Pareto Interaction Ensemble (PIE) Machine via a Feasible Solution Algorithm (FSA)

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Hello!

- Assistant Professor and Biostatistician
  - Within a College of Nursing
- I teach PhD students in Nursing Research
  - Little background in math or stats
- I consult with Facutly, Students and Staff within CoN
  - I'll discuss more later
- I conduct my own research in statistical methodology
  - Contents of this talk

Previous Research

- The Feasible Solution Algorithm (FSA) (Dissertation December 2017)
- R package rFSA (released in Jan 2018)
- rFSA R Journal Paper (Published December 2018)

Current Research: Big Data in Health Outcomes

- Working on problems in big data for health outcomes
- PI NIH R03 and R21 submissions to NIDA, NINR, and NICHD (currently under review)
- Applying FSA to identify subgroup specific effects in big data. These include
  - Maternal Morbidity (CSL data)
  - Outcomes of Children Prenatally Exposed to Opioids (MIDH data)
  - Telomere Length (CARDIA data)

Current Research: Biostatistics Methodology 😄

- Improving the FSA
- Using FSA for estimating pareto optimal regression models
- Pareto Interaction Ensemble (PIE) Machine ☕

The Feasible Solution Algorithm

- First introduced by Dr. Doug Hawkins (University of Minnesota) in 1993 paper "The feasible set algorithm for least median of squares regression".
- In 2015, Dr. Arnold Stromberg and I developed the current implementation of the algorithm for subset selection and interaction identification. The R package *rFSA* implements our algorithm in R.
- For m=2
- (Form 1) Subsets: $Y \sim \beta_0 + \beta_1 X_A + \beta_2 X_B$
- (Form 2) Interactions: $Y \sim \beta_0 + \beta_1 X_A + \beta_2 X_B + \beta_3 X_A X_B$

The Feasible Solution Algorithm

1. Randomly select m variables to compose either Form 1 or Form 2, and compute the objective function of choice.
2. Under each possible exchange of one of the m variables in the working model for a variable not contained in the model, compute the new value of the objective function.
3. Make the single exchange of variables from Step 2 that most improves the objective function.
4. Continue making exchanges until no single additional exchange improves the objective function. The variables composing the final model constitute a single feasible solution.
5. Return to (1) to search for another feasible solution.

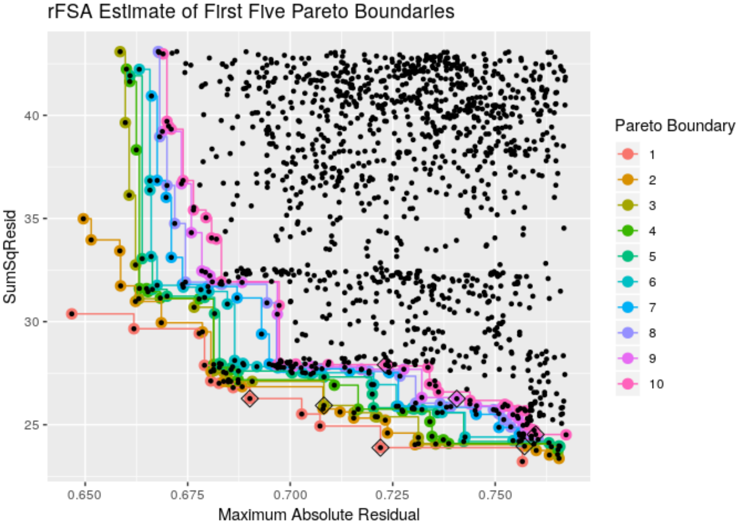
The Feasible Solution Algorithm

- How does it do?
- See Lambert rFSA R Journal paper 2018 (9000 downloads)
  - Fast, Flexible, » Interactions
- Featured in Kuhn and Johnson's 2019 book "Feature Engineering and Selection: A Practical Approach for Predictive Models"
- Properties of FSA in 2019 book "Modern Statistical Methods for Spatial and Multivariate Data" Dr. Norou Diawara
  - "Properties of the Number of Iterations of a Feasible Solutions Algorithm" by Janse and Thompson 2019
  - Determine the number of iterations of FSA needed to obtain the statistically optimal solution of an m-way interaction model with a certain probability (lower bound)
  - A lower bound on the probability of identifying optimal model in cp random starts is $1 - e^{-cm^2}$ where $0 < c < 1$.

Pareto Optimality

- During the process of model selection statisticians are often concerned with the model which has the single most optimal criterion (eg. AIC, R^2) before continuing to check several other diagnostics.
- This strategy is multi-objective in nature but single-objective in its numeric execution.
- Jin and Sendhoff, 2008 "Pareto-Based Multiobjective Machine Learning: An Overview and Case Studies"

Pareto Optimality: A Picture



Pareto Optimality: Great, but isn't this hard to estimate?

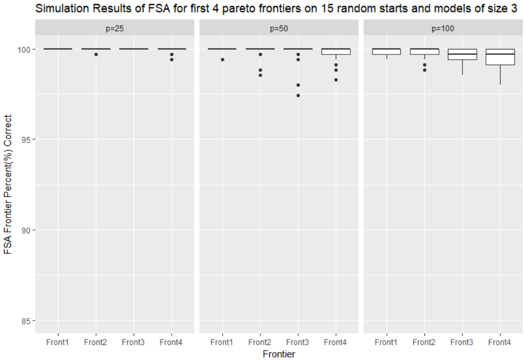
- Yes! Obtaining the the set of Pareto-optimal solutions and the frontiers is increasingly difficult as the number of solutions and criterion grow.
- Exhaustively searching will be difficult. For p variables, c criteria, identifying subsets of size m would require $choose(p, m)$ model checks and $choose(p, m) * c$ criteria checks.
- Sinha et. al. in "A Multiobjective Exploratory Procedure for Regression Model Selection" suggest a proceedure when the criteria are subset size, and one other model fit criteria (AIC, R^2).
  - not flexible

FSA and Pareto Optimality

- Given that FSA can identify *feasible solutions*, could we use it to estimate the pareto frontiers while remaining flexible to the criteria and regression strategy?
- Idea of FSA for Pareto Optimality:
  - Start with $1 \ldots c$ criteia
  - Use FSA to store models considered along the way to feasible solutions for criterion 1
  - Repeate this until completed for all c criteria.
  - At the end you will have a list of models considered by FSA along the path to the feasible solutions for criterion $1, \ldots, c$.
  - Calculate all criteria for all models considered.
  - Use this list as our estimate for Pareto Frontiers

FSA and Pareto Optimality

- How does this do? Under review at International Journal of Data Science and Analytics



Ensemble Learning

- Can we select a set of predictive models so that their “stacked”" performance is better then what we could have gotten from the single best model?
- We would like to be able to select a variety of models for our ensemble which predict different subsets of the data. Are the models predictions uncorrelated?
- When the uncorrelated models’ predictions are put together via a “Stacking” algorithm to predict the response will we get a good predictor?

Do you want to build an ensemble ☃?

- Can we use FSA to identify pareto optimal solutions along with a simple stacking algorithm to predict? Could it:
  - Compete with other machine learning techniques (RF, SVM, GBM, NN)?
  - Maintain high accuracy accross 2 or more criteria?
  - Interpretable?

Pareto Interaction Ensemble (PIE) Machine

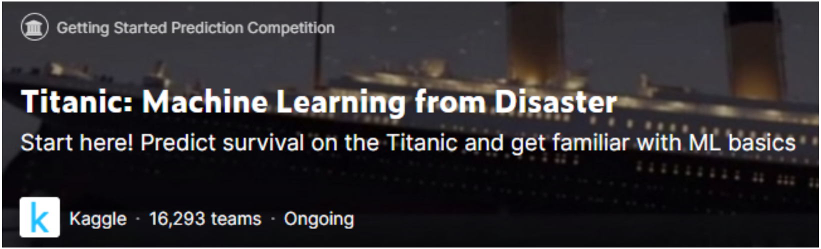
Concept of PIE Machine

- FSA can identify interactions
- FSA can also estimate interactions which are pareto optimal
- Can we use FSA to select a finite set of simple 2-way interaction models that predict different aspects of an outcome?
  - $Y \sim \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2$
- Then use a classification and regresison tree to combine these predictions in an interpeatable way?
- Where will we find a dataset to predict with and a community of data scientist to compete with?

Kaggle! Kaggle is a place to ...

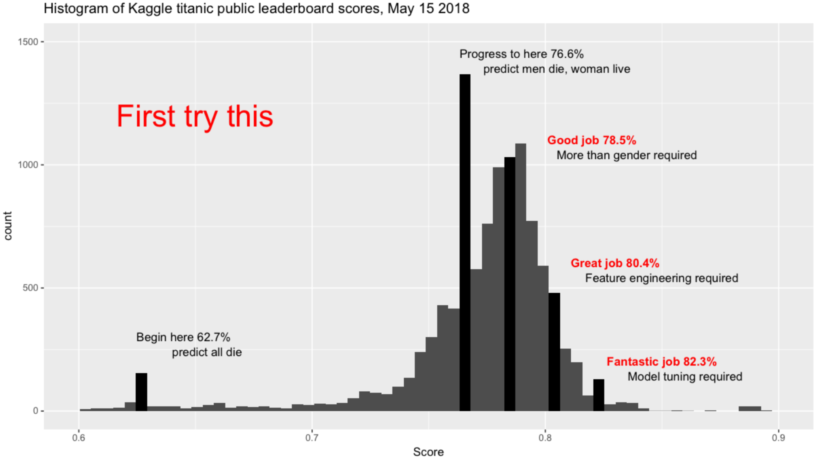
- learn, challenge, and improve data science, statistics, and computer science skillz.
- access numerous:
  - datasets
  - code
  - data scientists
- get answers
- drum up new ideas
- make money (??)

Kaggle: Titanic Challenge



- Your score is the percentage of passengers you correctly predict (Surivived, or Deceased).
- Challenge offers nice sandbox for testing new ML algorithms.

Kaggle: Cheaters of Titanic Proportions



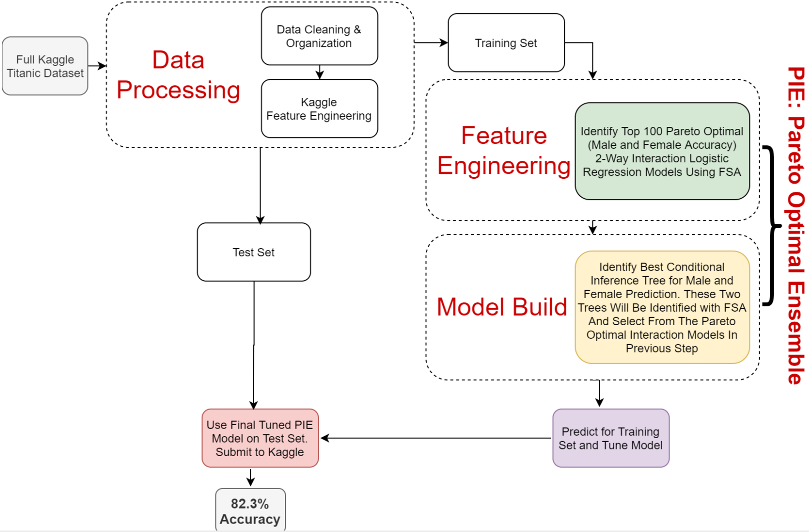
Motivation of a New ML Approach and Titanic Data

- RF model (ranger package in R) with 500 trees for Titanic Data
  - Training accuracy is 78.9% for Females
  - Training Accuracy is 83.7% for Males
- We would prefer a model that predicts well for both Females and Males.
- Also, it is difficult to tease out exactly why it is making this mistake.
- Real World Example: Recently Reuters reported that Amazon has been trying to develop a tool to automate resume screening and hiring. The project had to be scrapped because it showed a heavy prejudice against women. cite

Summary of PIE strategy for Titanic

- Predict Survival
- Want: model accurate predictions for males and females (pareto optimal)
- Use FSA to identify interactions which are estaimted to be pareto optimal
- Use FSA to select a finite (# of models < 5) set of which when used in a tree predict the response well in the training set. (We will call this PIE machine)
- Apply test set to PIE machine and submit findings to Kaggle. Hope it competes with other machine learning methods.

PIE & Kaggle Workflow



PIE in R with rFSA: Setup

Kudos to @reisel https://www.kaggle.com/reisel/imputation-and-feature-engineering/data for the feature engineering and data cleaning. Please see their kaggle RMD at the link for more info on how they engineered the dataset.

PIE in R with rFSA: Setup Code

```r
passenger<-read.csv("data/passenger.csv")

#assigning categorical variables as factors
passenger$Survived<-as.factor(passenger$Survived)
passenger$Pclass<-as.factor(passenger$Pclass)
passenger$SpouseSurvivedDiff<-as.factor(passenger$SpouseSurvivedDiff)
passenger$SiblingSurvivedDiff<-as.factor(passenger$SiblingSurvivedDiff)
passenger$ChildrenSurvivedDiff<-as.factor(passenger$ChildrenSurvivedDiff)
passenger$ParentsSurvivedDiff<-as.factor(passenger$ParentsSurvivedDiff)
passenger$FatherSurvivedDiff<-as.factor(passenger$FatherSurvivedDiff)
passenger$MotherSurvivedDiff<-as.factor(passenger$MotherSurvivedDiff)
passenger$RelativesSurvivedDiff<-as.factor(passenger$RelativesSurvivedDiff)
passenger$SameTicketNumber<-as.factor(passenger$SameTicketNumber)
passenger$HasAge<-as.factor(passenger$HasAge)
passenger$HasCabin<-as.factor(passenger$HasCabin)
passenger$Deck<-as.factor(passenger$Deck)
passenger$CabinSide<-as.factor(passenger$CabinSide)

#There aren't many Dr or Rev, so lets set them to RareTitle and refactor
passenger$Title[which(passenger$Title=="Dr")]<-"RareTitle"
passenger$Title[which(passenger$Title=="Rev")]<-"RareTitle"
passenger$Title<-factor(passenger$Title)

train<-passenger[passenger$DataSet=="Training",-1]
test<-passenger[passenger$DataSet=="Test",-1]
```

PIE in R with rFSA: Overview of Variables

```
#variables we'd like to use for predictions (note: this doesn't include all variables available)
vars<-c("Survived","Pclass","Sex","Age","SibSp",
        "Parch","Fare","Embarked","Title",
        "SpouseNumber","SpouseSurvivedDiff",
        "SiblingNumber","SiblingSurvivedDiff",
        "ChildrenNumber","ParentsNumber",
        "ChildrenSurvivedDiff","ParentsSurvivedDiff",
        "FatherSurvivedDiff","FatherNumber",
        "MotherSurvivedDiff","MotherNumber",
        "RelativesSurvivedDiff","SameTicketNumber",
        "FamilySize","FarePerPerson","HasAge",
        "HasCabin","Deck","CabinSide"
        #,"SiblingAgeMin","SiblingAgeMax","SiblingAgeMean",
        #"ParentAgeMin","ParentAgeMax","ParentAgeMean",
        #"ChildrenAgeMin","ChildrenAgeMax","ChildrenAgeMean",
        #"SameTicketAgeMin","SameTicketAgeMax","SameTicketAgeMean","SpouseAge"
        )
```

PIE in R with rFSA: Required Libraries

```r
library(rFSA)
library(ggplot2)
library(rPref)
library(partykit)
```

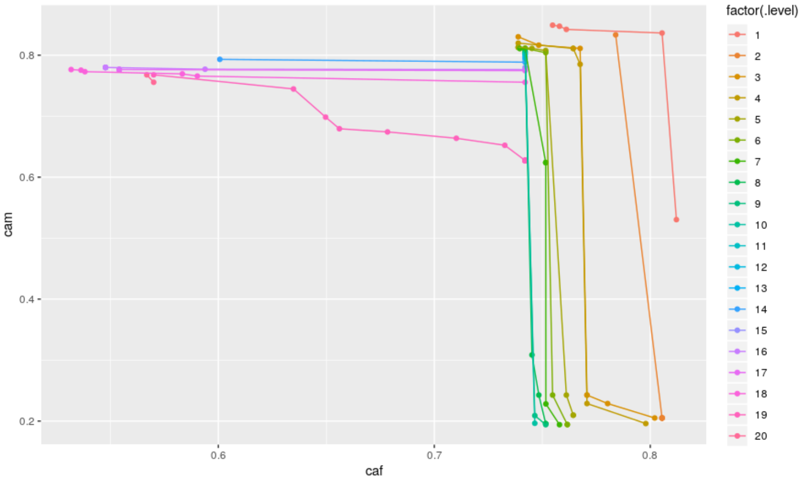
PIE in R with rFSA: FSA code

```
caf<-function(model){
  if(!typeof(model)=="list"|any(is.na(model$coefficients))){return(0)}
  tab<-table(factor(round(as.numeric(predict(model,type="response",newdata = train)>0.35)),levels = c(0,1)
  sum(diag(tab[,,"female"]))/sum(tab[,,"female"])
}

cam<-function(model){
  if(!typeof(model)=="list"|any(is.na(model$coefficients))){return(0)}
  tab<-table(factor(round(as.numeric(predict(model,type="response",newdata = train)>0.35)),levels = c(0,1)

  sum(diag(tab[,,"male"]))/sum(tab[,,"male"])
}

start<-Sys.time()
sln <- pFSA(formula =  "Survived~1", data = train[,vars], m = 2,fitfunc = glm, family="binomial", criteri
end<-Sys.time()
end-start
```

PIE in R with rFSA: make predictions using pareto models

- Left out some code here. Check github if you are interested in the code to do this.
- Select top 100 models that are pareto optimal. Turns out to estimated the first approx 20 pareto boundaries.

PIE in R with rFSA: ploting the estimates of the pareto boundary



PIE in R with rFSA: Putting it together CART

```
cam.tree<-function(tree){
  if(is.null(tree)){return(0)}
  tab<-table(predict(tree,type="response"),train[,"Survived"], train[,"Sex"])
  sum(diag(tab[,,"male"]))/sum(tab[,,"male"])
}

caf.tree<-function(tree){
  if(is.null(tree)){return(0)}
  tab<-table(predict(tree,type="response"),train[,"Survived"], train[,"Sex"])
  sum(diag(tab[,,"female"]))/sum(tab[,,"female"])
}

ctree2<-function(formula,data){
  ctree(formula,data,control = ctree_control(minsplit = 10, minbucket = 5, maxdepth = 4))
}

tree_fsa_2way<-FSA(formula = Survived~.,data = pred_mat,fitfunc = ctree2,
              fixvar = NULL, quad = FALSE,
              m = 3, numrs = 40, cores = 40, interactions = FALSE,
              criterion = c(caf.tree, cam.tree), minmax = c('max', 'max'),checkfeas = NULL,var4int = NULL
              )

tree_fsa_2way$table[which.max(tree_fsa_2way$table$criterion.1),]$formula #female
tree_fsa_2way$table[which.max(tree_fsa_2way$table$criterion.2),]$formula #male

tree.male<-ctree(formula = Survived~SibSp_Title+Embarked_Title+Age_CabinSide,data = pred_mat,control = ctr
tree.female<-ctree(formula = Survived~Age_Title+Sex_FarePerPerson+Pclass_Fare,data=pred_mat,control = ctre
cam.tree(tree.male)
caf.tree(tree.female)
```

PIE in R with rFSA: make predictions

```
pred_mat_test$Sex<-test$Sex
male_pred<-predict(object = tree.male, type="response", newdata=pred_mat_test[pred_mat_test$Sex=="male",])

female_pred<-predict(object = tree.female, type="response", newdata=pred_mat_test[pred_mat_test$Sex=="fema
table(male_pred)
table(female_pred)

pred_mat_test$pred<-NA
pred_mat_test[pred_mat_test$Sex=="male",]$pred<-male_pred
pred_mat_test[pred_mat_test$Sex=="female",]$pred<-female_pred
pred_mat_test$pred<-pred_mat_test$pred-1
table(pred_mat_test$pred,pred_mat_test$Sex)


pie_results<-cbind(test$PassengerId,pred_mat_test$pred)
colnames(pie_results)<-c("PassengerId","Survived")
table(pie_results[,2])
write.csv(pie_results,file = "PIEmachineMaleFemale.csv",row.names = FALSE)
```

PIE in R with rFSA: Upload to Kaggle

PIE in R with rFSA: Shiny App for Titanic Example

- App code is on Github page. Need *library(shiny)* to run.
- Run App Now!

Summary

- Used FSA to find models with 2-way interactions.
- Used FSA to estimate the parto boundaries for models that have high female and male accuracy.
- Used FSA to pick the best 3 models to use in a CART model for final ensemble prediction.
- We called all this PIE. Why would we want to use PIE?
  - Have a model which performs well on mulitple critiera
  - Interpretable model
  - Similar performance to other ML results on Kaggle. Top 4%.
- This is in pre-alpha stages. So user beware on other datasets.
- Working on paper now, should be submitted soon(ish).

Thank you!

- https://github.com/joshuawlambert/PIEtalk
- Remember: "All models are wrong, but some are useful -Dr. George Box".