Project

Chris Meade

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Abstract

Diabetes occurs more often in the Pima Indian tribe of southern Arizona than any other population of people in the world. By selecting the optimal parameters for three machine learning algorithms – Random Forest decision trees, a Support Vector Machine (SVM) with a radial basis function kernel, and a Multilayer Perceptron (MLP) neural network – this paper proves that diabetes can be accurately diagnosed in Pima women. The results also indicate that classification accuracy is maximized with the neural network algorithm.

1. Introduction

This paper attempts to explore the viability of the application machine learning to the medical field and human health. Can statistical learning algorithms be utilized by doctors to help make accurate diagnoses and aid in decision making as it pertains to patient health? To attempt to answer this question, we train three distinct machine learning algorithms – Random Forest decision trees, a Support Vector Machine (SVM) with a radial basis function kernel, and a Multilayer Perceptron (MLP) neural network – using data about diabetes occrance in Pima Indian Women. All analysis was performed with the R statistical computing software package and associated machine learning packages in the RStudio integrated development enviornment. Our results clearly indicate that all three algorithms had a high success rate in correctly diagnosing diabetes in Pima women. This lends support to the proposed hypothesis that machine learning does have a place in doctors' arsenal.

1.1 About the Data

The data about diabetes incidence in Pima women used in our analysis are freely avaiable from the University of California, Irvine machine learning repository at http://archive.ics.uci.edu/ml/. The dataset contains 768 observations of nine features. The features in the order they appear in the dataset are as follows:

Feature Description	Feature name in dataset
Number of times pregnant	timePregnant
Plasma glucose concentration at 2 hours in an oral glucose tolerance test	plasmaGlucose
Diastolic blood pressure (mm Hg)	diastolicPressure
Triceps skin fold thickness (mm)	tricepThickness
2-Hour serum insulin (mu U/ml)	serumInsulin
Body mass index (weight in kg/(height in m)^2)	bmi
Diabetes pedigree function	pedigreeFunction
Age (years)	age
Class variable (diabetic or not diabetic)	diabetes

1.2 Software Used in Analysis

All analysis was performed with the R statistical computing environment. The functionality of R was extended by importing the following software libraries: `caret`, `mice`, `randomForest`, `kernlab` `VIM`, and `RSNNS`. These librarys add support for data imputation and for the three machine learning algorithms used in our analysis.

The analysis was written in the RStudio integrated development enviornment. This package was generated using the 'rmarkdown' R package.

2. Data Processing

2.1 Data Aquisition

We must first import our data into R and load the required R packages used in our analysis.

```
library(caret)
library(mice)
library(randomForest)
library(kernlab)
library(RSNNS)
library(VIM)

#Create a vector of the feature names
headers <- c("timesPregnant", "plasmaGlucose", "diastolicPressure", "tricepThickness",
             "serumInsulin", "bmi", "pedigreeFunction", "age", "diabetes")

#Import data
www <- paste0("http://archive.ics.uci.edu/ml/machine-learning-databases/",
              "pima-indians-diabetes/pima-indians-diabetes.data")

data <- read.csv(url(www),
                 header = FALSE,
                 col.names = headers)
```

We examine the structure of our data table to ensure that it was imported correctly.

```
str(data)
```

```
## 'data.frame':    768 obs. of  9 variables:
##  $ timesPregnant    : int  6 1 8 1 0 5 3 10 2 8 ...
##  $ plasmaGlucose    : int  148 85 183 89 137 116 78 115 197 125 ...
##  $ diastolicPressure: int  72 66 64 66 40 74 50 0 70 96 ...
##  $ tricepThickness  : int  35 29 0 23 35 0 32 0 45 0 ...
##  $ serumInsulin     : int  0 0 0 94 168 0 88 0 543 0 ...
##  $ bmi              : num  33.6 26.6 23.3 28.1 43.1 25.6 31 35.3 30.5 0 ...
##  $ pedigreeFunction : num  0.627 0.351 0.672 0.167 2.288 ...
##  $ age              : int  50 31 32 21 33 30 26 29 53 54 ...
##  $ diabetes         : int  1 0 1 0 1 0 1 0 1 1 ...
```

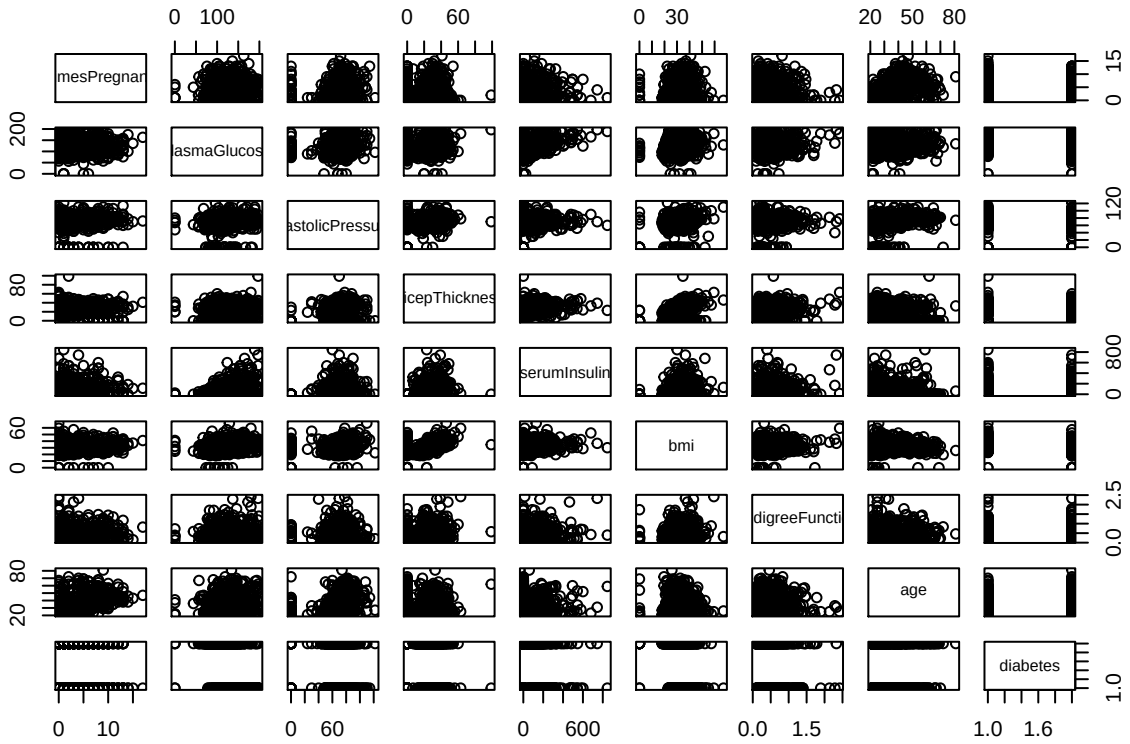
Next, we encode the class label of the `diabetes` feature to be more reable by changing `0` to `notDiabetic` and `1` to `Diabetic`. We then covert this feature to a factor.

```
data$diabetes <- as.factor(ifelse(data$diabetes == 0, "notDiabetic", "Diabetic"))
```

2.2 Exploratory Analysis

Now that we have our data and have imported all required software libraries, we perform some exploratory analysis. We begin by constructing a scatterplot matrix.

```
pairs(data)
```



From this scatterplot matrix we make the following observations:

1. Several features have `0` valued observation.
2. There does not appear to be strong linearity between any two features. We confirm this later in the analysis.

2.3 Missing Data

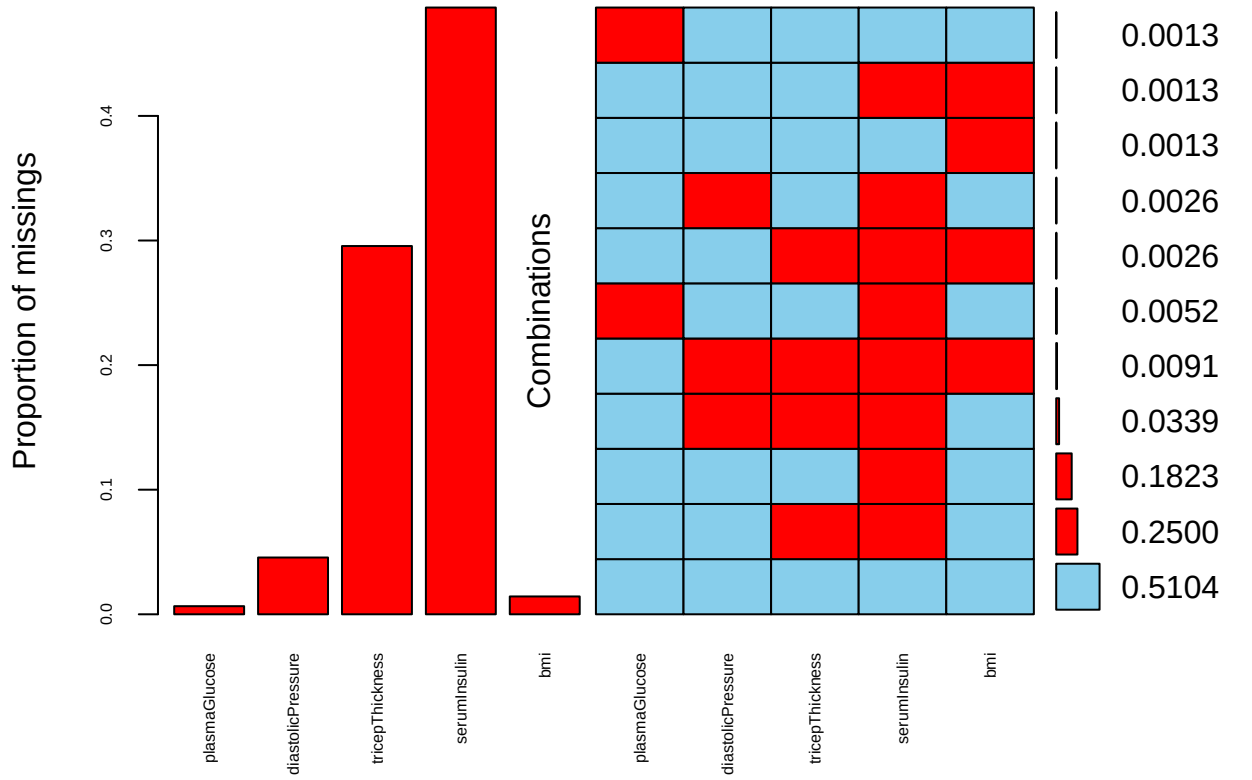
From our exploratory analysis, we found the several features contain values of `0`. For several of the features, a `0` value is biologically impossible, namely in `plasamaGlucose`, `diastolicPressure`, `tricepThickness`, `serumInsulin`, `bmi`. We conclude that although the dataset does not explicitly contain missing values, it does contain implicity missing values encoded as `0`s.

We decide to explictily encode the missing values in the five listed features as `NA`s.

```
for (i in 2:6){
  for (n in 1:nrow(data)){
    if (data[n, i] == 0){
      data[n, i] <- NA
    }
  }
}
```

Now that missing data is correcty encoded as `NA`'s, we construct an aggregation plot to count the precise number of missing values.

```
aggr(data[,2:6], cex.lab=1, cex.axis = .5, numbers = T, gap = 0)
```



The left plot shows the proportion of missing values to total observations for each feature. We note that over half of all observations for `serumInsulin` and nearly a third `tricepThickness` observations are missing.

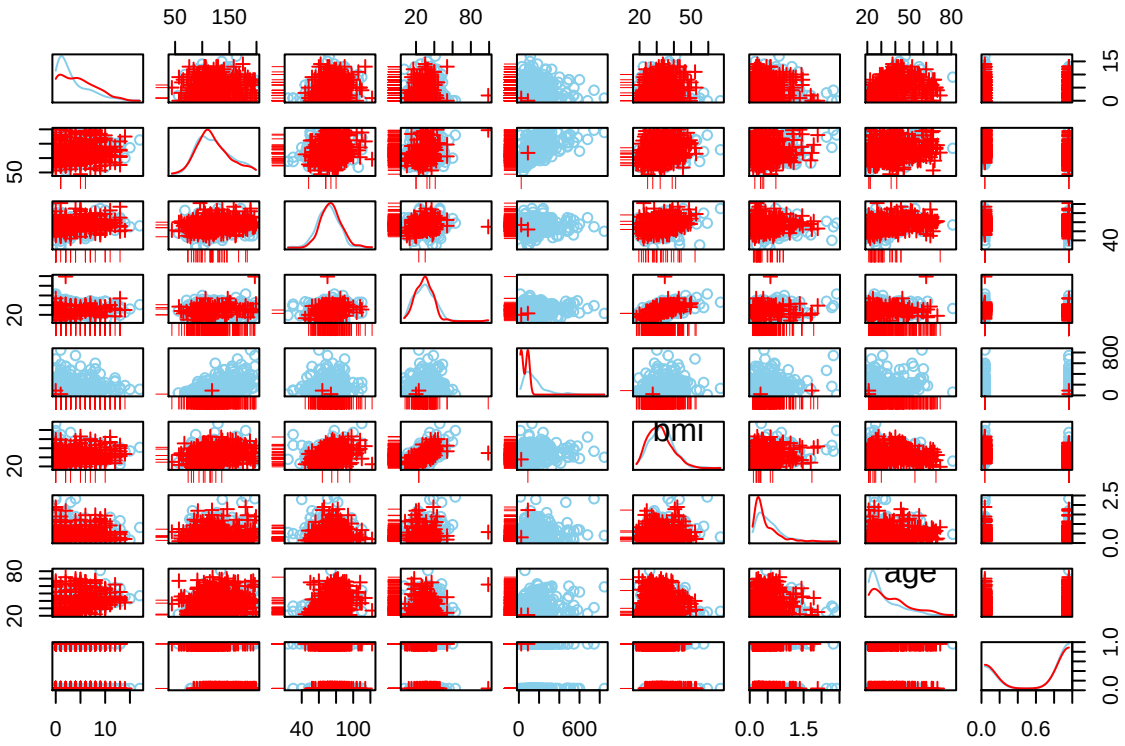
The plot on the right indicates that only little over half of the observations are complete. Due to the number of observations with missing values, we choose not to drop these observations from our analysis. Instead, we will impute missing values using a technique called Imputation by Predicted Mean matching, which "imputes missing values by means of the nearest-neighbor donor with distance based on the expected values of the missing variables conditional on the observed covariates."(1)

Imputation by Predicted Mean Matching is advantagous over other methods of data imputation because it "can provide valid inference when data are missing at random." (2)

This introduces an assumption: that data are at least missing at random. That is, we must be sure that our data are not Missing Not at Random (MNAR). In the case of MNAR,

To test if this is a reasonable assumption, we construct a scatterplot matrix highlighting missing values.

```
scattmatrixMiss(data)
```



We note no relationship between variables and missing values, so our assumption is valid. We proceed with the Imputation by Predictive Mean Matching.

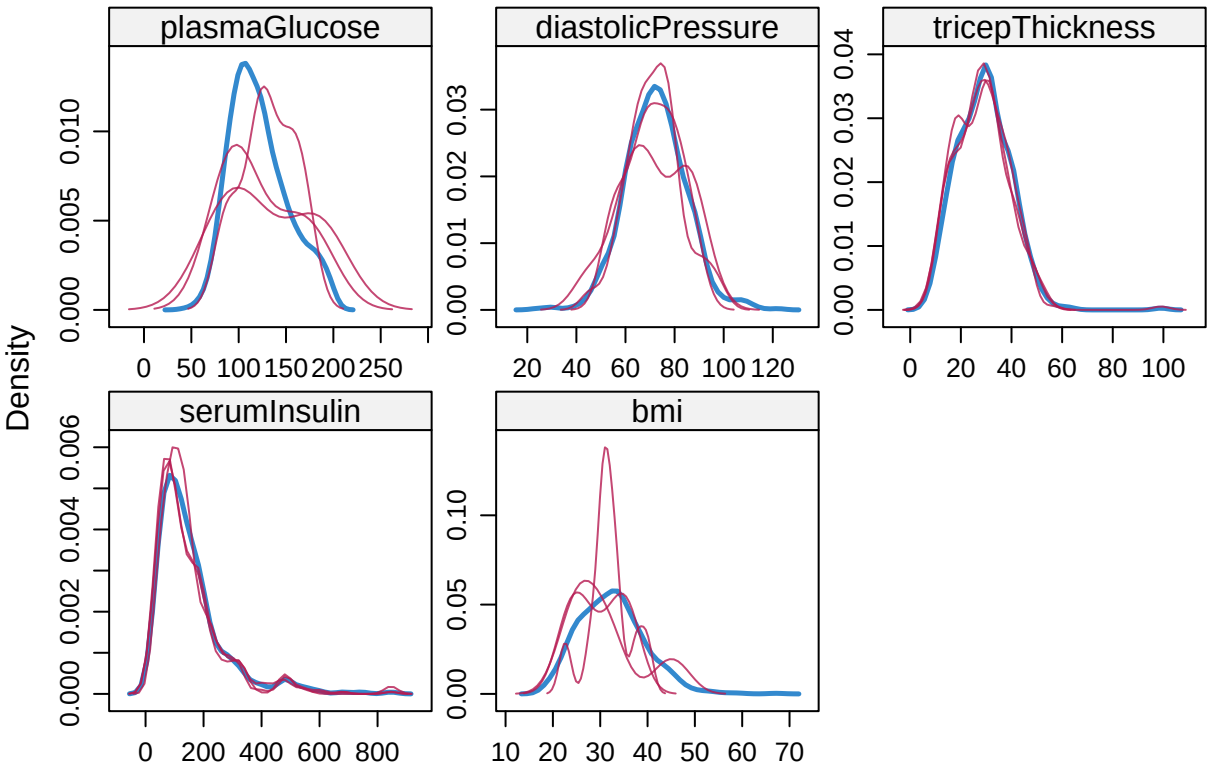
```
tempdata <- mice(data, m = 3, method = 'pmm', seed = 100)
```

```
##
##  iter imp variable
##    1   1  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    1   2  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    1   3  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    2   1  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    2   2  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    2   3  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    3   1  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    3   2  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    3   3  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    4   1  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    4   2  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    4   3  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    5   1  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    5   2  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
##    5   3  plasmaGlucose  diastolicPressure  tricepThickness  serumInsulin  bmi
```

```
data <- complete(tempdata)
```

We examine the distributions of our imputed data (red) compared to the original data (blue).

```
densityplot(tempdata)
```



The distributions are approximately equal, so we may proceed to feature selection.

2.4 Feature Selection

We ensure that no two features are too highly correlated by constructing a scatterplot matrix. If any two features have a correlation coefficient greater than `0.7`, we will consider removing one of them.

```
correlationMatrix <- cor(data[,1:8])
findCorrelation(correlationMatrix, cutoff=0.7)
```

```
## integer(0)
```

This is not necessary, though, as no two features are that highly correlated. Consequently, we choose not to eliminate any features from our analysis.

2.5 Data Standardization

Since the features of the dataset represent different units, we choose to standardize the data but making the mean of each column `0` with a standard deviation of `1`.

This is accomplished with a very simple algorithm:

Replace each observation of a random variable with the output of the following function:

$$f(x_i) = \frac{x_i - mean(X)}{sd(X)}$$

Repeat for each random variable.

This standardization is easily performed with R.

```
data[, 1:8] <- scale(data[, 1:8], center = TRUE, scale = TRUE)
```

3. Training the Algorithms

With our exploratory analysis and data processing complete, we being our analysis. Models for each of our three methods will be constructed from a training set of observations using 10-fold cross validation to prevent overfitting. This is easily implemented using the `caret` package.

```
tenFoldCV <- trainControl(method = "repeatedcv",
                          number = 10,
                          repeats = 10,
                          classProbs=TRUE,
                          summaryFunction=twoClassSummary)
```

The best model for each of the three methods will then be selected by its area under the ROC curve. This score, $x \in [0, 1]$ represents model accuracy. A score close to `1` indicates high accuracy.

3.1 Predicting the most common label

Of the 768 observations, about 65% have class label 'notDiabetic' and the remaining 35% have class label 'Diabetic'. So by predicting 'notDiabetic' for every class, one will already be 65% accurate. Thus any model must have an accuracy greater than 65% to be viable.

3.2 Training and Test Sets

We use 70% of the observations to train the models and reserve the remaining 30% to test performance.

```
sampleSize <- floor(.7 * nrow(data))

set.seed(131)
trainIndices <- sample(seq_len(nrow(data)), size = sampleSize)

x.train <- data[trainIndices, 1:8]
y.train <- data[trainIndices, 9]

x.test <- data[-trainIndices, 1:8]
y.test <- data[-trainIndices, 9]
```

3.3 Random Forest

This algorithm presents a tree-based classification method. It is unique from other tree-based methods because whenever a split in the tree is considered, the algorithm may only random subset of predictor variables as split candidates. Then only one predictors in the random subset is used in the split.(3)

References

(1) http://www.stefvanbuuren.nl/publications/2014%20Semicontinuous%20-%20Stat%20Neerl.pdf
(2) http://bmcmedresmethodol.biomedcentral.com/articles/10.1186/1471-2288-14-75
(3) Introduction to Statistical Learning