Tree-based Alternatives to Generalized Linear Models

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Introduction

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  - The roles of individual predictors are clearly understood
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  - The roles of individual predictors are clearly understood
  - The models can be used for statistical inference
- These models can be poorly suited for applications with a high degree of interaction between predictors, or a high degree of non-linearity

Well Switching

At the end of Lab #9, you saw an application involving households in Bangladesh switching from high arsenic wells to safer ones:

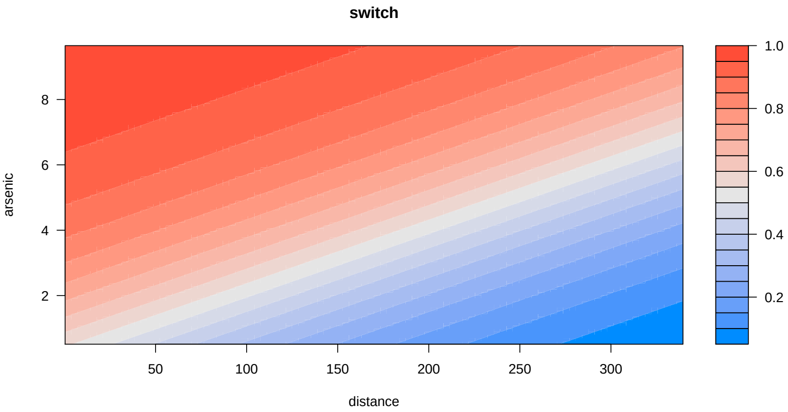
Well Switching - Logistic Regression

Looking at the logistic regression model: `switch ~ distance + arsenic`, how do these predictors influence the likelihood of switching?

```
##
## Call:
## glm(formula = switch ~ distance + arsenic, family = "binomial",
##     data = Wells)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -2.6351  -1.2139   0.7786   1.0702   1.7085
##
## Coefficients:
##              Estimate Std. Error z value Pr(>|z|)
## (Intercept)  0.002749   0.079448   0.035    0.972
## distance    -0.008966   0.001043  -8.593   <2e-16 ***
## arsenic      0.460775   0.041385  11.134   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##     Null deviance: 4118.1  on 3019  degrees of freedom
## Residual deviance: 3930.7  on 3017  degrees of freedom
## AIC: 3936.7
##
## Number of Fisher Scoring iterations: 4
```

Well Switching - Logistic Regression (Visualization)

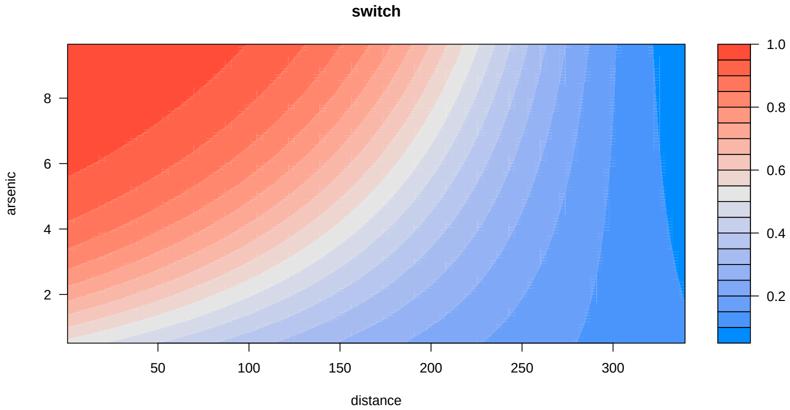
```r
library(visreg)
m <- glm(switch ~ distance + arsenic, data = Wells, family = "binomial")
visreg2d(m, xvar = "distance", yvar = "arsenic", scale = "response")
```



Interactions

However, perhaps there's an interaction between these two variables? How can we determine if this interaction is real?

```r
m <- glm(switch ~ distance*arsenic, data = Wells, family = "binomial")
visreg2d(m, xvar = "distance", yvar = "arsenic", scale = "response")
```



Interactions

A likelihood ratio test provides borderline statistical evidence of an interaction…

```r
library(lmtest)
m1 <- glm(switch ~ distance + arsenic, data = Wells, family = "binomial")
m2 <- glm(switch ~ distance*arsenic, data = Wells, family = "binomial")
lrtest(m1, m2)
```

```
## Likelihood ratio test
##
## Model 1: switch ~ distance + arsenic
## Model 2: switch ~ distance * arsenic
##   #Df  LogLik Df  Chisq Pr(>Chisq)
## 1   3 -1965.3
## 2   4 -1963.8  1 3.0399    0.08124 .
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Alternatives to Logistic Regression

- In some circumstances, it might make sense to change the modeling approach rather than include numerous interactions in a logistic regression model
  - Logistic regression coefficients can already be difficult to interpret, and interactions will make interpreting the model even more complicated

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- In some circumstances, it might make sense to change the modeling approach rather than include numerous interactions in a logistic regression model
  - Logistic regression coefficients can already be difficult to interpret, and interactions will make interpreting the model even more complicated
- Classification and Regression Trees (CART) are a type of *non-parametric* model that are well-suited for applications involving many interactive features
  - As you'll soon see, CART models are easily interpreted (even while including numerous interactions between features)

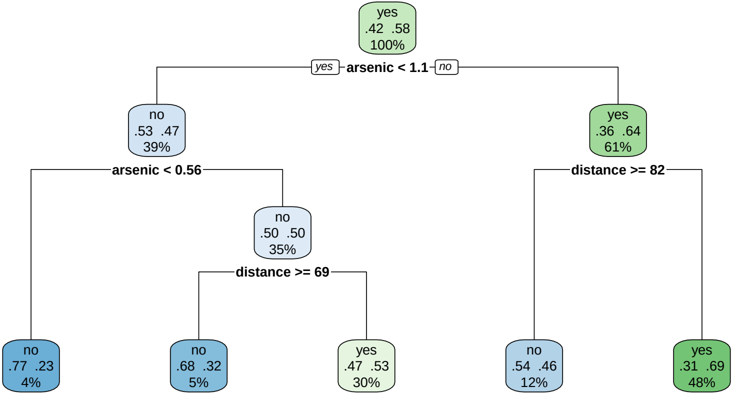
The CART Algorithm

The CART algorithm relies on a procedure known as *recursive binary splitting*:

1) Starting with a "parent" node, search for a splitting rule that maximizes the *homogeneity* or *purity* of the "child" nodes
2) Next, considering each node that hasn't yet been split, find another splitting rule that maximizes *purity*
3) Repeat until a stopping criteria has been reached

Example - CART

```r
library(rpart)
library(rpart.plot)
mytree <- rpart(switch ~ distance + arsenic, data = Wells)
rpart.plot(mytree, extra = 104)
```



How are Splits Determined?

- The CART algorithm works to split parent nodes into child nodes that are as homogeneous (or "pure") as possible
- There are dozens of ways to measure *purity*, but a couple popular ones are:
  - *Gini Index*: a criteria based upon the binomial variance, $p * (1 - p)$ - nodes that are more "pure" have less variance
  - *Information Gain*: A more sophisticated theoretical construct that compares the divergence of two probability distributions

Additional information:

- More on CART splits: http://pages.stat.wisc.edu/~loh/treeprogs/guide/wires11.pdf
- More on Information Gain: https://en.wikipedia.org/wiki/Information_gain_in_decision_trees

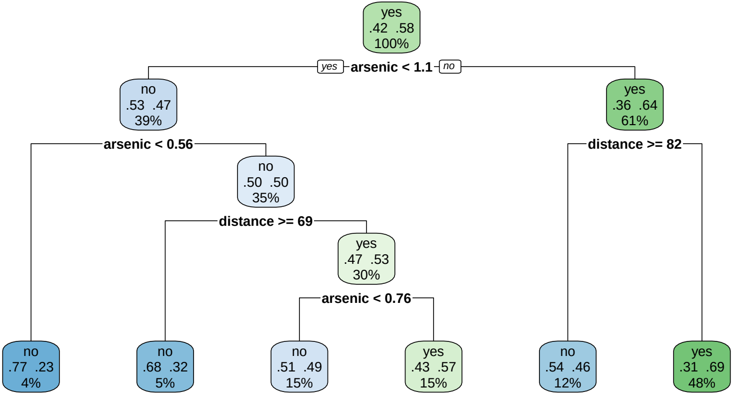
When does Splitting Stop?

There are two factors which determine when the CART algorithm terminates:

1) The *complexity parameter*, *cp*, a minimum factor improvement in the purity measure that most be achieved in order for a split to be considered "worthwhile" (1% by default in `rpart()`)
2) The *minimum node size*, the minimum number of data-points that must belong to a node for it to be deemed eligible for splitting (20 by default in `rpart()`)

Tuning the CART Algorithm

```
mytree <- rpart(switch ~ distance + arsenic, data = Wells,
                control = rpart.control(cp = 0.008, minsplit = 100))
rpart.plot(mytree, extra = 104)
```



Comments on Splitting/Tuning

- In the previous example, notice our new tree is merely our first tree with one additional split
  - This is not a coincidence, the CART algorithm is greedy
- An implication is that we can always go from a larger CART model to a smaller one by ignoring splits that are beneath a certain depth
  - This idea is called "pruning", and is discussed in greater detail in this week's lab
  - Pruning is unique to CART models, we couldn't do the same thing in logistic regression

Can CART Outperform Logistic Regression?

- In our well switching application, how might we determine whether our CART model is better than a logistic regression model?
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  - Can we use a model selection criterion like AIC or BIC? No, the CART model doesn't involve a likelihood.
  - Can we compare performance summaries like classification accuracy, Cohen's kappa, or AUC? Yes, but we should be careful not to reward overfitting the sample data

Comparison Using Cross-Validation

```r
### Setup
set.seed(123)
fold_id <- sample(rep(1:5, length.out = nrow(Wells)), size = nrow(Wells))
preds1 <- preds2 <- preds3 <- preds4 <- numeric(nrow(Wells))

## Loop across CV folds
for(k in 1:5){

  ## Subset the data
  train <- Wells[fold_id != k, ]
  test <- Wells[fold_id == k, ]

  ## Fit models on the data
  m1 <- glm(switch ~ arsenic*distance, data = train, family = "binomial")
  m2 <- glm(switch ~ arsenic + distance, data = train, family = "binomial")
  m3 <- rpart(switch ~ distance + arsenic, data = train)
  m4 <- rpart(switch ~ distance + arsenic, data = train,
              control = rpart.control(cp = 0.008, minsplit = 100))

  ## Store predictions
  preds1[fold_id == k] <- predict(m1, newdata = test, type = "response")
  preds2[fold_id == k] <- predict(m2, newdata = test, type = "response")
  preds3[fold_id == k] <- predict(m3, newdata = test, type = "prob")[,2]
  preds4[fold_id == k] <- predict(m4, newdata = test, type = "prob")[,2]
}
```

Comparison Using Cross-Validation (continued)

Unfortunately both of our CART models have lower *out-of-sample* accuracy than either logistic regression model

```
## Out-of-sample accuracy
pred_class1 <- ifelse(preds1 >= .5, "yes", "no")
out_acc1 <- sum(pred_class1 == Wells$switch)/nrow(Wells)
pred_class2 <- ifelse(preds2 >= .5, "yes", "no")
out_acc2 <- sum(pred_class2 == Wells$switch)/nrow(Wells)
pred_class3 <- ifelse(preds3 >= .5, "yes", "no")
out_acc3 <- sum(pred_class3 == Wells$switch)/nrow(Wells)
pred_class4 <- ifelse(preds4 >= .5, "yes", "no")
out_acc4 <- sum(pred_class4 == Wells$switch)/nrow(Wells)
c(out_acc1, out_acc2, out_acc3, out_acc4)
```

```
## [1] 0.6215232 0.6201987 0.6152318 0.6115894
```

In-sample Prediction?

It's worthwhile noting our the CART model *does* have higher *in-sample accuracy* than the logistic regression model with an interaction...

```
## Larger tree
mytree <- rpart(switch ~ distance + arsenic, data = Wells,
                control = rpart.control(cp = 0.008, minsplit = 100))
preds_tree <- predict(mytree, newdata = Wells, type = "prob")[,2]
preds_tree_class <- ifelse(preds_tree >= .5, "yes", "no")

## Larger Logistic Regression
lreg <- glm(switch ~ arsenic*distance, data = Wells, family = "binomial")
preds_lreg <- predict(lreg, newdata = Wells, type = "response")
preds_lreg_class <- ifelse(preds_lreg >= .5, "yes", "no")

## In-sample accuracy
c(sum(preds_tree_class == Wells$switch)/nrow(Wells),
  sum(preds_lreg_class == Wells$switch)/nrow(Wells))
```

```
## [1] 0.6307947 0.6241722
```

Pros and Cons of Tree-based Models

Pros:

- Work great on highly interactive data
- Doesn't require the user to specify a parametric model (or perform model selection)
- Easy to visualize and understand
- Easily generalized to nominal or numeric outcomes

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Cons:

- Tend to overfit the sample data, leading a greater disparity between in-sample and out-of-sample performance (we'll talk more about this next time)
- Effects of individual predictors aren't distinct

Additional Comments

- It isn't necessary to use CART as a "final model", the method used to help discover interactions or non-linear relationships
  - So, even if your application suggests using regression, trees are a useful an exploratory method

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- It isn't necessary to use CART as a "final model", the method used to help discover interactions or non-linear relationships
  - So, even if your application suggests using regression, trees are a useful an exploratory method
- Alternatively, even if logistic regression offers superior predictive performance, a CART model is sometimes still preferable due to its simplicity
  - It's much easier to explain a set of splitting rules to most non-statisticians than it is to explain log-odds or odds ratios