Parameters Estimation for the Cosmic Microwave Background with Bayesian Neural Networks

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In this paper, we present the first study that compares different models of Bayesian Neural Networks (BNNs) to predict the posterior distribution of the cosmological parameters directly from the Cosmic Microwave Background (CMB) map. We focus our analysis on four different methods to sample the weights of the network during training: Dropout, DropConnect, Reparameterization Trick (RT), and Flipout. We find that Flipout outperforms all other methods regardless of the architecture used, and provides tighter constraints for the cosmological parameters. Additionally, we describe existing strategies for calibrating the networks and propose new ones. We show how tuning the regularization parameter for the scale of the approximate posterior on the weights in Flipout and RT we can produce unbiased and reliable uncertainty estimates, i.e., the regularizer acts as a hyper parameter analogous to the dropout rate in Dropout. The best performances are nevertheless achieved with a more convenient method, in which the network is let free during training to achieve the best uncalibrated performances, and the confidence intervals are then calibrated in a subsequent phase. Furthermore, we claim that the correct calibration of these networks does not change the behavior for the epistemic and aleatoric uncertainties provided for BNNs when the training dataset size changes. The results reported in the paper can be extended to other cosmological datasets in order to estimate confidence regions for features that can be extracted directly from the raw data, such as non-Gaussianity signals or foreground emissions.

I. INTRODUCTION

The Cosmic Microwave Background (CMB) is by far one of the most powerful datasets available in cosmology for understanding the Universe [1, 2]. Measurements within the last decade have yielded strong support of the standard cosmological spatially-flat ΛCDM model and provided precise estimates for its cosmological parameters [3–5]. This base model is described by six parameters divided into two groups: the primordial given by \((n_s, A_s)\) that describe the initial state of perturbations produced by quantum fluctuation during inflation, and the late-time group formed by \((\omega_c, \omega_b, \tau, \theta_{MC})\) which trace the linear evolution of perturbations after reentering the Hubble radius [6, 7]. In addition to the standard cosmological model, other parameters might provide a wealth of new information on cosmology e.g., the total mass of neutrinos, the effective extra relativistic degrees of freedom, the tensor-to-scalar ratio, non-Gaussianity parameters, among others [8–12]. These parameters have been of great interest for cosmologists because they could produce significant departure from the standard model and represent new physics in the early Universe. Combining the next-generation of CMB experiments along with large scale structure (LSS) probes will be the next step toward a precision cosmology that will allow us to constrain these fundamental physics parameters and find out extensions to the ΛCDM model [13]. However, the combination of these probes will also require more advanced statistical methods to analyze the dataset and an enormous computational effort. From the Bayesian statistics viewpoint, the estimation of the cosmological parameters demands the calculation of theoretical temperature and polarisation CMB power spectra, which is obtained through an Einstein-Boltzmann Solvers (EBS) like camb [14] or CLASS [15,16]. Usually, these codes require few seconds for computing the observables, depending on the complexity of the cosmological model. Afterward, a comparison between the predictions at various points in the parameter space with the available observations is done, and based on the likelihood a best-fit of the parameters is obtained. Packages like cosmoMC [17] or montepython [18] use MCMC algorithms to sample from the posterior distribution and fulfil this task [19]. However, this process is computationally expensive for theoretical models that include large amount of parameters or contain “slow parameters” (most of them are late-time and delay the calculation of the power spectrum) since the EBS is executed each step in the parameter space.

In recent years, deep neural networks have been used successfully in the field of cosmology as a way to confront the upcoming computational challenges. Originally inspired by neurobiology, deep neural network models have become a powerful tool in machine learning due to their capacity of approximating functions and dynamics by learning from examples [20, 21]. Using deep learning
methods as emulators for computing the cosmological observables has become a very popular application in cosmology. Different authors have proposed to implement deep neural networks emulators for the EBS [22,23], either totally or even partially, i.e., only in places where traditional estimations are more time-consuming [24, 25]. Deep neural networks have been also used for extracting the observables directly from the raw data without requiring the power spectrum or other compressed information. Based on this strategy, deep learning has been employed in classification tasks for detecting strongly lensed systems [26, 27], discriminating cosmological models [28, 29], or detecting cosmic strings in the CMB maps [30]. Additionally, for regression tasks deep learning provides a way to make inference either in gravitational lensing systems [31, 32], weak lensing or LSS data [33–37], reionization and 21cm observations [38, 39], and CMB data [40–43], also in generative models as a powerful alternative to cosmological numerical simulations [44]. However, the use of Deep neural networks may rise some problems. They are prone to over-fitting, so analyzing the results based on only point estimates, they might produce unreliable predictions with spuriously high confidence [45, 46]. Therefore, the following question naturally arises: how can we be sure that our model is certain about its outcomes? This fundamental concern has been object of study in the machine learning community and one of the most attractive approaches to address this issue relies on the Bayesian Neural Networks (BNNs) [47]. BNNs represent the probabilistic version of the traditional neural networks capturing the posterior probability of the outcomes and estimating their predictive uncertainties. One of the most popular techniques used to obtain the uncertainties in the Bayesian framework is called Dropout. Initially, Dropout was proposed in [48] as a regularisation scheme, subsequently the authors in [47] developed a theoretical framework casting dropout in neural networks as approximate variational inference for deep Gaussian processes. Applications of BNNs using Dropout in cosmology are shown in [32, 40, 49]. Recent studies (see [50] and references therein) have found that other techniques can remarkably improve the performances of Bayesian neural networks and reduce the variance of the estimates. Furthermore, in [51] the authors have claimed that Dropout fails in some architectures while others discuss the reliability of this method [52]. Moreover, in general neural networks predictions suffer from a poor calibration over their uncertainty estimations and tend to be overconfident in their predictions, i.e., predicted posterior distributions do not reflect actual correctness probabilities [53]. Different strategies and metrics have been proposed to calibrate these networks and to be able to evaluate the accuracy of the obtained uncertainties, some of these methods will be analyzed in this paper.

Based on the aforementioned discussion, our goal is twofold. Firstly, we want to show an appealing application of deep learning in cosmology by estimating the posterior distribution of the cosmological parameters directly from simulated CMB maps. Secondly, we want to describe different techniques employed to generate reliable uncertainty estimates of the predicted parameters and discuss their performance for the CMB dataset.

The paper is organized as follows. In Sec. II we describe the two sources of uncertainty in neural networks: aleatoric/epistemic and their importance for quantifying confidence intervals. In Sec. III we briefly summarize the framework of variational inference, and how to produce estimates of the uncertainties and correlations of the physical parameters. Sec. IV contains a description of different methods used in the literature to approximate the posterior over the weights of the networks. Some of them have been frequently used because of their simplicity of implementation, while other more recent techniques lead to better interpretation under the Bayesian framework and improved performance. We then describe the generation of the synthetic maps used to train the inference models, including the network architectures in Sec. V. In Sec. VI we discuss the calibration methods used to assess the reliability of uncertainty estimates, and in Sec. VII we show our main results related to use of BNNs in a cosmological context, as well as the credible cosmological parameter contours for our model. Finally, we present our conclusions and final remarks in Sec. VIII.

II. EPISTEMIC AND ALEATORIC UNCERTAINTY

There are many sources of uncertainty in model prediction of physical phenomena, and their nature depend on the context and the application. However, these uncertainties have been categorized in two groups: aleatoric and epistemic [54]. Aleatoric uncertainties represent the intrinsic randomness in the input dataset [55] and they can be reduced enhancing the quality of the data. Moreover, this uncertainty can be heteroscedastic, i.e., the variability of the residuals does vary as the independent variable does, or the uncertainty can be homoscedastic when it does not.

For any neural network, the aleatoric uncertainty can be obtained by computing the variance of the conditional distribution of the predictions given the features [56]. If such conditional distribution is Gaussian, the output of the network can be split into mean predictions and their variance. Then, the variance is learned implicitly from the minimization of the Gaussian log-likelihood while we supervise the learning of the regression task [55, 57]. Further methods to estimate and model the aleatoric uncertainty are given in [40, 56, 58, 59].

On the other hand, epistemic uncertainty quantifies the ignorance about the correct model that generated the data, it includes the uncertainty in the model, parameters, convergence, among the others [54]. This uncertainty is caused by the limited training data with respect to the entire feature space. Collecting more data in regions where there is low density of training examples will
reduce this uncertainty, while the aleatoric will remain unchanged [55]. Methods for estimating epistemic uncertainties are different from the aleatoric ones, and this is where BNNs can offer a mathematically grounded base for computing this uncertainty and be able to estimate the performance of the model [55]. Alternatives techniques for obtaining this uncertainty can be seen in [60]. Deep neural networks involve both types of uncertainties and determine whether a particular uncertainty is aleatoric or the epistemic but sometimes could be confused [54]. However, for BNNs the authors in [61–63] rewrote the estimator for the variance such that it can split in two terms associated to the epistemic and aleatoric uncertainty. We will see in the Sec. VII that this split allow us to evaluate the quality of the predictive uncertainty estimates. A more complete discussion of the nature of uncertainties can be found in [54].

III. CAPTURING UNCERTAINTY IN NEURAL NETWORK INFERENCE

In this section we will briefly introduce some variational inference techniques for dealing with non-tractable posterior distributions. We remind the reader to refer to [55, 57, 61] for additional details.

Let \( D = \{(x_i, y_i)\}^D \) be a dataset formed by \( D \) couples of inputs \( x_i \in \mathbb{R}^M \) and their respective targets \( y_i \in \mathbb{R}^N \), and \( f_w(x_i) \) be the output of the neural network with parameters (weights and biases) \( w \in \Omega \), where \( \Omega \) is the parameter space.

Traditional neural networks are trained by Maximum Likelihood Estimation (MLE), i.e., the parameters \( w \) are estimated in such a way that the likelihood of the observations in \( D \) is maximized. In the Bayesian setting, we choose a prior on the weights \( p(w) \), and a model which allows the definition of the likelihood \( p(y|x, w) \) capturing the predictive probability of the model given \( w \). The aim then is to find the posterior distribution given the observed dataset \( p(w|D) \), which using Bayes’ theorem can be written as

\[
p(w|D) = \frac{p(D|w)p(w)}{p(D)} = \frac{\prod_{i=1}^{D} p(y_i|x_i, w)p(x_i)p(w)}{p(D)},
\]

where \( p(D) = \int_{\Omega} p(D, w) dw \) is the evidence, and the second equality holds assuming that \( D \) is a realization of i.i.d. random variables [61]. Once the posterior has been computed, the probability distribution of \( y^* \) for a new input \( x^* \) can be obtained by integrating out the parameter \( w \) as

\[
p(y^*|x^*, D) = \int_{\Omega} p(y^*|x^*, w)p(w|D) dw.
\]

Unfortunately, the posterior \( p(w|D) \) usually cannot be obtained analytically and thus approximate methods should be used to perform the inference task. Here we will focus on a variational inference approach which approximates the posterior distribution \( p(w|D) \) by a variational distribution \( q(w|\theta) \), chosen in a well behaved functional space and depending on a set of variational parameters \( \theta \). The objective can then be formalized as finding \( \theta \) that makes \( q \) as close as possible to the true posterior, for instance by minimizing the Kullback-Leibler (KL) divergence between the two distributions

\[
KL(q(w|\theta)||p(w|D)) = \int_{\Omega} q(w|\theta) \ln \frac{q(w|\theta)}{p(w|D)} dw. \tag{3}
\]

By substituting the true posterior given in Eq. (1) into Eq. (3), we can observe that minimizing the KL divergence is equivalent to minimizing the following objective function

\[
F(D, \theta) = KL(q(w|\theta)||p(w))
- \sum_{(x, y) \in D} \int q(w|\theta) \ln p(y|x, w) dw, \tag{4}
\]

which is often known as the variational free energy [57]. The first term is the KL divergence between the variational distribution and the prior that acts as an Occam razor term, i.e., penalising complexity priors, while the second term drives the variational distribution to place as close as possible to the true posterior, for instance by choosing \( \theta \) such that \( E_q [\|\theta\|] \leq \text{KL}(q(w|\theta)||p(w)) \) for a fixed \( \theta \), where

\[
E_q [\|\theta\|] = \int_\Omega \|\theta\| q(w|\theta) dw,
\]

and

\[
E_q [\|\theta\|] = \frac{1}{K} \sum_{k=1}^{K} p(y^*|x^*, \tilde{w}_k), \quad \text{with} \quad \tilde{w}_k \sim q(w|\theta), \tag{6}
\]

where \( K \) is the number of samples. We can also compute the covariance of the variational predictive distribution, for a fixed \( x \), by invoking the total covariance law

\[
\text{Cov}_{q_{\theta}}(y^*, y^*|x) \equiv E_{q_{\theta}}[y^*y^*|x] - E_{q_{\theta}}[y^*|x]E_{q_{\theta}}[y^*|x]^T
= \int_{\Omega} \text{Cov}_{p}(y^*, y^*|x) q(w|\theta) dw + \int_{\Omega} \left[ \left( E_{p}[y^*|x] - E_{q_{\theta}}[y^*|x]\right) \times \left( E_{p}[y^*|x] - E_{q_{\theta}}[y^*|x]\right)^T \right] q(w|\theta) dw,
\]

where \( E_{q_{\theta}}[y|x] = \int y q_{\theta}(y|x) dy \), \( y^T \) is the transpose of the vector \( y \), and \( E_p[y|x] = \int y p(y|x) dy \) [61, 63]. The
first term in Eq. (7) collects the variability of the output coming from the training dataset which corresponds to the aleatoric uncertainty as it was mentioned in the previous section, while the second term encodes the variability of the output coming from the model, which it should be associated to the epistemic uncertainty. Following [64], we assume that the last layer of the network consists of a mean vector $\boldsymbol{\mu} \in \mathbb{R}^N$ and a covariance matrix $\Sigma \in \mathbb{R}^{N(N+1)/2}$. Suppose that for a given fixed input $\mathbf{x}^*$, $T$ forward passes of the network are computed, obtaining for each of them a mean vector $\boldsymbol{\mu}_t$ and a covariance matrix $\Sigma_t$. Then, an estimator for Eq. (7) can be written as

$$
\widehat{\text{Cov}}(y^*, y^*| \mathbf{x}^*) \approx \frac{1}{T} \sum_{t=1}^{T} \Sigma_t + \frac{1}{T} \sum_{t=1}^{T} (\boldsymbol{\mu}_t - \mathbf{p})(\boldsymbol{\mu}_t - \mathbf{p})^T,
$$

(8)

with $\mathbf{p} = \frac{1}{T} \sum_{t=1}^{T} \boldsymbol{\mu}_t$. Notice that in case $\Sigma$ is diagonal, the last equation reduces to the variance of the variational predictive distribution given in [61, 64] with both aleatoric and epistemic uncertainties

$$
\widehat{\text{Var}}(y^*_t| \mathbf{x}^*) \approx \frac{1}{T} \sum_{t=1}^{T} \sigma_{t,t}^2 + \frac{1}{T} \sum_{t=1}^{T} \mu_{t,t}^2 - \mathbf{p}^2.
$$

(9)

The aforementioned results allow the neural network to be able to learn the joint distribution for the targets and produce estimates of the uncertainties and correlations of the physical parameters.

**IV. VARIATIONAL DISTRIBUTIONS**

In this section we will review different types of neural networks, all characterized by a common Gaussian layer (aleatoric) in output. Deterministic neural networks (Fig. 1a) have a fixed value of their weights, after training. On the other side, Bayesian Neural Networks (Fig. 1b) have a prior and a posterior distribution defined over their weights (Sec. III), which is usually chosen to belong to any well behaved family of distributions. Two popular approximations for BNN are Dropout and DropConnect. In Dropout (Fig. 1c) each neuron is dropped with a certain probability, while in DropConnect (Fig. 1d) each weight-connection is dropped instead. The most popular approaches for BNNs present in the literature are briefly summarized in the following.

**A. Bernoulli via Dropout**

Dropout was first proposed in [48] as regularisation method in neural networks which helps to reduce co-adaptations amongst the neurons. During training, each neuron in the $j$-th layer $h^{(j)}$ of size $H_j$ is dropped from the network with probability $p$ (commonly known as dropout rate). The application of dropout can be expressed as

$$
h^{(j+1)} = \sigma \left( \mathbf{m}^{(j+1)} \odot (\mathbf{W}^{(j)} h^{(j)}) \right), \quad \mathbf{m}^{(j+1)} \sim \text{Ber}(p),
$$

(10)

where $\odot$ corresponds to the Hadamard product, $\sigma(\cdot)$ is a nonlinear activation function, $\mathbf{W}^{(j)}$ is the weight $(H_{j+1} \times H_j)$-matrix for the layer $j$, and $\mathbf{m}^{(j+1)}$ a vector mask of size $H_{j+1}$, which is sampled from a Bernoulli distribution which return 1 with probability $p$ and 0 with probability $(1-p)$. Once trained, the entire network is used although neurons are scaled using the factor $p$, this compensates for the larger size of the network compared to the one used during training. Interestingly, the authors in [65] have shown a connection between Dropout and approximate variational inference for Gaussian processes, allowing the neural network to be interpreted as an approximate Bayesian model. In this case, the variational distribution $q(\mathbf{W}^{(j)})$ for the $j$-th layer associated to Eq. (10) can be written as [66]

$$
\mathbf{W}^{(j+1)} = \mathbf{V}^{(j+1)} \text{diag} \left( \mathbf{m}^{(j+1)} \right), \quad \mathbf{m}^{(j+1)} \sim \text{Ber}(p),
$$

(11)

being $\mathbf{V}^{(j+1)}$ a $(H_{j+1} \times H_j)$-matrix of variational parameters to be optimised. Inserting this variational distribution into Eq. (4), we obtain an unbiased estimator for the objective function [65]

$$
- \hat{\mathcal{F}} = \sum_{i=1}^{D} p(y_i|x_i, \mathbf{w}) - \lambda \sum_{j=1}^{L} ||\mathbf{W}^{(j)}||^2,
$$

(12)

where the weights $\mathbf{w}$ are sampled at each layer from $q(\mathbf{W}^{(j)})$ defined in Eq. (11) and $\lambda$ is a positive constant. The first term corresponds to the likelihood that encourages $\mathbf{w}$ to explain well the observed data, while the second term is a $L_2$ regularization, weighted by the weight decay parameter $\lambda$, which mimics the KL term in Eq. (4).
Therefore, training such neural network using Dropout has the same effect as minimizing the KL in Eq. (3). This scheme, besides working similar to a Bayesian Neural Network, acts also as a regularization method which prevents over-fitting. After training the neural network, Dropout remains active and we follow Eqs. (6) and (8) to perform inference and estimate the uncertainties of the network, respectively. Such procedure is known in literature as Monte Carlo Dropout.

B. Bernoulli via DropConnect

DropConnect is a generalization of Dropout used for regularizing in deep neural networks [67]. In this scheme, each weight-connection is dropped with probability $p$, differently from DropConnect were neurons are dropped.

$$h^{(j+1)} = \sigma \left((M^{(j)} \odot W^{(j)}) h^{(j)}\right), \quad M^{(j)} \sim \text{Ber}(p),$$

(13)

where $M^{(j)}$ a matrix mask of size $H_{j+1} \times H_j$. In [68, 69] the authors use DropConnect to obtain approximated uncertainties. Here, the mask is applied directly to each weight, differently from Dropout where the weights are not sampled. The variational distribution for the weights of the $j$-th layer is given by

$$W^{(j)} = W^{(j)} \odot M^{(j)}, \quad M^{(j)} \sim \text{Ber}(p),$$

(14)

where $m_{rs}^{(j)}$ is the element of the mask $M^{(j)}$ connecting the $r$-th neuron of the $(j+1)$-th layer to the $s$-th neuron of the $j$-th layer. Similarly to the previous case, during training the network weights are adjusted to minimize Eq. (12), while at test time each input is passed through the network multiple times. It allows to capture both the epistemic and aleatoric uncertainties via Eq. (8).

C. Reparameterization Trick and Flipout Technique

So far we have seen two methods to provide the networks with stochastic weights. Dropout deals with stochastic activations (drop neurons), the weights are not sampled independently however it is easy to implement and quite cheap to compute. On the other hand, DropConnect drops directly the weights which in most cases are far more than the number of neurons, i.e. it is more expensive and has a higher variance. Recently, different works have proposed to sample the weights from Gaussian distributions instead. The Reparameterization Trick (RT), allows to generate samples which are differentiable with respect to the the parameters of the distribution from which they were drawn [70]. If the weights are considered as a continuous random variable drawn from $w \sim q(w|\theta)$, thanks to the RT we might express it as a deterministic function $w = g(\epsilon, \theta)$ of a fixed random auxiliary variable $\epsilon$, i.e., $\epsilon \sim \rho(\epsilon)$ has a probability density function $\rho$ independent of $\theta$, and $q$ is parameterized by $\theta$. This implies that any expectation with respect to $q(w|\theta)$, can be estimated as [70, 71]

$$\int_\Omega q(w|\theta) f(w) dw \approx \frac{1}{K} \sum_{k=1}^K f(g(\epsilon_k, \theta))$$

(15)

In the multivariate Gaussian case $w \sim \mathcal{N}(\mu, \Sigma)$ [72], we have the usual reparameterization given by $w = \mu + L \epsilon$, where $\epsilon \sim \mathcal{N}(0, I)$ and $L$ has the property that $\Sigma = LL^T$, a noteworthy example being the lower triangular Cholesky factorization. Given this reparameterization along with Eq. (15), we can get the approximated value of the second term in Eq. (4) and thus, be able to derive the unbiased estimates of the gradient of the variational free energy [70].

The downside of RT is that the sampled weights are the same for all the examples of the batch, thus correlating the gradients between different examples in the same batch. To overcome this limitation and thus reduce the gradient variance, the authors of [50] propose the Flipout method as an efficient way to provide pseudo-independent weights perturbations. Methods like Flipout or Local Reparameterization Trick [71] are some of the strategies used today for variance reduction. Flipout assumes that the variational distribution can be written as a mean $\overline{W}$ plus a perturbation with symmetric distribution around zero

$$W = \overline{W} + \Delta W$$

(16)

and proposes to decorrelate the noise inside a mini-batch with pseudo-random sign matrices, to randomly flip the symmetric perturbation of the weights. For an example $n$ in the batch

$$\Delta W_n = \Delta \overline{W} \odot (r_n s_n^\top)$$

(17)

where $r_n$ and $s_n$ are random vectors whose entries are uniformly sampled from $\pm 1$ and $\Delta \overline{W}$ is a perturbation sampled only once for the whole mini-batch. Remarkably this approach can be easily vectorized in a given batch and thus be used to efficiently obtain pseudo-random weights perturbations [71].

V. DATASET AND NETWORK

We have generated 50,000 independent realizations of simulated CMB full-sky maps and extracted from them images of $20 \times 20$ deg$^2$ with $256 \times 256$ pixels (the CMB data generator code is available at [73]). From the total dataset, 70% is for training, 20% for testing, and 10% for validation. These simulations were created given the temperature angular power spectra generated by CLASS and healpy [74], by originating a realisation on the HEALPix grid. The choice of the resolution for the maps comes from the analysis displayed in Fig. 2. Here we can see
that for small angular sizes, the power spectrum obtained from the patches cannot retain enough information from the original spectrum produced by CLASS, in contrast to images with angular size equal or larger than 10×10 deg². However for large angular size, the assumption of flat approximation cannot be valid and distortions produced by the projection of the spherical data into the flat sky could lead to undesirable effects, that is, the resolution leads to a trade-off between accuracy of the recovered power spectrum and execution time (speed) of the neural network. One alternative to deal with large angular size images is to create CMB maps from the lens-tools package [75] which produces a Gaussian random field directly over the pixels of the flat image.

FIG. 2. Power spectra generated from patches with different angular scales (Field: [5,10,20] deg²) and pixelized into (pixel-size: [128,256,512] pixels). The shadow region corresponds to an average of 500 samples. The red line shows the power spectrum obtained from theory. We use lens-tools to compute the power spectrum of the CMB patches.

In this paper we assume a minimal version of the ΛCDM model where each power spectrum generated in CLASS differs in three parameters: baryon density \( \omega_b \in [0.019, 0.031] \), cold dark matter density \( \omega_{cdm} \in [0.06, 0.22] \), and primordial spectrum amplitude \( A_s \in [1.01 \times 10^{-9}, 4.01 \times 10^{-9}] \), sampled over a uniform 3D grid, while the rest of the ΛCDM parameters are fixed with the values reported by the Planck mission [7]. The multiple generation of the power spectra should gather the cosmic variance that will contribute to the aleatoric uncertainty. The images and the parameters are normalized between -1 and 1, without any additional data augmentation.

Architecture

We have implemented our models in TensorFlow [76]. The API tf.Keras and the library TensorFlow-Probability [77] have been also used for developing RT and Flipout, while Dropout and DropConnect were implemented in the higher-level library Sonnet [78]. We implement a modified version of the VGG [79] and AlexNet [80] networks illustrated in Fig. 3. We choose to have all the architectures with roughly the same number of weights so that the analysis carried out for all BNN methods depends only on their performance, and not on the size or complexity of the network. The VGG network consists of ten convolutional layers with a fixed kernel size 3×3, using LeakyReLU as the activation function. Each convolutional layer, except for the last one, is followed by a batch renormalization layer, which ensures that the activations computed in the forward pass of the training depend only on a single example and are identical to the activations computed in testing [81]. We apply zero padding in each convolution layer, and we downsample using max pooling, allowing the network to learn correlations at large angular scales. Additionally, for AlexNet the input is convolved with six convolutional layers of kernel size (11, 5, 3, 3, 3, 1), with the same activation function after each layer and without batch (re)normalization. The downsampling is done using max pooling as before for three of the six layers as we can see in Fig. 3. One critical modification with respect to AlexNet consists in the change of the fully connected layers at the end of the network which are replaced by convolutional layers. Indeed, we observed that in our configuration, for the CMB dataset, the presence of the dense layers deteriorates the performances. At the end of the convolutional part for both architectures, a dense layer with nine neurons is built, three of them correspond to the means of the cosmological parameters used to generate the maps, and the other six compose a lower triangular matrix \( L \). This last layer yields to a multivariate Gaussian distribution with mean \( \mu \) and covariance \( \Sigma = LL^\top \) to guarantee positive definiteness.

Training

The negative log-likelihood (NLL) of our neural network, used to estimate the cosmological parameters and their uncertainties, is given by

\[
\mathcal{L} \sim \frac{1}{2} \log |\Sigma| + \frac{1}{2}(y - \mu)\Sigma^{-1}(y - \mu)^\top, \tag{18}
\]

averaged over the mini-batch. The objective function differs depending on the method employed. For example, for Dropout and DropConnect, it will be expressed as the sum of the negative log-likelihood in Eq. (18) plus
a L2-regularization term from Eq. (12). Here we used $\lambda = 0.001$ for the weights and $\lambda = 0.0001$ for the bias.

In the case of RT and Flipout, the optimization is based on the KL divergence written in Eq. (4). The prior that we have chosen is a normal distribution under the mean field approximation initialized with mean 0 and variance 1, while the posterior is given by the same distribution but initialized with the Glorot normal initializer for the mean, and the variance is sampled from a Gaussian distribution $N(-9, 0.01)$. Furthermore, the weights of the posterior are controlled by a L2-regularization term and the bias in both cases is taken as a deterministic function. Different experiments using (non)-trainable prior distributions showed that training both the posterior and prior parameters turned out in better performances. Furthermore, a deterministic dense layer as last layer of the network (outputting mu and sigmas) instead of a probabilistic one produces better results. The algorithm used to minimize the objective function is the Adam optimizer [82] with first and second moment exponential decay rates of 0.9 and 0.999, respectively, a learning rate of $10^{-4}$ and decay rate of 0.9. The decay step has been tuned based on the method: for Flipout it is 6,000, for Dropout and DropConnect it is 8,000, and for RT 2,000. We trained the network for 400 epochs with batches of 32 samples.

Validation and Testing

We have fed each input image from the test set 2,500 times to the network, essentially getting enough samples from the posterior of the network and hence being able to capture the epistemic uncertainty. Each sample produces nine variables corresponding to the cosmological parameter values and its covariance matrix. The former represents the aleatoric uncertainty learned from optimizing the objective function, hence, the total uncertainty reported for each example is provided via Eq. (8).

VI. CALIBRATION

The issue of the calibration of neural networks has gained interest in the recent years, since it has been shown that deep neural networks tend to be overconfident in their predictions [83]. Different works have been addressed to identify why neural networks may become miscalibrated (see, e.g., [53], and references therein). One of the ways to diagnostic the quality of the uncertainty estimates is through reliability diagrams. Fig. 4 displays the confidence intervals against the expected coverage probabilities defined as the $x\%$ of samples for which the true value of parameters falls in the $x\%$-confidence interval. If the network is well calibrated, then the diagram should correspond to a straight line and any deviation from it represents a miscalibration. As we will show

FIG. 3. Illustration for the modified versions of the (a) AlexNet and (b) VGG architectures. The input of the networks are images of $256 \times 256$ pixels and the output consists of nine values. Both architectures have around $\sim 60,000$ weights, being batch normalization in VGG the most remarkable difference between them.

FIG. 4. Reliability diagrams for CMB maps before (solid lines with marks) and after calibration (dashed lines). The black dashed line stands for the perfect calibration, while the other color lines represent different BNNs. For some hyperparameters values in AlexNet (Alex), the model underestimates its errors, while for VGG all models are overconfident in their predictions. We have implemented beta calibration for obtaining these curves [84].
later, the methods employed to adjust the predicted uncertainties can be applied during or after training. During the training process, we just need to adapt some hyper parameters in the model in order to achieve the good calibration. For example, in the Dropout case the authors in [32] found out that the Dropout rate should be tuned to produce high accuracy uncertainty estimations (see AlexNet with dropout rate 7% in Fig. 4). Moreover, the authors in [85] introduced Concrete Dropout which allows for the dropout probabilities to be automatically tuned, improving the performance and getting calibrated uncertainties. Additionally, we will show in the next section that the hyper parameters related to Flipout correspond to the regularization parameters for the scale of the approximate posterior over weights and bias. However, calibrating the network during training is not efficient in all cases. Tuning hyper parameters could drastically affect the performance of the model and besides this, the method depends strongly on the architecture of the network. An example on this issue will be shown later when we observe that this technique fails on the VGG architecture. On the other hand, it has been noticed that methods for calibrating the network after training indeed preserve the accuracy of the predictions achieved during training. Histogram Binning [86], Isotonic Regression [87], Platt Scaling [84, 88, 89], and Temperature Scaling are some of the most common methods used for calibrating the networks in regression tasks. In this work we will use an extended version of the parametric Platt Scaling method described in [84]. Basically, we build the reliability diagram to be then fitted with respect to the calibrated map [84]

\[
\beta(x; a, b, c) = \frac{1}{1 + (e^c + \alpha) - x)}
\]

with the scalar parameters \(a, b, c \in \mathbb{R}\). Hence, we apply the following transformation to the covariance matrix \(\Sigma \rightarrow s \Sigma\) in the evaluation of the coverage probabilities (see Eq. (20)), being \(s \in \mathbb{R}^+\) a scalar parameter. Finally, we will choose the value of \(s\) used for the calibration of the network by minimizing the calibrated maps with respect to a diagonal line. Fig. 4 displays the results of the beta calibration for different BNN models for VGG and AlexNet. For example, a dropout rate of 1% using AlexNet or using Flipout on AlexNet without regularization on their posterior weights, will produce underestimation in their errors. This means that most of the true value does not fall in its corresponding confidence interval, as we can see in Fig. 5. On the other hand, overconfident networks (like VGG, as we see in Fig. 4) are very conservative in their errors, therefore they produce weak constraints on the parameter space, as it shows in Fig. 5. Although the beta calibrated method works relatively well, it is considered less robust than the Temperature scaling, where the previous transformation is applied directly to the NLL in Eq. (18) in the validation set. Finally, let us discuss about the evaluation of the coverage probabilities. We have found out that all models used in this work produce an approximately Gaussian joint distribution (higher-order statistical moments are very close to zero). Therefore, we can assume that the predictive distribution obey to a multivariate Gaussian distributions whose confidence interval can be computed through

\[
C \geq (y - \hat{y})\Sigma^{-1}(y - \hat{y})^T
\]

which is basically an ellipsoidal confidence set with coverage probability \(1 - \alpha\). The quantity \(C\) has the Hotelling’s T-squared distribution \(T_{k, D-k}^2(1 - \alpha)/D\) with \(k\) degrees of freedom, being \(D\) the number of samples [91]. For large samples, the Hotelling’s \(T^2\) tends to the more common \(\chi^2\) distribution [92], which is the distribution of a sum of the squares of \(k\) independent standard normal random variables. This is indeed the distribution which we will use in the calculation of our confidence intervals. Therefore, the coverage probabilities correspond to the percentage of samples satisfying Eq. (20), in other words, the fraction of examples where the true value lies into the 3D-ellipsoidal region. This evaluation generalizes the current methods in the literature in which we must bin the samples in order to estimate the region that contains \((1 - \alpha)\) of the test dataset, as long as the joint distribution is almost Gaussian. In Appendix A, we compute the coverage
probabilities from the histograms as it is usually done in literature [26], finding consistence results when we used ellipsoidal confidences.

VII. ANALYSIS AND RESULTS

In this section we describe the results we obtained with different architectures and types of BNNs. We compare all experiments in terms of performance, i.e., the precision of their predictions for the cosmological parameters quantified through Mean Square Error (MSE), and their values achieved in the NLL. Furthermore, we analyze the quality of the uncertainty estimates in each experiment and its appropriate calibration, if needed.

A. Dropout and DropConnect

We begin by comparing the performance of Dropout and DropConnect. The best results are displayed in Table I. As it can be seen, DropConnect does not exhibit particularly exciting performances for any architecture. Even for a vast range of regularization and initialization values, we could not achieve good results, as was reported in [68]. It seems that DropConnect injects large noise on convolutional layers until this unstabilizes the training process. Nonetheless, in contrast to the DropConnect technique, Dropout effectively improves the performance of VGG by a noticeable margin, while for AlexNet it works roughly well. Indeed, many works have shown that dropping weights (or neurons) does not bring much performance improvement in convolutional neural networks. Some authors attribute this failure to the incorrect placement in the convolutional blocks [93], while others assert that these methods fail in some network architectures [51]. Since our aim is searching for a good BNN model useful to analyse the CMB dataset, hereafter, we will mostly focus on Dropout for both architectures. Now, to understand the impact of the Dropout rate on the training process, we plot the NLL for different values of the parameter in Fig. 6 for AlexNet, and in Fig. 7 for VGG.

We can directly observe in Fig. 6 that large values of Dropout rates are required to decrease the gap between training and validation, and dropping 10% of the neurons yields the highest performances. Conversely, besides producing better results with respect to AlexNet, VGG also reduces notably the training/validation gap, and only 1% of Dropout rate is required to score the best performance in the model, as we can observe in Fig. 7. We can ascribe this favorable behavior to batch renormalization which acts not only as a regularizer, but also avoids extra normalisation calculations during the forward pass that yield to a quick convergence. On the other hand, as discussed in Sec. VI, often neural networks are miscalibrated. We then estimate the coverage probabilities corresponding to confidence intervals of 68%, 95.5%, and 99.7% (i.e., 1σ, 2σ, and 3σ, respectively). Some authors attribute this failure to the incorrect placement in the convolutional blocks [93], while others assert that these methods fail in some network architectures [51].
$\sigma$, and $3\sigma$) in order to verify the accuracy of the uncertainty estimates. The results using AlexNet are shown in Table II. We can notice that firstly as expected the coverage probability is proportional to the Dropout rate, since this variable is associated to the stochasticity of the model.

| Rate C.I | $\sigma$=1% | $\sigma$=5% | $\sigma$=7% | $\sigma$=10% | $\sigma$=20% |
|----------|-------------|-------------|-------------|-------------|-------------|
| $\sigma$=O. | 0.024 | 0.080 | 0.104 |
| $\sigma$=C. | 0.002 | 0.013 | 0.051 |
| $\sigma$=O. | 0.003 | 0.004 | 0.003 |
| $\sigma$=C. | 0.006 | 0.006 | 0.006 |

TABLE II. Estimation of coverage probabilities corresponding to confidence intervals of $1\sigma$, $2\sigma$, and $3\sigma$. Dropout rate ($dr$) becomes a hyper parameter which should be tuned in order to calibrate the network. $Dr \sim 0.07$ and $dr \sim 0.05$ yield to accurate uncertainties for Dropout and DropConnect, respectively.

FIG. 8. Training (solid lines) and validation (dotted lines) for AlexNet. Negative log-likelihood for Dropout method as a function of the epoch. The colors represent the training dataset size used for a dropout rate of $dr = 0.07$.

Interestingly, the Dropout rate that leads to the correct calibration is not necessarily equal to that one which yields to the best performance. This result supports the fact that calibration of deep neural networks after training becomes the most effective. Additionally, we observe that the Dropout rate used to calibrate DropConnect models is smaller than the one used in Dropout, suggesting that a stronger stochasticity is involved in DropConnect networks (since there are more weights than neurons). The behavior in the VGG architecture is substantially different, we observe that is not possible to calibrate the network during training. Tuning the hyper parameters (Dropout rate or posterior regularization) is not enough to tune the uncertainties and thus calibrate the confidence intervals. This is due to the batch (re)normalization layers in the VGG architecture, the normalization applied at each layer indeed standardizes the activations (mean close to 0 and standard deviation close to 1), reducing or even nullifying the effect of the hyper parameters tuning on the epistemic uncertainties. Re-calibration after training must be applied in networks with batch (re)normalization layers. Therefore, an important result obtained so far is that calibrating networks during training is sometimes not enough, this necessarily depends on the architecture of the network, especially if the former contains transformation techniques on the weights like batch (re)normalization. We further plot the NLL curves of networks for different trained dataset size in Fig. 8. As we might expect, the performance of the network depends on the amount of images used for training the network. We also computed the aleatoric and epistemic uncertainties for those experiments (see Table III). Results show that reducing the training dataset size appreciable increases the epistemic uncertainty, while the aleatoric remains roughly constant, as discussed in Sec. II. Thereby, observing the effect of the training dataset size on uncertainties should reflect the quality of the uncertainty measurement.

B. Reparameterization Trick and Flipout

In this section we evaluate the use of Flipout compared to RT on both architectures. The performance of both methods are shown in Table I. We have found that Flipout outperforms all other methods regardless the network architecture and also it has achieved significant speedups during the training process. As mentioned above, VGG tends to produce more miscalibrated networks. This effect was also observed using either Flipout or RT, while for AlexNet we have found out that calibration can be achieved by regularizing the scale parameter of the approximate posterior of the weights and biases. If the initially trained network is overestimating the error, we want to add a regularization reducing the variance of the approximate posterior. In the case in which the scale of the approximate posterior is parametrized with a softplus function, we can use a SUM regularizer on the parameters...
of the scale (before the softplus) to reduce the variance and an L2 regularizer to increase it (since the parameters of the scales are negative for a prior with scale around 1). See also Appendix B. We experimented also by varying the prior scale, but we have found this approach not effective. The amount of regularization on the parameters of the posterior scale thus play the role the hyper parameter required to calibrate the network.

| Coverage probability estimation for Flipout and RT. |
|---|---|---|---|---|---|---|
| C.L. | Reg | Non-Reg | Reg=1e-7 | Reg=6e-8 | Reg=1e-5 | Reg=1e-4 |
| Flip | Flip | Flip | Flip | Flip | Flip | Flip |
| 68.3% | 65.1 | 65.1 | 65.1 | 65.1 | 65.1 | 65.1 |
| 95.5% | 95.2 | 95.2 | 95.2 | 95.2 | 95.2 | 95.2 |
| 99.7% | 99.4 | 99.4 | 99.4 | 99.4 | 99.4 | 99.4 |

TABLE IV. Estimation of coverage probabilities corresponding to the confidence intervals of 1σ, 2σ, and 3σ. The regularizer (Reg) becomes an hyper parameter which should be tuned in order to calibrate the network. Reg = 6e-6 and Reg=1e-5 yield to roughly accurate uncertainties for Flipout and RT respectively. The bias used here is 0.001.

In fact, regularizing the posterior allows to reduce the width of the posterior distribution, producing more accurate confidence estimates. A visualization of this effect can be seen in Appendix B. Table IV reports the coverage probabilities corresponding to confidence intervals of 1σ, 2σ, and 3σ for different values of the regularization. We have found out that without any regularizer, the estimation of the error is permissive and enhancing this hyper parameter increases the coverage probability estimation until arriving at values very close to their corresponding confidence intervals. The values reached to calibrate the network are ~ 6e-6 and ~ 1e-5 for Flipout and RT, respectively. Fig. 9 displays the performance of the network for the models used in Table IV only for Flipout. Despite the fact that BNNs incorporate some degree of regularization, we observed that for AlexNet the gap between training/validation still remains, while for VGG it becomes small. Additionally, we can estimate both the epistemic and aleatoric uncertainties from the calibrated Flipout network. The results are shown in Table III. As before, epistemic uncertainty increases with the size of the training dataset. However, we do observe that the epistemic uncertainties becomes smaller for Flipout compared to Dropout, implying that Flipout indeed achieves the largest variance reduction. Conversely, aleatoric uncertainty seems to be unaffected by the size of the training dataset and its value remains similar to that obtained in Dropout, concluding that this type of uncertainty does not depend on the variability of the weights in the network. The performance of the network using different training dataset sizes can be seen in Fig. 10. Although the use of batch (re)normalization produces reduction on the training/validation gap, it also leads to large fluctuations due to the fact that it is constantly readjusting the layers to new distributions.

C. Approximated posterior distribution of the cosmological parameters

So far we have analyzed the performance of different BNNs for each architecture. We have found out that Flipout and Dropout are methods which work really well to carry out parameter inference using our CMB dataset.
After calibrating the network with the approach introduced in Sec. VI, we can visualize the performance of the above methods in terms of precision of their cosmological parameters predictions. Fig. 11 shows the predictions for each method on the test CMB maps and its accurate uncertainties. As mentioned in the previous section, implementing Dropout in the AlexNet architecture leads to large MSE values and larger uncertainties observing sparsely data in the parameter space, while Flipout keeps excellent performance regardless the architecture, and its uncertainties are notably reduced. Finally, we constraint the dark-energy density written as \( \Omega_\Lambda \approx 1 - \Omega_b - \Omega_{cdm} \), being \( \omega_i \equiv \Omega_i h^2 \) with \( h = 0.6781 \) [6], just to examine the posterior distribution for the derived parameters. The triangle plots of Figs. 12 and 15 show our main results for one example randomly picked from the CMB test dataset. We use the Python GetDist package for creating the triangular plot [90]. Fig. 12 displays the four best accurate BNNs which yield to suitable credible cosmological parameter contours. Here, the true value corresponds to \( \omega_b = 0.02590 \), \( A_s = 3.65653 \), and \( \omega_{cdm} = 0.15773 \), and the derived parameter \( \Omega_\Lambda = 0.59761 \). Table V gives marginalized parameter constraints from the CMB maps, including one derived parameter. The credible intervals shown in the table are consistent with the one reported in the literature although for \( \omega_b \) which was the most difficult parameter to be learned by the network, becomes one order of magnitude larger. In fact, the networks used in this paper have reduced capacity to reach the high accuracy for all parameters obtained by standard techniques like MCMC, but a robust network can indeed reduce significantly the credible intervals. In Appendix C we show the results for all the BNNs introduced in this paper.

| BNN         | Marginalized parameter constraints |
|-------------|-----------------------------------|
| \( \Omega_\Lambda \) | 0.597 \( \pm \) 0.034 |
| \( A_s \)   | 3.659 \( \pm \) 0.049 |
| \( \omega_{cdm} \) | 0.158 \( \pm \) 0.043 |
| \( \Omega_\Lambda \) | 0.598 \( \pm \) 0.043 |
| \( A_s \)   | 3.656 \( \pm \) 0.047 |
| \( \omega_{cdm} \) | 0.157 \( \pm \) 0.042 |
| \( \Omega_\Lambda \) | 0.604 \( \pm \) 0.042 |

Table V. Parameters 95% intervals for the minimal base- \( \Lambda \)CDM model from our synthetic CMB dataset using Flipout, RT, and Dropout with the AlexNet and VGG architectures.
among four methods. The diagonal plots are the marginalized values and the black solid line corresponds to the true values. We have compared them by implementing two architectures and several training methods. Flipout emerged as the most reliable and effective method, achieving best performances across architectures, while DropConnect had worse performances. Furthermore, we observed that Flipout manifests a significant speedup during training and a notable reduction in the credible contours for the parameters. Additionally, in Sec. V, we introduced the problem of calibration in deep neural networks. In fact, we have showed that all models are (under)over-confident in their predictions unless some hyper parameters such as the Dropout rate or the regularization parameter are tuned. However, we have found out that hyper parameter tuning during training is not sufficient in the cases where batch (re)normalization is present in the architecture. Therefore, calibration in these architectures is only possible after training. Despite this, using batch (re)normalization is advantageous since it allows us to obtain the best performances and the highest speed of convergence during training while focusing on calibration after. The calibration method used here is simple but quite successful. Generalization of this method will be reported in a future paper. Finally, we have noted that for a well-calibrated network, the aleatoric and epistemic uncertainties behave consistently when the training dataset size is reduced. As mentioned in Sec. II, we expect that the epistemic uncertainty reduces its value, while the aleatoric one remains unchanged. This behavior was indeed observed in Table III. Furthermore, the aleatoric uncertainty is approximately the same regardless of the method or the architecture used, as expected since it does depend only on the stochasticity of the input dataset.

On the other hand, the epistemic one is very small when Flipout is used, finding again that this method reduces the variance compared to the others. Since we have verified that BNNs are able to capture the total uncertainty of the predictions, we have proceeded to compute the posterior distributions of the parameters. The results are displayed in Fig. 12. We observed that all methods work well, and they predict roughly the same marginalized posterior. We also obtained the binding intervals shown in Table V, finding consistence with the ranges reported in the literature. The \( \omega_b \) parameter produced a less binding uncertainty because it was the hardest parameter to be learned by the network. We expect that this estimation can be easily improved by using more complex neural network architectures. The research showed in this paper will allow a direct comparison with the current techniques used so far in Cosmology. Moreover, this methodology will allow the estimation of confidence regions for features that can be extracted directly from the raw data such as non-Gaussian signals [94] or foreground emissions [95, 96]. In future work, we plan to carry out this comparison improving the architecture and using other cosmological datasets such as CMB polarization with large-scale matter distribution and 21cm maps. The latter allows to obtain complementary information on processes related to reionization history or inflation, while the former will improve the constraints on cosmological parameters and help to break some partial parameter degeneracies.

VIII. CONCLUSIONS

In this paper we have presented Bayesian neural networks as a reliable and accurate tool to estimate the marginalized posterior distribution of the cosmological parameters directly from simulated CMB maps. BNNs, when properly set and calibrated, offer the capability to estimate the total uncertainty (aleatoric and epistemic) of their predictions by imposing a prior distribution on the parameters of the network (weights) and approximating the posterior distribution using variational inference. Different assumptions about the distribution over the weights have been proposed, and four of them were used in this work: Dropout, DropConnect, Flipout, and Reparameterization Trick. We have compared them by implementing two architectures and several training methods. Flipout emerged as the most reliable and effective method, achieving best performances across architectures, while DropConnect had worse performances. Furthermore, we observed that Flipout manifests a significant speedup during training and a notable reduction in the credible contours for the parameters. Additionally, in Sec. V, we introduced the problem of calibration in deep neural networks. In fact, we have showed that all models are (under)over-confident in their predictions unless some hyper parameters such as the Dropout rate or the regularization parameter are tuned. However, we have found out that hyper parameter tuning during training is not sufficient in the cases where batch (re)normalization is present in the architecture. Therefore, calibration in these architectures is only possible after training. Despite this, using batch (re)normalization is advantageous since it allows us to obtain the best performances and the highest speed of convergence during training while focusing on calibration after. The calibration method used here is simple but quite successful. Generalization of this method will be reported in a future paper. Finally, we have noted that for a well-calibrated network, the aleatoric and epistemic uncertainties behave consistently when the training dataset size is reduced. As mentioned in Sec. II, we expect that the epistemic uncertainty reduces its value, while the aleatoric one remains unchanged. This behavior was indeed observed in Table III. Furthermore, the aleatoric uncertainty is approximately the same regardless of the method or the architecture used, as expected since it does depend only on the stochasticity of the input dataset. On the other hand, the epistemic one is very small when Flipout is used, finding again that this method reduces the variance compared to the others. Since we have verified that BNNs are able to capture the total uncertainty of the predictions, we have proceeded to compute the posterior distributions of the parameters. The results are displayed in Fig. 12. We observed that all methods work well, and they predict roughly the same marginalized posterior. We also obtained the binding intervals shown in Table V, finding consistence with the ranges reported in the literature. The \( \omega_b \) parameter produced a less binding uncertainty because it was the hardest parameter to be learned by the network. We expect that this estimation can be easily improved by using more complex neural network architectures. The research showed in this paper will allow a direct comparison with the current techniques used so far in Cosmology. Moreover, this methodology will allow the estimation of confidence regions for features that can be extracted directly from the raw data such as non-Gaussian signals [94] or foreground emissions [95, 96]. In future work, we plan to carry out this comparison improving the architecture and using other cosmological datasets such as CMB polarization with large-scale matter distribution and 21cm maps. The latter allows to obtain complementary information on processes related to reionization history or inflation, while the former will improve the constraints on cosmological parameters and help to break some partial parameter degeneracies.

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[1] M. Giovannini, *A Primer on the Physics of the Cosmic Microwave Background* (World Scientific, 2008).
[2] P. Naselsky, D. Novikov, and I. Novikov, *The Physics of the Cosmic Microwave Background*, Cambridge Astrophysics (Cambridge University Press, 2006).
[3] P. Collaboration, Planck 2015 results - xiii. cosmological parameters, *A&A* **594**, A13 (2016).
[4] M. Giovannini, Why CMB physics?, *Int. J. Mod. Phys. A* **22**, 2697 (2007), arXiv:astro-ph/0703730 [astro-ph].
[5] S. Dodelson and A. P. L., 1941-1969), *Modern Cosmology* (Elsevier Science, 2003).
[6] P. Collaboration (Planck), Planck 2018 results. VI. Cosmological parameters, arXiv:1807.06209v1 (2018).
[7] P. Collaboration, Planck 2018 results. X. Constraints on inflation, arXiv e-prints , arXiv:1807.06211 (2018), arXiv:1807.06211 [astro-ph.CO].
[8] S. Mishra-Sharma, D. Alonso, and J. Dunkley, Neutrino masses and beyond- ΛCDM cosmology with lst and future cmb experiments, *Phys. Rev. D* **97**, 123544 (2018).
[9] W. Deng, Dark energy constraints in light of pantheon sne ia, bao, cosmic chronometers and cmb polarization and lensing data, *Phys. Rev. D* **97**, 123507 (2018).
[10] C. Pitrou, A. Coc, J.-P. Uzan, and E. Vangioni, Precision big bang nucleosynthesis with improved helium-4 predictions, *Physics Reports* **754**, 1 (2018), precision big bang nucleosynthesis with improved helium-4 predictions.
[11] H. J. Hortáu and L. Castaneda, Reduced bispectrum solving system (CLASS). part II: Approximation schemes, *Journal of Cosmology and Astroparticle Physics* **2011** (07), 034.
[12] M. Shiraishi, Probing the early universe with the cmb scalar, vector and tensor bispectrum, *Springer Theses 10.1007/978-4-431-54180-6* (2013).
[13] http://www.cfhtlens.org/
http://kids.strw.leidenuniv.nl/index.php
http://www.darkenergysurvey.org
http://hsc.ntk.nao.ac.jp/zsp/
http://www.lsst.org
http://sci.esa.int/euclid/
http://ufirst.gafc.nasa.gov
https://cmb-s4.org/
https://www.litebird-europe.eu/
https://www.core-mission.org/
https://simonsobservatory.org/
[14] https://camb.info/.
[15] http://class-code.net.
[16] D. Blas, J. Lesgourgues, and T. Tram, The cosmic linear anisotropy solving system (CLASS), part II: Approximation schemes, *Journal of Cosmology and Astroparticle Physics* **2011** (07), 034.
[17] https://cosmologist.info/cosmomc/.
[18] http://baudren.github.io/montepython.html.
[19] R. Trotta, Bayes in the sky: Bayesian inference and model selection in cosmology, *Contemporary Physics* **49**, 71 (2008), https://doi.org/10.1080/00107510802066753.
[20] N. Kriegeskorte and T. Golan, Neural network models and deep learning - a primer for biologists, arXiv e-prints , arXiv:1902.04704 (2019), arXiv:1902.04704 [q-bio.NC].
[21] H. W. Lin, M. Tegmark, and D. Rolnick, Why does deep and cheap learning work so well?, *Journal of Statistical Physics* **168**, 1223 (2017).
[22] https://github.com/marius311/pypico.
[23] W. A. Fendt and B. D. Wandelt, Pico: Parameters for the Impatient Cosmologist, *Astrophys. J.* **654**, 2 (2006), arXiv:astro-ph/0606709 [astro-ph].
[24] J. Albers, C. Fidler, J. Lesgourgues, N. Schöneberg, and J. Torrado, CosmicNet I: Physics-driven implementation of neural networks within Boltzmann-Einstein solvers, arXiv e-prints , arXiv:1907.05764 (2019), arXiv:1907.05764 [astro-ph.CO].
[25] A. Manrique-Yus and E. Sellentin, Euclid-era cosmology for everyone: Neural net assisted MCMC sampling for the joint 3x2 likelihood, arXiv e-prints , arXiv:1907.05881 (2019), arXiv:1907.05881 [astro-ph.CO].
[26] F. Lanusse, Q. Ma, N. Li, T. E. Collett, C.-L. Li, S. Ravanbakhsh, R. Mandelbaum, and B. Poczoz, CMU DeepLens: deep learning for automatic image-based galaxygalaxy strong lens finding, *Mon. Not. Roy. Astron. Soc.* **473**, 3895 (2018), arXiv:1703.02642 [astro-ph.IM].
[27] C. E. Petrillo, C. Tortora, S. Chatterjee, G. Vernardos, L. V. E. Koopmans, G. Verdoes Kleijn, N. R. Napolitano, G. Covone, P. Schneider, A. Grado, and J. McFarland, Finding strong gravitational lenses in the Kilo Degree Survey with Convolutional Neural Networks, *mnras* **472**, 1129 (2017), arXiv:1702.07675 [astro-ph.GA].
[28] J. Schmelze, A. Luchci, T. Kacprzak, A. Amara, R. Sgier, R. Rfrgier, and T. Hofmann, Cosmological model discrimination with Deep Learning, arXiv1707.05167 (2017).
[29] N. Perraudin, M. Defferrard, T. Kacprzak, and R. Sgier, DeepSphere: Efficient spherical Convolutional Neural Network with HEALPix sampling for cosmological applications, *Astron. Comput.* **27**, 130 (2019), arXiv:1810.12186 [astro-ph.CO].
[30] R. Ciucu, O. F. Hernández, and M. G. Wolman, A convolutional neural network for cosmic string detection in cmb temperature maps (2017).
[31] Y. D. Hezaveh, L. Perreault Levasseur, and P. J. Marshall, Fast Automated Analysis of Strong Gravitational Lenses with Convolutional Neural Networks, *Nature* **548**, 555 (2017), arXiv:1708.08842 [astro-ph.IM].
[32] L. Perreault Levasseur, Y. D. Hezaveh, and R. H. Wechsler, Uncertainties in Parameters Estimated with Neural Networks: Application to Strong Gravitational Lensing, *Astrophys. J.* **850**, L7 (2017), arXiv:1708.08843 [astro-ph.CO].
[33] A. Gupta, J. M. Z. Matilla, D. Hsu, and Z. Haiman, Non-Gaussian information from weak lensing data via deep learning, *Phys. Rev. D* **97**, 103515 (2018), arXiv:1802.01212 [astro-ph.CO].
[34] D. Ribli, B. Árnin Pataki, J. M. Zorrilla Matilla, D. Hsu, Z. Haiman, and I. Csaibai, Weak lensing cosmology with convolutional neural networks on noisy data, arXiv e-prints , arXiv:1902.03663 (2019), arXiv:1902.03663 [astro-ph.CO].
15

[35] J. Fluri, T. Kacprzak, A. Refregier, A. Amara, A. Lucchi, and T. Hofmann, Cosmological constraints from noisy convergence maps through deep learning, Phys. Rev. D98, 123518 (2018), arXiv:1807.08732 [astro-ph.CO].

[36] A. Mathur, D. Bard, P. Mendygral, L. Meadows, J. Arnenmann, L. Shao, S. He, T. Karna, D. Moise, S. J. Pennycook, K. Masoff, J. Sewall, N. Kumar, S. Ho, M. Ringenberg, Prabhat, and V. Lee, CosmoFlow: Using Deep Learning to Learn the Universe at Scale, arXiv e-prints , arXiv:1808.04728 (2018), arXiv:1808.04728 [astro-ph.CO].

[37] N. Perraudin, M. Defferrard, T. Kacprzak, and R. Sgier, DeepspHERE: Efficient spherical convolutional neural network with healpix sampling for cosmological applications, Astronomy and Computing 27, 130 (2019).

[38] A. Doussot, E. Eames, and B. Semelin, Improved supervised learning methods for EoR parameters reconstruction, arXiv e-prints , arXiv:1904.04106 (2019), arXiv:1904.04106 [astro-ph.CO].

[39] N. Gillet, A. Mesinger, B. Greig, A. Liu, and G. Ucci, Deep learning from 21-cm tomography of the cosmic dawn and reionization, mnras 484, 282 (2019), arXiv:1805.02699 [astro-ph.CO].

[40] S. He, S. Ravanbakhsh, and S. Ho, Analysis of cosmic microwave background with deep learning (2018).

[41] J. Caldeira, W. Wu, B. Nord, C. Avestruz, S. Trivedi, and K. Story, Deepcmb: Lensing reconstruction of the cosmic microwave background with deep neural networks, Astronomy and Computing 28, 100307 (2019).

[42] N. Krachmalnicoff and M. Tomasi, Convolutional Neural Networks on the HEALPix sphere: a pixel-based algorithm and its application to CMB data analysis, A&A 628, A129 (2019), arXiv:1902.04083 [astro-ph.IM].

[43] H. U. Norgaard-Nielsen, Excess b-modes extracted from the planck polarization maps, Astronomische Nachrichten 337, 662 (2016).

[44] S. He, Y. Li, Y. Feng, S. Ho, S. Ravanbakhsh, W. Chen, and B. Póczos, Learning to predict the cosmological structure formation, Proceedings of the National Academy of Sciences 116, 13825 (2019).

[45] Y. Kwon, J.-H. Won, B. J. Kim, and M. C. Paik, Uncertainty quantification using bayesian neural networks in classification: Application to biomedical image segmentation, Computational Statistics and Data Analysis 142, 106816 (2020).

[46] G. Pereyra, G. Tucker, J. Chorowski, L. Kaiser, and G. E. Hinton, Regularizing neural networks by penalizing confident output distributions, CoRR abs/1701.06548 (2017), arXiv:1701.06548.

[47] Y. Gal and Z. Ghahramani, Dropout as a Bayesian approximation: Insights and applications, in Deep Learning Workshop, ICML (2015).

[48] N. Srivastava, G. Hinton, A. Krizhevsky, I. Sutskever, and R. Salakhutdinov, Dropout: A simple way to prevent neural networks from overfitting, Journal of Machine Learning Research 15, 1929 (2014).

[49] W. R. Morningstar, Y. D. Hezaveh, L. Perreault Levasseur, R. D. Blandford, P. J. Marshall, P. Putzky, and R. H. Wechsler, Analyzing interferometric observations of strong gravitational lenses with recurrent and convolutional neural networks, arXiv e-prints , arXiv:1808.00011 (2018), arXiv:1808.00011 [astro-ph.IM].

[50] Y. Wen, P. Vicol, J. Ba, D. Tran, and R. Grosse, Flipout: Efficient pseudo-independent weight perturbations on mini-batches, in International Conference on Learning Representations (2018).

[51] Y. Gal and Z. Ghahramani, Bayesian convolutional neural networks with bernoulli approximate variational inference (2015), arXiv:1506.02158 [stat.ML].

[52] I. Osband, J. Aslanides, and A. Cassirer, Randomized Prior Functions for Deep Reinforcement Learning, arXiv e-prints , arXiv:1806.03335 (2018), arXiv:1806.03335 [stat.ML].

[53] C. Guo, G. Pleiss, Y. Sun, and K. Q. Weinberger, On calibration of modern neural networks, in Proceedings of the 34th International Conference on Machine Learning - Volume 70, ICML'17 (JMLR.org, 2017) pp. 1321–1330.

[54] A. D. Kiureghian and O. Ditlevsen, Aleatory or epistemic? does it matter?, Structural Safety 31, 105 (2009), risk Acceptance and Risk Communication.

[55] Y. Gal, Uncertainty in Deep Learning, Ph.D. thesis, University of Cambridge (2016).

[56] N. Tagasovska and D. Lopez-Paz, Single-model uncertainties for deep learning (2018), arXiv:1811.00908 [stat.ML].

[57] A. Graves, Practical variational inference for neural networks, in Advances in Neural Information Processing Systems 24, edited by J. Shawe-Taylor, R. S. Zemel, P. L. Bartlett, F. Pereira, and K. Q. Weinberger (Curran Associates, Inc., 2011) pp. 2348–2356.

[58] G. Wang, W. Li, M. Aertsen, J. Deprest, S. Ourselin, and T. Vercauteren, Aleatoric uncertainty estimation with test-time augmentation for medical image segmentation with convolutional neural networks, Neurocomputing 338, 34 (2019).

[59] J. Fluri, T. Kacprzak, A. Lucchi, A. Refregier, A. Amara, T. Hofmann, and A. Schneider, Cosmological constraints with deep learning from kids-450 weak lensing maps, Phys. Rev. D 100, 063514 (2019).

[60] B. Lakshminarayanan, A. Pritzel, and C. Blundell, Simple and scalable predictive uncertainty estimation using deep ensembles (2016), arXiv:1612.01474 [stat.ML].

[61] Y. Kwon, J.-H. Won, B. Joon Kim, and M. Paik, International conference on medical imaging with deep learning , 13 (2018).

[62] F. Laumann, K. Shridhar, and A. L. Maurin, Bayesian convolutional neural networks, (2018), arXiv:1806.05978.

[63] K. Shridhar, F. Laumann, and M. Liwicki, Uncertainty Estimations by Softplus normalization in Bayesian Convolutional Neural Networks with Variational Inference, arXiv e-prints , arXiv:1806.05978 (2018), arXiv:1806.05978 [cs.LG].

[64] A. Kendall and Y. Gal, What uncertainties do we need in bayesian deep learning for computer vision? (2017), arXiv:1703.04977 [cs.CV].

[65] Y. Gal and Z. Ghahramani, Dropout as a bayesian approximation: Representing model uncertainty in deep learning, in Proceedings of The 33rd International Conference on Machine Learning, Proceedings of Machine Learning Research, Vol. 48, edited by M. F. Balcan and K. Q. Weinberger (PMLR, New York, New York, USA, 2016) pp. 1050–1059.

[66] Y. Gal and Z. Ghahramani, Bayesian convolutional neural networks with Bernoulli Approximate Variational Inference, in 4th International Conference on Learning Representations (ICLR) workshop track (2016).
[67] L. Wan, M. Zeiler, S. Zhang, Y. L. Cun, and R. Fergus, Regularization of neural networks using dropconnect, in *Proceedings of the 30th International Conference on Machine Learning*, Proceedings of Machine Learning Research, Vol. 28, edited by S. Dasgupta and D. McAllester (PMLR, Atlanta, Georgia, USA, 2013) pp. 1058–1066.

[68] M. Aryan, N. H. V., M. Supratak, G. Naveen, and W. C. C., Dropconnect is effective in modeling uncertainty of bayesian deep networks, arXiv e-prints, arXiv:1906.04569 (2019), arXiv:1906.04569 [cs.LG].

[69] P. McClure and N. Kriegeskorte, Robustly representing uncertainty in deep neural networks through sampling, (2016), arXiv:1611.01639 [cs.LG].

[70] K. D. P. and W. Max, Auto-encoding variational bayes, arXiv e-prints, arXiv:1312.6114 (2013), arXiv:1312.6114 [stat.ML].

[71] D. P. Kingma, T. Salimans, and M. Welling, Variational Dropout and the Local Reparameterization Trick, arXiv e-prints, arXiv:1506.02557 (2015), arXiv:1506.02557 [stat.ML].

[72] W. J. T. M. Riccardo, H. Frank, and D. M. Peter, The reparameterization trick for acquisition functions, arXiv e-prints, arXiv:1712.00424 (2017), arXiv:1712.00424 [stat.ML].

[73] https://github.com/JavierOrjuela/BayesianNN_CMB.

[74] A. Zonca, L. Singer, D. Lenz, M. Reinecke, C. Rosset, E. Hivon, and K. Gorski, healpy: equal area pixelization and spherical harmonics transforms for data on the sphere in python, Journal of Open Source Software 4, 1298 (2019).

[75] A. Petri, Mocking the weak lensing universe: The LensTools Python computing package, Astronomy and Computing 17, 73 (2016), arXiv:1606.01903.

[76] https://www.tensorflow.org/.

[77] https://www.tensorflow.org/probability.

[78] https://sonnet.readthedocs.io/en/latest/.

[79] S. Liu and W. Deng, Very deep convolutional neural network based image classification using small training sample size, in *2015 3rd IAPR Asian Conference on Pattern Recognition (ACPR)* (2015) pp. 730–734.

[80] A. Krizhevsky, I. Sutskever, and G. E. Hinton, ImageNet classification with deep convolutional neural networks, in *Proceedings of the 25th International Conference on Neural Information Processing Systems - Volume 1*, NIPS'12 (Curran Associates Inc., USA, 2012) pp. 1097–1105.

[81] S. Ioffe, Batch renormalization: Towards reducing mini-batch dependence in batch-normalized models, in *NIPS* (2017).

[82] D. P. Kingma and J. Ba, Adam: A Method for Stochastic Optimization, arXiv e-prints, arXiv:1412.6980 (2014), arXiv:1412.6980 [cs.LG].

[83] Y. Ovadia, E. Fertig, J. Ren, Z. Nado, D. Sculley, S. Nowozin, J. V. Dillon, B. Lakshminarayanan, and J. Snoek, Can You Trust Your Model’s Uncertainty? Evaluating Predictive Uncertainty Under Dataset Shift, arXiv e-prints, arXiv:1906.02530 (2019), arXiv:1906.02530 [stat.ML].

[84] M. Kull, T. S. Filho, and P. Flach, Beta calibration: a well-founded and easily implemented improvement on logistic calibration for binary classifiers, in *Proceedings of the 20th International Conference on Artificial Intelligence and Statistics*, Proceedings of Machine Learning Research, Vol. 54, edited by A. Singh and J. Zhu (PMLR, Fort Lauderdale, FL, USA, 2017) pp. 623–631.

[85] Y. Gal, J. Hron, and A. Kendall, Concrete Dropout, arXiv e-prints, arXiv:1705.07832 (2017), arXiv:1705.07832 [stat.ML].

[86] B. Zadrozny and C. Elkan, Obtaining calibrated probability estimates from decision trees and naive bayesian classifiers, in *Proceedings of the Eighteenth International Conference on Machine Learning*, ICML ’01 (Morgan Kaufmann Publishers Inc., San Francisco, CA, USA, 2001) pp. 609–616.

[87] B. Zadrozny and C. Elkan, Transforming classifier scores into accurate multiclass probability estimates, in *Proceedings of the Eighth ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, KDD ’02 (ACM, New York, NY, USA, 2002) pp. 694–699.

[88] J. C. Platt, Probabilistic outputs for support vector machines and comparisons to regularized likelihood methods, in *ADVANCES IN LARGE MARGIN CLASSIFIERS* (MIT Press, 1999) pp. 61–74.

[89] V. Kuleshov, N. Fenner, and S. Ermon, Accurate Uncertainties for Deep Learning Using Calibrated Regression, arXiv e-prints, arXiv:1807.00263 (2018), arXiv:1807.00263 [cs.LG].

[90] A. Lewis, Getdist: a python package for analysing monte carlo samples (2019), arXiv:1910.13970 [astro-ph.IM].

[91] J. Sanchez, Mardia, k. v., j. t. kent, j. m. bibby: Multivariate analysis, *Biometrical Journal* 24, 502 (1982).

[92] H. Hotelling, The generalization of student’s ratio, *Ann. Math. Statist.* 2, 360 (1931).

[93] S. Cai, J. Gao, M. Zhang, W. Wang, G. Chen, and B. C. Ooi, Effective and efficient dropout for deep convolutional neural networks, CoRR abs/1904.03392 (2019), arXiv:1904.03392.

[94] C. P. Novaes, A. Bernui, I. S. Ferreira, and C. A. Wuen-sche, A neural-network based estimator to search for primordial non-Gaussianity in Planck CMB maps, *jcap* 2015, 064 (2015), arXiv:1409.3876 [astro-ph.CO].

[95] H. U. Nørgaard-Nielsen, Foreground removal from wmap 5yr temperature maps using an mlp neural network (2010).

[96] H. U. Nørgaard-Nielsen, Confirmation of the detection of b modes in the planck polarization maps, *Astronomische Nachrichten* 339, 432 (2018).

[97] P. Graff, F. Feroz, M. P. Hobson, and A. Lasenby, BAMBI: blind accelerated multimodal Bayesian inference, *mnras* 421, 169 (2012), arXiv:1110.2907 [astro-ph.IM].

[98] B. Phan, R. Salay, K. Czarnecki, V. Abdelzad, T. Denouden, and S. Vernekar, Calibrating Uncertainties in Object Localization Task, arXiv e-prints, arXiv:1811.11210 (2018), arXiv:1811.11210 [cs.LG].

[99] D. Levi, L. Gispan, N. Giladi, and E. Fetaya, Evaluating and Calibrating Uncertainty Prediction in Regression Tasks, arXiv e-prints, arXiv:1905.11659 (2019), arXiv:1905.11659 [cs.LG].

[100] A. D. Cobb, S. J. Roberts, and Y. Gal, Loss-Calibrated Approximate Inference in Bayesian Neural Networks, arXiv e-prints, arXiv:1805.03901 (2018), arXiv:1805.03901 [stat.ML].

[101] D. Hendrycks, K. Lee, and M. Mazeika, Using pretraining can improve model robustness and uncertainty, CoRR abs/1901.09960 (2019), arXiv:1901.09960.

[102] D. Hendrycks, K. Lee, and M. Mazeika, Using pre-training can improve model robustness and uncertainty,
Appendix A: Evaluation of coverage probabilities through binned samples

As mentioned in Sec. V, if the distribution that describes the samples drawn from the posterior is Gaussian, we can compute the coverage probabilities from the ellipsoidal confidence. However, this distribution sometimes is not restricted to be Gaussian, especially for Dropout. In this case, we can follow the method used in [32] and generate a histogram from binned samples drawn from the posterior. Since this histogram is expected to be unimodal, we can compute the interval that contains the (100α)% of the samples around the mode, with α ∈ [0, 1]. Fig. 13 shows the histogram for ωb where we can observe the difference by using both architectures, while Table VI reports the coverage probability for individual parameters. We can observe that the values are consistent with the ones expected for a calibrated network.

| C.I. | VGG-Dropout | Alex-Dropout |
|-----|-------------|--------------|
| 68.3% | 68.1 ± 0.7 | 67.1 ± 0.6 |
| 95.5% | 95.1 ± 0.5 | 94.5 ± 0.6 |
| 99.7% | 99.6 ± 0.5 | 99.4 ± 0.4 |

TABLE VI. Estimation of coverage probabilities corresponding to confidence intervals of 1σ, 2σ and 3σ. AlexNet was trained with 7% dropout rate, while for VGG we used the network calibrated after training.

Fig. 13. Histogram generated from binned samples drawn from the posterior of the parameter ωb using Dropout with the VGG (green) and AlexNet (blue) architectures. The mode for Dropout with VGG is 0.04478 while for the one with AlexNet is 0.04349. The true value is ωb = 0.04492.

Fig. 14. Variation of the mean and variance or “scale” (before applying Softplus) for the approximated posterior in the top panel and for prior in bottom panel during training. (a) Initializer distributions. (b) Distributions for calibrated networks after 300 epochs. (c) and (d) posterior for uncalibrated networks. Colors refer to each layer in the network.

In order to analyze the calibration of BNNs for Flipout and RT methods through their hyper parameters, we need to visualize the behavior of the approximated posterior of the weights during training. The results are shown in Fig. 14. At the beginning, we see that the prior dominates the distribution (see Fig. 14-a), but its evolution will depends on the degree of regularization. For models
without batch normalization and without regularization which underestimate their uncertainties, we observe that the posterior scale moves to small values, as in Fig. 14-c. While in presence of batch normalization, the posterior always tends to produce large variance as we note in Fig. 14-d.

Appendix C: Triangle plots for CMB maps from different BNNs methods

Fig. 15 displays the results for all BNNs methods introduced in this paper. We can observe that the AlexNet architecture does not work well for RT and Dropout, while for RT we obtained low performance with respect to Flipout and Dropout. In Table VII we report the marginalized parameter constraints from the CMB maps. What we can conclude from these results is that the performance for both RT and Dropout depends strongly of the architecture used, as was reported in [51], while for Flipout we do not find this issue. Therefore, Flipout is a more flexible and robust method for obtaining uncertainties at least for CMB dataset.

FIG. 15. Minimal base-ΛCDM 68% and 95% parameter constraint contours from our synthetic CMB dataset using Flipout with Alexnet (blue), VGG (magenta); Dropout with Alexnet (green), VGG (orange); and RT with Alexnet (red), VGG (cyan) architectures. The diagonal plots are the marginalized parameter constraints, the dashed lines stand for the predicted values and the black solid line corresponds to the true values $\omega_b = 0.02590$, $A_s = 3.65653$. 
| Parameter       | HNN          | Drop-Alex    | RT-Alex     |
|-----------------|--------------|--------------|-------------|
| $\omega_b$      | 0.0245$^{+0.0040}_{-0.0039}$ | 0.0247$^{+0.0045}_{-0.0044}$ |              |
| $A_s$           | 3.59$^{+0.12}_{-0.14}$ | 3.63$^{+0.088}_{-0.092}$ |             |
| $\omega_{cdm}$  | 0.137$^{+0.038}_{-0.038}$ | 0.140$^{+0.036}_{-0.037}$ |             |

TABLE VII. Parameter 95\% intervals for the minimal base-$\Lambda$CDM model from our synthetic CMB dataset using RT and Dropout with Alexnet.