# Notes 7 - Advanced Regression

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Math 3190

1. Weighted Least Squares
2. Regularization – Ridge Regression, LASSO, and Elastic Net
3. Poisson Regression
4. Partial Least Squares Regression

# Introduction

In MATH 2140 or 3150 - Applied Statistics, we discussed many topics in regression. We'll discuss a few more advanced regression techniques:

- Weighted least squares
- Regularization
  - Ridge regression
  - LASSO
  - Elastic net
- Poisson regression
- Partial least squares regression

Section 1

# Weighted Least Squares

# WLS - Matrix Formulation

We are used to regression models being written

$$\hat{y}_i = \hat{\beta}_0 + \hat{\beta}_1 x_{i1} + \cdots + \hat{\beta}_{p-1} x_{i,p-1}$$

We can write this in matrix-vector form. If we define $\hat{\boldsymbol{y}} = [\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_n]^T_{n\times 1}$, $\boldsymbol{\beta} = [\beta_0, \beta_1, \ldots, \beta_{p-1}]^T_{p\times 1}$, and $\mathbf{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1,p-1} \\ 1 & x_{21} & x_{22} & \cdots & x_{2,p-1} \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{n,p-1} \end{bmatrix}_{n\times p}$ then

that equation above can be written

$$\hat{\boldsymbol{y}}_i = \mathbf{X}_i \boldsymbol{\beta}$$

and then all $n$ equations for the $y$ values can be written

$$\hat{\boldsymbol{y}} = \mathbf{X}\boldsymbol{\beta}$$

# WLS - Matrix Formulation

In ordinary least squares (OLS) regression, we determine the estimates for the $\beta$ values by computing

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\boldsymbol{y}$$

Then we can compute standard errors for these estimates as long as the **linear regression assumptions** hold:

1. The residuals have zero mean (the relationship is linear).
2. The residuals are normally distributed.
3. The residuals have the same variance.
4. The residuals are independent.

If the homogeneity of variance assumption is violated, then the standard errors of the estimated $\beta_i$ values are usually incorrect and not especially helpful when constructing confidence intervals.

# WLS - Standard Errors

We can obtain the standard errors of the estimates by computing the variance-covariance matrix in the following manner:

$$\boldsymbol{\sigma^2_B} = \begin{bmatrix} \text{Var}(\hat{\beta}_0) & \text{Cov}(\hat{\beta}_0, \hat{\beta}_1) & \dots & \text{Cov}(\hat{\beta}_0, \hat{\beta}_{p-1}) \\ \text{Cov}(\hat{\beta}_1, \hat{\beta}_0) & \text{Var}(\hat{\beta}_1) & \dots & \text{Cov}(\hat{\beta}_1, \hat{\beta}_{p-1}) \\ \vdots & \vdots & \ddots & \vdots \\ \text{Cov}(\hat{\beta}_{p-1}, \hat{\beta}_0) & \text{Cov}(\hat{\beta}_{p-1}, \hat{\beta}_1) & \dots & \text{Var}(\hat{\beta}_{p-1}) \end{bmatrix} = \sigma^2_\epsilon (\mathbf{X}^T \mathbf{X})^{-1}$$

This means that the standard errors can be obtained by taking the square root of the diagonals of this matrix.

# WLS - Standard Errors

Consider this example of attempting to predict blood pressure using age.

```
library(tidyverse)
bp <- read_table("blood_pressure.txt") |>
  rename(bp = diastolic_blood_pressure)
bp_mod <- lm(bp ~ age, data = bp)
X <- model.matrix(bp_mod)
var_matrix <- summary(bp_mod)$sigma^2 * solve(t(X) %*% X)
std_errors <- var_matrix |> diag() |> sqrt()
std_errors
```

```
## (Intercept)         age
##  3.99367376  0.09695116
```

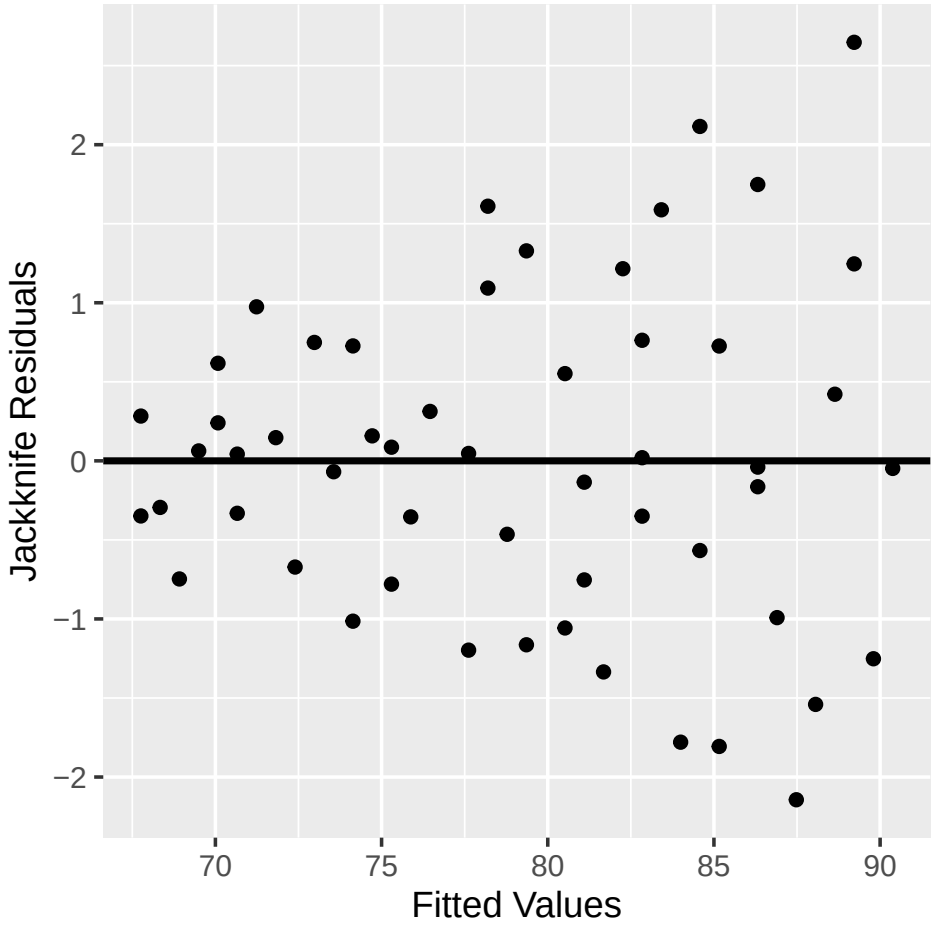
# WLS - Standard Errors

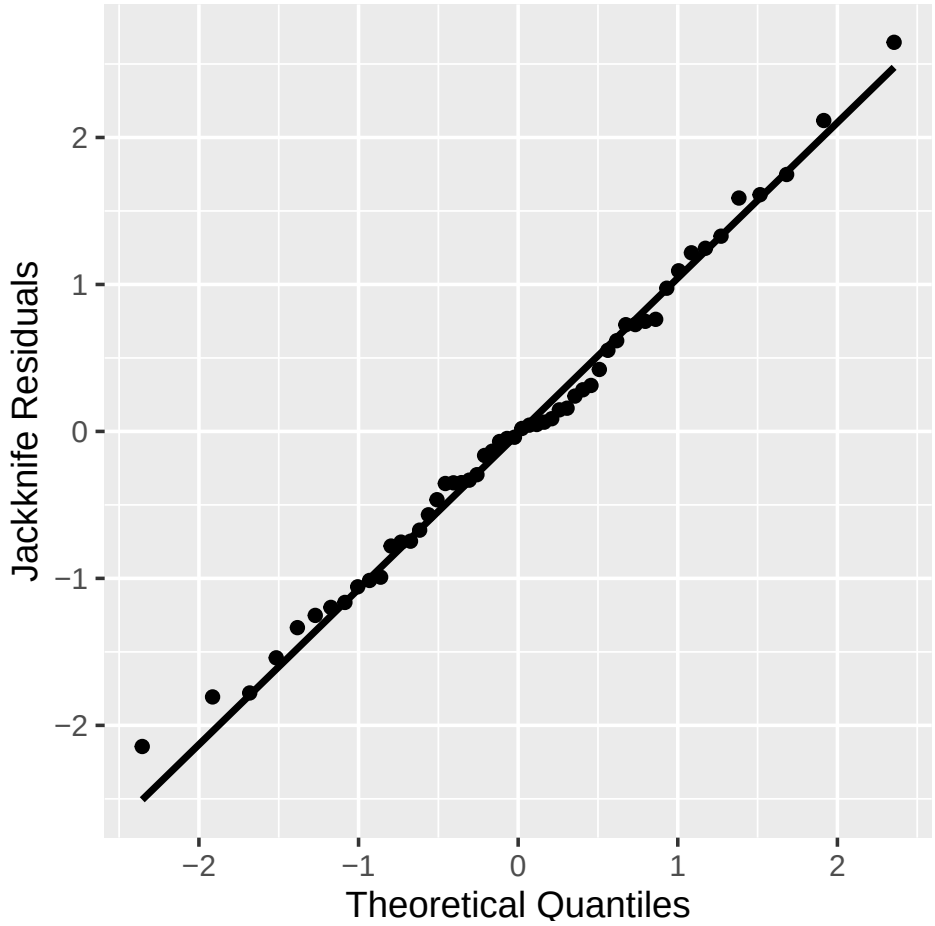
```
# Compare to summary output
summary(bp_mod)
```

```
##
## Call:
## lm(formula = bp ~ age, data = bp)
##
## Residuals:
##      Min       1Q   Median       3Q      Max
## -16.4786  -5.7877  -0.0784   5.6117  19.7813
##
## Coefficients:
##             Estimate Std. Error t value Pr(>|t|)
## (Intercept) 56.15693    3.99367  14.061  < 2e-16 ***
## age          0.58003    0.09695   5.983 2.05e-07 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 8.146 on 52 degrees of freedom
## Multiple R-squared:  0.4077, Adjusted R-squared:  0.3963
## F-statistic: 35.79 on 1 and 52 DF,  p-value: 2.05e-07
```

# WLS - Original Diagnostic Plots

Below is what the diagnostic plots looks like for this example:



# WLS - Weighted Least Squares

In order to adjust so the estimates and standard errors are not as effected by the points that have large residuals, we can **weight** each observation. We will define a vector of weights as $\boldsymbol{w} = [w_1, w_2, \ldots, w_n]^T$ and a matrix of the weights as

$$\mathbf{W} = \begin{bmatrix} w_1 & 0 \ldots & 0 & \\ 0 & w_2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & w_n \end{bmatrix}$$

We can then obtain the weighted estimates of the coefficients, called $\hat{\beta}_{\boldsymbol{w}}$, by computing

$$\hat{\beta}_{\boldsymbol{w}} = (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}\boldsymbol{y}$$

with variance-covariance matrix

$$\boldsymbol{\sigma}^2_{\boldsymbol{B}} = \sigma^2_\epsilon \cdot (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}.$$

# WLS - Selecting the Weights

In ordinary least squares (OLS), we assume $\text{Var}(\epsilon_i) = \sigma_\epsilon^2$ for all $i$. In WLS, we instead allow for each error to have its own variance. So, we have $\text{Var}(\epsilon_i) = \sigma_i^2 = \sigma_\epsilon^2 / w_i$. Our best guess for $\sigma_\epsilon^2$ is the mean square error (MSE). That is what we typically denote as $s_\epsilon^2$.

Now we need to determine the best values for the weights. First, we must obtain an estimate for the variance function for the residuals. This will depend on the residual plot(s), but the most common situation for using weighted least squares is when the residuals plotted against the fitted values has a fan shape. In this scenario, we can estimate the weights by:

1. Fit an ordinary least squares model (and verify that a residual plot against the fitted values has a fan shape).
2. Fit a new linear model by regressing the absolute value of the residuals on the fitted values. That is, use $|\hat{\epsilon}|$ as $y$ and $\hat{y}$ as $x$.
3. Let the weights be the reciprocals of the squares of the fitted values of that second model.

# WLS - Assessing the Adequacy of the Weights

Each of the following should be true when using weighted least squares:

1. The estimates of the $\beta$ values using WLS should be very close to the estimates of the $\beta$ values using OLS.
2. The weighted mean square error ($MSE_w$) should be close to 1.
3. The residual plot of the jackknife residuals should have constant variance.

Also note the following things about WLS:

1. $R^2$ has no real meaning in weighted least squares and should not be considered. We should use the $R^2$ from the OLS model.
2. Externally studentized (jackknife) residuals take into account the weights, so they should be used in residual plots for model diagnostics.
3. For QQ plots, use the unstudentized residuals. Either the raw of standardized are fine.

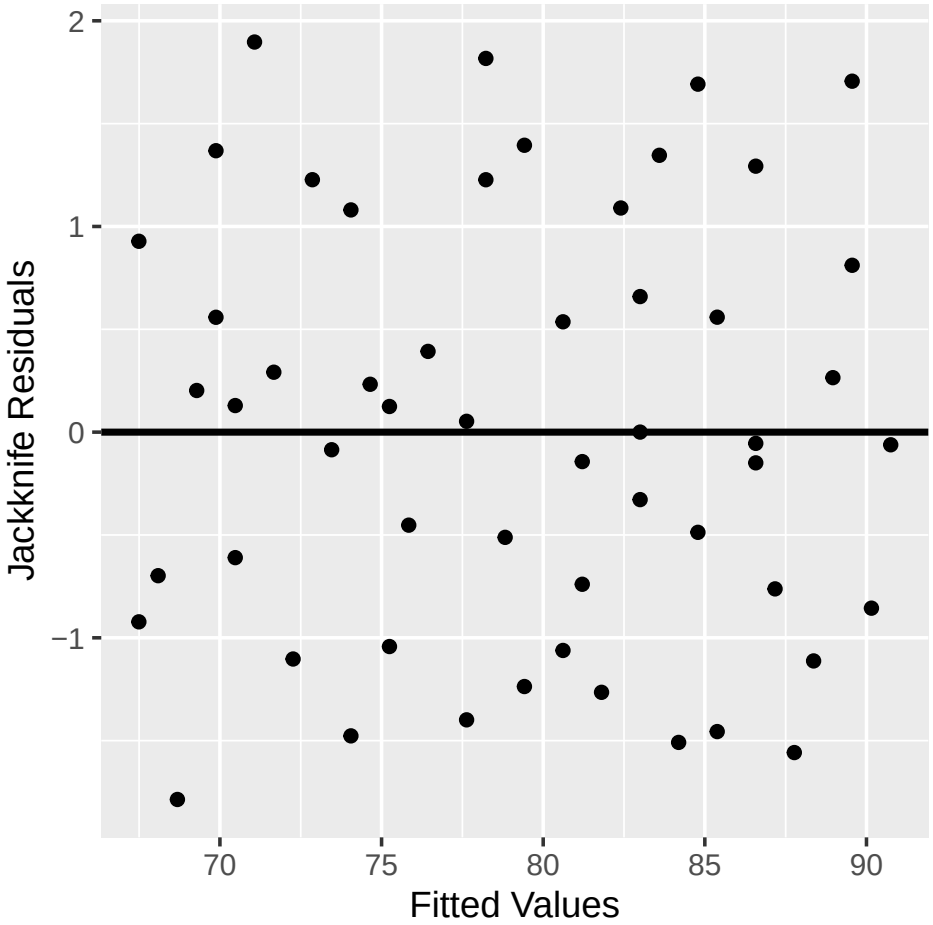
# WLS - Weighted Fit

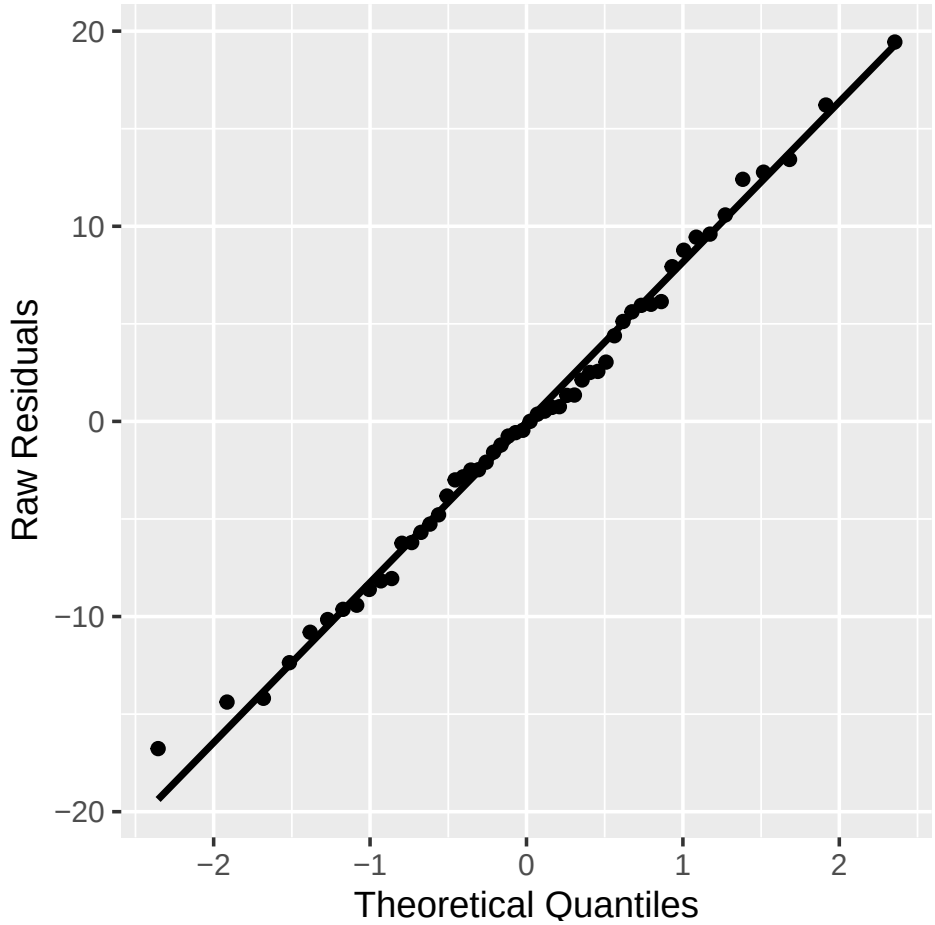
```
bp_mod <- lm(bp ~ age, data = bp)
e_mod <- lm(abs(bp_mod$residuals) ~ bp_mod$fitted.values)
w <- 1/e_mod$fitted.values^2
bp_mod_w <- lm(bp ~ age, data = bp, weights = w)
summary(bp_mod_w)
```

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 55.56577    2.52092  22.042  < 2e-16 ***
age          0.59634    0.07924   7.526 7.19e-10 ***
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 1.213 on 52 degrees of freedom
Multiple R-squared:  0.5214,    Adjusted R-squared:  0.5122
F-statistic: 56.64 on 1 and 52 DF,  p-value: 7.187e-10
```

# WLS - Weighted Diagnostic Plots



# WLS - Confidence Intervals

We can easily obtain confidence intervals for the $\beta$'s by using the `confint()` function. The variance-covariance matrix is now $\sigma_\epsilon^2(\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}$.

To obtain confidence intervals for predictions, that is, a confidence interval for $E(y|\mathbf{x}^*)$, we first consider what the CI looks like in the OLS case. For obtaining the $(1-\alpha)\cdot 100\%$ confidence interval for $E(y|\boldsymbol{x}^*)$ at a specific row vector $\boldsymbol{x}^* = \begin{bmatrix} 1 & x_1^* & \dots & x_n^* \end{bmatrix}$ is given by

$$\hat{y}|\boldsymbol{x}^* \pm t_{\alpha/2} s_\epsilon \sqrt{\boldsymbol{x}^*(\mathbf{X}^T\mathbf{X})^{-1}(\boldsymbol{x}^*)^T}$$

For weighted least squares, we just need to insert the weight matrix:

$$\hat{y}|\boldsymbol{x}^* \pm t_{\alpha/2} s_w \sqrt{\boldsymbol{x}^*(\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}(\boldsymbol{x}^*)^T}$$

where $s_w$ is the square root of the weighted MSE.

# WLS - Confidence Intervals

An example for obtaining the bounds for blood pressure at age 50:

```
W <- diag(w)
n <- nrow(bp)
alpha <- 0.05
x_star <- matrix(c(1, 50), nrow = 1)
yhat <- predict(bp_mod, data.frame(age = 50))
yhat_w <- predict(bp_mod_w, data.frame(age = 50))
se <- summary(bp_mod)$sigma
se_w <- summary(bp_mod_w)$sigma
# OLS Bounds
yhat - qt(1-alpha/2, n-2)*se*sqrt(x_star%*%solve(t(X)%*%X)%*%t(x_star))
```

```
##          [,1]
## [1,] 82.14817
```

```
yhat + qt(1-alpha/2, n-2)*se*sqrt(x_star%*%solve(t(X)%*%X)%*%t(x_star))
```

```
##          [,1]
## [1,] 88.16877
```

```
# Verify using the predict function
predict(bp_mod, data.frame(age = 50), interval = "confidence")
```

```
##        fit      lwr      upr
## 1 85.15847 82.14817 88.16877
```

# WLS - Confidence Intervals

```
# WLS Bounds - Confidence Interval
yhat_w - qt(1-alpha/2, n-2)*se_w*sqrt(
  x_star%*%solve(t(X)%*%W%*%X)%*%t(x_star))
```

```
##           [,1]
## [1,] 81.84106
```

```
yhat_w + qt(1-alpha/2, n-2)*se_w*sqrt(
  x_star%*%solve(t(X)%*%W%*%X)%*%t(x_star))
```

```
##           [,1]
## [1,] 88.92464
```

```
# Verify using the predict function
predict(bp_mod_w, data.frame(age = 50),
        interval = "confidence")
```

```
##        fit      lwr      upr
## 1 85.38285 81.84106 88.92464
```

# WLS - Prediction Intervals

The prediction interval for OLS is computed with

$$\hat{y}|\boldsymbol{x}^* \pm t_{\alpha/2} s_\epsilon \sqrt{1 + \boldsymbol{x}^*(\mathbf{X}^T\mathbf{X})^{-1}(\boldsymbol{x}^*)^T}$$

For weighted least squares, we just need to change that 1 to 1 over the weight for that particular $\boldsymbol{x}^*$:

$$\hat{y}|\boldsymbol{x}^* \pm t_{\alpha/2} s_w \sqrt{\frac{1}{w^*} + \boldsymbol{x}^*(\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}(\boldsymbol{x}^*)^T}$$

where $w^*$ is the weight for the value we are predicting.

# WLS - Prediction Intervals

```
# Prediction interval OLS
yhat - qt(1-alpha/2, n-2)*se*sqrt(
  1+x_star%*%solve(t(X)%*%X)%*%t(x_star))
```

```
##           [,1]
## [1,] 68.53795
```

```
yhat + qt(1-alpha/2, n-2)*se*sqrt(
  1+x_star%*%solve(t(X)%*%X)%*%t(x_star))
```

```
##           [,1]
## [1,] 101.779
```

```
predict(bp_mod, data.frame(age = 50),
        interval = "prediction")
```

```
##        fit      lwr     upr
## 1 85.15847 68.53795 101.779
```

# WLS - Prediction Intervals

```
# Prediction interval WLS
# Get new weight for x = 50:
new_fit <- predict(bp_mod, data.frame(age = 50))
new_weight <- 1/predict(e_mod, data.frame(fitted = new_fit))^2
# Construct Intervals
yhat_w - qt(1-alpha/2, n-2)*se_w*sqrt(
  1/new_weight + x_star%*%solve(t(X)%*%W%*%X)%*%t(x_star))
```

```
##           [,1]
## [1,] 64.72992
```

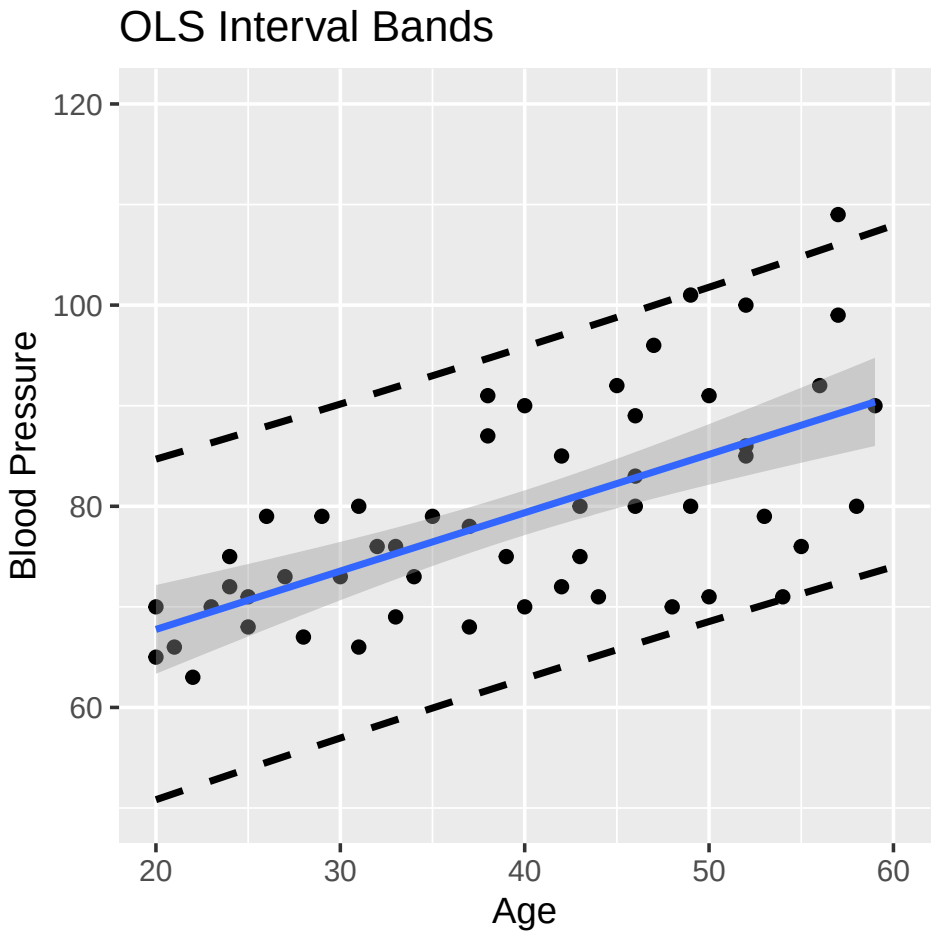
```
yhat_w + qt(1-alpha/2, n-2)*se_w*sqrt(
  1/new_weight + x_star%*%solve(t(X)%*%W%*%X)%*%t(x_star))
```

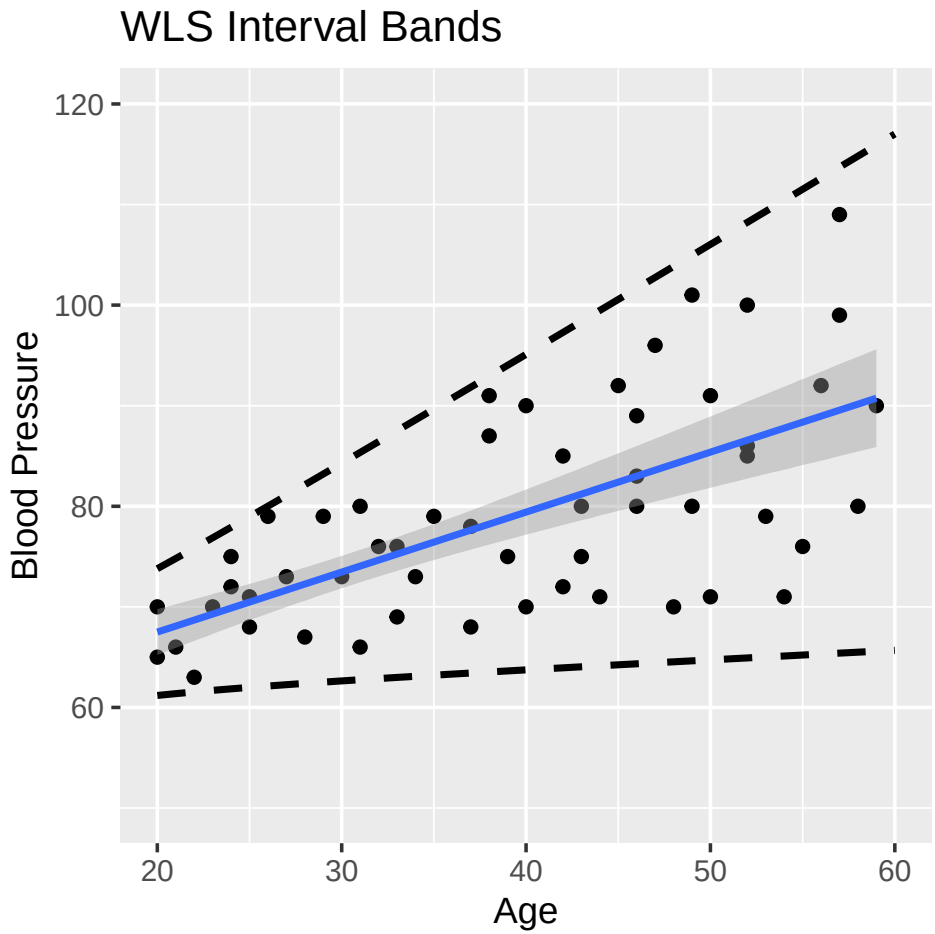
```
##           [,1]
## [1,] 106.0358
```

```
predict(bp_mod_w, data.frame(age = 50), interval = "prediction",
        weight = new_weight)
```

```
##        fit      lwr      upr
## 1 85.38285 64.72992 106.0358
```

# WLS - Interval Plots



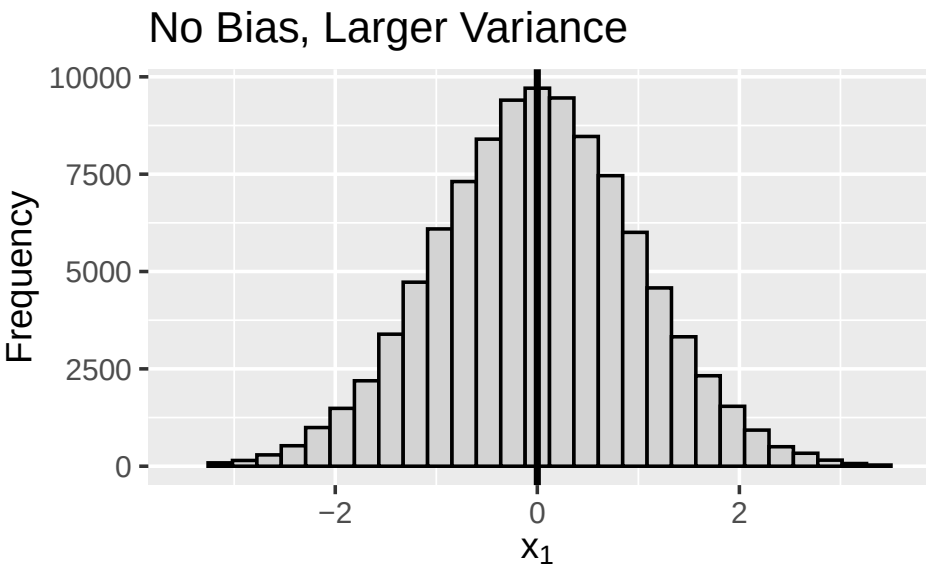
Section 2

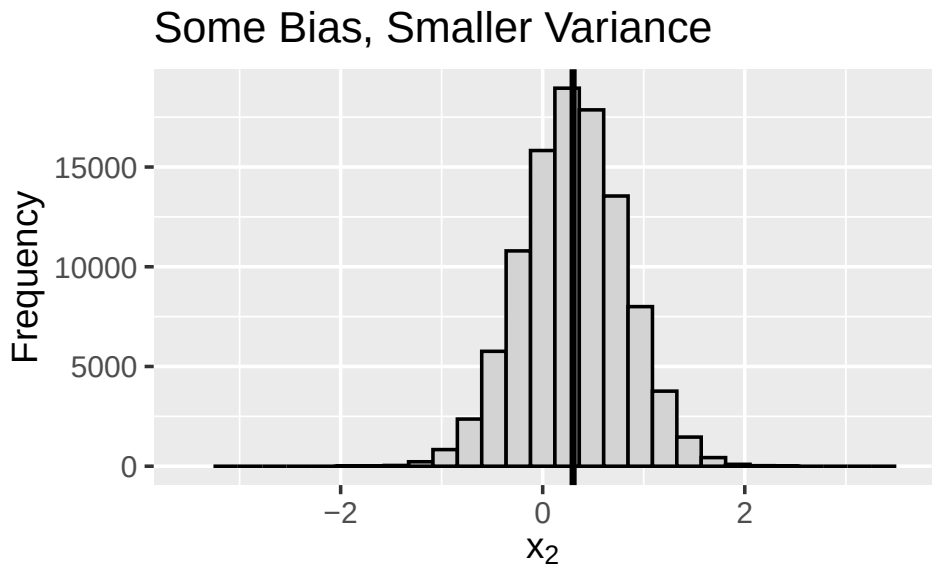
# Regularization – Ridge Regression, LASSO, and Elastic Net

# Bias-Variance Trade Off

In statistical estimation, there is often a trade off between bias and variance. Many statistical methods, like least squares regression, guarantee that the estimate is **unbiased**, which means that the sampling distribution of the statistic is centered at the parameter it is estimating.

However, these unbiased estimators will often have more uncertainty, a higher variance, than some biased estimators. When this is the case, the biased estimator that is more precise may be preferred.



# Bias-Variance tradeoff

In statistics and machine learning, the **bias–variance tradeoff** is the property of a model that the variance of the parameter estimated across samples can be reduced by increasing the bias in the estimated parameters.

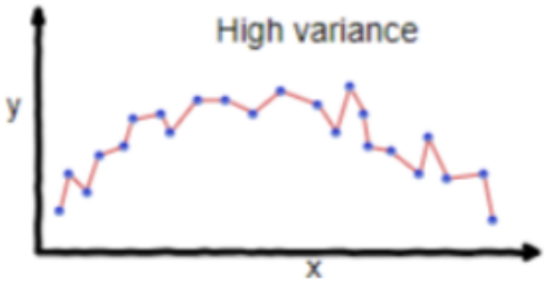
The **bias–variance dilemma** or **bias–variance problem** is the conflict in trying to simultaneously minimize these two sources of error that prevent supervised learning algorithms from generalizing beyond their training set

(Source: Wikipedia)

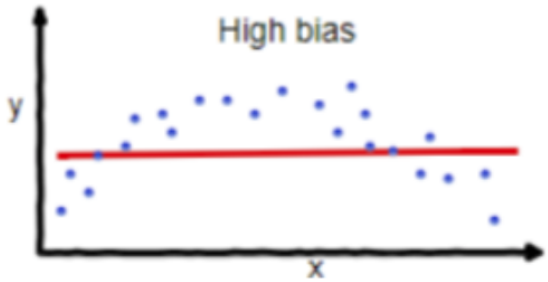
# Bias-Variance tradeoff

The **bias** is an error from faulty assumptions or mispecification of the learning algorithm. High bias can cause an algorithm to miss the relevant relations between features and target outputs (underfitting).

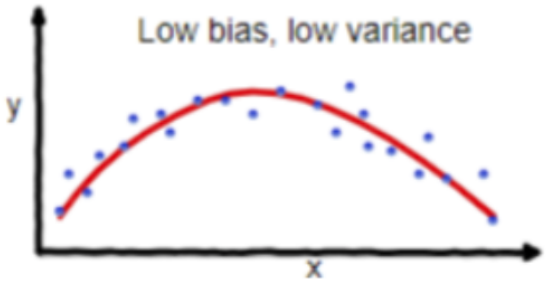
The **variance** is an error from sensitivity to small fluctuations in the training set. High variance may result from an algorithm modeling the random noise in the training data (overfitting).




**overfitting**

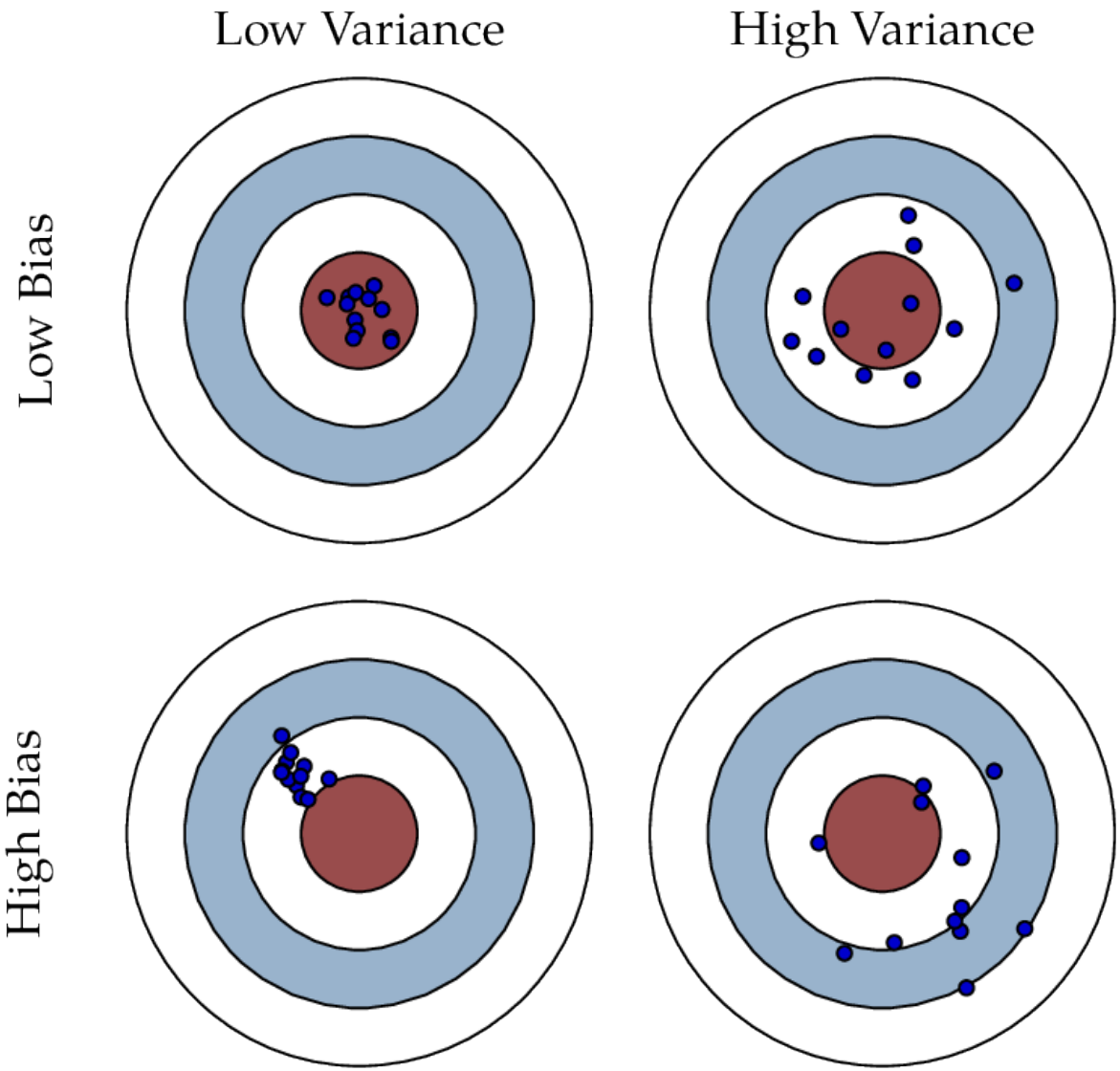



**underfitting**




**Good balance**

# Bias-Variance tradeoff



# Bias-Variance tradeoff

The bias–variance tradeoff is a central problem in supervised learning. Ideally, one wants to choose a model that both accurately captures the regularities in its training data, but also generalizes well to unseen data.

Unfortunately, it is typically impossible to do both simultaneously. High-variance learning methods may be able to represent their training set well but are at risk of overfitting to noisy or unrepresentative training data. In contrast, algorithms with high bias typically produce simpler models that may fail to capture important regularities (i.e. underfit) in the data.

# Regularization in Machine Learning

In regression analysis, the features are estimated using coefficients while modeling. In small sample sizes or noisy data coefficient estimates could be anecdotally incorrect (e.g., overfitting) or inaccurate.

If the estimates can be restricted, penalized, or shrunk towards zero, then the impact of insignificant features might be reduced and would prevent models from high variance with a stable fit.[1]

[1] Adapted from:
https://www.analyticssteps.com/blogs/l2-and-l1-regularization-machine-learning

# Regularization in Machine Learning

**Regularization** is the most used technique to penalize complex models in machine learning, it is deployed for reducing overfitting (or, contracting generalization errors) by putting small network weights into the model (adding a small amount of bias). Also, it enhances the performance of models for new inputs.

Examples of regularization in machine learning, include:

- K-means: Restricting the segments for avoiding redundant groups.
- Neural networks: Confining the complexity (weights) of a model.
- Random forests: Reducing the depths of tree and branches (new features).

# Ridge Regression

Ridge regression **regularizes** (shrinks) coefficients by imposing a penalty on their size. The ridge coefficients minimize a penalized sum of squared error:

$$\hat{\boldsymbol{\beta}}_{\text{ridge}} = \arg\min_{\boldsymbol{\beta}} \left\{ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{p-1} x_{ij}\beta_j)^2 + \lambda \sum_{j=1}^{p-1} \beta_j^2 \right\},$$

where $\lambda \geq 0$ is a parameter that controls the shrinkage. The larger the value of $\lambda$ the more shrinkage (towards 0).

# Ridge Regression

Or in matrix form, ridge regression minimizes:

$$\hat{\beta}_{\text{ridge}} = \arg\min_{\beta} \left\{ (\mathbf{y} - \mathbf{X}\beta)^T (\mathbf{y} - \mathbf{X}\beta) + \lambda \beta^T \beta \right\}.$$

With a little work, the ridge regression solution can be shown to be:

$$\hat{\beta}_{ridge} = (\mathbf{X}^T\mathbf{X} + \lambda \mathbf{I}_N)^{-1}\mathbf{X}^T\mathbf{y}$$

# Penalty Terms

The regularization for ridge regression, $\lambda\beta^T\beta$, is usually denoted as an **L2 regularization** or **L2 penalty**, as it adds a penalty which is equal to the square of the magnitude of coefficients. Both Ridge regression and Support Vector Machines (SVMs) implement this method.

L2 regularization can deal with multicollinearity problems (independent variables are highly correlated) through constricting the coefficient while keeping all the variables in a model.

However, L2 regularization is not an effective method for selecting relevant predictors (or removing redundant parameters). We will use a **L1 regularization** for this purpose.

# LASSO Regression

LASSO (Least Absolute Shrinkage and Selection Operator) regression also **regularizes** coefficients by imposing a penalty on their size, but it uses an **L1** penalty. The LASSO coefficients minimize the following cost function:

$$\hat{\beta}_{\text{lasso}} = \arg\min_{\beta} \left\{ \sum_{i=1}^{n} (y_i - \sum_{j=1}^{p-1} x_{ij}\beta_j)^2 + \alpha \sum_{j=1}^{p-1} |\beta_j| \right\},$$

where $\alpha \geq 0$ is a parameter that controls the shrinkage. The larger the value of $\alpha$ the more shrinkage (towards 0).

# LASSO Regression

Notice the similarity to the ridge regression problem: the L2 ridge penalty $\sum_{j=1}^{p-1} \beta_j^2$ is replaced by the L1 lasso penalty $\sum_{j=1}^{p-1} |\beta_j|$.

This latter constraint makes the solutions nonlinear in the $y_i$, and there is no closed form expression for the LASSO as was the case in ridge regression.

Because of the nature of the constraint, making $\alpha$ sufficiently small will cause some of the coefficients to be exactly zero. Thus the LASSO does a kind of continuous subset selection, or conducts a **variable selection**.

# LASSO vs Ridge Regression

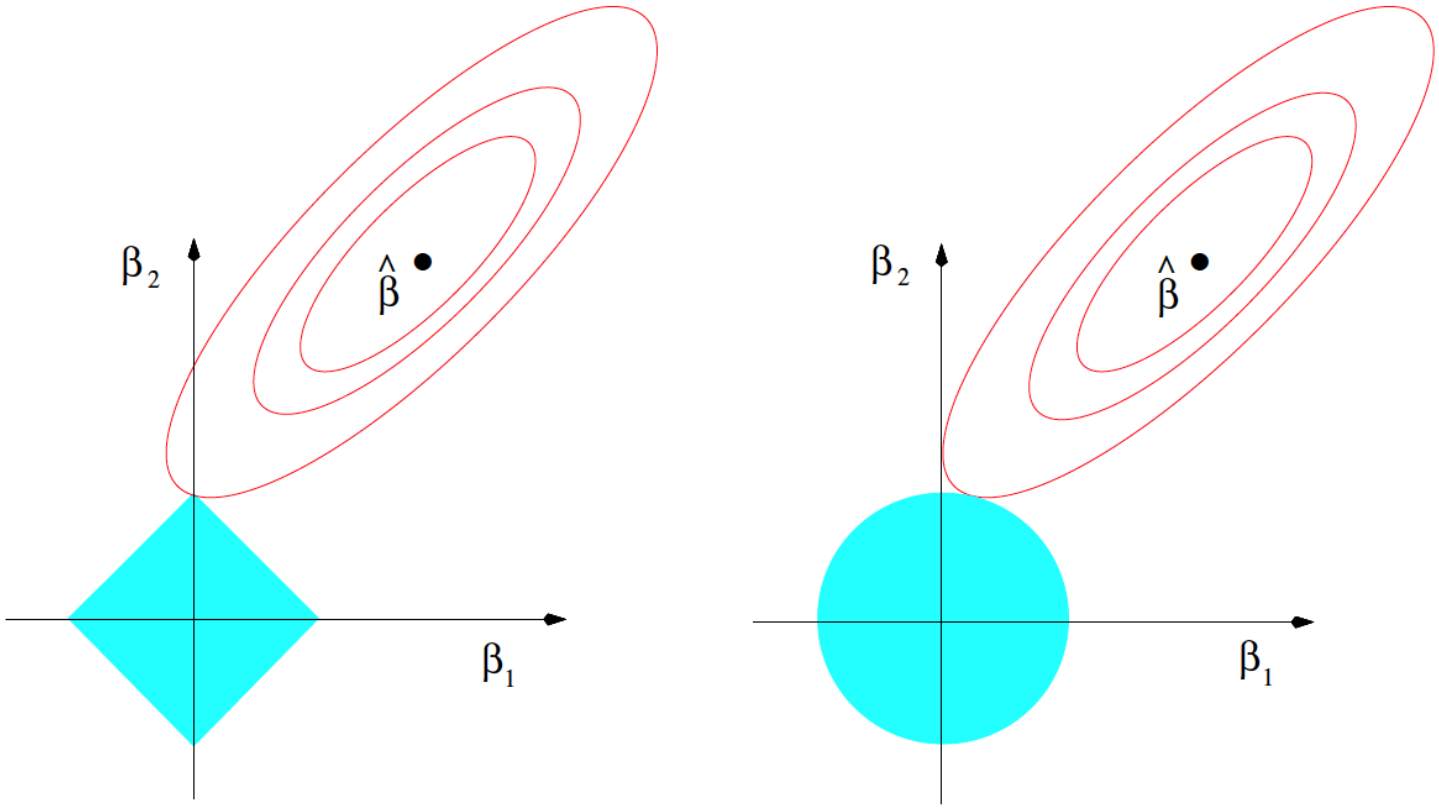



**FIGURE 3.11.** *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$*, respectively, while the red ellipses are the contours of the least squares error function.*

(Elements of Statistical Learning, Hastie, Tibshirani, Friedman, by Springer)

# LASSO vs Ridge Regression

| S.No | L1 Regularization | L2 Regularization |
|---|---|---|
| 1 | Panelizes the sum of absolute value of weights. | penalizes the sum of square weights. |
| 2 | It has a sparse solution. | It has a non-sparse solution. |
| 3 | It gives multiple solutions. | It has only one solution. |
| 4 | Constructed in feature selection. | No feature selection. |
| 5 | Robust to outliers. | Not robust to outliers. |
| 6 | It generates simple and interpretable models. | It gives more accurate predictions when the output variable is the function of whole input variables. |
| 7 | Unable to learn complex data patterns. | Able to learn complex data patterns. |
| 8 | Computationally inefficient over non-sparse conditions. | Computationally efficient because of having analytical solutions. |

(https://www.analyticssteps.com/blogs/l2-and-l1-regularization-machine-learning)

# Elastic Net Regularization

Which should we choose? Ridge or LASSO? Well, why do we have to choose?!

Instead use the **Elastic Net** that minimizes:

$$\hat{\beta}_{\text{elastic net}} = \arg\min_{\beta} \left\{ \sum_{i=1}^{n} \left( y_i - \sum_{j=1}^{p-1} x_{ij}\beta_j \right)^2 + \alpha_1 \sum_{j=1}^{p-1} |\beta_j| + \alpha_2 \sum_{j=1}^{p-1} \beta_j^2 \right\},$$

for some $\alpha_1 \geq 0$ and $\alpha_2 \geq 0$.

The quadratic penalty term makes the loss function strongly convex, and it therefore has a unique minimum. The elastic net method includes Ridge regression, LASSO, and OLS by setting either $\alpha_1 = 0$, $\alpha_2 = 0$, or both to 0.

# Regression Regularization in R: glmnet

We can use the **glmnet** package to apply regularization in R:

```
install.packages("glmnet")
```

The default model used in the package is the "least squares" regression model and glmnet actually optimizes:

$$\hat{\beta}_{\text{elastic net}} = \arg\min_{\beta} \left\{ \sum_{i=1}^{n} \left( y_i - \sum_{j=1}^{p-1} x_{ij}\beta_j \right)^2 + \lambda \left( \alpha \sum_{j=1}^{p-1} |\beta_j| + \frac{(1-\alpha)}{2} \sum_{j=1}^{p-1} \beta_j^2 \right) \right\},$$

with $\alpha = 1$ as a default (so LASSO!).

# Regression Regularization in R: glmnet

As an example, let's look at a dataset for predicting body fat of a person using a variety of variables:

```
library(glmnet) |> suppressPackageStartupMessages()
library(faraway) |> suppressPackageStartupMessages()
fat_mod <- lm(
  brozek ~ age + weight + height + neck + chest +
    + abdom + hip + thigh + knee + ankle + biceps +
    forearm + wrist, data = fat
  )
# Removes intercept column since that is automatically added
X <- model.matrix(fat_mod)[,-1]
y <- fat$brozek
```

# Regression Regularization in R: glmnet

We fit the model using the most basic call to glmnet. $\alpha = 1$ by default, but let's also specified it here.

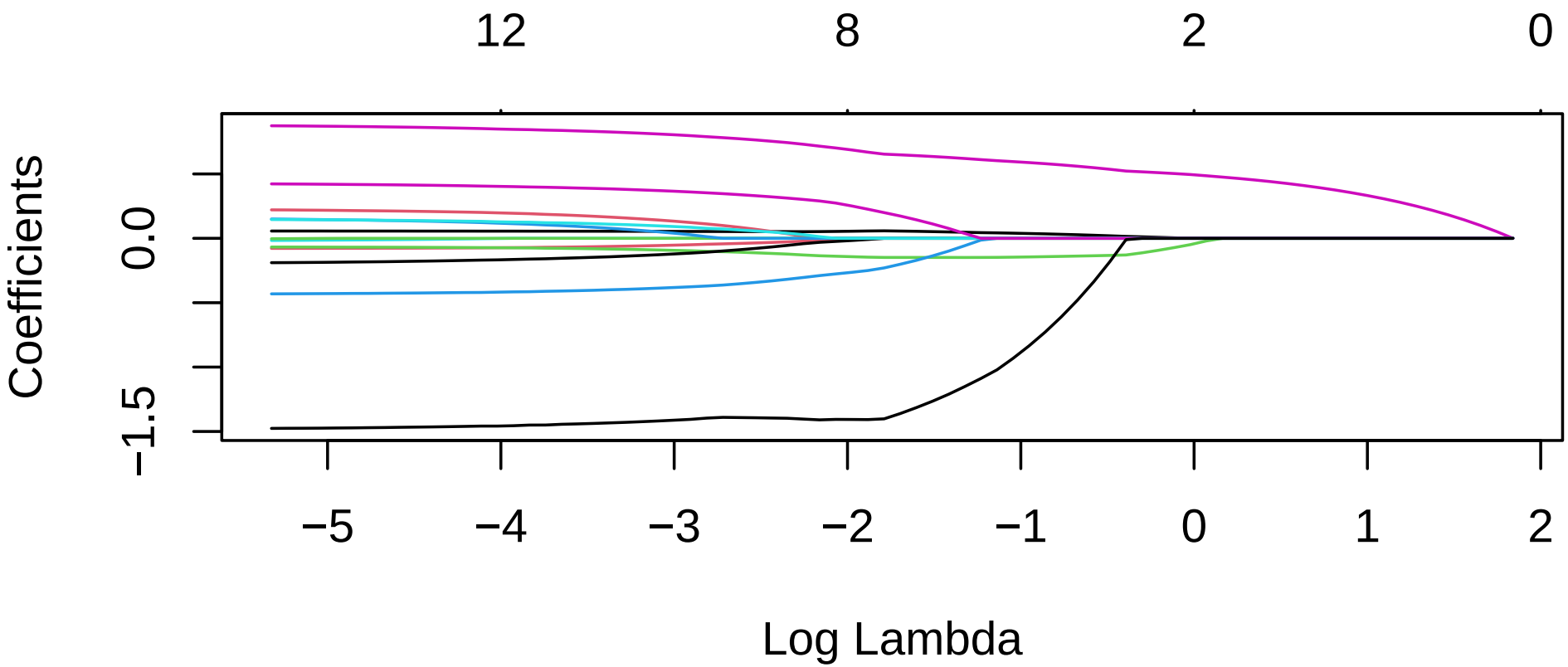
```
fit_lasso <- glmnet(X, y, alpha = 1) # Fits a LASSO
```

**fit_lasso** is now an object of class glmnet that contains all the relevant information of the fitted model for further use. There are various functions that work well with this class ob object such as `plot`, `print`, `coef` and `predict`.

# Regression Regularization in R: glmnet

We can visualize the size of the coefficients for different $\lambda$ values by using the `plot()` function:

```
plot(fit_lasso, "lambda")
```



# Regression Regularization in R: glmnet

A summary of the glmnet path at each step is displayed if we just enter the object name or use the print function:

```
print(fit_lasso)
```

```
##
## Call:  glmnet(x = X, y = y, alpha = 1)
##
##    Df  %Dev Lambda
## 1   0  0.00 6.2940
## 2   1 11.24 5.7350
## 3   1 20.57 5.2260
## 4   1 28.32 4.7610
## 5   1 34.76 4.3380
## 6   1 40.10 3.9530
## 7   1 44.53 3.6020
## 8   1 48.21 3.2820
## 9   1 51.27 2.9900
## 10  1 53.80 2.7250
## 11  1 55.91 2.4830
```

# Regression Regularization in R: glmnet

We can obtain the model coefficients at one or more $\lambda$ values within the range of the sequence:

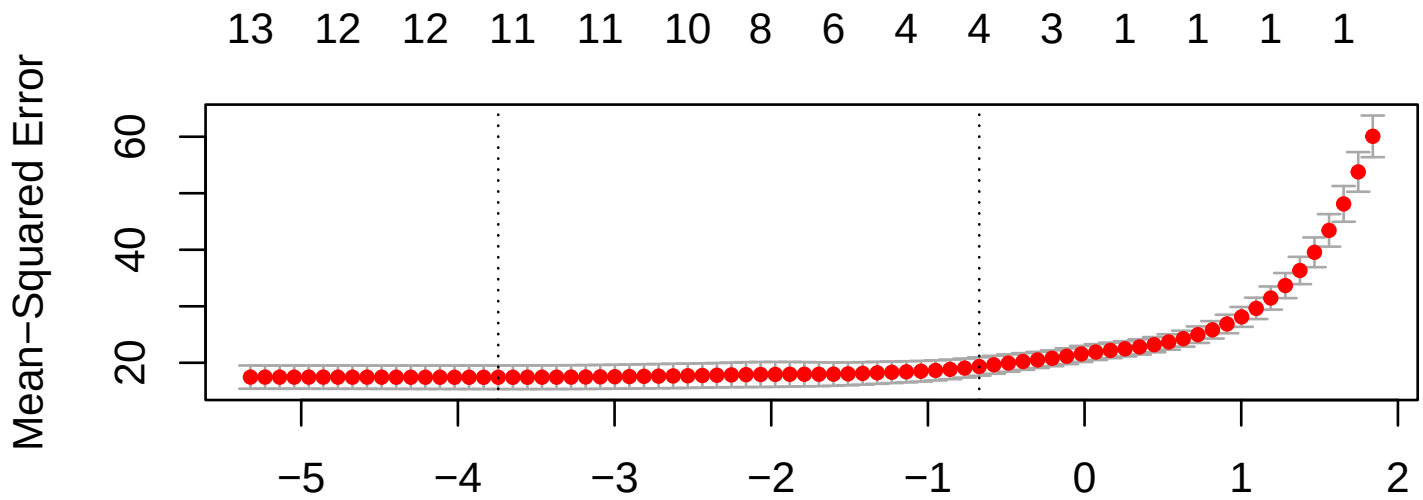
```
coef(fit_lasso, s = 0.1)
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                       s1
## (Intercept) -7.53281619
## age          0.05183206
## weight      -0.02504372
## height      -0.12561764
## neck        -0.31157363
## chest        .
## abdom        0.73717170
## hip         -0.04875740
## thigh        0.02570643
## knee         .
## ankle        .
## biceps       0.03422877
## forearm      0.30749547
## wrist       -1.40042018
```

# Regression Regularization in R: glmnet

The function **glmnet** returns a sequence of models for the users to choose from. **Cross-validation** is perhaps the simplest and most widely used method to select a model. **cv.glmnet** is the main function to do cross-validation here, along with various supporting methods such as plotting and prediction.

```
set.seed(2024)
cvfit_lasso <- cv.glmnet(X, y)
plot(cvfit_lasso)
```



# Coefficients Using Minimum Lambda

We can get the value of $\lambda_{min}$ and the model coefficients:

```
cvfit_lasso$lambda.min
```

```
## [1] 0.02369799
```

```
coef(cvfit_lasso, s = "lambda.min")
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                       s1
## (Intercept) -14.33408980
## age           0.05544891
## weight       -0.06937774
## height       -0.07673409
## neck         -0.41139197
## chest         .
## abdom         0.84027230
## hip          -0.15870755
## thigh         0.18612695
## knee          .
## ankle         0.10359361
## biceps        0.12109209
## forearm       0.39664464
## wrist        -1.45008669
```

# Coefficients Using Lambda within 1 SE of Min

The output of the `cv.glmnet()` function also gives us the largest $\lambda$ that is within 1 SE of the $\lambda$ that gave the smallest MSE. This $\lambda_{1se}$ value penalizes the coeficicients more and therefore choses a simpler model.

```
cvfit_lasso$lambda.1se
```

```
## [1] 0.5105576
```

```
coef(cvfit_lasso, s = "lambda.1se")
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                        s1
## (Intercept) -15.69396000
## age           0.02757973
## weight        .
## height       -0.13800356
## neck          .
## chest         .
## abdom         0.55983870
## hip           .
## thigh         .
## knee          .
## ankle         .
## biceps        .
## forearm       .
```

# Fitting Model with Selected $\lambda$

Then we can fit our model using the $\lambda$ value that we choose.

```
fit_min <- glmnet(X, y, lambda = cvfit_lasso$lambda.min)
fit_min
```

```
##
## Call:  glmnet(x = X, y = y, lambda = cvfit_lasso$lambda.min)
##
##    Df  %Dev Lambda
## 1 11 74.83 0.0237
```

```
fit_1se <- glmnet(X, y, lambda = cvfit_lasso$lambda.1se)
fit_1se
```

```
##
## Call:  glmnet(x = X, y = y, lambda = cvfit_lasso$lambda.1se)
##
##    Df %Dev Lambda
## 1   4 69.5 0.5106
```

# LASSO vs Stepwise Selection

Since LASSO is primarily used for model selection, it makes sense to compare it to another common model selection tool: the step wise selection.

```
# step(fat_mod) # Using AIC
# step(fat_mod, k = log(nrow(fat))) # Using BIC
# coef(cvfit_lasso, s = "lambda.min") # LASSO
# coef(cvfit_lasso, s = "lambda.1se") # LASSO
```

# LASSO vs Stepwise Selection

| Method | Model |
|---|---|
| Stepwise AIC | $-20.1 + 0.059 \cdot \text{age} - 0.084 \cdot \text{weight}$ $-0.432 \cdot \text{neck} + 0.877 \cdot \text{abdom}$ $-0.186 \cdot \text{hip} + 0.286 \cdot \text{thigh}$ $+0.483 \cdot \text{forearm} - 1.40 \cdot \text{wrist}$ |
| Stepwise BIC | $-31.3 - 0.126 \cdot \text{weight} + 0.921 \cdot \text{abdom}$ $+0.446 \cdot \text{forearm} - 1.39 \cdot \text{wrist}$ |
| LASSO (min $\lambda$) | $-14.3 + 0.055 \cdot \text{age} - 0.069 \cdot \text{weight}$ $-0.077 \cdot \text{height} - 0.411 \cdot \text{neck} + 0.840 \cdot \text{abdom}$ $-0.159 \cdot \text{hip} + 0.186 \cdot \text{thigh} + 0.104 \cdot \text{ankle}$ $+0.121 \cdot \text{biceps} + 0.397 \cdot \text{forearm} - 1.45 \cdot \text{wrist}$ |
| LASSO (1 SE $\lambda$) | $-15.7 + 0.028 \cdot \text{age} - 0.138 \cdot \text{height}$ $+0.560 \cdot \text{abdom} - 0.479 \cdot \text{wrist}$ |

# LASSO vs Stepwise Selection

Note that the variables selected by the LASSO are **not unique** due to the randomness associated with choosing $\lambda$. The cross-validation randomly selects groups from the data to fit the model and that can lead to a different "best" $\lambda$ value. For example, if our seed is set to a different number, we obtain a different result. The $\lambda$ can change in ridge regression as well, but the number of variables will not change with ridge.

```
set.seed(2024)
cv.glmnet(x = X, y = y, alpha = 1)$lambda.min
```

```
## [1] 0.02369799
```

```
set.seed(1)
cv.glmnet(x = X, y = y, alpha = 1)$lambda.min
```

```
## [1] 0.03132734
```

# Ridge Regression Example

Now let's use ridge regression to get estimates for the coefficients. We will set $\alpha = 0$ here. This does not reduce the number of predictors at all.

```
cvfit_ridge <- cv.glmnet(X, y, alpha = 0)
fit_ridge <- glmnet(X, y, alpha = 0, lambda = cvfit_ridge$lambda.min)
coef(cvfit_ridge)
```

```
## 14 x 1 sparse Matrix of class "dgCMatrix"
##                         s1
## (Intercept) -12.175488520
## age           0.103330254
## weight        0.006785216
## height       -0.192995854
## neck         -0.209769836
## chest         0.148121060
## abdom         0.364746908
## hip           0.052400618
## thigh         0.154209341
## knee          0.005875661
## ankle        -0.066339490
## biceps        0.069643584
## forearm       0.217379435
## wrist        -1.288686182
```

# Ridge Regression VIF Reduction

One common use of ridge regression is eliminating some problems causes by multicollinearity, which occurs when the predictors are highly correlated with each other. When this is the case, the slopes are difficult to interpret and the standard errors in the slope estimates get inflated. Let's check this in our model for body fat.

```
options(width = 70)
library(car) # vif() function is in the car package
vif(fat_mod)
```

```
##       age    weight    height      neck     chest     abdom       hip
##  2.250450 33.509320  1.674591  4.324463  9.460877 11.767073 14.796520
##     thigh      knee     ankle    biceps   forearm     wrist
##  7.777865  4.612147  1.907961  3.619744  2.192492  3.377515
```

The VIF tells us how much the variance of the estimates of the slopes are inflated. For example, the variance of the abdom variable is 11.767 times higher (so the SE is about 3.43 times larger) than it would be if multicollinearity was not present.

# Ridge Regression VIF Reduction

```
summary(fat_mod)
```

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -15.29255   16.06992  -0.952  0.34225
age           0.05679    0.02996   1.895  0.05929 .
weight       -0.08031    0.04958  -1.620  0.10660
height       -0.06460    0.08893  -0.726  0.46830
neck         -0.43754    0.21533  -2.032  0.04327 *
chest        -0.02360    0.09184  -0.257  0.79740
abdom         0.88543    0.08008  11.057  < 2e-16 ***
hip          -0.19842    0.13516  -1.468  0.14341
thigh         0.23190    0.13372   1.734  0.08418 .
knee         -0.01168    0.22414  -0.052  0.95850
ankle         0.16354    0.20514   0.797  0.42614
biceps        0.15280    0.15851   0.964  0.33605
forearm       0.43049    0.18445   2.334  0.02044 *
wrist        -1.47654    0.49552  -2.980  0.00318 **
```

# Ridge Regression VIF Reduction

While there is not a closed-form expression for the standard error of the ridge regression estimates, we can obtained estimated standard errors using either bootstrapping or Bayesian methods (we must wait until Notes 9 for Bayesian!). Let's look at an example using bootstrapping:

```
set.seed(2024)
nboot <- 1000
coefs <- matrix(rep(0, nboot*14), nrow = nboot)
for(i in 1:nboot) {
  index <- sample(1:nrow(X), nrow(X), replace = T)
  mod <- cv.glmnet(X[index,], y[index], alpha=0)
  coefs[i,] <- coef(mod, s = "lambda.min")[1:14]
}
sd(coefs[,2]); sd(coefs[,3]); sd(coefs[,7])
```

```
## [1] 0.02120437; 0.01584251; 0.04055876
```

# Ridge Regression VIF Reduction

The standard errors for the slope of `age` decreased from 0.02996 to 0.02120 (a factor of about 1.41). The SE for the slope for `weight` decreased from 0.04958 to 0.01584 (a factor of about 3.13), and the SE for the slope of `abdom` decreased from 0.08008 to 0.04056 (a factor of about 1.97).

Of course, these estimates are now biased. By exactly how much is hard to determine.

# Ridge Regression VIF Reduction

Another way to obtain the VIF values in OLS is by computing the diagonals of the inverse of the correlation matrix for the predictors: $\mathbf{r}_{xx}^{-1}$.

In ridge regression, the VIF values can be computed by taking the diagonal elements of

$$(\mathbf{r}_{xx} - \lambda\mathbf{I})^{-1}\mathbf{r}_{xx}(\mathbf{r}_{xx} - \lambda\mathbf{I})^{-1}.$$

The original VIF values:

```
options(width = 70)
r_xx <- cor(X)
r_xx |> solve() |> diag() |> round(5)
```

```
##      age   weight   height     neck    chest    abdom      hip
##  2.25045 33.50932  1.67459  4.32446  9.46088 11.76707 14.79652
##    thigh     knee    ankle   biceps forearm    wrist
##  7.77786  4.61215  1.90796  3.61974  2.19249  3.37751
```

# Ridge Regression VIF Reduction

In our case for this toy example, a good $\lambda$ value was 0.6294.

The reduced ridge regression VIF values:

```
options(width = 70)
diag(
  solve(r_xx + 0.6294*diag(rep(1, 13))) %*%
    r_xx %*%
    solve(r_xx + 0.6294*diag(rep(1, 13)))
  ) |> round(5)
```

```
##     age  weight  height    neck   chest   abdom     hip   thigh
## 0.33414 0.08150 0.36442 0.29041 0.21550 0.18218 0.16728 0.21672
##    knee   ankle  biceps forearm   wrist
## 0.28443 0.36689 0.30987 0.35652 0.31358
```

We actually obtain VIF values less than 1. This can happen under ridge regression and indicates that the multicollinearity issue has likely been resolved. There are some articles that propose different ways to calculate VIF in ridge regression, however, like this one here.

# glmnet in the caret package

While we were able to obtain an "optimal" $\lambda$ value using the `cv.glmnet()` function, it did not have an option to optimize $\alpha$ as well. If all we care about are predictions and are not trying to use LASSO for model selection or ridge regression for VIF reduction, then choosing $\alpha$ via cross validation can make sense.

```
library(caret) |> suppressPackageStartupMessages()
set.seed(2024)
search_grid <- expand.grid(alpha = seq(0, 1, length = 20),
                           lambda=seq(0, 1, by = 0.1))
train_glmnet <- train(
  brozek ~ age + weight + height + neck + chest +
    + abdom + hip + thigh + knee + ankle + biceps +
    forearm + wrist, data = fat, method = "glmnet",
  tuneGrid = search_grid, trControl = trainControl(method = "cv", number = 5)
  )
train_glmnet$bestTune
```

```
##        alpha lambda
## 56 0.2631579      0
```

# glmnet in the caret package

The best $\lambda$ was chosen to be zero, which likely means are search grid steps were too large.

```
library(caret) |> suppressPackageStartupMessages()
set.seed(2024)
search_grid <- expand.grid(alpha = seq(0, 1, length = 20),
                           lambda=seq(0, 0.1, by = 0.001))
train_glmnet <- train(
  brozek ~ age + weight + height + neck + chest +
    + abdom + hip + thigh + knee + ankle + biceps +
    forearm + wrist, data = fat, method = "glmnet",
  tuneGrid = search_grid, trControl = trainControl(method = "cv", number = 5)
  )
train_glmnet$bestTune
```

```
##         alpha lambda
## 514 0.2631579  0.008
```

This found that an elastic net with $\alpha = 0.2616$ and $\lambda = 0.008$ is best in terms of minimizing the MSE.

# Example: Logistic Regression Elastic Net

We can do regularization using ridge regression, LASSO, or elastic net in other models as well, like logistic regression.

Logistic regression is a widely-used model when the response is binary. Suppose the response variable $y$ takes values $\{0,1\}$. We model

$$P(y = 1|\mathbf{X}_i) = \frac{e^{\mathbf{X_i}\beta}}{1 + e^{X_i\beta}},$$

which can be written in the following form:

$$\log\left(\frac{P(y = 1|\mathbf{X}_i)}{P(y = 0|\mathbf{X}_i)}\right) = \mathbf{X}_i\beta,$$

the so-called "logistic" or log-odds transformation.

# Example: Logistic Regression Elastic Net

We seek to minimize the following loss function:

$$\arg\min_{\beta} \left\{ -\frac{1}{n}\sum_{i=1}^{n} y_i \log(\mathbf{X}\beta) - \log\left(1 + e^{\mathbf{X}\beta}\right) + \lambda\left(\alpha\sum_{j=1}^{p-1}|\beta_j| + \frac{(1-\alpha)}{2}\sum_{j=1}^{p-1}\beta_j^2\right)\right\},$$

where the left hand side is the loss function for standard logistic regression, and the right hand side is the elastic net regularization.

Logistic regression is often plagued with degeneracies when $p > n$ and exhibits wild behavior even when $n$ is close to $p$; the elastic net penalty alleviates these issues, and regularizes and selects variables as well.

# Example: Logistic Regression Elastic Net

Using the example data set from the glmnet package:

```
library(glmnet)
data(BinomialExample)
x <- BinomialExample$x
y <- BinomialExample$y
```

# Example: Logistic Regression without Elastic Net

Let's try to fit a logistic regression to this dataset with $n = 100$ and $p = 30$.

```
logistic_fit <- glm(y ~ x, family = "binomial")
```

```
## Warning: glm.fit: algorithm did not converge
## Warning: glm.fit: fitted probabilities numerically 0 or 1 occurred
```

```
summary(logistic_fit)
```

```
##
## Call:
## glm(formula = y ~ x, family = "binomial")
##
## Coefficients:
##               Estimate Std. Error z value Pr(>|z|)
## (Intercept)  7.815e+00  5.947e+04   0.000    1.000
## x1           1.536e+01  4.586e+04   0.000    1.000
## x2           4.219e+01  5.145e+04   0.001    0.999
## x3          -1.483e+01  5.276e+04   0.000    1.000
## x4          -2.831e+01  3.652e+04  -0.001    0.999
## x5          -4.968e+00  5.440e+04   0.000    1.000
## x6          -4.099e+01  5.211e+04  -0.001    0.999
## x7           1.176e+01  6.024e+04   0.000    1.000
## x8          -1.903e+01  6.449e+04   0.000    1.000
## x9           2.635e+01  6.535e+04   0.000    1.000
```

# Example: Logistic Regression Elastic Net

Now let's try with the elastic net with $\alpha = 1/3$ (equal weight on the L1 and L2 penalty).

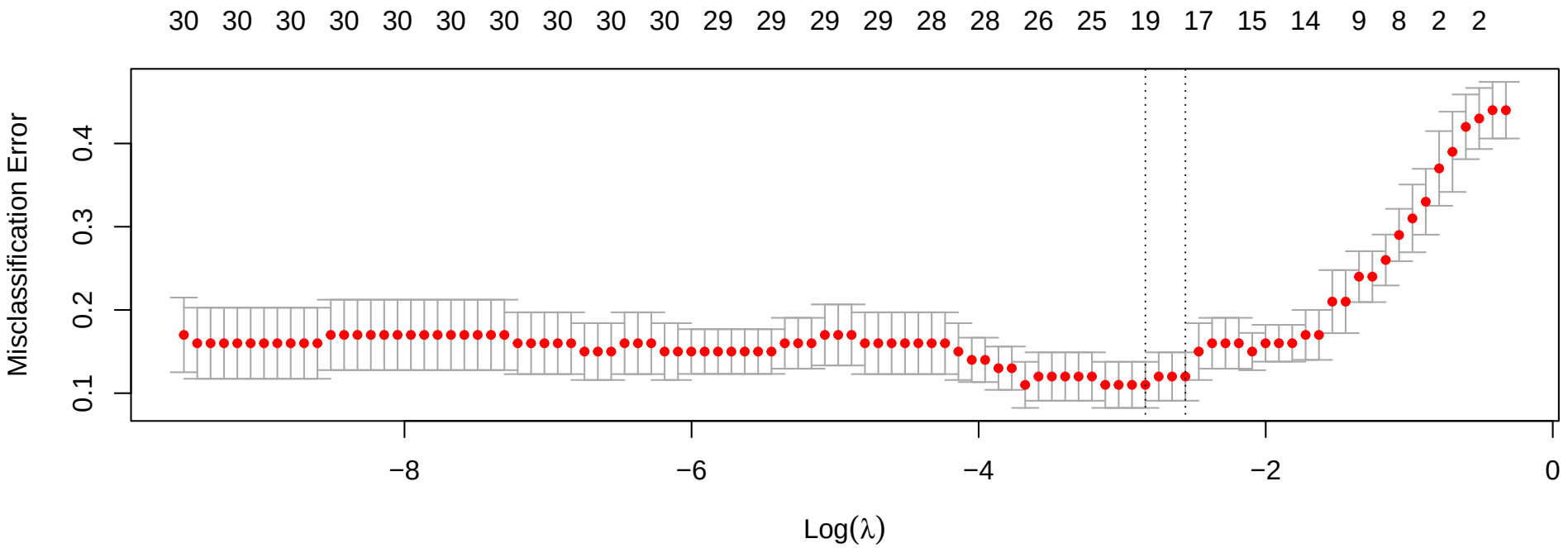
Set family option to "binomial" in the `glmnet` or `cv.glmnet` functions. The code below uses misclassification error as the criterion for 10-fold cross-validation:

```
set.seed(2024)
cvfit <- cv.glmnet(x, y, family = "binomial", alpha = 1/3,
                   type.measure = "class")
```

# Example: Logistic Regression Elastic Net

Now we can plot the cross-validation results and find the 'best' $\lambda_{min}$:

```
plot(cvfit)
```




```
cvfit$lambda.min
```

```
## [1] 0.05851731
```

# Example: Logistic Regression Elastic Net

```
fit <- glmnet(x, y, family = "binomial", alpha = 1/3,
              lambda = cvfit$lambda.min)
coef(fit)
```

```
## 31 x 1 sparse Matrix of class "dgCMatrix"
##                       s0
## (Intercept)  0.24276558
## V1           .
## V2           0.33757200
## V3          -0.26163948
## V4          -0.68663741
## V5          -0.19256156
## V6          -0.49550422
## V7           .
## V8          -0.32897557
## V9           0.33773353
## V10         -0.75247907
## V11         -0.09102764
## V12         -0.04228607
## V13          .
## V14          .
## V15          .
## V16          0.13059658
## V17          .
## V18          .
## V19          .
## V20         -0.01169230
## V21          .
## V22          0.16271574
## V23          0.23426330
## V24          .
## V25          0.37648053
## V26         -0.25867171
```

Section 3

# Poisson Regression

# Poisson Regression Intro

When doing regression analysis in Applied Statistics, we discussed linear regression with a continuous response variable, logistic regression where the response variable is binary, and multinomial logistic regression where the response variable is nominal with several (more than two) categories.

We did not discuss the best way to handle a discrete, quantitative response variable. If this is the case, the possible values range from 0 to infinity, and large counts are rare, then **Poisson regression** is most appropriate.

# Poisson Distribution

Recall the Poisson distribution from MATH 1040 or MATH 3700:

$$P(Y = y) = f(y) = \frac{e^{-\lambda}\lambda^y}{y!} \quad \text{for } y = 0, 1, 2, \ldots$$

with $E[Y] = \text{Var}(Y) = \lambda$. So, the variance increases as the mean of $Y$ increases.

We often use capital letters (like $Y$) to denote the variable name and lowercase letters (like $y$) to denote values of that variable.

# Poisson Link Function

Like when doing logistic regression, we need a link function for Poisson regression. In logistic regression, the most common link function is the logit function: $\log\left(\frac{\widehat{P(Y=1|\mathbf{X}_i)}}{1-\widehat{P(Y=1|\mathbf{X}_i)}}\right)$ and when using that function, the model becomes linear. That is, $\log\left(\frac{\widehat{P(Y=1|\mathbf{X}_i)}}{1-\widehat{P(Y=1|\mathbf{X}_i)}}\right) = \mathbf{X}_i\beta$.

The most common link function for Poisson regression is just the log function. Typically, we just write "log" to indicate the natural log function. That is,

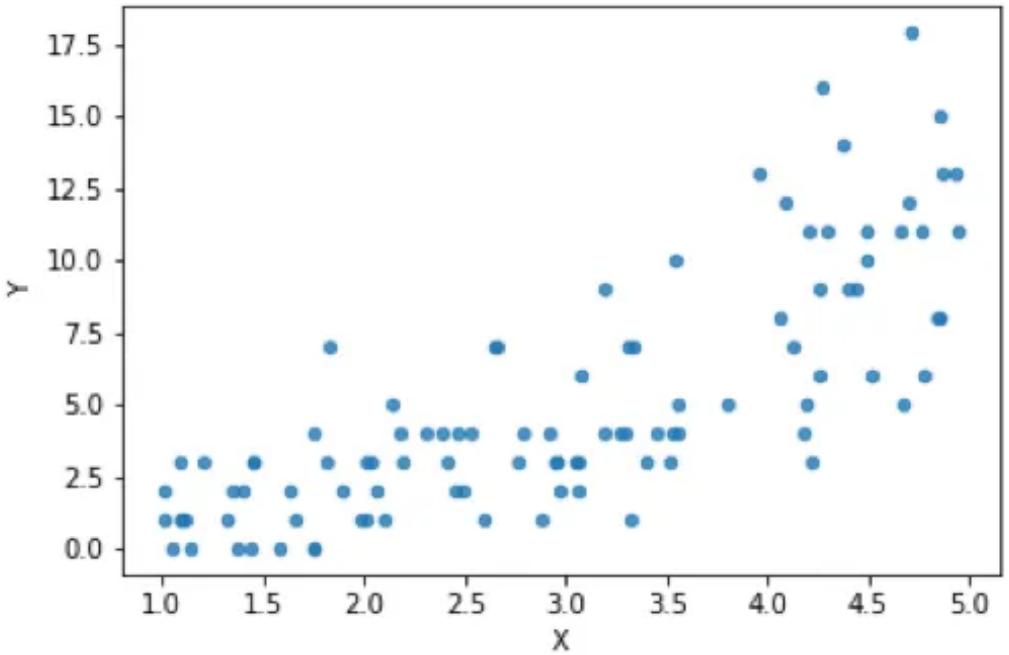
$$\log(\widehat{E[Y|\mathbf{X}_i]}) = \mathbf{X}_i\beta$$

where $\mathbf{X}_i$ is the $i$th row of the model matrix $\mathbf{X}$.

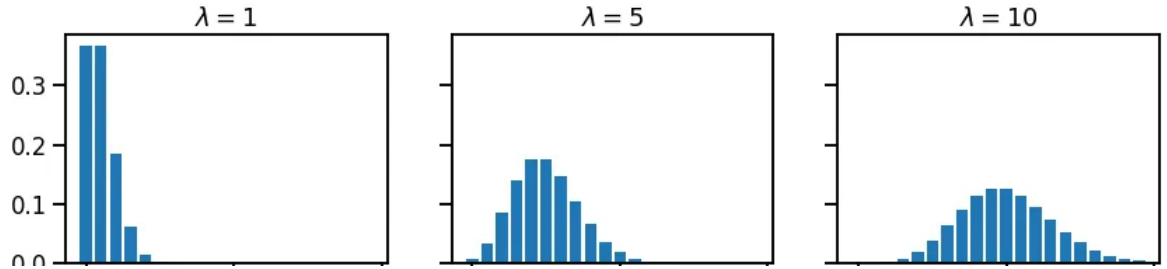
Of course, the expected value of $Y$ is $\lambda$, so this model is really for predicting $\lambda$ at certain values of $X$: $\log(\hat{\lambda}_i|x_i) = \beta_0 + \beta_1 x_i$ or $\hat{\lambda}_i|x_i = e^{\beta_0+\beta_1 x_i}$ in the SLR case.

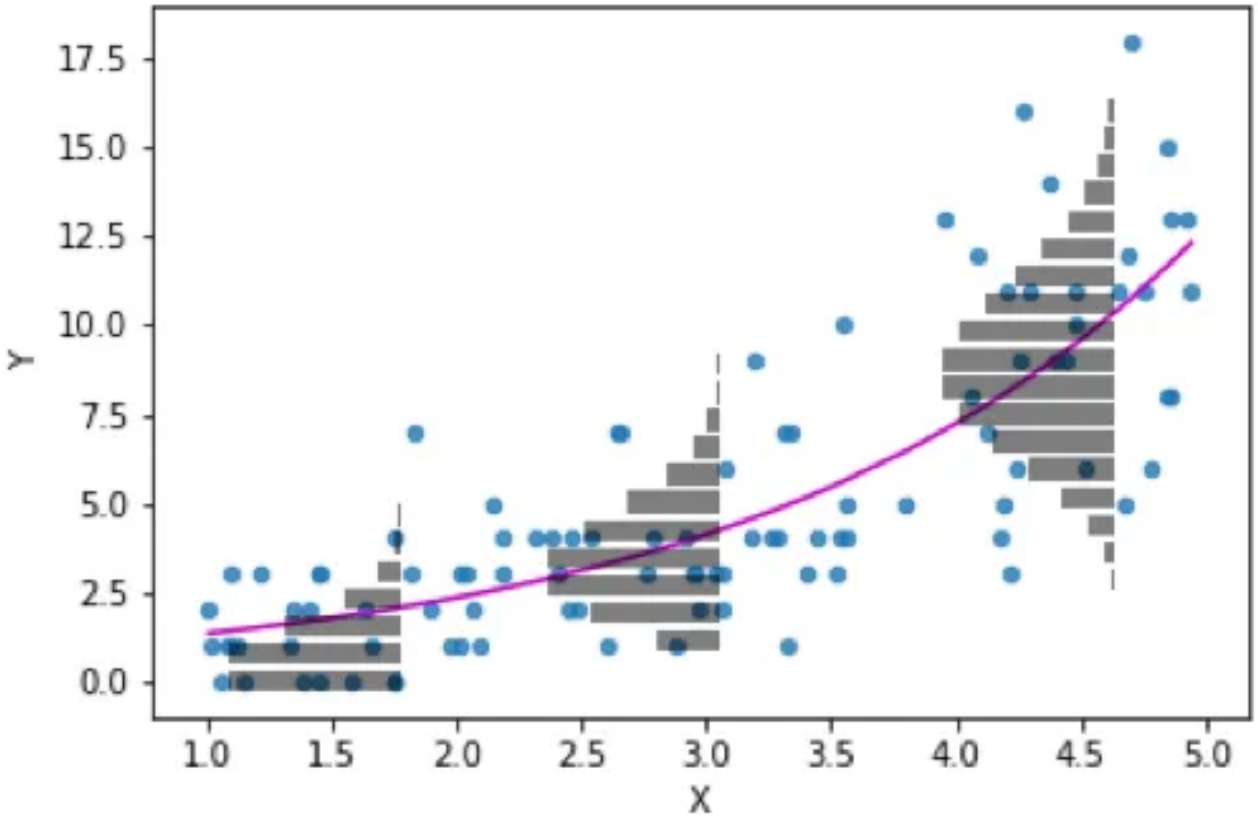
# Poisson Data Model

With the Poisson regression, we model the data by thinking about $Y$ as following a Poisson distribution with a different mean at every value of $x$. So, if we begin with a dataset that looks like the one in the image below, which is fairly common for Poisson regression, then we can imagine a different Poisson distribution at each $x$ value.



# Poisson Data Model



# Poisson Regression Assumptions

1. **Poisson Response**: The response variable is conditionally a count per unit of time or space, described by a Poisson distribution.
2. **Independence**: The observations must be independent of one another.
3. **Mean = Variance**: By definition, the mean of a Poisson random variable must be equal to its variance.
4. **Linearity**: The log of the mean rate, $\log(\lambda)$, must be a linear function of $x$.

# Finding Parameter Estimates

The parameters, $\beta_0, \beta_1, \ldots, \beta_{p-1}$ are not estimated using least squares. Instead, like for logistic regression, these are estimated using **maximum likelihood estimation** (MLE). The way MLE works is to determine the values of $\beta$ such that it maximizes the likelihood function of obtaining these data.

The likelihood function is essentially the joint probability density function (pdf), but we think of the data as fixed and the $\beta's$ as random. For the poisson, assuming independent data values, the likelihood function is

$$\begin{aligned} L(\beta) &= \prod_{i=1}^{n} f_i(y_i) = f_1(y_1) \cdot \cdots \cdot f_n(y_n) \\ &= \frac{e^{-\lambda_1}\lambda_1^{y_1}}{y_1!} \cdot \cdots \cdot \frac{e^{-\lambda_n}\lambda_n^{y_n}}{y_n!} \end{aligned}$$

Let's continue this on the next slide.

# Maximum Likelihood Estimation

$$L(\beta) = \prod_{i=1}^{n} f_i(y_i) = f_1(y_1) \cdot \cdots \cdot f_n(y_n)$$
$$= \frac{e^{-\lambda_1}\lambda_1^{y_1}}{y_1!} \cdot \cdots \cdot \frac{e^{-\lambda_n}\lambda_n^{y_n}}{y_n!}$$
$$= \frac{\prod_{i=1}^{n} \lambda_i^{y_i} \cdot \exp\{-\sum_{i=1}^{n} \lambda_i\}}{\prod_{i=1}^{n} y_i!}$$

Now it is common to take the log of the likelihood to make the actual maximizing easier:

$$\ln(L(\beta)) = \ell(\beta) = \ln\left(\frac{\prod_{i=1}^{n} \lambda_i^{y_i} \cdot \exp\{-\sum_{i=1}^{n} \lambda_i\}}{\prod_{i=1}^{n} y_i!}\right)$$
$$= \ln\left(\prod_{i=1}^{n} \lambda_i^{y_i}\right) + \ln\left(\exp\left\{-\sum_{i=1}^{n} \lambda_i\right\}\right) - \ln\left(\prod_{i=1}^{n} y_i!\right)$$
$$= \sum_{i=1}^{n} y_i \ln(\lambda_i) - \sum_{i=1}^{n} \lambda_i - \sum_{i=1}^{n} \ln(y_i!)$$

# Maximum Likelihood Estimation

Now we can substitute for $\lambda_i$. That is, $\lambda_i = E(Y|\mathbf{X}_i) = \exp(\mathbf{X}_i\beta)$:

$$\begin{aligned}
\ell(\beta) &= \sum_{i=1}^{n} y_i \ln(\lambda_i) - \sum_{i=1}^{n} \lambda_i - \sum_{i=1}^{n} \ln(y_i!) \\
&= \sum_{i=1}^{n} y_i \ln(\exp(\mathbf{X}_i\beta)) - \sum_{i=1}^{n} \exp(\mathbf{X}_i\beta) - \sum_{i=1}^{n} \ln(y_i!) \\
&= \sum_{i=1}^{n} y_i(\mathbf{X}_i\beta) - \sum_{i=1}^{n} \exp(\mathbf{X}_i\beta) - \sum_{i=1}^{n} \ln(y_i!)
\end{aligned}$$

Now, to maximize this, like in calculus, we take the derivative with respect to one of the parameters (one of the $\beta$'s) and set the equation equal to zero.

# Maximum Likelihood Estimation

Let's do an example in the SLR case where $\mathbf{X}_i\boldsymbol{\beta} = \beta_0 + \beta_1 x_i$.

$$\begin{aligned}\ell(\boldsymbol{\beta}) &= \sum_{i=1}^{n} y_i(\mathbf{X}_i\boldsymbol{\beta}) - \sum_{i=1}^{n} \exp(\mathbf{X}_i\boldsymbol{\beta}) - \sum_{i=1}^{n} \ln(y_i!) \\ &= \sum_{i=1}^{n} y_i(\beta_0 + \beta_1 x_i) - \sum_{i=1}^{n} \exp(\beta_0 + \beta_1 x_i) - \sum_{i=1}^{n} \ln(y_i!)\end{aligned}$$

Take the derivative with respect to $\beta_0$ and set it equal to zero:

$$\frac{\partial \ell}{\partial \beta_0} = \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} \exp(\beta_0 + \beta_1 x_i) = 0$$

Take the derivative with respect to $\beta_1$ and set it equal to zero:

$$\frac{\partial \ell}{\partial \beta_1} = \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \exp(\beta_0 + \beta_1 x_i) = 0$$

# Maximum Likelihood Estimation

Now, these equations need to be solved numerically (unlike ordinary least squares), so they do not have a closed-form solution. Just to verify that these are correct, though, let's simulate a little toy example:

```
set.seed(2024)
x <- rnorm(5) # Simulate 5 random values for x
# Simulate 5 random values for y (with a couple different means)
y <- c(rpois(3, 2), rpois(2, 6))
mod <- glm(y ~ x, family = "poisson") # Fit the Poisson model
b0 <- coef(mod)[1] # Extract the intercept
b1 <- coef(mod)[2] # Extract the slope
sum(y) - sum(exp(b0 + b1 * x)) # First MLE equation
```

```
## [1] -1.421085e-12
```

```
sum(x * y) - sum(x * exp(b0 + b1 * x)) # Second MLE equation
```

```
## [1] 1.314504e-13
```

# Other Poisson Regression Functions in **R**

In **R**, we can use the `glm()` function to fit a Poisson model. Like we do with logistic regression, we need to specify the family and the link function. By default, the link function in the "poisson" family is the log, so we will keep it as the default.

```
glm(y ~ x, data = poisson_df, family = "poisson")
```

# Illustrative Example - Lumber

The Miller Lumber Company is a large retailer of lumber and paint, as well as of plumbing, electrical, and other household supplies. During a representative two-week period, in-store surveys were conducted and addresses of customers were obtained. The addresses were then used to identify the metropolitan area census tracts in which the customers reside. At the end of the survey period, the total number of customers who visited the store from each census tract within a 10-mile radius was determined and relevant demographic information for each tract (average income, number of housing units, etc.) was obtained. Several other variables expected to be related to customer counts were constructed from maps, including distance from census tract to nearest competitor and distance to store.

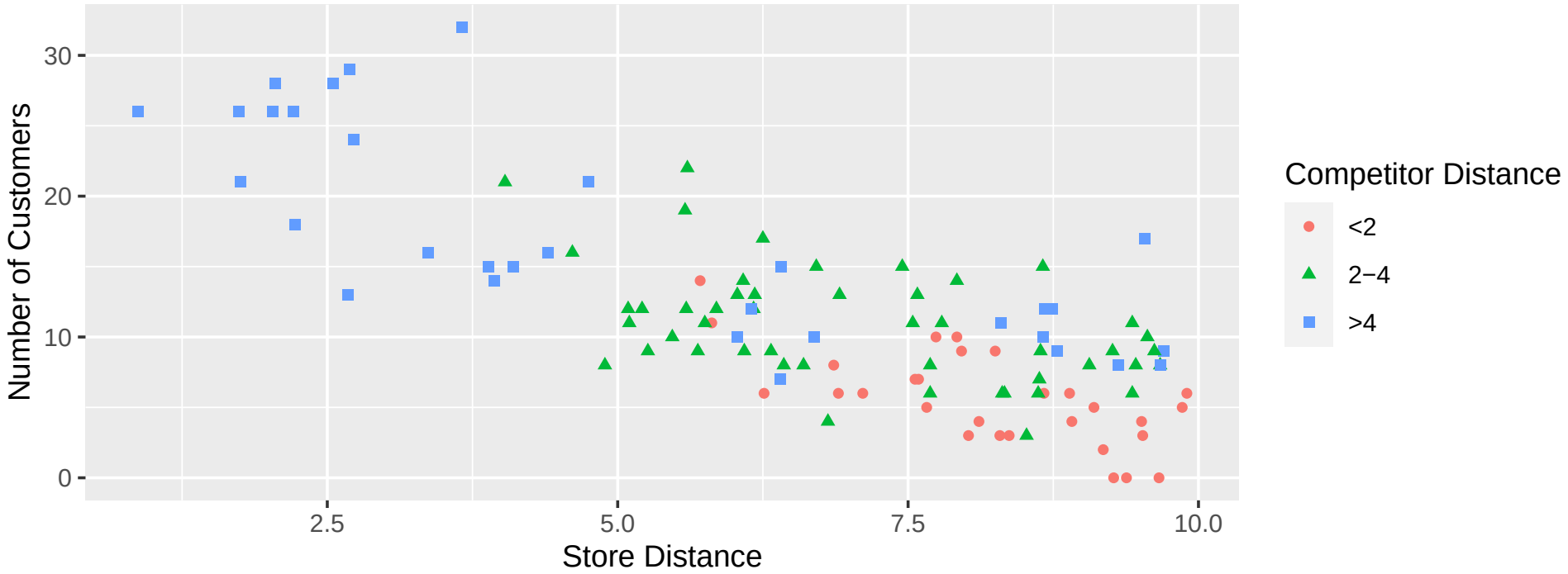
We will try to predict the number of customers from a Census tract using two variables: the distance the track is to the Miller Lumber Company store (quantitative in miles) and the distance from a competitor's store (categorical with categories "<2", "2-4", or "4+" miles.)

# Illustrative Example - Lumber Model

```
library(tidyverse) |> suppressPackageStartupMessages()
lumber <- read_table(
  paste0("~/My Drive/Math 3190 - Fundamentals of Data ",
         "Science/Data/lumber_company.txt")
  ) |>
  mutate(competitor_dist = factor(case_when(
    competitor_distance <= 2 ~ "<2",
    competitor_distance > 2 & competitor_distance <= 4 ~ "2-4",
    competitor_distance > 4 ~ ">4"
    ), levels = c("<2", "2-4", ">4"))
  )
lumber_mod <- glm(customers ~ store_distance * competitor_dist,
                  data = lumber, family = "poisson")
```

# Illustrative Example - Lumber Scatter Plot

```
ggplot(lumber, aes(x = store_distance, y = customers,
                   shape = competitor_dist,
                   color = competitor_dist)) +
  geom_point() +
  labs(x = "Store Distance", y = "Number of Customers",
       shape = "Competitor Distance", color = "Competitor Distance")
```



# Illustrative Example - Lumber Model Output

```
summary(lumber_mod)
```

```
Coefficients:
                                 Estimate Std. Error z value Pr(>|z|)
(Intercept)                       4.32561    0.50344   8.592  < 2e-16 ***
store_distance                   -0.32659    0.06425  -5.083 3.71e-07 ***
competitor_dist2-4               -1.12808    0.54137  -2.084  0.03718 *
competitor_dist>4                -0.89883    0.50992  -1.763  0.07795 .
store_distance:competitor_dist2-4  0.20830    0.07034   2.961  0.00306 **
store_distance:competitor_dist>4   0.19871    0.06623   3.000  0.00270 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for poisson family taken to be 1)

    Null deviance: 422.22  on 109  degrees of freedom
Residual deviance: 132.35  on 104  degrees of freedom
AIC: 588.39
```

# Illustrative Example - Lumber Model Equations

We will get one equation for each category of the categorical variable. Letting $x_i$ be the $i$th value of store_distance, we obtain:

Model 1 ($<$2 Group): $\ln(\hat{\lambda}_i) = 4.32561 - 0.32659 \cdot x_i$

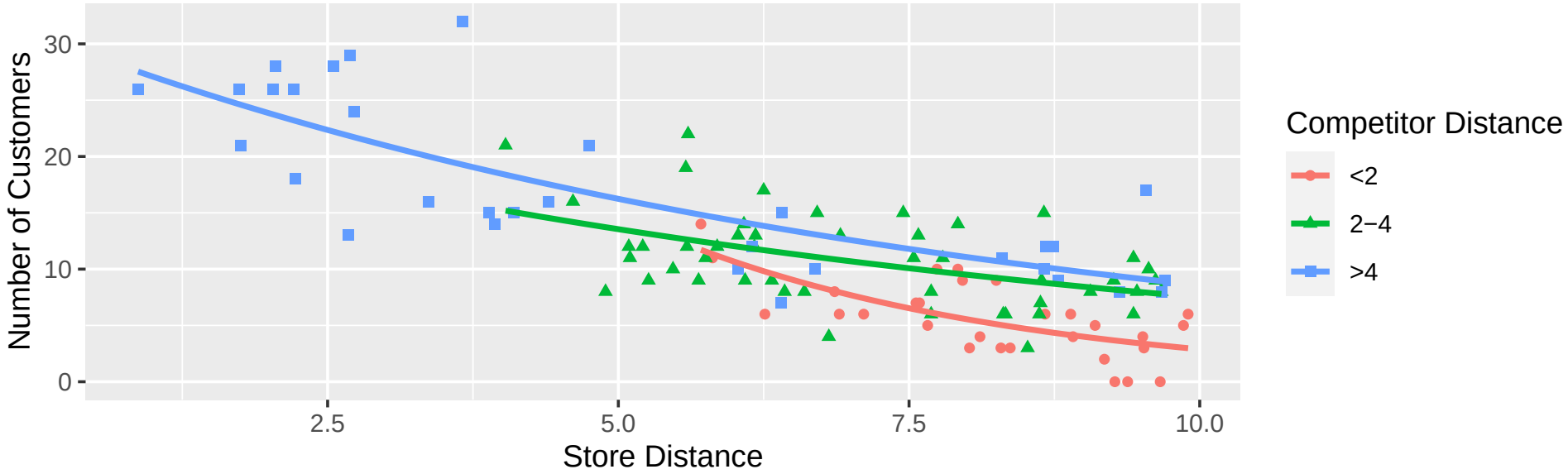
Model 2 (2-4 Group): $\ln(\hat{\lambda}_i) = 3.19753 - 0.11829 \cdot x_i$

Model 2 (4+ Group): $\ln(\hat{\lambda}_i) = 3.42678 - 0.12788 \cdot x_i$

# Illustrative Example - Lumber Model Plot with Models

We can use the geom_smooth() function to plot the models curves.

```
ggplot(lumber, aes(x = store_distance, y = customers,
                   shape = competitor_dist,
                   color = competitor_dist)) +
  geom_point() +
  labs(x = "Store Distance", y = "Number of Customers",
       shape = "Competitor Distance", color = "Competitor Distance") +
  geom_smooth(method = "glm", method.args = list(family = "poisson"),
              formula = "y ~ x", se = F)
```



# Interpreting the Model Coefficients

The interpretation of the coefficients here is quite similar to interpreting the coefficients of a log-transformed linear regression model.

**Intercept**: The predicted mean of the Poisson distribution when $x = 0$ is $\exp(\hat{\beta}_0)$.

**Slope**: The predicted change in the mean of the Poisson distribution when $x$ increases by one is $\exp(\hat{\beta}_1)$.

# Confidence Intervals for the Model Coefficients

We can obtain confidence intervals for the intercept and slope(s) using normal approximations as long as our sample size is fairly large:

$$\left(\hat{\beta}_i - z_{\alpha/2} \cdot SE(\hat{\beta}_i), \hat{\beta}_i + z_{\alpha/2} \cdot SE(\hat{\beta}_i)\right)$$

Then we can exponentiate these to get the confidence intervals back on the original scale:

$$\left(\exp\left\{\hat{\beta}_i - z_{\alpha/2} \cdot SE(\hat{\beta}_i)\right\}, \exp\left\{\hat{\beta}_i + z_{\alpha/2} \cdot SE(\hat{\beta}_i)\right\}\right)$$

Using the `confint()` function in **R** uses what is called the "profile likelihood" method for computing these intervals, which we will not discuss here, so the results will be a bit different. Note that the `MASS` package must be installed for this to work.

# Lumber Example Confidence Intervals

For the "store_distance" variable, the $\beta_1$ estiamte is $-0.32659$ with a standard error of 0.06425. We can obtain an approximate 95% interval using

```
-0.32659 - qnorm(1-0.05/2) * 0.06425
```

```
## [1] -0.4525177
```

```
-0.32659 + qnorm(1-0.05/2) * 0.06425
```

```
## [1] -0.2006623
```

So the interval is $-0.453 < \beta_1 < -0.201$.

Using the `confint()` function:

```
confint(lumber_mod)[2,]
```

```
## Waiting for profiling to be done...
##      2.5 %     97.5 %
## -0.4522654 -0.2001689
```

We obtain an interval of $-0.452 < \beta_1 < -0.200$.

# Confidence Intervals for the Mean Response

We can obtain an approximate confidence interval for $E(Y_i|\boldsymbol{x}_i)$ using the `predict()` function with the options `type = "response"` and `se.fit = T`. This won't create for CI for us, though. We can approximate using a normal distribution. This approximation is better for larger values of $\lambda_i$.

```
lumber_pred <- predict(lumber_mod,
                       data.frame(store_distance = 5,
                                  competitor_dist = "2-4"),
                       type = "response", se.fit = T)
lumber_pred$fit - 1.96 * lumber_pred$se.fit
lumber_pred$fit + 1.96 * lumber_pred$se.fit
```

```
11.7594; 15.33278
```

So, the interval is $11.76 < E(Y^*|\boldsymbol{x}^*) < 15.33$ or $11.76 < \lambda^*|\boldsymbol{x}^* < 15.33$.

# Confidence Intervals for Predictions

These confidence intervals are for the mean Poisson response at a given row vector $\boldsymbol{x}$. Then, to get predictions for the actual count, we can use percentiles for Poisson distribution.

For the lower bound of a $(1-\alpha)\times 100\%$ confidence interval, we can use the $\alpha/2 \times 100$th percentile using the lower bound of the CI for the mean.

For the upper bound of a $(1-\alpha)\times 100\%$ confidence interval, we can use the $(1-\alpha/2) \times 100$th percentile using the upper bound of the CI for the mean.

```
qpois(0.025, 11.7594)  # 2.5th percentile using lower mean
```

```
## [1] 6
```

```
qpois(0.975, 15.33278) # 97.5th percentile using upper mean
```

```
## [1] 23
```

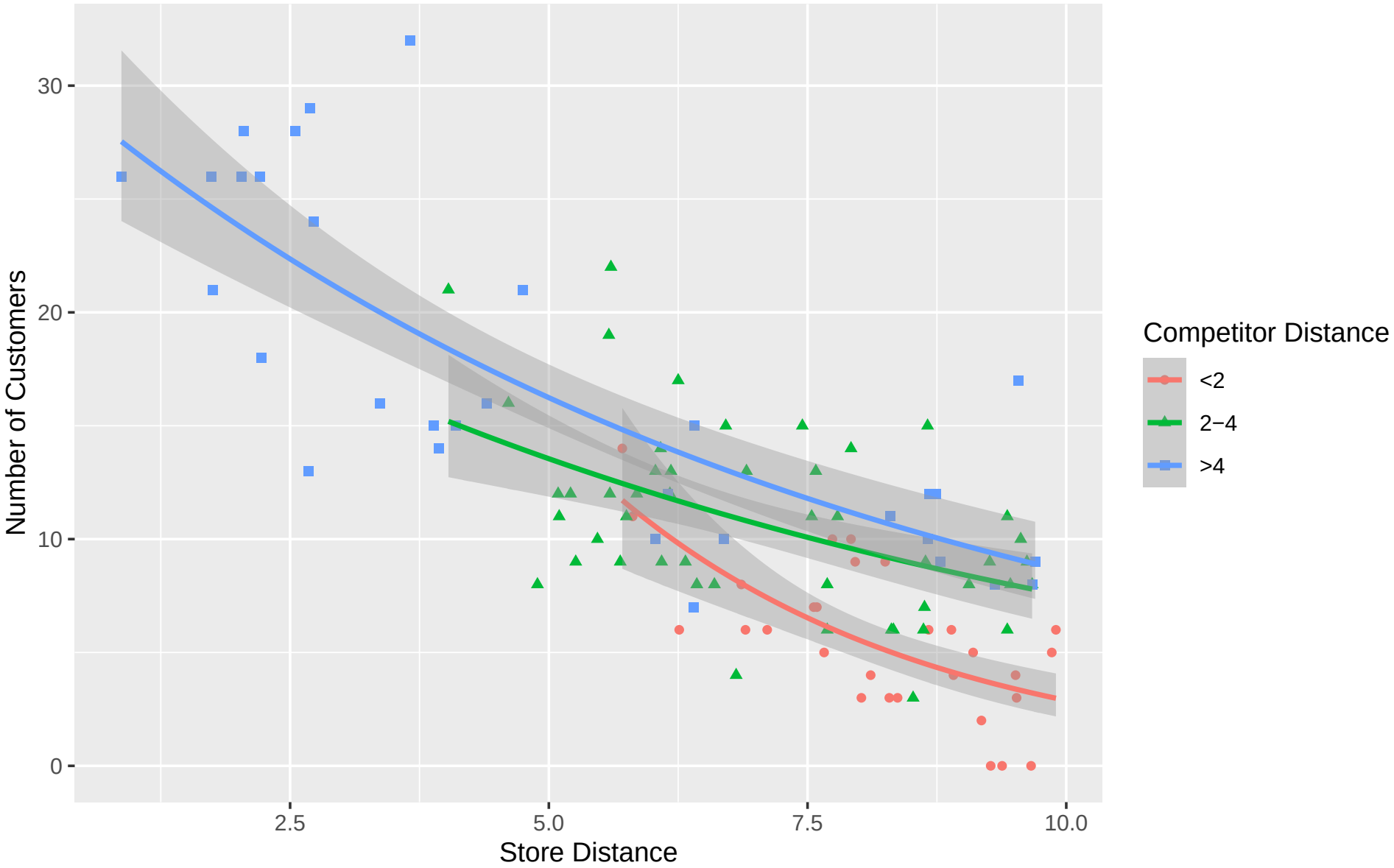
That gives an interval of $6 < y^*|\boldsymbol{x}^* < 23$.

# Lumber Model Plot with CI

We can plot the CI for the mean with the geom_smooth() function as well. These intervals are constructed using the profile likelihood method rather than normal approximations, but they are similar.

```
ggplot(lumber, aes(x = store_distance, y = customers,
                   shape = competitor_dist,
                   color = competitor_dist)) +
  geom_point() +
  labs(x = "Store Distance",
       y = "Number of Customers",
       shape = "Competitor Distance",
       color = "Competitor Distance") +
  geom_smooth(method = "glm",
              method.args = list(family = "poisson"),
              formula = "y ~ x", se = T)
```

# Lumber Model Plot with CI



# Poisson Residuals

There are several different types of residuals for a Poisson regression model. The first is called the **Pearson residual**, which is computed using

$$\hat{\epsilon}_i^P = \frac{y_i - \hat{y}_i}{\sqrt{\hat{y}_i}}$$

where $\hat{y}_i = \exp(\mathbf{X}_i\hat{\beta}) = \hat{\lambda}_i$.

Then there is the **deviance residual**, which is computed using

$$\hat{\epsilon}_i^D = \text{sgn}(y_i - \hat{y}_i)\sqrt{2\left(y_i \cdot \ln\left(y_i/\hat{y}_i\right) - y_i + \hat{y}_i\right)}$$

where sgn is the sign function that is positive when its input is positive and negative otherwise. Note that when $y_i = 0$, we take $y_i \cdot \ln\left(y_i/\hat{y}_i\right)$ to also equal 0.

It can be shown that both of these residuals are approximately normally distributed.

# Other Poisson Regression Functions in **R**

To obtain the fitted values on the original data scale, we can either use the

```
fitted.values()
```

function or use

```
predict(model, type = "response")
```

If we just use

```
predict(model)
```

it will return the linear predictors. To get back to the original scale, we would need to exponentiation those values.

To obtain the Pearson residuals, we can use

```
residuals(model, type = "pearson")
```

The deviance residuals are the default, so they be obtained using either

```
residuals(model)
residuals(model, type = "deviance")
```

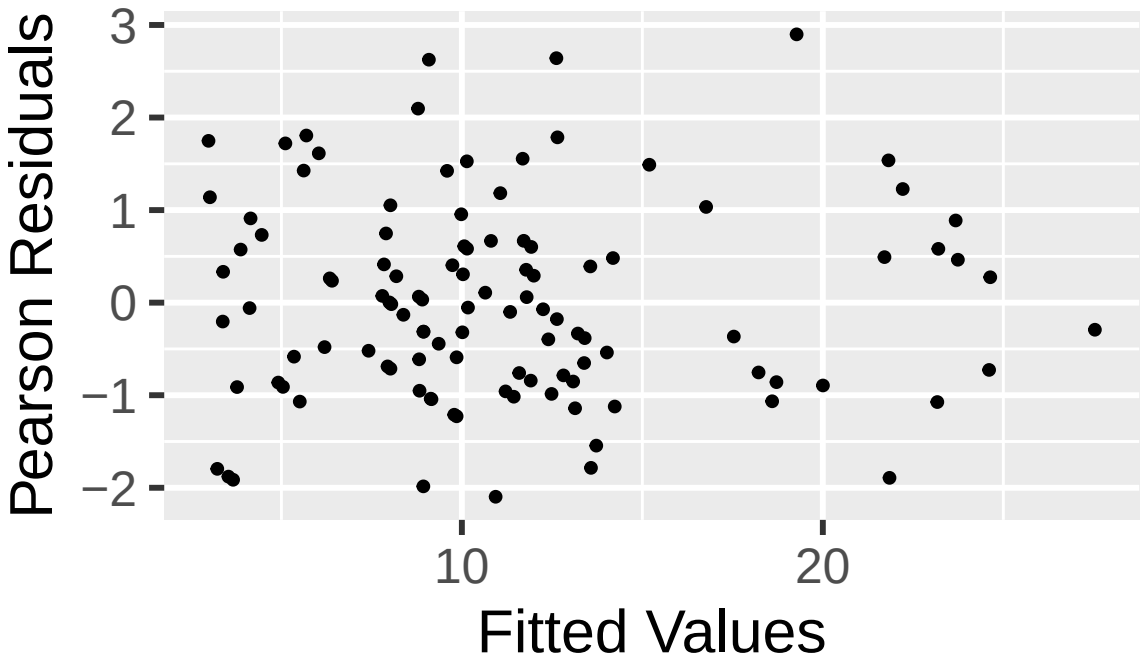
# Poisson Regression Diagnostics

We can perform **diagnostics** for Poisson regression using hypothesis tests and plots. Each of the following are helpful:

1. A residual plot of the Pearson residuals vs the predicted values. These residuals should appear randomly spread.
2. A QQ-plot of the Pearson or deviance residuals. These should be approximately normally distributed.
3. A deviance goodness-of-fit (GOF) test.
4. A check for overdispersion.

# Poisson Regression Diagnostics - Residual Plot

```
p_resids <- residuals(lumber_mod, type = "pearson")
resid_df <- data.frame(p_resids,
                       fitted = lumber_mod$fitted.values)
ggplot(resid_df, aes(x = fitted, y = p_resids)) +
  geom_point(size = 0.5) +
  labs(x = "Fitted Values", y = "Pearson Residuals")
```

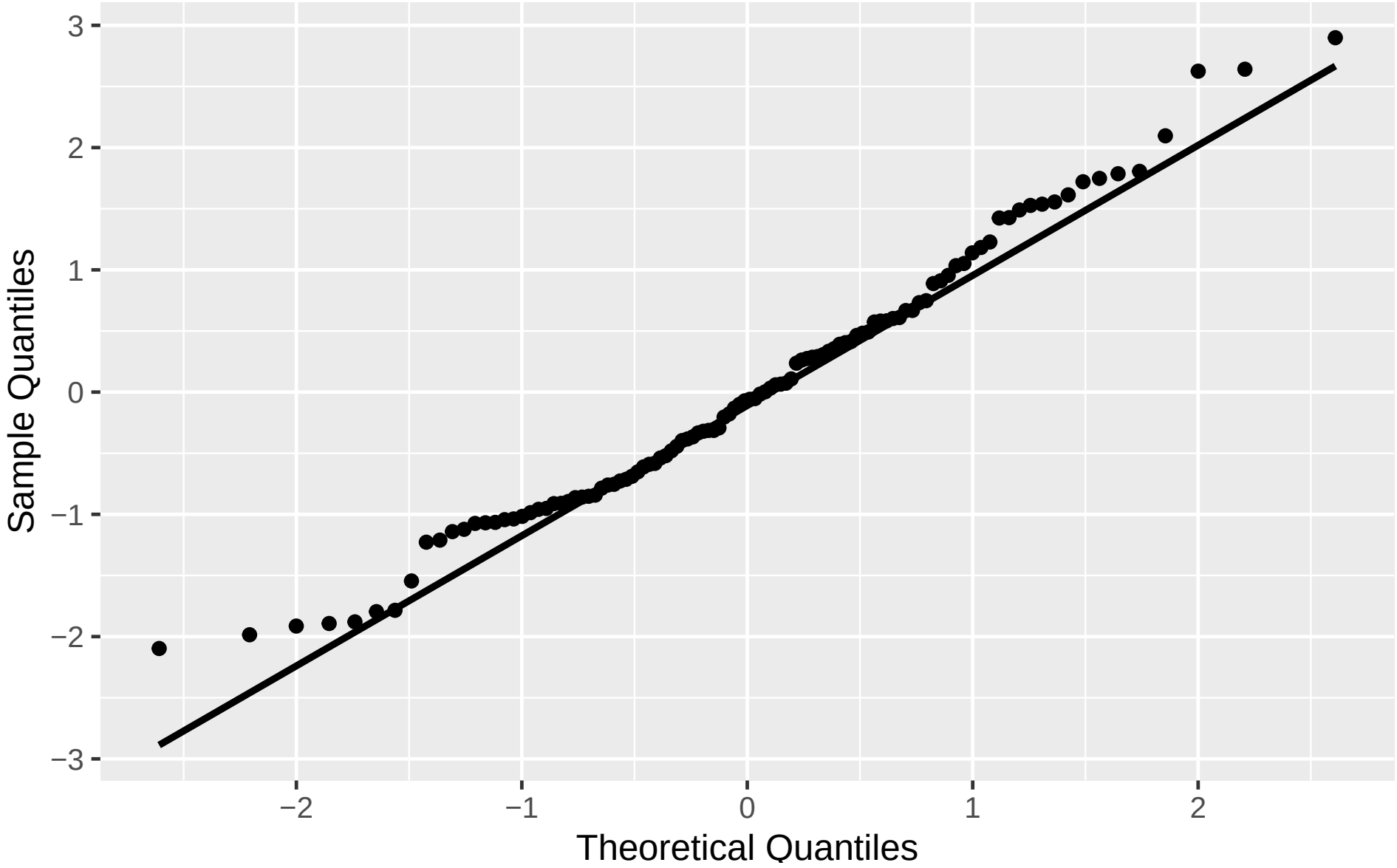


# Poisson Regression Diagnostics - QQ Plot

We can use a **QQ plot** to check if the Pearson residuals are approximately normal. This can be done with the `qqnorm()` and `qqline()` function in base **R** or the `geom_qq()` and `geom_qq_line()` in ggplot2. The closer to the line, the better.

```
ggplot(resid_df, aes(sample = p_resids)) +
  geom_qq() +
  geom_qq_line(linewidth = 1) +
  labs(x = "Theoretical Quantiles",
       y = "Sample Quantiles")
```

# Poisson Regression Diagnostics - QQ Plot



# Poisson Regression Diagnostics - GOF Test

A **deviance goodness-of-fit** (GOF) test tests the hypotheses

$H_0$ : The model is correctly specified.
$H_A$ : The model is incorrectly specified.

The test statistic is

$$D = 2\sum_{i=1}^{n}\left(y_i \ln(y/\hat{y}_i) - (y_i - \hat{y}_i)\right) = \sum_{i=1}^{n}\left(\hat{\epsilon}_i^D\right)^2,$$

the sum of the squared deviance residuals. This statistic approximately follows a $\chi^2$ distribution with $n - p$ degrees of freedom when the predicting means as not too small. It is also given in the output of the Poisson model as the "Residual deviance".

If this statistic is large relative to the degrees of freedom, we have evidence that the model does not fit well, and we would reject the null hypothesis. Therefore, this is a right-tailed test.

# Poisson Regression Diagnostics - GOF Test Example

```
1 - pchisq(lumber_mod$deviance, df = lumber_mod$df.residual)
```

```
## [1] 0.03169943
```

We have evidence here that this model does not fit well. In this case, that is likely becuase the model is **overdispersed**. We can alleviate this issue by adding more important variables. If we add more variables, we lose evidence the model is poorly fitting.

```
lumber_mod2 <- glm(customers ~ store_distance + competitor_dist +
                     average_income + average_age + housing_units,
                   data = lumber, family = "poisson")
1 - pchisq(lumber_mod2$deviance, df = lumber_mod2$df.residual)
```

```
## [1] 0.2755826
```

# Poisson Regression Diagnostics - Overdispersion

One important property of a Poisson distribution is that $E(Y) = \lambda$ and $Var(Y) = \lambda$. That is, both the mean and the variance are equal. **Overdispersion** occurs when the variance of a model is greater than its mean.

- Overdispersion is caused by a positive correlation between responses or by too much variation between response probabilities or counts. Overdispersion also arises when there are violations in the distributional assumptions of the data as well as when the data are prone to it (i.e., when earlier events cause or influence the existence of subsequent events).
- Overdispersion is an issue because it may cause standard errors of the estimates to be underestimated (i.e., a variable may appear to be a significant predictor when it is in fact not significant).

# Poisson Regression Diagnostics - Overdispersion

- A model may be overdispersed if the value of the sum of the squared Pearson residuals divided by the degrees of freedom (df) is greater than 1.0. This quotient is called the dispersion. Small amounts of overdispersion are of little concern; however, if the dispersion statistic is greater than 1.25 for moderate-sized models, then a correction may be warranted. Models with large numbers of observations may be overdispersed with a dispersion statistic of 1.05.
- We can alleviate the issue overdispersion issue by adding other predictors, transforming the count data, or **changing models**.

If we are using Poisson regression in its proper context, than the most common way to alleviate overdispersion is to change from a Poisson model to a **quasi-Poisson model**.

# Quasi-Poisson Regression

The quasi-Poisson distribution is very similar to the Poisson, except it allows for the mean and variance to differ:

$$E[Y] = \lambda$$
$$Var(Y) = \phi\lambda$$

where $\phi$ is known as the dispersion parameter that is estimated from the data.

In particular, $\phi = \frac{1}{n-p}\sum_{i=1}^{n}\hat{\epsilon}_i^P$, the sum of the squared Pearson residuals divided by the residual degrees of freedom.

# Quasi-Poisson Example

In our example, let's check the estimate for $\phi$:

```
sum(residuals(lumber_mod, type = "pearson")^2)
```

```
## [1] 124.7268
```

```
lumber_mod$df.residual # n - p = 110 - 6
```

```
## [1] 104
```

```
phi <- sum(residuals(lumber_mod, type = "pearson")^2)/lumber_m
phi
```

```
## [1] 1.199297
```

The dispersion estimate of 1.199 is not above the 1.25 cutoff, but it fairly large. Let's fit a new model using a "quasi-poisson" family.

```
lumber_mod_quasi <- glm(
  formula = customers ~ store_distance * competitor_dist,
  family = "quasipoisson", data = lumber)
```

# Quasi-Poisson Example - Poisson Output

```
summary(lumber_mod)
```

```
Coefficients:
                                 Estimate Std. Error z value Pr(>|z|)
(Intercept)                       4.32561    0.50344   8.592  < 2e-16 ***
store_distance                   -0.32659    0.06425  -5.083 3.71e-07 ***
competitor_dist2-4               -1.12808    0.54137  -2.084  0.03718 *
competitor_dist>4                -0.89883    0.50992  -1.763  0.07795 .
store_distance:competitor_dist2-4  0.20830    0.07034   2.961  0.00306 **
store_distance:competitor_dist>4   0.19871    0.06623   3.000  0.00270 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for poisson family taken to be 1)

    Null deviance: 422.22  on 109  degrees of freedom
Residual deviance: 132.35  on 104  degrees of freedom
AIC: 588.39
```

# Quasi-Poisson Example - Quasi-Poisson Output

```
summary(lumber_mod_quasi)
```

```
Coefficients:
                                 Estimate Std. Error t value Pr(>|t|)
(Intercept)                       4.32561    0.55133   7.846 3.99e-12 ***
store_distance                   -0.32659    0.07036  -4.642 1.01e-05 ***
competitor_dist2-4               -1.12808    0.59287  -1.903  0.05984 .
competitor_dist>4                -0.89883    0.55843  -1.610  0.11052
store_distance:competitor_dist2-4  0.20830    0.07703   2.704  0.00800 **
store_distance:competitor_dist>4   0.19871    0.07253   2.740  0.00724 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

(Dispersion parameter for quasipoisson family taken to be 1.199297)

    Null deviance: 422.22  on 109  degrees of freedom
Residual deviance: 132.35  on 104  degrees of freedom
AIC: NA
```

# Quasi-Poisson Regression

Some things to notice:

- The parameter estimates are the same.
- We estimate the standard errors of the $\hat{\beta}_i$ coefficients by taking the SE estimates in the regular Poisson regression model and multiplying them by $\sqrt{\phi}$.
- These estimates for the quasi-Poisson approximately follow a $t$ distribution rather than a normal distribution.
- AIC is not defined for the quasi-Poisson family.

An alternative to using the quasi-Poisson is to use **negative binomial regression**. Poisson regression is actually just a special case of negative binomial regression regression and the latter has more than one parameter to allow for the mean and variance to differ.

# Just for Fun - Poisson Bootstrap

The bootstrap never (or at least rarely) lies! Compare these standard errors to the Poisson and quasi-Poisson ones.

```
nsims <- 5000
betas <- matrix(rep(0, 6*nsims), nrow = nsims)
for(i in 1:nsims) {
  index = sample(1:nrow(lumber), nrow(lumber), replace = T)
  betas[i,] <- coef(
    glm(customers ~ store_distance * competitor_dist,
        family = "poisson", data = lumber[index,])
    )
}
apply(betas, 2, mean) |> round(4) # Take mean of each column
```

```
## [1]  4.3218 -0.3267 -1.1252 -0.8973  0.2081  0.1989
```

```
apply(betas, 2, sd) |> round(4)   # Take SD of each column
```

```
## [1] 0.5368 0.0720 0.5747 0.5441 0.0776 0.0739
```

Section 4

# Partial Least Squares Regression

# PLS Intro

**Partial Least Squares** (PLS) Regression is a **dimension reduction** tool similar to **Principal Component Analysis** (PCA). Let's first review PCA.

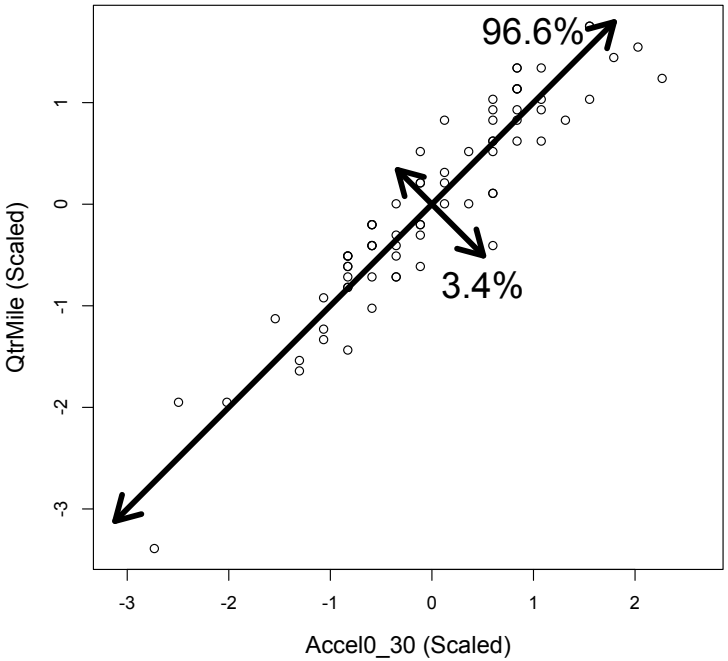
# PCA Review

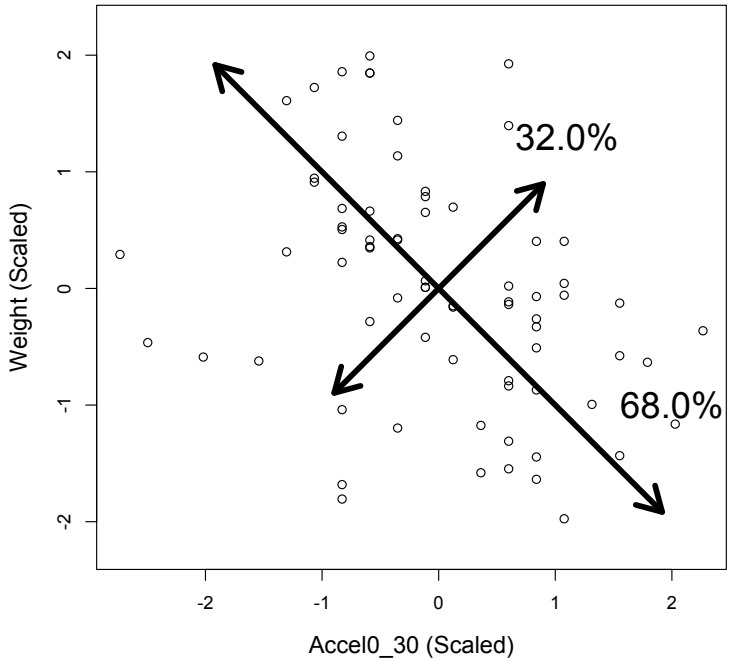
The idea of PCA is to obtain $k$ new predictors, called components, with $k < p - 1$ where each new predictor is a linear combination of the original predictor variables. PCA is useful for:

- Reducing the dimension of the problem so we are using $k$ predictors instead of $p - 1$ predictors.
- Reducing problems associated with multicollinearity.
  - Slopes being hard to interpret.
  - Standard errors being inflated.

# PCA Review

The way PCA works is that we create orthogonal predictor components using information from all the original predictors. The first component explains as much of the variation (or information) as possible in the original explanatory variables. The second component then explains as much as possible of the remaining variation, and so on. The more correlated the original variables are, the more variation can be explained with each new linear combination.



# PCA Review

Those images came from the PCA on the cars99 dataset that is in the Math3190_Sp24 GitHub repo.

```
cars <- read_csv(
  "~/My Drive/Math 3190 - Fundamentals of Data Science/Data/cars99.txt"
  ) |>
  na.omit()
head(cars)
```

```
## # A tibble: 6 x 11
##   Model        PageNum CityMPG HwyMPG FuelCap Weight FrontWt Accel0_30
##   <chr>          <dbl>   <dbl>  <dbl>   <dbl>  <dbl>   <dbl>     <dbl>
## 1 Buick Centu~      74      20     29    17.5   3350      64       3.3
## 2 Buick Regal       77      19     30    17.5   3325      63       3.3
## 3 Chevrolet L~      89      20     29    16.6   3350      64       3.4
## 4 Chevrolet M~      90      22     30    15     3040      64       3.3
## 5 Chrysler Ci~     101      19     27    16     3170      64       3.5
## 6 Daewoo Lang~     108      20     28    15.8   3185      60       4
## # i 3 more variables: Accel0_60 <dbl>, QtrMile <dbl>, Type <chr>
```

# PCA Review

We can find the components using the `prcomp()` function in **R**. Let's use PCA to try to predict highway mpg using fuel capacity, weight, front weight, 0-30 mph acceleration time, 0-60 mph acceleration time, and quarter mile time. Since the scale is so vastly different between the variables, we will center and scale them.

```
X <- cars[,5:10]
y <- cars$HwyMPG
pca <- prcomp(X, scale = T)
```

# PCA Review

The amount of variation explained by each component can be found using the standard deviations of the components.

```
round(pca$sdev, 3)
```

```
## [1] 1.941 1.147 0.839 0.350 0.288 0.074
```

```
round(pca$sdev^2/sum(pca$sdev^2), 3)
```

```
## [1] 0.628 0.219 0.117 0.020 0.014 0.001
```

```
round(cumsum(pca$sdev^2/sum(pca$sdev^2)), 3)
```

```
## [1] 0.628 0.847 0.965 0.985 0.999 1.000
```

# PCA Review

```
round(pca$rotation, 3)
```

```
##                PC1   PC2    PC3    PC4    PC5    PC6
## FuelCap     -0.349 0.597 -0.127  0.681  0.203 -0.028
## Weight      -0.345 0.602 -0.140 -0.698 -0.104  0.023
## FrontWt      0.268 0.353  0.896 -0.014  0.033  0.001
## Accel0_30    0.461 0.287 -0.219  0.182 -0.789  0.045
## Accel0_60    0.486 0.193 -0.240 -0.069  0.444  0.683
## QtrMile      0.487 0.196 -0.237 -0.102  0.357 -0.728
```

# PCA Review

These components are related to how correlated the predictor variables are. The way we find these components is by finding the eigenvectors of the correlation matrix (for scaled PCA) or the covariance matrix (for un-scaled). Then the standard deviations are the square roots of the eigenvalues.

```
eig <- eigen(cor(X))
sqrt(eig$values) |> round(3)
```

```
## [1] 1.941 1.147 0.839 0.350 0.288 0.074
```

```
eig$vectors |> round(3)
```

```
##        [,1]   [,2]   [,3]   [,4]   [,5]   [,6]
## [1,] -0.349 -0.597 -0.127  0.681 -0.203  0.028
## [2,] -0.345 -0.602 -0.140 -0.698  0.104 -0.023
## [3,]  0.268 -0.353  0.896 -0.014 -0.033 -0.001
## [4,]  0.461 -0.287 -0.219  0.182  0.789 -0.045
## [5,]  0.486 -0.193 -0.240 -0.069 -0.444 -0.683
## [6,]  0.487 -0.196 -0.237 -0.102 -0.357  0.728
```

# Unsupervised vs Supervised Learning

Notice that the response variable, $y$, is never used to find the components in PCA. Because of this, PCA is known as an **unsupervised** statistical learning algorithm.

However, a natural idea is to do something similar to PCA, but to make the algorithm **supervised**. That is, we can try to find these components using information from $\boldsymbol{y}$ in addtion to $\mathbf{X}$. This is essentially what partial least squares (PLS) is. We will find these components by balancing explaining variation in the predictors and correlation with the response variable.

# PLS and PCA in **R**

We can use the `plsr()` function in the `pls` package to perform partial least squares regression. There is also a `pcr()` function to implement PCA.

```
library(pls) |> suppressPackageStartupMessages()
cars_pls <- plsr(HwyMPG ~ FuelCap + Weight + FrontWt +
       Accel0_30 + Accel0_60 + QtrMile,
       data = cars, scale = TRUE)
cars_pcr <- pcr(HwyMPG ~ FuelCap + Weight + FrontWt +
       Accel0_30 + Accel0_60 + QtrMile,
    data = cars, scale = TRUE)
```

# pcr Function Output

Let's compare the output of the pcr() function to our PCA.

```
summary(cars_pcr)
```

```
Number of components considered: 6
TRAINING: % variance explained
        1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
X         62.81    84.74    96.49    98.53    99.91   100.00
HwyMPG    38.86    56.53    66.22    71.13    71.14    71.87
```

```
round(cars_pcr$projection, 3)
```

```
##             Comp 1 Comp 2 Comp 3 Comp 4 Comp 5 Comp 6
## FuelCap     -0.349  0.597 -0.127  0.681  0.203 -0.028
## Weight      -0.345  0.602 -0.140 -0.698 -0.104  0.023
## FrontWt      0.268  0.353  0.896 -0.014  0.033  0.001
## Accel0_30    0.461  0.287 -0.219  0.182 -0.789  0.045
## Accel0_60    0.486  0.193 -0.240 -0.069  0.444  0.683
## QtrMile      0.487  0.196 -0.237 -0.102  0.357 -0.728
```

# plsr Function Output

Let's check out the plsr() output.

```
summary(cars_pls)
```

```
Number of components considered: 6
TRAINING: % variance explained
        1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
X         60.26    82.64    95.66    98.53    98.91   100.00
HwyMPG    53.42    66.40    68.78    71.22    71.74    71.87
```

```
round(cars_pls$projection, 3)
```

```
##             Comp 1 Comp 2 Comp 3 Comp 4 Comp 5 Comp 6
## FuelCap    -0.519 -0.382  0.501  0.787  0.049 -0.102
## Weight     -0.600 -0.679 -0.366 -0.793 -0.031  0.032
## FrontWt     0.291  0.179  0.810 -0.144  0.004 -0.028
## Accel0_30   0.281 -0.400  0.006  0.182 -0.155  0.545
## Accel0_60   0.319 -0.389 -0.198 -0.114 -0.619 -1.475
## QtrMile     0.324 -0.373 -0.137  0.022  0.775  0.920
```

# `plsr` Function Output Interpretation

# More Differences Between PCA and PLS

In PCA, the loading matrix comes from the eigenvectors, which are orthogonal, so if we call the loading matrix $\mathbf{P}$ (as is common in the literature), we have that $\mathbf{P}^{-1} = \mathbf{P}^T$.

We can obtain the components (also called the scores) using $\mathbf{T} = \mathbf{XP}$. That means $\mathbf{X} = \mathbf{TP}^T$. Then we regress $\boldsymbol{y}$ on the first $k$ columns of $\mathbf{T}$ instead of $X$. That gives us

In PLS, the loadings are not orthogonal. So, while we can still decompose $\mathbf{X}$ using $\mathbf{X} = \mathbf{TP}^T$, the components can be found using $\mathbf{T} = \mathbf{X}\left(\mathbf{P}^T\right)^{-1}$. That matrix, $\left(\mathbf{P}^T\right)^{-1}$, is sometimes called the **projection** matrix and it gives the linear combinations needed to obtain the components. For PCA, the loading and projection matrix are the same.

# PLS Algorithm Part 1

Unlike PCA, the PLS projection matrix is obtained iteratively rather than using eigenvalues. Here is one way to obtain the scores:

1. Center and scale the original data matrix $\mathbf{X}$ (without an intercept column) by column. We will still call this scaled matrix $\mathbf{X}$. $\boldsymbol{y}$ need not be centered or scaled.
2. Obtain the first column of the project matrix, $\phi_1$, by setting the $j$th entry of $\phi_1$ equal to the slope from the simple linear regression of $\boldsymbol{y}$ onto $\mathbf{X}_j$, the $j$th column of $\mathbf{X}$.
   - This is equivalent to taking $\phi_1 = \mathbf{X}^T \boldsymbol{y}$ (up to a constant).
3. Then normalize these values so the length of the vector $\phi_1$ is 1.
4. Compute the first column of the scores matrix: $\mathbf{V}_1 = \sum_{j=1}^{p-1} \phi_{j1} X_j = \mathbf{X}\phi_1$.

# PLS Algorithm Part 2

5. Adjust each of the variables, $\mathbf{X}_1, \ldots \mathbf{X}_{p-1}$, for $\mathbf{V}_1$ by regressing each variable on $\mathbf{V}_1$ and taking the residuals.
   - These residuals can be interpreted as the remaining information that has not been explained by the first PLS direction.
6. Create a new matrix, $\mathbf{R}$ with columns equal to the residuals of each regression conducted in step 5.
7. Obtain $\tilde{\phi}_2 = \mathbf{R}^T \boldsymbol{y}$ and normalize it.
   - Note: this $\tilde{\phi}_2$ is not exactly equal to the second column of the projection matrix, but can be used to obtain the second column of the scores.
8. Compute the second column of the scores matrix: $\mathbf{V}_2 = \mathbf{R}\tilde{\phi}_2$.
9. Repeat steps 5-8 until all columns of the scores matrix have been obtained.

# PLS Algorithm in **R**

```
y <- cars$HwyMPG # y need not be scaled. It doesn't matter.
X_s <- scale(as.matrix(X)) # Scale X
R <- X_s # Initialize R matrix
# Initialize scores matrix
Scores <- matrix(rep(0, nrow(X_s)*ncol(X_s)), ncol = ncol(X_s))

for(i in 1:6) {
  phi <- t(R) %*% y # Find phi. First time through, R = X_s
  phi <- phi/sqrt(sum(phi^2)) # Normalize phi
  v <- R %*% phi # Get column of scores
  Scores[,i] <- v # Update scores matrix
  for(j in 1:ncol(X_s)) {
    R[,j] <- lm(R[,j] ~ v)$residuals # Update R matrix
  }
}
# Get projections
Proj <- solve(t(X_s) %*% X_s) %*% t(X_s) %*% Scores
# Get loadings
P <- t(solve(Proj))
```

# PLS Algorithm in **R**

```
round(Proj, 3)
```

```
##                [,1]   [,2]   [,3]   [,4]   [,5]   [,6]
## FuelCap      -0.519 -0.382  0.501  0.787  0.049 -0.102
## Weight       -0.600 -0.679 -0.366 -0.793 -0.031  0.032
## FrontWt       0.291  0.179  0.810 -0.144  0.004 -0.028
## Accel0_30     0.281 -0.400  0.006  0.182 -0.155  0.545
## Accel0_60     0.319 -0.389 -0.198 -0.114 -0.619 -1.475
## QtrMile       0.324 -0.373 -0.137  0.022  0.775  0.920
```

# PLS Algorithm

Note: typically the algorithm used in software finds the loadings first and then inverts the transpose of that matrix to give the projections. More info on the algorithm can be found in the "pls" package documentation.

I implemented their method in the notes in the R Markdown file, but I will not show it here since the one I showed above makes more sense (to me).

# PLS Surrogates

Like with PCA, we can obtain surrogates using PLS. We don't want to ignore any with a loading around 0.3 or higher unless others are quite a bit larger. Let's think about what they would be in this case:

# PLS Surrogates

Creating these surrogates in **R**:

```
X_s <- scale(as.matrix(X))
surrogate1 <- (X_s[,1] + X_s[,2])/2 -
                (X_s[,3] + X_s[,4] + X_s[,5] + X_s[,6])/4
surrogate2 <- (X_s[,1] + X_s[,2] + X_s[,4] + X_s[,5] + X_s[,6])/5
surrogate3 <- (X_s[,1] + X_s[,3])/2
surrogate4 <- X_s[,1] - X_s[,2]
surrogate5 <- X_s[,6] - X_s[,5]
surrogate6 <- (X_s[,4] + X_s[,6])/2 - X_s[,5]
```

# Cross Validation in PLS

The `plsr()` function has an option built in for cross validation to pick the number of components. The options are "none", "CV" for 10-fold cross validation (by default, using the `segments` option can change how many folds are used), and "LOO" for leave-one-out cross validation.

The "adjCV" is a biased-corrected CV estimate.

```
set.seed(2024)
cars_pls_cv <- plsr(HwyMPG ~ FuelCap + Weight + FrontWt +
       Accel0_30 + Accel0_60 + QtrMile,
       data = cars, scale = TRUE, validation = "CV")
summary(cars_pls_cv)
```

# Cross Validation in PLS

```
## Data:    X dimension: 73 6
##  Y dimension: 73 1
## Fit method: kernelpls
## Number of components considered: 6
##
## VALIDATION: RMSEP
## Cross-validated using 10 random segments.
##        (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps
## CV           3.085    2.180    1.895    1.841    1.799    1.848
## adjCV        3.085    2.174    1.889    1.834    1.791    1.832
##        6 comps
## CV       1.831
## adjCV    1.819
##
## TRAINING: % variance explained
##         1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
## X         60.26    82.64    95.66    98.53    98.91   100.00
## HwyMPG    53.42    66.40    68.78    71.22    71.74    71.87
```

# Cross Validation in PLS with Caret

The caret package also has pls and pcr methods for partial least squares and PCA, respectively.

```
set.seed(2024)
cars_pls_train <- train(HwyMPG ~ FuelCap + Weight + FrontWt +
       Accel0_30 + Accel0_60 + QtrMile,
       data = cars, method = "pls", scale = T,
       trControl = trainControl(method = "cv", number = 10),
       tuneGrid = data.frame(ncomp = 1:6))
summary(cars_pls_train$finalModel)
```

```
## Data:    X dimension: 73 6
##  Y dimension: 73 1
## Fit method: oscorespls
## Number of components considered: 6
## TRAINING: % variance explained
##           1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
## X           60.26    82.64    95.66    98.53    98.91   100.00
## .outcome    53.42    66.40    68.78    71.22    71.74    71.87
```

# Fitting Final PLS Model

```
car_pls_mod <- lm(
  HwyMPG ~ surrogate1 + surrogate2 + surrogate3 + surrogate4,
  data = cars)
summary(car_pls_mod)
```

```
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept)  28.9726     0.1983 146.103  < 2e-16 ***
surrogate1   -1.7875     0.1528 -11.699  < 2e-16 ***
surrogate2   -2.4234     0.4767  -5.084 3.11e-06 ***
surrogate3    0.8460     0.4053   2.087  0.04060 *
surrogate4    1.1692     0.4205   2.780  0.00702 **
---
Signif. codes:  0 ‘***’ 0.001 ‘**’ 0.01 ‘*’ 0.05 ‘.’ 0.1 ‘ ’ 1

Residual standard error: 1.694 on 68 degrees of freedom
Multiple R-squared:  0.7112,    Adjusted R-squared:  0.6942
F-statistic: 41.87 on 4 and 68 DF,  p-value: < 2.2e-16
```

# Conclusion

Regression is fun!

# Session

```
sessionInfo()
```

```
## R version 4.3.2 (2023-10-31)
## Platform: aarch64-apple-darwin20 (64-bit)
## Running under: macOS Sonoma 14.2.1
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.3-arm64/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.3-arm64/Resources/lib/libRlapack.dylib;  LAPACK version 3
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## time zone: America/Denver
## tzcode source: internal
##
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets  methods
## [7] base
##
## other attached packages:
##  [1] pls_2.8-3       caret_6.0-94    lattice_0.21-9  car_3.1-2
##  [5] carData_3.0-5   faraway_1.0.8   glmnet_4.1-8    Matrix_1.6-1.1
##  [9] gridExtra_2.3   lubridate_1.9.3 forcats_1.0.0   stringr_1.5.1
## [13] dplyr_1.1.4     purrr_1.0.2     readr_2.1.5     tidyr_1.3.1
## [17] tibble_3.2.1    ggplot2_3.4.4   tidyverse_2.0.0
##
## loaded via a namespace (and not attached):
##  [1] tidyselect_1.2.0     timeDate_4022.108    farver_2.1.1
##  [4] fastmap_1.1.1        pROC_1.18.5          digest_0.6.34
##  [7] rpart_4.1.21         timechange_0.3.0     lifecycle_1.0.4
## [10] survival_3.5-7       magrittr_2.0.3       compiler_4.3.2
## [13] rlang_1.1.3          tools_4.3.2          utf8_1.2.4
```