

Week 11: Binary Classification Decision Trees

Predicting Classes rather than Numeric Values

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Decision Trees

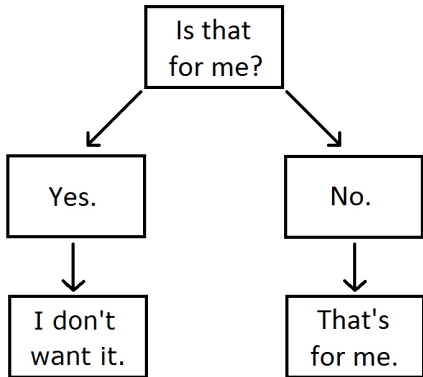


Decision Trees



Binary Classification Decision Trees

My Cat's Decision-Making Tree.



Statistical Inference

- Hypothesis Testing
 - One sample simulation p-values
 - Two sample permutation p-values
- Estimation
 - Bootstrap Confidence Intervals
- Prediction
 - Simple Linear Regression: real-valued outcome predictions with one predictor
 - Multivariate Linear Regression: real-valued outcome predictions with many predictors
 - **Classification**: class prediction with many predictors

Statistics and Data Science

Statistics: Inference

- Hypothesis Testing
- Estimation (Confidence Intervals)

Data Science: Machine Learning

- Prediction
 - Regression
 - Classification

- Hypothesis Testing and Estimation are both aspects of Simple Linear and Multivariate Regression
 - The same is true for a related Classification method called Logistic Regression
- Our Machine Learning (ML) focus is on the Decision Tree Classification
 - but there are many other ML Classification methods and also many ML Regression methods beyond Simple Linear and Multivariate Regression models from Statistics

Trouble Sleeping?

```
# https://cran.r-project.org/web/packages/NHANES/NHANES.pdf
# Random sample of n=2500 observations from the
# US National Health and Nutrition Examination Study (NHANES)
library(tidyverse); NHANES <- read_csv("NHANES_data.csv")
NHANES %>% select(Age, Race3, Work, DaysMentHlthBad, DaysPhysHlthBad,
                  Depressed, SleepHrsNight, SleepTrouble) %>% glimpse()

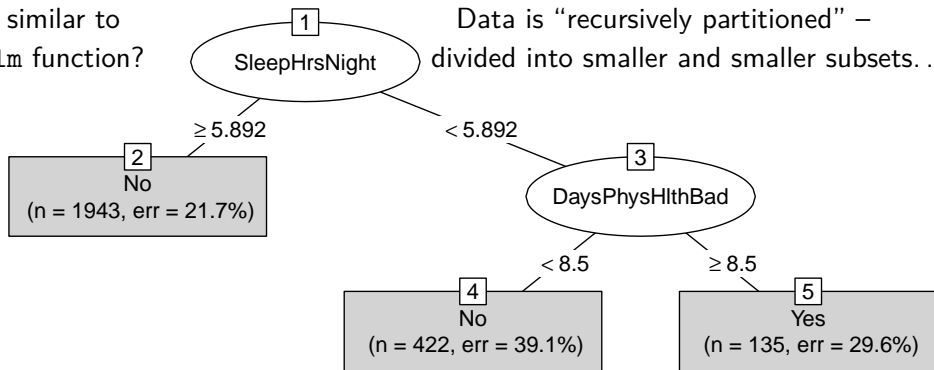
## Rows: 2,500
## Columns: 8
## $ Age          <dbl> 64, 32, 67, 43, 75, 21, 30, 79, 37, 60, 27, 45, 26, 47~
## $ Race3        <chr> "Hispanic", NA, NA, NA, "White", "Hispanic", "White", ~
## $ Work         <chr> "NotWorking", "Working", "Working", "NotWorking", "Not~
## $ DaysMentHlthBad <dbl> 0, 0, 0, 30, 0, 0, 2, 0, 30, 3, 4, 26, 3, 0, 30, 2, 30~
## $ DaysPhysHlthBad <dbl> 0, 0, 0, 21, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 10, 3~
## $ Depressed     <chr> "None", "None", "None", "Most", "None", "None", "None"~
## $ SleepHrsNight <dbl> 5.477751, 6.819995, 5.852940, 5.721259, 8.071489, 6.39~
## $ SleepTrouble  <chr> "Yes", "No", "No", "Yes", "Yes", "No", "Yes", "No", "N~
```

Who reports sleep trouble?

```
library(rpart) #install.packages("rpart") # for the `rpart()` function
tree <- rpart(SleepTrouble ~ SleepHrsNight + DaysPhysHlthBad, data=NHANES)
library(partykit) #install.packages("partykit") for `as.party()` & `plot()`
plot(as.party(tree), gp=gpar(cex=1), type="simple")
```

Very similar to
the `lm` function?

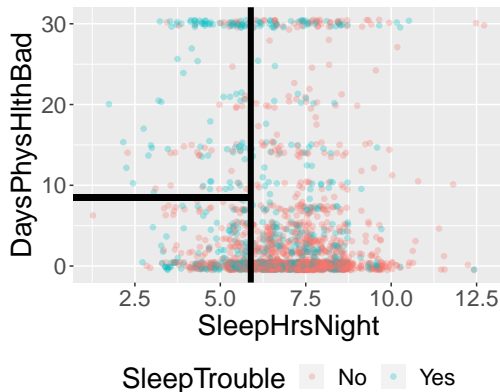
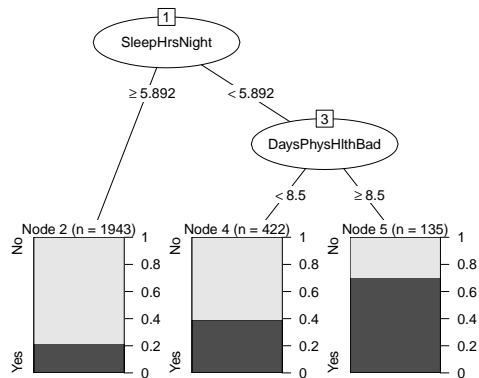
Data is “recursively partitioned” –
divided into smaller and smaller subsets...



Geometric Interpretation

Data is "recursively partitioned"

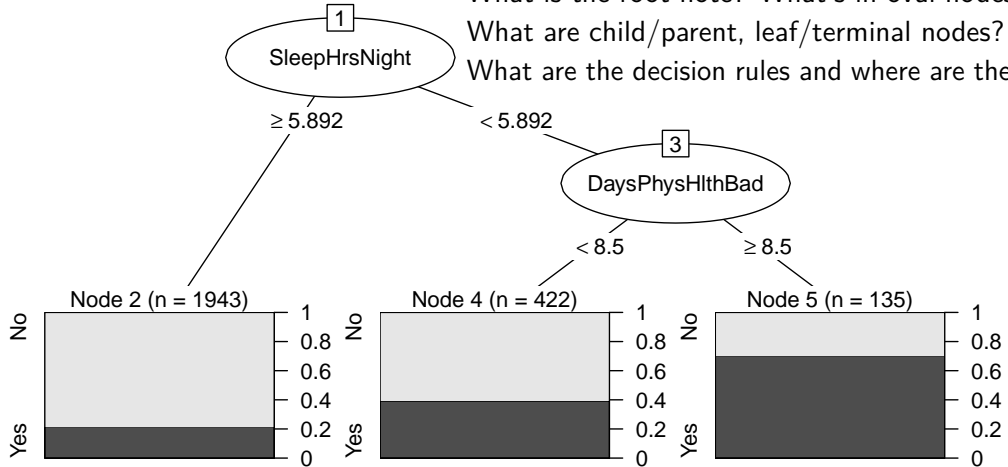
Divided into smaller and smaller subsets...



Who reports sleep trouble?

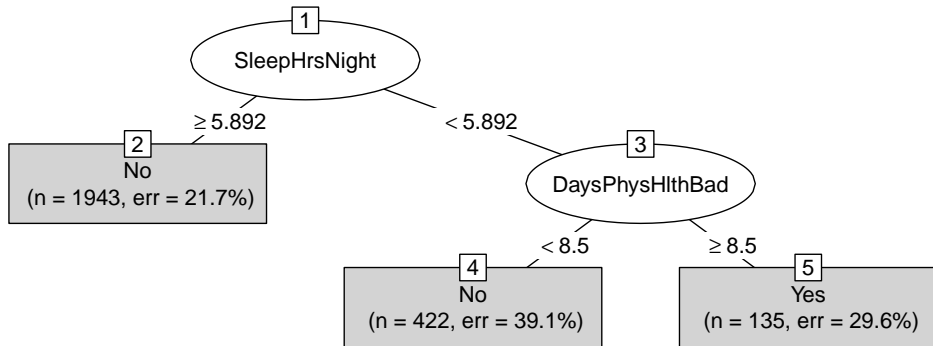
```
plot(as.party(tree), type="extended")
```

What is the root node? What's in oval nodes?
What are child/parent, leaf/terminal nodes?
What are the decision rules and where are they?



How do you use a decision tree?

```
plot(as.party(tree), gp=gpar(cex=1), type="simple")
```

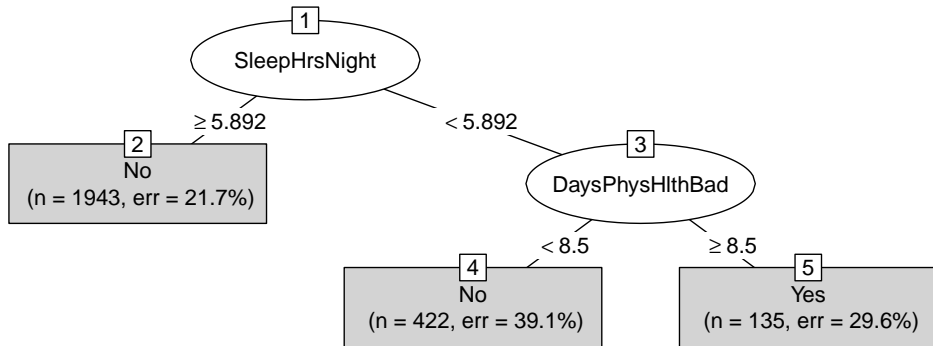


Does someone have trouble sleeping if

- they typically get 5.2 hours of sleep on weeknights ? (**and**)
- report having 4 days of poor physical health over the past month ?

What kind of things could be different here?

```
plot(as.party(tree), gp=gpar(cex=1), type="simple")
```



Does someone have trouble sleeping if

- they typically get 5.2 hours of sleep on weeknights ? (**and**)
- report having 4 days of poor physical health over the past month ?

What kind of things could be different here?

Nonstandard Binary Classification Decision Trees?

- Why are there two branches only?
 - Why are decision rules only a single cutoff?
 - Why are decision rules based on one variable only?
 - Are “composite” decision rules possible?
- How would we use a nonbinary categorical variable?

```
MaritalStatus <-  
  as.factor(NHANES$MaritalStatus)  
  
MaritalStatus2 <-  
  as.numeric(MaritalStatus)  
  
tibble(level_text=MaritalStatus,  
        level_numeric=MaritalStatus2) %>%  
  unique() %>% arrange(level_numeric)
```

```
## # A tibble: 6 x 2  
##   level_text    level_numeric  
##   <fct>          <dbl>  
## 1 Divorced             1  
## 2 LivePartner          2  
## 3 Married              3  
## 4 NeverMarried         4  
## 5 Separated            5  
## 6 Widowed             6
```

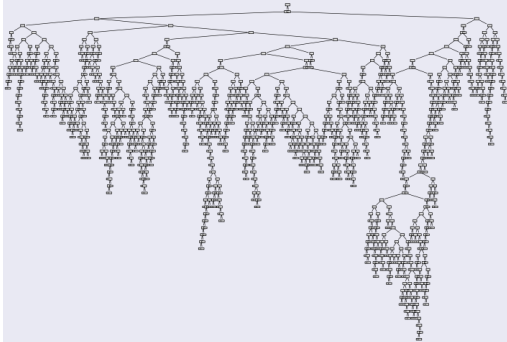
How are decision trees constructed?

- 1 All possible **variables** and all their possible **decision rules** are considered
 - Each **variable** and **decision rule** creates two new child nodes
- 2 All **variable** and **decision rule** violating **stopping rules** are discarded
 - node must be large enough to split, resulting nodes must be large enough
 - maximum tree depth, and maximum node count must not be exceeded
- 3 Of those remaining, the **variable** and **decision rule** producing the lowest *entropy/gini impurity* nodes is selected (for possible addition into the tree)
 - $\text{entropy}(p) = -p \log(p) - (1 - p) \log(1 - p)$ • $\text{gini}(p) = 1 - p^2 - (1 - p)^2$
(*entropy* and *gini impurity* are highest if $p = 0.5$ and lowest if $p = 1$ or $p = 0$)
- 4 A **variable** and **decision rule** giving “sufficient improvement” is added to the tree
 - The `cp` parameter in the `rpart()` function defines “sufficient improvement”:
 $\text{Error}(T) + \text{cp} \times \text{splits} \times \text{Error}(T_0)$ must improve (T_0 is the no splits tree)

Model complexity

Why are we so careful with deciding if a split should be added to a decision tree?

Why don't we just grow the tree as big as possible?



Decision trees too easily ***overfit*** the data...

“If *this* and *this* and *this* and *this* and ... are *true*, then conclude *this*...”

At some point we're just ***memorizing*** the data...

How are decision trees evaluated?

The outcome/response y_i (and hence \hat{y}_i) is re-coded as 0 (negative) or 1 (positive)

- \hat{y}_i either *predicts* or *does not predict* the positive event
- \hat{y}_i for “Do you have sleep trouble? Yes or No?” is 1 if “Yes” is predicted

- | | | |
|------------------------|---|---|
| 1. Accuracy: | $\frac{\sum_{i=1}^n 1_{y_i}(\hat{y}_i)}{\sum_{i=1}^n 1_{y_i}(\hat{y}_i) \times 1_1(\hat{y}_i)}$ | where $1_{y_i}(\hat{y}_i) = 1$ if $\hat{y}_i = y_i$ |
| 2. Precision: | $\frac{\sum_{i=1}^n \hat{y}_i}{\sum_{i=1}^n 1_{y_i}(\hat{y}_i) \times 1_1(\hat{y}_i)}$ | where $1_1(\hat{y}_i) = 1$ if $\hat{y}_i = 1$ |
| 3. Sensitivity/Recall: | $\frac{\sum_{i=1}^n y_i}{\sum_{i=1}^n 1_{y_i}(\hat{y}_i) \times 1_1(\hat{y}_i)}$ | |
| 4. Specificity: | $\frac{\sum_{i=1}^n 1_{y_i}(\hat{y}_i) \times 1_0(\hat{y}_i)}{\sum_{i=1}^n (1 - y_i)}$ | where $1_0(\hat{y}_i) = 1$ if $\hat{y}_i = 0$ |

For even more versions see: https://en.wikipedia.org/wiki/Sensitivity_and_specificity

What is the meaning of Accuracy, Precision, Sensitivity/Recall, and Specificity?

What do the expressions mean? $\sum_{i=1}^n y_i$, $\sum_{i=1}^n (1 - y_i)$, $\sum_{i=1}^n 1_{y_i}(\hat{y}_i) \times 1_1(\hat{y}_i)$, etc.?

How are decision trees evaluated?

The outcome/response y_i (and hence \hat{y}_i) is re-coded as 0 (negative) or 1 (positive)

- \hat{y}_i either *predicts* or *does not predict* the positive event
- \hat{y}_i for “Do you have sleep trouble? Yes or No?” is 1 if “Yes” is predicted

TP, TN, FP, FN, and Confusion Matrices – What are each of these things?

	$y_i = 0$	$y_i = 1$
$\hat{y}_i = 0$	n_{TN}	n_{FN}
$\hat{y}_i = 1$	n_{FP}	n_{TP}

	$y_i = 0$	$y_i = 1$
$\hat{y}_i = 0$	✓	×
$\hat{y}_i = 1$	×	✓

$$n = n_{TN} + n_{FN} + n_{FP} + n_{TP}$$

This is like *Type I* and *Type II* errors from the *Hypothesis Testing* context!

- What do FP, FN, TP, or TN predictions mean practically in different contexts?

How are decision trees evaluated?

The outcome/response y_i (and hence \hat{y}) is re-coded as 0 (negative) or 1 (positive)

- \hat{y}_i either *predicts* or *does not predict* the positive event
- \hat{y}_i for “Do you have sleep trouble? Yes or No?” is 1 if “Yes” is predicted

TP, TN, FP, FN, and Confusion Matrices – What are each of these things?

	$y_i = 0$	$y_i = 1$
$\hat{y}_i = 0$	n_{TN}	n_{FN}
$\hat{y}_i = 1$	n_{FP}	n_{TP}

$$n = n_{TN} + n_{FN} + n_{FP} + n_{TP}$$

$$1. \text{ Accuracy: } \frac{n_{TP} + n_{TN}}{n}$$

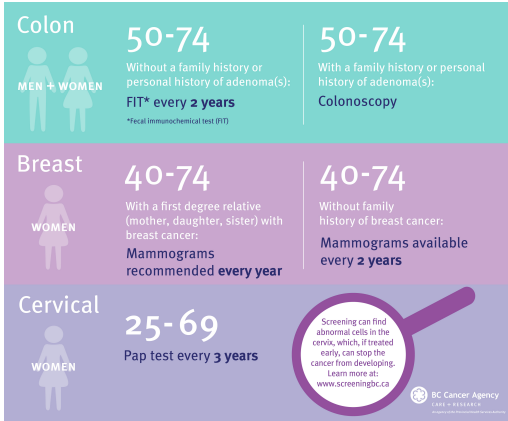
$$2. \text{ Precision: } \frac{n_{TP}}{n_{TP} + n_{FP}}$$

$$3. \text{ Sensitivity/Recall: } \frac{n_{TP}}{n_{TP} + n_{FN}}$$

$$4. \text{ Specificity: } \frac{n_{TN}}{n_{TN} + n_{FP}}$$

For more information see: https://en.wikipedia.org/wiki/Confusion_matrix#Example

What's Worse? FN or FP?



Is it more costly to wrongly ignore cancer (FN)?



Is it more costly to approve bad applicants (FP)?

What's Worse? FN or FP?

Sometimes it's not immediately clear which may be better or worse

Regarding self-quarantine, some questions

- Does FN meaningfully increase transmission?
- Does FP meaningfully decrease well-being?

Regarding hospitalization, some questions

- Does FN significantly worsen outcomes?
- Does FP prohibitively burden medical care?



This depends on the costs and benefits of the intervention/failure to intervene

What's Worse? FN or FP?

- **Sensitivity/Recall** is also called the **True Positive Rate (TPR)**
 - The **FALSE Negative Rate (FNR)** is $1 - \text{TPR}$
FNR tells you the proportion of negatives that are missed
- **Specificity** is also called the **True Negative Rate (TNR)**
 - The **FALSE Positive Rate (FPR)** is $1 - \text{TNR}$
FPR tells you the proportion of positives that are missed

For more information see: https://en.wikipedia.org/wiki/Confusion_matrix#Example

How are decision trees evaluated?

- 1 Decide what matters: accuracy, precision, sensitivity/recall, or specificity?

Accuracy is often a good choice, but not for some **class imbalance** contexts

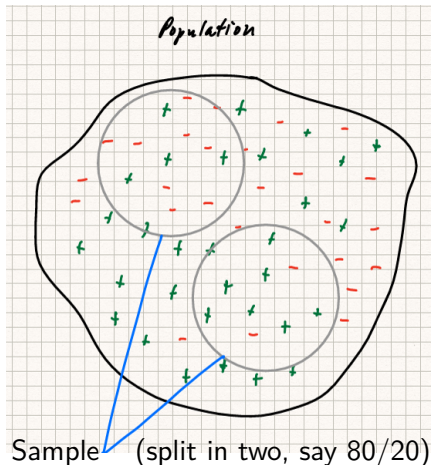
- If you care about FP but they're rare, then accuracy overemphasizes FN
 - If most predictions are negative, then most errors are FN, so FN drives accuracy...
- If you care about FN but they're rare, then accuracy overemphasizes FP
 - If most predictions are positive, then most errors are FP, so FP drives accuracy...

- 2 Use the 80-20 train-test split methodology to compare competing models

- Build the classification model with 80% of the data
- Score the predictions on the remaining 20% of the data
- This suggests how well a model will actually generalize and perform on new data

Review: The 80/20 Train-Test Split

- Classification is about doing something (predicting) in the sample
- *So you should try to see how well you can do that thing in the population...*



← **Here we split a "representative" population sample into two "representative" samples**

- 1 You fit the model based on a "representative" sample
- 2 So subsamples are "representative of the population"
- 3 Use 80% of the data to fit the "representative" model
- 4 Use 20% to see if the model's actually "representative"

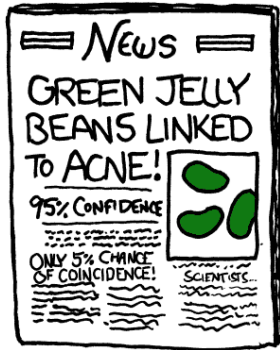
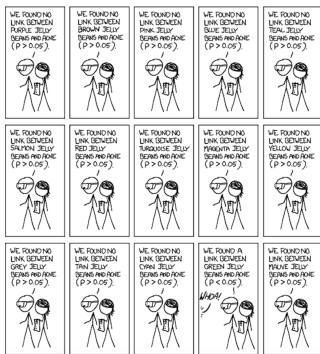
This strategy shows when the model for 80% of the data doesn't work well for the remaining 20% of the data, which could happen if

- The subsamples aren't 'representative' to start with
- The model is overly specific to 80% of the data

Review: The 80/20 Train-Test Split

Fit a model on 80% of the data → "score" the model on the remaining 20%

- The train-test method is a wonderful tool in LARGE data contexts
 - when there's enough data so the random train-test split isn't just "lucky"
- In its more advanced (data science) forms, train-test is a powerful model tuning tool

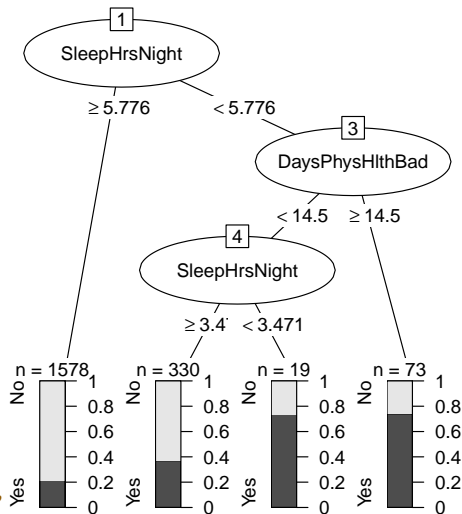


- Like Hypothesis Testing, it is subject to "random chance" (of the test-train split)
- Unlike Hypothesis Testing, it is based on observed out of sample generalizability, rather than tests based on modeling assumptions
- It's not about parameters or 'right' or 'wrong', but picking models predicting new data 'well'

Trouble Sleeping: 80-20 Train-Test Split

```
NHANES %>% rowid_to_column() ->  
  NHANES; n <- nrow(NHANES)  
set.seed(1002); train_ids <-  
  sample(1:n, size=round(0.8*n))  
train <- NHANES %>%  
  filter(rowid %in% train_ids)  
test <- NHANES %>%  
  filter(!(rowid %in% train_ids))
```

```
tree <- rpart(SleepTrouble ~  
  SleepHrsNight + DaysPhysHlthBad,  
  data=train)  
tree %>% as.party() %>%  
plot(type="extended", #gp=gpar(cex=0.8),  
  tp_args=list(id=FALSE))
```



Trouble Sleeping: Confusion Matrices

```
tree_train_pred <- predict(  
  tree, type="class")  
train_confusion_matrix <- table(  
  `y-hat`=tree_train_pred,  
  `observed y`=train$SleepTrouble)  
train_confusion_matrix
```

```
##           observed y  
## y-hat      No  Yes  
## No  1447  461  
## Yes   24   68
```

```
train_confusion_matrix/sum(  
  train_confusion_matrix)
```

```
##           observed y  
## y-hat      No  Yes  
## No  0.7235 0.2305  
## Yes 0.0120 0.0340
```

```
tree_test_pred <- predict(  
  tree, type="class", newdata=test)  
test_confusion_matrix <- table(  
  `y-hat`=tree_test_pred,  
  `observed y`=test$SleepTrouble)  
test_confusion_matrix
```

```
##           observed y  
## y-hat      No  Yes  
## No   339  133  
## Yes    9   19
```

```
test_confusion_matrix/sum(  
  test_confusion_matrix)
```

```
##           observed y  
## y-hat      No  Yes  
## No  0.678 0.266  
## Yes 0.018 0.038
```

Trouble Sleeping: Metrics (Accuracy, etc.)

```
n_TN <- train_confusion_matrix[1,1]
n_FN <- train_confusion_matrix[1,2]
n_FP <- train_confusion_matrix[2,1]
n_TP <- train_confusion_matrix[2,2]
# accuracy
(n_TP+n_TN)/sum(train_confusion_matrix)
```

```
## [1] 0.7575
```

```
# precision
(n_TP)/(n_TP+n_FP)
```

```
## [1] 0.7391304
```

```
# sensitivity/recall:  $TPR = 1-FNR$ 
(n_TP)/(n_TP+n_FN)
```

```
## [1] 0.1285444
```

```
# specificity:  $TNR = 1-FPR$ 
(n_TN)/(n_TN+n_FP)
```

```
## [1] 0.9836846
```

```
n_TN <- test_confusion_matrix[1,1]
n_FN <- test_confusion_matrix[1,2]
n_FP <- test_confusion_matrix[2,1]
n_TP <- test_confusion_matrix[2,2]
# accuracy
(n_TP+n_TN)/sum(test_confusion_matrix)
```

```
## [1] 0.716
```

```
# precision
(n_TP)/(n_TP+n_FP)
```

```
## [1] 0.6785714
```

```
# sensitivity/recall:  $TPR = 1-FNR$ 
(n_TP)/(n_TP+n_FN)
```

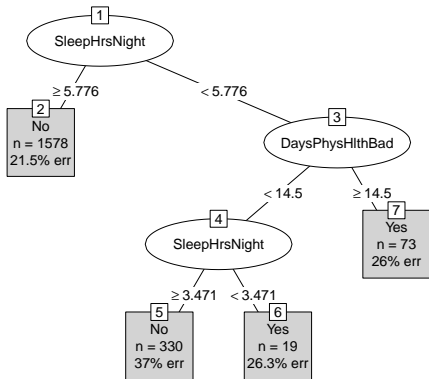
```
## [1] 0.125
```

```
# specificity:  $TNR = 1-FPR$ 
(n_TN)/(n_TN+n_FP)
```

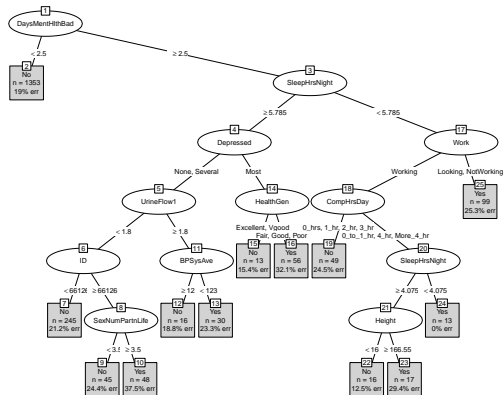
```
## [1] 0.9741379
```

Trouble Sleeping: Comparing Models

```
tree1 <- rpart(SleepTrouble~SleepHrsNight+DaysPhysHlthBad,
  data=train)
tree1 %>% as.party() %>% plot(type="simple",
  tp_args = list(FUN = function(info)
    list(format(info$prediction), format(paste("n =",info$n)),
      format(paste(round(info$err,1), "% err", sep="")))))
```



```
tree2 <- rpart(SleepTrouble ~ ., data=train)
tree2 %>% as.party() %>% plot(type="simple",
  ep_args = list(justmin=15),
  tp_args = list(FUN = function(info)
    list(format(info$prediction), format(paste("n =",info$n)),
      format(paste(round(info$err,1), "% err", sep="")))))
```



Trouble Sleeping: Comparing Models

Let's just compare the out of sample generalizability

```
tree1_test_pred <- predict(tree1,  
                           type="class",  
                           newdata=test)  
tree1_test_confusion_matrix <-  
  table(`y-hat`=tree1_test_pred,  
        `observed y`=test$SleepTrouble)  
n <- sum(tree1_test_confusion_matrix)  
tree1_test_confusion_matrix
```

```
##      observed y  
## y-hat  No Yes  
##   No  339 133  
##   Yes   9  19
```

```
# accuracy  
sum(diag(tree1_test_confusion_matrix))/n
```

```
## [1] 0.716
```

```
tree2_test_pred <- predict(tree2,  
                           type="class",  
                           newdata=test)  
tree2_test_confusion_matrix <-  
  table(`y-hat`=tree2_test_pred,  
        `observed y`=test$SleepTrouble)  
n <- sum(tree2_test_confusion_matrix)  
tree2_test_confusion_matrix
```

```
##      observed y  
## y-hat  No Yes  
##   No  320 116  
##   Yes  28  36
```

```
# accuracy  
sum(diag(tree2_test_confusion_matrix))/n
```

```
## [1] 0.712
```

Trouble Sleeping: Comparing Models

Let's just compare the out of sample generalizability

```
tree1_test_pred <- predict(tree1,  
                           type="class",  
                           newdata=test)  
tree1_test_confusion_matrix <-  
  table(`y-hat`=tree1_test_pred,  
        `observed y`=test$SleepTrouble)  
n <- sum(tree1_test_confusion_matrix)  
tree1_test_confusion_matrix/n
```

```
##      observed y  
## y-hat    No    Yes  
##   No  0.678 0.266  
##   Yes 0.018 0.038
```

```
# accuracy  
sum(diag(tree1_test_confusion_matrix))/n
```

```
## [1] 0.716
```

```
tree2_test_pred <- predict(tree2,  
                           type="class",  
                           newdata=test)  
tree2_test_confusion_matrix <-  
  table(`y-hat`=tree2_test_pred,  
        `observed y`=test$SleepTrouble)  
n <- sum(tree2_test_confusion_matrix)  
tree2_test_confusion_matrix/n
```

```
##      observed y  
## y-hat    No    Yes  
##   No  0.640 0.232  
##   Yes 0.056 0.072
```

```
# accuracy  
sum(diag(tree2_test_confusion_matrix))/n
```

```
## [1] 0.712
```

Trouble Sleeping: Comparing Models

```
n_TN <- tree1_test_confusion_matrix[1,1]
n_FN <- tree1_test_confusion_matrix[1,2]
n_FP <- tree1_test_confusion_matrix[2,1]
n_TP <- tree1_test_confusion_matrix[2,2]
# accuracy
(n_TP+n_TN)/sum(tree1_test_confusion_matrix)
```

```
## [1] 0.716
```

```
# precision
(n_TP)/(n_TP+n_FP)
```

```
## [1] 0.6785714
```

```
# sensitivity/recall: TPR = 1-FNR
(n_TP)/(n_TP+n_FN)
```

```
## [1] 0.125
```

```
# specificity: TNR = 1-FPR
(n_TN)/(n_TN+n_FP)
```

```
## [1] 0.9741379
```

```
n_TN <- tree2_test_confusion_matrix[1,1]
n_FN <- tree2_test_confusion_matrix[1,2]
n_FP <- tree2_test_confusion_matrix[2,1]
n_TP <- tree2_test_confusion_matrix[2,2]
# accuracy
(n_TP+n_TN)/sum(tree2_test_confusion_matrix)
```

```
## [1] 0.712
```

```
# precision
(n_TP)/(n_TP+n_FP)
```

```
## [1] 0.5625
```

```
# sensitivity/recall: TPR = 1-FNR
(n_TP)/(n_TP+n_FN)
```

```
## [1] 0.2368421
```

```
# specificity: TNR = 1-FPR
(n_TN)/(n_TN+n_FP)
```

```
## [1] 0.9195402
```

Comparing Models

Which of the two models above do we prefer? [Use generalizability on *test* data...]

How to choose between models: Rationale 1

- If a FP is costly, then low FPR (high TNR, since $FPR = 1 - TNR$) is important
 - So high specificity = $TNR = 1 - FPR$ is important
- If a FN is costly, then low FNR (high TPR, since $FNR = 1 - TPR$) is important
 - So high sensitivity/recall = $TPR = 1 - FNR$ is important
- Accuracy is a weighted average of sensitivity/recall and specificity
 - sensitivity/recall gets more weight if positive outcomes are more prevalent
 - specificity gets more weight if negative outcomes are more prevalent

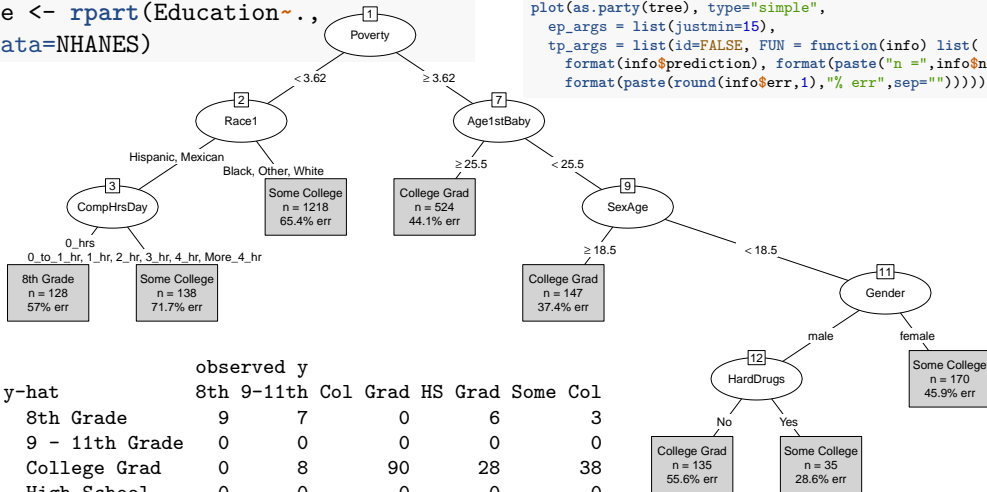
How to choose between models: Rationale 2

- Less complex models are less likely to overfit the data
 - Less complex model performance tends to generalize better
- Less complex models tends be easier to interpret than more complex models

Multi-Class (Non-Binary) Outcomes

```
tree <- rpart(Education~.,
  data=NHANES)
```

```
plot(as.party(tree), type="simple",
  ep_args = list(justmin=15),
  tp_args = list(id=FALSE, FUN = function(info) list(
    format(info$prediction), format(paste("n =",info$n)),
    format(paste(round(info$err,1),"% err",sep="")))))
```



##		observed y				
##	y-hat	8th	9-11th	Col	Grad	HS Grad
##	8th Grade	9	7	0	6	3
##	9 - 11th Grade	0	0	0	0	0
##	College Grad	0	8	90	28	38
##	High School	0	0	0	0	0
##	Some College	18	49	54	72	117

Controlling FP and FN with Thresholding

```
tree2_test_pred <-  
  predict(tree2, type="class",  
          newdata=test)  
table(`y-hat`=tree2_test_pred,  
      `observed y`=test$SleepTrouble)
```

```
##           observed y  
## y-hat   No Yes      FNR: 8%  
##   No  320 116      TPR: 24%  
##   Yes   28  36
```

```
predict(tree2, newdata=test) %>%  
  as_tibble() -> tree2_test_pred  
tree2_test_pred %>% head(3)
```

```
## # A tibble: 3 x 2  
##       No    Yes  
##   <dbl> <dbl>  
## 1 0.810 0.190  
## 2 0.253 0.747  
## 3 0.810 0.190
```

```
threshold_20 <- tree2_test_pred %>%  
  mutate(prediction=ifelse(  
    Yes>=0.20, "Yes", "No"))  
table(`y-hat`=threshold_20$prediction,  
      `observed y`=test$SleepTrouble)
```

```
##           observed y  
## y-hat   No Yes      FNR: 25%  
##   No  261  94      TPR: 38%  
##   Yes   87  58
```

```
threshold_70 <- tree2_test_pred %>%  
  mutate(prediction=ifelse(  
    Yes>=0.70, "Yes", "No"))  
table(`y-hat`=threshold_70$prediction,  
      `observed y`=test$SleepTrouble)
```

```
##           observed y  
## y-hat   No Yes      FNR: 5%  
##   No  333 127      TPR: 17%  
##   Yes   15  25
```