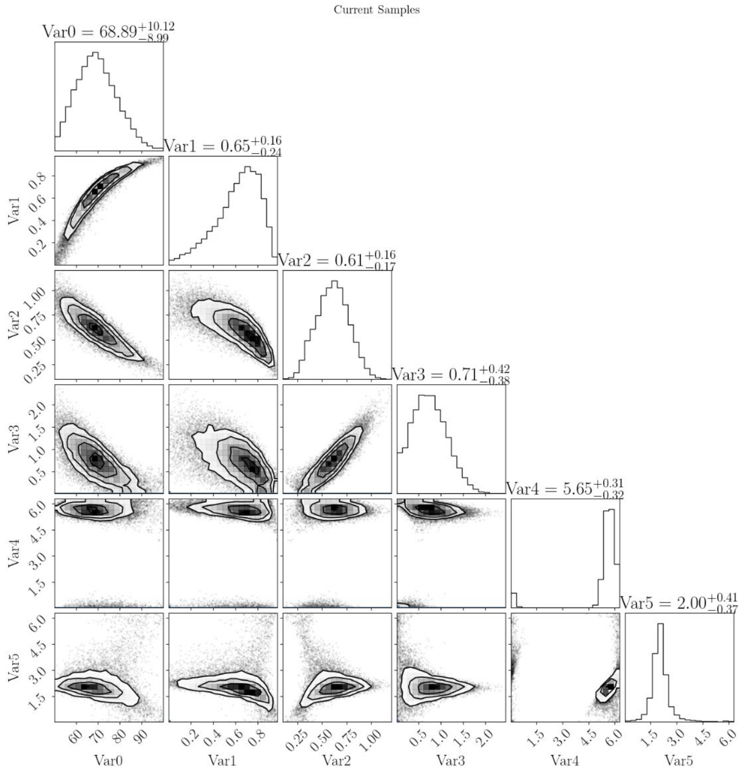


Applications: GW Ringdown

Bayes factor in favor of the presence of the higher 221 overtone in GW150914

Fundamental Mode vs Fundamental Mode w/ Overtone





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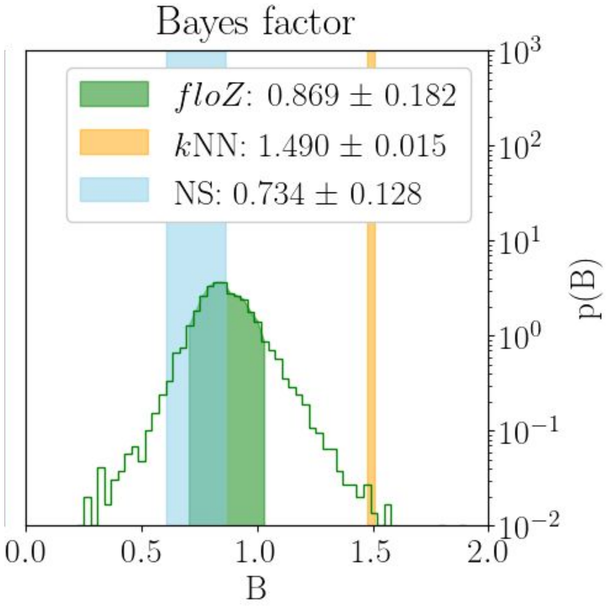
floZ estimates is compatible with nested sampling within their 1σ uncertainties.

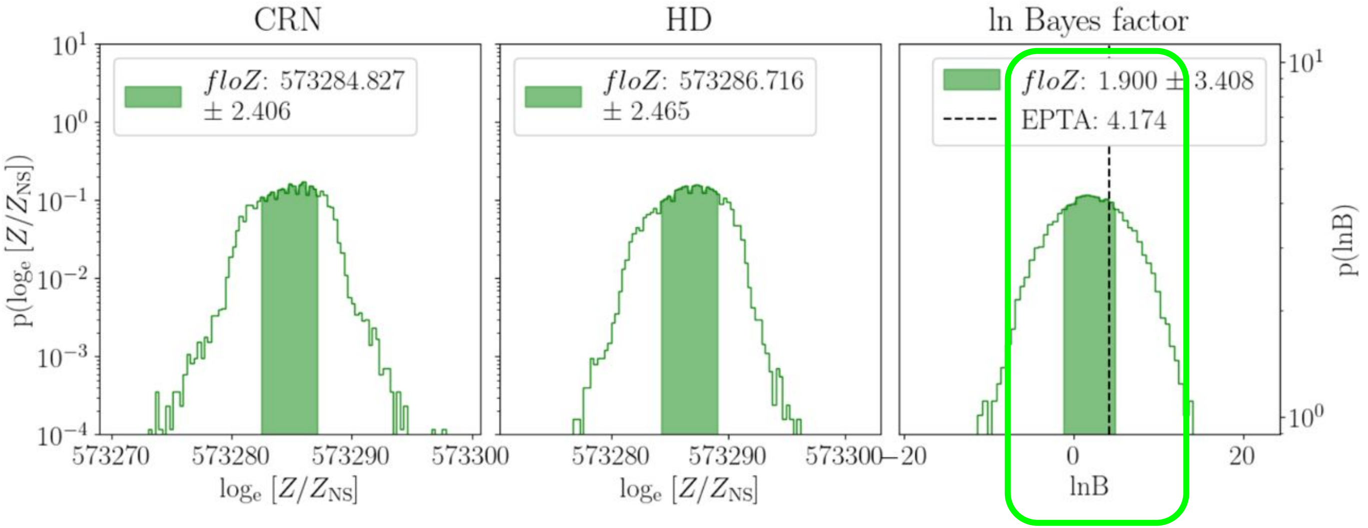


Applications: Pulsar Timing Array

Bayes factor in favor of the presence of Hellings-Downs relation in EPTA data

70 dimensional samples, with **1e5 samples**.

Compatible with EPTA within the 1σ.
Very non-gaussian distribution → **Need more samples** (ongoing analysis)



Samples provided by the EPTA collaboration

Convergence Test

How do we know that the flow is correct?

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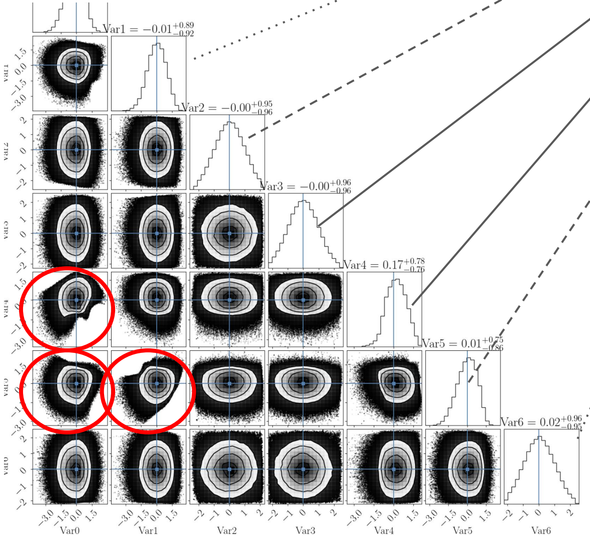
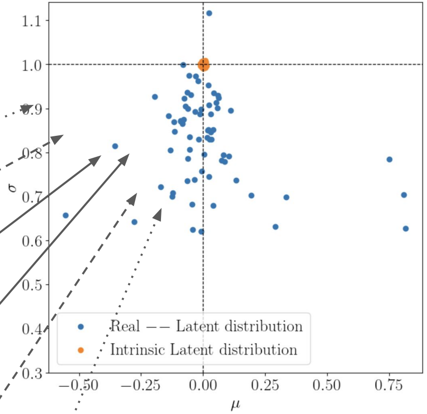
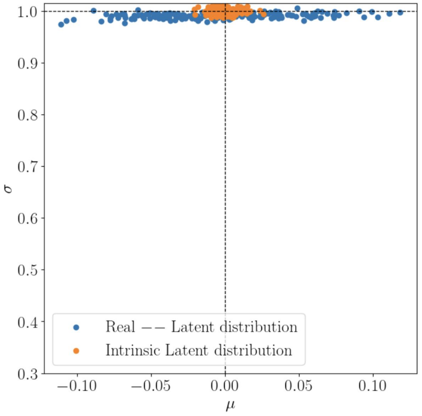
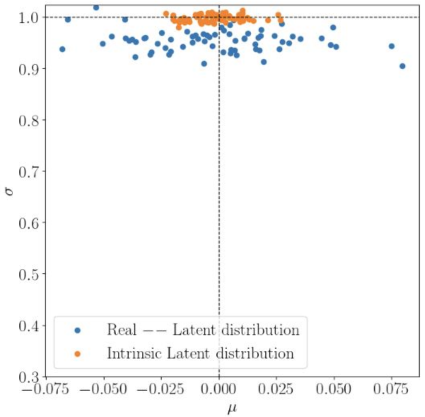
μ - σ plot

Mapping to Latent space should be a gaussian









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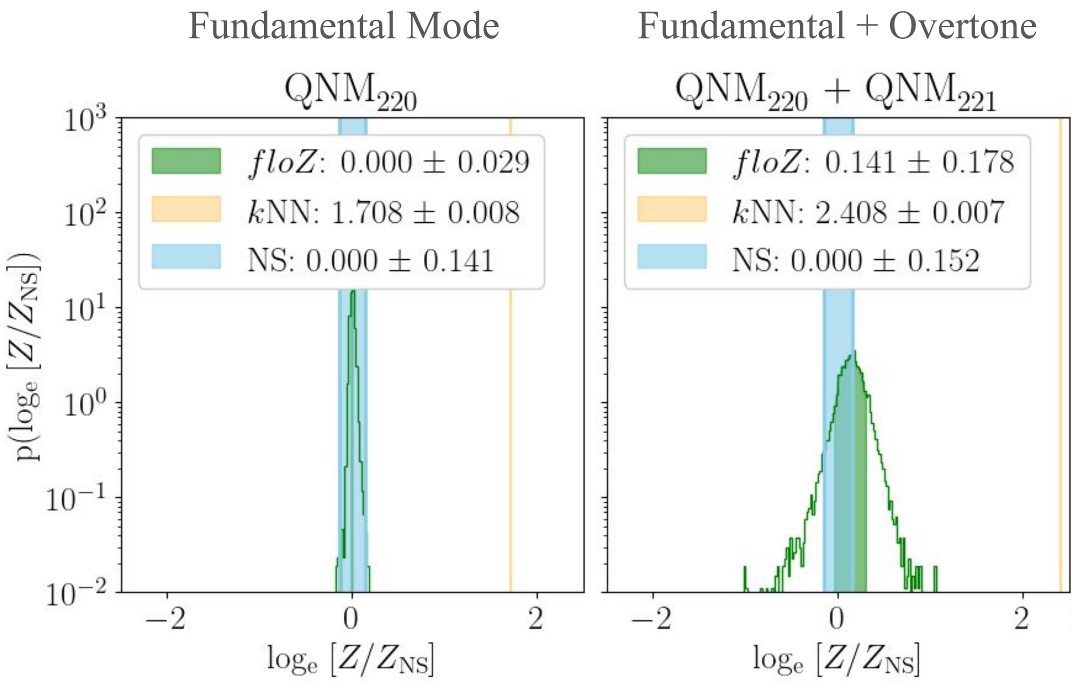

Samples from a nested sampler: CPNest [1]

1. W. Del Pozzo and J. Veitch, “CPNest: Parallel nested sampling.” Astrophysics source code library, record ascl:2205.021, May, 2022.

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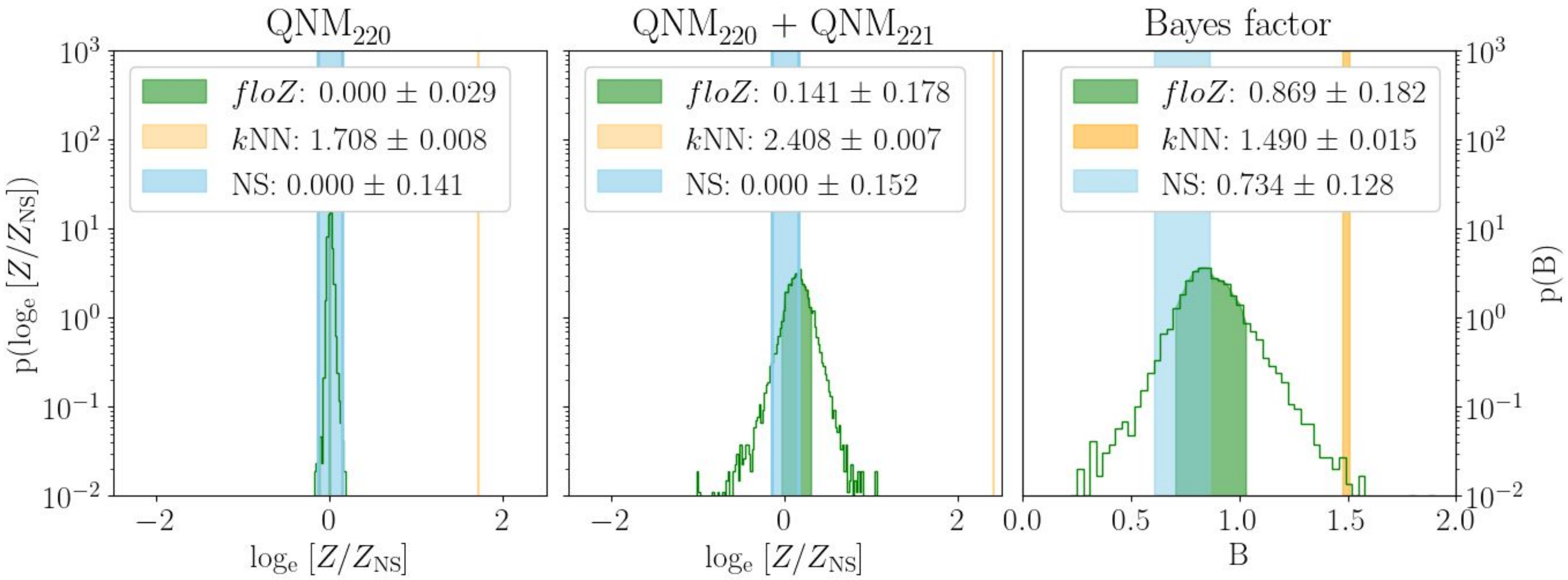

Alternatives?

Reweighting by fraction of outliers