THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL

STOR 320 Modeling I

Lecture 15

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Introduction

- Read
  - Part IV in R4DS
  - Chapters 6 and 7 in ModernDive
- 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:

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

Linear Regression

- 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/Explanation

Linear Regression

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

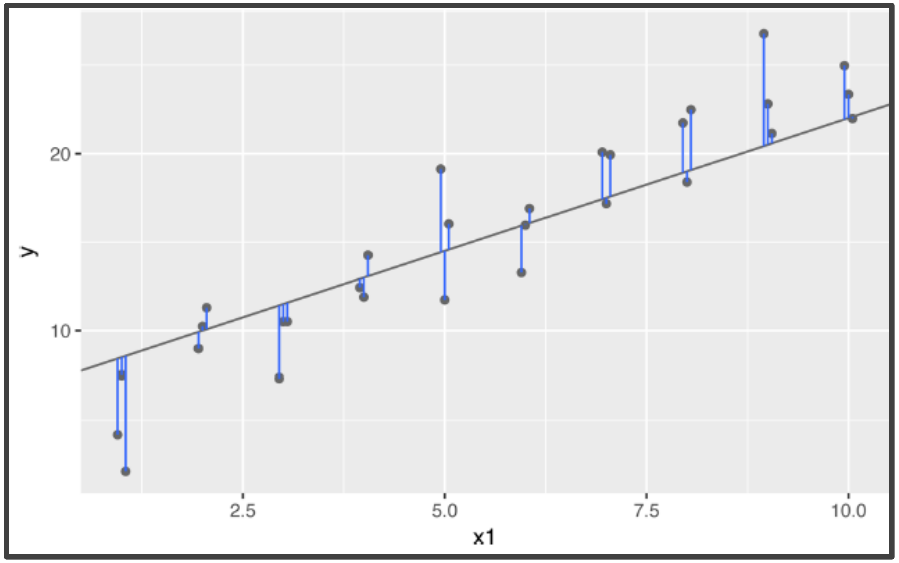
Optimization

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

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

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

    $$\begin{aligned}\hat{\varepsilon}_k &= y_k - \hat{y}_k \\ &= y_k - (\hat{\beta}_0 + \hat{\beta}_1 x_k)\end{aligned}$$



Optimization

- 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 $\mathrm{MAE} = \frac{1}{N}\sum |\hat{\varepsilon}_k|$

Family of Models

- 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

Data Partition

- 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

Example

- Modeling Real Experimental Data
  - Question: What Factors Improve Hourly Salary?
    - Hypothesis 1: Experience

    - Hypothesis 2: Education

Example

- Modeling Real Experimental Data
  - Data From 10,000 Individuals
    - X_1= Experience (# of Years)
    - X_2= Education (# of Years)
    - Y= Salary (dollars/hour)
    - Preview of Data:

```
## # A tibble: 6 x 3
##   salary experience education
##    <dbl>      <int>     <int>
## 1   47.9         27         9
## 2   37.8         24         2
## 3   35.6         19         7
## 4   34.0         17         8
## 5   39.7         25         4
## 6   37.4         23         5
```

Example

```
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)
```

```
## Rows: 8,525
## Columns: 4
## $ salary     <dbl> 37.78150, 39.69892, 37.43090, 43.21785, 25.81015, 30.99309…
## $ experience <int> 24, 25, 23, 27, 8, 17, 23, 15, 28, 20, 13, 29, 19, 24, 29,…
## $ education  <int> 2, 4, 5, 4, 5, 5, 3, 7, 0, 3, 4, 7, 6, 7, 4, 3, 6, 7, 5, 7…
## $ SPLIT      <chr> "TRAIN", "TRAIN", "TRAIN", "TRAIN", "TRAIN", "TRAIN", "TRA…
```

```
glimpse(TEST)
```

```
## Rows: 1,475
## Columns: 4
## $ salary     <dbl> 47.88340, 35.60634, 34.00961, 39.45598, 38.36103, 50.13343…
## $ experience <int> 27, 19, 17, 22, 21, 30, 21, 24, 22, 16, 13, 20, 31, 21, 23…
## $ education  <int> 9, 7, 8, 8, 8, 9, 15, 8, 9, 8, 11, 9, 7, 10, 13, 8, 10, 8,…
## $ SPLIT      <chr> "TEST", "TEST", "TEST", "TEST", "TEST", "TEST", "TEST", "T…
```

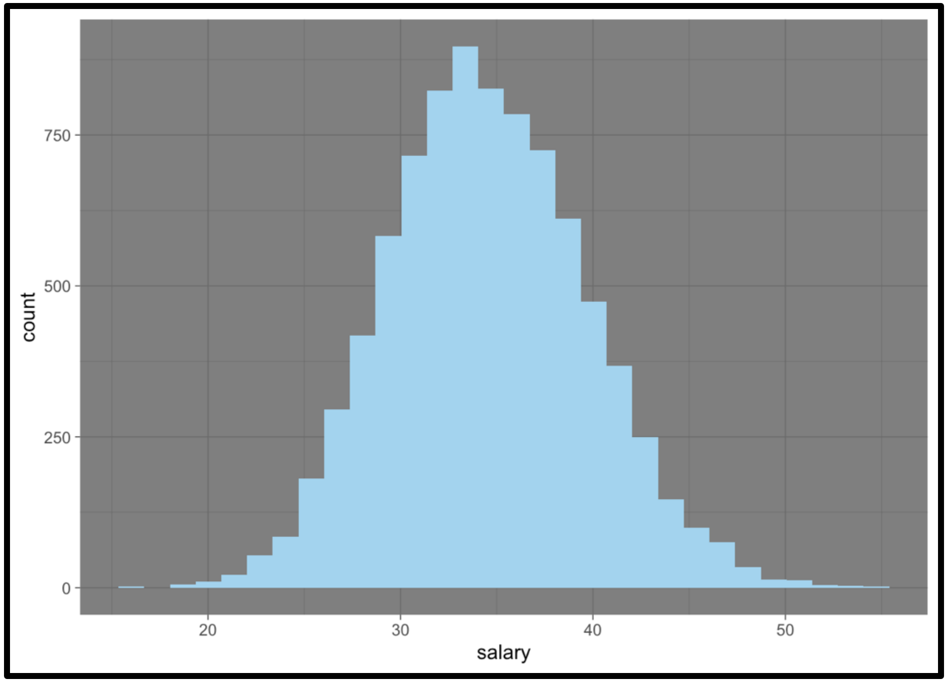
Empty Model (MODEL 0)

- MODEL 0

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

- Summary of Salary

```
## # 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:

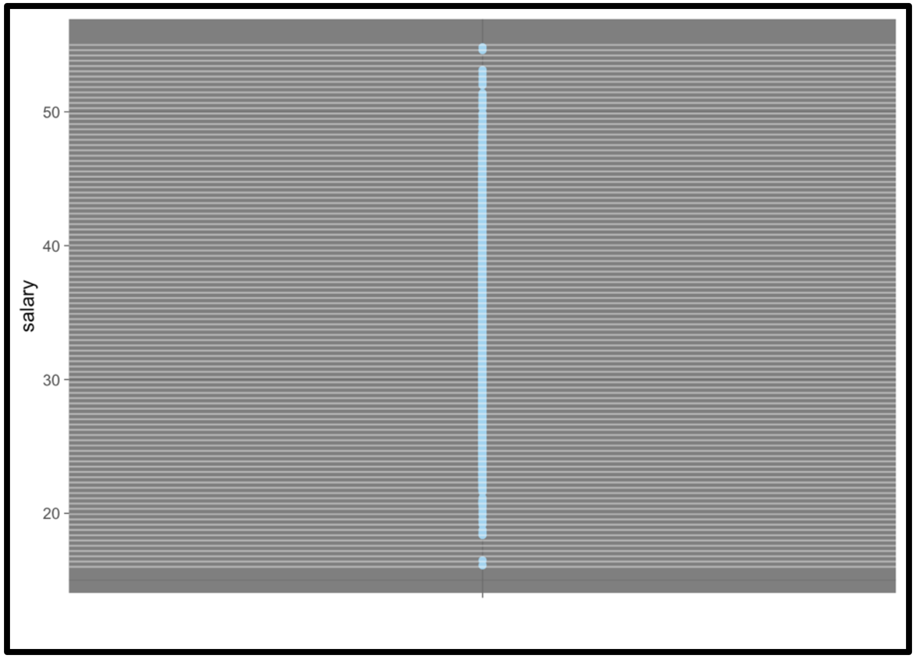
```
MSE0=function(DATA,COEF){
  ERROR=DATA$salary-MODEL0(DATA,COEF)
  LOSS=mean(ERROR^2)
  return(LOSS)
}
MAE0=function(DATA,COEF){
  ERROR=DATA$salary-MODEL0(DATA,COEF)
  LOSS=mean(abs(ERROR))
  return(LOSS)
}
```

Empty Model: Optimization

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

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

  - All Possible Models



Empty Model: Optimization

- 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: Optimization

- 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(salary~1,data=TRAIN)
coef(LM0)
```

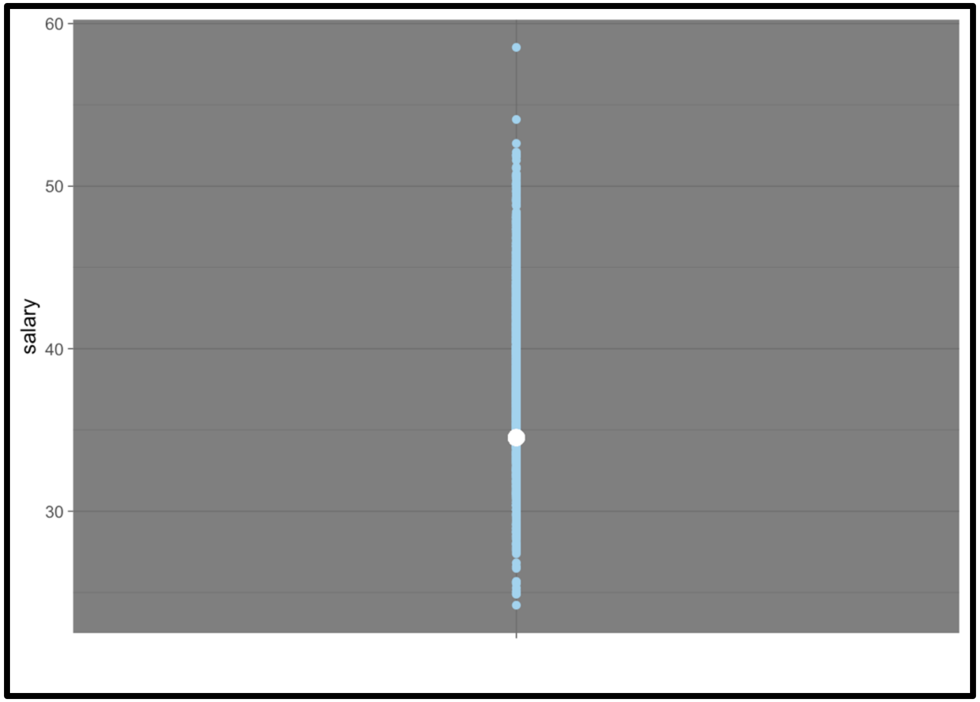
```
## (Intercept)
##    34.53428
```

Empty Model: Final Model

- Final MODEL 0

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

- Prediction on Test Data:

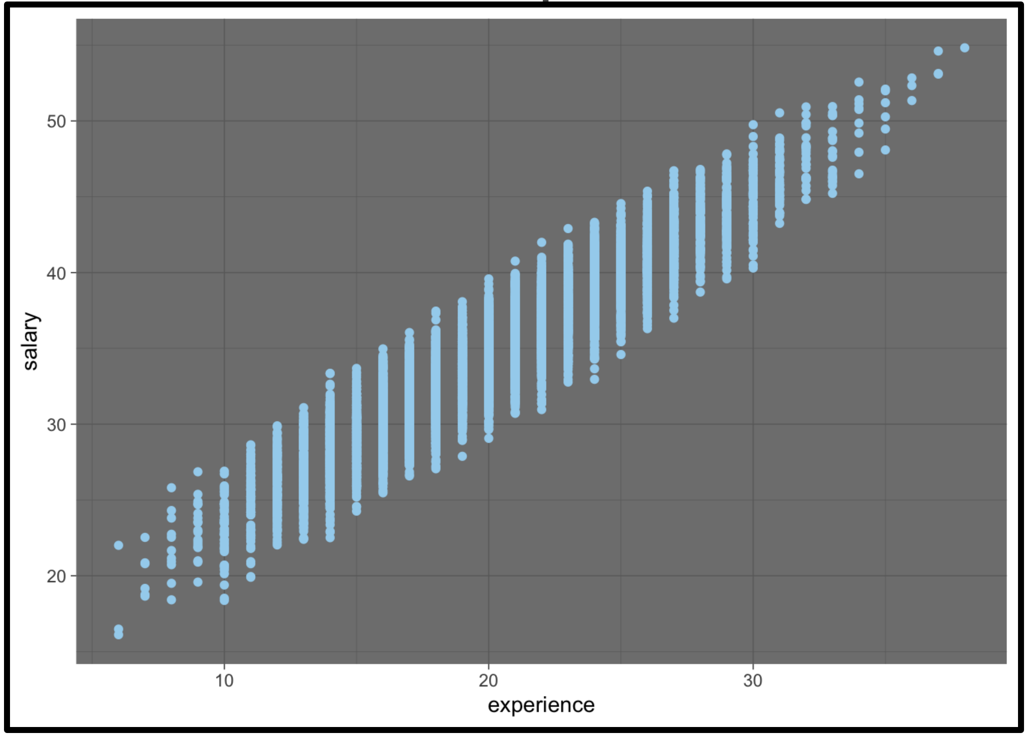


Model 1A

- MODEL 1A

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

- Visualization of Relationship



Model 1A

- Function to Get Fitted Values

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

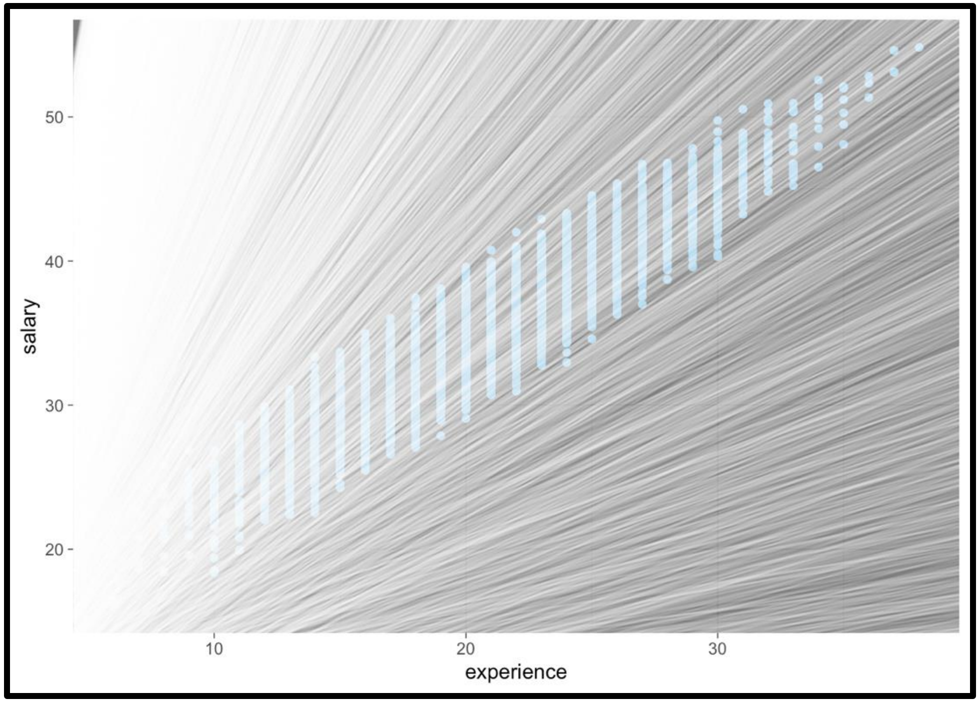
- Functions to Evaluate Model

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

Model 1A: Optimization

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

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



Model 1A: Optimization

- 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
```

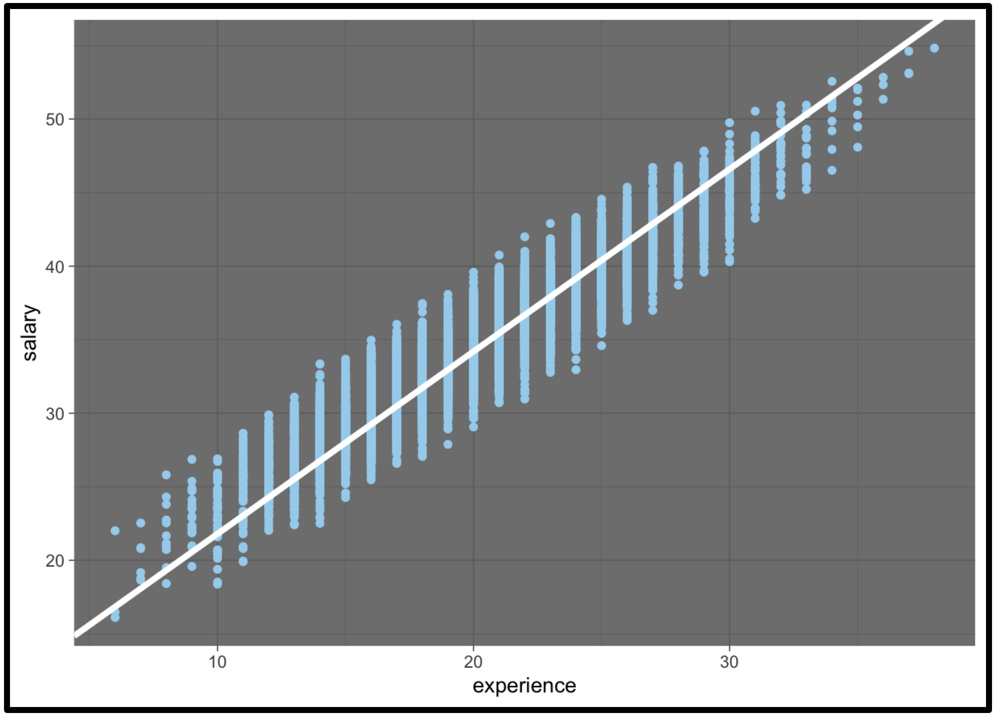
Model 1A: Final Model

- Final MODEL 1A

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

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

- Fitted on Train Data



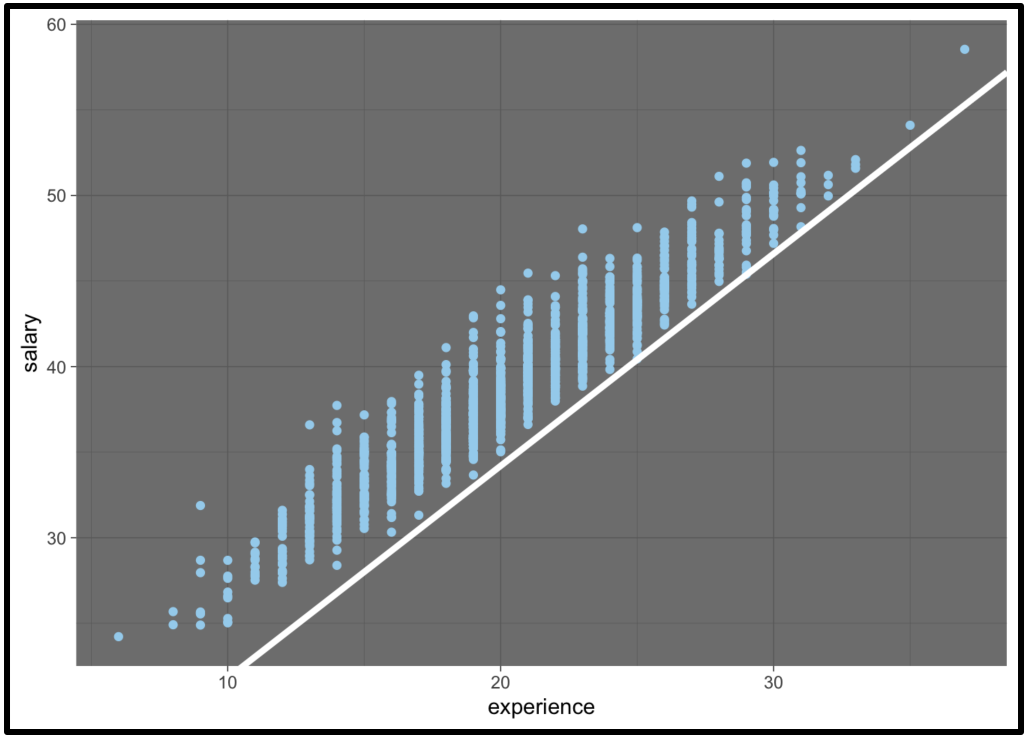
Model 1A: Final Model

- Final MODEL 1A

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

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

- Prediction on Test Data

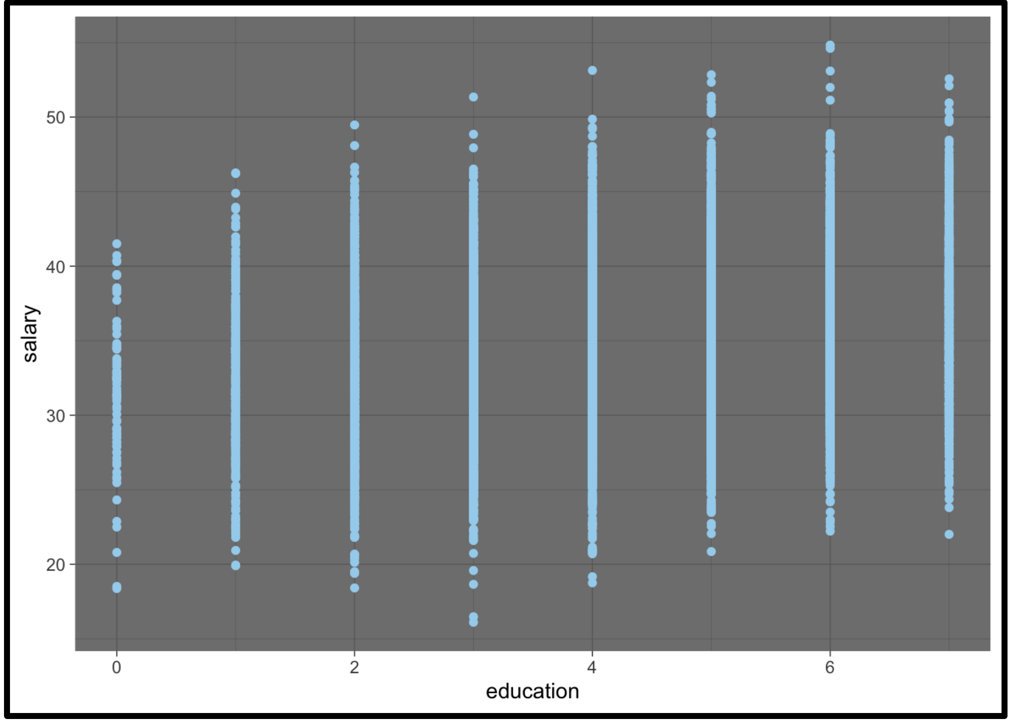


Model 1B

- MODEL 1B

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

- Visualization of Relationship



Model 1B

- Function to Get Fitted Values

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

- Functions to Evaluate Model

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

Model 1B: Optimization

- Optimization
  - Use of optim() Function

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

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

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

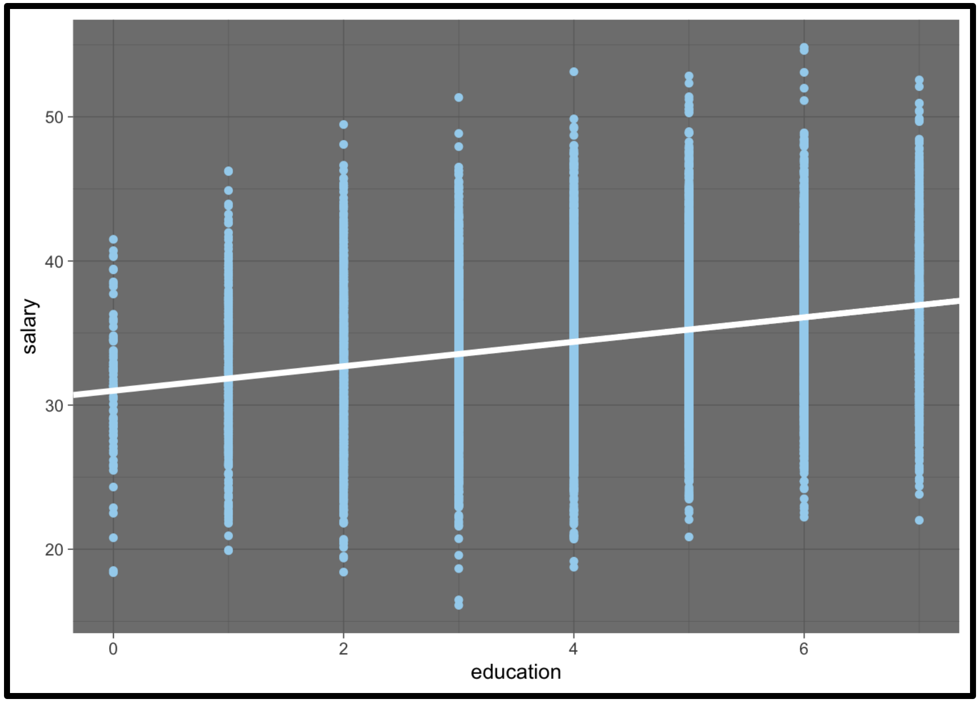
```
## [1] 30.6619753  0.8512186
```

Model 1B: Final Model

- Final MODEL 1B

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

- Fitted on Train Data

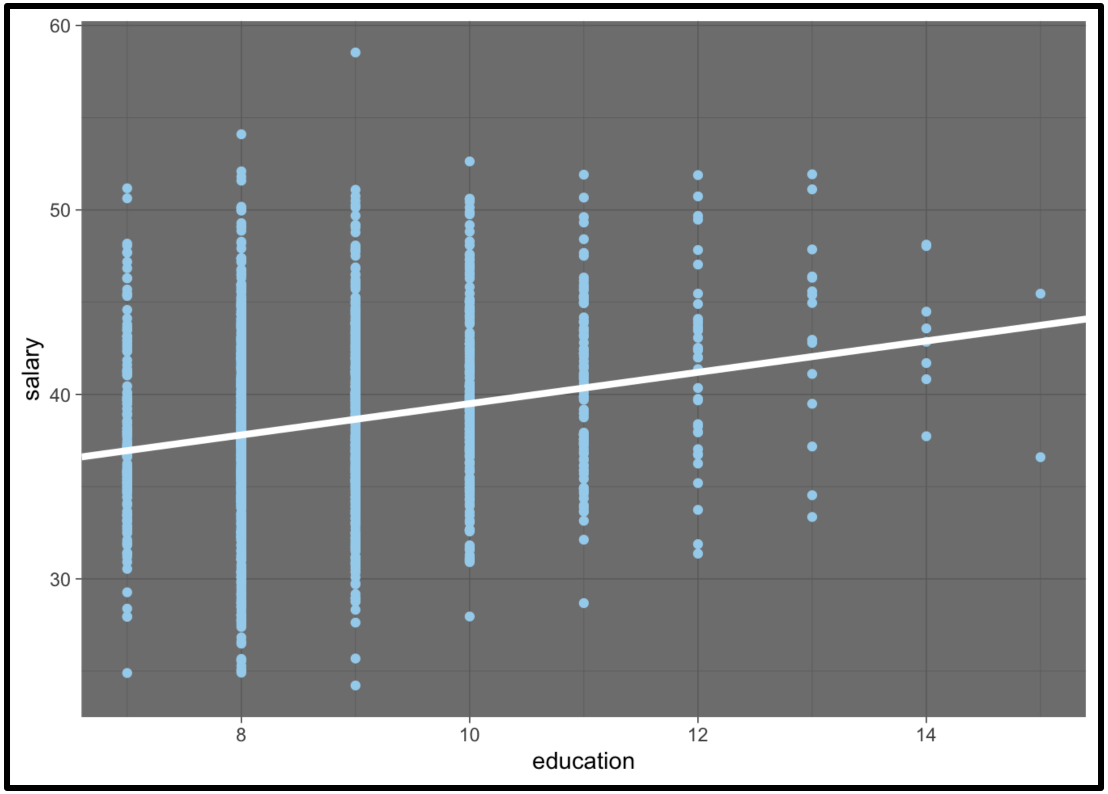


Model 1B: Final Model

- Final MODEL 1B

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

- Prediction on Test Data

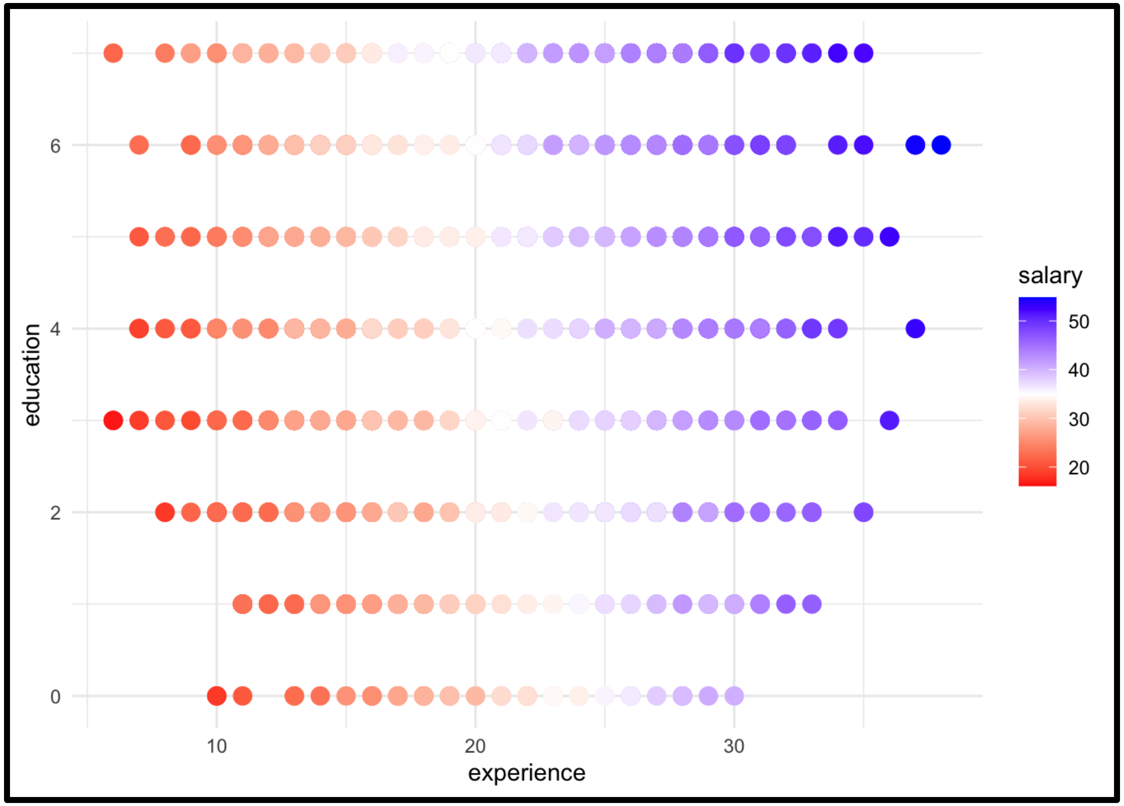


MODEL 2

- 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



MODEL 2

- Function to Get Fitted Values

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

- Functions to Evaluate Model

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

Multiple Regression

- Use lm() with summary()
- Final MODEL 2

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

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

```
LM2=lm(salary~experience+education,data=TRAIN)
summary(LM2)
```

```
##
## Call:
## lm(formula = salary ~ experience + education, 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 ***
## experience  1.079243   0.002474   436.3 <0.0000000000000002 ***
## education   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
```

Model Summary

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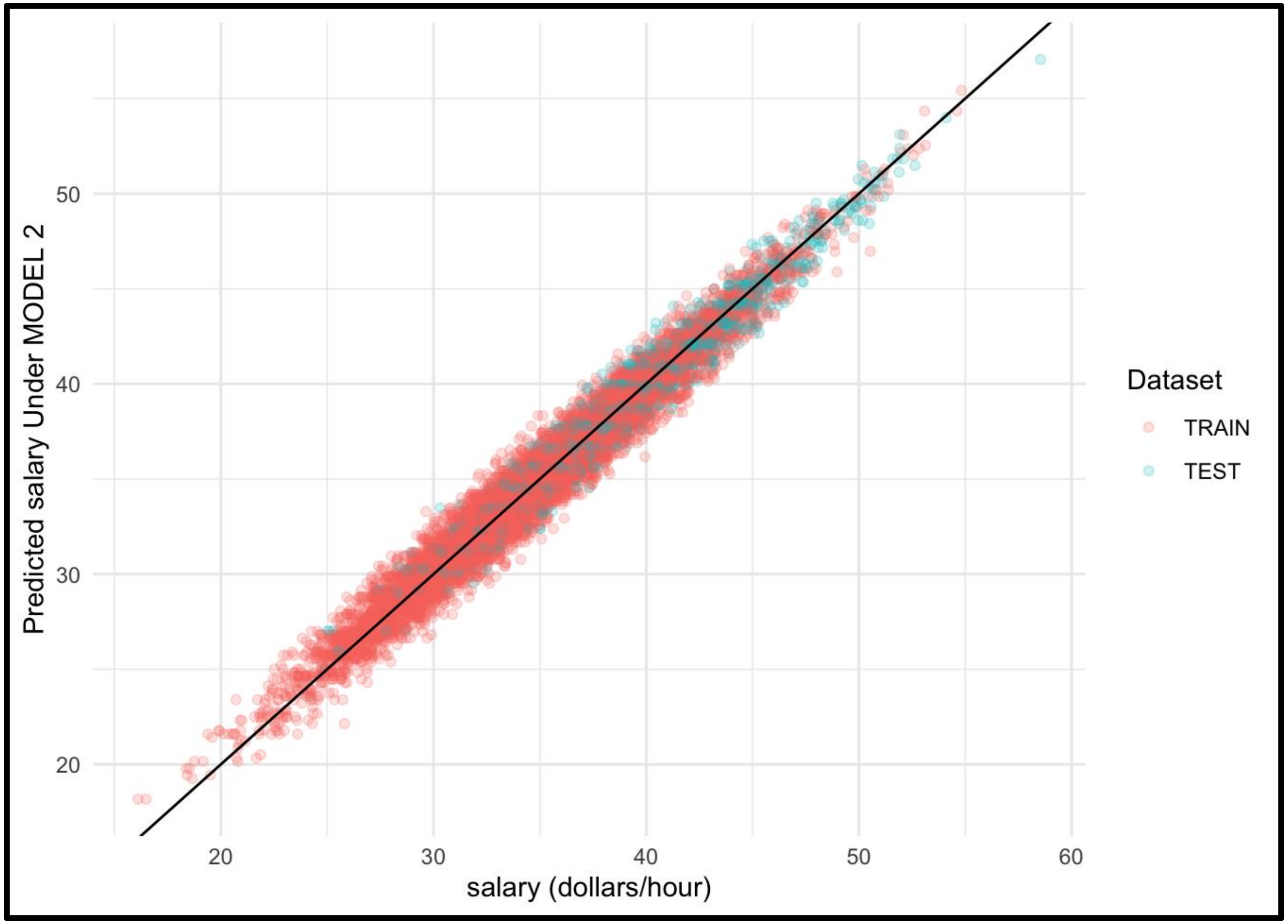
```
LM2=lm(salary~experience+education,data=TRAIN)
summary(LM2)
```

```
##
## Call:
## lm(formula = salary ~ experience + education, 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 ***
## experience  1.079243   0.002474   436.3 <0.0000000000000002 ***
## education   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
```

Visualization

- Comparing Predicted Values to Actual Values for MODEL 2



Model Evaluation

- Out-of-Sample Evaluation

```
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
```