Advanced R: Statistical Machine Learning

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Zoom Workshop for SJRWMD
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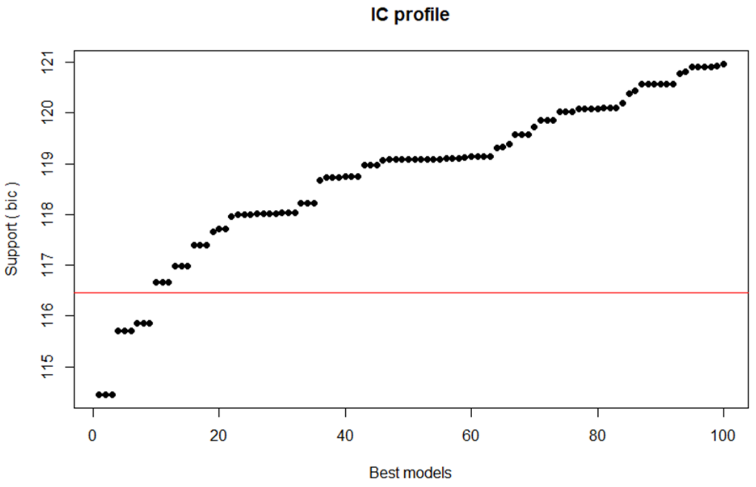
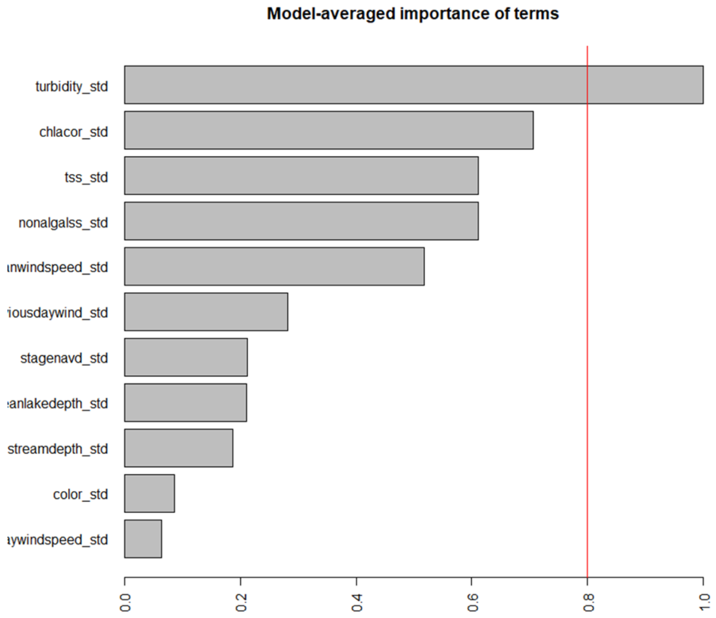
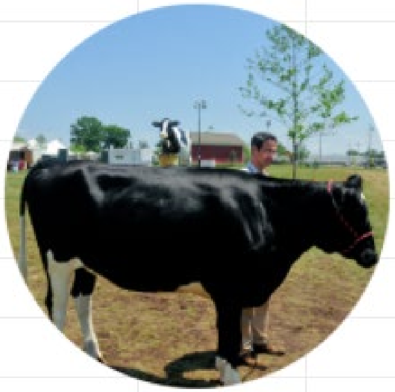




Ensembles and Random Forest

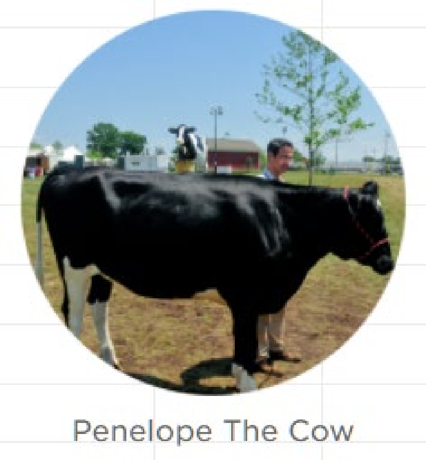
How much does this cow weigh?



Penelope The Cow

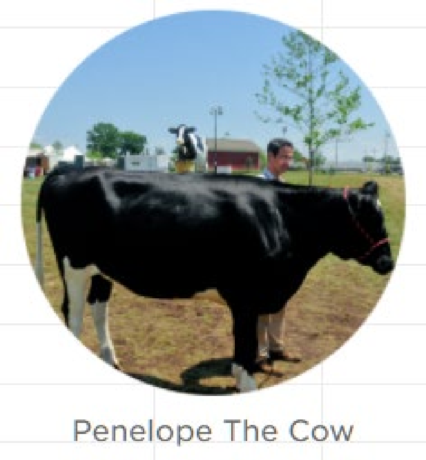
How much does this cow weigh?

- Google says depends on gender…

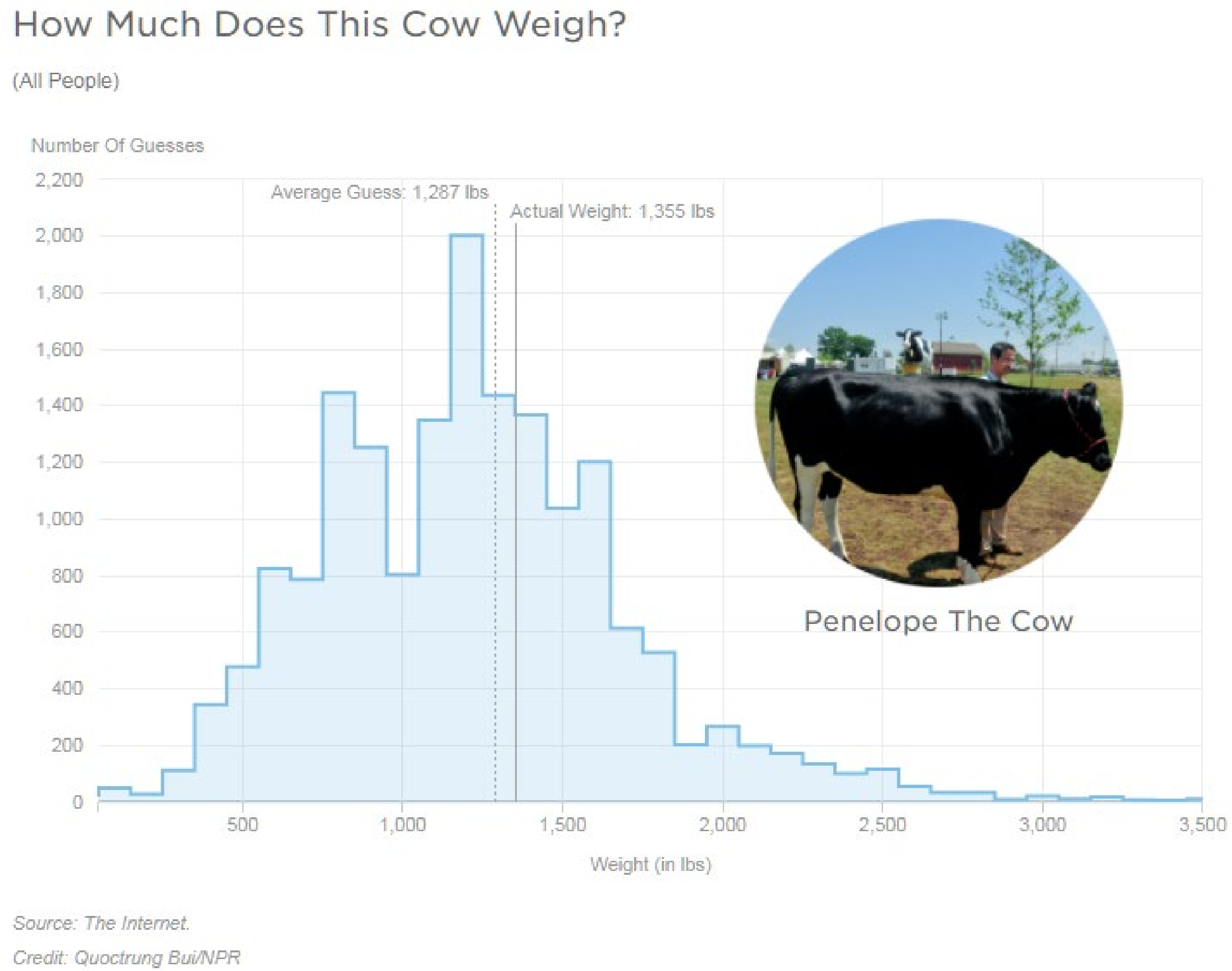


How much does this cow weigh?

- Google says depends on gender…sounds like Google has been doing some machine learning…



The wisdom of crowds in machine learning: ensemble techniques (bagging and boosting)



https://www.npr.org/sections/money/2015/08/07/429720443/17-205-people-guessed-the-weight-of-a-cow-heres-how-they-did

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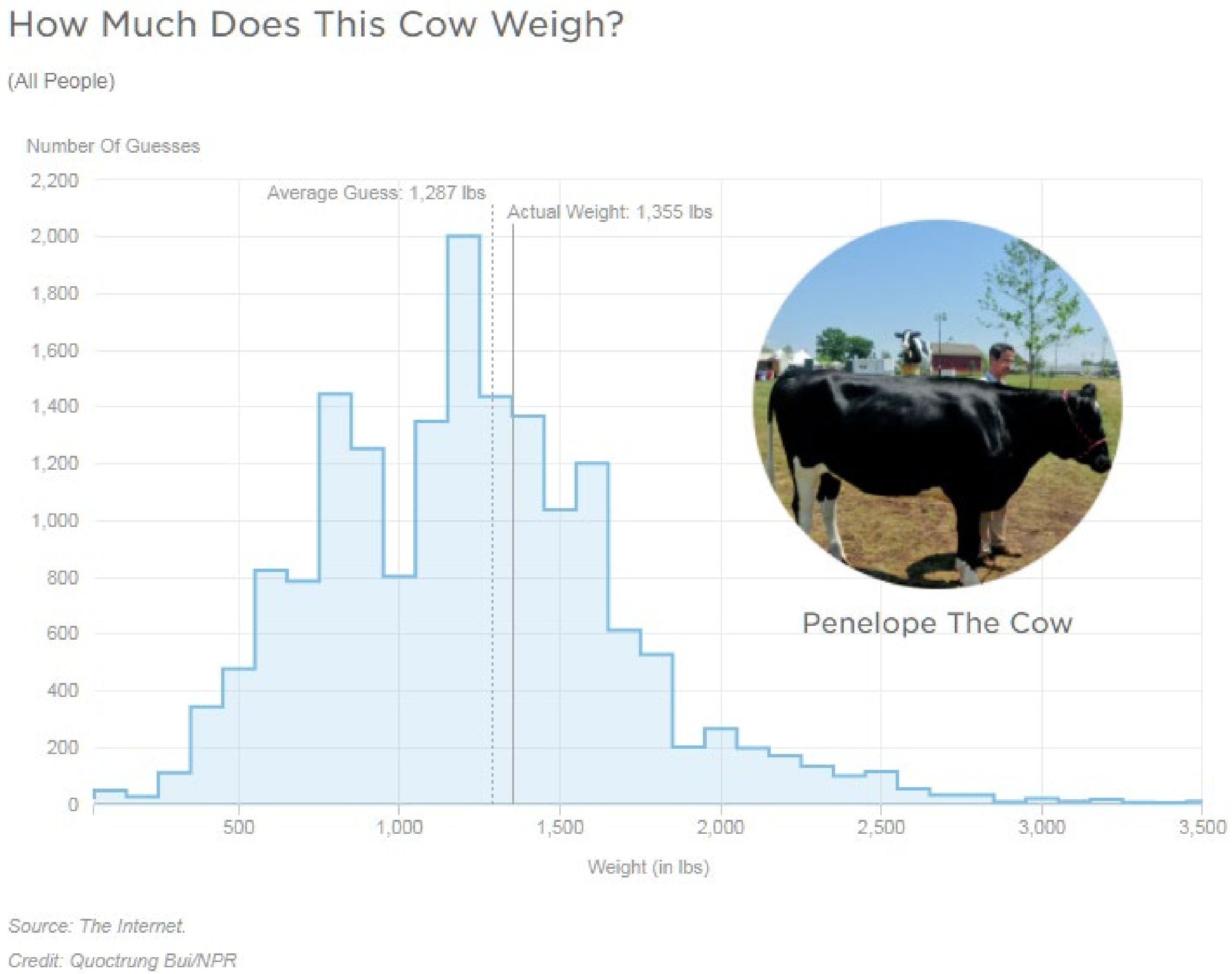
The wisdom of crowds in machine learning: ensemble techniques (bagging and boosting)



Idea is that a group of "weak learners" will average out to a better answer than a typical expert!

Can think of this as the large positive and negative errors of the "uneducated" canceling out.

https://www.npr.org/sections/money/2015/08/07/429720443/17-205-people-guessed-the-weight-of-a-cow-heres-how-they-did

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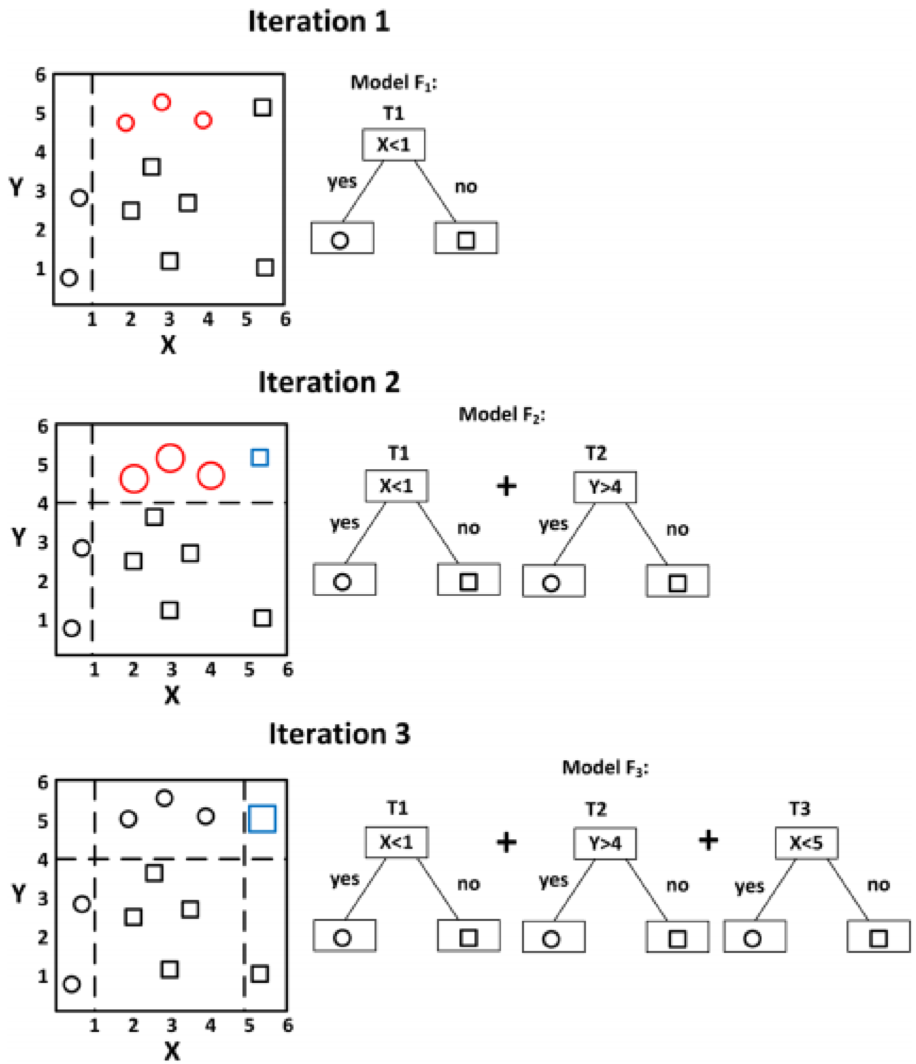
Types of ensembles: bagging

- Bagging – bootstrap aggregation. Subsample rows of a dataset (bootstrapping) repeatedly and then average responses (regression) or majority vote (classification).
  - Decreases the variance in the prediction by generating additional data from training dataset (sampling with replacement)
  - Interestingly, by chance if you sample the same number of rows with replacement on average each bootstrap sample contains 63.2% of the original observations and omits 36.8%
  - The omitted observations from each sample are called out-of-bag observations and can be used as a kind of hold-out sample

Types of ensembles: boosting

XGBoost is a superstar in the machine learning world!

- Boosting – fitting successive models which address residual variation by increasing the weight of poorly fit observations in successive models. This is a sequential method.



https://www.researchgate.net/publication/326379229_Exploring_the_clinical_features_of_narcolepsy_type_1_versus_narcolepsy_type_2_from_European_Narcolepsy_Network_database_with_machine_learning

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Types of ensembles: stacking

- Stacking – a method of combining heterogenous models. Train several models, then train a metamodel on the outputs of the group of models.

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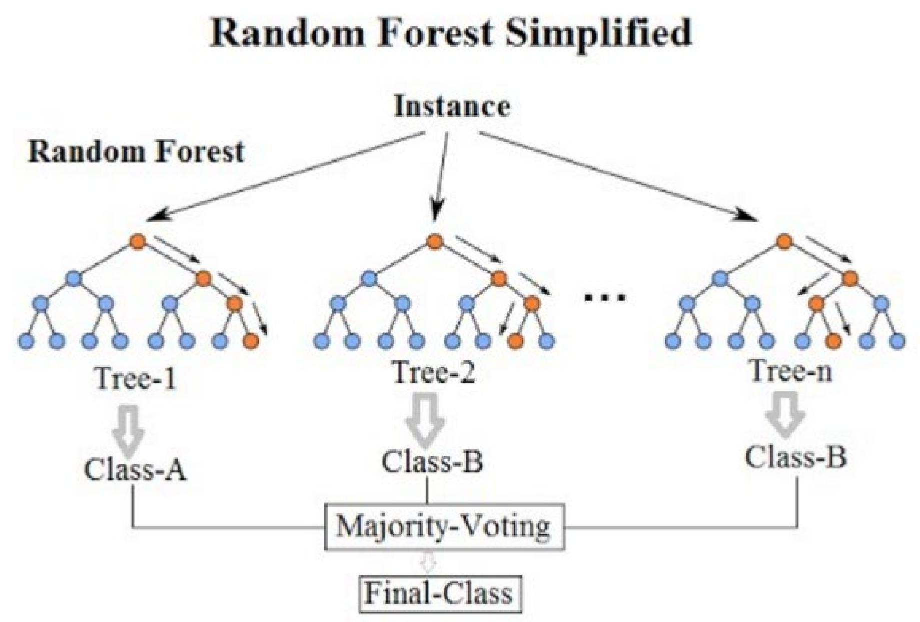
Random Forest Algorithm: a modified bagged decision tree

- Can be used for classification or regression
- Creates “forest” of decision trees using subset of cases and variables (bootstrap aggregation or “bagging”)
- Predictions are made by running case through all trees (e.g., 500) and taking an average for regression
- Each tree is grown with only about 60% of the data, so the remaining data provide a realistic “out-of-bag” error estimate
- Robust to outliers and noise
- Allows complex interactions
- No statistical assumptions
- Handles datasets >1000 variables
- Avoids overfitting
- Minimal tuning required
- Limitations
  - Can’t extrapolate
  - May overestimate lows/underestimate highs



https://community.tibco.com/wiki/random-forest-template-tibco-spotfirer-wiki-page

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Random Forest Algorithm Pseudocode

```
1.  Given a training data set
2.  Select number of trees to build (n_trees)
3.  for i = 1 to n_trees do
4.  |  Generate a bootstrap sample of the original data
5.  |  Grow a regression/classification tree to the bootstrapped data
6.  |  for each split do
7.  |  | Select m_try variables at random from all p variables
8.  |  | Pick the best variable/split-point among the m_try
9.  |  | Split the node into two child nodes
10. |  end
11. | Use typical tree model stopping criteria to determine when a
    | tree is complete (but do not prune)
12. end
13. Output ensemble of trees
```

Random Forest hyperparameters worth tuning

- mtry – number of variables tried at each split on tree, typical default values are
  - Number of parameters/3 (regression)
  - Number of paramerers^0.5 (classification)
- ntree – number of trees in the forest
  - default value is 500
  - may be useful to tune mtry at 500 trees, then boost number of trees to see if any improvement

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Less frequently tuned hyperparameters

- The complexity of each tree
  - node size, max depth, max number of terminal nodes, or the required node size to allow additional splits
- The sampling scheme
  - Bootstrap with replacement is the norm but if you have many categorical features with a varying number of levels, sampling with replacement can lead to biased variable split selection
- The splitting rule to use during tree construction
  - The splitting is based usually on Gini impurity (in the case of classification) and the SSE (in case of regression), but it can be changed.

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Tuning mtry using caret on ttrain4

```
# code below used to identify optimal mtry hyperparameter for tuning using caret
seed<-42
set.seed(seed)
control <- trainControl(method="repeatedcv", number=10, repeats=3, search="grid", classProbs = TRUE)
tunegrid <- expand.grid(.mtry=c(1:7))
metric<-"Accuracy"
rf_gridsearch <- train(Survived2~., data= ttrain4rf, method="rf", metric=metric, tuneGrid=tunegrid, trControl=control)

print(rf_gridsearch)
plot(rf_gridsearch)
print(rf_gridsearch)
```

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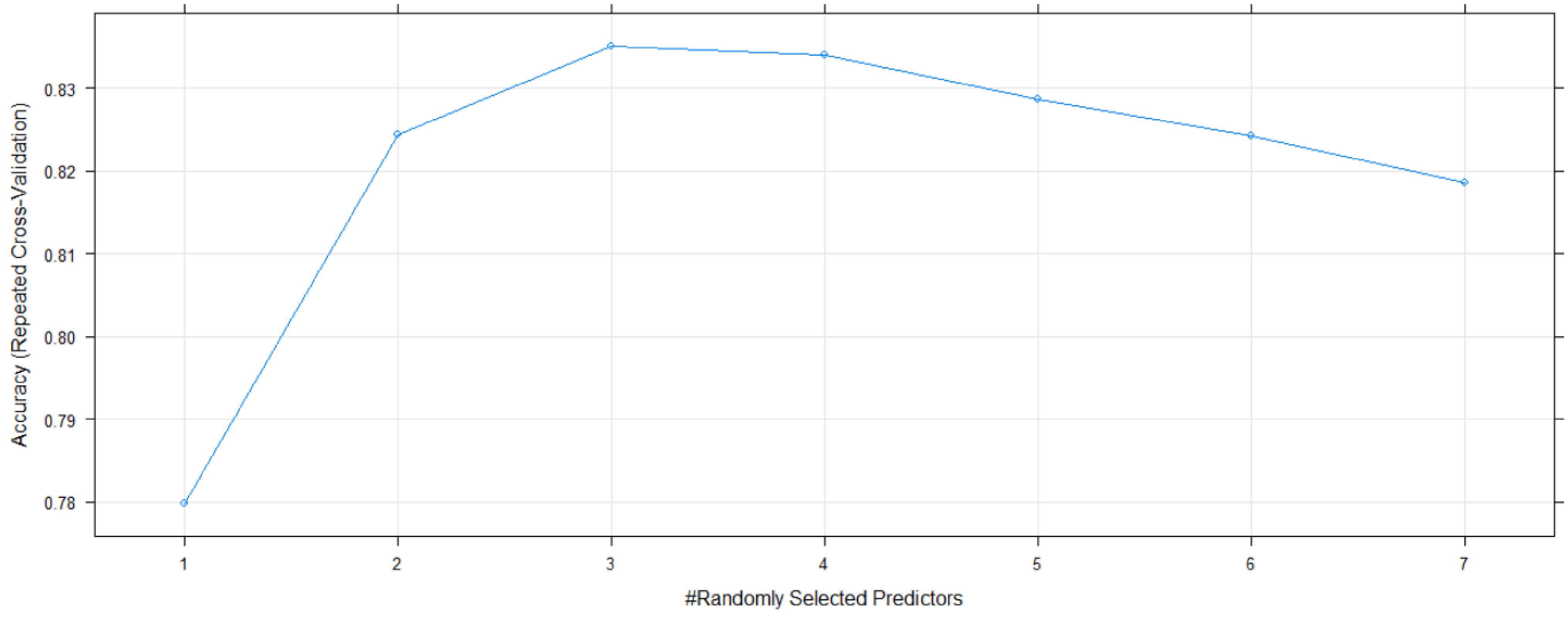
mtry=3 results in highest accuracy

plot(rf_gridsearch)



Out-of-bag performance on ttrain4, ntree=500

- OOB accuracy of 100-16.39 = 83.61%
- OOB is usually conservative compared to test set results

```
> print(rfm_ttrain4_500) # view OOB estimate of error rate

Call:
 randomForest(formula = Survived2 ~ ., data = ttrain4rf, mtry = 3,      ntree = 500)
               Type of random forest: classification
                     Number of trees: 500
No. of variables tried at each split: 3

        OOB estimate of  error rate: 16.39%
Confusion matrix:
    X0  X1 class.error
X0 496  53  0.09653916
X1  93 249  0.27192982
> 
```

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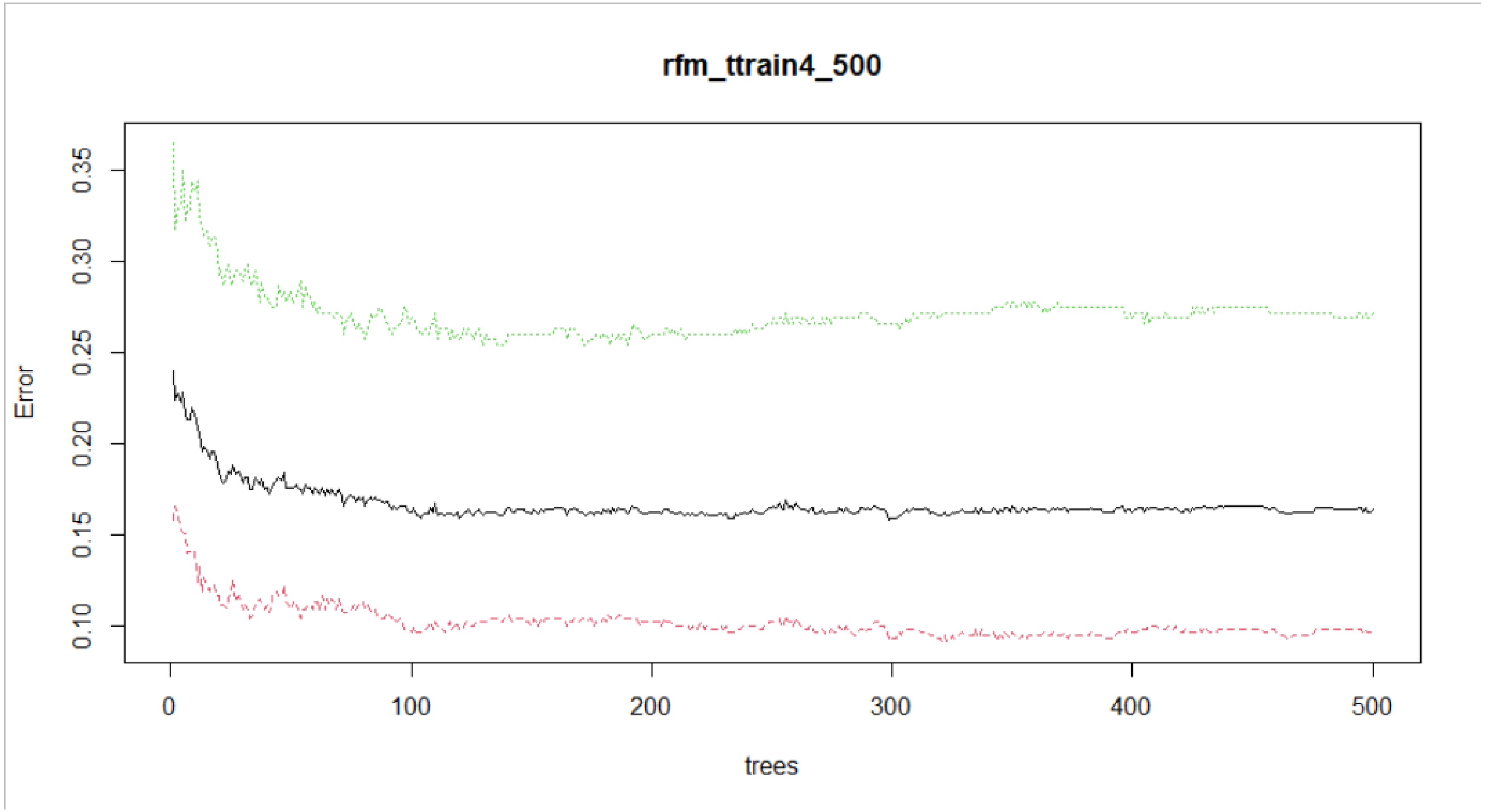
Plotting the randomForest object gives idea of changing error rates with ntree

plot(rfm_ttrain4_500)



Out-of-bag performance on ttrain4 for ntree=10000

- OOB accuracy of 100-16.61 = 83.39%
- No improvement over model with default 500 trees in this case

```
> print(rfm_ttrain4_10000) # view OOB estimate of error rate

Call:
 randomForest(formula = Survived2 ~ ., data = ttrain4rf, mtry = 3,      ntree = 10000)
               Type of random forest: classification
                     Number of trees: 10000
No. of variables tried at each split: 3

        OOB estimate of  error rate: 16.61%
Confusion matrix:
    X0  X1 class.error
X0 494  55   0.1001821
X1  93 249   0.2719298
> plot(rfm_ttrain4_10000)
```

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Test set performance ntree=500

confusionMatrix(pred_rfm_500_test,ttest4rf$Survived2) # evaluating performance on out-of-sample test dataset

- 76% accuracy
- Not as good as knn

```
> confusionMatrix(pred_rfm_500_test,ttest4rf$Survived2) #
 evaluating performance on out-of-sample test dataset
Confusion Matrix and Statistics

          Reference
Prediction  X0  X1
        X0 210  54
        X1  40  91

               Accuracy : 0.762
                 95% CI : (0.7169, 0.8032)
    No Information Rate : 0.6329
    P-Value [Acc > NIR] : 2.664e-08

                  Kappa : 0.4773

 Mcnemar's Test P-Value : 0.18

            Sensitivity : 0.8400
            Specificity : 0.6276
         Pos Pred Value : 0.7955
         Neg Pred Value : 0.6947
             Prevalence : 0.6329
         Detection Rate : 0.5316
   Detection Prevalence : 0.6684
      Balanced Accuracy : 0.7338

       'Positive' Class : X0

>
```

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Test set performance ntree=10000

confusionMatrix(pred_rfm_10000_test,ttest4rf$Survived2)

```
> confusionMatrix(pred_rfm_10000_test,ttest4rf$Survived2)

Confusion Matrix and Statistics

          Reference
Prediction  X0  X1
        X0 212  53
        X1  38  92

               Accuracy : 0.7696
                 95% CI : (0.7249, 0.8103)
    No Information Rate : 0.6329
    P-Value [Acc > NIR] : 3.776e-09

                  Kappa : 0.4932

 Mcnemar's Test P-Value : 0.1422

            Sensitivity : 0.8480
            Specificity : 0.6345
         Pos Pred Value : 0.8000
         Neg Pred Value : 0.7077
             Prevalence : 0.6329
         Detection Rate : 0.5367
   Detection Prevalence : 0.6709
      Balanced Accuracy : 0.7412

       'Positive' Class : X0
```

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Peeking into the random forest– a “black box” model

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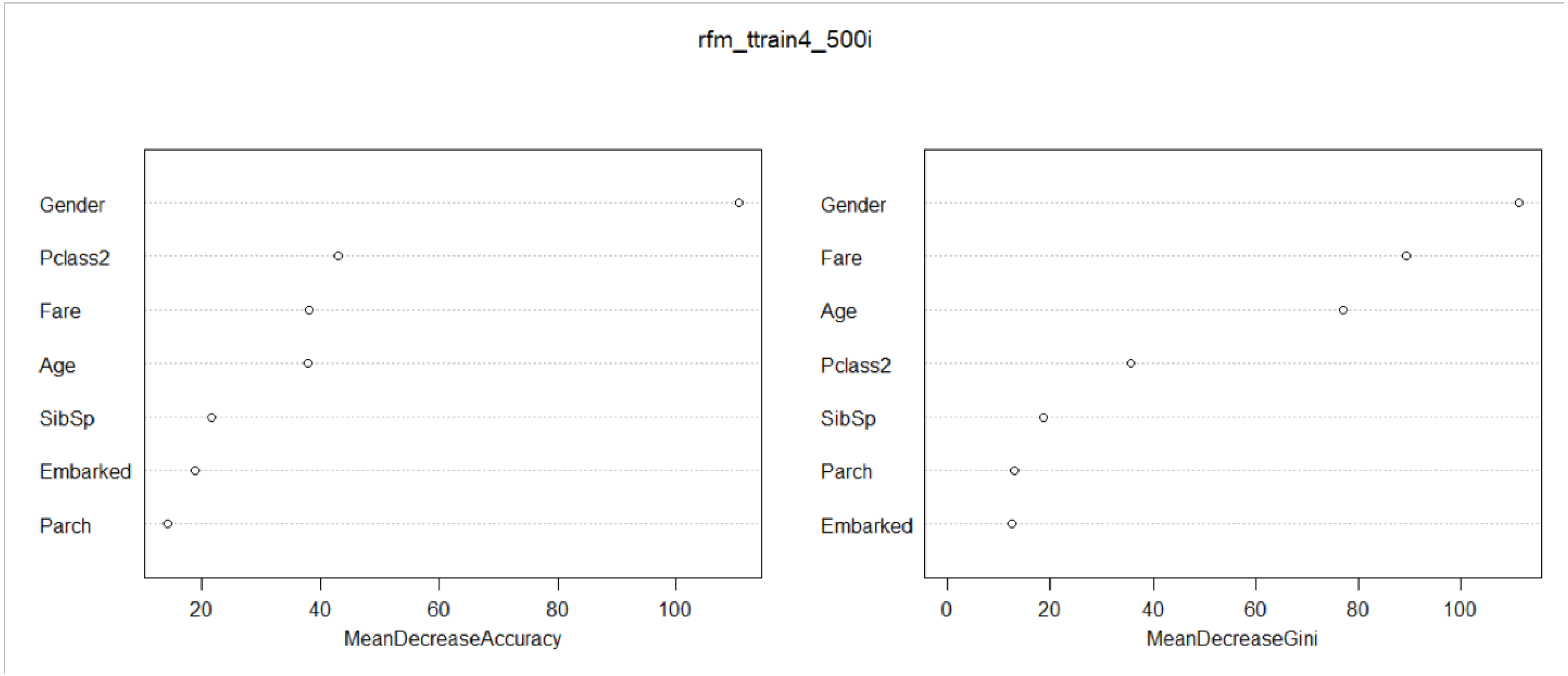
Two types of importance available for randomForest

rfm_ttrain4_500i<-randomForest(Survived2~.,ttrain4rf,mtry=3,ntree=500, importance=T)

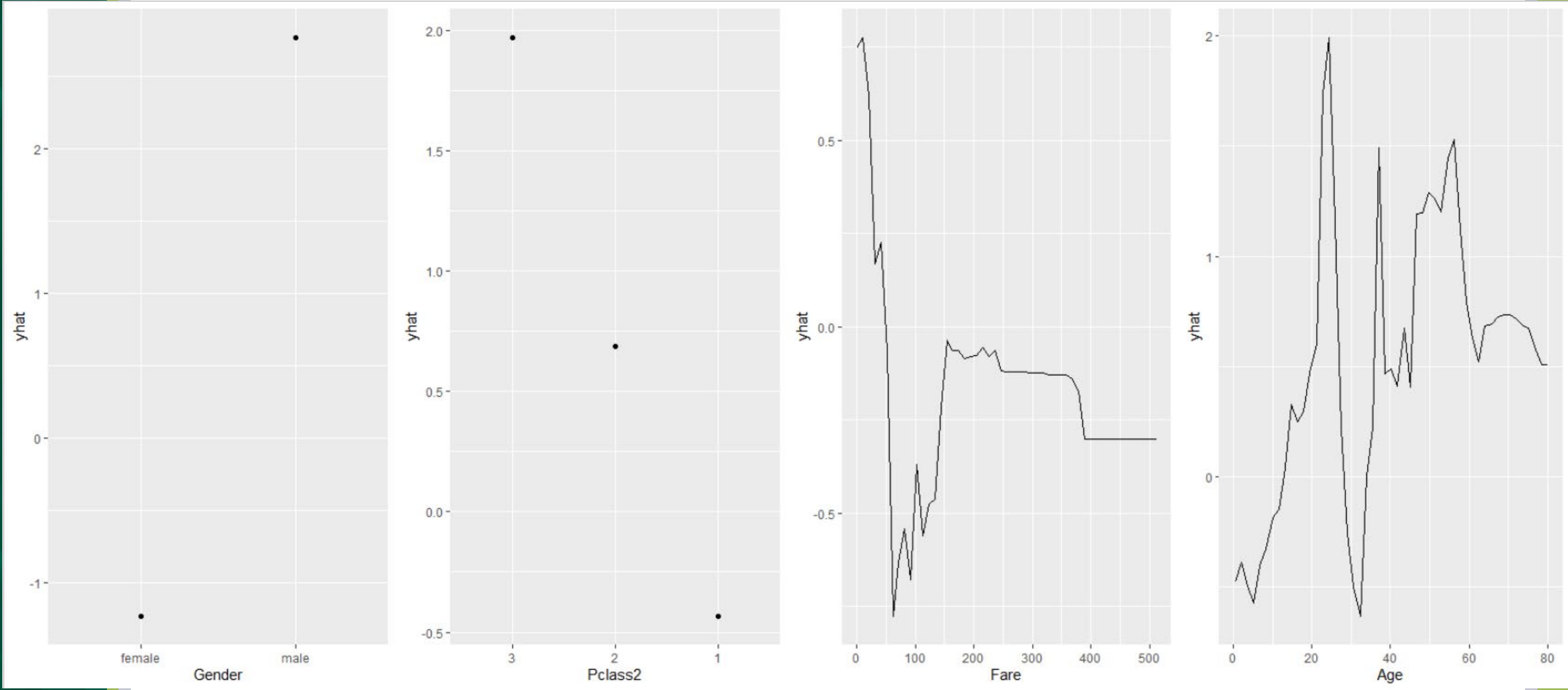
- varImpPlot(rfm_ttrain4_500i)



Randomization-based

Importance for tree-splitting

Dependence plots



randomForest on ames train_3

- 90.51% out-of-bag estimate of variance explained

```
> m_rf_ames_v1<-randomForest(Sale_Price~., data=train_3)
> print(m_rf_ames_v1)

Call:
 randomForest(formula = Sale_Price ~ ., data = train_3)
               Type of random forest: regression
                     Number of trees: 500
No. of variables tried at each split: 26

          Mean of squared residuals: 592460699
                    % Var explained: 90.51
> 
```

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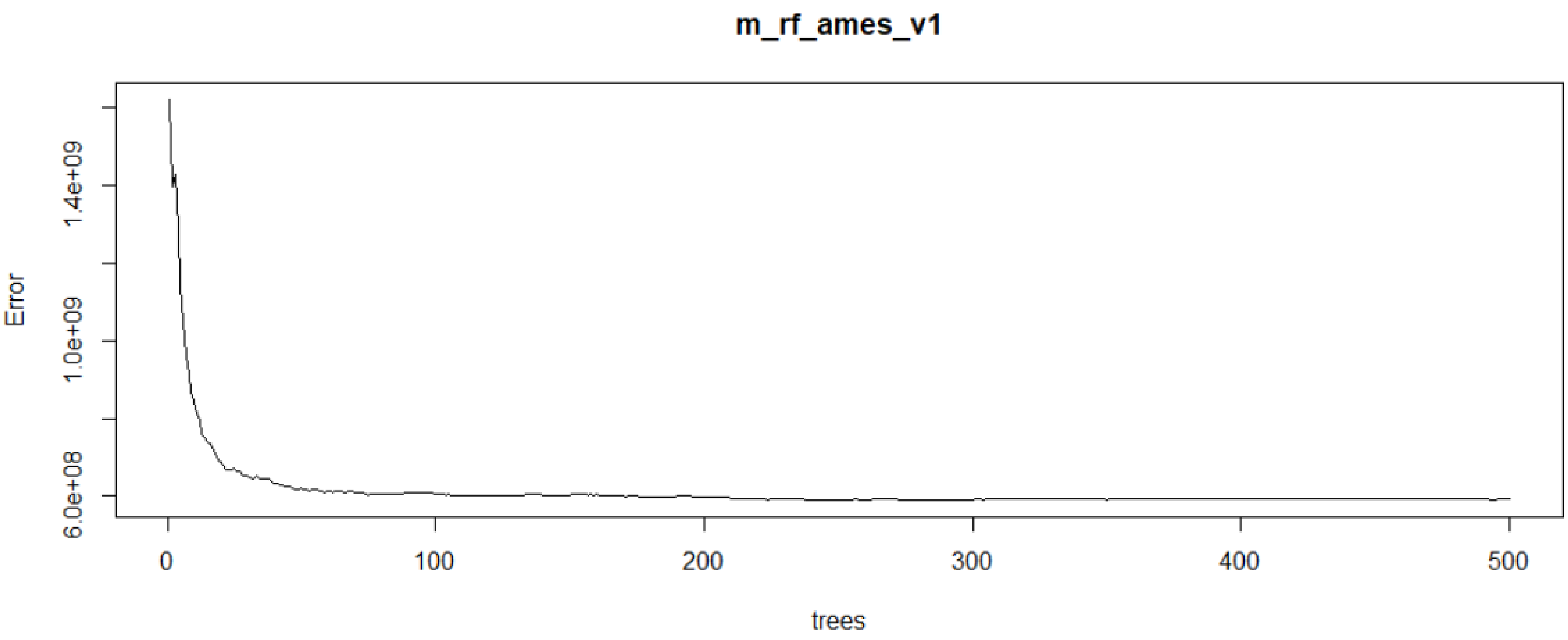
Results from ames train

plot(m_rf_ames_v1)



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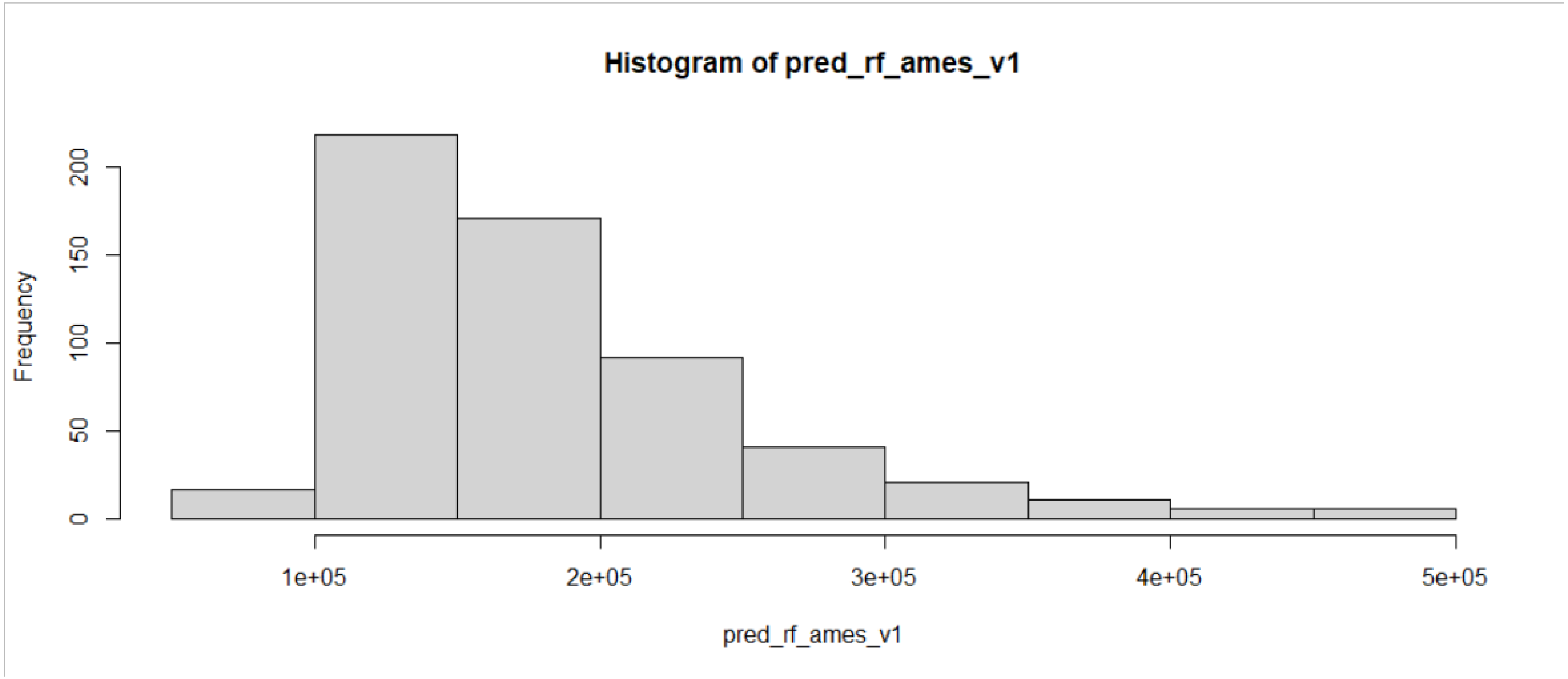
Predicting test_3

```
pred_rf_ames_v1<-predict(m_rf_ames_v1,newdata=test_3)
hist(pred_rf_ames_v1)
```



rf train and test RMSE

```
> RMSE(m_rf_ames_v1$predicted, train_3$Sale_Price)
[1] 24340.52
> RMSE(pred_rf_ames_v1, test_3$Sale_Price)
[1] 31741.76
> test_3aug$predrf1<-pred_rf_ames_v1
> ggplot(test_3aug,aes(x=predrf1,y=Sale_Price))+
+   geom_point()+stat_smooth(method=lm)+geom_abline(slope=1, intercept=0, col
='red')
`geom_smooth()` using formula 'y ~ x'
> cor(test_3aug$predrf1,test_3aug$Sale_Price)^2
[1] 0.8597779
> res_predrf1<-test_3aug$Sale_Price-test_3aug$predrf1
> (mean((res_predrf1)^2))^0.5
[1] 31741.76
>
```

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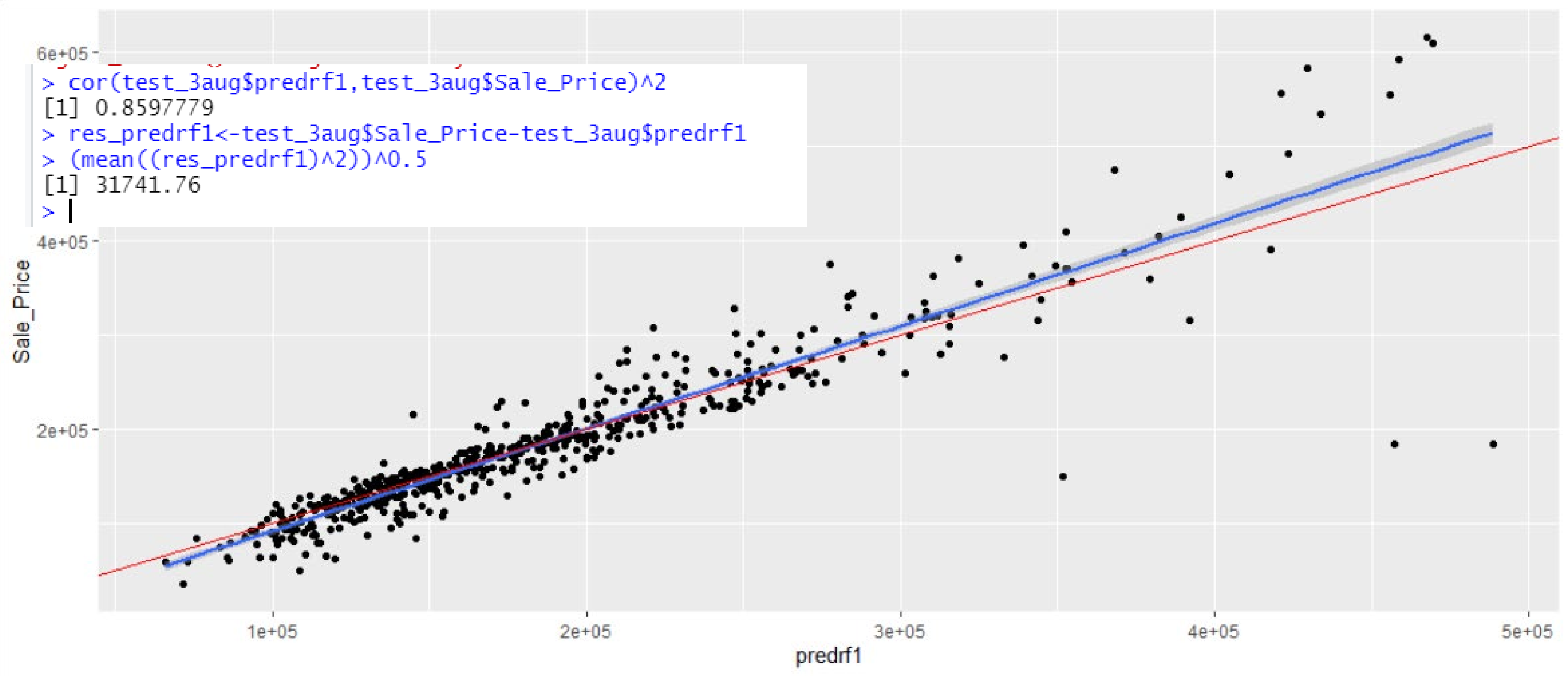
rf excellent performance on test set with RMSE 31741.76 and r^2 of 6%

- randomForest algorithm well suited to this problem



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