COSMOPower-JAX: High-Dimensional Bayesian Inference with Differentiable Cosmological Emulators

D. Piras†,‡ and A. Spurio Mancini‡,⋆

1 Département de Physique Théorique, Université de Genève, 24 quai Ernest Ansermet, 1211 Genève 4, Switzerland and 2 Mullard Space Science Laboratory, University College London, Holmbury St. Mary, Dorking, Surrey, RH5 6NT, UK

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Abstract

We present CosmoPower-JAX, a JAX-based implementation of the CosmoPower framework, which accelerates cosmological inference by building neural emulators of cosmological power spectra. We show how, using the automatic differentiation, batch evaluation and just-in-time compilation features of JAX, and running the inference pipeline on graphics processing units (GPUs), parameter estimation can be accelerated by orders of magnitude with advanced gradient-based sampling techniques. These can be used to efficiently explore high-dimensional parameter spaces, such as those needed for the analysis of next-generation cosmological surveys. We showcase the accuracy and computational efficiency of CosmoPower-JAX on two simulated Stage IV configurations. We first consider a single survey performing a cosmic shear analysis totalling 37 model parameters. We validate the contours derived with CosmoPower-JAX and a Hamiltonian Monte Carlo sampler against those derived with a nested sampler and without emulators, obtaining a speed-up factor of $O(10^3)$. We then consider a combination of three Stage IV surveys, each performing a joint cosmic shear and galaxy clustering (3x2pt) analysis, for a total of 157 model parameters. Even with such a high-dimensional parameter space, CosmoPower-JAX provides converged posterior contours in 3 days, as opposed to the estimated 6 years required by standard methods. CosmoPower-JAX is fully written in Python, and we make it publicly available to help the cosmological community meet the accuracy requirements set by next-generation surveys.

1. INTRODUCTION

Bayesian inference of cosmological parameters from next-generation large-scale structure (LSS) and cosmic microwave background (CMB) surveys such as Euclid (Laureijs et al. 2011),1 the Vera Rubin Observatory (Ivezić et al. 2019)2, the Nancy Grace Roman Space Telescope (Spergel et al. 2015)3, the Simons Observatory (Adé et al. 2019)4, CMB-S4 (Abazajian et al. 2016)5, and CMB-HD (Sehgal et al. 2019)6, will require the exploration of high-dimensional parameter spaces – $O(100)$ parameters and higher – necessary to accurately model the physical signals and their several systematic contaminants. Sampling the posterior distribution in these high-dimensional spaces represents a significant computational challenge for Markov Chain Monte Carlo (MCMC) algorithms (Roberts et al. 1997; Katafygiotis & Zuev 2008; Liu 2009), which are traditionally used in cosmological analyses (Lewis & Bridle 2002; Audren et al. 2013; Brinckmann & Lesgourgues 2019; Torrado & Lewis 2021). Gradient-based inference methods, such as Hamiltonian Monte Carlo (HMC, Duane et al. 1987; Neal 1996) and variational inference (VI, Hoffman et al. 2013; Blei et al. 2017), manage to concentrate the sampling in regions of high posterior mass, even in large parameter spaces, provided one has efficient access to accurate derivatives of the likelihood function with respect to the model parameters (Brooks et al. 2011; Neal 2011; Zhang et al. 2017; Betancourt 2017). Combining differentiable and computationally inexpensive likelihood functions with gradient-based inference techniques is thus crucial to efficiently obtain unbiased posterior distributions in high-dimensional parameter spaces.

Recently, there has been growing interest in the use of machine learning emulators to accelerate cosmological parameter estimation (e.g. Mootoovaloo et al. 2020; Aricò et al. 2022; Zennaro et al. 2021; Nygaard et al. 2022; Günter et al. 2022; Bonici et al. 2022; Eggemeier et al. 2022). Spurio Mancini et al. (2022) (SM22 hereafter), in particular, developed CosmoPower, a suite of neural network emulators of cosmological power spectra that replaces the computation of these quantities traditionally performed with Einstein-Boltzmann solvers such as the Code for Anisotropies in the Microwave Background (CAMB, Lewis & Challinor 2011) or the Cosmic Linear Anisotropy Solving System (CLASS, Blas et al. 2011). In SM22 the authors show how Bayesian inference of cosmological parameters can be accelerated by several orders of magnitude using CosmoPower; the speed-up becomes particularly relevant when the emulators are employed within an inference pipeline that can be run on graphics processing units (GPUs).

An additional advantage in using machine learning emulators is that they efficiently provide accurate derivatives with respect to their input parameters. This is made possible by the automatic differentiation features implemented in the libraries routinely used to build these emulators, such as TensorFlow (Abadi et al. 2015), JAX
In this paper, we first develop an implementation of CosmoPower built using purely JAX primitives. We train the neural network emulators on the same data used in SM22, achieving an accuracy similar to that obtained by the TensorFlow-based implementation of SM22. We additionally compare the derivatives of the power spectra with respect to the input cosmological parameters computed using autodiff against those obtained with numerical differences and CAMB, showing a good agreement overall. We then couple CosmoPower-JAX with jax-cosmo to build likelihood functions completely written using the JAX library; this allows us to run parameter estimation pipelines using gradient-based algorithms on GPUs over very large parameter spaces. In particular, we consider two examples of future Stage IV survey configurations. In the first one, we study a single cosmic shear survey with typical Stage IV specifications; we compare the posterior contours obtained with our JAX-based pipeline against those obtained with a standard pipeline based on CCL, CAMB and the nested sampler PolyChord (Handley et al. 2015a,b). In the second case, we consider a joint analysis of three Stage IV surveys, each carrying out a joint shear - galaxy clustering (3x2pt) analysis. We show how CosmoPower-JAX enables efficient exploration of the 157-dimensional parameter space required for the modelling of the observables at a fraction of the time that would be required with traditional methods. In both experiments, inference is performed using the No U-Turn Sampler (NUTS) HMC variation (Hoffman & Gelman 2014), as implemented in the NumPyro library (Bingham et al. 2019; Phan et al. 2019).

The structure of this paper is as follows. In Sec. 2 we first describe our new JAX emulators and how they are trained on the same data used in SM22. We then review gradient-based methods for posterior inference and describe our JAX-based cosmological likelihoods. In Sec. 3 we validate the accuracy of our emulators and report our inference results in the two simulated Stage IV configurations described above. We conclude in Sec. 4. We make CosmoPower-JAX, which is fully written in Python, publicly available.  

7 https://github.com/dpiras/cosmopower-jax

2. METHODS

2.1. CosmoPower-JAX

CosmoPower is a suite of neural network emulators of cosmological power spectra, namely matter and cosmic microwave background power spectra (albeit the emulation framework is highly flexible and can be used to emulate any other cosmological quantity; see e.g. Burger et al. 2023; Gong et al. 2023). Power spectra represent the key component of 2-point statistics analysis of cosmological fields, and are typically computed by Einstein-Boltzmann solvers such as CAMB or CLASS. These computations usually represent the main bottleneck in parameter estimation pipelines, particularly when high accuracy is required or when the cosmological scenario considered is not standard (see e.g. Spurio Mancini & Pour- sidou 2022; Balkenhol et al. 2022; Bolliet et al. 2023). CosmoPower-JAX is a JAX-based implementation of CosmoPower: as such, it implements the same two emulation methods present in the original CosmoPower software. These are either a direct neural network mapping between cosmological parameters and logarithmic spectra, or a neural network mapping between cosmological parameters and the coefficients of a principal component analysis (PCA) of the spectra; we refer to SM22 for a detailed discussion. In our release version of CosmoPower-JAX these differences are dealt with internally; therefore, the user can simply obtain fast predictions of cosmological power spectra in three lines of code.

The neural networks we employ are made of four layers of 512 nodes each, with the same activation function described in SM22. In the case of the CMB temperature-polarisation and lensing power spectra, we preprocess the spectra using PCA, keeping 512 and 64 components, respectively. We optimise the mean-squared-error loss function using Adam (Kingma & Ba 2015), and keep a constant batch size of 512. The starting learning rate is $10^{-2}$, which we decrease by a factor of 10 (until $10^{-6}$) every time the validation loss does not improve for more than 40 consecutive epochs.

We choose to re-implement and re-train the CosmoPower emulators in JAX to demonstrate that it is possible to build neural networks with this library; nonetheless, in our public implementation of CosmoPower-JAX it is also possible to upload weights and biases from previously-trained models and obtain JAX predictions using only the forward pass of the network. Building the emulators using the JAX library unlocks its automatic-differentiation features, as well as the efficient batch evaluation and just-in-time compilation. Importantly, JAX is built around the popular NumPy library (Harris et al. 2020), which facilitates its use and portability. We refer the reader to Frostig et al. (2018) and Campagne et al. (2023) for a complete description of the features of JAX, especially in the context of cosmological analyses.

2.2. Data

We consider the same datasets as in SM22 to train and validate our emulators. Using CAMB, we produce a total of $\sim 2 \times 10^5$ matter power spectra at 420 wavenumbers in the interval $k \in [10^{-5} - 10] \text{Mpc}^{-1}$ and with varying redshift $z \in [0, 5]$. We consider both the linear matter power spectrum $P_L$ and the non-linear correc-
tion $P_{\delta \delta}^{\text{NL-CORR}}$, such that the non-linear matter power spectrum $P_{\delta \delta}$ can be written as:

$$P_{\delta \delta}(k, z) = P_{\delta \delta}^{\text{NL-CORR}}(k, z) \times P_{\delta \delta}(k, z),$$

where $P_{\delta \delta}^{\text{NL-CORR}}$ is computed with HMC code (Mead et al. 2015, 2016). This non-linear correction introduces two extra baryonic parameters: the minimum halo concentration $c_{\text{min}}$, and the halo bloating $\eta_0$, which we vary when performing Bayesian inference.

Using CAMB we also produce $5 \times 10^5$ CMB power spectra, including the temperature $C^{\text{TT}}$, polarisation $C^{\text{EE}}$, temperature-polarisation $C^{\text{TE}}$ and lensing potential $C^{\text{\phi \phi}}$ power spectra in the interval $\ell \in [2, 2508]$. All emulators are trained on the same parameter range indicated in table 1 of SM22. In both cases, we use $\sim 90\%$ of the data to train the neural networks (of which we leave 10\% for validation), and evaluate the trained models on the remaining $\mathcal{O}(10^3)$ test spectra.

2.3. Gradient-based Bayesian inference

The goal of Bayesian inference is to sample the posterior distribution $p(\theta | d)$ of some parameters $\theta$ given observed data $d$. Bayes’ theorem relates the posterior distribution to the likelihood function $p(d | \theta)$:

$$p(\theta | d) = \frac{p(d | \theta) p(\theta)}{p(d)},$$

where $p(\theta)$ expresses prior knowledge on the parameters $\theta$, and the evidence $p(d)$ is a normalisation factor commonly ignored in parameter estimation tasks.

Drawing from $p(\theta | d)$ requires the use of stochastic samplers to generate a list of samples drawn from the posterior distribution. MCMC and nested sampling algorithms are the two main classes of samplers typically used in cosmological applications. Widely used examples of MCMC methods in cosmology include the Metropolis-Hastings and affine ensemble algorithms (Lewis & Bridle 2002; Lewis 2013; Karamanis et al. 2022; Goodman & Weare 2010; Foreman-Mackey et al. 2013), whereas the most widely adopted nested sampling algorithms are multimodal nested sampling and slice-based nested sampling (Feroz & Hobson 2008; Feroz et al. 2009, 2019; Handley et al. 2015a,b).

Metropolis-Hastings and nested sampling methods can struggle to explore large parameter spaces, since, as the dimensionality increases, sampling from the typical set of the posterior distribution becomes exponentially harder (Betancourt 2017). In these challenging inference scenarios, it is useful to resort to gradient-based algorithms, which manage to concentrate the sampling in regions of high posterior mass despite the large number of model parameters. A popular gradient-based method is Hamiltonian Monte Carlo (HMC, Duane et al. 1987; Neal 1996), which formulates the problem of sampling the posterior distribution as the dynamical evolution of a particle with position $\theta$ and momentum $p$. The Hamiltonian of the system is written as:

$$H(\theta, p) = \frac{1}{2}p^T M^{-1} p + U(\theta),$$

where $M$ is a “mass matrix”, which is assumed to be the covariance matrix of a zero-mean multivariate Gaussian distribution used to sample $p$, and the potential energy $U(\theta)$ is defined as:

$$U(\theta) \equiv -\ln p(\theta | d).$$

Starting from an initial point in the phase space $(\theta, p)$, it is possible to collect samples of the posterior distribution by numerically solving the Hamilton’s equations using a leapfrog algorithm. A new proposed state $(\theta^*, p^*)$ is then either accepted or rejected based on the new energy value $H(\theta^*, p^*)$. HMC can thus be seen as a modification to the original Metropolis-Hastings algorithm, which leverages the analogy with a Hamiltonian system to find a better proposal distribution and results in a higher acceptance rate.

A practical difficulty of HMC is the need for tuning of the hyperparameters governing the leapfrog numerical integration of the Hamiltonian dynamics. These are the number and the size of steps to be taken by the integrator before the sampler changes direction to a new random one. These numbers can be particularly hard to tune and lead to inefficient sampling of the posterior. The No-U-Turn Sampler (NUTS, Hoffman & Gelman 2014) tackles this issue by forcing the sampler to avoid U-turns in parameter space. In particular, rather than fixing the number of integration steps, NUTS adjusts the integration length by running the leapfrog algorithm until the trajectory starts to return to previously-visited regions of the parameter space; while the number of model evaluations increases, this leads to a higher acceptance rate, and therefore to faster and more reliable convergence.

In our experiments, we use the NUTS implementation provided by the NumPyro library (Bingham et al. 2019; Phan et al. 2019). We set the integration step size to $10^{-3}$, and find no difference in the final results by increasing or decreasing this value by one order of magnitude. Additionally, we set the maximum number of model evaluations before sampling a new momentum to $2^7$, and specify a block mass matrix according to the expected correlations among parameters. Finally, to further improve the geometry of the problem we perform a reparameterisation of the inference variables: all of the parameters with a Gaussian prior distribution are centered (Gorinova et al. 2020), while all of those with a uniform prior are rescaled to $U[-5, 5]$. All original prior distributions are reported in Table 1.

We run the NUTS algorithm on three NVIDIA A100 GPUs with 80 GB of memory. Using multiple GPUs allows us to showcase the pmapped feature of JAX to distribute the NUTS chains over multiple GPU devices. We report below an example snippet to run inference over multiple GPUs using NumPyro, where the parallelisation happens simultaneously over a single device and across multiple devices.
In this example, 8 chains are run on each GPU, and the total number of GPUs available is determined at run time.

2.4. Likelihoods

To test the computational efficiency and accuracy of our CosmoPower-JAX emulators, we run examples of cosmological inference on large parameter spaces, such as those that will characterise the analysis of future surveys. We consider a power spectrum analysis of both cosmic shear alone, as well as in cross-correlation with galaxy clustering (3x2pt), which in recent years has become the standard method to combine information on the cosmic shear and galaxy clustering field (e.g. Joachimi & Bridle 2010; Sanchez et al. 2021; Heymans et al. 2021; Abbott et al. 2022). Redshift information is included in the analysis through tomography, assigning galaxies to one of \( N_{\text{bins}}\) bins based on their photometric redshift. The angular power spectra of the probes are jointly modelled computing all of the unique correlations between tomographic bins \( i,j \), weighted by pairs of window functions \( W \) and redshift \( z \). In the following we briefly review the modelling of the power spectra for cosmic shear, galaxy clustering and their cross-correlation (“galaxy-galaxy lensing”), as well as describe the Stage IV surveys we take into consideration. We follow the notation of SM22.

Angular power spectra for the three probes can be expressed as integrals of the matter power spectrum \( P_{\delta \delta}(k, z) \) (a function of wavevector \( k \) and redshift \( z \)), weighted by pairs of window functions \( W \) for the shear \( (\gamma) \), clustering \( (n) \) and intrinsic alignment \( (I) \) fields:

\[
C_{ij}^{AB}(\ell) = \int_0^{\chi_m} d\chi \frac{W_i^A W_j^B}{\chi^2} P_{\delta \delta} \left( k = \frac{\ell + 1/2}{\chi}, z \right),
\]

where \( \{A,B\} = \{\gamma,n,I\} \), \( \chi \) is the comoving distance (itself a function of redshift), and the upper limit of integration is the Hubble radius \( \chi_H = c/H_0 \), with \( c \) the speed of light and \( H_0 \) the Hubble constant. In Eq. (5) we assumed the extended Limber approximation (LoVerde & Ashordi 2008) which connects Fourier scales \( k \) with angular multipoles \( \ell \).

The angular power spectrum \( C_{ij}^{\gamma}(\ell) \) of the cosmic shear signal for tomographic bins \( i,j \) is a combination of a pure shear contribution and an intrinsic alignment contamination:

\[
C_{ij}^{\gamma}(\ell) = C_{ij}^{\gamma}(\ell) + C_{ij}^{\gamma}(\ell) + C_{ij}^{\gamma}(\ell) + C_{ij}^{\gamma}(\ell). \tag{6}
\]

For a tomographic redshift bin distribution \( n_{i,\text{source}}(z), i = 1, \ldots, N_{\text{bins}} \), the weighting function

\[
W_i^{\gamma}(\chi) \text{ for the cosmic shear field } \gamma \text{ is given by:}
\]

\[
W_i^{\gamma}(\chi) = \frac{3 H_0^2 \Omega_m}{2 c^2} \int_0^\chi d\chi' n_{i,\text{source}}(\chi') \frac{\chi' - \chi}{\chi'}, \tag{7}
\]

where \( \Omega_m \) is the matter density parameter and \( a \) is the scale factor. To model the window function for the intrinsic alignment field \( I \), we start from the commonly-used non-linear alignment model (Hirata & Seljak 2004; Joachimi et al. 2011):

\[
W_i^I(\chi) = -A_{IA} \left( 1 + z_a \right)^{n_{i,\text{source}}(\chi)}, \tag{8}
\]

with two free parameters \( A_{IA} \) and \( n_{IA} \); the linear growth

\[
\begin{array}{lll}
\text{Parameter} & \text{Prior range} & \text{Fiducial value} \\
\hline
\omega_b & \mathcal{U}(0.01875, 0.02625) & 0.02242 \\
\omega_{cdm} & \mathcal{U}(0.05, 0.255) & 0.11933 \\
\eta_0 & \mathcal{U}(0.64, 0.82) & 0.6766 \\
\ln 10^{10} A_b & \mathcal{U}(1.61, 3.91) & 3.047 \\
\end{array}
\]

\begin{tabular}{lll}
\hline
\text{Cosmology} & \\
\hline
\omega_b & \mathcal{U}(0.01875, 0.02625) & 0.02242 \\
\omega_{cdm} & \mathcal{U}(0.05, 0.255) & 0.11933 \\
\eta_0 & \mathcal{U}(0.64, 0.82) & 0.6766 \\
\ln 10^{10} A_b & \mathcal{U}(1.61, 3.91) & 3.047 \\
\end{tabular}

\begin{tabular}{lll}
\hline
\text{Baryons} & \\
\hline
\omega_b & \mathcal{U}(0.01875, 0.02625) & 0.02242 \\
\omega_{cdm} & \mathcal{U}(0.05, 0.255) & 0.11933 \\
\eta_0 & \mathcal{U}(0.64, 0.82) & 0.6766 \\
\ln 10^{10} A_b & \mathcal{U}(1.61, 3.91) & 3.047 \\
\end{tabular}

\begin{tabular}{lll}
\hline
\text{Vacuum} & \\
\hline
\omega_b & \mathcal{U}(0.01875, 0.02625) & 0.02242 \\
\omega_{cdm} & \mathcal{U}(0.05, 0.255) & 0.11933 \\
\eta_0 & \mathcal{U}(0.64, 0.82) & 0.6766 \\
\ln 10^{10} A_b & \mathcal{U}(1.61, 3.91) & 3.047 \\
\end{tabular}

Table 1: Prior distributions and fiducial values of the cosmological and nuisance parameters for the simulated analyses performed in this work. Uniform (Gaussian) prior distributions are indicated with \( \mathcal{U} \) (\( \mathcal{N} \)). For the cosmological parameters and the baryonic feedback parameters (\( \epsilon_{\min}, \eta_0 \)) the prior range corresponds to the range of validity of our emulators. The superscripts S1, S2 and S3 refer to three simulated Stage IV surveys, whose details we discuss in Sect. 2.4.
Finally, the galaxy-galaxy lensing power spectrum is given by

\[ C_{ij}^\ell (\chi) = C_{ij}^{\gamma\gamma} (\ell) + C_{ij}^{\gamma I} (\ell) . \]  

The first experiment we run is a simulated cosmic shear analysis of a Stage IV survey (dubbed “S1”). We assume 10 tomographic bins for \( n_{\text{source}}(z) \), with galaxies following the distribution:

\[ n(z) \propto z^2 \exp \left( - (z/z_0)^{1.5} \right) . \]  

with \( z_0 = 0.64 \) (Smail et al. 1994; Joachimi & Bridle 2010). We consider a Gaussian covariance matrix (e.g. Tutusaus et al. 2020) with a sky fraction \( f_{\text{sky}} = 0.35 \), a surface density of galaxies \( n_{\text{source}} = 30 \) galaxies per arcmin\(^2\), and an observed ellipticity dispersion \( \sigma_\epsilon = 0.3 \). The \( C(\ell) \) spectra are computed for 30 bin values between \( \ell_{\text{min}} = 30 = \ell_{\text{max}} = 3000 \).

We use the nested sampler PolyChord to sample the posterior distribution and run the inference pipeline within Cobaya (Lewis 2013). To compute the theoretical predictions for the cosmological observables we use the Cosmo Core Cosmology Library (CCL, Chisari et al. 2019). The three upper blocks of Table 1 summarise the prior distributions assumed for the parameters used in this analysis. These include:

- five standard ΛCDM cosmological parameters, namely the baryon density \( \omega_b = \Omega_b h^2 \), the cold dark matter density \( \omega_cdm = \Omega_cdm h^2 \), the Hubble parameter \( h \), the scalar spectral index \( n_s \), and the primordial power spectrum amplitude \( \ln 10^{10} A_s \);
- the ΛCDM parameters \( c_{\text{min}} \), \( \eta_0 \);
- one intrinsic alignment amplitude \( A_{IA} \) for each of the ten redshift bins;
- one shift parameter \( D_{z_{\text{source}}} \) for each of the ten source redshift distributions;
- one multiplicative bias coefficient \( m \) for each of the ten redshift bins,

for a total of 37 model parameters.

We run a second experiment in which we consider the joint analysis of three surveys, dubbed “S1”, “S2” and “S3”, each one performing a 3x2pt analysis over 10 redshift bins over different \( z \) ranges, \( n_{\text{source}}(z) \) and \( n_{\text{lens}}(z) \) are sampled from Eq. (12), with different galaxy densities \( n_{\text{source}} \) and \( n_{\text{lens}} \) reported in Table 2. In this analysis, the cosmological and baryon parameters are unique, while each survey has its own set of nuisance parameters to model redshift distribution shifts, multiplicative biases and galaxy bias. With respect to the cosmic shear analysis, for each survey we add:

- one shift parameter \( D_{z_{\text{lens}}} \) for each of the ten lens redshift distributions;
- one linear galaxy bias coefficient \( b \) for each of the ten redshift bins,

for a total of 157 parameters. The prior distributions and fiducial values of the nuisance parameters for all surveys are reported in Table 1, while we report all survey specifications in Table 2.

### 3. RESULTS

#### 3.1. Emulator accuracy

Having used the same dataset and training settings, the accuracy of our JAX emulators is in excellent agreement with the results presented in SM22, i.e. the difference with respect to the CAMB test spectra is always

<table>
<thead>
<tr>
<th>( f_{\text{sky}} )</th>
<th>0.35</th>
<th>0.05</th>
<th>0.45</th>
</tr>
</thead>
<tbody>
<tr>
<td>( n_{\text{source}} ) [gal/arcmin(^2)]</td>
<td>30</td>
<td>50</td>
<td>50</td>
</tr>
<tr>
<td>( n_{\text{lens}} ) [gal/arcmin(^2)]</td>
<td>40</td>
<td>55</td>
<td>60</td>
</tr>
<tr>
<td>( \sigma_\epsilon )</td>
<td>0.30</td>
<td>0.25</td>
<td>0.35</td>
</tr>
</tbody>
</table>

Table 2: Specifications for the three Stage IV surveys S1, S2 and S3 that we consider in this work. All details can be found in Sect. 2.4.
Figure 1. Derivatives of the matter power spectrum components as defined in Eq. (1) with respect to cosmological parameters for random samples in the test set. Solid red lines represent finite differences calculated using CAMB and a five-point stencil as in Eq. (13), while dashed blue lines are obtained with the CosmoPower-JAX emulator and automatic differentiation (autodiff). A single derivative computed with finite differences requires $O(10)$ s, as opposed to the $O(0.1)$ s required for the derivatives with respect to all cosmological parameters obtained using CosmoPower-JAX.

Figure 2. Same as in Fig. 1 for the CMB temperature power spectrum $C_{\ell}^{TT}$. 
Figure 3. Inference results for the cosmic shear analysis of a simulated Stage IV survey with a total of 37 parameters. The contours show the 68% and 95% credibility contours and 1-D marginals for all of the parameters. The inset table reports the plot range and corresponding parameter name of every axis symbol; all parameters are described in Sect. 2.4, while in Table 1 we report the prior distributions and fiducial values. The contours in blue are obtained with the No U-Turn Sampler (NUTS) combined with our CosmoPower-JAX emulators. The contours in red are produced using the PolyChord sampler together with the Boltzmann code CAMB. The CosmoPower-JAX results are obtained over 3 graphics processing units (GPUs) in about 1 day, while the PolyChord+CAMB chain ran on 48 CPU cores for about 4 months, so that the total speed-up factor in terms of CPU/GPU hours is $O(10^3)$. When replacing CAMB with the original CosmoPower emulator (Spurio Mancini et al. 2022), we obtain the contours in grey, which required about 8 days on 48 CPU cores, and show an excellent agreement overall. All of the contours shown in this paper are plotted using GetDist (Lewis 2019).
sub-percent for both the matter power spectrum and the CMB probes. We do not show the accuracy plots here for brevity, and refer the reader to SM22 for an extended comparison.

In Fig. 1 we then compare the derivatives of the linear matter power spectrum and the non-linear boost with respect to cosmological parameters, using CAMB and finite differences with a five-point stencil as a benchmark. These numerical derivatives rely on a simple Taylor expansion of the function $f(x)$ being considered, and are calculated as:

$$f'(x) \simeq -f(x + 2s) + 8f(x + s) - 8f(x - s) + f(x - 2s),$$

where $s$ is a small step size. We choose the step size for each derivative by ensuring that the numerical derivative would only change at the sub-percent level, or within machine precision, when increasing or decreasing $s$ by one order of magnitude.

The derivatives computed by our JAX emulators are efficient to obtain and show excellent agreement with the numerical ones, despite the latter being prone to numerical instabilities due to the choice of the step size. A single derivative of the linear matter power spectrum with finite differences takes $O(10)$ s on a CPU core, since it requires four independent calls to CAMB. On the other hand, on the same CPU core we can obtain derivatives with respect to all cosmological parameters and for batches of tens of spectra in $O(0.1)$ s; we expect the speed-up to be even more substantial when running on GPU. In Fig. 2 we repeat this comparison for the $C_l^{TT}$ power spectrum, showing again good agreement and high computational efficiency for all cosmological parameters.

### 3.2. Bayesian inference

Here we present and comment on the results of running our gradient-based inference pipelines. We emphasise that, while the survey configurations that we consider are representative of the ones expected from upcoming surveys, our goal is not to obtain official forecast predictions, but rather to focus on the challenge represented by the large parameter space required by these analyses, and how to implement viable solutions to efficiently explore these spaces.

In Fig. 3 we show the posterior contours for the cosmological and nuisance parameters in the case of a cosmic shear analysis of a single Stage IV-like survey. The results obtained with NUTS and the CosmoPower-JAX emulators on three GPUs in one day are in excellent agreement with those yielded by the PolyChord sampler using CAMB and CCL, which however require about 4 months on 48 2.60 GHz Intel Xeon Platinum 8358 CPU cores. The total speed-up factor is then $O(10^3)$ in terms of CPU/GPU hours, and $O(10^3)$ in terms of actual elapsed time. We also run PolyChord with the original CosmoPower emulator (written using TensorFlow) on the same 48 CPU cores, obtaining overlapping contours in about 8 days. This suggests that a $O(10)$ acceleration is provided by the neural emulator, with the NUTS sampler and the GPU hardware providing the remaining $O(10)$ speed-up (in terms of the actual elapsed time).

In Fig. 4 and Fig. 5 we then show the posterior contours for the 7 cosmological parameters and the 150 nuisance parameters, respectively, of the joint analysis of the three Stage IV-like surveys described in Sect. 2.4. Obtaining the corresponding contours using PolyChord and CAMB would be extremely computationally expensive: optimistically, assuming a linear (rather than exponential, see e.g. Bishop 1995) scaling of the run time with the number of inference parameters, we would expect to be able to obtain such contours in at least 6 years on

<table>
<thead>
<tr>
<th>Parameter</th>
<th>$\omega_b$</th>
<th>$\omega_{cdm}$</th>
<th>$h$</th>
<th>$n_s$</th>
<th>$\ln(10^{10}A_s)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>0.02</td>
<td>$2 \cdot 10^{-5}$</td>
<td>$1 \cdot 10^{-5}$</td>
<td>$2 \cdot 10^{-5}$</td>
<td>$4 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>(b)</td>
<td>0.1</td>
<td>$2 \cdot 10^{-5}$</td>
<td>$1 \cdot 10^{-5}$</td>
<td>$2 \cdot 10^{-5}$</td>
<td>$3 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>(c)</td>
<td>0.02</td>
<td>0.02</td>
<td>0.02</td>
<td>0.03</td>
<td>0.03</td>
</tr>
<tr>
<td>(d)</td>
<td>0.03</td>
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**Table 3:** Effective sample size per likelihood call (in percentage) $\eta$, as defined in Eq. (14), for: (a) PolyChord+CAMB, cosmic-shear only; (b) PolyChord+CosmoPower, cosmic-shear only; (c) NUTS+CosmoPower-JAX, cosmic-shear only; (d) NUTS+CosmoPower-JAX, joint analysis. Except for $\omega_b$, which is unconstrained in the case of the cosmic shear analysis, the combination of NUTS and CosmoPower-JAX yields values of $\eta$ higher by up to three orders of magnitude, confirming the higher efficiency of the sampling approach.

![Figure 4](image_url)  
**Figure 4.** Inference results for the joint analysis of three simulated Stage IV surveys, each performing a 3x2pt analysis, for a total of 157 model parameters. Here we show the posterior contours for the cosmological parameters, while we report the marginal distribution of the nuisance parameters in Fig. 5. The blue contours represent the 68% and 95% credibility contours and 1-D marginals. These are obtained with the No U-Turn Sampler (NUTS) combined with our CosmoPower-JAX emulators in about 3 days on 3 graphics processing units (GPUs). Dashed grey lines represent the fiducial values, reported in Table 1 together with the prior distributions.
Figure 5. Marginal posterior distributions obtained in about 3 days on 3 graphics processing units (GPUs) with our CosmoPower-JAX emulators and the No U-Turn Sampler (NUTS) for the nuisance parameters of the joint analysis of three simulated Stage IV surveys. Each survey performs a 3x2pt analysis, for a total of 157 parameters. The corresponding cosmological constraints can be found in Fig. 4. Dashed grey lines represent the fiducial values, reported in Table 1 together with the prior distributions.
48 CPU cores. Therefore, we only show the results with NUTS and CosmoPower-JAX, which we obtain in about 3 days over 3 GPUs, for a total speed-up factor of $O(10^4)$ in terms of CPU/GPU hours. These results are unbiased and in good agreement with the fiducial values of our analysis.

We further quantify the efficiency of the different sampling approaches by computing the effective number of samples per likelihood call, namely:

$$\eta = \frac{n_{\text{eff}}}{n_{\text{eval}}} ,$$  \hspace{1cm} (14)

where $n_{\text{eff}}$ is the effective sample size (ESS), computed with the ArviZ library (Kumar et al. 2019), and $n_{\text{eval}}$ is the total number of likelihood calls. As we report and discuss in Table 3, $\eta$ is almost always $O(10^3)$ times bigger when using the NUTS sampler with CosmoPower-JAX with respect to the PolyChord sampler, and does not degrade even when considering 157 inference parameters.

4. CONCLUSIONS

We presented CosmoPower-JAX, a JAX-based implementation of the cosmological neural emulator CosmoPower (Spurio Mancini et al. 2022). CosmoPower-JAX adopts the same emulation methods of the original TensorFlow-based version of CosmoPower, but implements them using the JAX library. The key feature of JAX is the ability to automatically differentiate functions written in common Python libraries, such as NumPy. Additionally, JAX allows NumPy software to be dynamically compiled, evaluated in batch, and run on graphics processing units (GPUs) and tensor processing units (TPUs). In this paper, we made use of these JAX features to show how they can accelerate Bayesian cosmological inference by orders of magnitude.

We started by training a set of CosmoPower-JAX emulators of matter and cosmic microwave background (CMB) power spectra, using the same datasets of Spurio Mancini et al. (2022). We compared the accuracy of our JAX-based emulators with the Boltzmann code CAMB, showing excellent agreement both at the power spectra level as well as at the level of their derivatives. Crucially, rather than being obtained with finite differences, which are prone to numerical instabilities and require fine-tuning of the step size, derivatives of the power spectra with CosmoPower-JAX are obtained straightforwardly and efficiently with the built-in automatic differentiation (autodiff) features provided by JAX. We note that the usefulness of our differentiable power spectra emulators is not limited to 2-point-statistics analyses of cosmological fields: for example, field-level inference pipelines (e.g. Makinen et al. 2021, 2022; Loureiro et al. 2023; Porqueres et al. 2023) greatly benefit from efficient access to power spectra and their gradients.

We combined our emulators with the JAX-based cosmological library jax-cosmo (Campagne et al. 2023) to write likelihood functions that are fully differentiable by virtue of their pure-JAX implementation. Running these likelihoods within inference pipelines using gradient-based Monte Carlo algorithms like the No U-Turn Sampler (NUTS), we showed how to use CosmoPower-JAX to perform cosmological Bayesian inference over parameter spaces with $O(100)$ parameters, using multiple graphics processing units (GPUs) in parallel.

We performed a cosmic shear analysis for a Stage IV-like survey configuration with a total of 37 parameters, showing good agreement with standard nested sampling inference performed with CAMB, while being $O(10^3)$ times faster. We finally showed that with CosmoPower-JAX and NUTS it is possible to perform a combined Bayesian inference on three different Stage IV-like surveys, each performing a joint cosmic shear and galaxy clustering analysis (3x2pt), for a total of 157 parameters, of which 150 represent nuisance parameters used to model systematic effects for each survey. We obtained unbiased posterior contours in about 3 days on 3 GPUs, as opposed to an optimistic estimate of at least 6 years needed to obtain the same results with traditional sampling methods and standard Boltzmann codes, for a total speed-up factor of $O(10^4)$ in terms of CPU/GPU hours.

Developing fully differentiable, GPU-accelerated implementations of key analysis pipelines is of the utmost importance to tackle the massive computational requirements imposed by upcoming Stage IV surveys. To this purpose, we envision the use of differentiable libraries such as TensorFlow, JAX and PyTorch to become standard practice in cosmological software implementations, not least because they can all be used within the Python programming language, which is becoming the de facto standard programming language in both the cosmological and machine learning communities.

Libraries such as CosmoPower-JAX and jax-cosmo are therefore of paramount importance for the success of next generation surveys. To this purpose, we plan to integrate the public release of CosmoPower-JAX with the jax-cosmo library. In parallel, we will explore improved gradient-based posterior samplers, such as those described in Ver Steeg & Galstyan (2021); Park (2021); Robnik et al. (2022); Wong et al. (2023), to further improve the sampling efficiency, and thus the usefulness of our differentiable emulators.

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DATA AVAILABILITY

We make the CosmoPower-JAX emulators available in this GitHub repository (https://github.com/dpiras/cosmopower-jax, also accessible by clicking the icon [github](https://github.com/dpiras/cosmopower-jax)).
This paper was built using the Open Journal of Astrophysics \LaTeX{} template. The OJA is a journal which