mGPS Interface Tutorial

1. Introduction

mGPS interface is a web program based on the mGPS application created by Shiny. It can build a microbial origin prediction model and predict the origin of microbes. To learn more about mGPS, please visit mGPS.

2. Function and Output

2.1 Function 1: Build a new prediction model using mGPS

Geographical origin prediction of microbiome

Prediction program	Welcome HELP Result Plot Output				
Build a new prediction model using mGPS ▼	Build a new prediction model using mGPS				
Input file Merged metadata and abundance file Separate metadata and abundance fil	Function description This model can use the mGPS tool to build a microbial source prediction model based on the microbial				
Upload the reference merged dataset file Browse No file selected	abundance data and coordinates data uploaded by the user.				
Enter the main locality level	Usage				
	In left side bar:				
Enter the locality hierarchy	1. Select Prediction program as Build a new prediction model using mGPS				
	2. Input file(s): Upload data file(s) (in .csv format) containing microbial abundance data and metadata.				
Column range of abundance data	In metadata, at least one locality (eg. continent, city) and coordinates (necessary) data columns should be included. The metadata and abundance data of the sample can be merged into one file (Merged metadata and abundance data), or uploaded as two files (Separate metadata and abundance data)				
☐ Locality sample size cut off (Optional)	When Separate metadata and abundance file is selected. Merge column name in metadata/abundance file: Input the header name of column which is the merged column in two files.				
☐ Remove values (Optional) ☐ Subsets in feature elimination (Optional)	 Enter the main locality level: Input the main locality target. It should same as that column header. (eg. city) 				

2.1.1 Function 1 introduction

In this mode, you can use the mGPS tool to build a microbial source prediction model based on the microbial abundance data and coordinates data uploaded by the user.

2.1.2 Output plots

Geographical origin prediction of microbiome

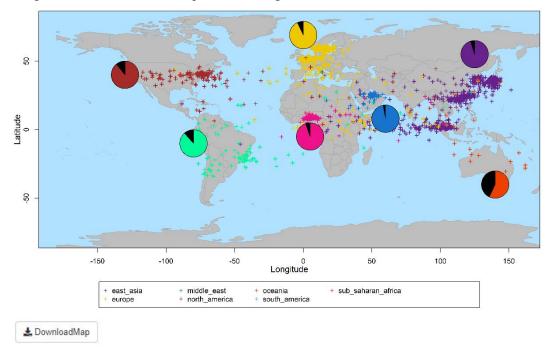


The "Result Plot" of this mode will show the accuracy of the prediction model trained by the mGPS tool and based on the reference microbial database you uploaded.

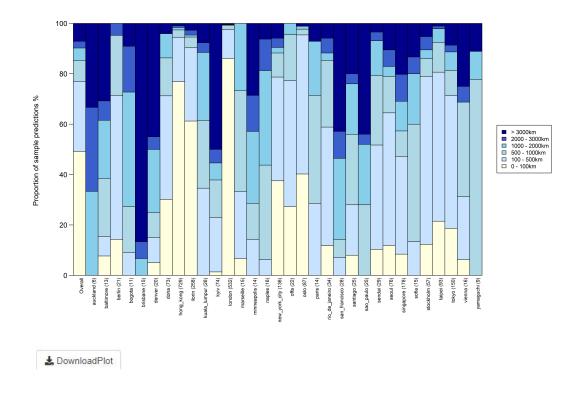
The original database will be divided into 5 folds, and mGPS will use 4 of these folds to train the model, and the resulting model will be used to predict the microbial source of the remaining fold. Iteratively obtain the prediction result of the original database and compare it with the actual location of the microorganism.

Example output plot:

a. World map: samples' prediction origins are plotted on the world map. By adjusting the range of longitude and latitude, you can select the plotting area of the figure on the map. In addition, you can choose whether to pull the predicted point into the continent or the ocean. The predicted origin of original samples will be mapped onto the world map. The pie charts with colors divided by geographic area represent the proportion of samples in the area whose origin region is predicted to be the same continent as the true location. You can download and save the png file of this map through the button 'DownloadMap' below the figure.

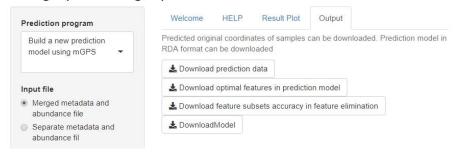


b. Prediction accuracy bar plot: The prediction accuracy of the model is shown per-site as the distances between the predicted and true sampling sites for the reference samples. The average prediction accuracy across all samples with each population given equal weight is shown on the left. You can download and save the png file of this plot through the button 'DownloadPlot' below the figure.

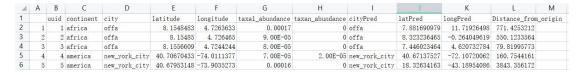


2.1.3 Output files

Geographical origin prediction of microbiome



a. Prediction data: Records the predicted original coordinates of the reference samples (columns: LatPred and LongPred). Also contains the distance between the predicted and true sampling site for the reference samples (column: Distance_from_origin). The original metadata and abundance data will be merged.



b. Optimal features in prediction model: Records the optimal features (microorganism) used to predict the original coordinates that selected by the mGPS algorithm. The column "Overall" records the importance value of each feature. The higher the value, the more important the feature in the prediction algorithm.

4	A	В	C	D	E	
1		Overal1	taxa			
2	Acetobacter. pasteurianus	0.0889962	Acetobacter. pasteurianus			
3	Acetobacter. aceti	0.0728943	Acetobacter. aceti			
4	Acetobacterium. woodii	0.0474666	Acetobacterium. woodii			
5	Acholeplasma.brassicae	0.0429964	Acholeplasma.brassicae			

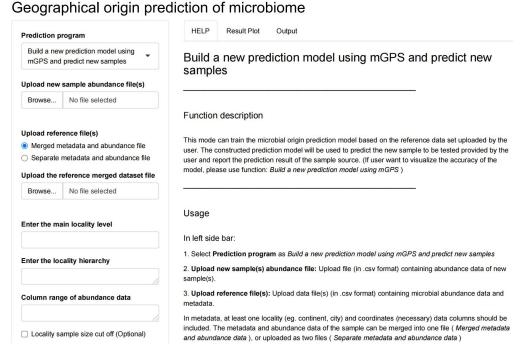
c. Feature subsets accuracy in feature elimination: Records the accuracy of the prediction model with different features (microorganisms) subset size (column: n_vars). The algorithm will use the subset size with the highest accuracy (column: accuracy). For example, the subset with a size of 100 has the highest accuracy value, and then it is used in the prediction algorithm.

4	Α	В	C		
1		n_vars	accuracy		
2	1	50	0.643030303		
3	2	100	0.764242424		
4	3	150	0. 723838384		
5	4	200	0. 731919192		
6					

d. Model: The origin prediction model built by mGPS algorithm saved in Rda format. You can download the model to view the details of the model through load into r. Also, this model can be uploaded to predict the origin of new samples through function 3 "Use an existing model to predict new samples".

load('Outputs/Prediction_model.R)

2.2 Function 2: Build a new prediction model using mGPS and predict new samples



2.2.1 Function 2 introduction

In this mode, you can train the microbial origin prediction model based on the reference data set uploaded by the user. The constructed prediction model will be used to predict the new sample to be tested provided by you and report the prediction result of the sample source. (If you want to

visualize the accuracy of the model, please use the function: Build a new prediction model using mGPS)

2.2.2 Output plot

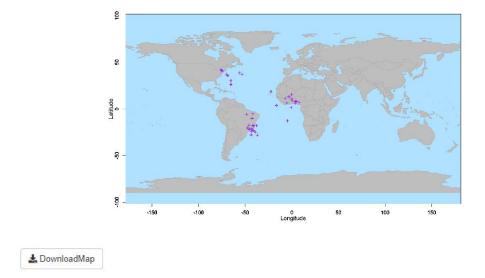




The reference datasets will be used to construct an origin prediction model by mGPS. Then this model will be used to predict the origin of new samples.

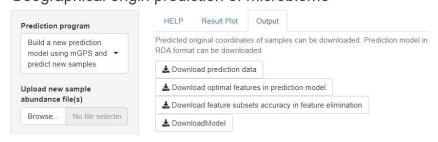
Example output plot:

a. World map: samples' prediction origins are plotted on the world map. By adjusting the range of longitude and latitude, you can select the plotting area of the figure on the map. In addition, you can choose whether to pull the predicted point into the continent or the ocean. You can download and save the png file of this map through the button 'DownloadMap' below the figure.



2.2.3 Output files

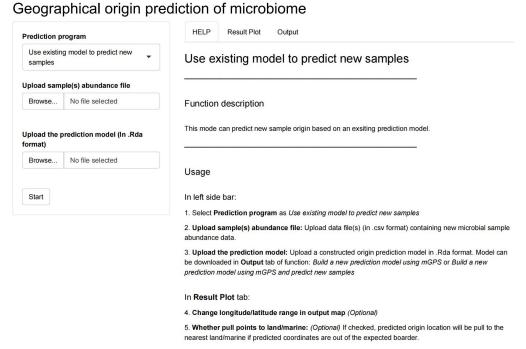
Geographical origin prediction of microbiome



a. Prediction data: Records the predicted original coordinates of the new samples. (columns: LatPred and LongPred).

4	Α	В	С	D	E	F	G
1		taxa1_abundance	taxa2_abundance	taxan_abundance	cityPred	latPred	longPred
2	1	0.00017	0	0	offa	7.881690979	11.71926498
3	2	9. 00E-05	0.00023	0	offa	8. 323236465	-0. 264049619
4	3	8. 00E-05	0	0	offa	7. 446023464	4. 620732784
5	4	7. 00E-05	2. 00E-05	2. 00E-05	new_york_	40. 67137527	-72. 10720062
6	5	0.00016	1. 00E+00	0	new_york_	18. 32634163	-43. 18954086

- b. Optimal features in prediction model: Same content as this file in function 1: Build a new prediction model using mGPS. Jump
- c. feature subsets accuracy in feature elimination: Same content as this file in function 1: Build a new prediction model using mGPS. <u>Jump</u>
- d. Model: Same content as this file in function 1: Build a new prediction model using mGPS. Jump
- 2.3 Function 3: Use an existing model to predict new samples



2.3.1 Function 3 introduction

In this mode, you can predict new sample origin based on an existing prediction model. You can download the model in the Output tab of functions: Build a new prediction model using mGPS or Build a new prediction model using mGPS and predict new samples. Jump to model

2.3.2 Output plot

Geographical origin prediction of microbiome

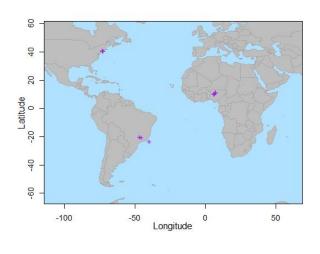


The model uploaded will be used to predict the origin of new samples.

Example output plot:

a. World map:

new samples' prediction origins are plotted on the world map. By adjusting the range of longitude and latitude, you can select the plotting area of the figure on the map. In addition, you can choose whether to pull the predicted point into the continent or the ocean. You can download and save the png file of this map through the button 'DownloadMap' below the figure.



2.3.3 Output files

♣ DownloadMap

Geographical origin prediction of microbiome



a. Prediction data: Records the predicted original coordinates of the new samples. (columns: LatPred and LongPred).

A	В	С	D	E	F	G
	taxa1_abundance	taxa2_abundance	taxan_abundance	cityPred	latPred	longPred
1	0.00017	0	0	offa	7. 881690979	11.71926498
2	9. 00E-05	0.00023	0	offa	8. 323236465	-0. 264049619
3	8. 00E-05	0	0	offa	7. 446023464	4. 620732784
4	7. 00E-05	2. 00E-05	2. 00E-05	new_york_	40. 67137527	-72. 10720062
5	0.00016	1. 00E+00	0	new_york_	18. 32634163	-43. 18954086
	1 2 3 4 5	1 0.00017 2 9.00E-05 3 8.00E-05 4 7.00E-05	1 0.00017 0 2 9.00E-05 0.00023 3 8.00E-05 0 4 7.00E-05 2.00E-05	1 0.00017 0 0 0 2 9.00E-05 0.00023 0 3 8.00E-05 0 0 4 7.00E-05 2.00E-05 2.00E-05	1 0.00017 0 0 offa 2 9.00E-05 0.00023 0 offa 3 8.00E-05 0 0 0 offa 4 7.00E-05 2.00E-05 2.00E-05 new_york	2 9.00E-05 0.00023 0 offa 8.323236465 3 8.00E-05 0 0 offa 7.446023464 4 7.00E-05 2.00E-05 2.00E-05 new_york 40.67137527

3. Reference

3.1 If you meet error:

```
> runApp('mGPS_interface.r')
Warning in file(con, "w"):
cannot open file 'C:\Users\Temp\...': No such file or directory
Error in file(con, "w"): cannot open the connection
```

Try to restart the R (Rstudio). Sometimes this error is due to caching in Rstudio.

3.2 If you meet error:

```
Error in file(file, ifelse(append, "a", "w")):

Cannot open the file:'.....': Permission denied

Warning: Error in file: cannot open the connection
```

Try to see if you have the file open in another program, so the file cannot be modified by the R application.