Mechanistic interpretation of feature importance

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June 9, 2016

Feature importance analysis from Random forest using Gini index (i.e., variance of the responses).

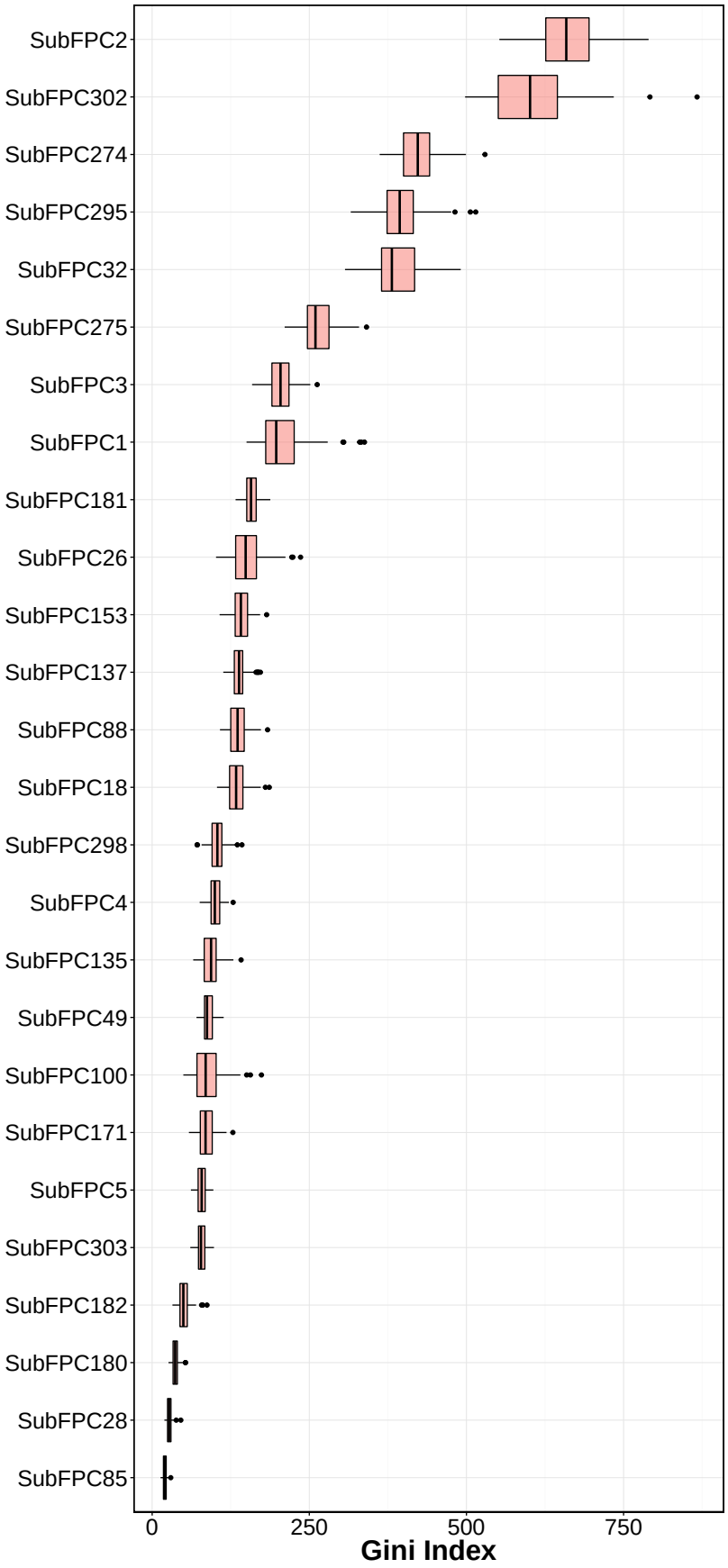
Creating a R function to perform feature importance

```
randomForest_feature_importance <- function(x) {
  library(doSNOW)
  library(foreach)
  library(parallel)
  cl <- makeCluster(8)
  registerDoSNOW(cl)

  results <- list(100)
  results <- foreach (i = 1:100) %dopar% {
    x <- na.omit(x)
    set.seed(i)
    para <- dplyr::sample_n(x, size = 2570, replace = TRUE)
    set.seed(i)
    in_train_para <- sample(nrow(para),
                            size = as.integer(nrow(para) * 0.8),
                            replace = FALSE)
    Train <- para[in_train_para, ]
    Test <- para[-in_train_para, ]
    rm(in_train_para)
    rm(Test)
    set.seed(i)
    model <- ranger::ranger(pIC50~., data = Train, importance = 'impurity',
                                  write.forest = TRUE, save.memory = TRUE)
    rm(Train)
    importance <- model$variable.importance
    results[[i]] <- importance
  }
  return(results)
  stopCluster(cl)
}
```

Generating the plot of feature importance

```
input <- readRDS(file = "data.Rds")
SubStructure_fingerPrintCount <- input$Substructure_fingerPrintCount
set.seed(10)
results_feature_importance_RF <- randomForest_feature_importance(SubStructure_fingerPrintCount)
data1 <- data.frame(results_feature_importance_RF)
data1 <- cbind(features = rownames(data1), data1)
library(reshape2)
data_melt <- suppressWarnings(melt(data1, id.vars = "features"))
#data_melt <- melt(data1, id.vars = "features")
```

```r
data_melt$features <- factor(data_melt$features)
library(ggplot2)
set.seed(1)
plot_feature <- ggplot(data_melt, aes(x = reorder(features, value, FUN = median), y = value)) +
  geom_boxplot(fill = "#F8766D", colour = "black", alpha = 0.5) +
  theme_bw() + xlab("") + ylab("Gini Index") + coord_flip() + theme(
    axis.text.y = element_text(size = 20, colour = "black"),
    axis.text.x = element_text(size = 20, colour = "black"),
    #axis.title.x = element_blank(),
    plot.margin = unit(c(1, 1, 1, 1), "cm"),
    panel.border = element_rect(linetype = "solid", colour = "black", fill = NA, size = 1),
    axis.title = element_text(size = 25, face = "bold", colour = "black")
  )

plot_feature
```


SubFPC2
SubFPC302
SubFPC274
SubFPC295
SubFPC32
SubFPC275
SubFPC3
SubFPC1
SubFPC181
SubFPC26
SubFPC153
SubFPC137
SubFPC88
SubFPC18
SubFPC298
SubFPC4
SubFPC135
SubFPC49
SubFPC100
SubFPC171
SubFPC5
SubFPC303
SubFPC182
SubFPC180
SubFPC28
SubFPC85
0
250
500
750
Gini Index