Final_project_Bottino_Poetto_Spagliardi

Manuel Bottino, Patrick Poetto, Jacopo Spagliardi

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1 References

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2 Review

2.1 Why it works

First of all let's introduce the general idea of bagging. Given a dataset $L = \{(x_n, y_n),\ n = 1, \dots, N\}$ we try to improve a predicting procedure in a "naive" way, ideally we would like to have a sequence of datasets $\{L_k\}$ of training sets each containing N independent observations, then take the average of the sequence $\{\phi(x, L_k)\}$.

$$\phi_A(x, P) = E_L[\phi(x, L)] \tag{1}$$

.

Because ϕ_A depends not only on x but also the underlying probability distribution P from which L is drawn. Since we are missing this last information the only tool we are left with is our dataset L, we instead use P_L the bootstrap approximation of P, it can be defined as the probability mass function with equal probability of extracting each element of the dataset (x_n, y_n). Finally we can define the bootstrap aggregate predictor as:

$$\phi_B(x) = \phi_A(x, P_L) \tag{2}$$

.

In order to understand why bagging works theoretically it can be proved that mean-squared error (MSE) of $\phi_A(x)$ is lower than the mean-squared error averaged over L of $\phi(x, L)$. How much lower the two sides are depends on the inequality:

$$[E_L\phi(x, L)]^2 \leq E_L\phi^2(x, L) \tag{3}$$

This result is true taking advantage of the Jensen's inequality for the specific case in which $g(X) = X^2$, this function is convex ($g'' > 0$), thus $E[Z^2] \geq (E[Z])^2$

2.2 Instability

The inequality @ref(eq:ineq) is a nice starting point to explain what role instability plays. In fact, If $\phi(x, L)$ does not change too much with replicate L the two sides will be nearly equal, and aggregation will not help. The more highly variable the $\phi(x, L)$ are, the more improvement aggregation may produce. Applying this reasoning to our $\phi_B(x)$, if the procedure is unstable, it can give improvement through aggregation. However, if the procedure is stable, then $\phi_B(x) = \phi_A(x, P_L)$ will not be as accurate for data drawn from P as $\phi_A(X, P) \sim \phi(x, L)$.

Let's see how this concept can be translated when we look at a more specific context, like classification. In this instance the predictor $\phi(\boldsymbol{x}, L)$ predicts a label $j \in \{1, ..., J\}$. We first define $Q(j|x) = P(\phi(x, L) = j)$, over many independent replicates of the learning set L, ϕ predicts class label j at input x with relative frequency $Q(j|x)$, and let $P(j|x)$ be the probability that input x generates class j. At this point we can set $\phi^*(x) = \arg\max_j P(j|x)$ (the Bayes predictor) which leads to the following expression for $Q(j|x)$:

$$\begin{cases} 1\ if\ P(j|x) = max_i P(i|x) \\ 0\ elsewhere \end{cases}$$

Now we have all the ingredients to show the maximum classification rate where:

$$r^* = \int \max_j P(j|x) P_X(dx) \tag{4}$$

where $P_X(dx)$ is the probability distribution of X.

If we know focus on the aggregate of ϕ and define it following the procedure described above $\phi_A(x) = \arg\max_j Q(j|x)$. We have the maximum attainable correct-classification rate of $\phi(x)$, we are missing the corret-classification for x, which for $\phi_A(x)$ is $\sum_j I(\arg\max_j Q(j|x) = j)P(j|x)$ Where I is the indicator function. *Putting all the pieces together* the correct-classification rate for $\phi_A(x)$ is:

$$r_A = \int_{\boldsymbol{x}\in C} max_j P(j|\boldsymbol{x})P_X(d\boldsymbol{x}) + \int_{\boldsymbol{x}\in C'} [\sum_j (I(\phi_A(\boldsymbol{x}) = j)P(j|\boldsymbol{x})]P_X(\boldsymbol{x}) \tag{5}$$

Even if ϕ is order correct at x its correct classification rate can be far from optimal, but ϕ_A is optimal. Only if ϕ is order-correct for most input of x (it is good), then aggregation can transform it into a nearly optimal predictor. On the other hand, unlike the numerical prediction situation, poor predictors can be transformed into worse ones if we use bagging.

2.3 Model - Decision Tree-Based Methods

Tree-based methods partition the feature space into a set of rectangles, and then fit a simple model, say a constant, in each one. This is a simple yet powerful procedure since it is able to disentangle a model into simpler and smaller models and describe his features more accurately than global models do basically using binary conditional clustering. The geometric perspective described before can be seen as a tree where data are run and at each node a test is conducted to see what is the path a covariate should follow until reaching a leaf, which represents the final prediction explained by the constant model. For example, let's say we have p inputs and a response, for each of N observations: that is, (x_i, y_i) for $i = 1, 2, ..., N$, with $x_i = (x_{i1}, x_{i2}, ..., x_{ip})$. The algorithm has decide on the splitting variables and split points, as well as what shape the tree should have. Suppose first that we have a partition into M regions $R_1, R_2, ..., R_M$, and we model the response as a constant c_m in each region: As a criterion for optimal partitional we can minimize the sum of squares $\sum(y_i - f(x_i))^2$. In this way the best $\hat{c}_m$ is just the average of y_i in region R_m: $\hat{c}_m = av(y_i|x_i \in R_m)$. Our model will be then: $f(x) = \sum_{m=1}^{M} c_m \cdot I(x \in R_m)$.

Now finding the best binary partition in terms of minimum sum of squares is generally computationally infeasible so we can set up a CART (classification and regression tree) algorithm starting with the data, a splitting variable j, a split point s, and defining the half planes as: $R_1(j, s) = \{X \mid X_j \leq s\}$ and $R_2(j, s) = \{X \mid X_j > s\}$. Then we seek j and s that solve

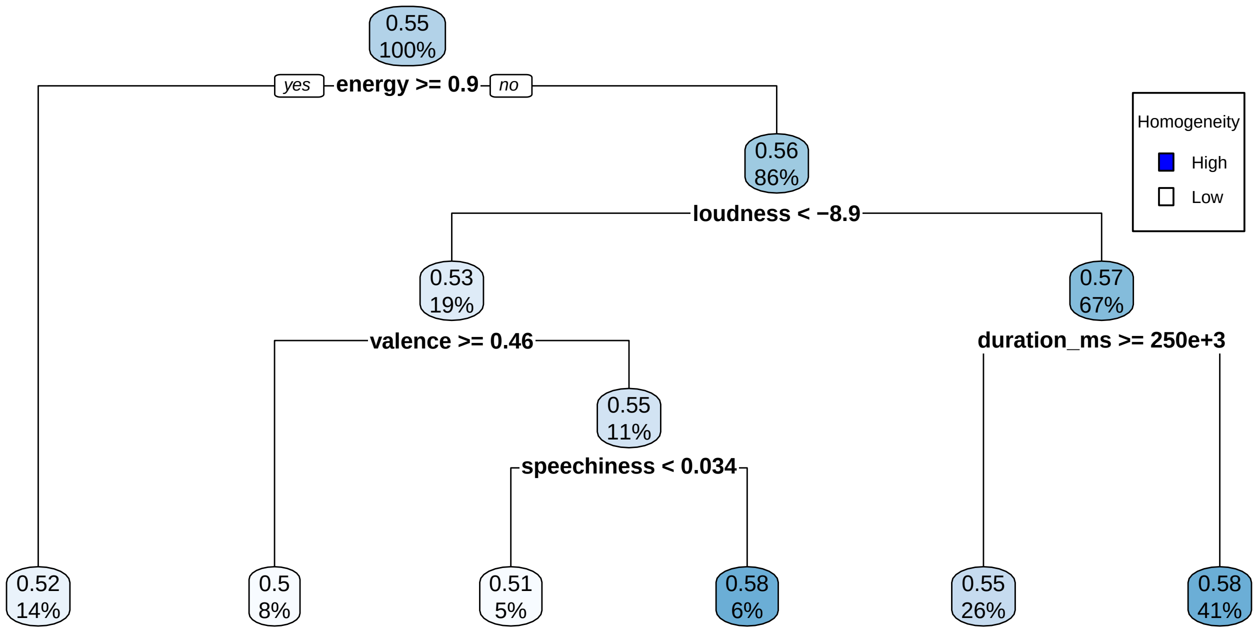
$$\min_{j,s}\left[\min_{c_1} \textstyle\sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2\right]$$

For any choice j and s, the inner minimization is solved by:

$$\hat{c}_1 = \mathrm{av}(y_i \,|\, x_i \in R_1(j,s)) \quad \text{and} \quad \hat{c}_2 = \mathrm{av}(y_i \,|\, x_i \in R_2(j,s))$$

For each j, the split point s can be found very quickly and hence determination of the best pair (j, s) is feasible by brute force. Having found the best split, we partition the data into the two resulting regions and repeat the splitting process on each of the two regions. Then this process is repeated on all of the resulting regions. The question now become: how large should we grow the three? It is pretty straightforward that too many nodes (splits) may overfit the data while doing vice versa may end up not being able to capture them well, resulting in misprediction. One strategy could be to set a lower threshold for the decrease of the sum of squares and stop the splitting when this is reached. However this strategy is too short sighted since a seemingly worthless split may lead to a very good one below. A more robust strategy may be to do kind of the opposite: grow a very large tree and then use a cost-complexity pruning criterion to collapse one internal node at a time from the full tree until the single node tree so that we find a sequence. It is intuitive that the optimal tree must be somewhere in the sequence. Now, with a cross validation selection method, we can find the actual optimal tree just minimizing the cross validated sum of squares.

This is how the CART algorithm for growing decision trees basically works. Note that decision trees are divided in classification and regression trees if the response is a factor or a numerical or continous variable.



Predicted Value	Median Value
0.5845508	0.55

We used the well known Spotify dataset to grow a basic tree with the function “rpart”. The thresholds at each node are defined by the algorithm which minimizes the MSE of the model. The color of each nodes represent homogeneity across data which have been classified in a node. Each node show the percentage of observations that it contains and the outcome prediction for that node. Then we used the function “predict” applied to our grown tree to make prediction on a virtual new observation, providing the median of each variable as a new value and getting predicted popularity of a song which have the median as each feature available in the dataset. Not surprisingly, the predicted value for popularity is near the median of the covariate popularity itself.

2.4 Algorithm Setup

Bootstrap aggregating Regression Trees can be done following the procedure proposed by **(Breiman, 1996)**:

1. Randomly divide a real dataset into a 10% test $\mathcal{T}$ and a 90% learning set $\mathcal{L}$. If the dataset is simulated then we can consider a $15-85$ or a $20-80$ proportion.

2. Grow a regression tree from $\mathcal{L}$ using a 10-fold cross validation, then run $\mathcal{T}$ down the tree to obtain the squared error $e_S(L,T)$. Using che k-folds cross validation means that $\mathcal{L}$ is divided into 10 folds, and for each iteration, a regression tree is trained on 9 folds and evaluated on the remaining fold. The process is repeated 10 times, such that each fold is utilized as the test set once. Ultimately, the best model, i.e. the regression tree with the best average performance across all test folds, is selected as the final result. At the end of the 10 iterations, the squared errors obtained for each test fold are used to calculate the mean squared error $e_S(L,T)$, which represents the average squared difference between the predictions of the regression tree and the actual values of the test set.

3. Select a bootstrap sample $\mathcal{L}_B$ from $\mathcal{L}$ and use it to grow a tree. Then use $\mathcal{L}$ to prune the tree avoiding overfitting. Repeat this step 25 times to obtain predictors $\phi_1(\mathbf{x}), ..., \phi_{25}(\mathbf{x})$.

4. For $(y_n, \mathbf{x_n}) \in \mathcal{T}$, the bagged predictor will be $\hat{y}_n = av_k \phi_k(\mathbf{x_n})$, and the squared error $e_B(\mathcal{L}, \mathcal{T}) = av_n(y_n - \hat{y}_n)^2$.
5. Divide the data into $\mathcal{L}$ and $\mathcal{T}$ for 100 times and average the errors to obtain $\bar{e}_S$ and $\bar{e}_B$.

2.5 Application of algorithm

Try to replicate the algorithm provided by the paper for regression trees using 10-fold cross-validation and bagging

```r
# Function that randomize learning and testing datasets, point 5 of algorithm
# performs this 100 time and only then the author applies both methods (cross validation
# and bagging). After this he recreates the division and compute the mean squared
# errors
random_training_test=function(df,k){
  fold_indices <- sample(cut(seq(1, nrow(df)), breaks = k, labels = FALSE,
                             ordered_result = FALSE))
  i=sample(1:k, 1)
  test_indices <- which(fold_indices == i)
  train_i <- df[-test_indices, ]
  test_i <- df[test_indices, ]
  return(list(train_i,test_i))
}



k_fold_reg_tree= function(df,k, y){
  formula <- as.formula(paste(y, "~", "."))

  # 1. take the dataset and divide it into learning and testing (90% - 10%)
  # which is already done by the function random_training_test
  train_i=df[[1]]
  test_i=df[[2]]

  # 2. take the learning set and apply 10-fold cv to find the model with lowest MSE

  # In this step we are dividing the training set in 10 folds to apply 10-fold cross validation
  fold_indices <- sample(cut(seq(1, nrow(train_i)), breaks = k, labels = FALSE,
                             ordered_result = FALSE))

  cv_result=Inf

  for (i in 1:k) {


  # Split the data into training and testing sets (10-fold cross validation)
  test_indices <- which(fold_indices == i)
  train_data <- train_i[-test_indices, ]
  test_data <- train_i[test_indices, ]




  # Train a regression tree on the training set
  model <- rpart(formula, data = train_data)

  # Predict the target variable for the testing set
  predictions <- predict(model, newdata = test_data)


  #Calculate the evaluation metric (e.g., mean squared errors
  result <- mean((predictions - test_data[[y]])^2)
  # 3. For every candidate we compute the MSE compered to the original test

  if(result<cv_result){
    cv_result=result
    # Compute mse of this model using the original test set as comparison
    predictions <- predict(model, newdata = test_i)
    final_res=mean((predictions - test_i[[y]])^2)
  }
  }
  return(final_res)
}

reg_tree_boot= function(df,b, y){
  formula <- as.formula(paste(y, "~", "."))

  # 1. take the dataset and divide it into learning and testing (90% - 10%)
  # which is already done by the function
  train_i=df[[1]]
  test_i=df[[2]]
  predictions=0

  # 2. compute 25 predictions with different bootstrap samples
  for (i in 1:b) {
  train_data=slice_sample(train_i,n=nrow(train_i), replace=TRUE)
  model <- rpart(formula, data = train_data)


  # Predict the target variable for the testing set
  predictions <- predictions + predict(model, newdata = test_i)

  }
  # 3. take the mean of these predictors and compute the MSE
  predictions=predictions/b
  final_res=mean((predictions - test_i[[y]])^2)
  return(final_res)
}

# I wrote down y instead of the standard MEDV (median of prices) so my lapply below
# can be computed
housing <- read.table("housing.csv", quote="\"", comment.char="")
colnames(housing)=c('CRIM', 'ZN', 'INDUS', 'CHAS', 'NOX', 'RM', 'AGE', 'DIS',
                    'RAD', 'TAX', 'PTRATIO', 'B', 'LSTAT', 'y')

# I wrote down y instead of the standard O3 (ozone levels) so my lapply below
# can be computed
```

```r
colnames(ozone)[1]="y"

fried1=mlbench.friedman1(n=200, sd=1)
friedman1=data.frame(cbind(fried1$x,fried1$y))
colnames(friedman1)=c("x_1","x_2","x_3","x_4","x_5","x_6","x_7","x_8","x_9","x_10","y")

fried2 <- mlbench.friedman2(n = 200)
friedman2=data.frame(cbind(fried2$x,fried2$y))
colnames(friedman2)=c("x_1","x_2","x_3","x_4","y")

fried3 <- mlbench.friedman3(n = 200)
friedman3=data.frame(cbind(fried3$x,fried3$y))
colnames(friedman3)=c("x_1","x_2","x_3","x_4","y")


B=1000
datasets=list(housing, ozone, friedman1, friedman2, friedman3)


# the list in which we will store all of our mse (both from cross validation and
# bagging) for each dataset, and the decrease in mse (computed below).
e_bar_global=list()


# Now that we have a function that takes the dataset as input, performs 10-fold cv
# on the learning set, selects the best fold and use it to make predictions.
# Only then we can compute the MSE that we are going to use
e_bar_global=lapply(datasets, function(data){
  colMeans(t(replicate(B, {
  df=random_training_test(data,10)
  mse_cv=k_fold_reg_tree(df,10,"y")
  mse_bag=reg_tree_boot(df,25,"y")
  c(mse_cv, mse_bag)
})))
})

e_bar_global=lapply(e_bar_global,
                    function(data){data[3]=((data[1]-data[2])/data[1])*100
                                   round(data,2)
  })
```

Dataset name	$\bar{e}_S$	$\bar{e}_B$	Decrease
Boston Housing	23.06	16.56	28.19
Ozone	23.04	18.14	21.25
Friedman #1	10.44	7.21	30.98
Friedman #2	2.987378×10^4	2.174148×10^4	27.22
Friedman #3	0.05	0.03	28.68

Do the same but this time we use libraries that simplifies the coding part a lot

3 Application