THIRD YEAR LABORATORY

STUDY OF MUON NEUTRINO OSCILLATIONS USING MICROBOONE DATA

This experiment has a significant computer programming component in python.

1 Aims

- 1. **Introduction to neutrino physics at MicroBooNE:** To use and understand data analysis techniques employed in measurements of neutrino properties. These techniques can be applied both to general neutrino experiments, but some that are specific to MicroBooNE.
- 2. **Neutrino Oscillations:** To understand the theory behind neutrino oscillations and how neutrino oscillations can be observed and measured in the lab.
- 3. **MicroBooNE detector:** Understand the MicroBooNE detector as well as general modern neutrino detectors.

2 Objectives

In this experiment, we learn about the basics of neutrino physics and then combine this knowledge with computational techniques to investigate neutrino oscillations. This experiment assumes basic knowledge of the python syntax.

- 1. You will learn some basic neutrino physics and observe some digital images of neutrino events from the MicroBooNE experiment. With these images, you will get the chance to look through different events and attempt to recognise when you see a neutrino event, as well as to identify particles by their topologies (e.g. showers and/or tracks).
- 2. You will use data frames to sort and analyse the data. This is where you will start doing some coding in python, and will provide good experience in data manipulation within a particle physics context.
- 3. You will be given a brief introduction to machine learning, including implementing decision trees.
- 4. You will apply a selection to the provided data (informally called 'cuts'), where you will try to keep events desired in our sample and remove background events. Applying effective cuts requires an understanding of the variables describing the data. After applying these requirements, you will write a python program to calculate the reconstructed neutrino energy.
- 5. You will plot the neutrino energy for different data sets as histograms and scale them correctly according to their weight.
- 6. You will apply an oscillation analysis to the simulated sample while doing a χ^2 test between the data and the simulation.

3 Background reading

Potential sources for background reading:

- A good summary document on neutrino oscillations written by Dr Steve Boyd can be found here.
- The MicroBooNE website also contains valuable information about the experiment, and can be found here.
- *PDG Review of Particle Physics* is an exceptionally rigorous review documenting the current state of Particle Physics, including Neutrino Masses, Mixing and Oscillations (page 285). The document can be found here.

The relevant PDFs from these sites are also saved locally under the *Background Reading* directory.

4 Neutrinos

Neutrinos are neutral leptons with spin quantum number 1/2 that only interact weakly and were originally assumed to be massless in the standard model [11]. The first indication of neutrinos came in studies of β decays in the early 1900s. There are two separate type of β decays; β^{\pm} , with β^+ decays being when a proton within the atomic nucleus decays to a neutron, emitting a positron and neutrino: $p \to n + e^+ + \nu_e$

Lepton	Charge	Spin	Mass (GeV/c ²)	Generation
electron (e^-)	-1	1/2	0.00051	1
muon (μ^-)	-1	1/2	0.10565	2
tau (au^-)	-1	1/2	1.77686	3
electron-neutrino (ν_e)	0	1/2	Non-zero	1
muon-neutrino ($ u_{\mu}$)	0	1/2	Non-zero	2
tau-neutrino ($\nu_{ au}$)	0	1/2	Non-zero	3

Table 1: Table of general lepton properties, including the different **flavours**: electron, muon, and tau

Early experiments on β decays found that the emitted electron does not have a discrete energy as predicted, but instead follows a continuous distribution. In 1930 Wolfgang Pauli proposed a solution to this problem in which the nucleus also emits a particle with no electric charge and spin quantum number 1/2 to conserve angular momentum. By 1934, Enrico Fermi published a famous paper detailing his β decay theory in which he incorporated the neutrino [10]. It was not before 1956 that Los Alamos physicists Frederick Reines and colleague Clyde Cowan confirmed the existence of Neutrinos via the detection of antineutrinos [7].

4.1 The Solar neutrino problem

Nuclear fusion is another reaction known for its production of electron-neutrinos, which occurs in abundance within our own Sun. Due to their lack of interaction with matter, it was understood that neutrinos would pass through the Sun and reach Earth unperturbed. With this in mind, the 'expected electron-neutrino' flux arriving at Earth from the Sun was determined. This computation was shown to be at odds with experimental data, as approximately a third of the expected flux was detected across multiple experiments [4].

A solution to this discrepancy between the data and theory was the introduction of **neutrino oscillation**, in which the individual neutrino flavours can oscillate between one another ($\nu_e \rightarrow \nu_\mu$, $\nu_\mu \rightarrow \nu_\tau$, etc). This was verified by multiple neutrino experiments and resulted in the 2015 Nobel Prize being awarded to Takaaki Kajita and Arthur McDonald for 'the discovery of neutrino oscillations, which shows that neutrinos have mass' [1].

4.2 Neutrino Oscillation

As stated above, the existence of neutrino oscillation necessitates that they must have mass, as the theory posits that **neutrino flavour eigenstates** are considered as combinations of **mass eigenstates**. We will not go into detail on how this works, but if you wish, you can explore this topic on your own. Let us, for now, assume that neutrinos have a non-zero mass. Neutrino oscillation, the phenomenon of one flavour of neutrino (ν_e, ν_μ, ν_τ) oscillating into another flavour, was proposed by Bruno Pontecorvo in 1967 [9]. In this framework it is important to distinguish between flavour eigenstates as (ν_e, ν_μ, ν_τ), produced in **weak interactions** and the mass eigenstates which are the those with definite masses (ν_1, ν_2, ν_3). The flavour eigenstates can be thought of as linear superpositions of the mass states described by the PMNS matrix [8], $U^{\rm PMNS}$:

$$\begin{pmatrix} \nu_e \\ \nu_\mu \\ \nu_\tau \end{pmatrix} = U^{\text{PMNS}} \begin{pmatrix} \nu_1 \\ \nu_2 \\ \nu_3. \end{pmatrix}$$
 (1)

In the two-flavour approximation, we can write the relation between the flavour eigenstates and the mass eigenstates as [6]

$$\begin{pmatrix} \nu_{\alpha} \\ \nu_{\beta} \end{pmatrix} = \begin{pmatrix} \cos \theta & \sin \theta \\ -\sin \theta & \cos \theta \end{pmatrix} \begin{pmatrix} \nu_{1} \\ \nu_{2} \end{pmatrix} \tag{2}$$

From this, we can find the time propagation of a weak state as

$$|\nu(t=0)\rangle = |\nu_{\alpha}\rangle = \cos\theta |\nu_{1}\rangle + \sin\theta |\nu_{2}\rangle,$$
 (3)

$$|\nu(t)\rangle = e^{iq_1 \cdot x} \cos \theta |\nu_1\rangle + e^{iq_2 \cdot x} \sin \theta |\nu_2\rangle,$$
 (4)

where $q_{1,2}$ are the time propagated four momenta of the two states $q_i \cdot x = E_i t - \bar{P} \cdot \bar{x}$

If you are unfamiliar with bra-ket notation ($|\nu_{\alpha}\rangle$), please check the appendix subsection 16.1

Exercise 1: From this you should be able to derive the probability of the two-flavour oscillation formula $P(\nu_{\alpha} \to \nu_{\beta}) = |\langle \nu_{\beta} | \nu(t) \rangle|^2 = \sin^2(2\theta) \sin^2(\frac{\Delta m_{21}^2 L}{4E})$, where $\Delta m_{21}^2 = m_2^2 - m_1^2$.

Hint: first show that $q_i \cdot x = \frac{m_i^2 L}{2E}$ via the relativistic energy-momentum relation. Use Taylor expansions where needed.

Using natural units, this probability can be written as:

$$P(\nu_{\alpha} \to \nu_{\beta}) = \sin^2(2\theta)\sin^2\left(1.27 \frac{\Delta m_{21}^2 (\text{eV})^2 L(\text{km})}{E(\text{GeV})}\right)$$
 (5)

This will be useful in later exercises.

Write down what each of the variables in equation 5 mean. What is the significance of the two separate sine components? What effect do they have on the resultant probability?

To give a better feeling of said effect, plot the probability varying the parameters θ , Δm_{21}^2 , L and E respectively.

5 An Introduction to MicroBooNE

In this experiment, you will analyse data from the neutrino detector MicroBooNE. MicroBooNE is a 170-ton liquid argon time projection chamber (TPC). These detectors are some of the best detectors suited for modern neutrino experiments and therefore you should ensure you have an understanding of their operation and why they are the preferred method for emerging physics analyses. The MicroBooNE detector operates in a muon neutrino beam at Fermilab which is created by 'firing' protons at a Beryllium target.

5.1 Liquid-argon TPCs

Liquid-argon TPCs use a large container of liquid argon to analyse neutrino interactions. We cannot detect neutrinos directly as they have no charge and do not emit any Cherenkov or Bremsstrahlung radiation. Therefore, what we do is detect charged particles that have been created during an interaction of a neutrino with the argon and infer the neutrino's properties. An example of this is 'quasi-elastic scattering' where a neutrino interacts with a neutron from the liquid argon atoms producing a proton and a corresponding charged lepton. This interaction can be seen in Figure 1. This is a charged current (CC) interaction as it is mediated by a W boson and will be our signal in this analysis.

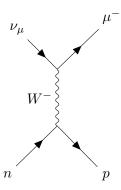


Figure 1: The quasi-elastic neutrino scattering of a neutron. This is a charged current interaction mediated by a W boson.

After a neutrino interaction has occurred within the argon, there will be both scintillation photons emitted and ionization electrons from the charged particles hitting the argon atoms. To analyse the charged particles involved in the neutrino interaction, an electric field is applied to the detector that will drift the particles to one side of the detector. The detector has three collection wire planes that together with the time projection obtained from the detection of scintillation photons can be used to obtain a 3-dimensional picture of a neutrino interaction. A diagram of the process can be seen in Figure 2, and an animation demonstrating the process can be seen here, courtesy of FermiLab.

Exercise 2: What other interactions can neutrinos undergo? Are any of these applicable within the detector? If you know how, draw those applicable as Feynmann diagrams.

6 Initial setup

6.1 Installing packages

When running through the code, you may find that your local machine does not have the required python packages. If you are using the 3rd year lab machines, this can be easily resolved. First, open the command terminal and using the command pip install type:

```
pip install jupyterlab
... numpy
... uproot3
... pandas
... seaborn
... scipy
... scikit-learn
... matplotlib
```

There may be more packages required for your code to run. If you have any issues with this, please contact any of the lab support.

6.2 Downloading and using the lab scripts

If you are using the 3rd year lab machines, it is recommended that you save all data from this lab within your 'onedrive' folder. First, download the uboone_lab_student_copy repository from github, found here and read through the README.md. Extract the repository to whatever directory you wish to work from. Make sure to save all your data externally at the end of each session, as these local one drives are wiped occasionally.

Then you will need to download a large data file: bnb_run3_mc_larcv.h5. This will be provided either via a usb stick or onedrive link. Insert this file into the above directory in the 'data' folder. If the files data_flattened.pkl & MC_EXT_flattened.pkl within the data folder appear to be very small (bytes rather than MB), it means they have been downloaded incorrectly and should be downloaded manually from their github pages linked above.

Once you have all of this installed, you should be able to open up jupyterlab within command prompt by typing: python -m jupyterlab. Then use the interface to navigate to the relevant directory with your lab data.

7 Event Displays

Event displays are a useful tool used by MicroBooNE researchers to visualise the data we obtain from reconstructed interactions. In these event displays, you can see coloured pictures of what is happening in the detector. The colour map from blue to red indicates the amount of charge deposited by the particles involved in an interaction. By observing these events, one can distinguish different interactions and properties such as how shower-like or track-like an interaction was.

Exercise 3:

Go to the event_display.ipynb file, run the code and look at the event display produced. You can select which wire plane to observe the event from, and can use the in-built plotting tools to look at individual interactions or 'tracks'. Use the function list_entries to look at different 'images' from the dataset.

- Due to MicroBooNE's location above ground, it detects an excess of cosmic muons.
 These muons are consequently very easy to identify within the event displays (being the most abundant particle tracks). What characteristics do they all have in common? Justify these characteristics using your knowledge of Muons¹.
- Look at different events and try to recognise specific features that can be used to characterise different particle interactions.

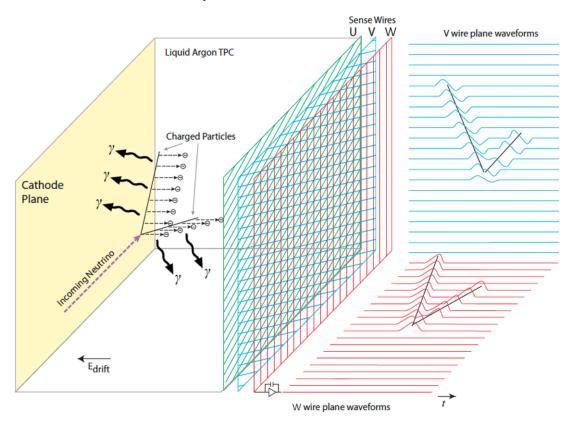


Figure 2: A schematic of the operation of a Liquid Argon Time Projection Chamber. The time projection from the scintillating photons together with the three wire planes are combined to produce a three-dimensional reconstruction of an interaction [2].

8 Variables

In the samples we will be using, many variables are defined, some of which we will not need. In Table 2 a list of the variables we will take into account is given with a description of what they do.

¹This paper may be useful for seeing some examples of what particles look like within the MicroBooNE detector.

Variable Name	Description
vertex _{x,y,z}	Reconstructed position of the vertex of an interaction
reco_nu_vtx_sce_x,y,z	in the detector (cm).
$\mathrm{track}^{\mathrm{start}}_{\mathrm{x,y,z}}$	Reconstructed position of the start of an identified
trk_sce_start_x,y,z_v	track in the detector. (cm)
$\mathrm{track_{x,y,z}^{end}}$	Reconstructed position of the end of an identified
trk_sce_end_x,y,z_v	track in the detector (cm).
$L_{distance}$	The distance between the longest track in an event
trk_distance_v	and the reconstructed neutrino vertex (cm).
$L_{ m length}$	The length of the detected neutrino interaction track.
trk_len_v	
d_{track}	Log likelihood score used to find the ID of the particle.
trk_llr_pid_score_v	For example, if it is a muon or a proton.
$L_{ u, cosmic}$	Distance between our detected Neutrino track and
_closestNuCosmicDist	closest cosmic muon track within the detector.
$S_{topological}$	A score which determines how much a signal in the
topological_score	detector looks like a muon neutrino track. This is also
	a variable that is determined by machine learning,
	where the machine has been trained with track-like
	events.
S_{track}	A score which determines how much a signal in the
trk_score_v	detector looks like a track (instead of a shower). This
	is also a variable that is determined by machine learn-
	ing, where the machine has been trained with track-
	like events.
$\mathbf{E_n}$	Reconstructed energy of the neutrino in the interac-
trk_energy_tot	tion.
P_{μ}^{range}	Muon momentum determined by the range (or length)
trk_range_muon_mom_v	of the muon track through the detector.
$P_{\mu}^{ m mcs}$	Muon momentum determined via Multiple coulomb
trk_mcs_muon_mom_v	scattering.

Table 2: A list of variables (and their names within the data structure) we are going to look at in this experiment and a description of their function.

9 Setting up

If you need to install any of the packages imported, you can type "pip install package" into an empty cell in the notebook or within your terminal, where "package" is the name of the package.

9.1 Running the example code

You are given a template for this lab in the form of *MainAnalysis.ipynb*, which will give you access to a couple of useful scripts as well as the code structure for some components of the lab.

Exercise 4: Run the example code. Look through the code and the figures that are produced and see if you can understand what the code does.

The samples used in this Python file are called "MC_EXT" and "data". The sample MC_EXT is a combination of the predicted distribution of the neutrino events from our detector, developed

using *Monte Carlo* simulations; and real data taken from MicroBooNE when the muon neutrino beam is turned off (interactions occurring due to EXTernal particles). The sample data is the real data taken at MicroBooNE. You may have noticed that within your MC_EXT data there are extra variables provided. Write down what these variables are called and try to determine what they mean? Recall that the MC_EXT data files are produced via Monte Carlo simulation.

10 Particle Identification within MicroBooNE

As shown in **exercise 3**, recognising different particle interactions within the detector for each and every event is a process that (by-hand) would take a very long time, but is key to particle physics analysis (what use is a detector if we don't know what its detecting?). Therefore, automation processes are implemented to increase the speed at which interactions within the detector can be 'classified' or categorised. These classification processes are relatively complex and use a variety of tools to identify as many particles within the detector as possible.

As is the case in most areas of cutting-edge research, machine learning is a tool that is used extensively throughout particle physics. Here we will be implementing a very simple machine learning method known as **Random Decision Forests** to try and classify our particle interactions, as well as determine what variables are most important in distinguishing between them.

10.1 Data visualisation and manipulation

First, lets look at our data and learn how to use pandas, a python library that allows for intuitive manipulation and analysis of data. You should have already seen pandas in action within the template, printing off the 'head' of our MicroBooNE and Monte Carlo data.

You may notice that we have some variables in our Monte Carlo dataframe that are not described in table 2, these being *weight & category*. Category tells us the type of interaction seen within the detector as shown in table 3, and weight is a scaling factor applied to each Monte Carlo event provided by the simulation framework.

Category	Interaction	Meaning
4	Mis-ID	Cosmic events misidentified as neutrino events
5	Out Fid. Vol.	Events occurring within the outer fiducial volume
7	EXT	Events detected when the neutrino beam is off
10	$ u_e$ CC	electron neutrino events
21	$ u_{\mu}$ CC	muon neutrino events
31	ν NC	neutral current neutrino events

Table 3: Different categories with respect to their interactions

Exercise 5:

- What is the meaning of outer fiducial volume? Why are these events categories separately from other events.
- · What sort of events would you expect to be contained within the EXT category?
- We will initially look at our data using the pairplot function from the seaborn package. pairplot shows pair-wise relationships in the dataset, which can be useful for trying to visualise correlations. Take some time to understand what the pairplot graph is showing you.

- Our signal events drown out any interesting trends that may be visible in the background events. Using pandas, create a dataframe that is *deep copy* of MC_EXT_VIS and remove all signal (category == 21) events from this dataframe. Plot another pairplot using this new dataframe.
- Are any trends/correlations visible within the data now? Why might it still be difficult to pick out trends by eye? How could this be resolved for visualisation purposes?
- Bonus 1: Try to apply some of your ideas to make visualising trends more clear.²
- Bonus 2: Add new variables to your plots to see if you can notice any other trends.

10.2 Decision Trees

Exercise 5 should have demonstrated that while visualising data can be useful for better understanding it, when working with large data sets and many parameters it becomes much more difficult to find trends or correlations by eye. This is were the application of machine learning becomes appropriate to find trends, correlations, and other dependencies/relations within our data that can help us better classify our particles.

Due to the nature of this lab, we will be looking at a rather simple example of machine learning, specifically **decision trees**. Decision trees (in this context) produce a collection of simple rules for partitioning our variable space that allow for the separation of our different interactions. For example, if we applied a selection partition on topological_score at 0.4 for our initial Monte Carlo data, we would see that the majority of our muon neutrino CC interactions would be on one side of our selection.

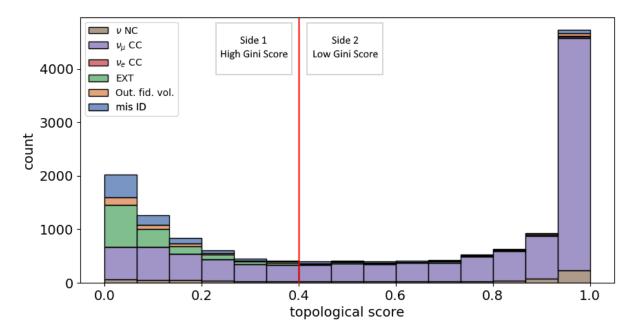


Figure 3: A plot of our topological score, now as a histogram for our different particle interactions, with the proposed partition at topological_score = 0.4. The hypothetical *Gini* scores for each side are represented in the plots as well.

Decision trees allow for such selection partitions to be made in sequence for large sets of data, across multiple variables for classification purposes. As this process of producing selection

²Be careful when playing around/reducing the size of dataframes in jupyter notebook! It's very easy to carry forward modifications to your dataframe that may be unintentional.

partitions is done automatically, we need a way to determine how good these partitions are at separating our different interactions. Decision trees do this by applying a 'criterion' for these selections that determine the 'accuracy' or how well the partitions classify the data, such as *Gini* or *Entropy*.

We will be using the *Gini* criterion: $G_{1,2}=1-\sum_{class}p_{class}^2$, where p_{class} is the probability of finding said class on one side of a partition (sides 1 & 2). *Gini* looks to minimise its own value with each partition, with 100% accuracy being when all partitions lead to $G_N=0$. This is a very brief explanation of *Gini*, so I would **highly** recommend looking at slides on Decision trees provided by Dr. Guillermo Hamity from the University of Edinburgh for a more in-depth look at how exactly such processes work and some excellent visualisation of the Decision Tree process, but for today we are just hoping to get to grips with implementing decision trees. His slides can be found here³.

A problem with decision trees is that they are very prone to **overfitting**, this is when the partitions are tailored very specifically for **only** one dataset due to too many partitions being allowed (too much training), meaning that you're model may be less accurate for another dataset of the same simulation. To counteract this issue, we will use a method of **bootstrap aggregation** or "bagging" called **random decision forests**. This is the process of producing multiple independent decision trees which will make different random choices for each tree across different features to ensure that they're distinct, and aggregating their results.

Exercise 6:

• To simplify the classification process, generate a new dataframe, MC_EXT_ML, that doesn't have any muon or electron neutrino events. This means we're only considering mis ID, Out Fid Vol, EXT and ν NC interactions.

For the decision trees to work, it needs 'training data' (X), which will be the interaction data we want to train or model on (MC_EXT_ML without the category column) and 'truth data' (y), or the true classifications of our interactions (the category column). The training and truth data have been separated for you already.

- Display the shape of X and y. Do these shapes make sense? Print them out and investigate to better understand the data.
- A good way to check for overfitting is to produce a 'test dataset'. We will use a slice of the training data that is kept aside (the model isn't trained on it) to validate that our random forest model works adequately on data it hasn't been trained on. Use the function train_test_split to produce 4 datasets: x_train, x_test, y_train, y_test, with the split between training and test being 80/20. Hint: Look up the documentation for scikit-learn functions when they're in use to understand what they're doing. This is generally good practice regardless of what you're doing.
- Now you can produce your RandomForestClassifier and fit/train it to your data! Create your model rf with 1000 trees, and a max_depth of 8, using the *Gini* criterion. Fit your RandomForestClassifier to your data using rf.fit.
- The code for determining the accuracy of your results for both your training and testing datasets has been provided. Comment on the accuracy.
- Bonus: What do you think would occur if you provided more trees/depth⁴ for your RandomForest model? You can try different depths and number of trees if you'd like, but don't spend too much time waiting for code to run!

 $^{^3}$ The link should start the PDF at page 28. Jump forward to this page if this doesn't work on your device.

⁴depth here means number of partitions

Now that you have a model that can be used to predict an interaction based on your variables, how well does it perform? Accuracy isn't the best way of quantifying this, so now lets produce a **confusion matrix**. A confusion matrix plots the probability that your truth data matches what your model predicts for your dataset. For a 100% accurate model, we would expect the diagonal boxes of a confusion matrix to contain 1s. An example can be seen in figure 4.

- Use the function ConfusionMatrixDisplay to produce a confusion matrix for model rf, using y_test & y_pred datasets.
- Comment on your results. Why might some interactions be confused with others by your model? Use your knowledge of each interaction category to justify the models (in)accuracy for each category.

Our model allows us to determine how **important** each variable is in classifying our data, as in which variables made the most impact on allowing the model to distinguish between interactions. This can be useful to know when planning to manipulate our real MicroBooNE data to single out certain interactions.

This is just a basic introduction to ML, with much more complex models implemented in the field to do what we've just done. MicroBooNE analysis often uses boosted decision trees and more complex neural networks to characterise tracks seen within the data, and determine what variables in real data affect said classifications. There are a myriad other uses and implementations of ML throughout physics, but sadly we don't have time to go into them here.

If you're curious at what a simple neural network model would look like when trying to complete the same task you've just done, look at the output of keras_example.ipynb, which is a basic neural network deployed to achieve the same goal of classification.

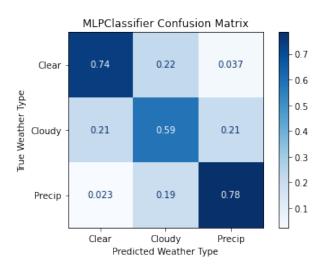


Figure 4: A confusion matrix for a model that predicts weather patterns.

11 Selection

From this section and onward, we will refer to limits and restrictions applied to the variables as selection cuts. We want to reduce the events induced by background processes while keeping as many signal CC ν_{μ} events as possible. One major component of the background (as described in **Exercise 3**) is cosmic rays. These interactions come from high-energy cosmic radiation. They will traverse most of the detector and usually be detected near the edge of the detector coordinates.

Exercise 7:

- Generate histograms of the various variables outlined in the previous section. Use seaborn.histplot and the example given within the template to help you.
- Once all variables have been plotted as histograms, identify appropriate cuts that can be used to remove background and apply them using the Selections function provided.

Suggestions:

- A good first cut to make is to reduce the total track energy to be less than a couple GeV, as most values larger than this are caused by tracks that are mis-interpreted or beyond the scope of what we're interested.
- Some of the variables detail the position of a vertex or the start/end points of a track. As described above, a lot of cosmic interactions occur near the edges of the detector (as should be clear in your variable histograms). Therefore, an initial cut that would make sense is to remove these interactions near the edge of the detector with cuts, consequently only considering the *fiducial volume*⁵ of the detector. You might have to adjust the bin width and limits on the axes to better represent the variables and make appropriate cuts.

11.1 Efficiency

It is worth monitoring the efficiency of the selection cuts you made. After each cut you lose some information, so you should see what selection cuts affect your efficiency the most. The efficiency of the selection cuts is defined as

$$\frac{\text{Signal events surviving the selections}}{\text{Total number of events}}.$$
 (6)

You should remove as many background events as possible while keeping a relatively high efficiency.

11.2 Purity

What fraction of all events is your signal? Purity describes it. You can use your simulated sample to assess the purity. The purity is defined as

$$purity = \frac{\text{The total number of signal events that pass your selection cuts}}{\text{Total events in selected sample}}.$$
 (7)

Exercise 8: Find a way to keep purity and efficiency high during your selection cuts. How does each cut effect the efficiency and purity?

12 Neutrino Energy

From the formula derived in Section 4.2, it is clear that the two parameters we can determine from the experiment are L and E. Since MicroBooNE has a defined baseline $L\approx 470m$, we will plot the number of events for various neutrino energies. Later on, we will use this plot to

⁵The fiducial volume of a detector is a sub-volume that will contain a specific number of events (usually 90%) that are present in the detector.

apply an oscillation analysis to the data. The systematic uncertainty in the experiment can be approximated to a flat 15% for each bin.

Exercise 9:

- Produce a histogram of the reconstructed neutrino energy (trk_energy_tot) for the predicted (Monte Carlo) sample. You should have done this in exercise 7.
- On top of this histogram, add the systematic uncertainty of the bins. Bonus: Include statistical uncertainty in your overall uncertainty of the bins.
- We want to compare the distribution of the reconstructed neutrino energy from our MicroBooNE data with that obtained from the simulated sample. Apply your MicroBooNE data to the histogram so that they can be visually compared.

Your result should look something like figure 5, but feel free to experiment with your cuts to see if you can improve the purity and efficiency!

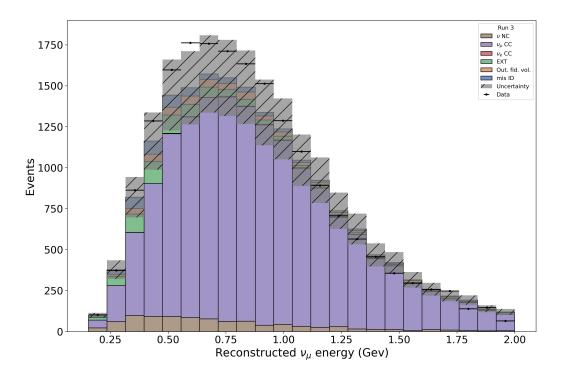


Figure 5: Reconstructed energy resolution for muon neutrinos, showing both MicroBooNE data and our Monte-Carlo Simulation Data.

13 Oscillation and fitting

In figure 5, you should see an excess of MicroBooNE (real) data compared to our Monte Carlo (simulated) data. The simulated data does not account for neutrino oscillation, so using the two-flavour oscillation probability derived in **exercise 1**, we can develop our own 'oscillation analysis', and see if including oscillations into our simulated data improves it's fit with respect to the real data.

We will do this by considering the occurrence of muon neutrino disappearance within our

data, where the muon neutrinos (ν_{μ}) oscillate into another neutrino flavour that MicroBooNE couldn't detect: $P(v_{\mu} \to v_{\beta})$. This oscillation probability can be applied to the data in figure 5 as a scaling factor, with the 'goodness' of fit determined via the minimisation of χ^2 between the real and simulated data.

Exercise 10:

- Write a function representing the two-flavour oscillation from exercise 1 within this new context. Recall that you are no longer looking for the probability of oscillation from $\nu_{\alpha} \rightarrow \nu_{\beta}$, but rather the 'disappearance' (or probability to *not* oscillate) for our muon neutrinos.
- What input variables are required for your oscillation function? The values for two
 of these parameters are not given and must be determined. Two of these parameters are given to you, what are they?
- Write a function that will apply the muon disappearance probability to your simulated data. This can be interpreted as the "scaling" of your Monte-Carlo data with respect to their true_E or true energy values. Why do we use true_E instead of trk_energy_tot to oscillate our data?
- BONUS: Try plotting your scaled or 'oscillated' energy as was done in exercise 9, or as shown in figure 6.
- Write a function for χ^2 that acts on the simulated data having undergone oscillation, and the real data.

$$\chi^2 = \sum_{i=1} \left(\frac{(\mu_i(\theta) - M_i)^2}{\sigma_i^2} \right) \tag{8}$$

Where $\mu_i(\theta)$ are the number of events in the ith bin for your Monte Carlo data (or MC_EXT) file, M_i are the number of events in the ith bin of your MicroBooNE data, and σ_i is your uncertainty across each bin (I'd recommend using the systematic error given previously).

14 Oscillation parameters

From **exercise 10**, you should know the two parameters that we are allowed to vary within the oscillation function of which we don't have 'set values'. These parameters impact the oscillation probability and consequently the shape of our energy curves as shown in Figure 6. So we can determine the most optimal parameters by varying each of them across a range and determining χ^2 for each combination.

14.1 Closure test

It is common practice to test your code's functionality before using it for its desired purpose. In **exercise 10**, you have developed a small section of code that allows you to oscillate (or 'scale') your data with respect to the true energy, and calculate a χ^2 which compares your Monte-Carlo data to the data taken from MicroBooNE.

You have been provided with a pickle file (oscillated_data.pkl) that is identical in format to MC_EXT, but it has already been oscillated with set values for Δm_{21}^2 and $\sin^2(2\theta)$. To demonstrate that the code you wrote in **exercise 10** works correctly, you should be able to determine what these set values are.

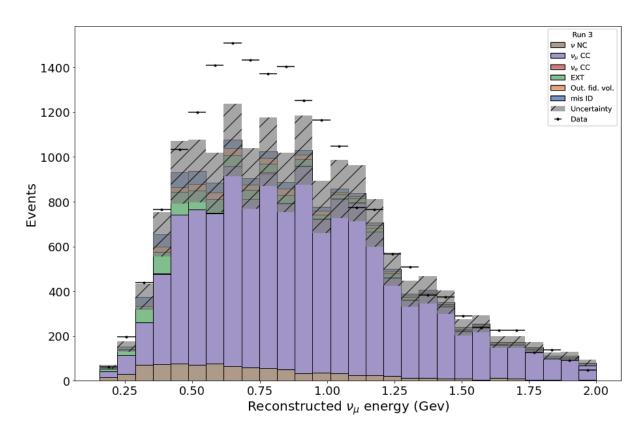


Figure 6: A demonstration of the simulated data modified by oscillation. Here it is clear that the parameters chosen do not produce a good fit between the simulated and real data, resulting in a large χ^2 .

Exercise 11a:

- Apply your selection cuts to oscillated_data.pkl.
- Write a function that oscillates MC_EXT data with respect to Δm^2_{21} and $\sin^2(2\theta)$, and calculates the χ^2 comparing your newly oscillated MC_EXT data to the data from oscillated_data.pkl
- Find values of χ^2 for varying values of Δm^2_{21} and $\sin^2(2\theta)$, and create a 2D contour plot of the χ^2 with the oscillation parameters as the axes. To start, you may choose a range for Δm^2_{21} and $\sin^2(2\theta)$ from (0.0001 \rightarrow 50) and (0.1 \rightarrow 1) respectively. Modify this range as you see fit. Use matplotlib's contourf function to help you.
- Produce a contourf plot, determine the point of lowest χ^2 either by eye or by creating smaller ranges to scan over. The minimum value of χ^2 should correspond with values of Δm_{21}^2 and $\sin^2(2\theta)$ which are those that <code>oscillated_data.pkl</code> was oscillated with. What are these values? Can you provide errors on your minimum χ^2 values?
- Add contours to these plots for 1, 2 and 3 σ . The values of χ^2 equivalent to these can be found in Ref [11], but can also be determined with *Chi-Square Tables* which are available online. For χ^2 , here we will consider the degrees of freedom as 2. Why do we use 2?

After being confident that your closure test shows that your code works as expected (you can obtain values for Δm^2_{21} and $\sin^2(2\theta)$ that are accurate to those used to oscillate oscillated_data.pkl), you can now move onto comparing the MC_EXT data to the data taken from MicroBooNE. This

will produce a very different contour plot to the closure test, so take your time to understand what exactly your scripts are doing with respect to the data.

Exercise 11b:

- Find the values of χ^2 for varying oscillation parameters Δm^2_{21} and $\sin^2(2\theta)$, and make a 2D contour plot of the χ^2 with the oscillation parameters as the axes. Use matplotlib's contourf function to help you.
- What characteristics can you see in your χ^2 plots? If no trends are visible, change your range of oscillation parameters.
- Bonus: Minimize χ^2 using a minimiser and extract the oscillation parameters that give the best fit for the Monte Carlo data against the real data. What do these values tell you about said parameters? Does this make sense within context to the applied oscillation?

Due to the nature of this analysis, we can't determine exact values for our desired parameters. Instead we can exclude certain parameter pairings based on their values of χ^2 , producing 'exclusion zones' of high χ^2 . These zones can be defined by **confidence levels** which we shall visualise as contour lines on our plots. Confidence levels act as 'upper limits' on our parameters, with a CL of 95% being equivalent to a 95% probability that our parameters allow for our simulated data to accurately describe our true data.

Exercise 12:

- Plot lines corresponding to confidence levels of 90, 95 and 99% using matplotlibs contour function as done in exercise 11.
- Find the oscillation parameters that give the smallest value of χ^2 within your range and plot the point on your contour or CL plot.

Hint: Restrain your oscillation parameters at least to between $10^{-4} \to 10^0$ for $\sin^2(2\theta)$ and $10^{-2} \to 10^2$ for Δm_{21}^2 , but play around with them a bit, as you may struggle to see certain features if your range is too large!

15 3+1 neutrino model

The 3+1 neutrino model assumes the existence of a fourth sterile neutrino, with a much larger mass than the other neutrinos that isn't able to be detected within the MicroBooNE detector (sound familiar?). The PMNS matrix from Equation 1 is modified by adding a 4th eigenstate:

$$\begin{pmatrix}
\nu_{e} \\
\nu_{\mu} \\
\nu_{\tau} \\
\nu_{s}
\end{pmatrix} = \begin{pmatrix}
U_{e1} & U_{e2} & U_{e3} & U_{e4} \\
U_{\nu 1} & U_{\nu 2} & U_{\nu 3} & U_{\nu 4} \\
U_{\tau 1} & U_{\tau 2} & U_{\tau 3} & U_{\tau 4} \\
U_{s1} & U_{s2} & U_{s3} & U_{s4}
\end{pmatrix} \begin{pmatrix}
\nu_{1} \\
\nu_{2} \\
\nu_{3} \\
\nu_{4}
\end{pmatrix},$$
(9)

where the relevant matrix elements we need are given by

$$|U_{e4}|^2 = \sin^2 \theta_{14},\tag{10}$$

$$|U_{\mu 4}|^2 = \sin^2 \theta_{24} \cos^2 \theta_{14}. \tag{11}$$

⁶scipy.optimize.curve_fit will be very beneficial here, but feel free to find your own solutions.

The probability of oscillation is now given as:

$$P(\alpha \to \beta) = \delta_{\alpha\beta} - 4(\delta_{\alpha\beta} - U_{\alpha4}^* U_{\alpha4}) U_{\beta4} U_{\beta4}^* \sin^2 \left(1.27 \frac{\Delta m_{14}^2 L}{E} \frac{(\text{eV}^2)(\text{km})}{(\text{GeV})} \right)$$

$$= \delta_{\alpha\beta} - \sin^2 (2\theta_{\alpha\beta}) \sin^2 \left(1.27 \frac{\Delta m_{14}^2 L}{E} \right).$$
(12)

Exercise 13:

- Derive the probability of $\nu_{\mu} \to \nu_{\mu}$ disappearance for 3+1 model, and consequently find a relation for $\sin^2 2\theta_{\mu\mu}$ with respect to $\sin^2(\theta_{24})$ and $\cos^2(\theta_{14})$.
- Derive the probability of $\nu_e \to \nu_e$ disappearance for 3+1 model, and consequently find a relation for $\sin^2 2\theta_{ee}$ with respect to $\sin^2(\theta_{14})$.
- Derive the probability of $\nu_{\mu} \to \nu_{e}$ appearance for 3+1 model, and consequently find a relation for $\sin^{2}2\theta_{\mu e}$ with respect to $\sin^{2}(\theta_{24})$ and $\sin^{2}(2\theta_{14})$.

Hint: Use trig identities (specifically double angle identities) to help you. Equate the two parts of equation 12 and rearrange for your $\sin 2\theta$ components.

15.1 LSND and MiniBooNE

One of the MicroBooNE experiment's searches is for possible neutrino oscillations involving a fourth sterile state [5]. This has been motivated by previous experiments such as MiniBooNE and LSND which found anomalies in their results that can indicate a fourth neutrino favour. The "allowed" parameter space that these experiments determined for this fourth sterile state can be seen as they are plotted at the end of the notebook. The MiniBooNE and LSND data are stored as 'MiniBooNEdata.csv' and 'LSNDdata.csv', respectively.

These experiments were looking for ν_e appearance from our muon beam, while the signal in our data is of ν_μ events [3]. We therefore have to consider how our two flavour estimation of $\nu_\alpha \to \nu_\beta$ can be used equivalently to describe this four flavour model, in which it is assumed that muon neutrinos are oscillated to sterile neutrinos ($|U_{\mu 4}|$) and then oscillated back into electron neutrinos ($|U_{e4}|$). The parameter we are then considering is $\sin^2 2\theta_{\mu e}$, which describes this resulting oscillation.

This is done by considering our oscillation parameter $\sin^2(2\theta)$ for " $P(\alpha \to \alpha) = 1 - P(\alpha \to \beta)$ " (survival of the α flavour) to be equivalent to $\sin^2(2\theta_{\mu\mu})$ (survival of the muon flavour) with some scaling factor. With this, we can now describe the parameter space of $\sin^2 2\theta_{\mu e}$.

Exercise 14:

- You have already determined $\sin^2 2\theta_{\mu e}$ with respect to $\sin^2(\theta_{24})$ & $\sin^2(\theta_{14})$. Relate this result to $|U_{\mu 4}|$ & $|U_{e4}|$ (you should have already done this).
- Do the same for $\sin^2 2\theta_{\mu\mu}$ & $\sin^2 2\theta_{ee}$ such that the the equation for $\sin^2 2\theta_{\mu e}$ contains within it both $\sin^2 2\theta_{ee}$ & $\sin^2 2\theta_{\mu\mu}$. This will require use of the quadratic formula to rearrange the relevant sine and cosine mass and flavour components.
- Using the value for $\sin^2 2\theta_{14} = \sin^2 2\theta_{ee} =$ 0.24 result from MicroBooNE [5], compare your result with LSND and MiniBooNE.
- If your cuts and analysis are well-tuned, you should see that your confidence levels overlap or exclude the results from MiniBooNE and LSND. What does this tell you about the previous MiniBooNE and LSND anomalies?

*Hint: In practice, this means replacing your previous oscillation parameter of $\sin^2 2\theta$ with $\sin^2 2\theta_{\mu e}$. To do this, derive $\sin^2 2\theta_{\mu e} = 4|U_{\mu 4}|^2|U_{e 4}|^2$ with respect to parameters we know:

- $\sin^2 2\theta_{\mu\mu}$ (which can be considered as your original oscillation parameter range)
- $\sin^2 2\theta_{ee} = \sin^2 2\theta_{14} = 0.24$

16 Appendix

16.1 Bra-ket

Bra-ket notation is a method for manipulating vectors, particularly in quantum physics.

In principle, column vectors can be considered as *kets*, and row vectors as *bras*:

$$|A\rangle = \begin{bmatrix} 1\\2\\3 \end{bmatrix} \qquad \langle B| = \begin{bmatrix} 4 & 5 & 6 \end{bmatrix} \tag{13}$$

The *bra* and the *ket* above can each be used to describe a 3-dimensional space, but they can have any number of dimensions, and not necessarily in space. In our case, they are considered as quantum states of a system. They can also be complex numbers (and usually they are), with the *bra* being the **complex conjugate** of the corresponding *ket*. For example:

$$|A\rangle = \begin{bmatrix} 1 - 2i \\ 3 - 4i \\ 5 + 6i \end{bmatrix}$$
 $\langle A| = \begin{bmatrix} 1 + 2i & 3 + 4i & 5 - 6i \end{bmatrix}$ (14)

In our case here, the important thing to know about bra-ket notation is how they multiply with one another:

$$\langle A|B\rangle = ? \tag{15}$$

As we don't have any operators or non-commuting terms in our equations (eg: \hat{O}), we're free to manipulate our *bras* and *kets* with respect to the content within them freely, as such:

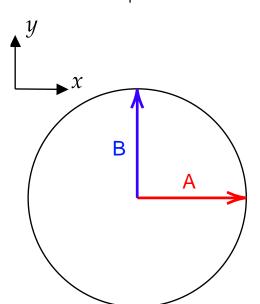
$$\langle A|\sin\theta|B\rangle = \langle B|\sin\theta|A\rangle = \sin\theta\langle A|B\rangle \tag{16}$$

In comparison:

$$\langle A|\hat{O}|B\rangle \neq \langle B|\hat{O}|A\rangle \tag{17}$$

In extension of this, if we know that our two vectors are orthogonal, we know that their multiplication produces a zero, and a 1 if they're perpendicular (and normalised).

Lets take an example of two vectors in 2D space:



$$|A\rangle = \begin{bmatrix} 1\\0 \end{bmatrix}$$
 $|B\rangle = \begin{bmatrix} 0\\1 \end{bmatrix}$ (18)

$$\langle A|B\rangle = 0 \tag{19}$$

$$\langle A|A\rangle = \langle B|B\rangle = 1$$
 (20)

Use this information to complete the **exercise** 1.

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