Homework 3

Insert your name here

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! Important

Please read the instructions carefully before submitting your assignment.

1. This assignment requires you to only upload a `PDF` file on Canvas
2. Don't collapse any code cells before submitting.
3. Remember to make sure all your code output is rendered properly before uploading your submission.

Please add your name to the author information in the frontmatter before submitting your assignment

For this assignment, we will be using the Wine Quality dataset from the UCI Machine Learning Repository. The dataset consists of red and white *vinho verde* wine samples, from the north of Portugal. The goal is to model wine quality based on physicochemical tests

We will be using the following libraries:

```r
library(readr)
library(tidyr)
library(dplyr)
```

```
Attaching package: 'dplyr'

The following objects are masked from 'package:stats':

    filter, lag

The following objects are masked from 'package:base':

    intersect, setdiff, setequal, union
```

```r
library(purrr)
library(car)
```

```
Loading required package: carData

Attaching package: 'car'

The following object is masked from 'package:purrr':

    some

The following object is masked from 'package:dplyr':

    recode
```

```r
library(glmnet)
```

```
Loading required package: Matrix
```

```
Attaching package: 'Matrix'

The following objects are masked from 'package:tidyr':

    expand, pack, unpack

Loaded glmnet 4.1-8
```

```r
library(broom)
library(corrplot)
```

```
corrplot 0.92 loaded
```

Question 1

> 50 points
>
> Regression with categorical covariate and t-Test

1.1 (5 points)

Read the wine quality datasets from the specified URLs and store them in data frames `df1` and `df2`.

```r
url1 <- "https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequalit

url2 <- "https://archive.ics.uci.edu/ml/machine-learning-databases/wine-quality/winequalit


df1 <- read.csv(url1, sep = ";")
df2 <- read.csv(url2, sep = ";")
```

1.2 (5 points)

Perform the following tasks to prepare the data frame `df` for analysis:

1. Combine the two data frames into a single data frame `df`, adding a new column called `type` to indicate whether each row corresponds to white or red wine.
2. Rename the columns of `df` to replace spaces with underscores
3. Remove the columns `fixed_acidity` and `free_sulfur_dioxide`
4. Convert the `type` column to a factor
5. Remove rows (if any) with missing values.

```
#1
df1$type <- "white"
df2$type <- "red"
df <- rbind(df1, df2)

#2
colnames(df) <- gsub("\\.", "_", colnames(df))

#3
df <- df %>%
  select(-fixed_acidity, -free_sulfur_dioxide)

#4
df$type <- as.factor(df$type)

#5
nrow(df)
```

```
[1] 6497
```

```
df <- na.omit(df)
dim(df) #none were removed
```

```
[1] 6497   11
```

Your output to `R dim(df)` should be

```
[1] 6497   11
```

```
head(df)
```

```
  volatile_acidity citric_acid residual_sugar chlorides total_sulfur_dioxide
1             0.27        0.36           20.7     0.045                  170
2             0.30        0.34            1.6     0.049                  132
3             0.28        0.40            6.9     0.050                   97
4             0.23        0.32            8.5     0.058                  186
5             0.23        0.32            8.5     0.058                  186
6             0.28        0.40            6.9     0.050                   97
  density   pH sulphates alcohol quality  type
1  1.0010 3.00      0.45     8.8       6 white
2  0.9940 3.30      0.49     9.5       6 white
3  0.9951 3.26      0.44    10.1       6 white
4  0.9956 3.19      0.40     9.9       6 white
5  0.9956 3.19      0.40     9.9       6 white
6  0.9951 3.26      0.44    10.1       6 white
```

1.3 (20 points)

Recall from STAT 200, the method to compute the t statistic for the the difference in means (with the equal variance assumption)

1. Using `df` compute the mean of `quality` for red and white wine separately, and then store the difference in means as a variable called `diff_mean`.
2. Compute the pooled sample variance and store the value as a variable called `sp_squared`.
3. Using `sp_squared` and `diff_mean`, compute the t Statistic, and store its value in a variable called `t1`.

```r
# 1
mean_red <- mean(df$quality[df$type == "red"])
mean_white <- mean(df$quality[df$type == "white"])
diff_mean <- mean_red - mean_white

# 2
n_red <- sum(df$type == "red")
n_white <- sum(df$type == "white")
var_red <- var(df[df$type == "red", "quality"])
var_white <- var(df[df$type == "white", "quality"])
sp_squared <- ((n_red - 1) * var_red + (n_white - 1) * var_white) / (n_red + n_white - 2)
sp = sqrt(sp_squared)

# 3
```

```r
t1 <- diff_mean / sqrt(sp_squared * (1/n_red + 1/n_white))
```

1.4 (10 points)

Equivalently, R has a function called `t.test()` which enables you to perform a two-sample t-Test without having to compute the pooled variance and difference in means.

Perform a two-sample t-test to compare the quality of white and red wines using the `t.test()` function with the setting `var.equal=TRUE`. Store the t-statistic in `t2`.

```r
t_test <- t.test(quality ~ type, data = df, var.equal = TRUE)
t2 <- t_test$statistic
```

1.5 (5 points)

Fit a linear regression model to predict `quality` from `type` using the `lm()` function, and extract the t-statistic for the `type` coefficient from the model summary. Store this t-statistic in `t3`.

```r
fit <- lm(quality ~ type, data = df)

summary_coef <- summary(fit)$coefficients
t_stat <- summary_coef["typewhite", "t value"]
t3 <- t_stat
```

1.6 (5 points)

Print a vector containing the values of `t1`, `t2`, and `t3`. What can you conclude from this? Why?

```r
c(t1, t2, t3) # Insert your code here
```

```
                 t
-9.68565 -9.68565  9.68565
```

Since t1 and t2 are postive while t3 is negative we see that there is a significant difference in mean quality between red and white wines.

Also, since the magnitive of each is the same we know that Welch's t-test and the two-sample t-test yield similar results.

Question 2

25 points

Collinearity

2.1 (5 points)

Fit a linear regression model with all predictors against the response variable `quality`. Use the `broom::tidy()` function to print a summary of the fitted model. What can we conclude from the model summary?

```r
lm_model <- lm(quality ~ ., data = df)

summary(lm_model)
```

```
Call:
lm(formula = quality ~ ., data = df)

Residuals:
    Min      1Q  Median      3Q     Max 
-3.3415 -0.4725 -0.0405  0.4573  3.1140 

Coefficients:
                       Estimate Std. Error t value Pr(>|t|)    
(Intercept)           5.753e+01  9.331e+00   6.166 7.44e-10 ***
volatile_acidity     -1.609e+00  8.057e-02 -19.965  < 2e-16 ***
citric_acid           2.721e-02  7.833e-02   0.347  0.72827    
residual_sugar        4.509e-02  4.158e-03  10.844  < 2e-16 ***
chlorides            -9.639e-01  3.328e-01  -2.897  0.00378 ** 
```

```
total_sulfur_dioxide -3.289e-04  2.623e-04  -1.254  0.20995
density              -5.520e+01  9.320e+00  -5.922 3.34e-09 ***
pH                    1.885e-01  6.613e-02   2.850  0.00438 **
sulphates             6.620e-01  7.584e-02   8.730  < 2e-16 ***
alcohol               2.767e-01  1.418e-02  19.514  < 2e-16 ***
typewhite            -3.858e-01  5.493e-02  -7.023 2.39e-12 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.7371 on 6486 degrees of freedom
Multiple R-squared:  0.2887,    Adjusted R-squared:  0.2876
F-statistic: 263.3 on 10 and 6486 DF,  p-value: < 2.2e-16
```

```r
tidy(lm_model)
```

```
# A tibble: 11 x 5
   term                   estimate std.error statistic  p.value
   <chr>                     <dbl>     <dbl>     <dbl>    <dbl>
 1 (Intercept)           57.5       9.33         6.17  7.44e-10
 2 volatile_acidity      -1.61      0.0806     -20.0   4.07e-86
 3 citric_acid            0.0272    0.0783       0.347 7.28e- 1
 4 residual_sugar         0.0451    0.00416     10.8   3.64e-27
 5 chlorides             -0.964     0.333       -2.90  3.78e- 3
 6 total_sulfur_dioxide  -0.000329  0.000262    -1.25  2.10e- 1
 7 density              -55.2       9.32        -5.92  3.34e- 9
 8 pH                     0.188     0.0661       2.85  4.38e- 3
 9 sulphates              0.662     0.0758       8.73  3.21e-18
10 alcohol                0.277     0.0142      19.5   1.87e-82
11 typewhite             -0.386     0.0549      -7.02  2.39e-12
```

I found that volatile acidity, residual sugar, chlorides, density, sulphates, alcohol, and the type of wine are significant predictors of wine quality. On the other hand, variables like citric acid and total sulfur dioxide do not seem to have a significant effect on quality.

2.2 (10 points)

Fit two **simple** linear regression models using `lm()`: one with only `citric_acid` as the predictor, and another with only `total_sulfur_dioxide` as the predictor. In both models, use `quality` as the response variable. How does your model summary compare to the summary from the previous question?

```r
model_citric <- lm(quality ~ citric_acid, data = df)
```

```r
model_sulfur <- lm(quality ~ total_sulfur_dioxide, data = df)
```

```r
summary(model_citric)
```

```
Call:
lm(formula = quality ~ citric_acid, data = df)

Residuals:
    Min      1Q  Median      3Q     Max 
-2.9938 -0.7831  0.1552  0.2426  3.1963 

Coefficients:
            Estimate Std. Error t value Pr(>|t|)    
(Intercept)  5.65461    0.02602 217.343   <2e-16 ***
citric_acid  0.51398    0.07429   6.918    5e-12 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.8701 on 6495 degrees of freedom
Multiple R-squared:  0.007316,	Adjusted R-squared:  0.007163 
F-statistic: 47.87 on 1 and 6495 DF,  p-value: 5.002e-12
```

```r
summary(model_sulfur)
```

```
Call:
lm(formula = quality ~ total_sulfur_dioxide, data = df)

Residuals:
    Min      1Q  Median      3Q     Max 
-2.8866 -0.7971  0.1658  0.2227  3.1965 

Coefficients:
                       Estimate Std. Error t value Pr(>|t|)    
(Intercept)           5.8923848  0.0246717 238.831  < 2e-16 ***
total_sulfur_dioxide -0.0006394  0.0001915  -3.338 0.000848 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

```
Residual standard error: 0.8726 on 6495 degrees of freedom
Multiple R-squared:  0.001713,  Adjusted R-squared:  0.001559
F-statistic: 11.14 on 1 and 6495 DF,  p-value: 0.000848
```

The reuslts are very comparable to the previous one. They show that, variables like citric acid and total sulfur dioxide do not seem to have a significant effect on quality.

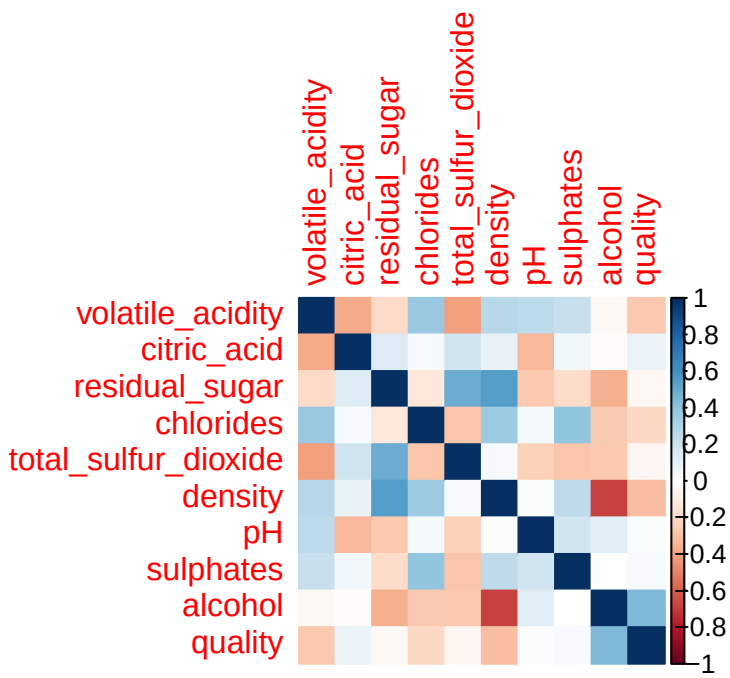
2.3 (5 points)

Visualize the correlation matrix of all numeric columns in `df` using `corrplot()`

```r
numeric_df <- df %>% select_if(is.numeric)

correlation_matrix <- cor(numeric_df)

corrplot(correlation_matrix, method = "color")
```



2.4 (5 points)

Compute the variance inflation factor (VIF) for each predictor in the full model using `vif()` function. What can we conclude from this?

```
lm_model <- lm(quality ~ ., data = df)

vif_scores <- vif(lm_model)
vif_scores
```

```
  volatile_acidity          citric_acid       residual_sugar
          2.103853             1.549248             4.680035
         chlorides total_sulfur_dioxide              density
          1.625065             2.628534             9.339357
                pH            sulphates              alcohol
          1.352005             1.522809             3.419849
              type
          6.694679
```

The VIF scores indicate that there is potential multicollinearity in density and type, where VIF values exceeded the common threshold of 10.

Question 3

40 points

Variable selection

3.1 (5 points)

Run a backward stepwise regression using a `full_model` object as the starting model. Store the final formula in an object called `backward_formula` using the built-in `formula()` function in R

```
full_model <- lm(quality ~ ., data = df)
```

```r
backward_model <- step(full_model, direction = "backward")
```

```
Start:  AIC=-3953.43
quality ~ volatile_acidity + citric_acid + residual_sugar + chlorides +
    total_sulfur_dioxide + density + pH + sulphates + alcohol +
    type

                       Df Sum of Sq    RSS     AIC
- citric_acid           1     0.066 3523.6 -3955.3
- total_sulfur_dioxide  1     0.854 3524.4 -3953.9
<none>                              3523.5 -3953.4
- pH                    1     4.413 3527.9 -3947.3
- chlorides             1     4.559 3528.1 -3947.0
- density               1    19.054 3542.6 -3920.4
- type                  1    26.794 3550.3 -3906.2
- sulphates             1    41.399 3564.9 -3879.5
- residual_sugar        1    63.881 3587.4 -3838.7
- alcohol               1   206.860 3730.4 -3584.8
- volatile_acidity      1   216.549 3740.0 -3567.9

Step:  AIC=-3955.3
quality ~ volatile_acidity + residual_sugar + chlorides + total_sulfur_dioxide +
    density + pH + sulphates + alcohol + type

                       Df Sum of Sq    RSS     AIC
- total_sulfur_dioxide  1     0.818 3524.4 -3955.8
<none>                              3523.6 -3955.3
- chlorides             1     4.495 3528.1 -3949.0
- pH                    1     4.536 3528.1 -3948.9
- density               1    20.794 3544.4 -3919.1
- type                  1    26.943 3550.5 -3907.8
- sulphates             1    41.491 3565.1 -3881.2
- residual_sugar        1    67.371 3590.9 -3834.3
- alcohol               1   235.151 3758.7 -3537.6
- volatile_acidity      1   252.565 3776.1 -3507.5

Step:  AIC=-3955.8
quality ~ volatile_acidity + residual_sugar + chlorides + density +
    pH + sulphates + alcohol + type

                    Df Sum of Sq    RSS     AIC
<none>                           3524.4 -3955.8
```

```
- pH                1     4.295 3528.7 -3949.9
- chlorides         1     4.523 3528.9 -3949.5
- density           1    21.540 3545.9 -3918.2
- sulphates         1    40.711 3565.1 -3883.2
- type              1    43.664 3568.0 -3877.8
- residual_sugar    1    66.572 3591.0 -3836.2
- alcohol           1   244.545 3768.9 -3521.9
- volatile_acidity  1   256.695 3781.1 -3501.0
```

```r
backward_formula <- formula(backward_model)

backward_formula
```

```
quality ~ volatile_acidity + residual_sugar + chlorides + density +
    pH + sulphates + alcohol + type
```

3.2 (5 points)

Run a forward stepwise regression using a `null_model` object as the starting model. Store the final formula in an object called `forward_formula` using the built-in `formula()` function in R

```r
null_model <- lm(quality ~ 1, data = df)

forward_model <- step(null_model, direction = "forward", scope = formula(~ .), data = df)
```

```
Start:  AIC=-1760.04
quality ~ 1
```

```r
forward_formula <- formula(forward_model)
forward_formula
```

```
quality ~ 1
```

3.3 (10 points)

1. Create a `y` vector that contains the response variable (`quality`) from the `df` dataframe.
2. Create a design matrix `X` for the `full_model` object using the `make_model_matrix()` function provided in the Appendix.
3. Then, use the `cv.glmnet()` function to perform LASSO and Ridge regression with `X` and `y`.

```
... # Insert your code here.
```

Create side-by-side plots of the ridge and LASSO regression results. Interpret your main findings.

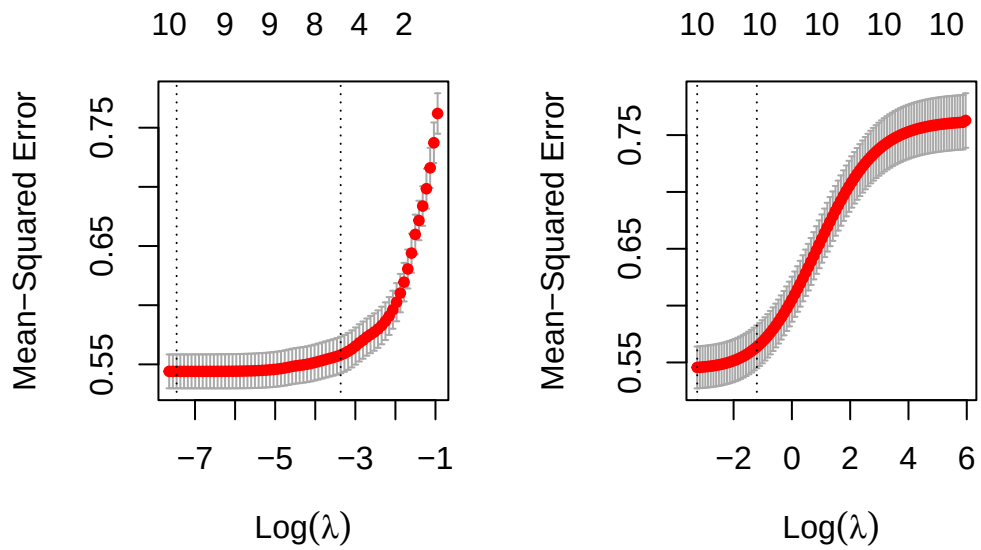
```r
# 1
y <- df$quality

# 2
X <- as.matrix(model.matrix(full_model))

# 3
lasso_model <- cv.glmnet(X, y, alpha = 1)

ridge_model <- cv.glmnet(X, y, alpha = 0)

par(mfrow=c(1, 2))
plot(lasso_model)
plot(ridge_model)
```



3.4 (5 points)

Print the coefficient values for LASSO regression at the `lambda.1se` value? What are the variables selected by LASSO?

Store the variable names with non-zero coefficients in `lasso_vars`, and create a formula object called `lasso_formula` using the `make_formula()` function provided in the Appendix.

```
# Extract coefficients at lambda.1se for LASSO model
lasso_coef <- coef(lasso_model, s = "lambda.1se")

# Print coefficient values
print(lasso_coef)

# Identify variables with non-zero coefficients
lasso_vars <- names(lasso_coef)[lasso_coef != 0]

# Remove the response variable "quality"
lasso_vars <- lasso_vars[!lasso_vars %in% "quality"]

# Create the LASSO formula
```

```r
lasso_formula <- as.formula(paste("quality ~", paste(lasso_vars, collapse = " + ")))

# Print LASSO formula
print(lasso_formula)
```

3.5 (5 points)

Print the coefficient values for ridge regression at the `lambda.1se` value? What are the variables selected here?

Store the variable names with non-zero coefficients in `ridge_vars`, and create a formula object called `ridge_formula` using the `make_formula()` function provided in the Appendix.

"'R# Extract coefficients at lambda.1se for Ridge model ridge_coef <- coef(ridge_model, s = "lambda.1se")

Print coefficient values

print(ridge_coef)

Identify variables with non-zero coefficients

ridge_vars <- names(ridge_coef)[ridge_coef != 0]

Create formula object using make_formula() function

ridge_formula <- make_formula(ridge_vars)

Print Ridge formula

print(ridge_formula)

```
---

###### 3.6  (10 points)

What is the difference between stepwise selection, LASSO and ridge based on your analyses abo
```



```
---

## Question 4
::: {.callout-tip}
## 70 points

Variable selection
:::

---


###### 4.1  (5 points)

Excluding `quality` from `df` we have $10$ possible predictors as the covariates. How many di

::: {.cell}

:::

---


###### 4.2  (20 points)

Store the names of the predictor variables (all columns except `quality`) in an object called
```

```
::: {.cell}

```{.r .cell-code}
x_vars <- colnames(df %>% select(-quality))

:::
```

Use:

- the `combn()` function (built-in R function) and
- the `make_formula()` (provided in the Appendix)

to **generate all possible linear regression formulas** using the variables in `x_vars`. This is most optimally achieved using the `map()` function from the `purrr` package.

```r
formulas <- map(
  1:length(x_vars),
  \(x){
    vars <- combn(x_vars, x)
    map(vars, \(var_set) make_formula(var_set))
  }
) %>% unlist()
```

If your code is right the following command should return something along the lines of:

```r
sample(formulas, 4) %>% as.character()
# Output:
# [1] "quality ~ volatile_acidity + residual_sugar + density + pH + alcohol"
# [2] "quality ~ citric_acid"
# [3] "quality ~ volatile_acidity + citric_acid + residual_sugar + total_sulfur_dioxide +
# [4] "quality ~ citric_acid + chlorides + total_sulfur_dioxide + pH + alcohol + type"
```

4.3 (10 points)

Use `map()` and `lm()` to fit a linear regression model to each formula in `formulas`, using `df` as the data source. Use `broom::glance()` to extract the model summary statistics, and bind them together into a single tibble of summaries using the `bind_rows()` function from `dplyr`.

```r
models <- map(formulas, ~lm(., data = df))
summaries <- map(models, glance)
```
```

```r
summaries <- bind_rows(summaries, .id = "model")
head(summaries)
```

4.4 (5 points)

Extract the `adj.r.squared` values from `summaries` and use them to identify the formula with the ***highest*** adjusted R-squared value.

```r
adj_r_squared <- summaries$adj.r.squared

best_model_index <- which.max(adj_r_squared)
```

Store resulting formula as a variable called `rsq_formula`.

```r
rsq_formula <- formulas[[best_model_index]]
```

4.5 (5 points)

Extract the `AIC` values from `summaries` and use them to identify the formula with the ***lowest*** AIC value.

```r
aic_values <- summaries$AIC

best_model_index <- which.min(aic_values)
```

Store resulting formula as a variable called `aic_formula`.

```r
aic_formula <- formulas[[best_model_index]]
print(aic_formula)
```

4.6 (15 points)

Combine all formulas shortlisted into a single vector called `final_formulas`.

```r
null_formula <- formula(null_model)
full_formula <- formula(full_model)

final_formulas <- c(
  null_formula,
  full_formula,
  backward_formula,
  forward_formula,
  lasso_formula,
  ridge_formula,
  rsq_formula,
  aic_formula
)
```

- Are `aic_formula` and `rsq_formula` the same? How do they differ from the formulas shortlisted in question 3?
- Which of these is more reliable? Why?
- If we had a dataset with $10,000$ columns, which of these methods would you consider for your analyses? Why?

4.7 (10 points)

Use `map()` and `glance()` to extract the `sigma, adj.r.squared, AIC, df`, and `p.value` statistics for each model obtained from `final_formulas`. Bind them together into a single data frame `summary_table`. Summarize your main findings.

```r
summary_table <- map(
  final_formulas,
  \(formula) {
    model <- lm(formula, data = df)
    glance(model)
  }
) %>%
bind_rows()

summary_table %>% knitr::kable()
```

Appendix

Convenience function for creating a formula object

The following function which takes as input a vector of column names `x` and outputs a `formula` object with `quality` as the response variable and the columns of `x` as the covariates.

```
make_formula <- function(x){
  as.formula(
    paste("quality ~ ", paste(x, collapse = " + "))
  )
}

# For example the following code will
# result in a formula object
# "quality ~ a + b + c"
make_formula(c("a", "b", "c"))
```

Convenience function for `glmnet`

The `make_model_matrix` function below takes a `formula` as input and outputs a **rescaled** model matrix `X` in a format amenable for `glmnet()`

```
make_model_matrix <- function(formula){
  X <- model.matrix(formula, df)[, -1]
  cnames <- colnames(X)
  for(i in 1:ncol(X)){
    if(!cnames[i] == "typewhite"){
      X[, i] <- scale(X[, i])
    } else {
      colnames(X)[i] <- "type"
    }
  }
  return(X)
}
```

Session Information

Print your `R` session information using the following command

```
sessionInfo()
```