

mGPS Algorithm Optimization

**Course: Bioinformatics Research Project (BINP37),
15 credits**

Student: Chandrashekar CR

(email: ch1131ch-s@student.lu.se)

Supervisor: Eran Elhaik

(email: eran.elhaik@biol.lu.se)

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Abstract

mGPS (microbiome Geographic Population Structure) is a novel algorithm designed to analyze the geographic distribution of microbial populations. This report details the optimization of the mGPS algorithm, focusing on enhancing its computational efficiency and accuracy in processing large datasets. The optimization process involved refining the algorithm's core functions, improving data handling capabilities, and implementing parallel processing techniques. The results demonstrate significant improvements in processing speed and accuracy, making mGPS a more robust tool for microbiome research. Future work will explore further enhancements and applications of mGPS in various biological contexts.

In this work I mainly focused on optimizing the mGPS algorithm to improve its performance in analyzing the geographic distribution of microbial populations. I primarily focussed on the Metasub dataset, which consists of around 4070 samples from 2016 to 2017. I implemented several models to optimize the algorithm, and compared the results with the original mGPS algorithm.

This research presents an enhanced version of the microbial Global Population Structure (mGPS) algorithm for predicting geographical origins of microbial samples. While previous implementations of mGPS achieved 92% accuracy at city-level prediction with a median error distance of 137 km, these metrics were interdependent, potentially masking true performance. Our study implements an ensemble learning approach combining XGBoost, CatBoost, TabPFN, neural networks, and GrowNets with a threshold-filtered meta-model architecture to improve prediction accuracy across hierarchical geographical scales. Using a dataset of 4,070 samples collected from 40 cities across 7 continents, we address class imbalance through SMOTE techniques and implement 5-fold cross-validation with stratification to minimize bias. A key contribution is our corrected calculation of error metrics, providing a more accurate assessment of model performance by considering the weighted contribution of different prediction scenarios. This refined methodology offers a more robust framework for microbial geolocation, with potential applications in forensic investigation, public health surveillance, and ecological monitoring.

1. Introduction

1.1 [First subsection title]

[Your introduction text here. This section should provide background information on your research topic.] The ability to predict the geographical origin of microbial communities has significant implications across multiple disciplines, including biosurveillance, forensic investigation, and public health monitoring. Microorganisms present in environmental samples can serve as biological signatures of specific locations, reflecting local environmental conditions, human activity patterns, and ecological factors unique to particular geographical regions.

The microbial Global Population Structure (mGPS) algorithm represents an innovative approach to leverage these microbial signatures for geographical prediction. By analyzing the relative sequence abundance (RSA) of microorganisms in samples, mGPS can infer the likely origin of a sample at multiple geographical scales—from continent to precise coordinates. The original implementation employed a hierarchical prediction model using XGBoost, where continent classification preceded city prediction, followed by latitude and longitude coordinates. This approach achieved notable success with 92% accuracy at the city level and a reported median error distance of 137 km.

However, the original methodology contained notable limitations. First, the reported error metrics were interdependent—the distance error calculation benefited from the high accuracy of continent and city predictions, potentially obscuring the true predictive performance. Second, the hierarchical nature of the model meant that errors propagated through prediction levels, with early misclassifications affecting subsequent predictions.

Our research addresses these limitations through several methodological improvements. Instead of relying on a single algorithm, we implement an ensemble approach combining multiple machine learning models: XGBoost, CatBoost, TabPFN, neural networks, and GrowNets. We introduce a threshold-filtering mechanism where only models achieving specified accuracy thresholds contribute to meta-model predictions at each geographical level. This selective ensemble approach helps mitigate error propagation through the hierarchical prediction chain.

To address dataset imbalances, we employ Synthetic Minority Over-sampling Technique (SMOTE) particularly at the continent level, ensuring more balanced training representations. Our implementation also incorporates 5-fold cross-validation with stratification to maintain consistent class distributions across training and testing splits, reducing potential biases in model evaluation.

A significant contribution of our work is the implementation of corrected error calculations that provide a more comprehensive understanding of model performance. By computing the expected coordinate error as a weighted sum over different correctness

67 combinations (continent and city predictions), we offer a more nuanced view of prediction
68 accuracy that accounts for the hierarchical nature of the geographical prediction task.

69 This research builds upon a dataset comprising 4,070 samples collected from train
70 stations and major urban centers across 40 cities and 7 continents, each geo-tagged with
71 precise latitude and longitude coordinates. Through our methodological enhancements,
72 we aim to optimize the mGPS algorithm to provide more accurate and reliable geograph-
73 ical predictions based on microbial community profiles.

2. Materials and Methods

2.1 Data collection

The data used for this study is part of the Metasub dataset, which includes approximately 4070 samples collected from various locations between 2016 and 2017. Subways stations from 40 cities were collected by standardized protocols. 16sRNA sequencing was performed on the samples, and the resulting data was processed to extract relevant microbial population information. The metagenome dataset was processed according using the standardized protocols, which included quality control, filtering, and normalization of the sequencing data. The sequences were then converted to their relative sequence abundances, which were used for further analysis. The dataset for this study was obtained from the previous work on the mGPS algorithm, which was designed to predict the location of the samples based on their microbial composition.

2.2 Preprocessing of the dataset

The preprocessing of the dataset involved several steps to ensure the data was suitable for analysis. This included quality control to remove locations that had less samples and corrections of co-ordinates where the samples were collected. This was done exactly the same way as described in the original mGPS paper. The code written in the original paper was in R, the similar code was written in Python to preprocess the dataset.

2.3 Optimization of the mGPS algorithm

The mGPS algorithm was optimized by implementing several strategies to enhance its performance. Since neural networks are considered to be the best approach for this kind of problem, I implemented several neural network models to optimize the algorithm. The following models were implemented:

- **Model 1: Separate Neural Networks** A completely disconnected neural network model which was built separately on predicting continent. Then another model was built to predict the city based on the predicted probabilities of the continent as augmented features. Then similarly the predicted probabilities of city were used to predict the exact location of the sample, i.e latitude and longitude. The model was trained according to the 60 20 20 split of the dataset, where 60% of the data was used for training, 20% for validation, and 20% for testing.
- **Model 2: Combined Neural Network** A single neural network model that was built to predict the continent, city, and exact location of the sample in a single pass. The loss function was designed to optimize the predictions for all three levels simultaneously.

- **Model 3: Grownnet** A neural network that was built using the Grownnet architecture, which is designed to handle hierarchical predictions. This is also a boosting model which uses shallow neural networks to predict the continent, city, and exact location of the sample in a single pass. The model was trained using the same 60 20 20 split of the dataset.
- **Model 4: XBNet** This is a neural network that was built using the XBNet architecture, This model uses a combination of XGBoost and neural networks to predict the exact location for the sample. This model was only trained to predict the exact location of the sample, i.e latitude and longitude. The classification model requires to see all the different classes in a batch, which is not possible in this case because the dataset is not balanced. Hence, this model was only limited to prediction the latitude and longitude for each sample. This uses XGBoost's feature importance to select the most important features for the prediction, to reweight the hidden layers of the neural network.
- **Model 5: Ensemble Model** This model consists of neural networks for classification of continent and city, and a regression model for predicting the latitude and longitude of the sample. A classification model in Grownnet, XGBoost, CatBoost, and LightGBM was used to predict the continent and city of the sample. The same models were also used to predict the latitude and longitude of the sample, but this time the output was a regression model. The final output of the continent layer was the predicted probabilities of the continent, which was then used to train a meta-model to get the best prediction for continent and city. The same was done for the latitude and longitude of the sample. A caveat was added that if each model performs at least at 93% accuracy, then the model will be used to predict the continent and city of the sample. or above, then the predicted probabilities will be added to the final prediction using the meta-model.

2.4 [Third methods subsection]

[Describe additional methods as needed.]