Glioma Grading using Machine Learning techniques: Model optimization and web deployment

Uriel Nguefack Yefou
African Institute for Mathematical Sciences
Limbe, Cameroon
uriel.nguefack@aims-cameroon.org

Solafa Fadlallah
African Institute for Mathematical Sciences
Mbour, Thies, Senegal
sfadlallah@aimsammi.org

Kobby Panford-Quainoo
African Institute for Mathematical Sciences
Mbour, Thies, Senegal
kpanford-quainoo@aimsammi.org

Phanie Dianelle Negho
African Institute for Mathematical Sciences
Limbe, Cameroon
phanie.negho@aims-cameroon.org

Dieu-Donné Fangnon
African Institute for Mathematical Sciences
Mbour, Thies, Senegal
fangnon.dieudonne@aims-senegal.org

***Abstract*—Detecting and grading glioma at an early stage to determine a tumor's severity is an important step in the treatment of this brain tumor. Although a lot of research on this subject has been based on the use of MRI images in the past few years, molecular markers have grown in their significance in tumor classification. Machine Learning(ML) algorithms have been proven to be very effective in solving problems in the Healthcare sector. This work aims to assess the performance of several ML methods for glioma grading. These ML models' hyperparameters are tuned using the framework Optuna. Using the publicly available TCGA dataset, six ML algorithms including Extreme Gradient Boosting (XGBoost), Categorical Boosting (CatBoost), Ridge Classifier(Ridge), Light Gradient Boosting Machine (LGBM), ExtraTreeClassifier (ExtraT) and Random Forest (RF). We also evaluate the carbon emission produced by each of these models during the training which is one of the important factors to consider when choosing the best model. After comparison of the models using six evaluation metrics such as accuracy, precision, recall, F1-score, AUC, and specificity, XGBoost emerged as the most performant technique with 89.27%, 85.64%, 93.44%, 91.49%, 88.08%, and 91.81% of F1-score, recall, precision, specificity, accuracy, and AUC respectively. We make our model accessible by designing a Web application using the framework Streamlit for real-time predictions and data collection.**

***Index Terms*—Glioma, Machine Learning, Optuna, Carbon emission, Optimization, streamlit**

I. Introduction

Glioma, also known as intra-axial brain tumors, grows within the brain's material and frequently mixes with regular brain cells, is one of the most frequent kinds of CNS (Central Nervous System) [1], [2] tumor arising from cells known as glial cells. In the United States, six gliomas are diagnosed for every 100,000 persons each year. The World Health Organisation (WHO) has traditionally divided gliomas into four categories: I, II, III, IV, based on histological findings [3]. However, the most recent WHO categorization of CNS tumors, released in 2016, includes both histological and genotypic criteria [4]. In this new classification, Grade I and II are grouped under the class LGG(Low Grade Glioma) whereas Grade III and IV are grouped under the class GBM(GlioBastoma Multiforme).

Grading glioma is a complex task, as it is based on a number of historical and molecular parameters [5]. To assist pathologists in this arduous task, the use of technologies based on artificial intelligence is considerably important in supporting their decision-making. The problem we hope to solve in this project is to be able to use patients' historical and molecular parameters to classify a brain tumor as LGG or GBM. The utilized data in this project has not been exploited in numerous studies yet. Hence, the intention behind this work is to elevate the previously achieved results.

The main goal of this work is to optimize ML models for better grading of Gliomas. The data we will use in this work is a public dataset that can be found in [6]. It is the same dataset used by [7] in their study. To attain our objective, we do the following:

- Design six ML models with some initial set of hyperparameters.
- Tune each model by finding the optimal hyperparameters using the Optuna Framework and therefore show the importance of hyperpapameter tuning.
- Make a comparison of the six models based on the evaluation metrics we have defined.

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- Measure the carbon emission of the six models during the training.
- Compare the best model with the current state-of-the-art model [7] .
- Deploy the best model in a web application using Streamlit

The rest of the paper is organized as follows. Section II presents related work on glioma grading. Section III is devoted to the materials and methodology used in this work and the description of the entire proposed framework. Section IV focuses on experiments and results using our framework. Section V concludes the paper and presents suggestions for future work.

II. Related Work

To grade a tumor, pathologists traditionally evaluate the tumor characteristics. To avoid wrong grading, the system in place needs a certain domain knowledge since the grading process will demand checking some requirements [8]. [8] proposed a method to grade glioma tumors using OWL-DL and the NCI Thesaurus which is the major ontological resource in the cancer domain. Their method succeeded in grading ten clinical reports correctly out of eleven.

For a while, ML has been employed in glioma tumor grading using MRIs images or historical and molecular parameters. [7] used four-dimensionality reduction techniques to develop a unique hierarchical voting-based method for boosting feature selection for stage performance and machine learning algorithms for glioma grading using clinical and genetic predictors. In their investigation, they employed the CGGA and TCGA databases. They obtained an accuracy of 87.606% on the TGCA dataset and 79.668% on the CGGA dataset using a total of 16 models. We believe the results can be improved using the method that is presented in this work to make the glioma grading task more accurate. [9] describes a unique two-phase classification system for glioma grading and detection using gradient-based characteristics extracted from structural magnetic resonance imaging (sMRI) images. They use the approach on brain image data from Wuhan University's Zhongnan Hospital as well as TCIA datasets containing glioblastomas (WHO IV) and low-grade gliomas (WHO II and III). For glioma detection, [10] employed a collection of MRI scans containing 34 glioblastomas and 73 diffuse lower-grade gliomas. The authors merged the global and local image feature sets and got an accuracy of 88%. [11] used MRI texture analysis (MRTA) to assess tumor heterogeneity in 95 patients with 68 High-Grade Gliomas (HGG) (grade III=34 and grade IV=34) and 27 LGG (grade II). Their proposed method had an AUC, sensitivity, and specificity of 91%, 93%, and 81%, respectively.

III. Materials and Methods

A. Dataset description

The Cancer Genome Atlas (TCGA) Project – NCI funded the creation of the data used in this work which is publicly available for research. The dataset contains 23 columns, we have 20 most frequently mutated genes which are all categorical variables: IDH1, TP53, ATRX, PTEN, EGFR, CIC, MUC16, PIK3CA, NF1, PIK3R1, FUBP1, RB1, NOTCH1, BCOR, CSMD3, SMARCA4, GRIN2A, IDH2, FAT4, PDGFRA, which can be mutated or not mutated and 3 clinical features: Age, Gender, Race considered from TCGA-LGG and TCGA-GBM brain glioma projects. We have 839 rows, of which 487 belong to LGG and 352 to GBM. Given this data, the goal is to grade the patient's glioma as either LGG or GBM given clinical and molecular/mutation features.

The ML algorithms are trained and evaluated on this data to grade the patient's glioma.

B. Proposed Method Framework

Here, we describe our proposed framework which is divided into the stages illustrated in Figure 1.

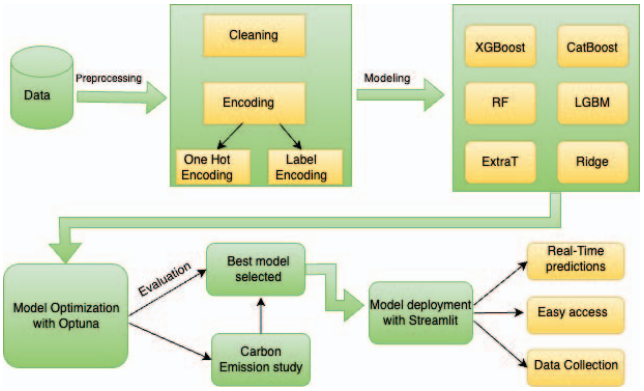

Fig. 1. Framework for Glioma grading.

- Data preprocessing: After retrieving the data, we represented our variables in datatypes suitable for computation. For instance, for each patient the age was given in years and months, we then converted the age to floating point values to take into account the information about the month. Rows where Gender, Age, or Race feature values were '–', or 'not reported' were removed from the dataset. Also, the columns Project, Case_ID, and Primary_Diagnosis were also removed since they add no values for the next stage. The 20 molecular features presented in Section III-A plus the race and gender attributes were encoded using One Hot Encoding. Finally, we also encoded the grade output variable using Label Encoding.
- Modeling: The data is split into a training set and a testing set with 80% being the former and 20%, the latter. The training set will be used with a 5-fold stratified cross-validation during the training. The six ML algorithms namely XGBoost [12], RF [13], ExtraT [14], CatBoost [15], LGBM [16] and Ridge Classifier are built using the training set.

- Model optimization with Optuna: Optuna [17] is a well-known framework used for ML models hyperparameters optimization and can be integrated with popular ML libraries like Tensorflow, Pytorch, and Scikit-learn.This framework uses the pruning technique which stops unpromising trials early and thereby reduces unnecessary computation and speeds up the optimization process which is the reason why we decided to work with it. For each model we designed, Optuna is used to find the best hyperparameters in a given number of trials.
- Carbon emission study: During the model training, we evaluated the carbon emissions of the different models using the Python library codecarbon. ML algorithms require significant computing resources. The energy consumption associated with training these models can lead to a substantial carbon footprint, contributing to Green House Gases(GHG) and Climate Change [18]. The carbon emission tracker was launched when we started to train the model and stopped at the end of the training.
- Model evaluation and best model selection: Out of the six models and after evaluation of their performance on the test set, we select one model that will be used during the model deployment phase. Combined with the carbon emission study, we chose the model not only having the best performance on the test set but also having a small carbon emission.
- Web application: The best model chosen with the above criteria is deployed using a Web Application through the framework Streamlit. The purpose of deploying the model is to enable researchers to be able to test the algorithm on their own to get real-time predictions and provide feedback on any amelioration. Since the data used was relatively small, the web application will also be used to collect data that pathologists will enter into the application and save it in a secure database that will further be used to improve the model performance.

IV. Experiments and Results

This section is organized into three distinct parts: the first part addresses the effectiveness of the optimization technique on the different models developed, the second part is dedicated to the confusion matrix and feature importance plot of the best model on the testing set. The web application developed with streamlit will be presented in the last part.

A. Comparison of our models

The obtained results from the different models are evaluated based on accuracy, precision, recall, F1-score, specificity, and AUC.

Optuna framework was employed to perform a hyperparameter optimization process for each model.

The best hyperparameters were subsequently used to train the models and the outcomes are reported in Table I. The term ”without optimization” refers to the fact that we are using the default parameters of each algorithm and the term ”with optimization” refers to the use of the Optuna framework. To use Optuna, we specify for each model parameter the possible range that the algorithm could take. We used 5-fold cross-validation for this implementation. The value in bold represents the best result for the corresponding metric.

This table indicates the efficiency of the hyperparameter tuning. It also shows that the XGBoost model outperforms the other models on four evaluation metrics: accuracy, recall, the F1 score, and the AUC. The best hyperparameter values of the XGBoost model are shown in Table II.

TABLE II
Best Hyperparameters for XGBoost

Hyperparameter	Value
max_depth	1
learning_rate	0.0872093937702263
n_estimators	988
min_child_weight	2
gamma	0.19742061908192798
subsample	0.9034895892313103
colsample_bytree	0.01446338279780691
reg_alpha	0.08929207215100589
reg_lambda	8.116062455767412e-07
seed	1808

Figure 2 shows the carbon emission of each of the models during the training phase that we obtained using the python library codecarbon. The CatBoost model produces a lot of carbon around 31 g CO2eq and the Ridge Classifier model produces the least carbon. By reducing carbon emissions or working with models producing less carbon emissions, we can help mitigate the environmental impact of the tech industry and address climate change concerns.

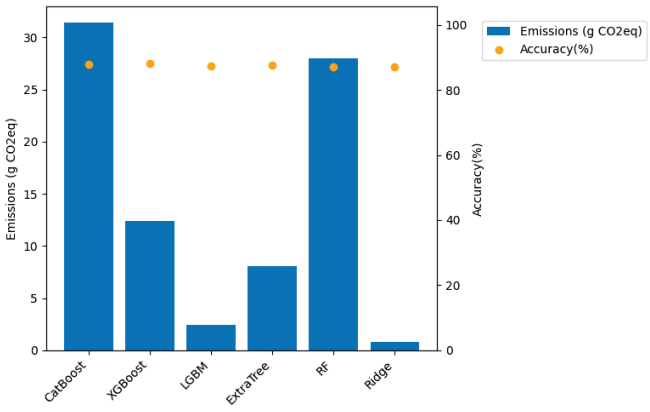

Fig. 2. Evaluation of carbon emission of ML models during training.

Based on the result of Table I and Figure 2, the XGBoost is our best model since it has good performance and relatively acceptable carbon emission.

Table III indicates that the XGBoost model outperforms the state-of-the-art model on five evaluation metrics namely the accuracy, the precision, the F1-score, the specificity, and the

TABLE I
COMPARISON OF THE MODELS WITH AND WITHOUT THE USE OF OPTUNA FRAMEWORK

Models		Accuracy	Precision	Recall	F1-score	Specificity	AUC
CatBoost	without optimization	86.53 ± 1.21	91.97 ± 3.35	84.40 ± 3.91	87.89 ± 1.27	89.50 ± 4.78	91.75 ± 1.04
	with optimization	87.84 ± 0.78	$\mathbf{93.96 \pm 2.18}$	84.61 ± 2.99	88.97 ± 0.88	92.33 ± 3.06	91.41 ± 1.03
XGBoost	without optimization	82.00 ± 0.55	85.50 ± 2.72	83.38 ± 4.36	84.28 ± 1.02	80.11 ± 5.11	89.69 ± 0.55
	with optimization	$\mathbf{88.08 \pm 0.83}$	93.44 ± 2.62	$\mathbf{85.64 \pm 3.31}$	$\mathbf{89.27 \pm 0.97}$	91.49 ± 3.67	$\mathbf{91.81 \pm 1.25}$
LGBM	without optimization	82.96 ± 1.55	86.66 ± 1.68	83.59 ± 3.61	85.03 ± 1.6	82.10 ± 3.02	89.37 ± 0.94
	with optimization	87.37 ± 0.67	92.91 ± 2.1	84.82 ± 2.93	88.61 ± 0.81	80.11 ± 5.11	91.71 ± 1.22
Ridge Classifier	without optimization	87.13 ± 1.14	93.86 ± 1.91	83.38 ± 3.45	88.23 ± 1.29	92.33 ± 2.61	91.25 ± 1.52
	with optimization	87.13 ± 1.14	93.86 ± 1.91	83.38 ± 3.45	88.23 ± 1.29	92.33 ± 2.61	91.25 ± 1.52
ExtraT	without optimization	81.29 ± 2.9	84.09 ± 3.68	83.78 ± 3.18	83.86 ± 2.45	77.87 ± 5.72	87.64 ± 1.85
	with optimization	87.61 ± 1.19	93.88 ± 1.5	84.19 ± 2.97	88.72 ± 1.25	$\mathbf{92.33 \pm 2.11}$	91.77 ± 1.15
RF	without optimization	83.32 ± 1.78	86.94 ± 3.94	84.2 ± 3.59	85.41 ± 1.5	82.13 ± 6.04	89.64 ± 1.49
	with optimization	87.01 ± 1	93.06 ± 1.83	83.99 ± 3.64	88.21 ± 1.21	91.19 ± 2.76	91.66 ± 1.32

AUC and we can also see that [7] did not provide a confidence interval for their results.

TABLE III
COMPARISON OF THE BEST MODEL WITH THE RESULT OF [7]

Models	Accuracy	Precision	Recall	F1-score	Specificity	AUC
XGBoost	$\mathbf{88.08 \pm 0.83}$	$\mathbf{93.44 \pm 2.62}$	85.64 ± 3.31	$\mathbf{89.27 \pm 0.97}$	$\mathbf{91.49 \pm 3.67}$	$\mathbf{91.81 \pm 1.25}$
[7]	87.6	81.5	**91.2**	85.8	85.2	91.4

In this work, it is crucial to achieve a balance between correctly identifying positive cases (recall) and minimizing false positives (precision), as we want to not only predict early LGG to take appropriate measures and avoid the tumor moving to the next level(GBM) but also efficiently predict GBM corresponding to the last stage of the tumor which can lead to the death of the patient. Therefore, the F1-score should be the most important metric to consider for that task, and we can clearly see that we have a very big improvement compared to [7] results.

B. Confusion matrix and Feature plot importance

Figure 3 shows the confusion matrix obtained using the best model, XGBoost on the testing set. In the matrix, each column corresponds to the model prediction, while each row represents the true label. The model accurately predicted 65 cases of GBM out of 70, and correctly identified 82 (out of 98) LGG.

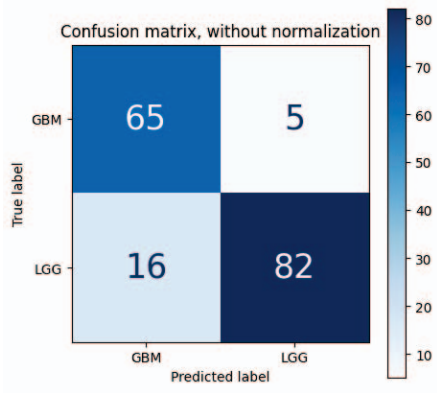

Fig. 3. Confusion matrix of the XGBoost model on the test set.

The feature importance plot shows the amount to which each of the features contributes to the model performance. Figure 4 shows the 10 highest features that influence the model performance.

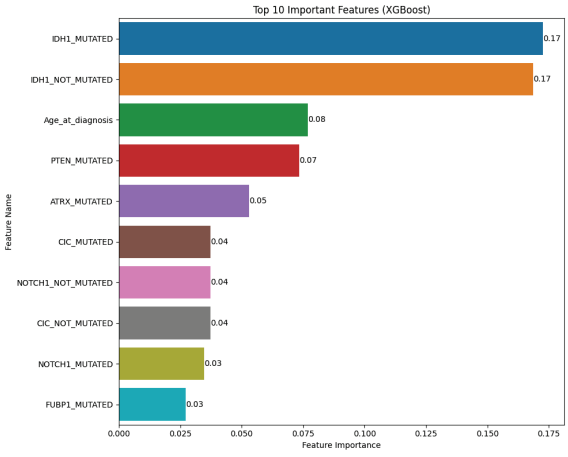

Fig. 4. Feature Importance on the XGBoost model.

The IDH1(isocitrate dehydrogenase) has the highest contribution followed by the CIC(capicua transcriptional repressor). whereas the variable NOTCH1(notch receptor 1) has the least contribution to the XGBoost model performance. Concerning the importance of the IDH1 variable, it was explained by [19] that IDH1 encourages the development of the tumor microenvironment, which is favorable for the growth of glioblastoma(GBM) stem cells; which is exactly what the feature importance plot shows us.

C. Web App presentation

The XGBoost model has been deployed in a web application using the framework streamlit. The Interface of the application is presented in Figure 5. With the information entered by the users in the web application, the model graded the tumor as GBM. To improve the model performance in the future, a system for data collection has been set up to collect and store -in a secure database- the information entered by the users in the web application. An example of how the database looks like is presented in Figure 6. We are planning to partner with some institutes and more precisely with pathologists who will give us their feedback on the prediction made by the model and their actual prediction, and get their suggestions on how we could improve the work.

V. Conclusion

In this work, we proposed multiple machine-learning models for glioma grading using the TCGA dataset. The models using the default hyperparameters were first designed after applying some data preprocessing techniques. The Optuna framework was used to find the best hyperparameters for each of the six models proposed and evaluate the models on a portion(20%) of the initial dataset and their performance compared using the accuracy, precision, recall, F1-score, specificity, and AUC. During the training, the carbon emission of the six models was evaluated and used as a criterion in the selection of the best model. The XGBoost model outperformed all other models and had relatively small carbon emissions. Using Streamlit, the XGBoost model was deployed to allow real-time prediction and data collection for model improvement in the future. For future work, we plan to collect more data, especially for patients underrepresented in the data. It is also planned to include a connection page for access to the web application only to pathologists to avoid collecting low-quality data in the database.

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Conflicts of interest statement
The authors declare no conflicts of interest.

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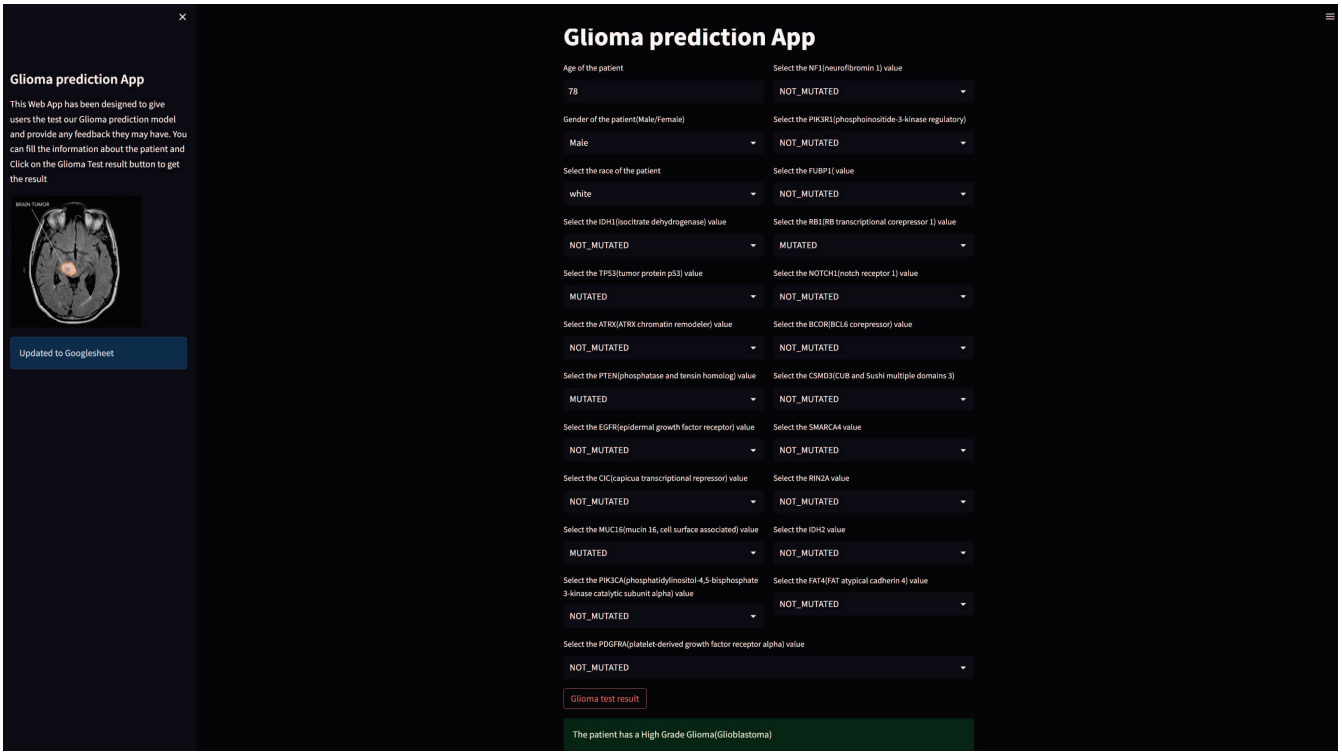

Fig. 5. Real-time prediction on the web application.

Fig. 6. Data Collection in a spreadsheet using data entered in the web application.

Glioma_Database

Age_at_diagnosis	Gender	Race	IDH1	TP53	ATRX	PTEN	EGFR	CIC	MUC16	PIK3CA	NF1	PIK3R1	FUBP1	RB1	NOTCH1	BCO
78	Male	white	NOT_MUTATED	MUTATED	NOT_MUTATED	MUTATED	NOT_MUTATED	NOT_MUTATED	MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	MUTATED	NOT_MUTATED	NOT
37.43	Female	white	MUTATED	MUTATED	MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT
44.75	Female	white	NOT_MUTATED	MUTATED	MUTATED	NOT_MUTATED	MUTATED	NOT_MUTATED	MUTATED	MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	MUTATED	NOT_MUTATED	NOT
85	Female	white	MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	MUTATED	NOT_MUTATED	NOT_MUTATED	MUTATED	NOT_MUTATED	NOT_MUTATED	NOT
79.4	Female	asian	MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	MUTATED	NOT_MUTATED	NOT_MUTATED	MUTATED	NOT_MUTATED	NOT_MUTATED	NOT
56.7	Female	white	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT
45	Male	white	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT
78.9	Female	white	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT
55	Male	white	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT_MUTATED	NOT