

# stsci3740 final project modeling

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```
# import datasets
red <- read.csv("C:/Users/xinya/Downloads/Cornell Classes/STSCI 3740/final project/winequality-red.csv")

white <- read.csv("C:/Users/xinya/Downloads/Cornell Classes/STSCI 3740/final project/winequality-white.csv")

wine <- read.csv("C:/Users/xinya/Downloads/Cornell Classes/STSCI 3740/final project/wine-quality-white.csv")
```

## Fitting a KNN Model

```
# normalize the data using z-score
normalize <- function(x) {
  return((x - mean(x)) / sd(x))
}

# wine_norm <- wine %>%
#   mutate(across(where(is.numeric) & !where(is.factor), normalize))

all_columns <- names(wine)
columns_to_normalize <- all_columns[all_columns != "quality" & sapply(wine, is.numeric)]
wine_norm <- wine
wine_norm[columns_to_normalize] <- lapply(wine[columns_to_normalize], normalize)

# change type of wine to white=1, red=2
wine_norm$type <- as.numeric(factor(wine_norm$type))

# split the dataset into train/test
set.seed(1)
index <- sample(1:nrow(wine_norm), size=nrow(wine_norm)*0.7, rep=FALSE)
training <- wine_norm[index, ]
testing <- wine_norm[-index, ]

training_X <- training %>% select(-quality)
testing_X <- testing %>% select(-quality)

# try different values of k
k.values <- 1:20
```

```

knn.errors <- sapply(k.values, function(k) {
  knn.pred <- knn(training_X, testing_X, training$quality, k=k)
  mean(knn.pred != testing$quality)
})

print(knn.errors)

```

```

## [1] 0.3989744 0.4794872 0.4707692 0.4574359 0.4482051 0.4456410 0.4507692
## [8] 0.4528205 0.4451282 0.4528205 0.4364103 0.4420513 0.4317949 0.4379487
## [15] 0.4358974 0.4358974 0.4461538 0.4415385 0.4389744 0.4405128

```

The value of k that seems to perform the best on this data is k=1.

## Choose the optimal k-value using Cross Validation

```

set.seed(1)
# 10-fold cross validation
control <- trainControl(method = "cv", number = 10)

knn_cv <- train(
  quality ~ .,
  data = wine_norm,
  method = "knn",
  trControl = control,
  tuneGrid = expand.grid(k = 1:20)
)

knn_cv

```

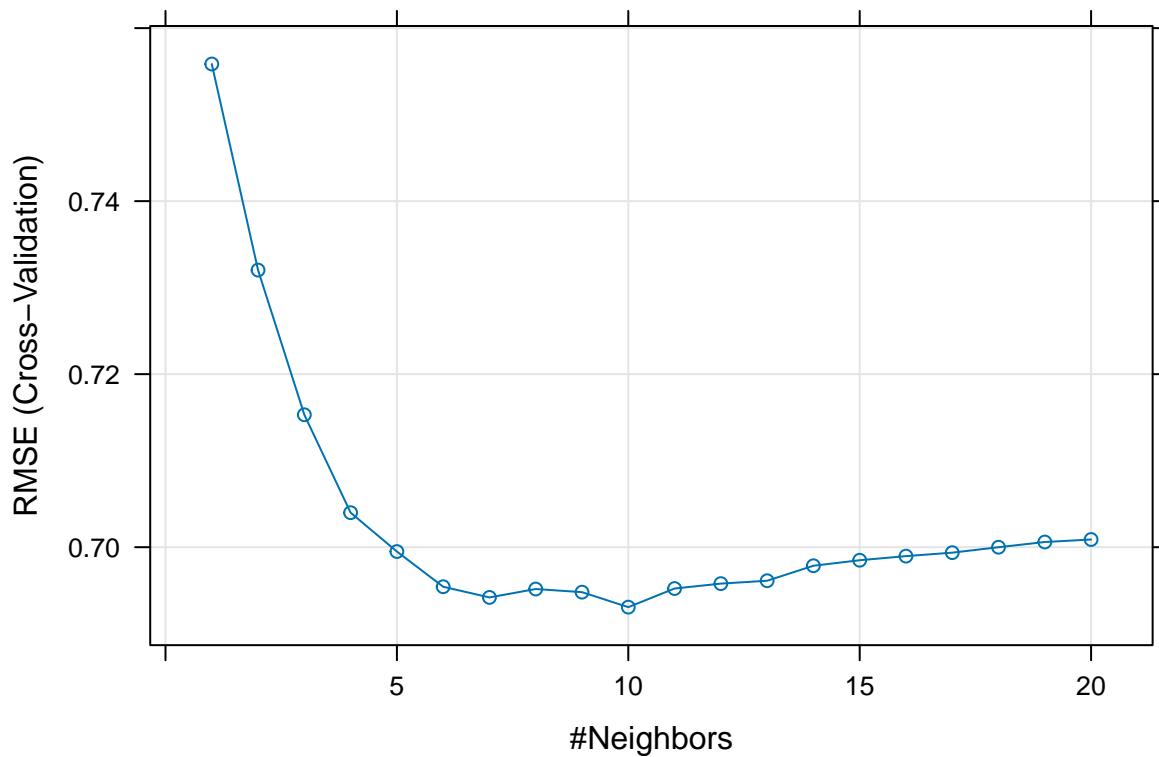
```

## k-Nearest Neighbors
##
## 6497 samples
## 12 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 5847, 5846, 5847, 5847, 5847, 5848, ...
## Resampling results across tuning parameters:
##
## k RMSE Rsquared MAE
## 1 0.7558513 0.3795189 0.4239693
## 2 0.7320306 0.3612061 0.4939238
## 3 0.7153067 0.3654421 0.5125768
## 4 0.7039897 0.3718375 0.5170525
## 5 0.6994976 0.3727748 0.5246780
## 6 0.6954288 0.3756623 0.5260905
## 7 0.6941926 0.3755005 0.5286038
## 8 0.6951634 0.3725416 0.5314023
## 9 0.6948018 0.3720174 0.5344289
## 10 0.6930709 0.3743660 0.5342596

```

```
## 11 0.6952228 0.3699285 0.5365115
## 12 0.6957883 0.3683444 0.5382253
## 13 0.6961228 0.3676329 0.5401778
## 14 0.6978546 0.3643808 0.5417053
## 15 0.6984920 0.3632550 0.5426139
## 16 0.6989681 0.3623560 0.5431027
## 17 0.6993684 0.3614560 0.5446430
## 18 0.6999960 0.3602518 0.5456382
## 19 0.7005973 0.3591466 0.5467203
## 20 0.7008890 0.3587130 0.5473792
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was k = 10.
```

```
plot(knn_cv)
```



## Fitting the best model

```
model <- knn(training_X, testing_X, training$quality, k=10)
confusion_matrix <- table(coPredicted = model, Actual = testing$quality)
print(confusion_matrix)
```

```
##           Actual
## coPredicted  3  4  5  6  7  8  9
##           3  0  0  0  0  0  0
##           4  0  2  5  0  0  0
##           5  4 32 392 186 16  4  0
##           6  4 33 219 547 155 22  1
##           7  0  0 19 123 144 31  1
##           8  0  0  0  5  2  2  1
##           9  0  0  0  0  0  0  0
```

```
accuracy <- sum(diag(confusion_matrix)) / sum(confusion_matrix)
accuracy
```

```
## [1] 0.5574359
```

## Apply PCA to reduce dimensionality

```
# apply PCA before fitting KNN
new_wine <- wine
new_wine$type <- as.numeric(factor(new_wine$type))

target <- new_wine$quality
predictors <- new_wine %>% select(-quality)

# standardize data
scaled_data <- scale(predictors)

# Perform PCA
pca_result <- prcomp(scaled_data, center = TRUE, scale. = TRUE)
summary(pca_result)
```

```
## Importance of components:
##              PC1    PC2    PC3    PC4    PC5    PC6    PC7
## Standard deviation  1.9518 1.5902 1.2496 0.9853 0.85077 0.78329 0.7324
## Proportion of Variance 0.3175 0.2107 0.1301 0.0809 0.06032 0.05113 0.0447
## Cumulative Proportion 0.3175 0.5282 0.6583 0.7392 0.79952 0.85065 0.8953
##              PC8    PC9    PC10    PC11    PC12
## Standard deviation  0.70921 0.59368 0.5068 0.34552 0.15539
## Proportion of Variance 0.04192 0.02937 0.0214 0.00995 0.00201
## Cumulative Proportion 0.93727 0.96664 0.9880 0.99799 1.00000
```

Decided to choose the first eight PCs

```
# reduce dimensionality
# choose the first eight PCs
pca_data <- pca_result$x[, 1:8]
```

## Fit KNN Model on PCA-reduced data

```

# apply KNN on PCA-reduced data
set.seed(1)
index_2 <- sample(1:nrow(pca_data), size=nrow(pca_data)*0.7, rep=FALSE)
training_data <- pca_data[index_2, ]
testing_data <- pca_data[-index_2, ]

training_target <- target[index_2]
testing_target <- target[-index_2]

# 10-fold cross validation to find the best k
control_new <- trainControl(method = "cv", number = 10)

knn_cv_2 <- train(
  training_data,
  training_target,
  method = "knn",
  trControl = control_new,
  tuneGrid = expand.grid(k = 1:20)
)

knn_cv_2

```

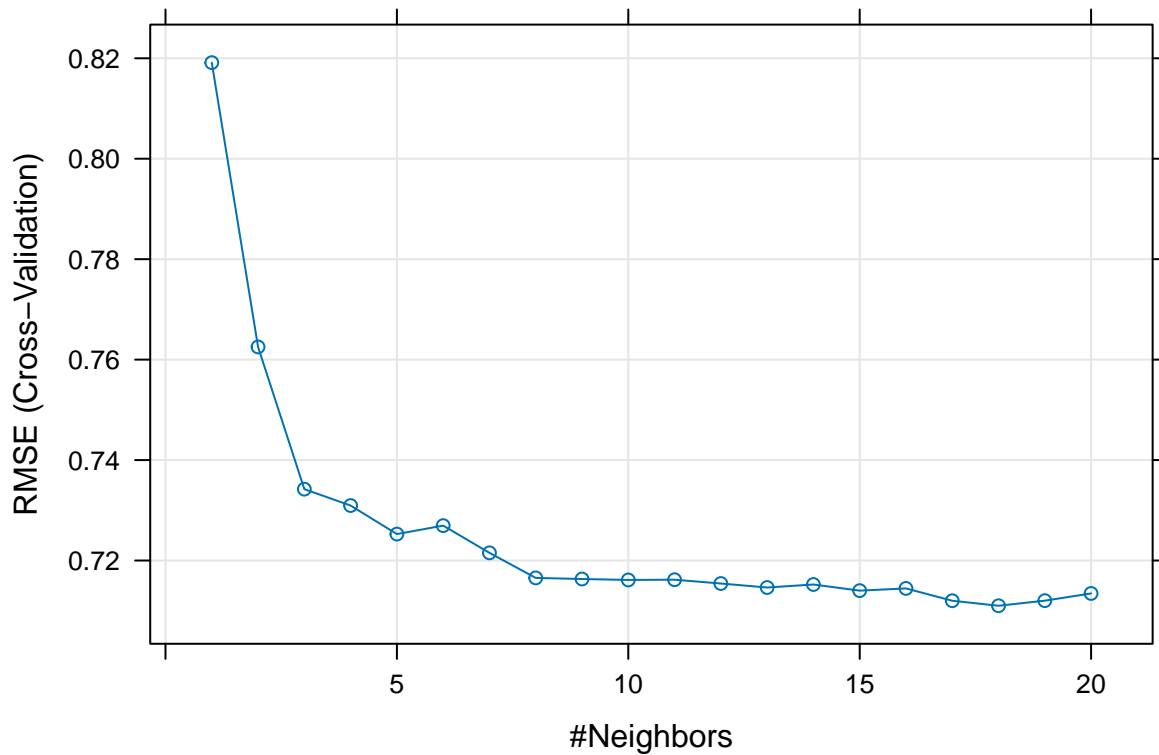
```

## k-Nearest Neighbors
##
## 4547 samples
##      8 predictor
##
## No pre-processing
## Resampling: Cross-Validated (10 fold)
## Summary of sample sizes: 4091, 4091, 4093, 4092, 4092, 4091, ...
## Resampling results across tuning parameters:
##
##   k    RMSE      Rsquared    MAE
##   1  0.8191349  0.2974479  0.4807663
##   2  0.7625294  0.3141066  0.5264729
##   3  0.7342127  0.3306869  0.5353884
##   4  0.7309495  0.3219460  0.5462665
##   5  0.7252672  0.3256003  0.5506567
##   6  0.7269512  0.3199774  0.5561480
##   7  0.7215278  0.3253284  0.5557852
##   8  0.7165359  0.3322161  0.5540389
##   9  0.7163207  0.3311995  0.5561248
##  10  0.7161339  0.3301913  0.5570248
##  11  0.7161817  0.3296976  0.5592316
##  12  0.7154242  0.3309020  0.5601571
##  13  0.7146273  0.3320483  0.5608825
##  14  0.7152282  0.3306918  0.5617482
##  15  0.7140067  0.3327959  0.5607729
##  16  0.7144465  0.3320431  0.5621654
##  17  0.7119925  0.3367552  0.5608877
##  18  0.7109959  0.3386110  0.5605507
##  19  0.7120115  0.3367728  0.5614468
##  20  0.7134455  0.3339659  0.5633644

```

```
##
## RMSE was used to select the optimal model using the smallest value.
## The final value used for the model was k = 18.
```

```
plot(knn_cv_2)
```



```
knn_model <- knn(train = training_data, test = testing_data, cl = training_target, k = 17)
confusion_matrix <- table(Predicted = knn_model, Actual = testing_target)
print(confusion_matrix)
```

```
##           Actual
## Predicted   3   4   5   6   7   8   9
##           3  0  0  0  0  0  0  0
##           4  0  1  2  1  0  0  0
##           5  5 34 367 200 14  3  0
##           6  3 30 247 566 176 25  2
##           7  0  2 19  94 126 31  1
##           8  0  0  0  0  1  0  0
##           9  0  0  0  0  0  0  0
```

```
accuracy <- sum(diag(confusion_matrix)) / sum(confusion_matrix)
accuracy
```

```
## [1] 0.5435897
```