# **Biodiverse Quick Start Guide**

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## 1 Quick Start Guide

Version 4.0

A tool for the spatial analysis of biological and related diversity

# Shawn W Laffan, Giovanni Di Virgilio & Hannah Beaton Dec 2022

This document is an update of the 2018 version.

There is also a blog that provides updates and tips about functionality. It can be accessed through http://biodiverse-analysis-software.blogspot.com.au/

If you have question about the software then please start a discussion at https://github.com/ shawnlaffan/biodiverse/discussions or post a question at https://groups.google.com/forum/#! forum/biodiverse-users

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## 2 Overview

### 2.1 What is Biodiverse?

Biodiverse is a free tool for the spatial analysis of diversity using indices based on taxonomic, phylogenetic, matrix and trait-based relationships. Analyses can be run on a wide range of variables that vary across space and/or time, whether they are biological (e.g., diversity distributions of marsupials across Australia), physical (e.g., variation in rainfall across continental US), or other systems (e.g., geographic and temporal distribution of various Mediterranean dialects).

### 2.2 What analyses can I do with Biodiverse?

You can run a range of spatial analyses, such as cluster, moving window and randomisation analyses, visualise analysis results in interactive diagrams and maps, and optionally export analysis results to a variety of formats (e.g. delimited text, geoTIFF, JSON) to third party software for further analysis, such as ESRI ArcGIS, R and Matlab.

## 2.3 What programming language is Biodiverse developed in?

Biodiverse is written in the Perl programming language. There are two parts: an analysis engine, which can be scripted using perl code, and a GUI which is developed using Gtk2 and which calls the analytical engine.

### 2.4 Which operating systems does Biodiverse support?

You can install and run binary and source code versions of Biodiverse on Windows, MacOS and Linux platforms. The analysis engine is also tested on the FreeBSD OS and source code installations can be used on that platform. Visit the Biodiverse Downloads page to obtain the version of Biodiverse you wish to install.

## 2.5 How do I install Biodiverse?

Follow the Installation instructions webpage for your selected version.

## 2.6 Using this guide

## 2.7 Where can I get additional help?

You can access a range of Biodiverse Help Topics by clicking on the Help option on the menu bar within the Biodiverse application (see image below). You can also hover the mouse pointer over most buttons and menu items in Biodiverse to view their associated tooltips.

This guide does not cover all the detailed aspects of Biodiverse functionality, so links to the online Biodiverse documentation covering more detailed information are provided throughout. Alternatively, visit the Biodiverse Project Home for more extensive software documentation.

You can also send questions to the Biodiverse discussion forum at https://github.com/ shawnlaffan/biodiverse/discussions or at https://groups.google.com/forum/#!forum/



## 2.8 Some key terminology

The two concepts below are important when using Biodiverse. For details of a fuller list of Biodiverse terminology, see the Data Structures page.

#### 2.8.1 .1 Labels

Typically labels represent species, but in reality they can be any named entity that is then aggregated, or 'binned', into a Group. Hence, an individual label could also represent other taxonomic levels, e.g. a genus, or distinct entities from other phenomena, such as lithological classes (e.g. different rock types) or linguistic structures (e.g. different phonemes).

#### 2.8.2 .2 Groups

Groups are cells into which the labels are aggregated (binned). These are usually square, but can represent any number of axes (x, y, z, time, population-ID, ...) with differing cell sizes (resolutions) and numeric or text types. The groups are plotted in the interactive maps that Biodiverse produces as outputs of data visualisation and spatial analyses, as in the example below. Groups are also integral to the spatial components of the moving window, cluster and randomisation analyses.

Please note however, that group coordinates are in the same coordinate system (map projection) as the input data. If you have input data in multiple files, with differing coordinate systems, then you can use GIS or other geospatial tools such as the sf library in R to project them into a common system.



The 'Groups' are the square cells representing the Australian mainland.

## **3 Starting Biodiverse**

Note that the first time you run the binary version it will take a little while before you see anything. This is because it is unpacking all the files into your temp directory (folder on Windows). Subsequent runs will be much faster as no unpacking is needed, but be aware that if you have tools that regularly clean your temp folders then the files will be deleted.

## 3.1 Windows

If you've installed the Binary version of Biodiverse, start the program by double clicking on BiodiverseGUI.exe in the Biodiverse installation folder (wherever you unzipped it).

If you have installed the source code version then you can double click the BiodiverseGUI.bat file in the Biodiverse installation folder.

## 3.2 Linux and MacOS

On Linux, the binary version of Biodiverse can be run by double clicking on BiodiverseGUI. On MacOS the installation process allows you to dock it, in which case you open it like any other application.

To run the source code version of Biodiverse, open a terminal window and change directory to the biodiverse/bin folder. If it is in your home folder and called biodiverse then type: cd ~/biodiverse/bin

Once you have done this, type the following command to open Biodiverse. perl BiodiverseGUI.pl

Alternately you can use the full path, e.g.: perl ~/biodiverse/bin/BiodiverseGUI.pl

## 4 Importing Data

Note: If all your files are in the same location then you can set the working directory under the File menu to save time finding them. You can also bookmark folders in the file selector to get back to them more easily. Right click on a folder to see the option.

### 4.1 Data structures

Before importing data it is important to understand the sorts of data supported by Biodiverse. There are four main types, each of which can be stored in native Biodiverse format.

**Projects** – (file extension **.bps**) are a composite structure and may consist of a set of any number of BaseData, Tree and Matrix objects and any associated analysis results. These are only used by the GUI.

**BaseData** – (file extension **.bds**) is the primary storage object used in Biodiverse. Base-Data stores your spatial data (e.g. different species and their XY locations), a set of analysis parameters, and any associated outputs from cluster, moving window and/or randomisation analyses.

**Trees** – (file extension .bts) these are hierarchical tree structures, e.g. phylogenies, taxonomies or word roots, which are imported from nexus and similar formats. These are used for analyses involving tree structures, e.g. phylogenetic diversity, linked by the matching labels in a BaseData.

**Matrices** – (file extension .**bms**) these are matrices of numeric values representing some relationship between pairs of labels or groups. These are used for analyses involving matrix structures linked by the matching labels in a BaseData. They are also used as part of cluster analyses, in which case they relate to pairs of groups in a BaseData object.

## 4.2 Opening data

To open pre-existing data (i.e. a Project, BaseData, Matrix or Tree saved to disk), select *Open* under the desired menu option and then navigate to the relevant file to load it:



evant menu bar.

Select the file you want to load, and click OK.

## 4.3 Importing data

BaseData, Matrix, and Tree object data can be imported from 'raw' data files (e.g. Tabular text, rasters, shapefiles, spreadsheets or CSV text files in the case of BaseData and Matrix

objects) by clicking on their respective import buttons on the main toolbar, or via the 'Import' command in their respective menus.

For BaseData objects, either a new object can be created, or an existing object can be added to. When adding data it is up to the user to ensure the new data are in the same coordinate system (i.e. Biodiverse does not check if you add data in UTM coordinates to a BaseData object using decimal degrees).

#### 4.3.1 BaseData

The default import file type for BaseData is delimited text (e.g. CSV files).

These instructions describe the process where an input text file is in list format and contains one record per observation, with separate columns for one or more labels (e.g. names such as genus and species) and groups (e.g. x and y coordinates of a data point). However you can also import data from raster, shapefile and spreadsheet formats. All formats except raster can also represent a matrix of data such as for a sites by species matrix (see Importing Data in Matrix Format).

See the *Example\_site\_data.csv* file in the data folder for an example of the file format. The columns of data can be separated by commas, spaces, tabs, semicolons or some other user defined character. There is no restriction on column names or how many columns there are in the file but it is up to the user to know what they represent. You can allow the system to determine the separator type or select from a range of options.

num	genus	species	х	у
1	Genus	sp1	8	8

num	genus	species	х	у
2	Genus	sp1	6	2
3	Genus	sp1	8	9
4	Genus	sp2	5	4

Select the import button on the BaseData toolbar (or use menu *Basedata>Import*) to open the *Import Data* dialogue window, from where you can select the input data file.

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Outputs
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The text box at the top right of the *Import Data* window allows you to name the output BaseData object that will be produced. Once you are finished, click **Next**.

Note: you can import more than one file at a time so long as the order of the columns is the same. Target Data Set One Basedata per file Format Text Desktop Places Name Size Modified Inknown Unknown	
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txt and csv files	

You will then see the Import Options window with various options you can set for the import:

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	Options		
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	Allow empty groups?		
	Data are in matrix form?		
	Skip lines with undef groups?		
	Convert sample counts to binary?		
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	Input quote character	guess 🗸	
	Maximum number of header columns to show options for (includes remap dialogues	s) 150 🔹	
	Number of decimal places used in cell sizes	7	
	<u>C</u> ancel	🛶 Next	

Details of all the import options are described in Import Options, but leave all of them unchecked for this tutorial, except '*Skip lines with undef groups*'. Checking this option allows you to ignore records where a group field is either undefined or non-numeric. Such records can occur where you do not know the coordinates for a sample, if you choose the wrong column to use for the groups, or if you have a series of lines with no data at the end of a file.

If you are not importing the *Example\_site\_data.csv* file, bear in mind you might need to check some of the other import options. A useful option is '*Allow empty groups*' which lets you have groups that are considered for analysis, but that have no labels themselves. This is useful when you wish to have moving window analyses extend beyond the sampled data to give a smoother result.

#### Click *Next*.

The *Choose columns* dialog box appears and allows you to select various options for each column in your input text file.

	\Desktop\Example site d	ata.csv			
			Set column options		
#	Column	Туре	Cell size	Cell origin	Data in degrees?
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1	genus	Label 🗸			
2	species	Label			
3	x	Group	100000.0000000	0.000000	~
4	У	Group	100000.0000000	0.0000000	~

You must set a *Type* value for at least one Group and one Label column, but more than one of each may be chosen.

All columns in your file that are irrelevant to the analysis should be set to *Ignore*, as is done for the **num** column in this case.

Select *Label* as the *Type* for the **genus** and **species** columns. This represents genus and species values for each record as one combined label, i.e. '*Genus species*'.

Select *Group* as the *Type* for the  $\mathbf{X}$  and  $\mathbf{Y}$  columns.

When a Group column has been set you will be given the option to select its cell size (in the same units as the group data is stored) and its origin. If you are not importing the *Example\_site\_data.csv* file, make sure these dimensions and units are appropriate to your data. You can specify if the group data are degrees using the *Data in degrees*? comboboxes. This allows you to import data in degrees minutes seconds (e.g. 22° 15' 10'' S) and decimal

degrees formats, as well as enabling some validation that the coordinate values are in the correct range for such units.

The Re-order Columns dialog box is the next window to appear. This allows you to order your labels and groups. For example, placing "y" above "x" makes the y column data the first dimension of a group's coordinates and x the second (useful if latitude precedes longitude in the column order of your input file). If you forget this step then the axis order can be changed later on using the *Duplicate with re-ordered axes* tool under the BaseData menu.

Since the columns in *Example\_site\_data.csv* are already in the correct order, we will accept the current column ordering. Click **OK**.

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			Up				
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Biodiverse now imports the data from the Example\_site\_data.csv input file and creates a new BaseData object. Once the import process is complete, the name of the new BaseData object ('My\_new\_basedata' in this case) appears in the top-left of the Biodiverse main window.

#### 4.3.1.1 Remap

The option to remap label names will appear after the re-order option.

The remap process can generate possible matches between spatial data and any tree, matrices, group properties and label properties automatically. While this section is focused on importing BaseData, any object can have its element names remapped during or after import, with the latter accessed through the Basedata, Tree and Matrix menus as appropriate. The centralised interface for automatic remaps can be accessed under the file menu, as below. There are panes listing exact matches, non-matches (i.e. differences were too great), punctuation matches and possible typos. Users can choose to ignore any of these sets, and also select subsets within the sets if, for example, there are false matches. See the blog for further remap information and examples.

Since we are just importing example base data we will not remap so choose "no".

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Having imported data into a BaseData object, you are now ready to run cluster, moving window and randomisation analyses, or you can **visualise** this data (see Visualising Data) or calculate a **spatial index** (see Building a Spatial Index) which helps run faster analyses when using this BaseData. Alternatively, you can now import additional data files (see importing Matrices and Trees below).

However, prior to doing anything else, it is a good idea to **Save** your newly imported data. Use the File > Save menu option to save the whole project. To save just the BaseData select the My\_new\_basedata object, and save it as a BaseData object, either via the *Basedata* menu

(Basedata > Save as) or the  $\square$  icon on the Basedata toolbar.

#### 4.3.2 Matrices

Matrix data can be imported at any time, although it can only be viewed with an existing (and selected) BaseData object. Currently only delimited text files can be imported (e.g. csv or txt files).

Remember that these matrices are not site by species matrices. These are matrices of numeric values representing some relationship between pairs of labels or groups, for example numbers of base pairs shared between pairs of labels. Site by species data are imported using the basedata import process.

Select the import button on the Matrix toolbar to open the Import Matrix dialogue window, from where you can select the input data file. Select *Example\_matrix.txt*, give the new Matrix a name if you like, and click **OK**.



After deciding if your matrix input file format is normal or sparse, you must now decide how the columns in the matrix file should be read. You must select at least one label column, and

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Column 35 Ignore® Label○ Matrix Start○	Genu:	• sp1	- anon_col	• anon_col! •	• •	6 anon_col?	7 anon_col: ● ○	<ul> <li>anon_cols</li> <li>O</li> </ul>	• •	0 anon_coli. •	• • •	2 an

only one "Matrix start" column. Any other columns in the file should be set to "Ignore".

Click Ok, then select No when prompted to *Remap element names and set include/exclude?* The matrix is imported and appears in the drop-down menu in the matrix toolbar at the top of the screen.

The matrix can only be visualised once a BaseData object has been imported and visualised as well. (it will only produce a useful display if the matrix and BaseData share at least some labels).



Note that you can either save the matrix as a Matrix .bms object ('Matrices > Save as' from the menu), or it can be saved as part of a Project see Saving a Project at the end of this guide.

#### 4.3.3 Trees

There are two options for creating Trees in Biodiverse:

- 1. Import a Tree into a project at any time
- 2. Derive a Tree at any time if you already have a BaseData and/or matrix object selected.

In both cases, a Tree can only be visualised with an existing BaseData object. A Tree is most useful if it shares some labels with the BaseData being displayed.

**Importing a Tree** A Tree can be imported from nexus (\*.nex or \*.tre), newick, "R json" or tabular formats. Once a tree is imported, it will be added to the project.

To import a Tree, select the import button on the Tree toolbar. A window will appear asking if your tree data are in a tabular format. After selecting YES or NO, you can select your file:

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Select your file and click OK. You will then have the option of choosing a label remap file. This is often needed so the node names match the relevant BaseData labels (see FAQ page: My phylogenetic analyses have empty results). In many cases a phylogenetic tree will have labels like "genus\_species", but if you imported data from a file that has genus and species in separate columns then the labels will look like "genus:species", which will not match. This is where remapping is needed.

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		Rema	p the node n	ames? <u>Y</u> es	<u>N</u> o			

Since we are using the example input data, we will remap (but if you don't wish to remap labels, simply click *Cancel* and the system will import the tree).

To remap the tree labels using an existing file, click **YES**. You are prompted to select a remap "label Source". Here we use "user derived file" to select our *Example\_tree\_remap.txt* file. Click **OK**, accept the column separator and quote defaults, click **Next**.

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lin z	Example_site_data_matrix_form.csv 3	3.5 kB Unknown
Deskton	Example_tree.nex 2	2.3 kB Unknown
Windows (C)	Example tree remap.txt	782 bytes Unknown
	Example_tree_with_colours.nex	2.8 kB Unknown
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A popup dialog now prompts you to specify the column types for the remap process. Specify as many *input\_element* columns as the tree labels have (i.e. one for nexus files) and then each label column in the BaseData object must be designated as a *remapped\_element*. Click **OK**. The system will import the tree and perform the remapping.

ita	Output Indices Typ	e			
imple_site_c	lata				
e pro	perty column types		×		
	,,	Select column types			
#	Column	Туре			
0	tree_name	Input_element ~			
1	genus	Remapped_element ~			
2	species	Remapped_element 🗸			

**Deriving a Tree** You can derive a Tree from a BaseData object or Matrix at any time. Select the "*Create tree from labels*" or "*Convert matrix to tree*" options under the BaseData and Matrix menus, respectively:



When generating a tree from the BaseData labels, labels are treated as taxonomic names, and thus are useful if the labels have at least two components (e.g. genus and species). A tree generated from a matrix is simply a cluster analysis using the average linkage function, so will only be valid for dissimilarity matrices.

## 5 Visualising Data

You can interactively visualise the relationships between the groups and labels once you have imported data or opened a pre-existing data set or project.

To visualise your data, either select the *Basedata->View Labels* menu option, or double-click on the basedata object under the Outputs tab. Depending upon which data objects you have imported (e.g. BaseData, Matrix, Tree), a maximum of 5 panes are viewable:



The panes constitute a linked visualisation system so that the selection (labels, groups, matrix cells or tree nodes) in one pane is reflected in the other panes. If more than one label is contained in the selection in any pane, the groups in the group grid are coloured with a hue of red according to the number of the selected labels they contain (dark red for more, lighter red for less, white for none).

Note that the sizes of the panes can be changed by clicking and dragging the dividing bars between them.

We now describe how each pane works.

#### 5.0.1 Label lists

Click on any row in the list to highlight a single label. Hold the shift key down to select a contiguous block, and the control key to select (or deselect) non-contiguous labels. The second list is only visible if the project has a selected matrix. The main use for the second list is to be able to select labels from each list to highlight specific cells – or columns of cells – in the matrix pane, if a matrix is currently selected. The first (top) label list represents matrix rows, while the second (bottom) label list represents matrix columns.



Sort the label lists by clicking on the column headers. The default order is by label, in a natural sort order. Re-ordering of these lists also re-orders the matrix plot (the upper list will sort the rows, the lower list will sort the columns). The current selection in the lists is updated whenever you select elements in one of the other panes.

The *Variety* column shows the number of groups (grid cells) each label occurs in.

The *Samples* column lists the number of times a label occurs across all groups.

The **Redundancy** column shows the sample redundancy for each label. This is calculated as (1 - variety / samples). A value close to one represents a good overall sample of a label relative to the number of groups it occurs in (many redundant samples). A value of zero means that there is only one sample per group the label occurs in, and it is therefore not well sampled.

The *Selected* / *Col selected* columns have a value of 1 when that label is selected, allowing the user to raise the selected set to the top of the list. The *Col selected* value is 1 only when one selects a matrix column, either through the lower Label List or on the matrix itself.

#### 5.0.2 Group grid

The group grid displays the groups. Normally this is a map of the data (e.g. if your group data consists of some form of geographic coordinates), but there is no reason that you are restricted to using geographic locations for your groups. If your data use text group axes then the system will assign them to cells on a grid based on an alphabetical sorting.

Hovering over a group will highlight in bold the nodes in the Tree corresponding to the labels it contains, if a tree is displayed.

Left-clicking on a group will highlight it in dark red. Other groups may also be highlighted depending on the number of labels they share with the selected group (darker red for more shared labels, lighter red for less, white for no labels in common). Groups will then be highlighted according to the number of labels they have in common with the selected group. Labels in selected groups will also be highlighted in the top label list (although the list does not automatically jump to them). Drawing a box over the grid with the left mouse button selects labels from all the groups in the box, allocating the hue based on the species richness of the selection rather than a single group.



While holding the control key down, click on a group to display a pop-up window that shows you a list of the labels it contains and the sample size in that group for each label. To bring up any group's detailed information without changing current highlighting, use the middle/wheel mouse button to select a group.



Alter the Group Grid zoom level using the three zoom buttons at the left of the pane. For more details about this see the relevant blog post.



#### 5.0.3 Tree

The tree is generally a representation of the phylogenetic similarities between labels, although it could be used for anything that uses such a structure. In this pane, you should see two sections (assuming a tree object is selected in the main toolbar at the top of the window). The upper section displays the relationship between labels as a dendrogram.

The dendrogram can be plotted by node depth or length via the *Options* button at the bottom of this pane. This menu also allows you to change highlighting settings.

Hovering over a tree node highlights the groups containing the node's labels in the group grid. It does this using a circular symbol. Right click on the node to fix the highlights until the next mouse click in the tree pane.

Left-clicking on a branch selects all labels in terminal descendants (single-label nodes) of that node in the tree that are also in the label lists. Any nodes containing a label that is not present in the BaseData will remain black in the tree.



Control-click on a node to display a pop-up window from which you can access lists of the labels, groups and branch characteristics (length, name, etc).



Note the blue vertical sliding bar on the right side of the tree pane. Hovering the mouse over this bar will display three numbers. The first two numbers indicate the quantity and percentage of nodes present to the right of the bar. If the tree is plotted by node depth, the third number indicates the depth at the current bar position. If the plot is by node length,

the third number indicates the distance from the bar position to the most distant (left-most) leaf node.

#### 5.0.3.1 Scree plot

The scree plot is hidden by default but can be dragged up from the bottom of the tree pane. This plot displays a simple graph of the proportion of nodes present to the left of an imaginary vertical line cut through the tree above. Move the mouse toward the bottom of the tree pane until it indicates a bar that you can click on and drag upward to reveal the graph.



#### 5.0.4 Matrix grid

Each matrix grid cell represents a pair of labels from the label lists, coloured according to the pair's matrix value, with a colour scale for these values on the right of the matrix.

Cells in the matrix grid are only coloured if both labels they represent are present in the BaseData label list. If one or both of its labels are not present in the BaseData, a cell remains white.

The system lists which element you are hovering over at the top of the pane, indicating the label pair and its matrix value.

Click on a single element (cell) to select one pair of labels. The two label lists will automatically adjust to show these two (the top list highlighting the label corresponding to the matrix row,

the bottom list highlighting the label corresponding to the matrix column). All cells in the group grid containing those labels will be highlighted in red as per the groups, as will the relevant nodes on the tree.

You can also click and drag the left mouse button to select a rectangular region in the matrix. This highlights the selected labels in the other panes, adjusting the label lists to reflect the new selection.



## 6 Data Analysis

## 6.1 Building a Spatial Index

We will build a **spatial index** for our new BaseData object. A spatial index enables analyses using this BaseData to run faster (though beware that some user-defined spatial conditions will not work with a spatial index). Note that an index can be deleted/rebuilt at any time, and these changes affect only subsequent analyses, not those that preceded any change.

Select Build Spatial Index from the Analyses menu option:



For most purposes, accept the index sizes suggested by the system (see Using the Spatial Index for additional details on setting optimal index sizes).

Click OK to build the spatial index. A pop-up dialog notifies you that the index has been built (OK).

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## 6.2 Running a Cluster Analysis

Once you have imported or opened a BaseData object, you can run cluster analyses to identify clusters in this data.

Biodiverse supports agglomerative clustering of the groups based on their labels, or some function of their labels such as the values of a linked matrix or tree.

We will run a cluster analysis on the BaseData imported earlier ' $Example\_new\_basedata$ ' (see Importing data). If  $My\_new\_basedata$  is not loaded, but you have saved it, open this file now by clicking on '*Open*' from the *Basedata* menu and navigating to the location of your bds file.

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	Transpose		
	Create tree from labels		
	Extract embedded trees		
	Extract embedded matrices		
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	Trim to match matrix elements		
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To run a cluster analysis on the currently selected BaseData object, select Cluster from the Analyses menu:

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The cluster analysis tab opens. It has three main sections where you can set options:

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Enter spatial constraints for the	Definition query			
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cluster those groups or clusters	Tie breakers	akers 1: random 🗸 maximi	e 🗸 2: random	✓ maximise ✓
with other groups that satisfy the spatial constraints.	Do not use caching	Build matrices and then stop Utput matrices direct to text files Output matrices direct to GDM compatible format	□ Keep spatial □ Do not clone matrices before clustering	Clear singleton nodes from tree
	Calculations to run fo	cluster node (optional)		
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e.g. just build matrices, and don't cluster;	PhyloCom Inc			
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Select the subsequent calculations which /	Phylogenetic	ver		~
will be run for each node in the tree /		Go!		
generated by the cluster analysis		001		

• The upper section (*Parameters*) determines the parameters used in the clustering to generate a tree. This includes options to control the cluster tie-breaker algorithm.

- There are check-boxes in the middle section that can be toggled to alter how the cluster analysis runs, e.g. by controlling aspects like process performance (e.g. memory usage), the automatic export of results, etc.
- The lower (*Spatial calculations to run for each cluster node*) determines what subsequent calculations will be run for each node in this tree, using the groups it contains to define the spatial sample. This allows you to, for example, calculate the phylogenetic diversity of the regions defined by each cluster node.

#### 6.2.1 Setting cluster analysis parameters

For the purposes of this guide, accept the default **name** for the cluster analyses (see diagram above) and also the default **metric** 'SORENSON' (the set of indices that can be used as the clustering metric is denoted by a column in the Indices list). We will also accept the default **linkage** of '*link\_average*', which calculates the dissimilarity of each newly created group with all other groups as the average value of the groups merged to form it, weighted by the number of terminal nodes they each include. In this way a merger between node A with 10 terminal nodes and node B with 1 terminal node will not be biased towards the labels in node B (see the Cluster parameters section of the Sample Session for details of the additional linkage functions that are available).

The **spatial conditions** can be used to control which Groups are considered candidates to be clustered together. The default condition in the 'Spatial conditions set 1' text box provided by the system is 'sp\_select\_all()'. This condition selects every group and is an appropriate condition to use for unconstrained clustering. If you wish to use a different spatial condition, for example to first cluster within geographic regions, then refer to Spatial Conditions for further details. The **definition query** serves a similar purpose, except that it can be used to restrict the clustering to only a subset of groups. For example you might have a data set for Europe but only want to cluster cells in regions above a specified elevation value. The Spatial Analysis section in this document has some more details about spatial conditions and definition queries.

Check the **option** or **calculations** boxes as appropriate. If you're curious as to what they do, hover over them with the mouse pointer to view a tooltip.

Click on the **Go!** button (keyboard shortcut *Control-G*). The system will first build the dissimilarity matrix (or matrices if you have several spatial conditions), then run the clustering using these matrices, and then any spatial calculations you have selected for each node. It will then prompt you to **display results**.

#### 6.2.2 Viewing the cluster results



There are three sub-panes within the display pane. On the left is the group grid, on the upper right is the tree representing the clustering, and on the lower right is the scree plot for the tree.

As with the visualisation of basedata/matrix/tree objects described earlier, the system is linked, and interactions in the group grid or tree of the cluster display are generally reflected in the other. Hovering the mouse over a node in the tree highlights the groups (in the group grid) that are contained in that node. Likewise, hovering the mouse over a group in the group grid will highlight the path (set of nodes/clusters) in the tree to which that group belongs.

Left click on a tree node to colour a set of subclusters (descendant nodes in the tree). These clusters are split into a number of coloured groupings based on the "*Clusters to colour*" parameter at the bottom of the pane. Note that some leaf nodes in the tree may have a length of zero (indicated by vertical bars at the leftmost side of the tree, longer vertical bars indicating more zero-length leaf nodes). Thus, if any such nodes occur under (to the left of) the node you have selected, their colouring will not be apparent if you are using "*Plot by Length*" mode. These nodes, along with their colouring (if selected) can be made apparent by switching to "*Plot by Depth*" mode under the tree options button under the *Display* menu at the left.

The blue sliding bar in the tree pane can be dragged across the tree to colour the nodes and groups at that level. The bar also displays the number of nodes it is crossing when the mouse is focused on it. The maximum number of contrasting colours the system will display is 13.

If the slider bar crosses more than 13 nodes, all nodes will be uniformly coloured red instead, and groups in the group grid will not be coloured.

It is also possible to assign your own colours to the clusters and to generate a geotiff (raster) to reproduce the coloured cells in other systems.

## 6.3 Running a Spatial (Moving Window) Analysis

#### 6.3.1 Introduction

The Spatial Analyses are a type of moving window analyses (because nearly all analyses in Biodiverse are spatial in some way), and are another method of identifying spatial patterns in your data. Depending upon the exact nature of your data, it is likely that the Groups comprising your BaseData constitute a geographic surface. Moving windows are used to systematically iterate across this space, with one or two **neighbourhoods** of the moving window being used to assess the labels/values aggregated in the Groups. The window might also consist only of the processing group, with no neighbours (each group is analysed separately).

To run a moving window analysis, you will need to have imported or loaded a BaseData object and ideally built a spatial index for this BaseData. These instructions assume you have either imported the sample data above, or you can open the example BaseData object 'example\_data.bds' in the Biodiverse data folder.

Select a Basedata object by clicking on it and open the menu option *Analyses -> Spatial* and the spatial tab appears:



The Spatial tab has two main sections where you can set options. The upper section (*Parameters*) determines the parameters used in defining the two neighbour sets used in the spatial analysis (the second is optional) as well as the definition query. The lower (*Calculations to run for each neighbourhood*) determines the subsequent calculations that will be run for the set of neighbours related to each group. You can select any number of calculations to perform.

#### 6.3.2 Setting the Spatial Analysis Options

The **Name** option is the name used in the system. You can accept the default, or enter a new name (you cannot have duplicate names within the same BaseData object).

The Neighbour set 1 and Neighbour set 2 text boxes allow you to define the neighbour sets used for the calculations (see Spatial Conditions for further details). The size and shape of the neighbourhoods defines the set of groups to be considered in an analysis and it is up to you to decide what sort of neighbourhoods and how many to use for your analysis. The system provides considerable flexibility in this regard: both neighbour sets may be arbitrarily defined independently of each other and you are not obliged to specify a second neighbourhood.

The default condition in the Neighbour set 1 text box is 'sp\_self\_only()'. This restricts the neighbourhood to one cell/group (the processing group, which is the group being processed at an iteration). The default condition in the Neighbour set 2 text box 'sp\_circle (radius => 100000)' defines a circular neighbourhood of 100000 units centred on the processing group. The units are whatever the original data used, and for the example data this is a 100 km or one cell radius.

These default conditions are appropriate for our sample data, but we will modify the second condition. Change the circle radius from 100000 to 200000.

See Spatial Conditions for more detail on defining the neighbourhood sets (e.g. for the range of functions that you can use to specify neighbourhoods).

Note that the use of neighbourhoods varies according to the type of calculation selected for analysis (see Selecting Indices below). Some calculations aggregate the neighbourhoods into a single set (e.g. endemism\_whole), others compare the labels in the first neighbour set with those in the second (e.g. Jaccard and other dissimilarity indices), while others use the first set to define the list of labels to use but then consider distributions across both neighbour sets (e.g. endemism\_central). Some will not be run unless two neighbour sets are defined, primarily the turnover calculations.

The **Definition query** text box allows the analysis to be applied to only a subset of groups (those which satisfy the criteria in the definition query, but note that all groups are still considered as possible neighbours). Leave this blank for this session. For details of setting a definition query see Definition Queries.

The Verify buttons let you know if the spatial conditions entered are syntactically valid.

#### 6.3.3 Selecting indices to calculate

Use the check boxes to select which calculations are to be calculated. Press the plus buttons next to the *Endemism*, *Lists and Counts* and *Taxonomic Dissimilarity and Comparison* sets to expand their trees. Check the boxes of *Endemism central*, *Redundancy* and *Richness* under *Lists and Counts* and *Sorenson* under the *Taxonomic Dissimilarity and Comparison* set.

Details about the full range of indices are available from the Indices page.

Click on the **Go!** button. The system will then run the selected spatial analyses.

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Absolute endemism lists	Lists underlying the absolute endemism scores.								
🗉 🗹 Endemism central	Calculate endemism for labels only in neighbour set 1, but with local ranges calculated using both neighbour sets								
🗉 🔲 Endemism central hierarchical partition	Partition the endemism central results based on the taxonomic hierarchy inferred from the label axes. (Level 0 is the highest).								
🗉 🔲 Endemism central lists	Lists used in endemism central calculations								
🗉 🔲 Endemism central normalised	Normalise the WE and CWE scores by the neighbourhood size.								
🗉 🔲 Endemism whole	Calculate endemism using all labels found in both neighbour sets								
🗉 🔲 Endemism whole hierarchical partition	Partition the endemism whole results based on the taxonomic hierarchy inferred from the label axes. (Level 0 is the highest).								
🗉 🔲 Endemism whole lists	Lists used in the endemism whole calculations								
Endemism whole normalised	Normalise the WE and CWE scores by the neighbourhood size.								
Hierarchical Labels									
Lists and Counts									
Element counts	Counts of elements used in neighbour sets 1 and 2.								
Element lists	Lists of elements used in neighbour sets 1 and 2.								
🗉 🗌 Label counts	Counts of labels in neighbour sets 1 and 2.								
I Label counts not in sample	Count of basedata labels not in either neighbour set (shared absence)								
Local range lists	Lists of labels with their local ranges as values.								
Image: Local range summary statistics	Summary stats of the local ranges within neighour sets.								
Image:	Counts of non-empty elements in neighbour sets 1 and 2.								
I 🗌 Rank relative sample counts per label	Find the per-group percentile rank of all labels across both neighbour sets, relative to the processing group. An absence is treated as a sample count of zero.								
🗉 🗹 Redundancy	Ratio of labels to samples.								
🗊 🔽 Richness	Count the number of labels in the neighbour sets								

## 6.3.4 Viewing the Spatial Analysis Results

Once the analysis is complete, the system asks you whether you want to display the results. Click *Yes* and you will be shown a map of the moving window analysis results. Pull the pane down to view the options you used, for example to change them and re-run the analysis.



Vector overlays from shapefiles can be plotted using the "overlays" interface at the bottom of the screen. Click the *Overlays...* button, click *Add*, navigate to the Biodiverse/data folder and select *coastline\_lamberts.shp*, click *OK*, highlight this file in the Select Overlay dialog box and click *OK*.

Nothe that Biodiverse is not yet aware of coordinate systems and only "sees" the coordinates as numbers. This means that the vector data MUST be in the same coordinate system as your basedata. If you have imported data as lat/long coordinates (a geographic coordinate system) then the vector data must also use geographic coordinates. If your basedata are in an equal area coordinate system then your vector data must also be in that coordinate system.



### 6.3.5 Running analysis with local neighbours

In the above moving window spatial analysis, the output visualisations only provided a single cell output of iterations within the map (black dot within the group cell).

However, altering the second neighbour entry to "sp\_circle (radius = > 500000)" when setting the initial analysis parameters (noted above), can identify aggregated relationships of these cells with their "neighbours".

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Neighbour set 1 sp_self_only () # sp_self_only will generate a single cell neighbour set									
Neighbour set 2	# Specify a neighbour set 2 for turnover and related window calculations # Uncomment the line for it to have an effect sp_circle (radius => 500000)								
Definition query	æ								
Calculations to ru	n for each neighbourhood								
🕀 🗌 Element P	roperties								

#### The result is a display like this:



Hovering over a group will highlight the groups used in the calculations – a solid circle for those in the first neighbourhood and a dash for those in the second neighbourhood. Right click on a group to keep the highlighting at that group until the mouse is left clicked on any group.

You can control whether these are displayed, or just display one set, by using the Neighbours selection options.

Holding the control key while clicking on a group, or clicking on a group with the middle mouse button, produces a pop-up list with all the results in it. It also includes lists of the elements (groups) in each neighbour set (Elements set1, set2 and all) and of the labels in these neighbour sets (Labels set1, set2 and all). The "All" list is the union of neighbour sets 1 and 2.

The tree branches are coloured according to whether they are found only in the first neighbour set (blue), the second neighbour set (red), both (black) or neither (grey). See also the blog post. Some indices can also be plotted on the tree.

### 6.4 Running a Randomisation Analysis

#### 6.4.1 Introduction

Randomisations in Biodiverse are used to assess the statistical significance of a set of analysis results given some randomisation scheme such as shuffling the species around the map (labels across groups in Biodiverse terms), subject to constraints such as each cell (group) must maintain the same number of species. Randomisations are key to interpreting where results differ from what would be expected, and are integral to protocols such as the Categorical Analysis of Paleo and Neo Endemism (CANAPE). The output can provide rank-relative scores from which significance can be derived as well as z-scores.

The default randomisation algorithm in Biodiverse is called rand\_structured.

The rand\_structured algorithm is so called because it maintains the structure of the original data, specifically the spatial distribution of the richness patterns, while randomly allocating taxa (labels) to groups (cells). By default, the richness patterns are matched exactly, but users also have the option to allow tolerances such as an additional number of labels per group (e.g. five extra), or some multiple of the observed (e.g. 1.5 times as many). The rand\_structured randomisation uses a filling algorithm, followed by a swapping algorithm to reach its richness targets. There is a series of blog posts describing the randomisation algorithms and visualisations.

The basic process of the randomisation is this. For each iteration of the randomisation analysis, Biodiverse will:

- 1. Create a new basedata object with a random allocation of labels to groups, according to the selected algorithm
- 2. For each analysis in the basedata:

- 1. Regenerate a version using the randomised basedata
- 2. Compare the values of the analyses from the original and randomised basedata and track if they are higher or lower, on a group by group basis
- 3. Track basic statistics of the distribution to allow the calculation of the mean and standard deviation, and thus z-scores.

Randomisations can be run by selecting the Analyses>Randomisation menu option:

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Outputs Labels - Example_site_data	Region <u>G</u> rower	Alt+G	example_data_x64_Spatial0 🕱
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Example_site_data	Build Spatial Index	Alt+I	
Example_	Delete Spatial Index		Cluster
Example_s	ite_data_Cluster0 SORENSON	Matrix_0	0 Matrix

Cluster and Region Grower trees are not rebuilt by default, partly for speed, partly because it is not normally needed. If you do want to do so then select the "build randomised tree outputs" checkbox. Note that any calculations per node are compared against the randomly generated basedata, though.

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Once the relevant parameters are specified, press "Randomise!".

Note that the randomisation analysis tab does not show maps or any other displays once the specified number of iterations have completed. The results are added as lists to any existing analysis objects and can be displayed by selecting from the "List and Indices" option on the relevant plots. You might need to close any open plots and re-open them to see the new lists. See the main help system.

A description of what the list and index names mean is also in the main help system. (Consider for example the Rand1»SPATIAL\_RESULTS list and C\_END\_CWE index below).



#### 6.4.2 Spatially Structured Randomisations

In the standard implementation of a randomisation, labels are randomly allocated to any group across the entire data set. This works well for many studies and is very effective, however, when one begins to scale analyses to larger extents, then the total pool of labels begins to span many different environments. The randomisations could allocate a polar taxon to the tropics, and a desert taxon to a rainforest. This does not make the randomisation invalid, but it is perhaps not as strict as it could be, and perhaps also not as realistic.

This can be readily fixed in Biodiverse by specifying a spatial condition to define subsets. Or, if you only want to randomise a subset of your data while holding the rest as-observed, you can use a *definition* query. You can specify spatial conditions using the same syntax as for the Spatial and Cluster analyses. The analytical decisions are yours but generally speaking it is better to use a condition that generates non-overlapping regions. Each group is allocated to only one subset, so in such overlapping cases it is the first one that contains a group "wins" that group.

To read more on spatially structured randomisations see this blog post.

<ul> <li>Biodiverse 4.0</li> </ul>	Madee Tree Andrew Hile	- 0 >	ζ.
Basedata examp	ie data x64 🗸 😭 🔚 는 🔶 Matrix Example_matrix 🗸 🍘 🔜 🌦 🔶 Tree Example_tree' 🛛 🖉 🔛 늘 💠		
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## 7 Export

## 7.1 Saving a Project

Exporting an entire project is done through the *File* menu using *Save* or *Save As.* This preserves all existing BaseData, matrix and tree objects – along with their associated analyses – as a ".bps" file.

## 7.2 Exporting results, groups and labels

Exporting a cluster or spatial analysis to be opened in a different software package is done through the Outputs tab, or via the Export menu at the left of the map display when viewing the result. Select the appropriate output and click *Export...* 

You can also export the groups or labels as a sites by species matrix (or similar) as per this example:

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<u>Eile B</u> asedata <u>M</u> atrices <u>I</u> rees <u>A</u> nalyses <u>H</u> elp			
Basedata Example_site_data 🗹 🗑 🔂 📄 🕂   Matrix (none) 🗸 🗑 🔜 🚔   Tree 'Example_tree' 🔽 🗑 🔂 🚔 🕂			
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Example_site_data		Sho	w
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Export Basedata X		Rena	me
What to export?		Descr	ibe
<u>G</u> roups <u>Labels</u>		Delet	e

Results can be exported to a range of formats. For example, to generate a set of geotiffs for display using a GIS, select the 'GeoTIFF' format from the drop-down and then click the **Next** button. Enter a filename (a file type extension is not required) for the exported results and a location where you would like them saved and click **OK**. (Note that currently the geotiff format generates one file for each index in a spatial result, and one for each label in a basedata if you chose to export the labels).

Tree based outputs like Cluster and RegionGrower objects can be exported to geospatial formats as well as to tree based formats like Nexus and Newick.

The examples below are for a Spatial Analysis exported to a delimited text file.

The first option is the type of file to export to.



The next window will show a large range of options, with the set of options changing depending on the type of file being exported to. Most will have popups that appear when you hover over them, so you should do this to see what is available.

🗢 Export format: Delimited text								×
Options		Filename						_
List to export	SPATIAL_RESULTS	Name:	example_export.csv					
Def query	•	Save in <u>f</u> older:	\ biodiv	erse			Create Fo	der
Force symmetric (matrix) format								
One value per line	0	Places	÷	Name	<b>^</b> 5	Size	Modified 4	*
Field separator	, 🗸	Search Recently Use	ed I	Can	ю	368.1 MB 52.0 kB	Unknown	1
Quote character	• v			🐒 can	ар	5.6 kB	Unknown	
NoData value	undef 🗸	Ph data		💌 can	ар	50.9 kB	Unknown	
Quote element names and headers	0	÷ -		🗋 clu	ste	36.9 kB	Unknown	
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The most important option is the choice of **List to export**. The analysis results in Biodiverse will be stored across several lists Most go in the SPATIAL\_RESULTS list, but list indices have their own. Each randomisation will also have several lists on each output (see Randomisation section above). This next example contains three calculation result lists from the PE clade contribution calculation, as well as three randomisation lists for each of the result lists.

A Export format: Delimited text				Х				
Options		Filename						
List to export	SPATIAL_RESULTS	Name: example_export.csv						
Def query	SPATIAL_RESULTS	Save in folder	diverse	County Falling				
	PE_CLADE_CONTR	Save in Tolder:	diverse	Create Poider				
Force symmetric (matrix) format	PE_CLADE_CONTR_P							
One value per line	PE_CLADE_SCORE	<u>P</u> laces	Name Size	Modified				
Field separator	Rand1>>PE_CLADE_CONTR	Search	1 Acaci 368.1 ME	Unknown				
Quote character NoData value Quote element names and headers	Rand1>>PE_CLADE_CONTR_P	W Recently Used	Canap 52.0 KB	Unknown Unknown Unknown				
	Rand1>>PE_CLADE_SCORE	biodiverse	Canap 5.0 kB					
	Rand1>>SPATIAL_RESULTS	<u>Asts</u>	Canap 50.9 kB					
	Rand1>>p_rank>>PE_CLADE_CONTR	<b>T</b> -	Cluste 30.9 KB	Unknown				
	Rand1>>p_rank>>PE_CLADE_CONTR_P		<u>C</u> ancel	<u>о</u> к				
	Rand1>>p_rank>>PE_CLADE_SCORE	RegionGrow	er					
	Rand1>>p_rank>>SPATIAL_RESULTS	Matrix						
•	Rand1>>z_scores>>PE_CLADE_CONTR	Spatial						
÷	Rand1>>z_scores>>PE_CLADE_CONTR_P	Spatial						
÷	Rand1>>z_scores>>PE_CLADE_SCORE	Spatial						
+	Rand1>>z_scores>>SPATIAL_RESULTS	Spatial						

The **Def query** is a definition query that allows only a subset of results to be exported. This follows the same syntax as all other definition queries.

## 8 Summary

The above is a very short and simplified introduction to what Biodiverse can do. As noted a few times already, if you would like more details then please start a discussion at https://github.com/shawnlaffan/biodiverse/discussions or post a question at https://groups.google.com/forum/#!forum/biodiverse-users

It is also useful to check the blog for other updates and tips about functionality. It can be accessed through http://biodiverse-analysis-software.blogspot.com.au/

The main help system can also be checked. There is always work to do on this and any contributions, for example new text or suggestions of things to add/clarify, are welcome.

# 9 Acknowledgements

Dr Israel Borokini provided very useful comments to clarify the document content.