Brain Tumor Identification in MRI Images using K-means Clustering and XGBoost

MS Machine Learning

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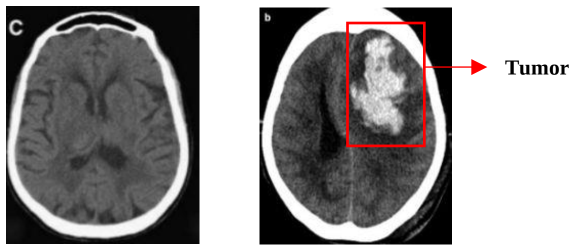
Abstract: Brain tumor is a cancerous or noncancerous mass or growth of abnormal cells in the brain. An estimated 700,000 Americans are living with a brain tumor. Of these, 69.8% tumors are benign and 30.2% tumors are malignant. Moreover, an estimated 87,240 people will receive a primary brain tumor diagnosis in 2020 [1]. Since these cases have an average survival rate for the malignant tumor cases is only 36%, early identification is very crucial for such situations. Brain tumors can be identified using MRI (Magnetic Resonance Imaging) diagnostic tests which is a time-consuming task for the doctors and healthcare specialists. Due to the high volume of MRI tests every year, an automated process of brain tumor identification from these images can help assist the pathology experts in speeding up the process of brain tumor identification. This study proposes the combination of supervised and unsupervised machine learning techniques to classify MRI images based on the presence of brain tumors. This crucial task requires high accuracy and therefore, we will have utilized the state-of-the-art techniques like XGBoost to achieve high specificity as well as high sensitivity.

I. Introduction

Brain tumors are the fifth-leading cause of cancer-related death in males age 40-59 years [1]. 3,657 children are estimated to be living with a brain tumor in the U.S. [1]. More than any other cancer, brain tumors can have lasting and life-altering physical, cognitive, and psychological impacts on a patient's life. In most people with primary brain tumors, the cause of the tumor is not clear, but the doctors have identified some factors that may increase your risk of a brain tumor which include Exposure to radiation and Family history of brain tumors [2].

Diagnosis of a brain tumor is done by a neurologic exam (by a neurologist or neurosurgeon), CT (computer tomography scan) and/or magnetic resonance imaging (MRI), and other tests like an angiogram, spinal tap and biopsy. Of these, magnetic MRI is commonly used to help diagnose brain tumors. It uses magnetic fields, not x-rays, to produce detailed images of the body. These tumors are mostly identifiable with the human eye but automating the process of tumor identification would require the use of complex machine learning techniques which we will introduce in this study.

Examples of MRI scans with and without brain tumor are depicted below:



MRI scan with no brain tumor | **MRI scan with brain tumor**

Figure 1.1 MRI Scans with and without tumor

Our approach to identify the tumors from MRI images is outlines below:

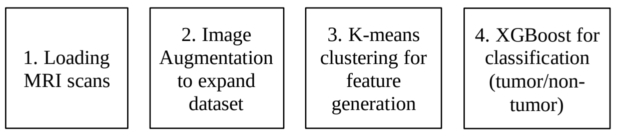

1. Loading MRI scans
2. Image Augmentation to expand dataset
3. K-means clustering for feature generation
4. XGBoost for classification (tumor/non-tumor)

Figure 1.2 Process flow

[1] Quick Brain Tumor Facts: https://braintumor.org/brain-tumor-information/brain-tumor-facts/
[2] Mayo Clinic: https://www.mayoclinic.org/diseases-conditions/brain-tumor/symptoms-causes/syc-20350084

II. Data Processing and Image Augmentation

A. *Data source*

A data source of 200 images was obtained from “Brain MRI Images for Brain Tumor Detection” [3] by Navoneel Chakrabarty. This dataset contains MRI images with the following summary statistics:

Data	**Attribute**
Total images	200
Tumor MRI images	100
Non-tumor MRI images	100
Image size	Varying

B. *Image resizing*

Since the images were of varying size, the images were transformed to have the same dimensions of 188 x 232.

C. *Image augmentation to expand dataset*

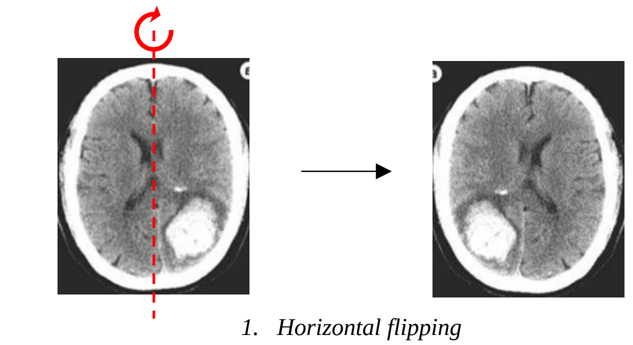
Due to the limitations in the size of the dataset (200 images), we performed image augmentation to expand our dataset for training. This involved rotating the images across various axes to obtain different versions of the same image which can then be utilized for training our model. Following transformations were performed for image augmentation:

1. Horizontal flipping
2. Vertical flipping
3. 180 degrees rotation

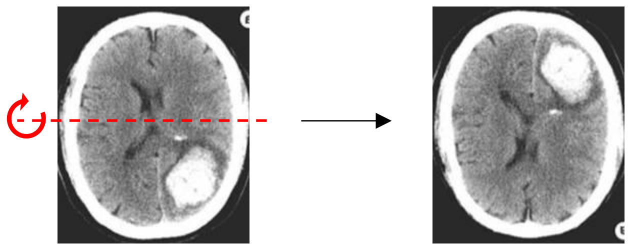
The image augmentation was carried out in R using the functions *“mirror”* and *“imrotate”* from the *“imager”* package. After obtaining our expanded dataset, we split it using *stratified sampling* into training (70%), validation (15%), and test (15%) sets. The final summary statistics of the data after image augmentations is given below:

Data	**Attribute**
Total images	800
Tumor MRI images	400
Non-tumor MRI images	400
Sampling method	Stratified sampling
Training set	560
Validation set	120
Test set	120
Event rate	50%
Image size	188 x 232

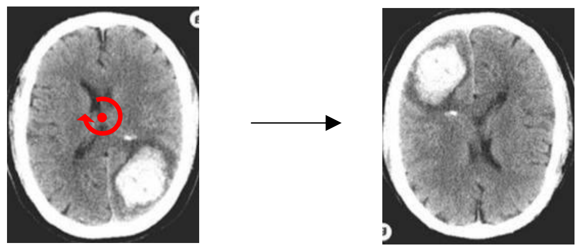
An example of image augmentation is depicted below:



1. *Horizontal flipping*



2. *Vertical flipping*



3. *180 degrees rotation*

Figure 2.1 Image augmentation

From the above MRI images, we make the following observations about the presence of tumors:

- ***Intensity:*** The tumor has a high color intensity then the rest of the image
- ***Size:*** The high intensity pixels for an image with tumor would he larger in number than an image with no tumor
- ***Centroid:*** The centroid for the pixels with high intensity can be a good indicator of the location of the tumor

Therefore, we use clustering method on these images to create feature sets which would take into account the above information and will then use these feature sets to solve the classification problem.

[3] https://www.kaggle.com/navoneel/brain-mri-images-for-brain-tumor-detection

III. K-means clustering for feature generation

A. Clustering process

In order to create features like intensity, size, and centroid, we used k-means clustering to cluster the pixels in the MRI images. The process is depicted below:

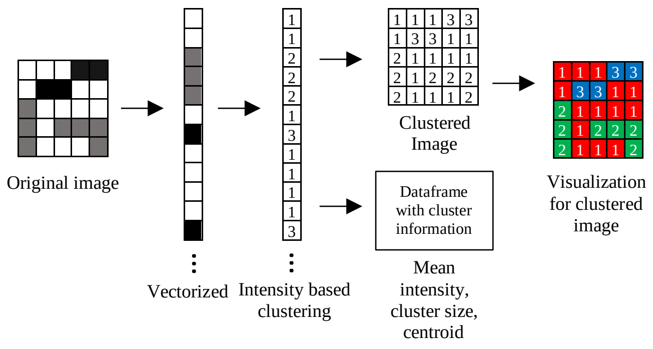

Original image
Vectorized
Intensity based clustering
Clustered Image
Dataframe with cluster information
Mean intensity, cluster size, centroid
Visualization for clustered image

Figure 3.1 Clustering process

The augmented images were read into R and each image was converted into a matrix of dimensions (height x width of image) containing the intensity values at each pixel. Each of these matrices were then vectorized in order to perform clustering on these images.

We chose k-means clustering for this purpose in order to:

- Speed up the process of clustering a total of 800 images and to have faster computations
- Large no. of pixel values (*high n*), hierarchical clustering would require in-memory *n* x *n* x *800* distance matrix

The cluster information from each image was then stored in a dataframe which included:

- Mean intensity at each cluster
- Size of each cluster (number of pixels)
- Centroid of each cluster (position in the image: x and y coordinate)
- Presence of tumor (binary: 0 or 1)
- Dataset label (train, validation, or test)

The vectors were then converted back to a matrix with cluster labels as the values and these matrices were then used to visualize the clustered image as depicted in the process above.

B. Determination of optimal number of clusters

In order to perform the clustering process efficiently, we use the elbow method to identify the optimal number of clusters. All the images were clustered using numbers of clusters from 1 to 10 and the average of the total within-clusters sum of squares was taken across all the images for each number of clusters. Finally, we plot the mean of total within-clusters sum of squares vs the number of clusters in order to determine the optimal number of clusters.

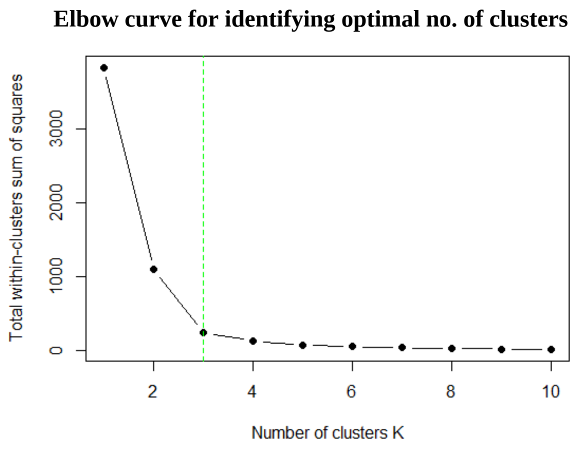


Figure 3.2 Elbow curve for K-means clustering

From the elbow curve, we identified the optimal number of clusters as 3.

A snapshot of the final dataframe obtained using K-means for feature extraction is shown below:

data_set	c1_size	c2_size	c3_size	c1_intensity
train	17607	20955	5054	0.0348607
train	16905	19751	6960	0.0655778
train	13714	23038	6864	0.0463897
train	10641	27462	5513	0.0217019
train	14514	18560	10542	0.0409230

c2_intensity	c3_intensity	c1_x_centroid	c2_x_centroid	c3_x_centroid
0.3471991	0.9332255	95.55342	93.76683	93.87000
0.3442183	0.9425208	98.41083	92.93332	89.44698
0.3662888	0.9529098	94.07255	94.85298	94.16929
0.4386409	0.9407041	90.59261	95.80537	95.53945
0.3548802	0.9439750	92.02039	95.83109	95.57039

c1_y_centroid	c2_y_centroid	c3_y_centroid	tumor
108.5343	122.3085	120.1672	0
104.9151	123.3934	125.0761	0
114.7050	116.6865	119.4605	0
109.5807	117.9369	122.6980	0
112.0284	121.7142	113.4764	0

Figure 3.3 Clustering features snapshot

An example of the input and the clustered image for tumor and non-tumor MRI scans is as follows:

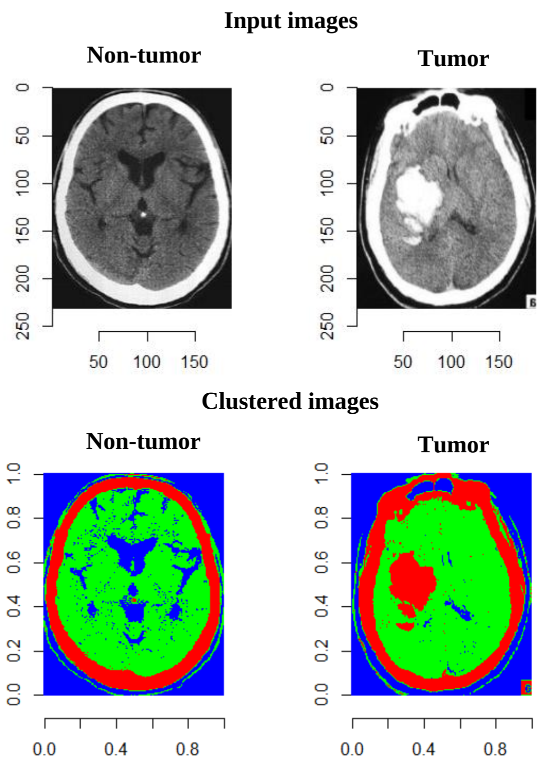


Figure 3.4 Visualization of clustered images

IV. XGBoost for Classification

After obtaining the features and labels, we now train an eXtreme Gradient Boosting (XGBoost) model to classify images based on the presence of brain tumor. XGBoost is a popular and efficient open-source implementation of the gradient boosted trees algorithm.

We choose an XGBoost model for this purpose because:

- This is a purely prediction problem. Our target is to make better predictions without analyzing the process of making these predictions
- XGBoost is known to produce best predictions in terms of accuracy. In healthcare problems, we need to be as accurate as possible in order to serve the patients better
- Since we are dealing with large number of images, we need to choose an algorithm which is hardware efficient. Being a powerful and fast machine learning library, XGBoost pushes the limit of computations resources to optimize the use of computer hardware

A. *Cross validation for no. of iterations*

One critical parameter which needs to be tuned in XGBoost is the number if iterations. We set the depth of trees to have sufficient interactions and the learning rate to be a low value and tune the number of iterations using cross validation. For this purpose, we trained the data using the training set and plot the validations error vs the number of iterations using the following hyperparameters:

Parameter	Value
Learning rate	0.01
Maximum depth of tree	6
Maximum iterations	2500
Objective	binary:logistic
Training observations	560
Validation obervations	120

Figure 4.1 Hyperparameters for cross validating XGBoost

The plot of validation error vs the number of iterations is depicted below:

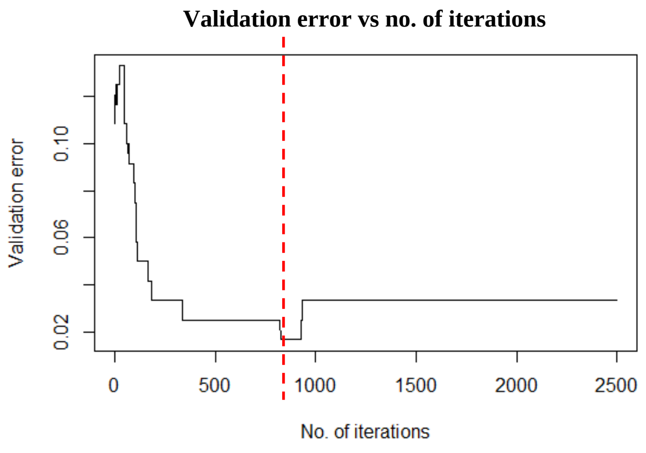


Figure 4.2 Cross validating no. of iterations

From this plot we observe that the minimum validation error occurs at 825 iterations

B. *Model training using cross validated hyperparameters*

We now retrain the model using the combination of training and validation sets and the optimum number of iterations identified using cross validation (825). The rest of the hyperparameter were set to be the same as mentioned in Figure 4.1. This time, we plot the training error vs. the number of iterations to monitor our XGBoost training process.

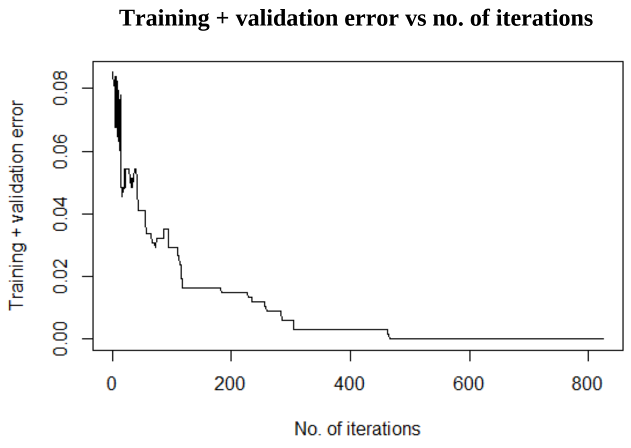


Figure 4.3 Training + validation error vs no. of iterations

V. Model performance and results

Finally, we make predictions on our training + validation set and test set and analyze their performance. The confusion matrices and results for both the sets are given below:

A. Training set

Training accuracy = 100%
Training Sensitivity = 1.0
Training Specificity = 1.0
Confusion Matrix:

N = 680	Actual: No	Actual: Yes
Predicted: No	340	0
Predicted: Yes	0	340

Figure 5.1 Confusion matrix for training + validation set

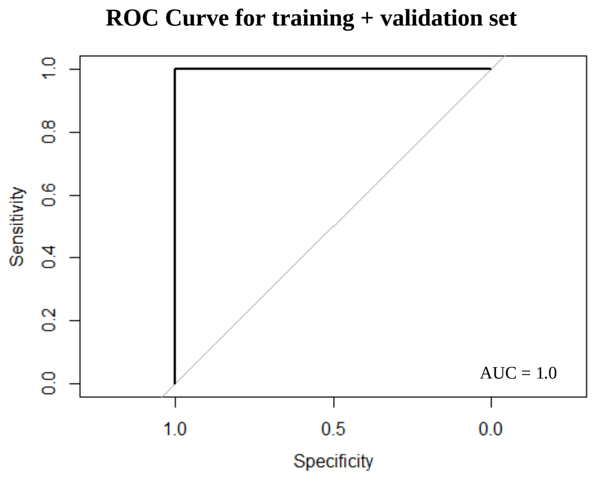


Figure 5.2 ROC curve for training + validation set

B. Test set

Test accuracy = 99.17%
Test Sensitivity = 0.9833
Test Specificity = 1.0
Confusion Matrix:

N = 120	Actual: No	Actual: Yes
Predicted: No	59	0
Predicted: Yes	1	60

Figure 5.2 Confusion matrix for test set

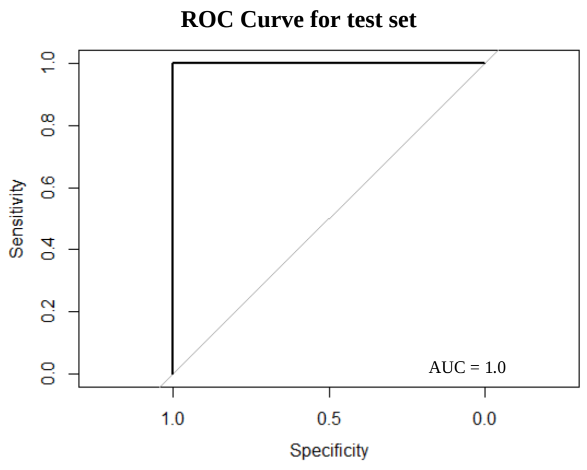


Figure 5.3 ROC curve for test set

The XGBoost model, known for its high predictive power is able to produce an accuracy of 99.17% on the test set.

VI. Discussion and Conclusions

A. Discussion

The model performance and results, at first, look too good to be true. An accuracy of 100% on the training set and 99.17% on the test seem very high. But it is important to note these numbers are usually dependent upon the context and the use case. Brain tumors are almost always identifiable with the naked eye and therefore, observing the same using machine learning is not a very difficult task. The actual value being created here is the automation of the process which saves a lot of time and a high accuracy is just a byproduct. The amount of time required to identify tumors in a large number of MRI images can now be reduced to a few seconds using this model. Moreover, the accuracy metrics indicate that the classification is indeed very reliable.

B. *Conclusions and future scope*

From this study, we observed the application of K-means clustering on image data which is very unique. Interestingly, one can infer that the features generated manually for using cluster analysis are similar to the ones generated using Convolutional Neural Networks which extracts image features at both micro and macro levels. In the case of MRI images, we are almost certain about the features which can be used to identify the tumors like cluster centroid, cluster size and intensity and therefore, we are able to create these features manually using K-means. This helps in reducing prediction time and makes the prediction process more intuitive than CNNs. In more complex applications like MRI of Alzheimer's disease, more complicated techniques and CNNs might be required for the classification problem but it would be interesting to observe the contribution of clustering technique in image feature extraction. Moreover, we conclude that eXtreme Gradient Boosting provides us with high prediction powers which cannot be obtained very easily using linear models.

VII. References

- T. M. Shahriar Sazzad, K. M. Tanzibul Ahmmed, M. U. Hoque and M. Rahman, "Development of Automated Brain Tumor Identification Using MRI Images," 2019 International Conference on Electrical, Computer and Communication Engineering (ECCE), Cox'sBazar, Bangladesh, 2019, pp. 1-4
- W. Chen, X. Qiao, B. Liu, X. Qi, R. Wang and X. Wang, "Automatic brain tumor segmentation based on features of separated local square," 2017 Chinese Automation Congress (CAC), Jinan, 2017, pp. 6489-6493.
- Z. Zulkoffli and T. A. Shariff, "Detection of Brain Tumor and Extraction of Features in MRI Images Using K-means Clustering and Morphological Operations," 2019 IEEE International Conference on Automatic Control and Intelligent Systems (I2CACIS), Selangor, Malaysia, 2019, pp. 1-5.

VIII. Resources

- Github link (with code and data) [4]

[4] https://github.com/skandupmanyu/Brain_Tumor_Identification_Kmeans_XGBoost

Appendix

R Script

```r
############################################
# Brain Tumor Identification in MRI Images #
#   using Kmeans Clustering and XGBoost    #
############################################

# 1. Load libraries
# -----------------

library(imager)
library(xgboost)
library(caret)
library(pROC)

# 2. Setup files
# --------------

# 2.a. Set working directory
setwd("E:/MS ML Project/Data/")

# 2.b. Extract all files
orig_tumor_files = paste("./tumor/",
                         list.files(path = "./tumor"), sep = "")

orig_non_tumor_files = paste("./non_tumor/",
                             list.files(path = "./non_tumor"), sep = "")

# 3. Image augmentation to expand our data
# ----------------------------------------

# 3.a. Function to create 4 rotated versions of the image -- #
augment_image = function(file, target)
{
  # Load image
  img_original = load.image(file)

  # Flip image horizontally
  img_flip_horizontal = mirror(img_original, "x")

  # Flip image vertically
  img_flip_vertical = mirror(img_original, "y")

  # 180 deegrees rotation
  img_x_y_mirror = imrotate(img_original, 180)

  # Create file names
  original_file_name = strsplit(strsplit(file, "\\/")[[1]][3], "\\.")[[1]][1]

  img_original_file_name = paste(target,
                               original_file_name, "_OR", '.jpg', sep = "")
  img_flip_horizontal_file_name = paste(target,
                                      original_file_name, "_FH", '.jpg', sep = "")
  img_flip_vertical_file_name = paste(target,
                                    original_file_name, "_FV", '.jpg', sep = "")
  img_x_y_mirror_file_name = paste(target,
                                 original_file_name, "_XY", '.jpg', sep = "")

  # Save images
  save.image(img_original, img_original_file_name)
  save.image(img_flip_horizontal, img_flip_horizontal_file_name)
  save.image(img_flip_vertical, img_flip_vertical_file_name)
  save.image(img_x_y_mirror, img_x_y_mirror_file_name)
}

# 3.b. Augment tumor files
for(file_name in orig_tumor_files)
{
  augment_image(file_name, "./augmented/tumor/")
}

# 3.c. Augment non-tumor files
for(file_name in orig_non_tumor_files)
{
  augment_image(file_name, "./augmented/non_tumor/")
}

# 4. Create training/validation/test set
# --------------------------------------

# 4.a. Read augmented files
tumor_files = paste("./augmented/tumor/",
                    list.files(path = "./augmented/tumor"), sep = "")

non_tumor_files = paste("./augmented/non_tumor/",
                        list.files(path = "./augmented/non_tumor"), sep = "")

# 4.b. Create training set
set.seed(2)
train_Y_indices = sample(1:length(tumor_files),
                         floor(0.7*(length(tumor_files))))

train_Y_files = tumor_files[train_Y_indices]

train_N_indices = sample(1:length(non_tumor_files),
                         floor(0.7*(length(non_tumor_files))))
```

```
train_N_files = non_tumor_files[train_N_indices]

val_test_tumor_files = tumor_files[-train_Y_indices]

val_test_non_tumor_files = non_tumor_files[-train_N_indices]

# 4.c. Create validation set
val_Y_indices = sample(1:length(val_test_tumor_files),
                       floor(0.5*(length(val_test_tumor_files))))

val_Y_files = val_test_tumor_files[val_Y_indices]

val_N_indices = sample(1:length(val_test_non_tumor_files),
                       floor(0.5*(length(val_test_non_tumor_files))))

val_N_files = val_test_non_tumor_files[val_N_indices]

# 4.d. Create test set
test_Y_files = val_test_tumor_files[-val_Y_indices]
test_N_files = val_test_non_tumor_files[-val_N_indices]

# 4.e. All files
train_files = c(train_Y_files, train_N_files)
val_files = c(val_Y_files, val_N_files)
test_files = c(test_Y_files, test_N_files)
all_files = c(train_files, val_files, test_files)

# 5. Identifying optimal number of clusters using elbow method
# ------------------------------------------------------------

# 5.a. Function to convert image to a vector
image_to_vec = function(file)
{
  # Load image
  im = load.image(file)

  # Convert to a greyscale intensity matrix
  mat = as.matrix(im[,,1,1])

  # Transpose and reverse to keep the aspect ratio intact
  mat = t(apply(mat, 1, rev))

  # Calculate aspect ratio
  asp_ratio = dim(mat)[2]/dim(mat)[1]

  # Convert to vector
  Vector = as.vector(mat)

  return(list(Vector, dim(mat)[2], dim(mat)[1], asp_ratio))
}

# 5.b. Function to calculate within sum of square distance for k means clustering
perform_k_means = function(Vector, k)
```

```r
{
  # Set seed
  set.seed(1)

  # Perform k means
  kmc = kmeans(Vector,
               nstart = 50,
               centers = k,
               iter.max = 50)

  # Calculate total within sum of squared distance
  tot_within_ss = kmc$tot.withinss

  # Return the value
  return(tot_within_ss)
}

# 5.c. Create an elbow curve
max_k = 10
wss = matrix(0, nrow = length(train_files), ncol = max_k)
for(i in 1:length(train_files))
{
  vec = image_to_vec(train_files[i])[[1]]
  for(j in 1:max_k)
  {
    wss[i,j] = perform_k_means(vec, j)
  }

}

# 5.d. Average across all training samples
wss_avg = apply(wss, MARGIN = 2, mean)

# 5.e. Plot the curve
plot(1:max_k, wss_avg,
     type ="b",
     pch = 19,
     xlab ="Number of clusters K",
     ylab ="Total within-clusters sum of squares",
     main = "Elbow curve for identifying optimal no. of clusters")
abline(v = 3, col = 'green', lty = 2)

# 5.f. Observe the graph and identify the optimal no. of clusters
opt_k = 3

# 6. Visualizing the results of k-means clustering
# ------------------------------------------------

Y_image_index = 40
N_image_index = 159

# 6.a. Non-tumor
vec_all_N = image_to_vec(train_N_files[N_image_index])
```

```r
vec_N = vec_all_N[[1]]
height_N = vec_all_N[[2]]
width_N = vec_all_N[[3]]
asp_ratio_N = vec_all_N[[4]]

set.seed(1)
kmc_N = kmeans(vec_N,
               nstart = 50,
               centers = opt_k,
               iter.max = 50)

clusters_N = kmc_N$cluster
dim(clusters_N) = c(width_N, height_N)

# 6.b. Tumor
vec_all_Y = image_to_vec(train_Y_files[Y_image_index])
vec_Y = vec_all_Y[[1]]
height_Y = vec_all_Y[[2]]
width_Y = vec_all_Y[[3]]
asp_ratio_Y = vec_all_Y[[4]]

set.seed(1)
kmc_Y = kmeans(vec_Y,
               nstart = 50,
               centers = opt_k,
               iter.max = 50)

clusters_Y = kmc_Y$cluster
dim(clusters_Y) = c(width_Y, height_Y)

# 6.c. Plot

# Input images
par(mfrow = c(1,2), oma = c(0, 0, 2, 0)) #outer margins
plot(load.image(train_N_files[N_image_index]), main = 'Non-tumor')
plot(load.image(train_Y_files[Y_image_index]), main = 'Tumor')
mtext('Input images', outer = T, cex = 1.5)

# Clustered images
image(clusters_N, col = c("green", "red", "blue"),
      asp = asp_ratio_N, main = 'Non-tumor', frame = F)

image(clusters_Y, col = c("green", "blue", "red"),
      asp = asp_ratio_Y, main = 'Non-tumor', frame = F)

mtext('Clustered images', outer = T, cex = 1.5)
par(mfrow = c(1,1))

# 7. Performing k-means using the optimal no. of clusters
# -------------------------------------------------------

# 7.a. Initialize a dataframe to store cluster results
cluster_data = data.frame(matrix(0, nrow = length(all_files), ncol = 4*opt_k + 2))
```

```r
colnames(cluster_data) = c('data_set',
                           'c1_size', 'c2_size', 'c3_size',
                           'c1_intensity', 'c2_intensity', 'c3_intensity',
                           'c1_x_centroid', 'c2_x_centroid', 'c3_x_centroid',
                           'c1_y_centroid', 'c2_y_centroid', 'c3_y_centroid',
                           'tumor')

# 7.b. Function to perform k-means and store clustering output to a dataframe
kmeans_insert_data = function(cluster_data, files, data_set_name, tumor, curr_row)
{
  for(i in 1:length(files))
  {
    # Convert image to vector
    vec_all = image_to_vec(files[i])
    vec = vec_all[[1]]
    height = vec_all[[2]]
    width = vec_all[[3]]
    asp_ratio = vec_all[[4]]

    # Set seed
    set.seed(1)

    # Perform k means
    kmc = kmeans(vec,
                 nstart = 50,
                 centers = opt_k,
                 iter.max = 50)

    # Extract cluster information
    centers = kmc$centers
    ordered_centers = order(centers)
    centers = centers[ordered_centers] #Intensity
    size = kmc$size[ordered_centers] #size

    # Extract centroids
    clusters = kmc$cluster
    dim(clusters) = c(width, height)
    x_centroids = c()
    y_centroids = c()
    for(j in 1:opt_k)
    {
      coords = which(clusters == j, arr.ind = T)
      x_centroid = apply(coords, MARGIN = 2, mean)[1]
      y_centroid = apply(coords, MARGIN = 2, mean)[2]
      x_centroids = c(x_centroids, x_centroid)
      y_centroids = c(y_centroids, y_centroid)
    }

    x_centroids = x_centroids[ordered_centers] #centroids
    y_centroids = y_centroids[ordered_centers] #centroids

    # Insert data
    cluster_data[curr_row,1] = data_set_name
    cluster_data[curr_row,2:(opt_k+1)] = size
    cluster_data[curr_row,(opt_k+2):(2*opt_k+1)] = centers
    cluster_data[curr_row,(2*opt_k+2):(3*opt_k+1)] = x_centroids
    cluster_data[curr_row,(3*opt_k+2):(4*opt_k+1)] = y_centroids
    cluster_data[curr_row,4*opt_k+2] = tumor

    # Increment row
    curr_row = curr_row + 1
  }
  return(list(cluster_data, curr_row))
}

# 7.c. Use the above function to create clustering output dataframe

# 7.c.1 Insert training data

# 7.c.1.a Non-tumor
curr_row = 1
cluster_output = kmeans_insert_data(cluster_data, train_N_files, 'train', 0, curr_row)
cluster_data = cluster_output[[1]]
curr_row = cluster_output[[2]]

# 7.c.1.b Tumor
cluster_output = kmeans_insert_data(cluster_data, train_Y_files, 'train', 1, curr_row)
cluster_data = cluster_output[[1]]
curr_row = cluster_output[[2]]

# 7.c.2 Insert validation data

# 7.c.2.a Non-tumor
cluster_output = kmeans_insert_data(cluster_data, val_N_files, 'val', 0, curr_row)
cluster_data = cluster_output[[1]]
curr_row = cluster_output[[2]]

# 7.c.2.b Tumor
cluster_output = kmeans_insert_data(cluster_data, val_Y_files, 'val', 1, curr_row)
cluster_data = cluster_output[[1]]
curr_row = cluster_output[[2]]

# 7.c.3 Insert test data

# 7.c.3.a Non-tumor
cluster_output = kmeans_insert_data(cluster_data, test_N_files, 'test', 0, curr_row)
cluster_data = cluster_output[[1]]
curr_row = cluster_output[[2]]

# 7.c.3.b Tumor
cluster_output = kmeans_insert_data(cluster_data, test_Y_files, 'test', 1, curr_row)
cluster_data = cluster_output[[1]]
curr_row = cluster_output[[2]]

# 7.d View data
knitr::kable(cluster_data[1:5, 1:5])
```

```r
knitr::kable(cluster_data[1:5, 6:10])
knitr::kable(cluster_data[1:5, 11:14])

# 8. Cross Validation for XGBoost
# -------------------------------

# 8.1. Create data matrix for XGBoost
X_train = data.matrix(cluster_data[cluster_data$data_set == 'train', c(-1, -14)])
X_val = data.matrix(cluster_data[cluster_data$data_set == 'val', c(-1, -14)])
X_test = data.matrix(cluster_data[cluster_data$data_set == 'test', c(-1, -14)])
Y_train = data.matrix(cluster_data[cluster_data$data_set == 'train', 14])
Y_val = data.matrix(cluster_data[cluster_data$data_set == 'val', 14])
Y_test = data.matrix(cluster_data[cluster_data$data_set == 'test', 14])

# 8.2. Create xgb matrix
train_data = xgb.DMatrix(X_train, label = Y_train)
val_data = xgb.DMatrix(X_val, label = Y_val)

# 8.3 Define model parameters
parameters = list(eta = 0.01,
                  max_depth = 6,
                  objective = "binary:logistic",
                  seed = 1)

# 8.4 Train model
set.seed(1)
model_xgb_cv = xgb.train(data = train_data,
                         params = parameters,
                         watchlist = list(eval = val_data, train = train_data),
                         nrounds = 2500,
                         verbose = 0)

# 8.5 Plot validation error vs. no. of iterations
plot(model_xgb_cv$evaluation_log$iter,
     model_xgb_cv$evaluation_log$eval_error,
     type = "l",
     main = "Validation error vs No. of iterations",
     xlab = "No. of iterations",
     ylab = "Validation error")

# 8.6 Find optimum no. of iterations
opt_iterations = model_xgb_cv$evaluation_log$iter[
  which(model_xgb_cv$evaluation_log$eval_error ==
          min(model_xgb_cv$evaluation_log$eval_error))[1]]

print(paste('Optimal no. of iterations:', opt_iterations))

# 9. Train final model using hyperparameters obtained from cross validation
# -------------------------------------------------------------------------

# 9.1 Append training and validation set
X_train_val = data.matrix(
  cluster_data[cluster_data$data_set %in% c('train','val'), c(-1, -14)])
```

```
Y_train_val = data.matrix(
  cluster_data[cluster_data$data_set %in% c('train','val'), 14])

# 9.2. Create xgb matrix
train_val_data = xgb.DMatrix(X_train_val, label = Y_train_val)

# 9.3 Train model
set.seed(1)
model_xgb = xgb.train(data = train_val_data,
                      params = parameters,
                      watchlist = list(train = train_val_data),
                      nrounds = opt_iterations,
                      verbose = 0)

# 9.4 Plot validation error vs. no. of iterations
plot(model_xgb$evaluation_log$iter,
     model_xgb$evaluation_log$train_error,
     type = "l",
     main = "Training + validation error vs No. of iterations",
     xlab = "No. of iterations",
     ylab = "Training + validation error")

# 10. Model performance
# ---------------------

# 10.1. Training + validation results

# 10.1.a Predictions
pred = predict(model_xgb, X_train_val)
pred_labels = as.factor(as.numeric(pred >= 0.5))
Y_train_val = as.factor(Y_train_val)

# 10.1.b Confusion matrix
confusion_matrix = confusionMatrix(pred_labels, Y_train_val)
print("Confusion matrix for training + validation data:")
print(confusion_matrix$table)

# 10.1.c Accuracy, sensitivity, and specificity
train_val_accuracy = confusion_matrix$overall['Accuracy']
train_val_sensitivity = confusion_matrix$byClass['Sensitivity']
train_val_specificity = confusion_matrix$byClass['Specificity']
print(paste('Training + validation accuracy:', train_val_accuracy))
print(paste('Training + validation sensitivity:', train_val_sensitivity))
print(paste('Training + validation specificity:', train_val_specificity))

# 10.1.d ROC
train_val_roc = roc(response = Y_train_val, predictor = pred)
plot(train_val_roc, main = "ROC Curve for training + validation set")

# 10.1.e AUC
train_val_AUC = train_val_roc$auc
print(paste('Training + validation set AUC:', train_val_AUC))
```

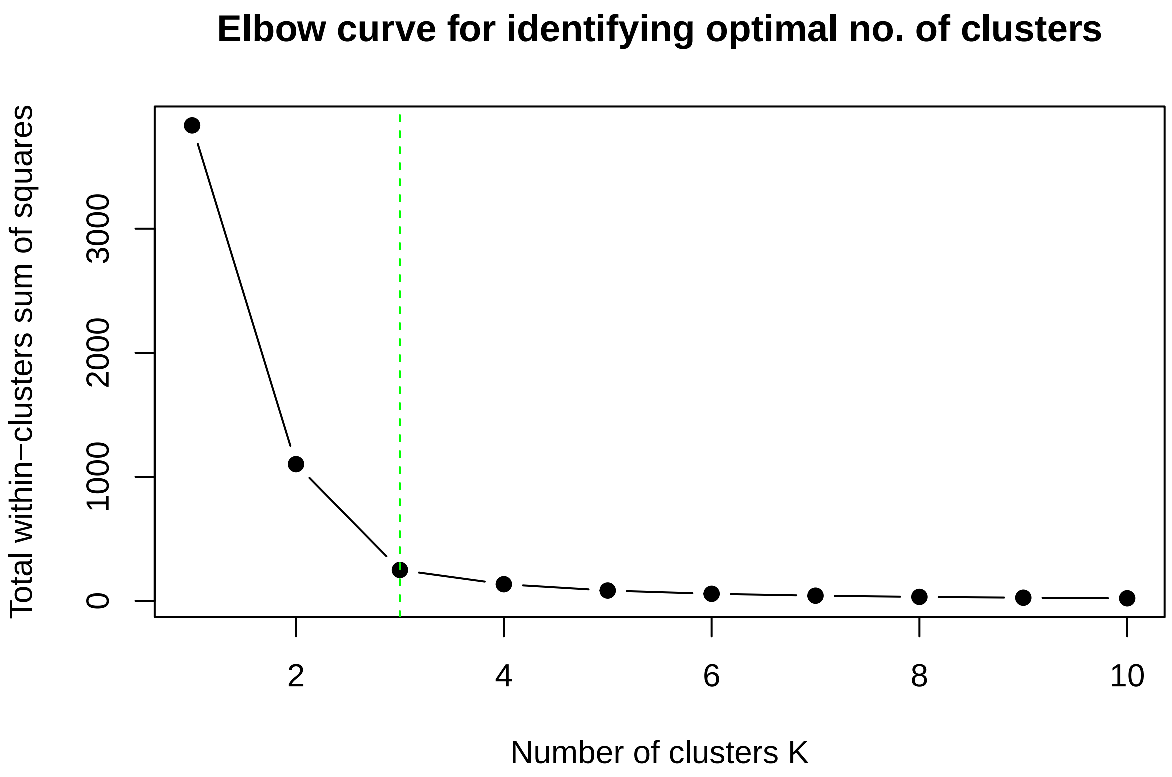
```r
# 10.2. Test results

# 10.2.a Predictions
pred = predict(model_xgb, X_test)
pred_labels = as.factor(as.numeric(pred >= 0.5))
Y_test = as.factor(Y_test)

# 10.2.b Confusion matrix
confusion_matrix = confusionMatrix(pred_labels, Y_test)
print("Confusion matrix for test data:")
print(confusion_matrix$table)

# 10.2.c Accuracy
test_accuracy = confusion_matrix$overall['Accuracy']
test_sensitivity = confusion_matrix$byClass['Sensitivity']
test_specificity = confusion_matrix$byClass['Specificity']
print(paste('Test accuracy:', test_accuracy))
print(paste('Test sensitivity:', test_sensitivity))
print(paste('Test specificity:', test_specificity))

# 10.2.d ROC
test_roc = roc(response = Y_test, predictor = pred)
plot(test_roc, main = "ROC Curve for test set")

# 10.2.e AUC
test_AUC = test_roc$auc
print(paste('Test AUC:', test_AUC))
```

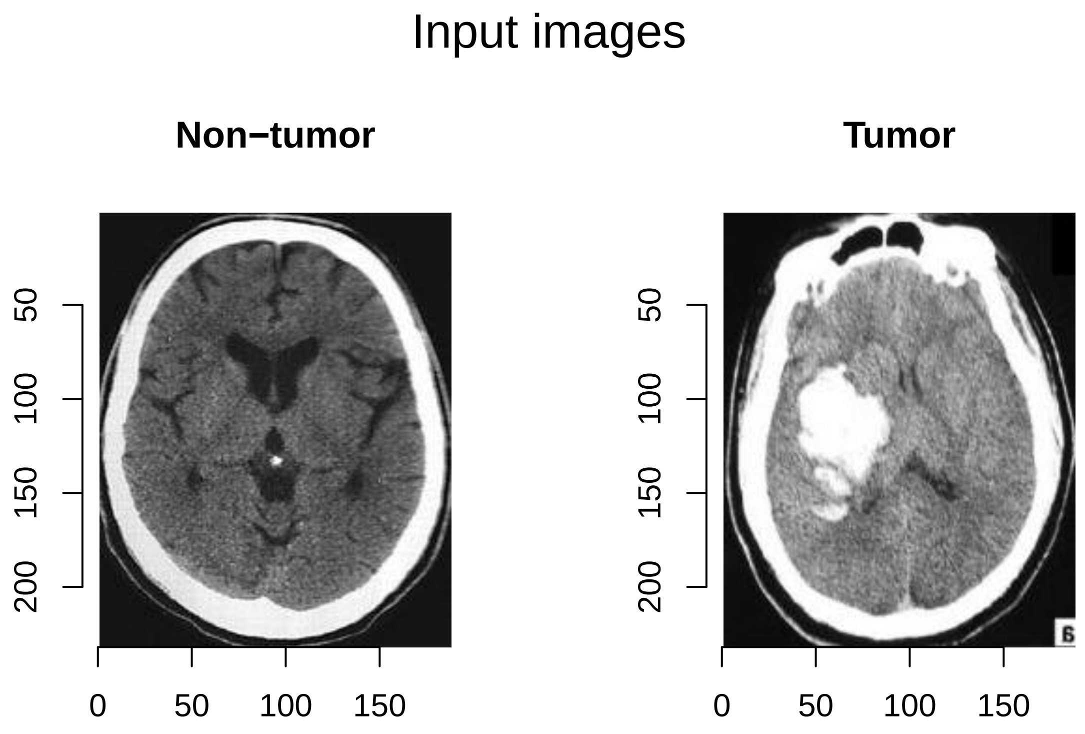
data_set	c1_size	c2_size	c3_size	c1_intensity
train	17607	20955	5054	0.0348607
train	16905	19751	6960	0.0655778
train	13714	23038	6864	0.0463897
train	10641	27462	5513	0.0217019
train	14514	18560	10542	0.0409230

c2_intensity	c3_intensity	c1_x_centroid	c2_x_centroid	c3_x_centroid
0.3471991	0.9332255	95.55342	93.76683	93.87000
0.3442183	0.9425208	98.41083	92.93332	89.44698
0.3662888	0.9529098	94.07255	94.85298	94.16929
0.4386409	0.9407041	90.59261	95.80537	95.53945
0.3548802	0.9439750	92.02039	95.83109	95.57039

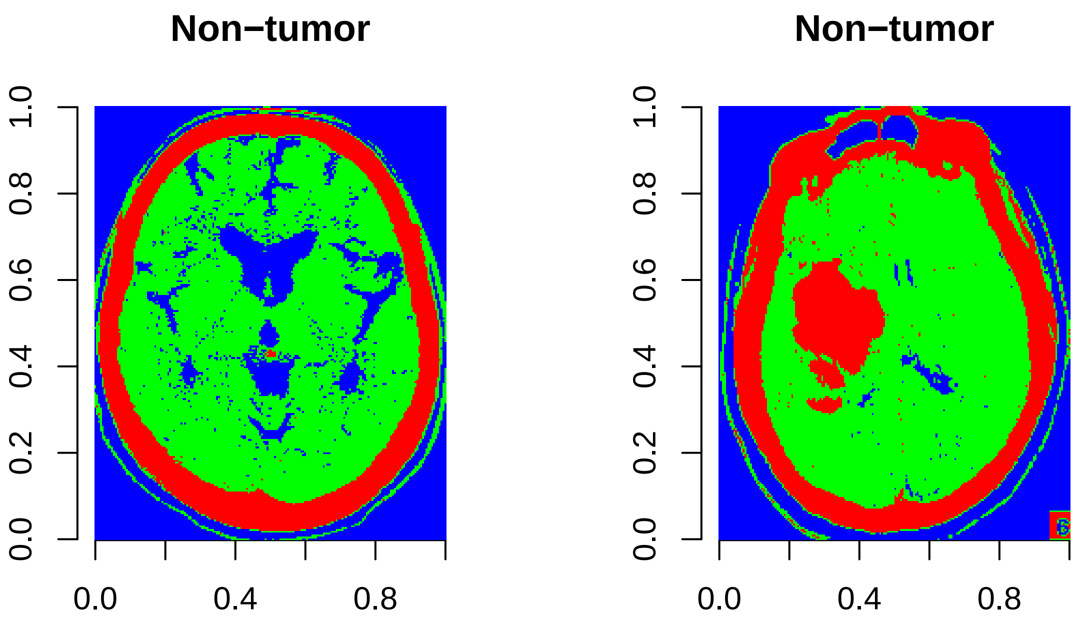
c1_y_centroid	c2_y_centroid	c3_y_centroid	tumor
108.5343	122.3085	120.1672	0
104.9151	123.3934	125.0761	0
114.7050	116.6865	119.4605	0
109.5807	117.9369	122.6980	0
112.0284	121.7142	113.4764	0

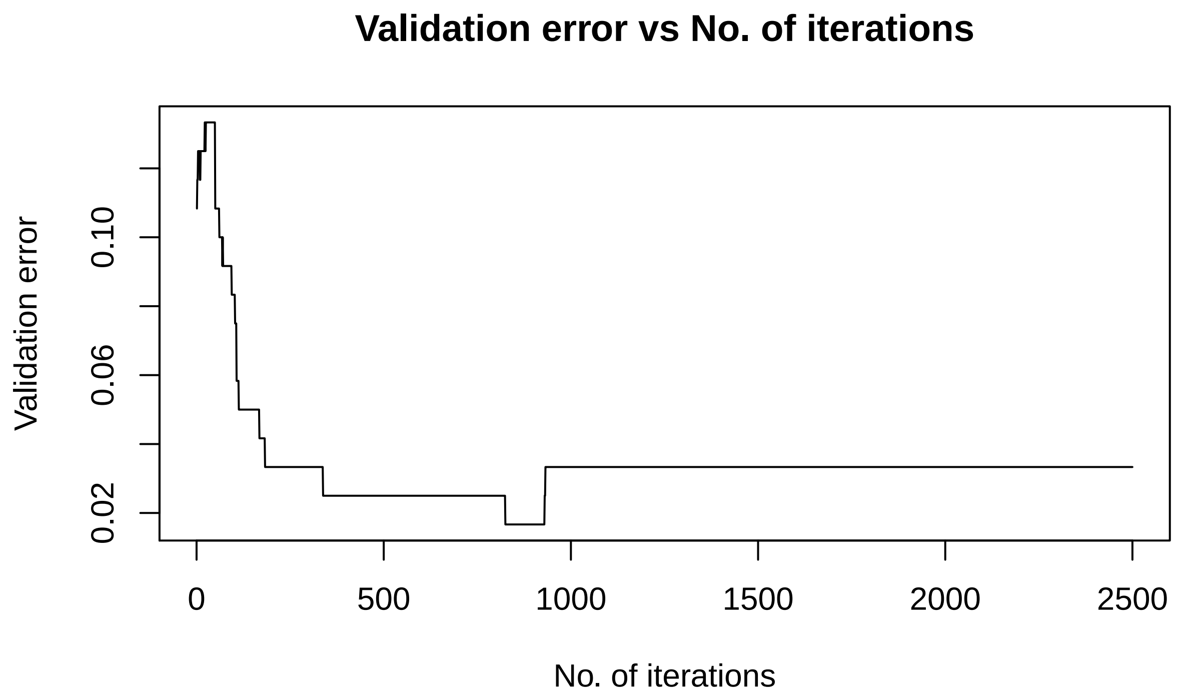
```
## [1] "Optimal no. of iterations: 825"
## [1] "Confusion matrix for training + validation data:"
##           Reference
## Prediction   0   1
##          0 340   0
##          1   0 340
## [1] "Training + validation accuracy: 1"
## [1] "Training + validation sensitivity: 1"
## [1] "Training + validation specificity: 1"
## [1] "Training + validation set AUC: 1"
## [1] "Confusion matrix for test data:"
##           Reference
## Prediction  0  1
##          0 59  0
##          1  1 60
## [1] "Test accuracy: 0.991666666666667"
## [1] "Test sensitivity: 0.983333333333333"
## [1] "Test specificity: 1"
## [1] "Test AUC: 1"
```

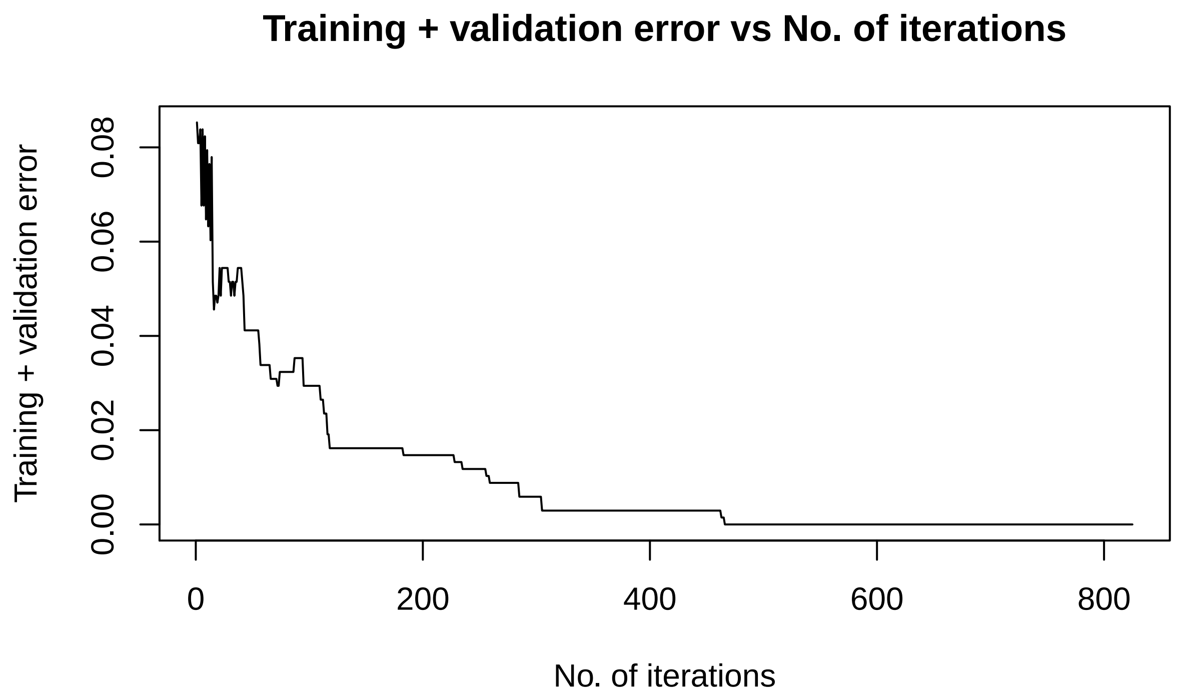


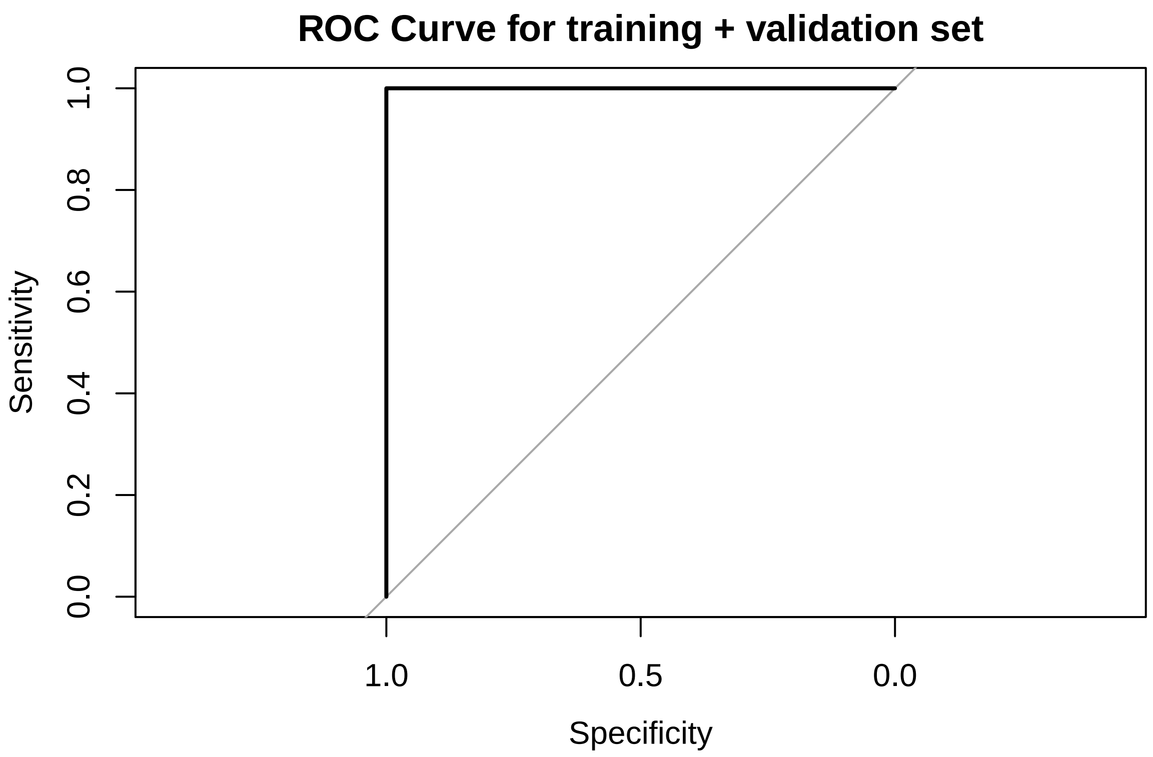

Input images
Non−tumor
Tumor
50
100
150
200
0
50
100
150
50
100
150
200
0
50
100
150
Б

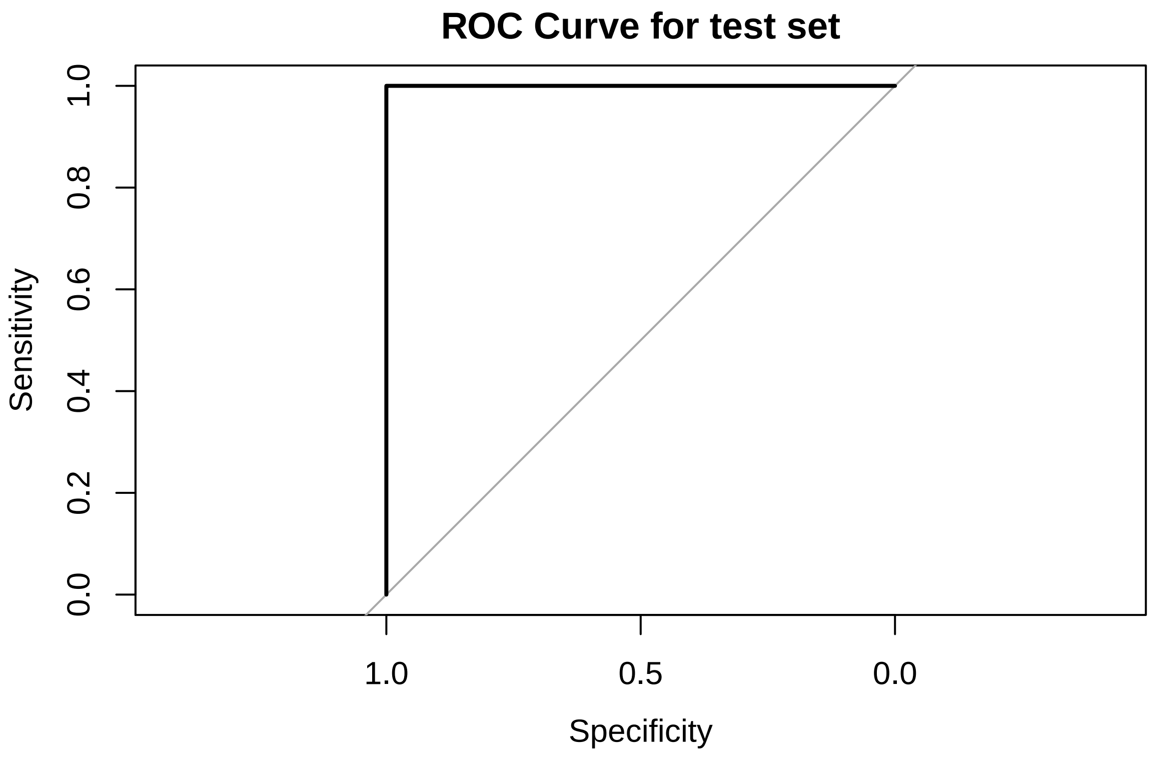
Clustered images




Validation error vs No. of iterations
Validation error
0.02
0.06
0.10
0
500
1000
1500
2000
2500
No. of iterations


Training + validation error vs No. of iterations
Training + validation error
0.00
0.02
0.04
0.06
0.08
0
200
400
600
800
No. of iterations


ROC Curve for training + validation set
Sensitivity
1.0
0.8
0.6
0.4
0.2
0.0
1.0
0.5
0.0
Specificity


ROC Curve for test set
Sensitivity
Specificity
1.0
0.8
0.6
0.4
0.2
0.0
1.0
0.5
0.0