The DNNLikelihood framework

4th ATLAS Machine Learning
Workshop – Public Session

11 November 2019

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Based on arxiv: 1911:03305 [hep-ph]

The DNNLikelihood: enhancing likelihood distribution with Deep Learning

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The Likelihood function

The Likelihood function is a central object in statistical inference

Bayes Theorem:

$$\mathcal{P}(\text{data}|\text{pars})\mathcal{P}(\text{pars}) = \mathcal{P}(\text{pars}|\text{data})\mathcal{P}(\text{data})$$

Likelihood function — Prior probability — Posterior probability — Bayesian evidence

Frequentist inference

e.g. Maximum Likelihood Estimation (MLE)

Pros:

- Does not require assumptions on the a-priori distribution of parameters
- Neyman-Pearson likelihood ratio
- Asymptotic formulae

Cons:

- Violates Likelihood principle
- Difficult (conceptually) to deal with nuisance parameters
- Coverage (pseudo-experiments)

Bayesian inference

e.g. Maximum A Posteriori (MAP)

Pros:

- Direct outcome of Bayes theorem
- When prior is known this is “the correct” inference procedure
- Simpler treatment of nuisance pars

Cons:

- Prior almost never known
- No reparametrization invariant uninformative priors

Distributing likelihoods

Different approaches (and frameworks) in presenting and distributing experimental information

Examples are:

1. Present just the results of the analysis (this was the approach until recent years)
2. Cross section measurements with uncertainties and possibly correlations
3. Measurements in (possibly uncorrelated) bins for several different signal regions, as, for instance Higgs Simplified Template Cross Sections (STXS)
4. Simplified Likelihood: parametrize the likelihood in terms of "combined" nuisance parameters using Gaussian approximation up to 3rd moment
5. HistFactory framework (ATLAS): this is going towards publishing all information that allows to reconstruct the full likelihood

Our approach: encode the full likelihood with all the dependence on elementary nuisance parameters into a DNN predictor. This allows for:

1. Encoding also unbinned likelihoods (especially, but not only, used in Flavor physics)
2. Re-sampling with custom priors to study the impact of different hypotheses on systematic unc.
3. Efficient combination of different likelihoods (when correlations are known)
4. Interpretation of results within different statistical approaches (Frequentist vs Bayesian)
5. Simple framework independent distribution through the ONNX format (this allows inference in any software environment (Python, R, Matlab, Mathematica, etc..)

A toy LHC-like New Physics search

Toy experiment already considered in the literature

Buckley, Citron, Fichet, Kraml, Waltenberger, Wardle, 1809.05548 [hep-ph]

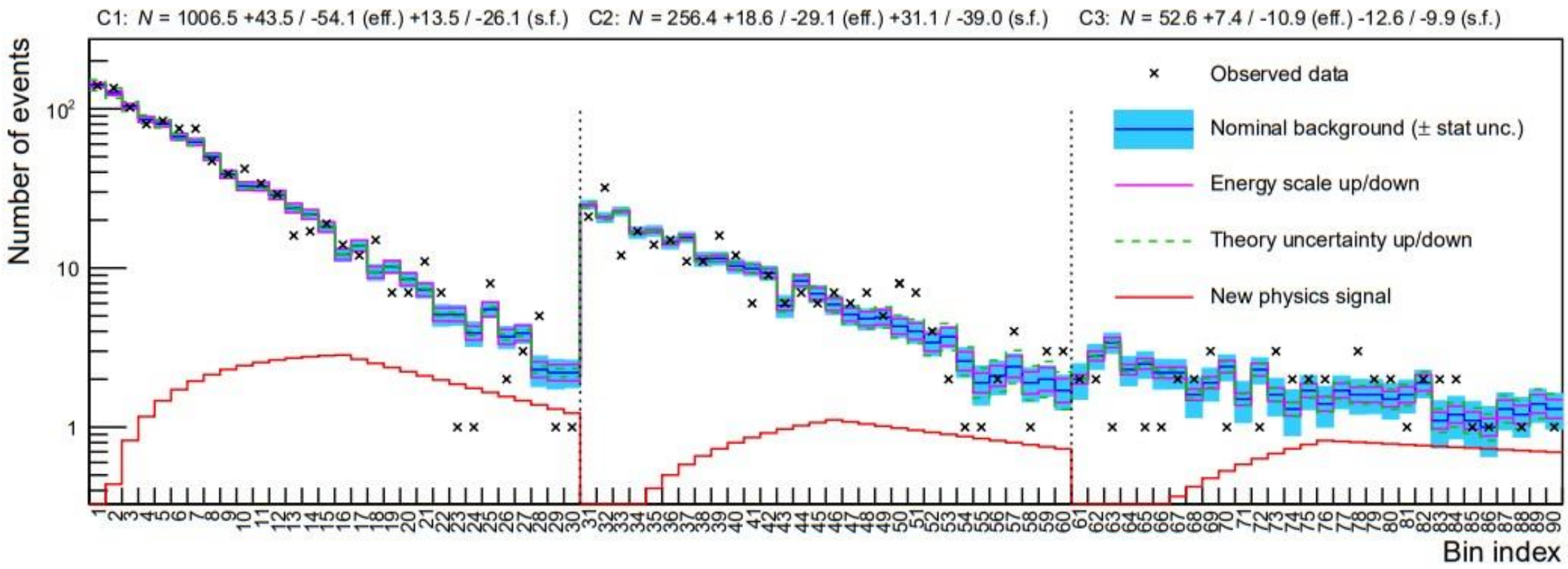


Figure 2. LHC-like search for new physics (mockup). The search is performed across three event categories, each divided into 30 bins to make a total of 90 search regions. The nominal expected contribution in each bin from the background and from the new physics signal is shown by the blue and red lines, respectively. The solid and dashed lines show the $\pm 1\sigma$ correlated variation in each bin expected due to an experimental and theoretical uncertainty while the blue shaded band shows the uncorrelated uncertainty in each bin due to limited MC simulation. The "observed" number of events in data in each bin is indicated by the black points.

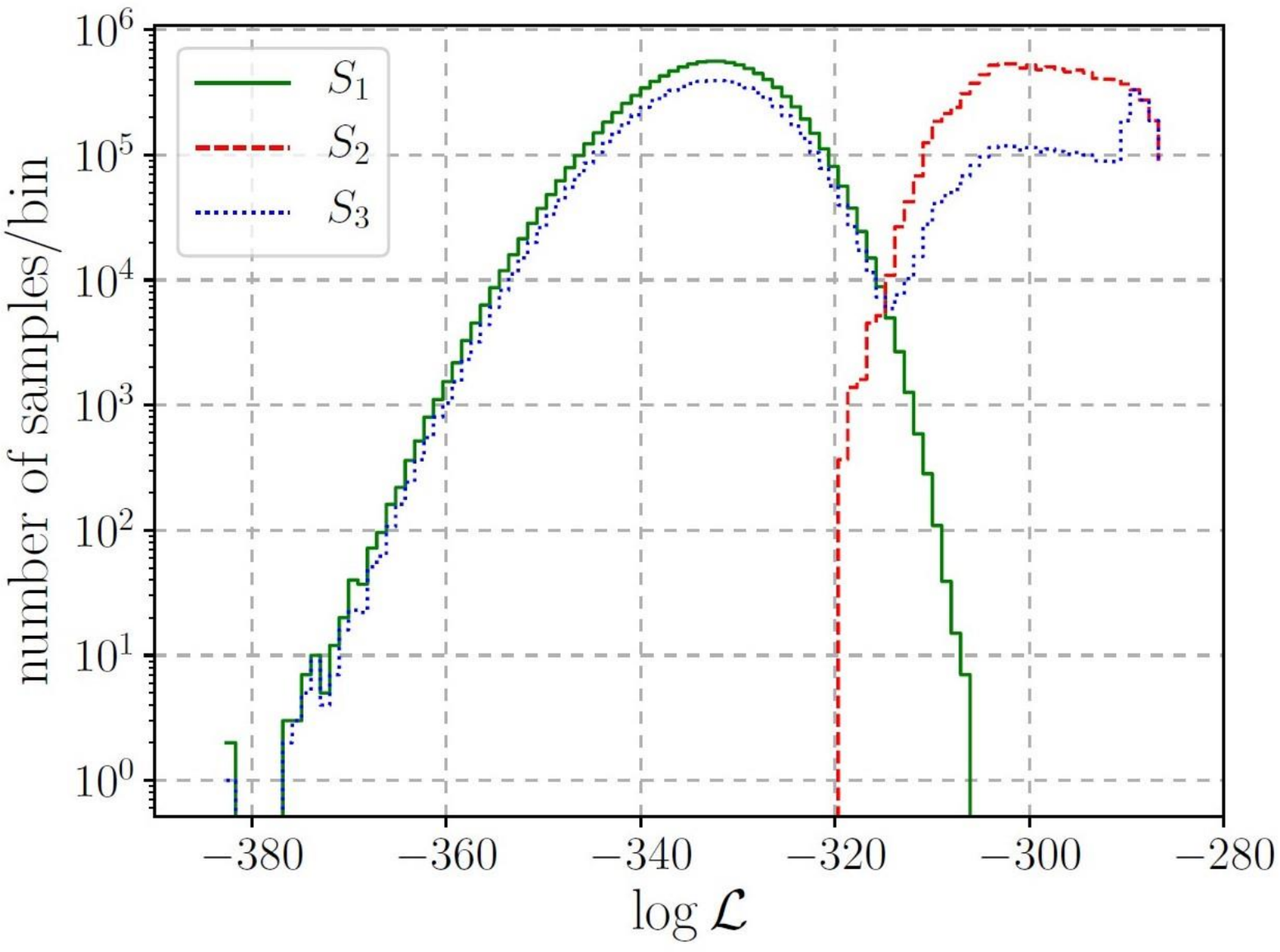
- One physical parameter (signal strength μ)
- 94 nuisance parameters (90 fully uncorrelated, two fully correlated, two normalizations)
- Non Gaussian (and not satisfying Wilks' hypotheses!)

Sampling

Supervised learning problem (interpolation) where high precision is needed

If we want to allow for both Frequentist and Bayesian inference, we need to know the LF well in very different regions (where prior volume is large and close to local maxima of the LF)

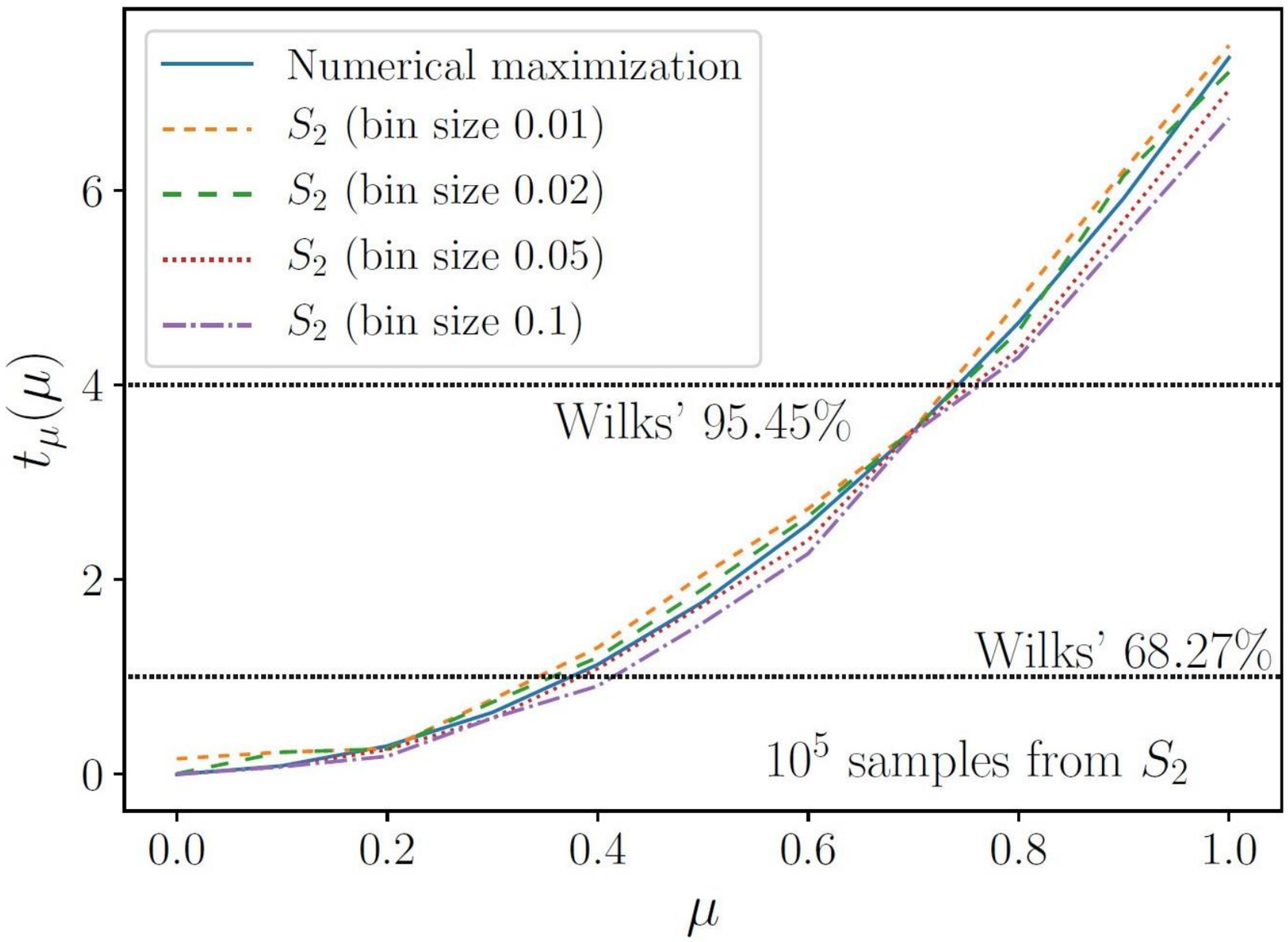
We sample with the emcee3 (ensemble sampling method) Python package (checking convergence with several different techniques)



Inference: Frequentist

For frequentist inference we construct the test statistics

$$t_\mu(\mu) = -2\log\frac{\mathcal{L}_{\text{prof}}(\mu)}{\mathcal{L}_{\max}}$$



Inference: Frequentist

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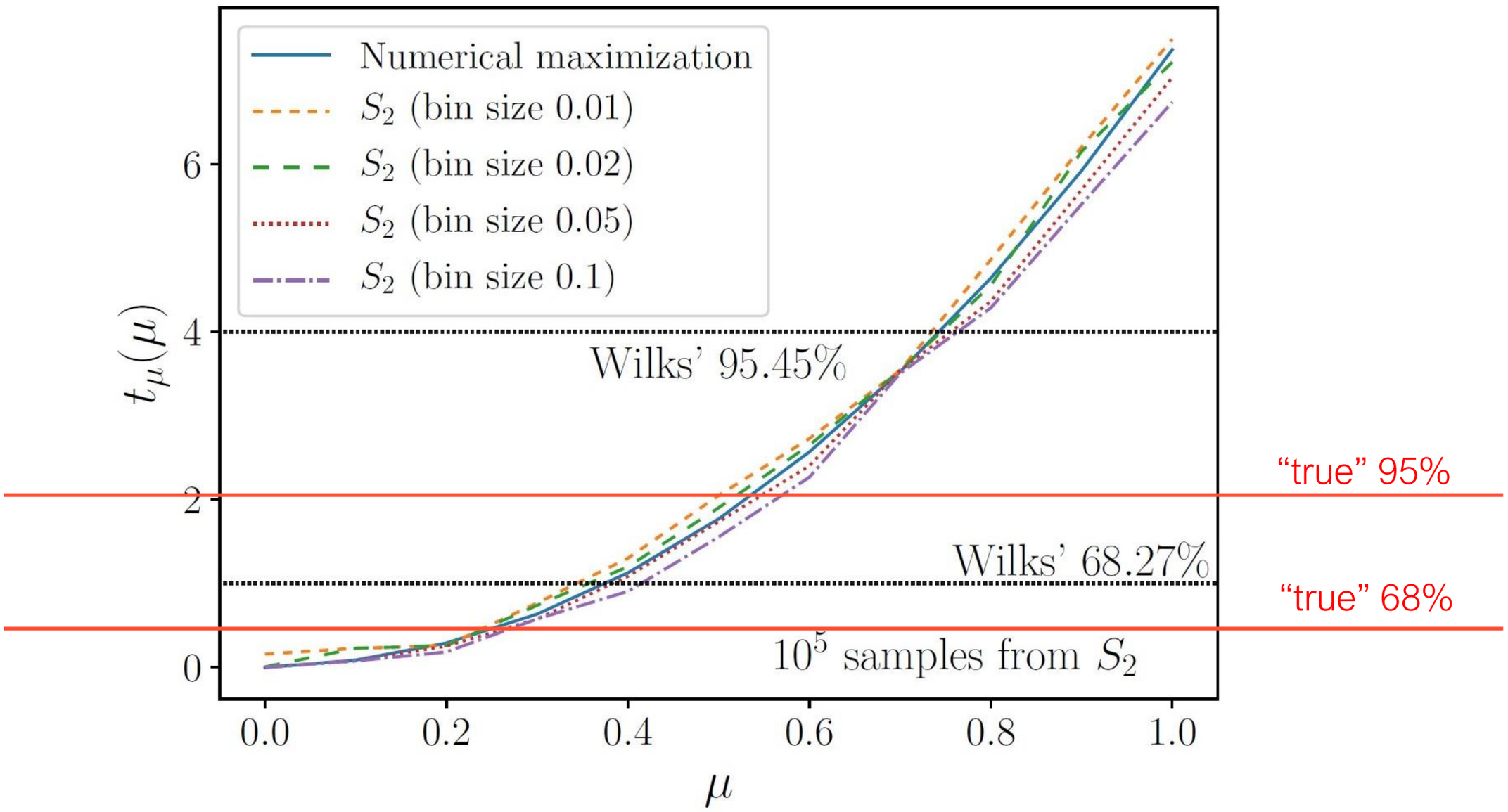
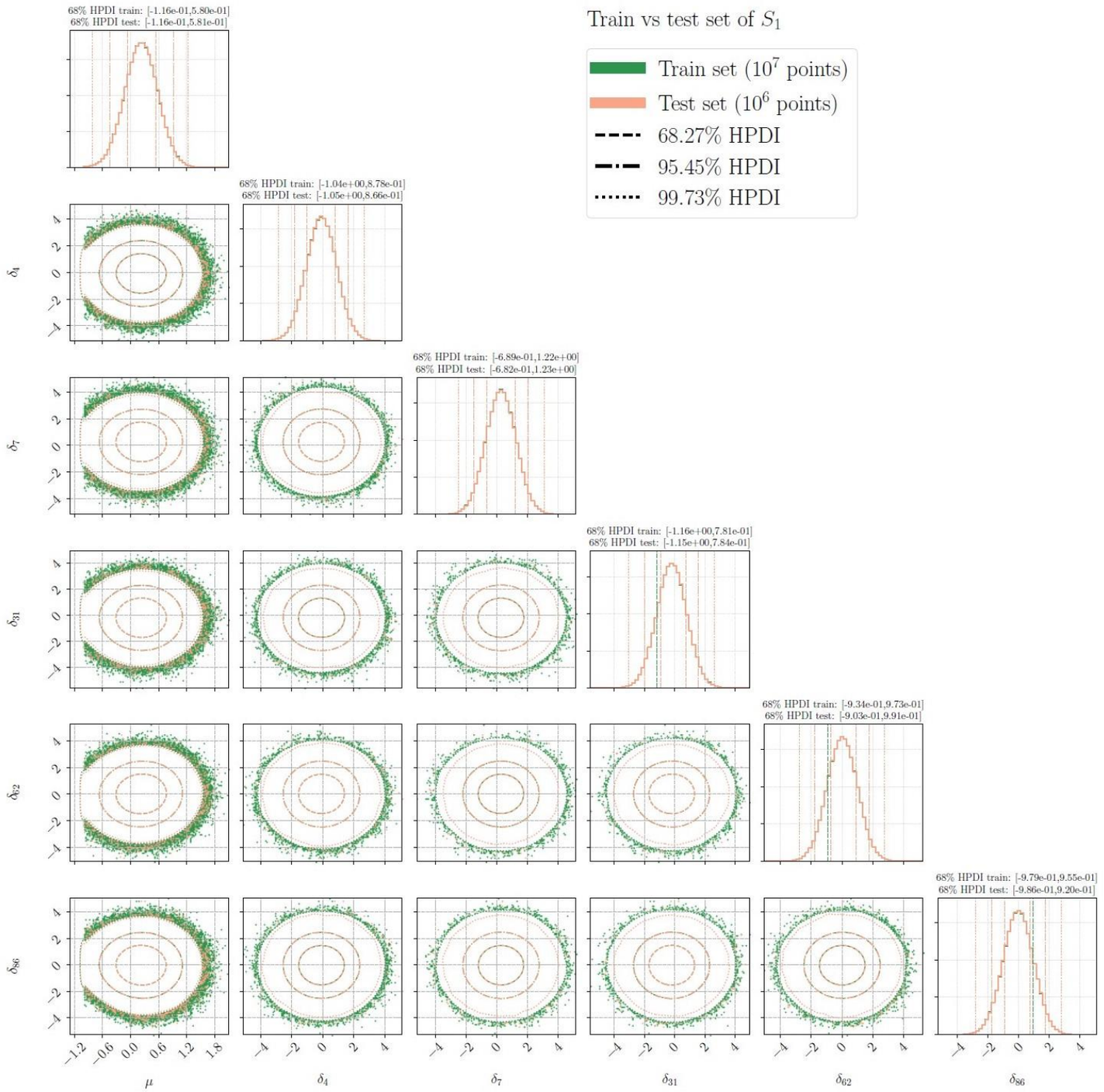
Pay attention with asymptotic statistics!



Inference: Bayesian

Bayesian inference is based on (marginal) posterior probability distributions

We quote results as marginalized Highest Posterior Density Intervals (HPDI)



HPDI	$\mu > -1$	$\mu > 0$
68.27%	$[-0.12, 0.58]$	0.48
95.45%	$[-0.47, 0.92]$	0.86
99.73%	$[-0.82, 1.26]$	1.22

The DNNLikelihood

We build and train a simple MLP model with Keras+TensorFlow with the following configurations (after a long phase of optimization):

- **Size of training set:** we consider 100K, 200K,and 500K training sets
- **Loss function:** mean squared error (mse)
- **Number of hidden layers:** usually 2 are enough, more complex problems can need more layers
- **Number of nodes per layer:** we consider 500, 1000, 2000, and 5000 nodes per layer
- **Activation functions:** Scaled Exponential Linear Unit (SELU)
- **Batch size:** we keep fixed the number of batches to around 200, and therefore vary batch size with training sample size: 512, 1024, 2048
- **Optimizer:** Adam with starting Learning Rate 0.001. Learning rate is decreased by a factor 0.2 every 40 epochs with no improvement in the validation loss within a tolerance of 1/N with N number of training events
- **Regularizer:** we do not need regularization! We cannot overfit, since we are doing interpolation and not regression. We just use early stopping to shorten training time. We stop after 48 epochs with no improvement in validation loss within a tolerance of 1/N with N number of training events
- **Ensembling:** for each architecture we train 5 identical models with randomly extracted training sets and take the best one to show results. We have experimented ensemble techniques, such as stacking, which are very promising but were not needed in this “relatively simple” case

The DNNLikelihood

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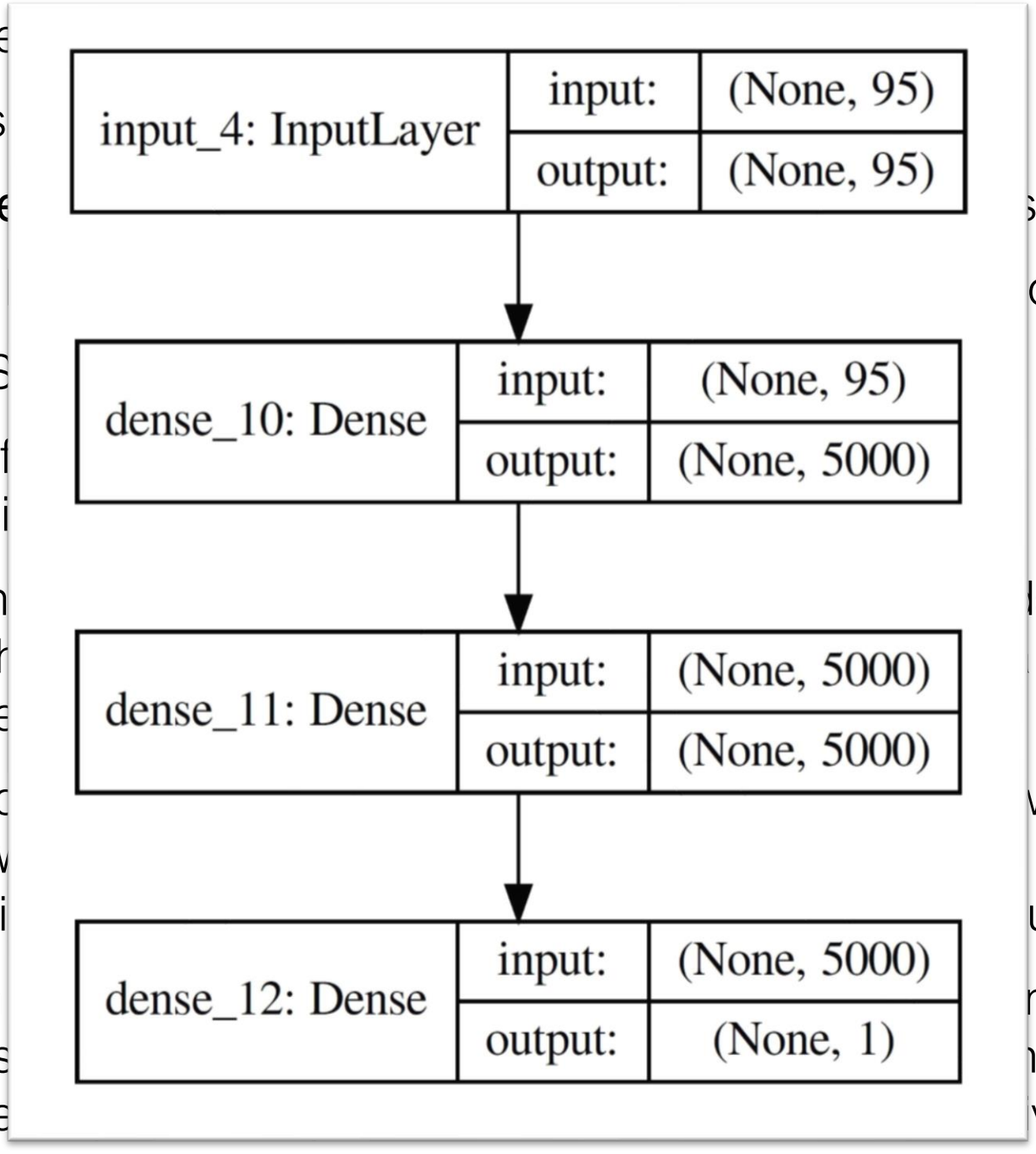
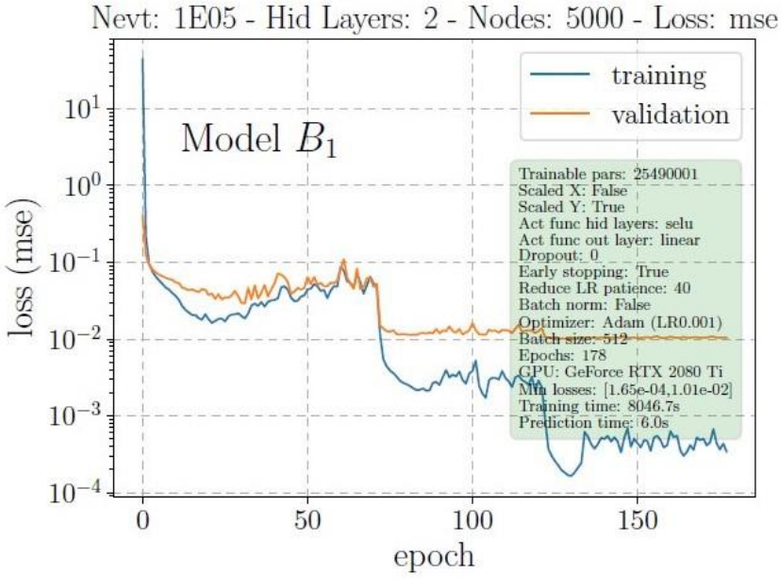
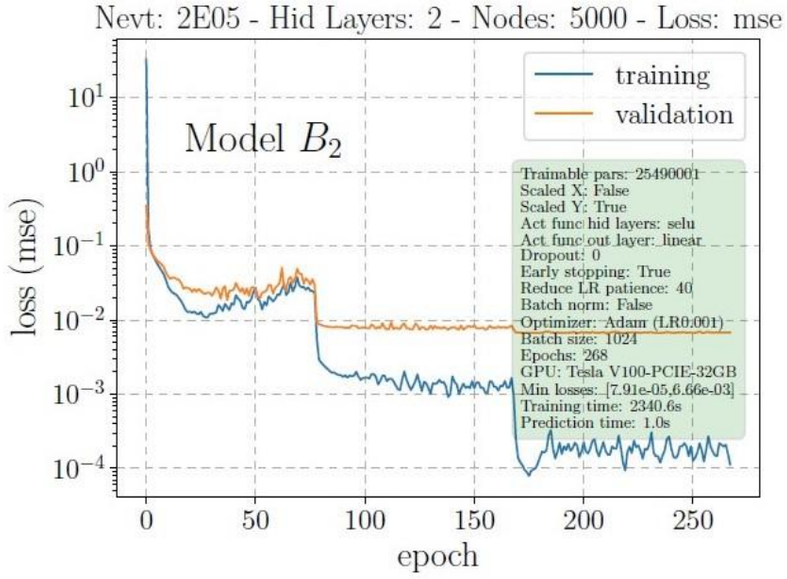
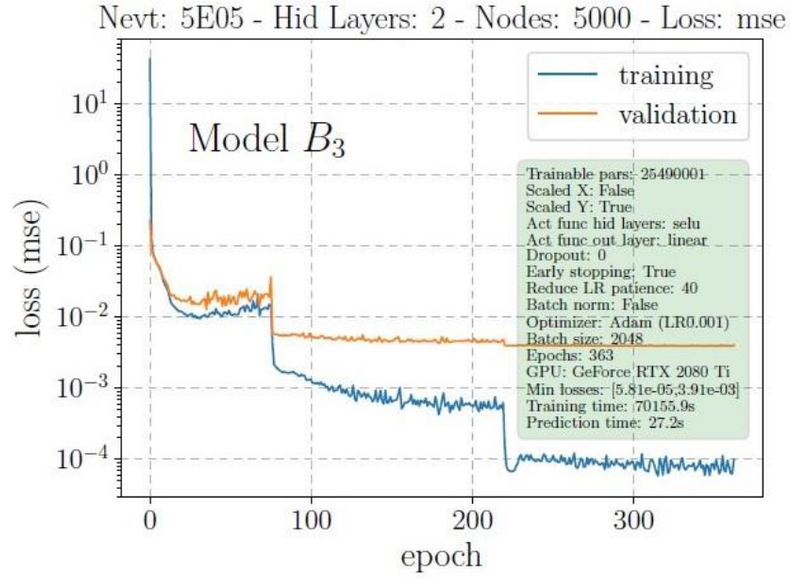


Results: Bayesian DNNLikelihood

Train with unbiased sampling S1







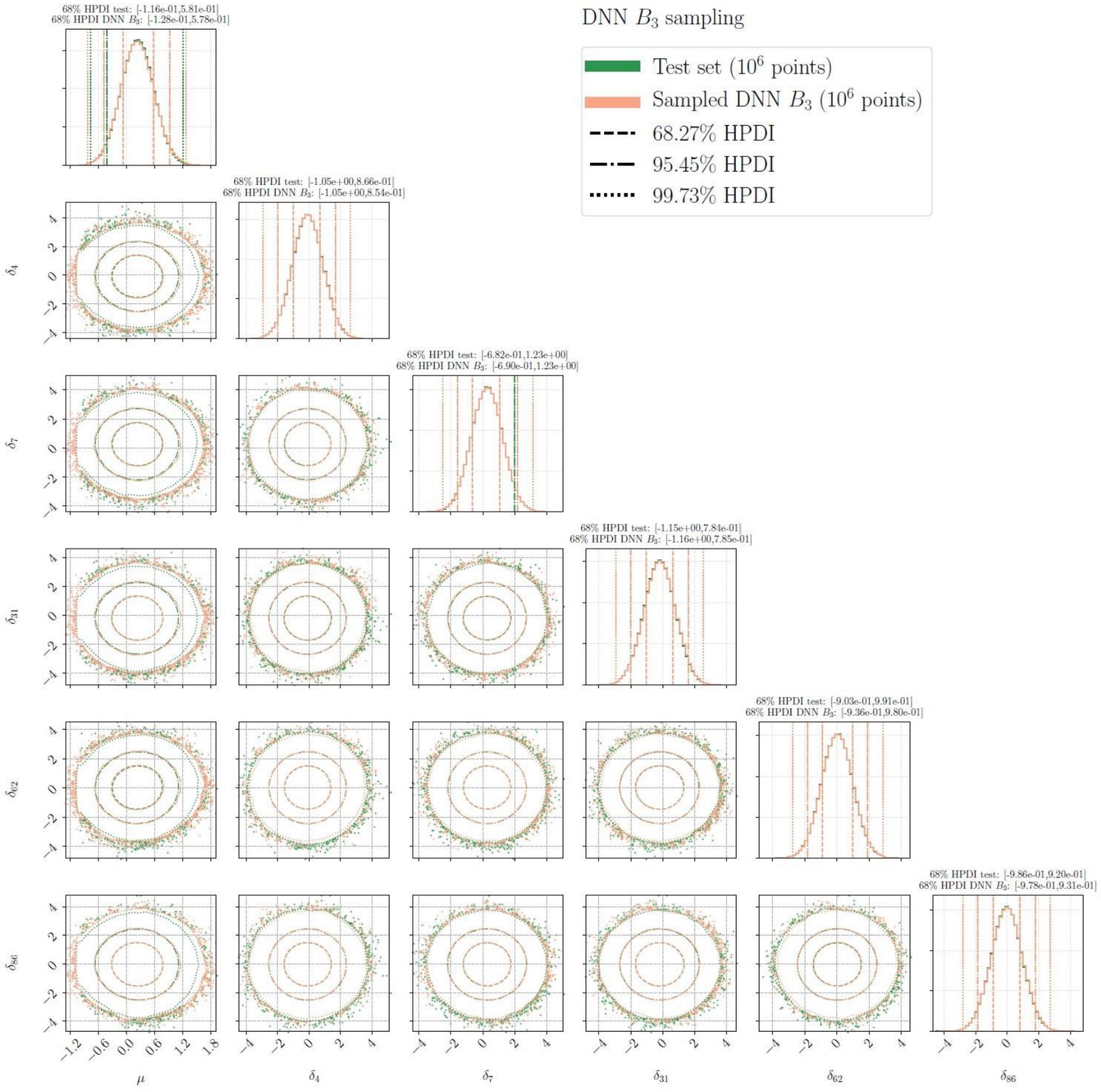
Metrics

Name	B_1	B_2	B_3
Sample size ($\times 10^5$)	1	2	5
Epochs	178	268	363
Loss train (MSE) ($\times 10^{-3}$)	0.14	0.088	0.054
Loss val (MSE) ($\times 10^{-3}$)	10.11	6.66	3.9
Loss test (MSE) ($\times 10^{-3}$)	10.02	6.64	3.9
ME train ($\times 10^{-3}$)	0.47	0.53	0.28
ME val ($\times 10^{-3}$)	5.44	2.58	1.76
ME test ($\times 10^{-3}$)	4.91	2.31	1.72
Median p-value of 1D K-S test vs pred. on train	0.41	0.46	0.39
Median p-value of 1D K-S test vs. pred. on val.	0.24	0.33	0.43
Median p-value of 1D K-S val vs. pred. on test	0.24	0.40	0.34
Training time (s)	1007	2341	8446
Prediction time (μs/point)	11.5	10.4	14.5

Results

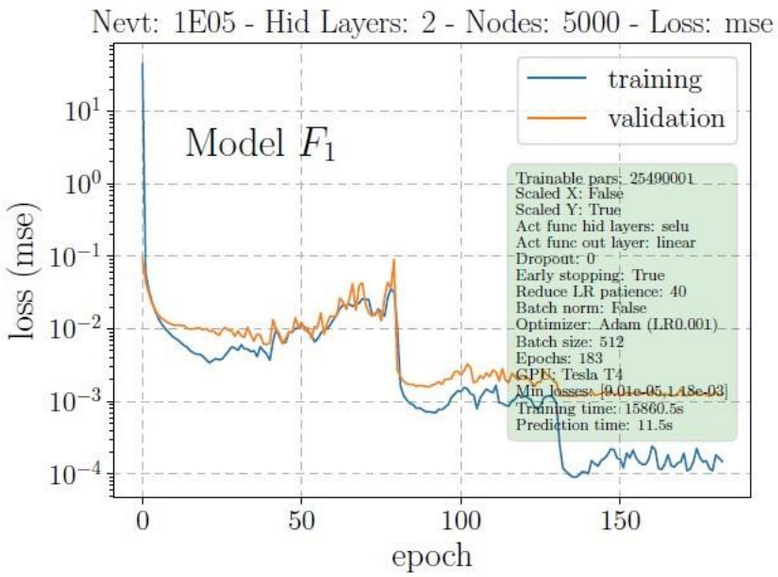
HPDI	$\mu > -1$	$\mu > 0$	B_1	B_2	B_3
68.27%	$[-0.12, 0.58]$	0.48	0.49	0.49	0.49
95.45%	$[-0.47, 0.92]$	0.86	0.92	0.91	0.88
99.73%	$[-0.82, 1.26]$	1.22	1.35	1.34	1.29

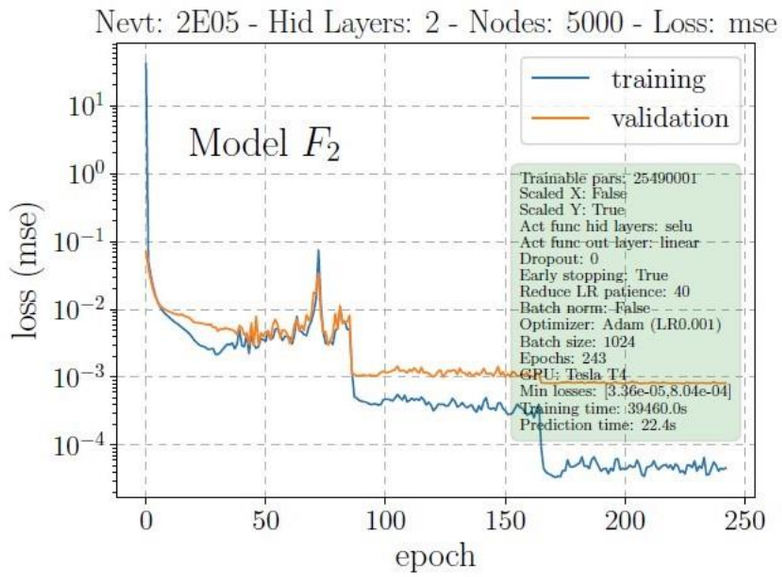
Results: Bayesian DNNLikelihood

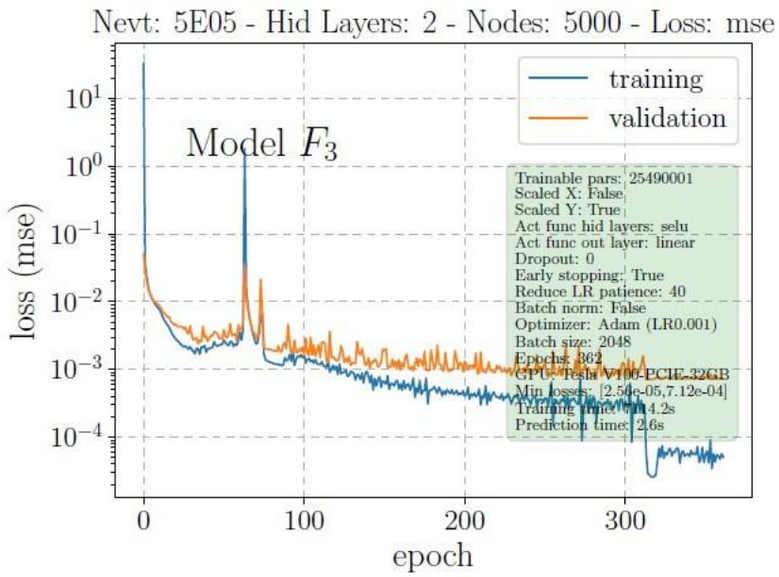


Results: full DNNLikelihood

Train with mixed sampling S3







Metrics

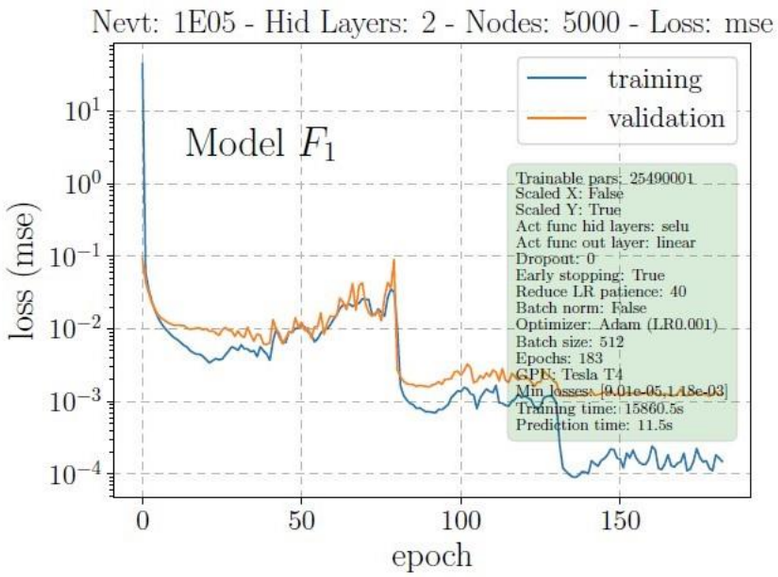
Name	F_1	F_2	F_3
Sample size ($\times 10^5$)	1	2	5
Epochs	183	243	362
Loss train (MSE) ($\times 10^{-3}$)	0.092	0.026	0.030
Loss val (MSE) ($\times 10^{-3}$)	1.18	0.80	0.71
Loss test (MSE) ($\times 10^{-3}$)	1.17	0.80	0.72
ME train ($\times 10^{-3}$)	3.07	0.47	1.1
ME val ($\times 10^{-3}$)	1.78	0.87	0.82
ME test ($\times 10^{-3}$)	1.50	0.68	0.86
Median p-value of 1D K-S test/pred-train	0.53	0.48	0.44
Median p-value of 1D K-S test/pred-val	0.15	0.27	0.20
Median p-value of 1D K-S val/pred-test	0.13	0.31	0.33
Mean error on $t_\mu(\mu)$	0.11	0.12	0.032
Training time (s)	1236	2819	7114
Prediction time (μs/point)	11.1	10.8	10.5

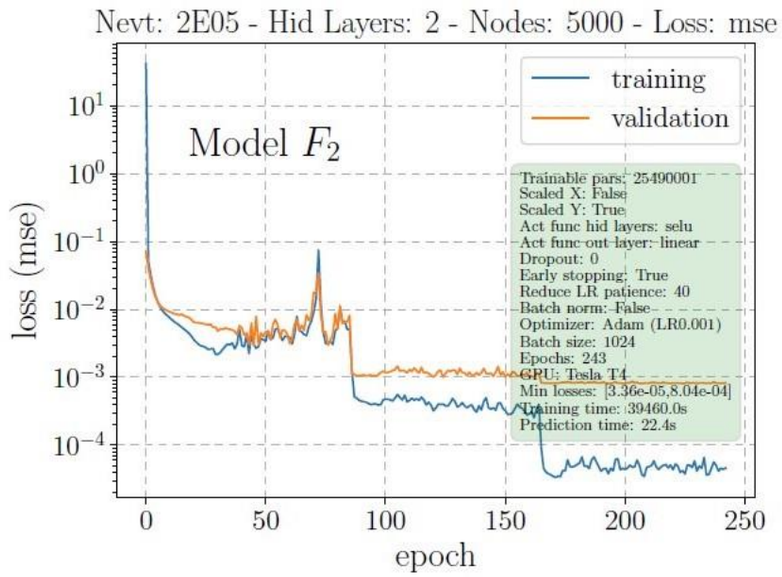
Results

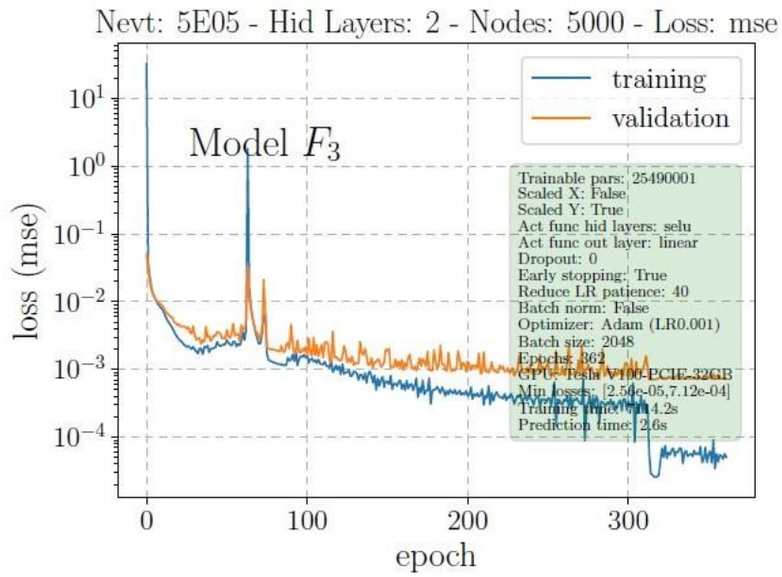
HPDI	$\mu > -1$	$\mu > 0$	F_1	F_2	F_3
68.27%	$[-0.12, 0.58]$	0.48	0.50	0.50	0.48
95.45%	$[-0.47, 0.92]$	0.86	0.93	0.93	0.88
99.73%	$[-0.82, 1.26]$	1.22	1.35	1.37	1.28

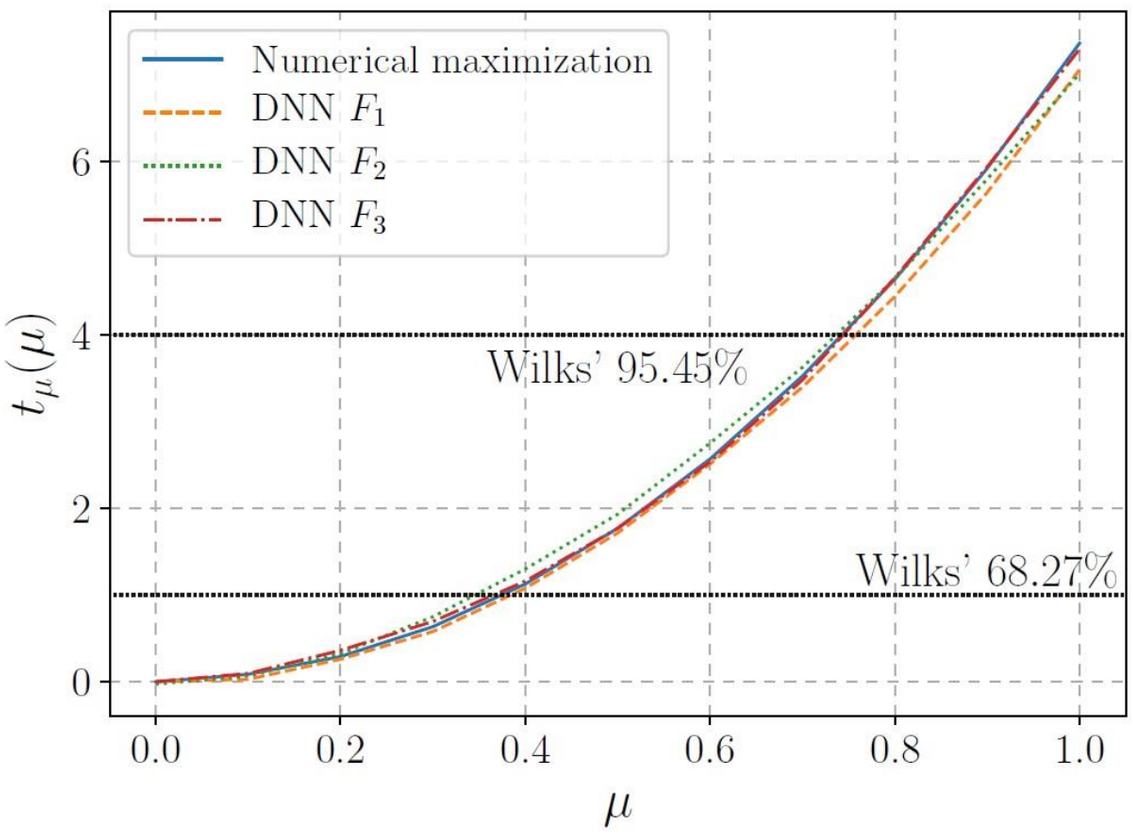
Results: full DNNLikelihood

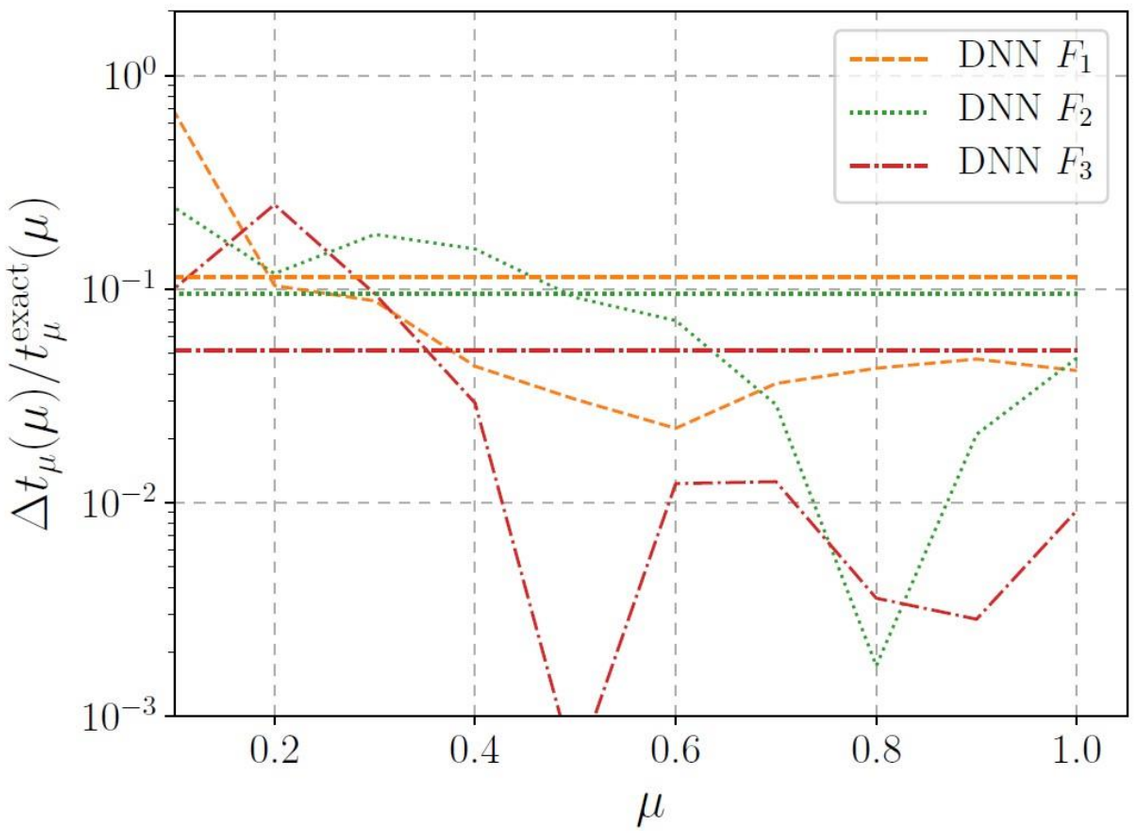
Train with mixed sampling S3











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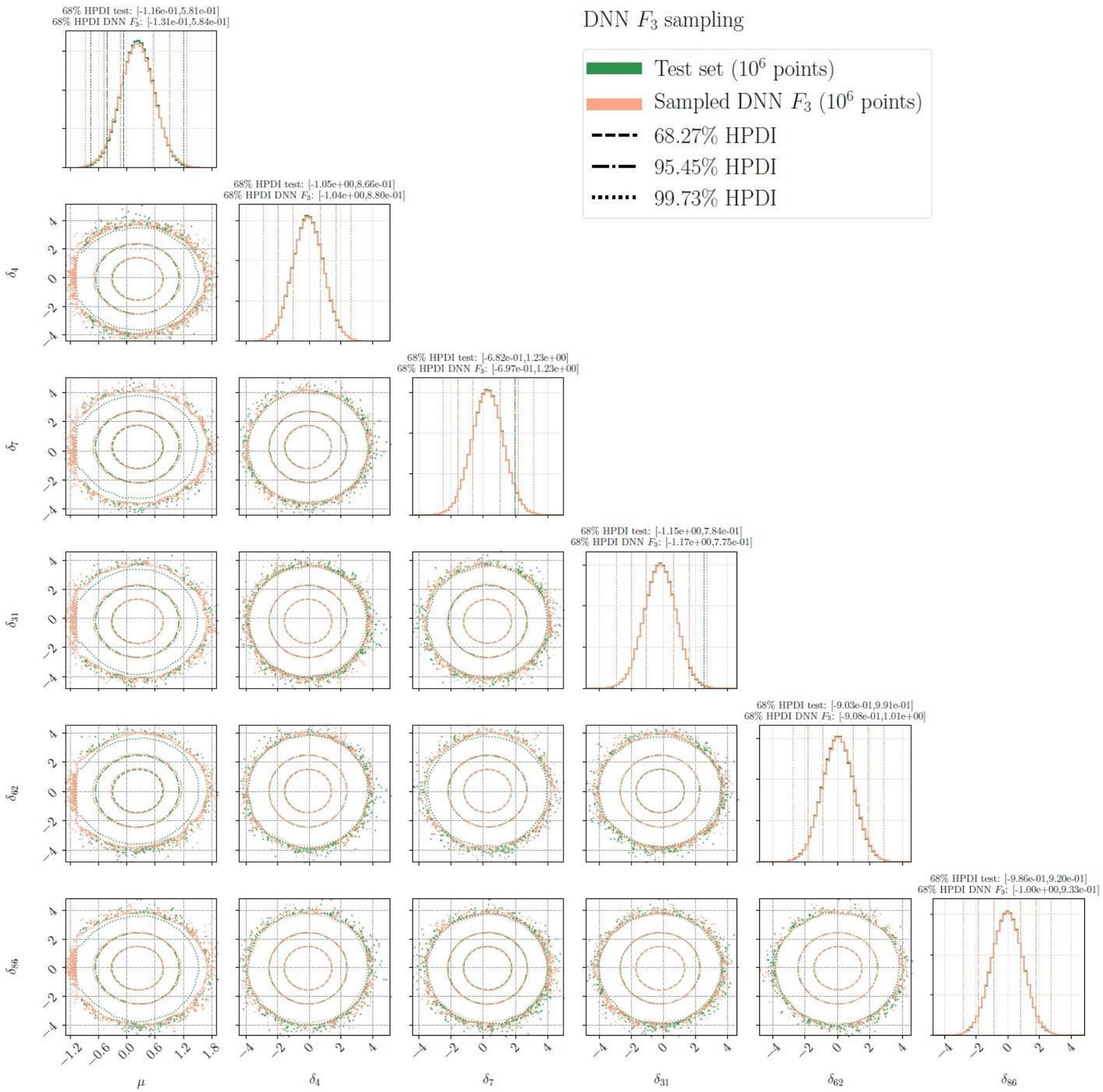

DNN F_3 sampling

- Test set (10^6 points)
- Sampled DNN F_3 (10^6 points)
- 68.27% HPDI
- 95.45% HPDI
- 99.73% HPDI

Conclusions

- We introduced the DNNLikelihood, a framework to encode, distribute, combine, and analyze likelihood functions
- In the realistic example we studied it seems to work extremely well without the need of too much hyperparameters tuning or advanced techniques (which may be necessary for very complicated multimodal function)
- All code used to produce the paper and all results are available on GitHub
- Together with the models our code always produces many auxiliary files keeping track of all parameters, metrics, results, etc. so that each model is carefully self documented
- We are preparing a more comprehensive Python module that will allow to sample likelihoods, build models (and ensembles of models), optimize, and analyze the results within different statistical frameworks. It is now in the phase of testing and we plan to release it by the end of the year
- Future plans are to present a few more example for real likelihoods (HepFit, Flavor)
- We got in touch with Zenodo group to identify the best strategy to store results on Zenodo

THANK YOU!