Modeling I

Some Dope Quotes

- George Box

  “All models are wrong, but some are useful”

- Mahatma Mario

  “The best model is the one you don’t have”

- Doctor Mario

  “If you can’t be a model, make a model”

Introduction to Modeling

- Read Vigorously
  - Part IV in R4DS
  - Chapters 6 and 7 in MD

- Goal: Understand the Relationship Between Variables

- Purpose:
  - Explanation
  - Prediction

- Classic Model:
  - Single Outcome Variable (Y)
  - Multiple Predictor Variables ($X_1, X_2, \ldots, X_P$)
  - Multiple Regression Model:

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_P X_P + \varepsilon$$

Introduction to Modeling

- Model Deconstruction:

$$Y = \underbrace{\beta_0 + \beta_1 X_1 + \cdots + \beta_P X_P}_{\text{Signal}} + \underset{\text{Noise}}{\varepsilon}$$

- Noise: Unexplainable Error
  - $E(\varepsilon) = 0$
  - $Var(\varepsilon) = \sigma^2$
- Signal: Helps Us Understand in the Variation in Y
  - $E(Y|X_1, \ldots, X_P) =$ Expected Value of Y Given Information about $X_1, \ldots, X_P$
  - Used For Prediction

Introduction to Modeling

- Once We Have Data
  - Estimate the Parameters $(\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_P)$
  - Use for Prediction $\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \cdots + \hat{\beta}_P X_P$
  - Obtain the Residuals $\hat{\varepsilon} = Y - \hat{Y}$
  - Evaluate the Noise $(\hat{\sigma}^2)$
- Key: Pick Estimates $(\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_P)$ where $\hat{\varepsilon} \approx 0$ and $\hat{\sigma}^2$ is Small

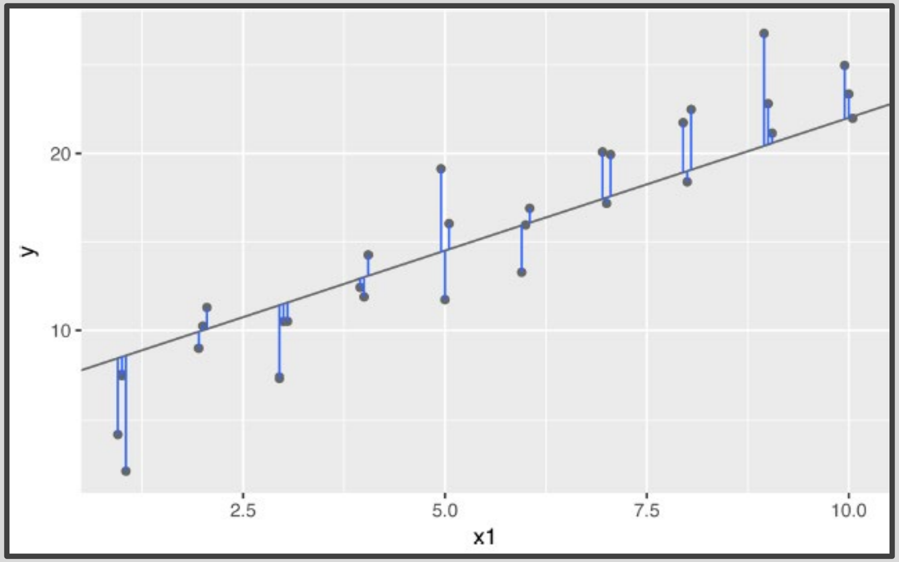
Introduction to Modeling

- Optimization Problem:
  - One Dependent Variable *(Y)*

    $y_1, y_2, y_3 \ldots, y_n$
  - One Independent Variable *(X)*

    $x_1, x_2, x_3 \ldots, x_n$
  - Choice of $\hat{\beta}_0$ and $\hat{\beta}_1$

    $$\hat{\varepsilon}_k = y_k - \hat{y}_k$$
    $$= y_k - (\hat{\beta}_0 + \hat{\beta}_1 x_1)$$



Introduction to Modeling

- Optimization Problem (Cont.):
  - Loss Functions:
    - Sum of Squared Errors $\mathrm{SSE} = \sum \hat{\varepsilon}_k^2$
    - Mean Squared Error $\mathrm{MSE} = \frac{1}{N} \sum \hat{\varepsilon}_k^2$
    - Root MSE $\mathrm{RMSE} = \sqrt{\frac{1}{N} \sum \hat{\varepsilon}_k^2}$
    - Mean Absolute Error $\mathrm{MAE} = \frac{1}{N} \sum |\hat{\varepsilon}_k|$

Introduction to Modeling

- Family of Models: $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$
  - Empty Model: $Y = \beta_0 + \varepsilon$
  - 1 Coefficient:
    - $Y = \beta_0 + \beta_1 X_1 + \varepsilon$
    - $Y = \beta_0 + \beta_2 X_2 + \varepsilon$
  - 2 Coefficients:
    - $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$
- Fact: Adding More Predictor Variables Will Always Cause the Loss Function to Decrease

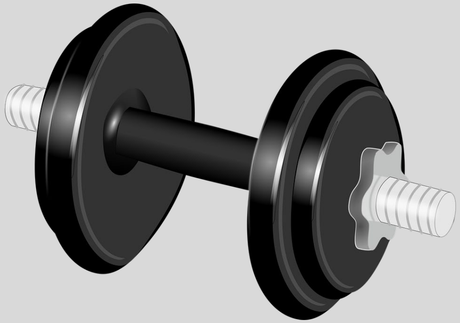
Introduction to Modeling

- Good Practice:
  - Randomly Split Full Dataset Into Two Datasets
  - Training Data
    - 80%-90% of Original Data
    - Used for Model Fitting
  - Testing Data
    - 20%-10% of Original Data
    - Used for Model Selection

Motivation

- Modeling Real Experimental Data
  - Question: What Factors Improve Vertical Jump?
    - Hypothesis 1:

    - Hypothesis 2:



Motivation

- Modeling Real Experimental Data
  - Data From 10,000 Individuals
    - X_1= Shrooms (#/Week)
    - X_2= Exercise (Hrs./Week)
    - Y= Vertical Jump (in.)
    - Preview of Data:

vert <dbl>	shroom <int>	exercise <int>
47.88340	27	9
37.78150	24	2
35.60634	19	7
34.00961	17	8
39.69892	25	4
37.43090	23	5

Motivation

- Modeling Real Experimental Data
  - Randomly Split Data

```
set.seed(216)
DATA$SPLIT=sample(x=c("TRAIN","TEST"),size=10000,
                  replace=T,prob=c(0.85,0.15))
TRAIN=DATA %>%  filter(SPLIT=="TRAIN")
TEST=DATA %>% filter(SPLIT=="TEST")
glimpse(TRAIN)
```

```
## Observations: 8,525
## Variables: 4
## $ vert     <dbl> 37.78150, 39.69892, 37.43090, 43.21785,
## $ shroom   <int> 24, 25, 23, 27, 8, 17, 23, 15, 28, 20,
## $ exercise <int> 2, 4, 5, 4, 5, 5, 3, 7, 0, 3, 4, 7, 6,
## $ SPLIT    <chr> "TRAIN", "TRAIN", "TRAIN", "TRAIN", "TR
```

```
glimpse(TEST)
```

```
## Observations: 1,475
## Variables: 4
## $ vert     <dbl> 47.88340, 35.60634, 34.00961, 39.45598,
## $ shroom   <int> 27, 19, 17, 22, 21, 30, 21, 24, 22, 16,
## $ exercise <int> 9, 7, 8, 8, 8, 9, 15, 8, 9, 8, 11, 9, 7
## $ SPLIT    <chr> "TEST", "TEST", "TEST", "TEST", "TEST",
```

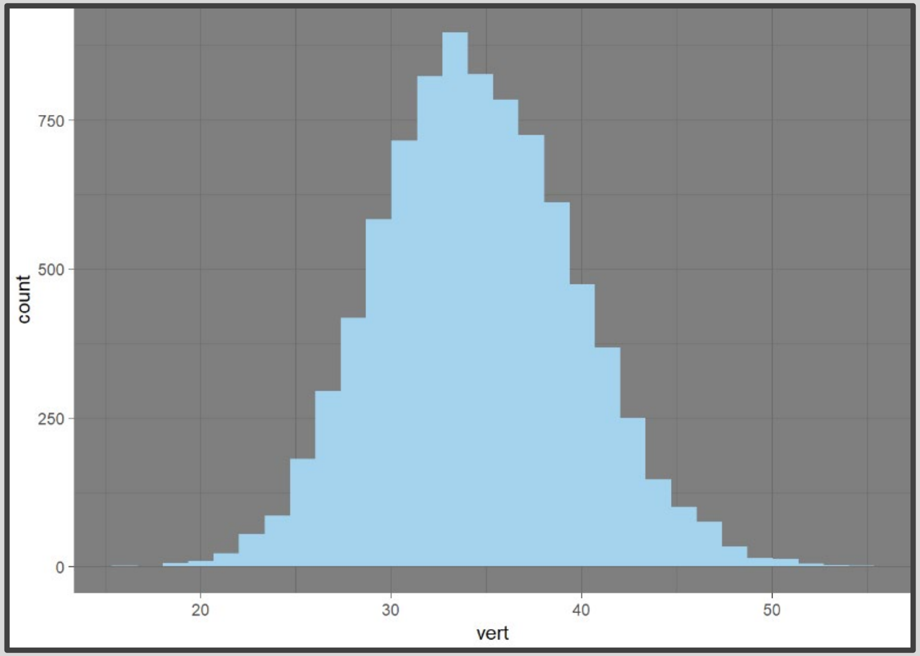
Empty Model (MODEL 0)

- MODEL 0

$$Y = \beta_0 + \varepsilon$$
$$E(Y) = \beta_0$$

- Summary of Vertical Jump

```
## # A tibble: 1 x 4
##    mean    sd   min   max
##   <dbl> <dbl> <dbl> <dbl>
## 1  34.5  5.15  16.1  54.8
```



Empty Model
(MODEL 0)

- Function to Get Fitted Values:

```
MODEL0 = function(DATA,COEF){
  FIT=COEF[1]
}
```

- Functions to Evaluate Model:

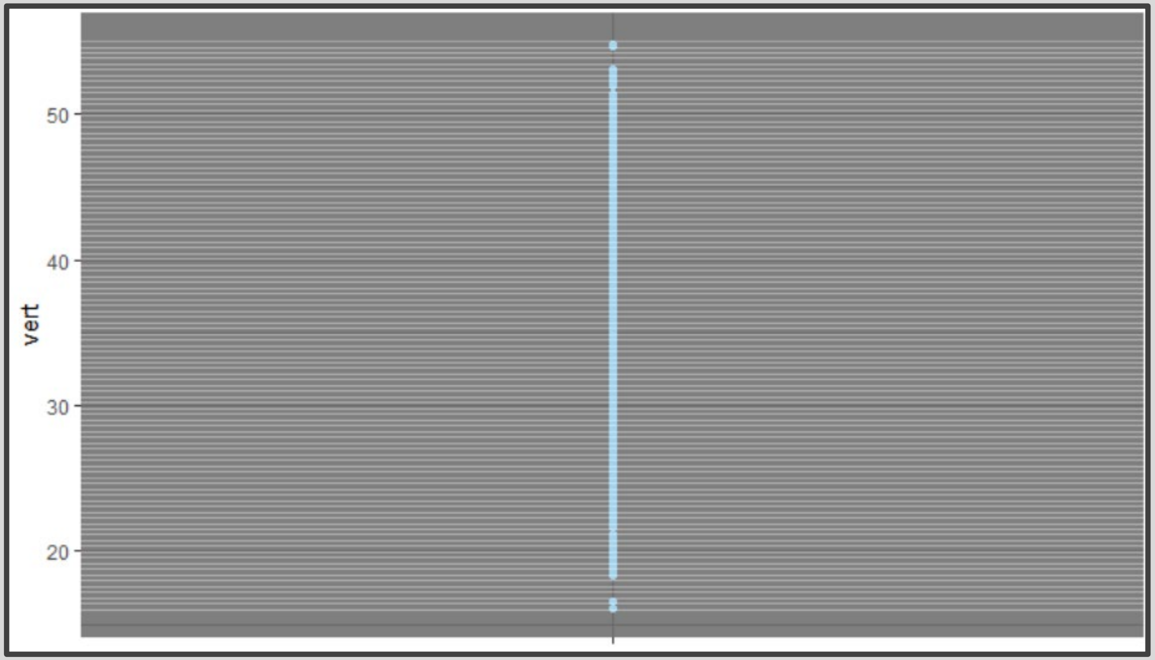
```
MSE0=function(DATA,COEF){
  ERROR=DATA$vert-MODEL0(DATA,COEF)
  LOSS=mean(ERROR^2)
  return(LOSS)
}
MAE0=function(DATA,COEF){
  ERROR=DATA$vert-MODEL0(DATA,COEF)
  LOSS=mean(abs(ERROR))
  return(LOSS)
}
```

Empty Model
(MODEL 0)

- Optimization
  - Specify Possible Values of $\hat{\beta}_0$

```
COEF0=tibble(
  beta0=seq(16,55,length=100)
)
```

  - All Possible Models



Empty Model (MODEL 0)

- Optimization
  - We Desire to Find the $\hat{\beta}_0$ that Minimizes MSE and MAE
  - map(): purr Package

```
COEF0 %>%
  mutate(MSE=purrr::map_dbl(beta0,MSE0,DATA=TRAIN),
         MAE=purrr::map_dbl(beta0,MAE0,DATA=TRAIN),
         rankMSE=rank(MSE),rankMAE=rank(MAE)) %>%
         filter(rankMSE<5,rankMAE<5)
```

```
## # A tibble: 3 x 5
##   beta0   MSE   MAE rankMSE rankMAE
##   <dbl> <dbl> <dbl>   <dbl>   <dbl>
## 1  34.1  26.7  4.13       3       2
## 2  34.5  26.5  4.13       1       1
## 3  34.9  26.7  4.15       2       3
```

Empty Model
(MODEL 0)

- Optimization
  - optim(): Base R

```
BESTMSE0=optim(par=16,fn=MSE0,DATA=TRAIN)
BESTMSE0$par
```

```
## [1] 34.53125
```

Starting Values

```
BESTMAE0=optim(par=16,fn=MAE0,DATA=TRAIN)
BESTMAE0$par
```

```
## [1] 34.34375
```

  - lm(): Base R (Linear Reg)

```
LM0=lm(vert~1,data=TRAIN)
coef(LM0)
```

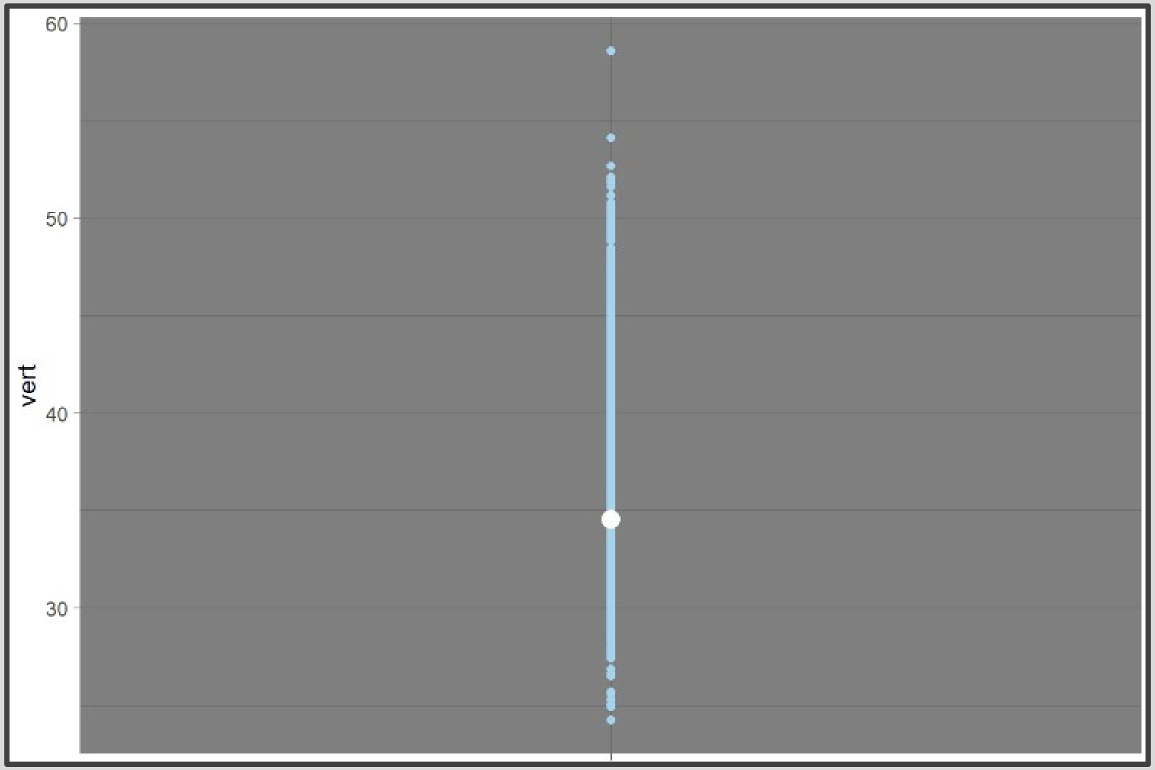
```
## (Intercept)
##    34.53428
```

Empty Model
(MODEL 0)

- Final MODEL 0

$$Y = 34.53 + \varepsilon$$
$$E(Y) = 34.53$$

- Prediction on Test Data:

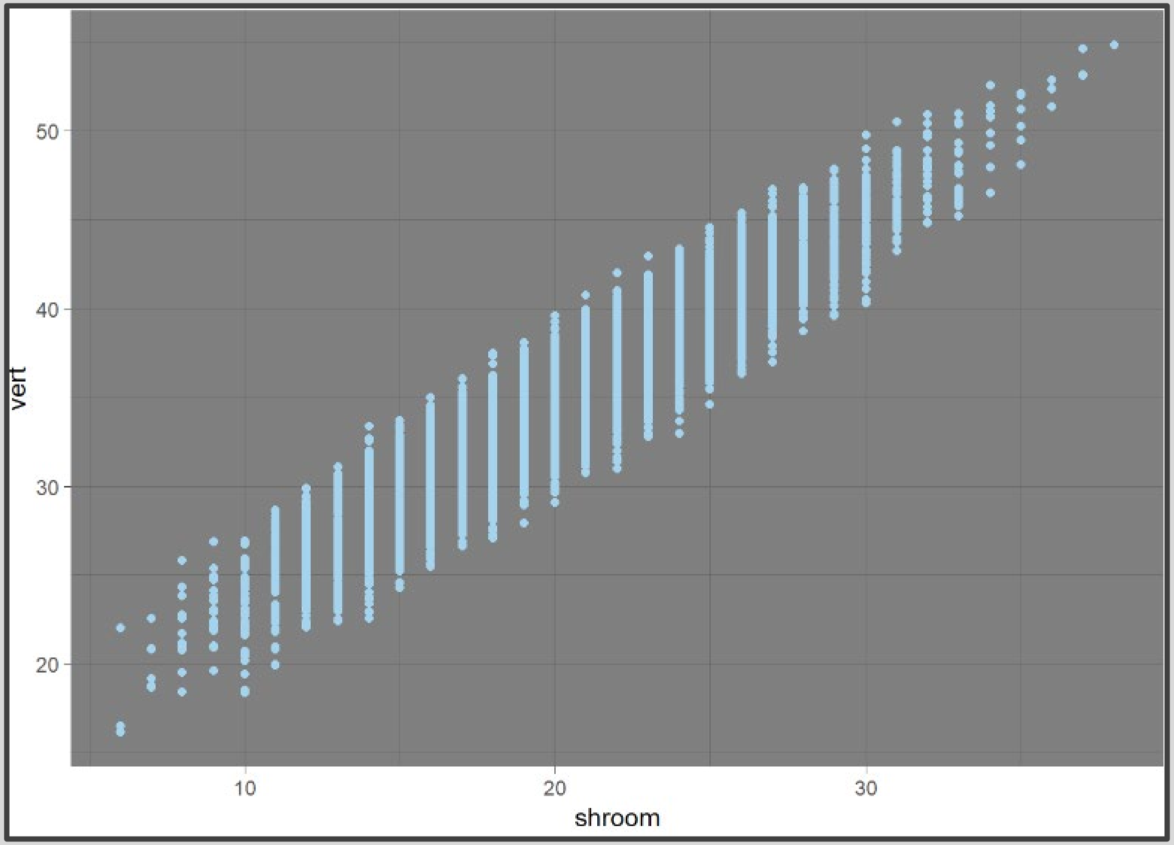


Linear Regression (MODEL 1A & 1B)

- MODEL 1A

$$Y = \beta_0 + \beta_1 X_1 + \varepsilon$$
$$E(Y) = \beta_0 + \beta_1 X_1$$

- Visualization of Relationship



Linear Regression
(MODEL 1A & 1B)

- Function to Get Fitted Values

```
MODEL1A = function(DATA,COEF){
  FIT=COEF[1]+COEF[2]*DATA$shroom
}
```

- Functions to Evaluate Model

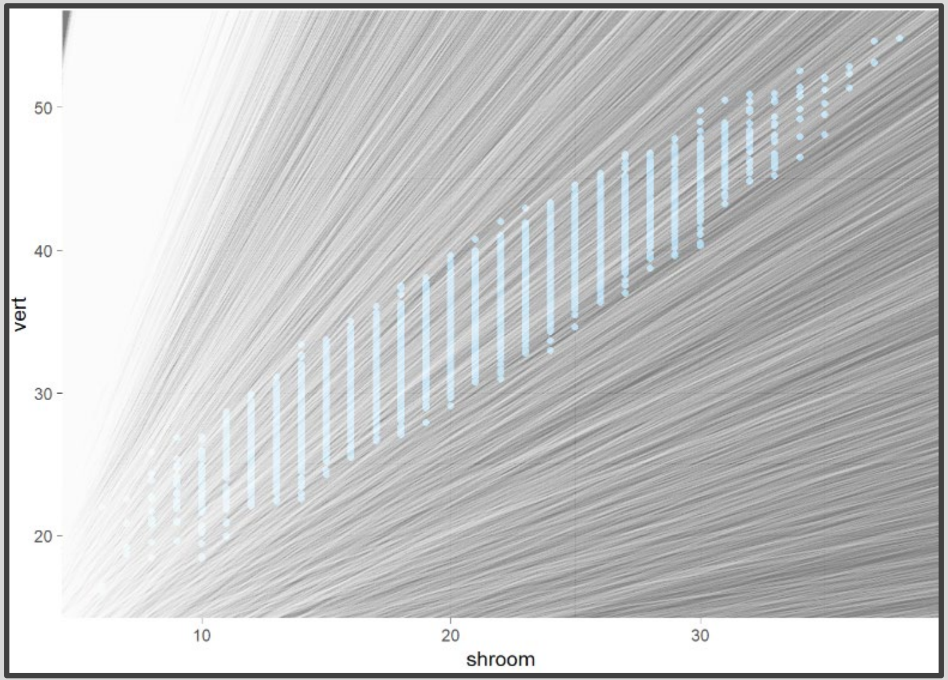
```
MSE1A=function(DATA,COEF){
  ERROR=DATA$vert-MODEL1A(DATA,COEF)
  LOSS=mean(ERROR^2)
  return(LOSS)
}
MAE1A=function(DATA,COEF){
  ERROR=DATA$vert-MODEL1A(DATA,COEF)
  LOSS=mean(abs(ERROR))
  return(LOSS)
}
```

Linear Regression (MODEL 1A & 1B)

- Optimization
  - Possible Values of $\hat{\beta}_0$ and $\hat{\beta}_1$

```
set.seed(216)
COEF1A=tibble(
  beta0=runif(10000,0,10),
  beta1=runif(10000,0,10)
)
```

  - All Possible Models



Linear Regression
(MODEL 1A & 1B)

- Optimization
  - Use of apply() Function

```
COEF1A %>%
  mutate(MSE=apply(COEF1A,1,MSE1A,DATA=TRAIN),
         MAE=apply(COEF1A,1,MAE1A,DATA=TRAIN),
         rankMSE=rank(MSE),rankMAE=rank(MAE)) %>%
         filter(rankMSE<5,rankMAE<5)
```

```
## # A tibble: 4 x 6
##   beta0 beta1   MSE   MAE rankMSE rankMAE
##   <dbl> <dbl> <dbl> <dbl>   <dbl>   <dbl>
## 1  9.48  1.26  4.09  1.63       3       3
## 2  9.46  1.23  4.00  1.62       2       2
## 3  9.84  1.20  4.12  1.65       4       4
## 4  9.40  1.24  3.96  1.61       1       1
```

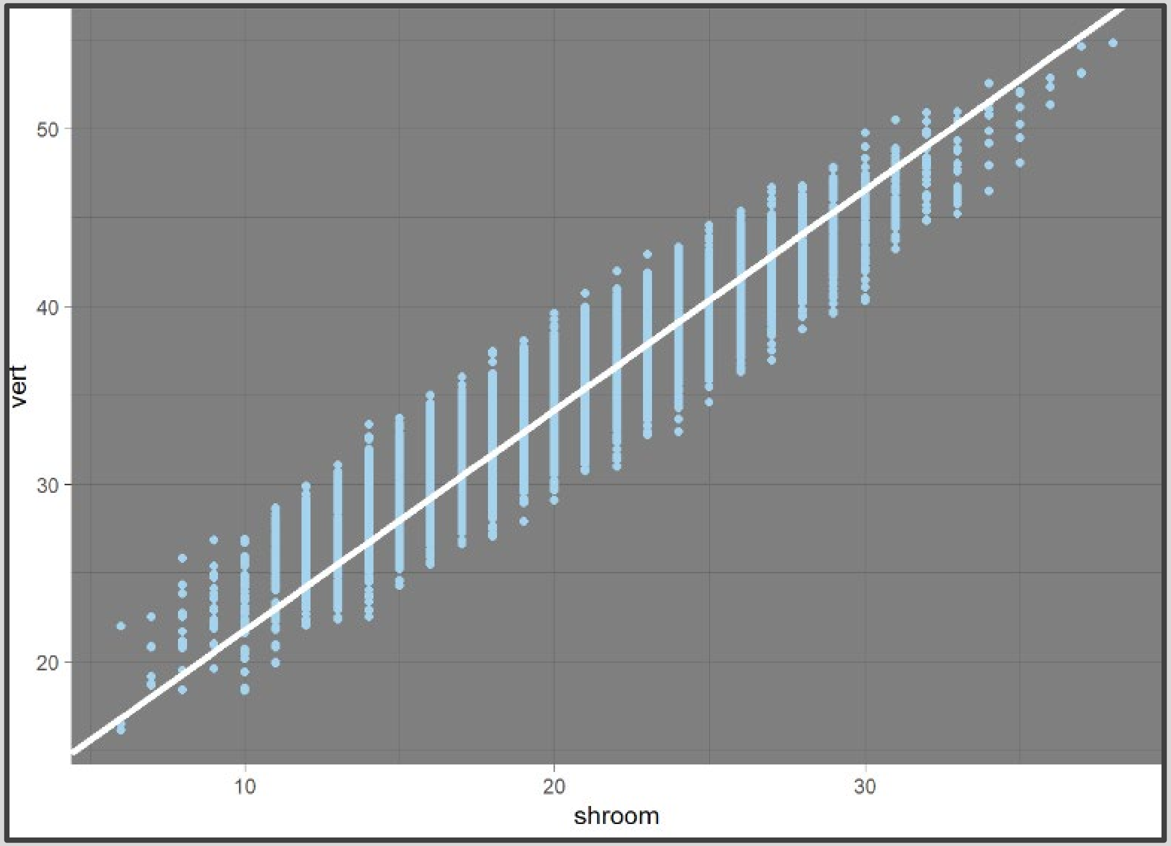
Linear Regression (MODEL 1A & 1B)

- Final MODEL 1A

$$Y = 9.4 + 1.24X_1 + \varepsilon$$

$$E(Y) = 9.4 + 1.24X_1$$

- Fitted on Train Data

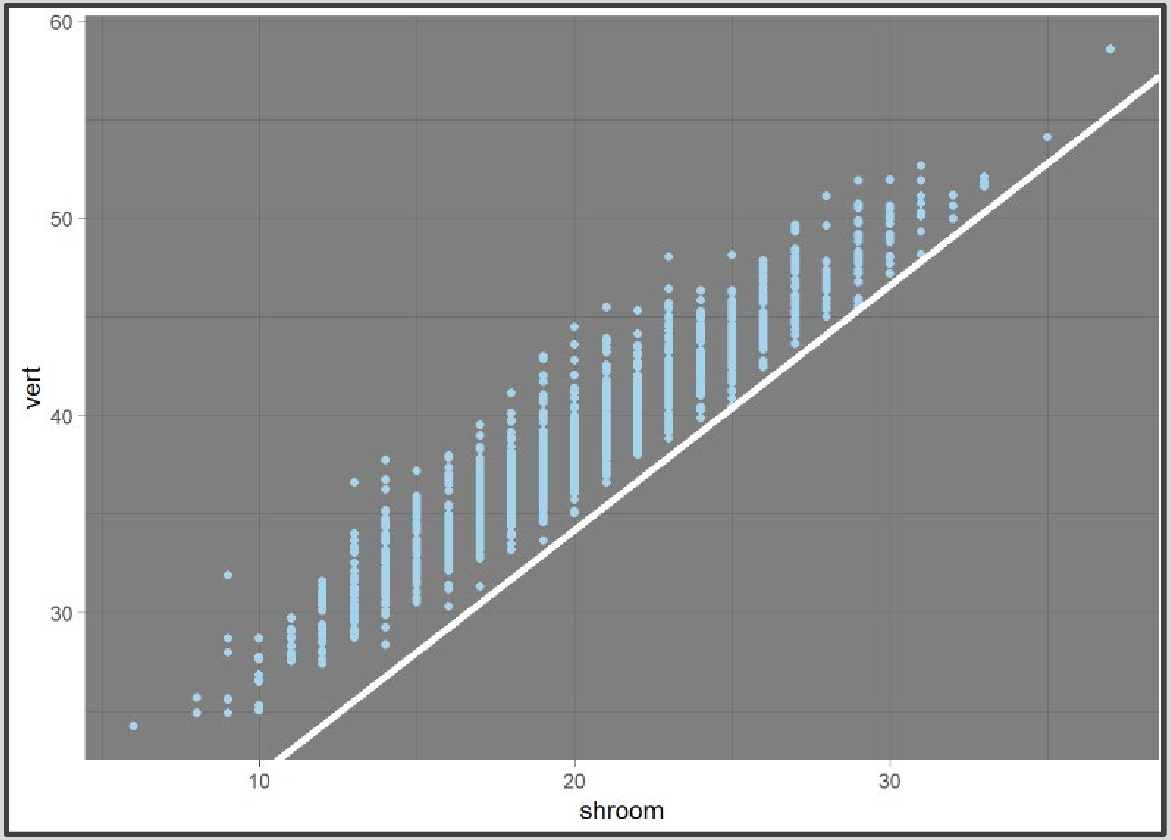


Linear Regression (MODEL 1A & 1B)

- Final MODEL 1A

$$Y = 9.4 + 1.24X_1 + \varepsilon$$
$$E(Y) = 9.4 + 1.24X_1$$

- Prediction on Test Data

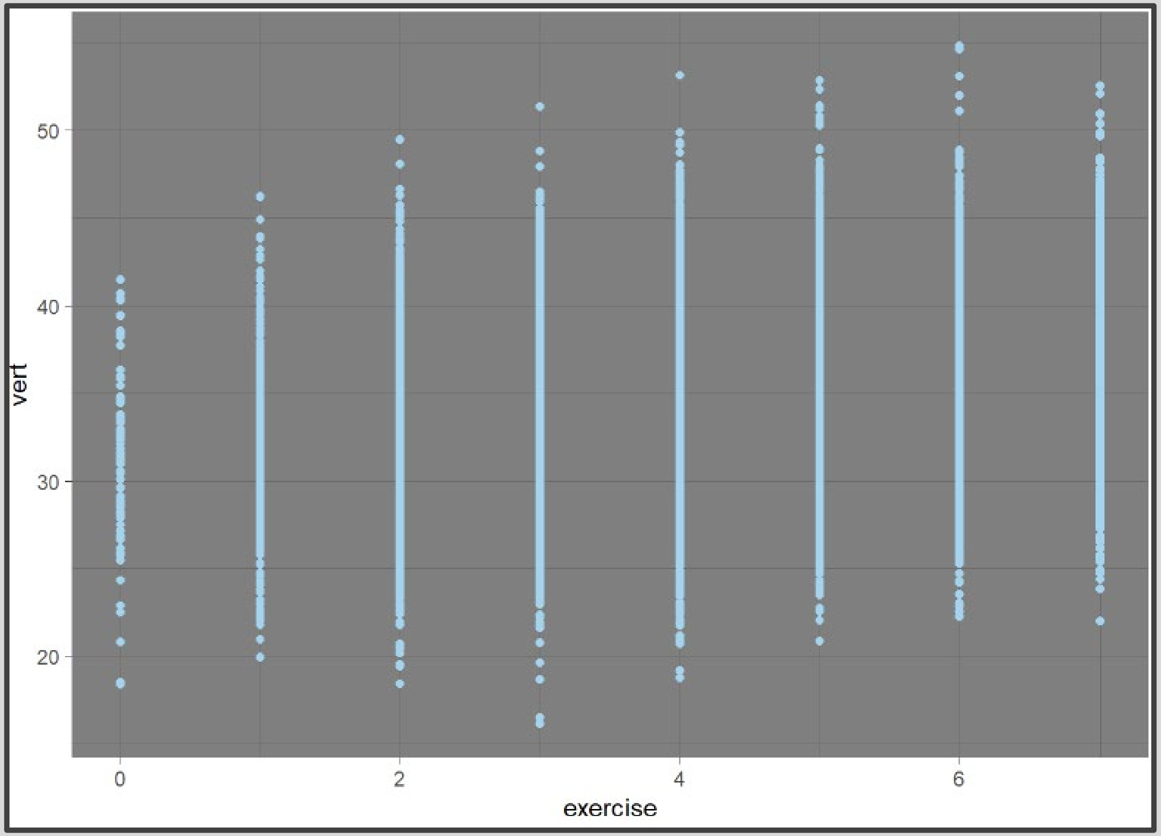


Linear Regression (MODEL 1A & 1B)

- MODEL 1B

$$Y = \beta_0 + \beta_1 X_2 + \varepsilon$$
$$E(Y) = \beta_0 + \beta_1 X_2$$

- Visualization of Relationship



Linear Regression (MODEL 1A & 1B)

- Function to Get Fitted Values

```
MODEL1B = function(DATA,COEF){
  FIT=COEF[1]+COEF[2]*DATA$exercise
}
```

- Functions to Evaluate Model

```
MSE1B=function(DATA,COEF){
  ERROR=DATA$vert-MODEL1B(DATA,COEF)
  LOSS=mean(ERROR^2)
  return(LOSS)
}
MAE1B=function(DATA,COEF){
  ERROR=DATA$vert-MODEL1B(DATA,COEF)
  LOSS=mean(abs(ERROR))
  return(LOSS)
}
```

Linear Regression (MODEL 1A & 1B)

- Optimization
  - Use of optim() Function

```
BESTMSE1B=optim(par=c(0,0),fn=MSE1B,DATA=TRAIN)
BESTMSE1B$par
```

```
## [1] 30.8323639  0.8543225
```

```
BESTMAE1B=optim(par=c(0,0),fn=MAE1B,DATA=TRAIN)
BESTMAE1B$par
```

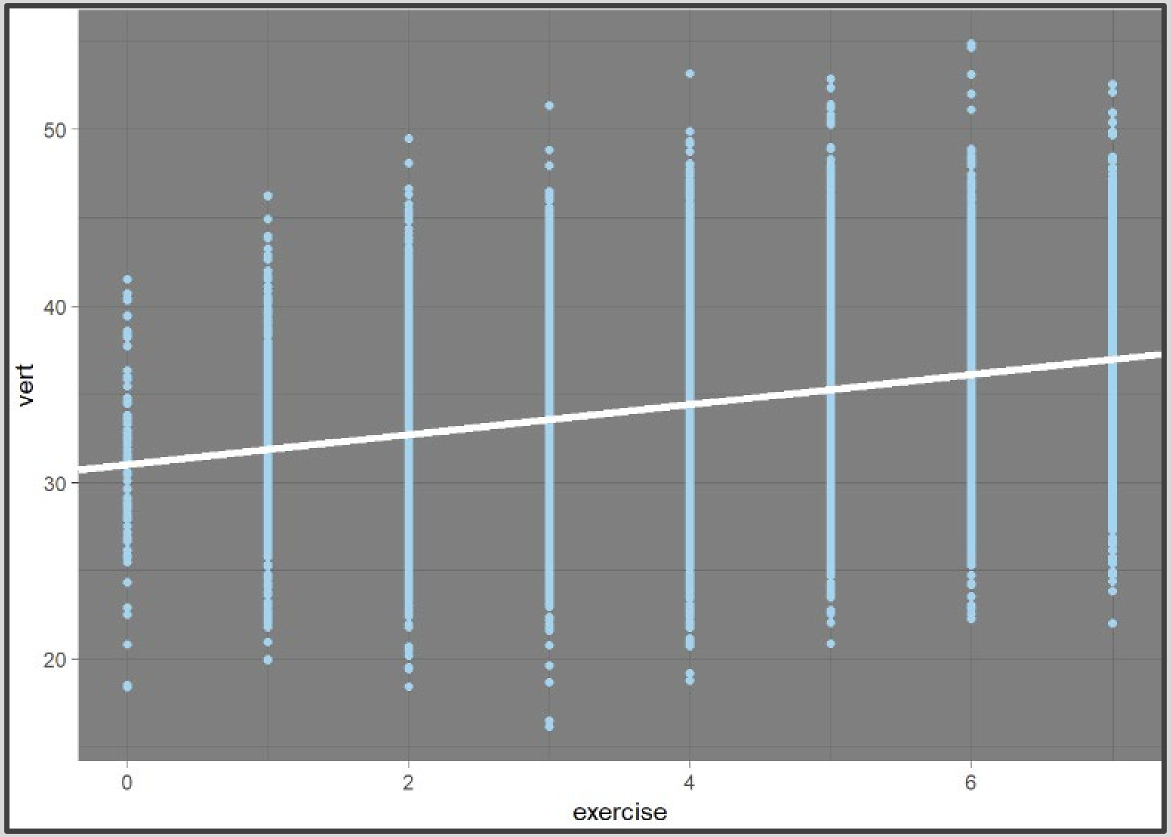
```
## [1] 30.6619753  0.8512186
```

Linear Regression (MODEL 1A & 1B)

- Final MODEL 1B

$$Y = 31 + 0.85X_2 + \varepsilon$$
$$E(Y) = 31 + 0.85X_2$$

- Fitted on Train Data

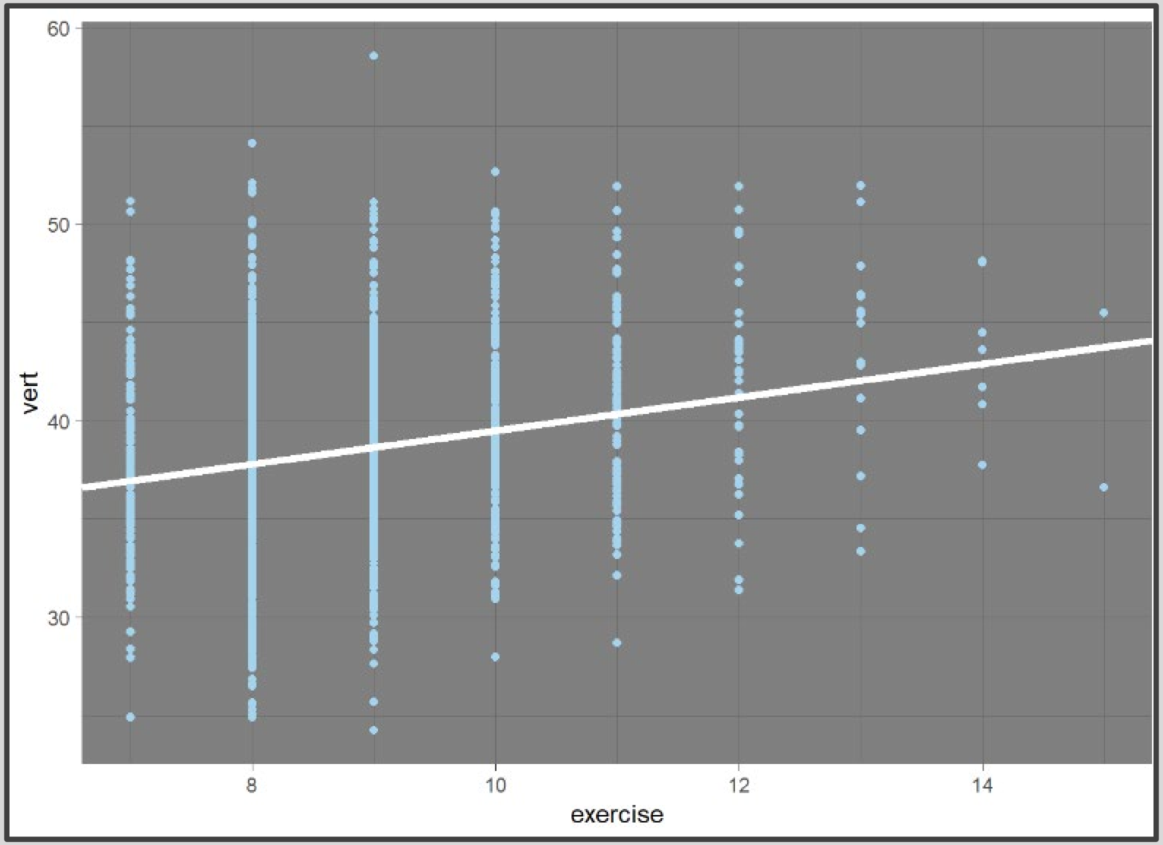


Linear Regression (MODEL 1A & 1B)

- Final MODEL 1B

$$Y = 31 + 0.85X_2 + \varepsilon$$
$$E(Y) = 31 + 0.85X_2$$

- Prediction on Test Data

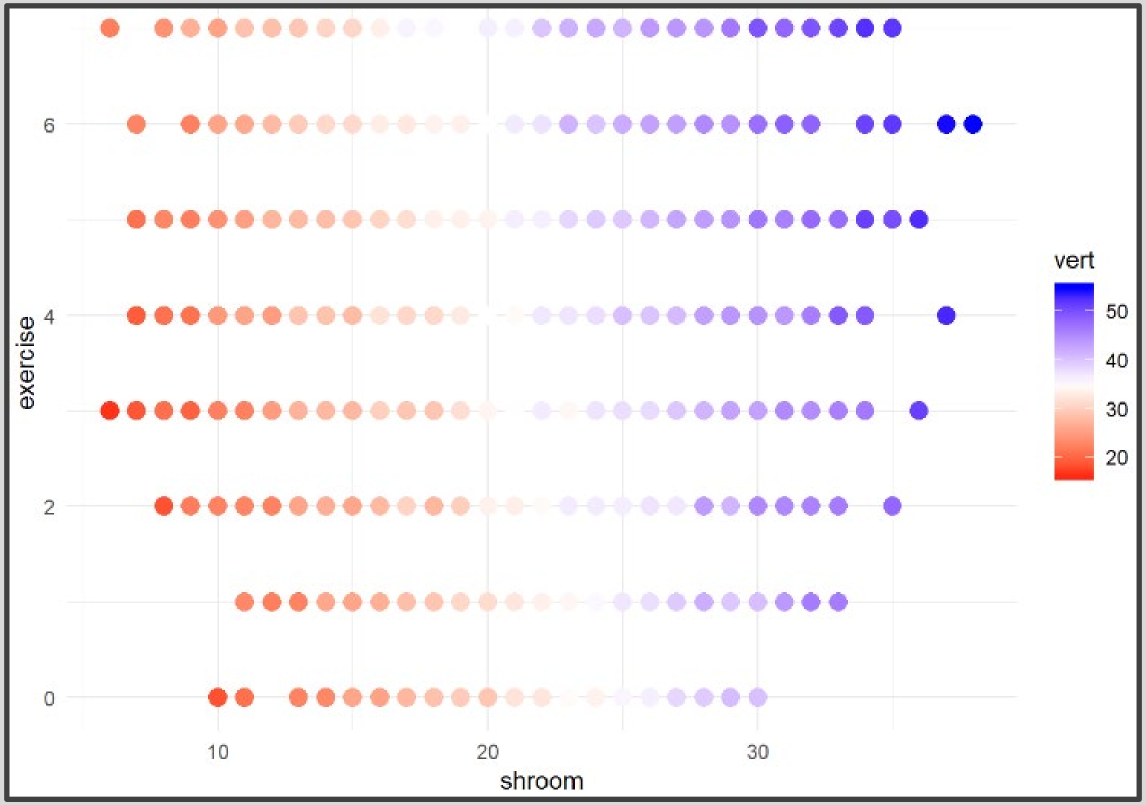


Multiple Regression (MODEL 2)

- MODEL 2

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \varepsilon$$
$$E(Y) = \beta_0 + \beta_1 X_1 + \beta_2 X_2$$

- Visualization of Relationship



Multiple Regression (MODEL 2)

- Function to Get Fitted Values

```
MODEL2 = function(DATA,COEF){
  FIT=COEF[1]+COEF[2]*DATA$shroom+COEF[3]*DATA$exercise
}
```

- Functions to Evaluate Model

```
MSE2=function(DATA,COEF){
  ERROR=DATA$vert-MODEL2(DATA,COEF)
  LOSS=mean(ERROR^2)
  return(LOSS)
}
MAE2=function(DATA,COEF){
  ERROR=DATA$vert-MODEL2(DATA,COEF)
  LOSS=mean(abs(ERROR))
  return(LOSS)
}
```

Multiple Regression (MODEL 2)

- Use lm() with summary()

```
LM2=lm(vert~shroom+exercise,data=TRAIN)
summary(LM2)
```

```
##
## Call:
## lm(formula = vert ~ shroom + exercise, data = TRAIN)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -3.6426 -0.6776 -0.0138  0.6838  3.7675
##
## Coefficients:
##             Estimate Std. Error t value             Pr(>|t|)
## (Intercept) 8.996672   0.058760   153.1 <0.0000000000000002 ***
## shroom      1.079243   0.002474   436.3 <0.0000000000000002 ***
## exercise    0.902851   0.006635   136.1 <0.0000000000000002 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 1.025 on 8522 degrees of freedom
## Multiple R-squared:  0.9605, Adjusted R-squared:  0.9604
## F-statistic: 1.035e+05 on 2 and 8522 DF,  p-value: < 0.00000000000000022
```

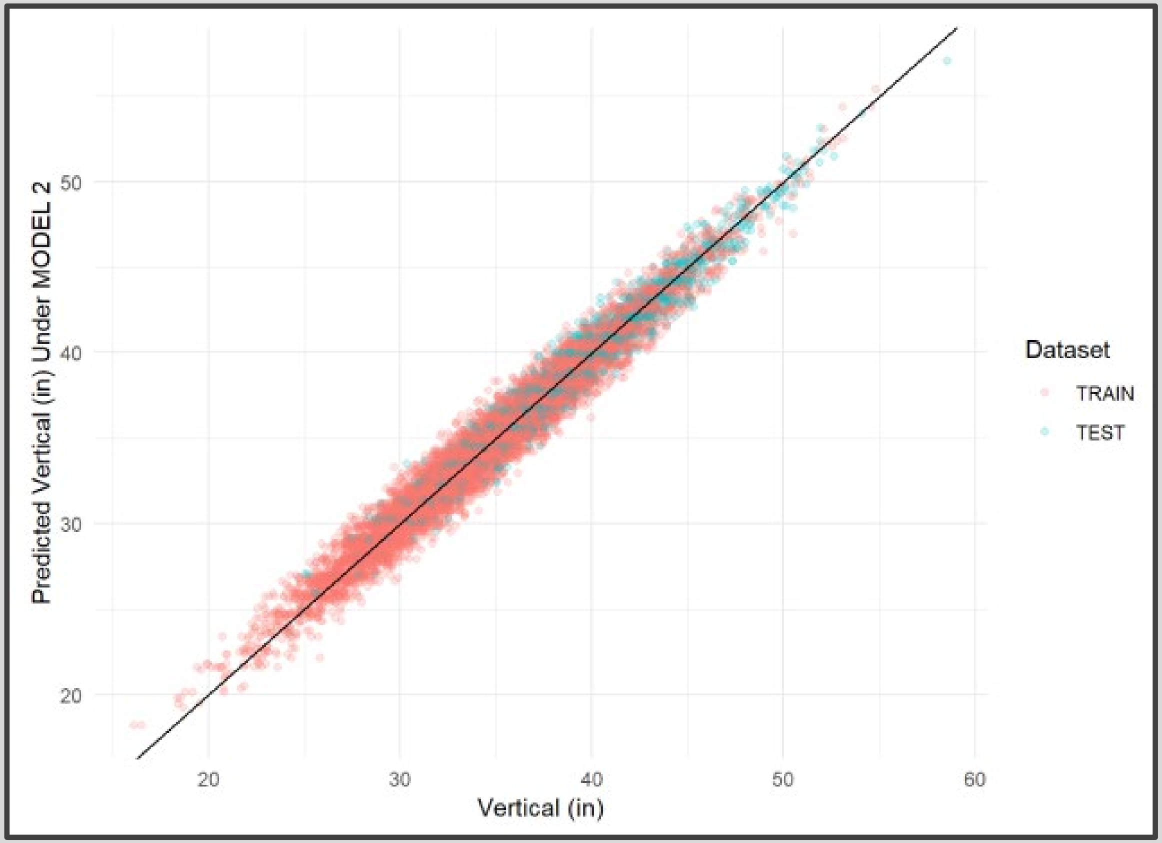
- Final MODEL 2

$$Y = 9 + 1.08X_1 + 0.9X_2 + \varepsilon$$

$$E(Y) = 9 + 1.08X_1 + 0.9X_2$$

Multiple Regression (MODEL 2)

- Comparing Predicted Values to Actual Values for MODEL 2



Model Evaluation

- Out-of-Sample Evaluation

```r
MODELS=c("MODEL 0","MODEL 1A","MODEL 1B","MODEL 2")
MSE=c(MSE0(TEST,c(34.53)),
      MSE1A(TEST,c(9.4,1.24)),
      MSE1B(TEST,c(31,0.85)),
      MSE2(TEST,c(9,1.07,0.9)))
MAE=c(MAE0(TEST,c(34.53)),
      MAE1A(TEST,c(9.4,1.24)),
      MAE1B(TEST,c(31,0.85)),
      MAE2(TEST,c(9,1.07,0.9)))
COMPARE=tibble(MODELS=MODELS,MSE=MSE,MAE=MAE)
print(COMPARE)
```

```
## # A tibble: 4 x 3
##   MODELS      MSE   MAE
##   <chr>     <dbl> <dbl>
## 1 MODEL 0  42.0   5.17
## 2 MODEL 1A 21.5   4.31
## 3 MODEL 1B 24.5   3.94
## 4 MODEL 2   0.965 0.786
```

Miss Universe

Da Truth

- Simulation Facts

$$Y = 8 + 1.08X_1 + 0.9X_2 + \varepsilon$$
$$E(Y) = 8 + 1.08X_1 + 0.9X_2$$
$$\varepsilon \sim N(\mu = 0, \sigma^2 = 1)$$
$$\sigma_y^2 = 5.15^2 = 26.5225$$

- Noise Variation

$$\sigma_{noise}^2 = 1$$

- Signal Variation

$$\sigma_{signal}^2 = 26.5225 - 1 = 25.5225$$

- Optimal R^2

$$R^2 = \frac{25.5225}{26.5225} = 0.96 = 96\%$$

Closing

Disperse and Make Reasonable Decisions