Neutrino oscillation parameter sampling with MonteCUBES

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Abstract

We present MonteCUBES (“Monte Carlo Utility Based Experiment Simulator”), a software package designed to sample the neutrino oscillation parameter space through Markov Chain Monte Carlo algorithms. MonteCUBES makes use of the GLoBES software so that the existing experiment definitions for GLoBES, describing long baseline and reactor experiments, can be used with MonteCUBES. MonteCUBES consists of two main parts: The first is a C library, written as a plug-in for GLoBES, implementing the Markov Chain Monte Carlo algorithm to sample the parameter space. The second part is a user-friendly graphical Matlab interface to easily read, analyze, plot and export the results of the parameter space sampling.

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After the firm establishment of neutrino oscillations from solar [1, 2, 3, 4, 5, 6], atmospheric [7, 8], reactor [9, 10, 11, 12] and accelerator [13, 14, 15] experiments, neutrino physics will enter a new precision age with future facilities aiming to measure the subleading unknown mixing parameters, such as $\theta_{13}$ and the $CP$-violating phase $\delta$ [16]. These forthcoming neutrino oscillation experiments, with unprecedented sensitivities, might also test new physics in the neutrino sector beyond the present constraints. It is then desirable to study the sensitivities of neutrino oscillation experiments to these non-standard parameters together with the improved constraints on the known mixing angles and mass squared differences and the possible correlations between the two.

The task of studying the combined sensitivity of neutrino facilities to both standard and new physics parameters and the degeneracies between them becomes prohibitively expensive in computer time as the number of parameters increases. Thus, it is common to “switch on” these new physics parameters only one or two at a time, which does not allow the exploration of correlations and degeneracies among them. In order to address this problem, we propose the use of Markov Chain Monte Carlo (MCMC) algorithms to explore these large parameter spaces (see, e.g., Ref. [17]). Contrary to sampling the $N$-dimensional parameter space through grids with $n$ samplings per parameter, which require $O(n^N)$ evaluations of the expected number of events and $\chi^2$ for the considered setup, the number of computations that MCMC sampling requires in order to achieve good convergence grows at most polynomially with $N$.

MonteCUBES [18] ("Monte Carlo Utility Based Experiment Simulator") contains a C library plug-in to implement MCMC sampling into the GLoBES [19, 20] software. It thus benefits from the flexibility of GLoBES in defining different experiments while implementing an efficient scanning of large parameter spaces. In addition to the MCMC sampling, MonteCUBES includes an intuitive and user-friendly graphical Matlab interface to interpret, plot and export the results of the MCMC sampling. It also incorporates a method to locate degenerate solutions in a simple way in order to tune the step proposal function of the MCMC sampling to efficiently explore all the degenerate solutions, with the correct weights, in the same run.

Not exclusive to the MCMC oriented functionalities of MonteCUBES, we have added two
extra utilities. The first is the implementation of two new physics scenarios: the NonUnitarity Engine (NUE), which allows the treatment of parameters describing the deviation from unitarity of the leptonic mixing matrix; and the non-Standard Interaction Event Generator Engine (nSIEGE), which describes non-standard neutrino interactions in matter. Calling these engines adds the dependence of the oscillation probabilities on the extra parameters along with useful functions in order to set their values and fix or free the several new parameters in the minimization algorithms and the MCMC samplings. The second functionality added is the possibility of specifying the observed number of events of a given experiment instead of computing them from the assumed “true” oscillation parameters. This allows the usage of GLoBES and MonteCUBES to analyze, not only forecasted data, but also real experimental data and study the resulting constraints on the neutrino oscillation parameters. Clearly, this feature requires extreme care when designing the experiment definition files in order for the experiment definition to coincide with the actual experiment.

II. MARKOV CHAIN MONTE CARLOS

Parameter determination through MCMC methods are based on Bayesian inference. The aim is to determine the probability distribution function (PDF) of the different model parameters $\theta$ given some data set $d$, i.e., the posterior probability $P(\theta|d)$. From Bayes’ theorem we have:

$$P(\theta|d) = \frac{P(d|\theta)P(\theta)}{P(d)} = \frac{L_d(\theta)\pi(\theta)}{M}.$$  

(1)

The starting point is the likelihood $L_d(\theta) = P(d|\theta)$, i.e., the probability of observing the data set $d$ given certain values of the parameters $\theta$. The prior $\pi(\theta) = P(\theta)$ is simply the probability of the parameters having the value $\theta$ regardless of the data $d$, i.e., our previous assumed knowledge of the parameters. Finally, the marginal probability $M$ is the probability $P(d)$ of measuring the values $d$. It does not depend on the parameters $\theta$ and can be disregarded as a normalization constant $M = \int L_d(\theta)\pi(\theta)d\theta$, which cancels when comparing the relative probabilities of different parameter values through the ratio of the posteriors.\(^1\)

Thus, in order to compare the relative posterior PDFs of different sets of parameters $\theta_1$\(^1\)

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\(^1\) This normalization is, however, the key parameter in Bayesian model selection \[21\].
and $\theta_2$ given the data $d$, we must compute the ratio

$$\frac{L_d(\theta_1)\pi(\theta_1)}{L_d(\theta_2)\pi(\theta_2)}.$$  \hspace{1cm} (2)

The $\chi^2$ functions defined in GLoBES actually provide the logarithm of the likelihood of the data $d$ following a Poisson distribution normalized to the distribution with mean $d$. Thus, computing the exponential of the difference between these GLoBES functions for $\theta_1$ and $\theta_2$ gives the desired likelihood ratio.

A. The algorithm

The aim of the MCMC is to create a Markov Chain that has the desired distribution (the posterior PDF for the oscillation parameters) as its equilibrium distribution. The most popular implementation, and the one used in MonteCUBES, is the Metropolis–Hastings algorithm. At each step, the chain moves from a point in the parameter space $\theta_1$ to another $\theta_2$ with a transition probability $T(\theta_1, \theta_2)$. This transition probability is the product of the proposal function $W(\theta_1, \theta_2)$ times the probability of accepting the new step:

$$\alpha(\theta_1, \theta_2) = \min \left( 1, \frac{P(\theta_2|d)W(\theta_2, \theta_1)}{P(\theta_1|d)W(\theta_1, \theta_2)} \right).$$  \hspace{1cm} (3)

This algorithm ensures that detailed balance

$$P(\theta_2|d)T(\theta_2, \theta_1) = P(\theta_1|d)T(\theta_1, \theta_2)$$  \hspace{1cm} (4)

is satisfied (while maximizing the acceptance) and thus, $P(\theta|d)$ is the equilibrium distribution of the chain.

In the original Metropolis algorithm, as well as in the default implementation of MonteCUBES, the proposal function $W(\theta_1, \theta_2)$ is symmetric so that the probability $\alpha(\theta_1, \theta_2)$ of accepting the new proposed step is simply given by the ratio of the posteriors, i.e., the exponential of the difference of the $\chi^2$ provided by GLoBES plus the prior.

In addition to using Gaussian proposal functions, MonteCUBES provides an easy way of treating degeneracies by changing the proposal function by randomly adding or subtracting steps with the correct length in the direction between the degeneracies. MonteCUBES can automatically search for degeneracies by increasing the temperature of the chain $T$ so that the likelihood is modified to $L_T \propto L^{1/T}$. This procedure flattens the likelihood distribution.
so that the chains can move between the different degeneracies. The temperature and step sizes are then decreased in successive steps and thus the different chains get stuck around different minima, unable to move through the disfavored regions when $T$ is too low. Finally, the points where the different chains have stopped are compared to decide how many different minima the chains have fallen into and a minimization of the log-likelihood is performed from those starting values so that the minima are reached. The difference between the minima, located in this manner, can then be used in the proposal function. Thus, when performing the MCMC sampling of the parameter space, the chains can jump freely between the degeneracies and sample them with the correct relative weights. Finally, the standard MonteCUBES proposal function can be replaced by an arbitrary user-defined proposal function, which does not necessarily need to be symmetric (as long as the user also implements the proper transition ratio function).

B. Interpreting the results

To test the convergence of the chains we use the method proposed in Ref. [22] with convergence criteria that can be specified by the user. The key parameter that controls the convergence speed and how well the chains will sample the distribution is the typical step sizes of the proposal function $W(\theta_1, \theta_2)$. Optimal step sizes are of the order of the expected $1\sigma$ allowed region.

If the steps are too small, the chains will sample small areas of the parameter space and take a very long time to cover the whole region of interest. Different chains will sample different regions, depending on their starting values, and will give different estimates of the means of the parameters, translating to very bad convergence. A good diagnose of too short a step in a given parameter is a long correlation length between the values sampled for this parameter as the chains progresses.

If the steps are too large, the chains will often propose jumps to regions of the parameter space which are very disfavored and the probability of accepting the step will be very small, requiring a long time to accumulate enough statistics to properly analyse the sampled probability. A good diagnose of too large steps is that the chains stop too many times at each accepted point.

The output of the MCMC sampling is several chain files, containing a list of the accepted
points in the parameter space together with the weight (the number of times the chain stayed at that point), since the equilibrium density of the chain is \( P(\theta) \) the density of points in the parameter space given by the chains will be proportional to the posterior probability we want to sample. Thus, simply binning the parameter space and distributing the points of the chains in their corresponding bins will provide the relative posterior probabilities of each bin in the multidimensional parameter space. Notice that the marginalization over nuisance parameters does not require a time-consuming minimization but is simply achieved by ignoring the corresponding parameters, effectively projecting the posterior PDF to the parameter subspace of interest.

### III. THE GRAPHIC USER INTERFACE

Even if the interpretation and analysis of the chains is straightforward, as outlined in the previous section, processing them can be cumbersome. For this task MonteCUBES includes an intuitive Matlab Graphic User Interface (GUI) that allows to read, combine, analyze, plot and export the results of the MCMC sampling. After opening the GUI the user can select the results of the run to be analyzed by opening the corresponding summary file generated by MonteCUBES together with the chains. The summary file contains the relevant information on the number of chains, number of samples, free parameters and convergence criteria required to properly read and analyze the results of the chains. After reading the summary file the GUI reads and processes the corresponding chains. The user can then either combine chains from further runs to increase the statistics of the chains or plot the results in several ways. The following plotting options are included in the GUI:

- **1D Histogram:** This plots a histogram of the number of points in the chains as a function of the parameter selected by the user in a range and with a number of bins that can be user-specified. The main application of this plot is to diagnose how well the chains have converged and sampled the chosen parameter. The histogram should resemble a Gaussian centered at the most likely value of the parameter or some multimodal distribution if that particular parameter presents degeneracies.

- **1D chain progression:** This plot also diagnoses the convergence and how well a parameter has been sampled. It plots the consecutive values of a parameter which
the chains have visited. For well sampled and converged chains these plots should resemble “white noise”, any residual correlation length in the form of oscillations in these plots indicate a poor sampling of the parameter and the typical size of the steps in the proposal function may need to be changed (typically increased) to achieve better sampling. Notice that the chain convergence can be defined in a quantitative way and that MonteCUBES can test the convergence of all the parameters in the chains and continue the sampling until the desired level of convergence is achieved. However, these plots constitute a useful tool to determine how to tune the steps in the proposal function to speed up the convergence of the chains and obtain better sampling of the parameter space.

- **1D confidence region:** This plots the posterior distribution marginalized in all the parameters except the one selected and highlights the most favored region at a user-defined confidence level.

- **2D scatter:** This draws a scatter plot in the specified parameters of the points which the chains have sampled. This can also be a good diagnosis of bad sampling, since the plot should be uniform with clearly visible denser regions corresponding to the best fit values that gradually thin when moving away from the favored area.

- **2D confidence contours:** This plots the isoprobability contours at the specified confidence levels for the specified parameters.

- **Triangle plot:** This option plots together the 1D confidence region and all the possible 2D confidence contours for a set of selected parameters.

- **3D surface:** This plots the isoprobability surface in the specified three parameters at the chosen confidence level.

For all of the above plotting options, except the two latter\(^2\), there is also the option of exporting the high-level data for the plots into text files. This functionality is provided so that the user can plot the data in a different graphical program if desirable.

\(^2\) All the plots from the triangle plot can be reproduced using the 1D confidence region and 2D confidence contour plots, while the 3D surface plot is not really suitable for the exporting of data.
In addition, all of the plotting functions provide the user with the choice of plotting the results against arbitrary transformations of the oscillation parameters. Since the Jacobian of these transformations may not be constant, the user-interface also provides the possibility of specifying an arbitrary weight function in order to compensate. This also allows to change the prior post-simulation.

IV. NEW PHYSICS IMPLEMENTATIONS

The MonteCUBES distribution includes two GLoBES implementations of new physics. Both of these contain nine extra parameters in addition to the six standard neutrino oscillation parameters. Thus, these scenarios are ideally suited for MCMC exploration of the parameter space, since a full scan quickly becomes inefficient.

The first implementation is the NonUnitarity Engine (NUE), which can be used together with GLoBES and MonteCUBES functions in order to include deviations from unitarity of the lepton mixing matrix parameterized in a completely general way. A non-unitary lepton mixing matrix in the charged-current interaction between neutrinos and charged leptons is a generic feature of models involving extra degrees of freedom that can mix with either of the left-handed lepton components. In particular, in the popular type-I seesaw models that accommodate the smallness of neutrino masses through the addition of heavy fermion singlets (right-handed neutrinos), these extra degrees of freedom will mix with the light active neutrinos, giving rise to a larger mixing matrix than the standard $3 \times 3$ matrix.

The $3 \times 3$ submatrix describing the mixing among the light mass eigenstates, accessible at low energies, and the three active flavour eigenstates will, in general, not be unitary. In standard seesaw models, this unitarity violation is expected to be unobservably small. However, these violations are induced by a lepton number conserving operator independent of the one that generates neutrino masses. The smallness of the neutrino mass can then be naturally accommodated through a slightly broken lepton number symmetry, as in the inverse or double seesaw models, with large potentially testable deviations from unitarity of the lepton mixing matrix.

A convenient way of parameterizing the effects of a non-unitary mixing in neutrino oscillations is splitting the general non-unitary matrix $N$ as the product of an Hermitian times a unitary matrix $N = (1 + \varepsilon)U$, where $\varepsilon^\dagger = \varepsilon$. Since strong constraints can be derived
on the unitarity deviations through electroweak decays [25, 26, 27, 28], $\varepsilon$ should be a small perturbation and $U \simeq U_{\text{PMNS}}$. The NUE adopts this parameterization, adding the six extra moduli and three extra phases included in the Hermitian $\varepsilon$ to the standard parameters of the unitary part of the general mixing matrix.

By using NUE, the oscillation probabilities are modified so that the dependence on these extra nine parameters is taken into account. The engine also includes useful functions in order to set the values of these parameters in the parameter vectors and fix or free them in GLoBES’ minimization functions or in MonteCUBES’ MCMC sampling.

The second new physics implementation is the non-Standard Interaction Event Generator Engine (nSIEGE). This engine is designed to treat non-standard neutrino interactions (NSI) with matter in their most general form. The formalism of NSI parametrises the effects from physics beyond the Standard Model on neutrino interactions through effective four-fermion operators

$$
\mathcal{L}_{\text{NSI}} = -2\sqrt{2} G_F \varepsilon^{P}[\bar{f} \gamma^\mu P f][\bar{\nu}_{\alpha} \gamma_\mu P_L \nu_{\beta}],
$$

where $f$ is a matter fermion, $P$ is either a left- or right-handed projector, and $\varepsilon^{P}$ parameterizes the strength of the NSI relative to the standard weak interactions. The new interactions give rise to non-standard matter interaction terms in the neutrino oscillation formalism, effectively leading to the replacement

$$
H_{\text{matter}} = \sqrt{2} G_F N_e \text{diag}(1, 0, 0) \to \sqrt{2} G_F N_e \text{diag}(1, 0, 0) + \varepsilon
$$

of the matter interaction term in the neutrino oscillation Hamiltonian. Here, $\varepsilon$ is a Hermitian matrix and $N_e$ is the electron number density.

This type of new physics has already been studied extensively with GLoBES [29, 30, 31, 32, 33, 34, 35, 36, 37] by several authors, but usually by fixing most of the parameters. The nSIEGE implementation is very similar to the that of the NUE in terms of the API.

V. CONCLUSIONS

We have presented a new software tool, MonteCUBES, which allows the exploration of the neutrino oscillation parameter space through Markov Chain Monte Carlo sampling. The MCMC algorithms are far more efficient than minimizations or grids over large parameters spaces and we therefore believe MonteCUBES to be a particularly powerful tool for the
investigation of the effects of new physics in neutrino oscillations, since they imply the addition of new parameters to the already high-dimensional standard parameter space. The simulation part of MonteCUBES is designed as a plug-in for the GLoBES software and thus benefits from a very flexible experiment definition. It includes a useful method to find degeneracies and allow a faster scan, taking all the allowed regions detected into account in the same sampling. We have also developed an intuitive graphic user interface for Matlab, which allows to easily read, combine, analyze, plot and export the results of the MCMC exploration of the parameter space in order to interpret the constraints that a given experiment can derive on the oscillation parameters.

Apart from the MCMC sampling, we incorporate two useful functionalities in the MonteCUBES software, both of them are compatible with the new MonteCUBES functions and the original functions defined in GLoBES. The first one is the implementation of two scenarios of new physics, the NonUnitarity Engine (NUE) that incorporates all the extra parameters required to study the effects that a deviation from unitarity of the lepton mixing matrix will have in neutrino oscillations, and the non-Standard Interaction Event Generator Engine (nSIEGE) that describes non-standard neutrino interactions in matter. These engines are examples of the kind of applications we believe MonteCUBES to be best suited to, namely the exploration of large parameter spaces. In both cases, six extra real parameters and three extra phases are required in order to take the new physics into account in the most general setting. Added to the six standard neutrino oscillation parameters, this results in 15-dimensional parameter spaces. Using MonteCUBES, a full scan of the unitarity violation parameter space in order to test the sensitivity of a Neutrino Factory \cite{38,39} to this particular scenario of new physics has been performed in Ref. \cite{40}.

The second additional functionality is the possibility to input the data of a given experiment so that GLoBES and MonteCUBES can be used to analyze real data and not only forecast the sensitivities by specifying some “true” oscillation parameters and predicting the event rates to be observed from them.

We conclude that the MCMC methods implemented in MonteCUBES constitute a powerful tool to explore the bounds on the neutrino oscillation parameters that different experimental setups can give, as well as possible degeneracies and correlations among them. In particular, they allow an easy and efficient way of treating all neutrino oscillation parameters simultaneously, as well as including additional parameters from different non-standard
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