

Guide to using project GUI:

Notes:

- Keep all code files in same directory to run GUI
- The GUI needs PyQt5 installed to run

There are three main pages in the GUI:

Front Page/Main page: Lets you create and upload tree data and configure your distance metrics

Result page: Shows the results of the distance metric in the form of a table

Center tree page: shows the result of the center tree analysis

To start GUI simply click the GUI.py module or type "GUI.py" into command prompt

Main Page

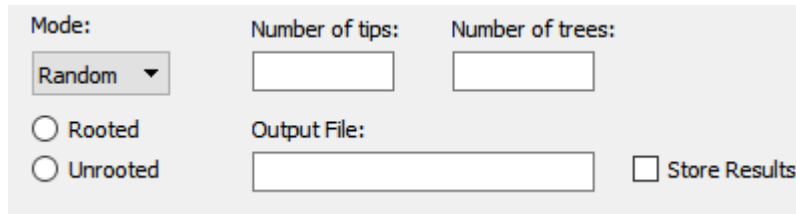
The image shows a software window titled "MainWindow" with a standard Windows title bar (minimize, maximize, close buttons). The window contains a "Set UP" section with the following controls:

- Rooted Metrics:** Includes radio buttons for "Kendall-Coljin" and "Triplet Distance". A "Lambda:" label is next to a text input field.
- Unrooted Metrics:** Includes radio buttons for "Robinson Fould" and "Quartet Distance".
- Tree Generator:** Contains a "Mode:" dropdown menu currently set to "Full". It also has input fields for "Number of tips:" and "Number of trees:". Below these are radio buttons for "Rooted" and "Unrooted".
- Output File:** A text input field for specifying the output file name.
- Store Results:** A checkbox.
- OK:** A button to confirm the settings.
- Input File:** A text input field for specifying the input file name.
- Find File:** A button to open a file selection dialog.
- Newick Trees:** A large text area for displaying or editing Newick tree format.
- Reset, OK, Quit:** Buttons at the bottom of the window.

Figure 1:MainPage

If creating trees for scratch:

1. Select mode: Full creates all trees of with the number of leaves indicated.
 - 1.a. If you change the Random the screen will change to let you set number of trees as well



Mode: Random ▼

Number of tips:

Number of trees:

☐ Rooted

☐ Unrooted

Output File:

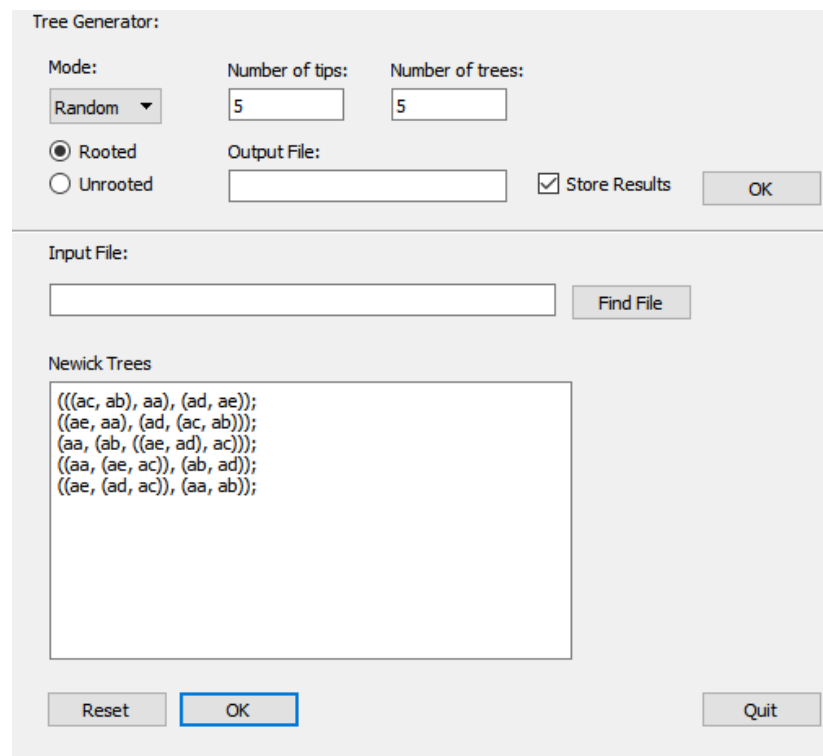
☐ Store Results

- 1.b. After picking mode set the number of trees and leaves you want (number of leaves limited to 20 for Full mode). Also decide whether you want to build Rooted or Unrooted trees by selecting the accurate radio button.

- 1.c. you can choose to save your data in an output file if prefer otherwise simply check “Store Results” and hit “OK”

- 1.d. If you selected “Store Results” then the resulting trees should appear in the Newick tree field.

Example:



Tree Generator:

Mode: Random ▼

Number of tips:

Number of trees:

☒ Rooted

☐ Unrooted

Output File:

☒ Store Results

Input File:

Newick Trees

```
(((ac, ab), aa), (ad, ae));  
((ae, aa), (ad, (ac, ab)));  
(aa, (ab, ((ae, ad), ac)));  
((aa, (ae, ac)), (ab, ad));  
((ae, (ad, ac)), (aa, ab));
```

If Uploading trees from file:

Use the “Find File” button to open file explorer. Then navigate and open desired file. The content of the file will display in the Newick trees field.

Input File:

C:/final/Random_200.txt Find File

Newick Trees

```
((ac, ad), (ab, ae)), aa;  
(((aa, ab), ac), (ad, ae));  
(((ae, ad), aa), (ab, ac));  
((ab, ac), (ae, (aa, ad)));  
(((ae, (aa, ad)), ac), ab);  
(ae, ((ac, (aa, ad)), ab));  
((((ac, ae), ad), aa), ab);  
(ac, ab), ((aa, ad), ae));  
(((ae, ac), ab), (aa, ad));  
(ae, ad), (ac, (ab, aa));  
(ae, (ac, aa)), (ad, ab));  
(ae, ((aa, ab), (ac, ad)));  
((aa, (ad, ac)), (ae, ab));
```

Reset OK Quit

Selecting Metric:

When you have your trees simply select you desired metric:

Rooted Metrics

Lambda:

☒ Kendall-Coljin

☐ Triplet Distance

Unrooted Metrics

☐ Robinson Fould

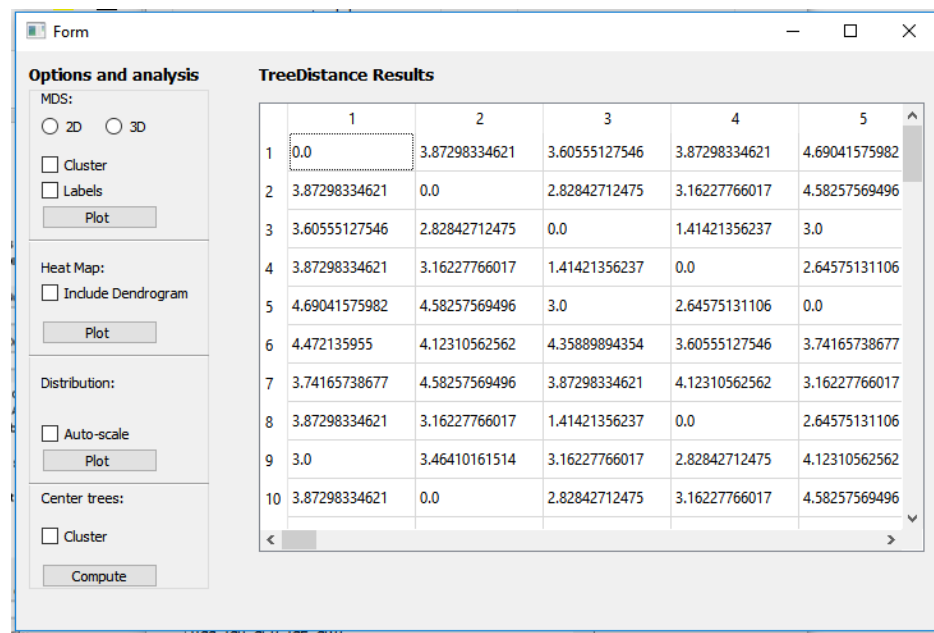
☐ Quartet Distance

Do this by selecting the radio button that corresponds to the metric of interest.

- if you select more then one then the program will pick whichever comes first in its code.
- Also make sure to set Lambda if using KC metric.

Select “ok” at the bottom of the page(next to “Reset”) when ready to compute distances.

Results page:



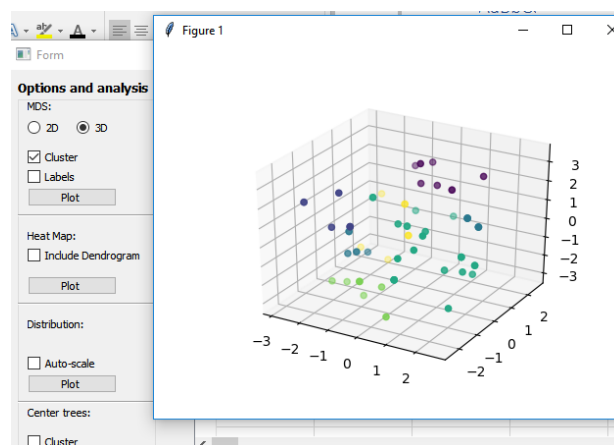
The results page contains the results of the selected distance metric in the form of a table.

From here you can produce visuals of the data:

For the MDS plots pick either 2D or 3D and select whether you want labels on the data points and colouring for the clusters.

Select "Plot" when ready.

A figure window(like the one shown below) will open and displayed the requested data.



When done, simply close window and produce more plots if desired.

For the Heatmaps select Include Dendrogram if you wish to see a dendrogram at the side of the heatmap. Then simply select plot.

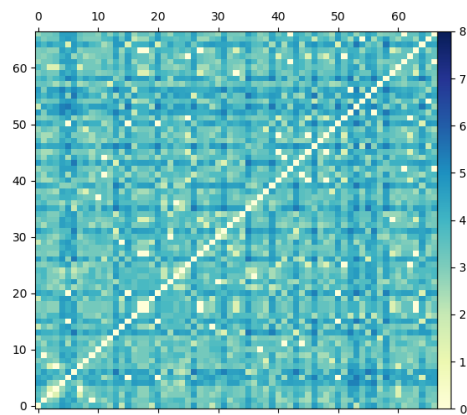


Figure 2: Without dendrogram

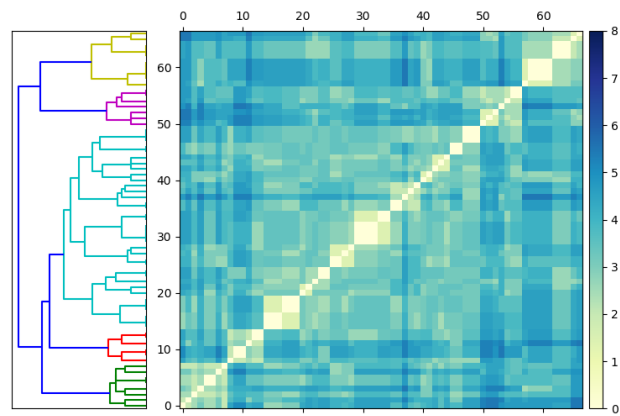


Figure 3: With Dendrogram

Likewise, for the Distribution plots you can chose to let the code auto scale the histogram(select the Auto-Scale checkbox) or use a constant value of 8 bins (Leave it unchecked). Then select “Plot”.

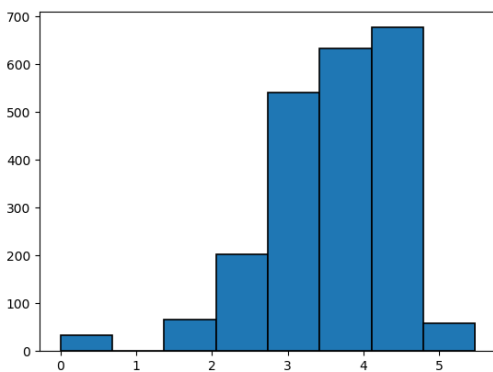


Figure 4: without Auto-Scale

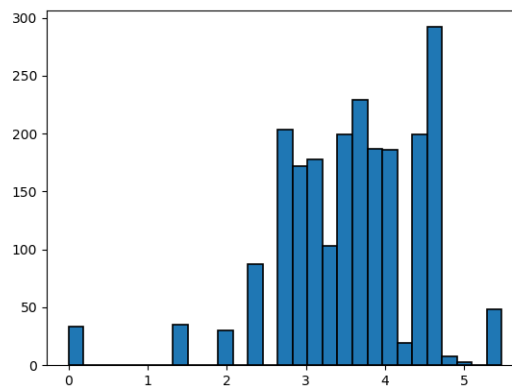


Figure 5: With Auto-Scale

The last available feature is the *Center Trees* option.

First select *Cluster* if you want the code to considered center trees for individual clusters as well the complete set. Otherwise it will only look at the total set of input trees.

After that, select “Compute”. This will open to the Center Tree Summary page and the requested data should be shown in the field on the page.

Form

Center tree Summary:

Center tree-approach #1:[4, 8]
Center tree-approach #2:[29]

Cluster ID:5
Cluster tree set:[1, 15, 20, 30, 54]
Center tree-approach #1:[20]
Center tree-approach #2:[20]

Cluster ID:6
Cluster tree set:[2, 3, 4, 8, 9, 10, 11, 13, 18, 19, 26, 28, 29, 33, 34, 38, 39, 41, 43, 46, 48, 49, 50, 52, 58, 60, 61, 62, 63, 64, 67]
Center tree-approach #1:[8, 13]
Center tree-approach #2:[29]

Cluster ID:4
Cluster tree set:[5, 7, 22, 24, 25, 36, 37, 40]
Center tree-approach #1:[24, 40]
Center tree-approach #2:[22]

Cluster ID:1
Cluster tree set:[6, 12, 16, 21, 27, 42, 45, 51, 56, 65]
Center tree-approach #1:[21, 51]
Center tree-approach #2:[16]

Cluster ID:2
Cluster tree set:[14, 23, 31, 32, 35, 44, 59]
Center tree-approach #1:[32]
Center tree-approach #2:[32]

Output to file

Save

If you wish to save this data:

1. Type in output filename
2. Select Save.