k-NN Implementation

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k-NN application to the dataset wisc_bc_data.csv on the variable diagnosis.

Pros and cons of k-NN algorithm

```
## Loading required package: 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
```

Table 1: **Strenghts and weaknesses of the k-NN algorithm**

Strengths	Weaknesses
Simple and effective	Does not produce a model, limiting the ability to understand how the features are related to the class
Makes no assumptions about the underlying data distribution	Requires selection of an appropriate k
Fast training phase	Slow classification phase
	Nominal features and missing data require additional processing

Data loading and first exploration

First of all, we upload the dataset. Specifying the file location is done under the hood (not shown).

```
dataset = read.csv(file, stringsAsFactors = T)
```

We explore the dataset using the str function.

```
str(dataset)
```

```
## 'data.frame':    569 obs. of  32 variables:
##  $ id                : int  87139402 8910251 905520 868871 9012568 906539 925291 87880 862989 89827 .
##  $ diagnosis         : Factor w/ 2 levels "B","M": 1 1 1 1 1 1 1 2 1 1 ...
##  $ radius_mean       : num  12.3 10.6 11 11.3 15.2 ...
##  $ texture_mean      : num  12.4 18.9 16.8 13.4 13.2 ...
##  $ perimeter_mean    : num  78.8 69.3 70.9 73 97.7 ...
##  $ area_mean         : num  464 346 373 385 712 ...
##  $ smoothness_mean   : num  0.1028 0.0969 0.1077 0.1164 0.0796 ...
##  $ compactness_mean  : num  0.0698 0.1147 0.078 0.1136 0.0693 ...
##  $ concavity_mean    : num  0.0399 0.0639 0.0305 0.0464 0.0339 ...
##  $ points_mean       : num  0.037 0.0264 0.0248 0.048 0.0266 ...
##  $ symmetry_mean     : num  0.196 0.192 0.171 0.177 0.172 ...
##  $ dimension_mean    : num  0.0595 0.0649 0.0634 0.0607 0.0554 ...
##  $ radius_se         : num  0.236 0.451 0.197 0.338 0.178 ...
##  $ texture_se        : num  0.666 1.197 1.387 1.343 0.412 ...
##  $ perimeter_se      : num  1.67 3.43 1.34 1.85 1.34 ...
##  $ area_se           : num  17.4 27.1 13.5 26.3 17.7 ...
##  $ smoothness_se     : num  0.00805 0.00747 0.00516 0.01127 0.00501 ...
##  $ compactness_se    : num  0.0118 0.03581 0.00936 0.03498 0.01485 ...
##  $ concavity_se      : num  0.0168 0.0335 0.0106 0.0219 0.0155 ...
##  $ points_se         : num  0.01241 0.01365 0.00748 0.01965 0.00915 ...
##  $ symmetry_se       : num  0.0192 0.035 0.0172 0.0158 0.0165 ...
##  $ dimension_se      : num  0.00225 0.00332 0.0022 0.00344 0.00177 ...
##  $ radius_worst      : num  13.5 11.9 12.4 11.9 16.2 ...
##  $ texture_worst     : num  15.6 22.9 26.4 15.8 15.7 ...
##  $ perimeter_worst   : num  87 78.3 79.9 76.5 104.5 ...
##  $ area_worst        : num  549 425 471 434 819 ...
##  $ smoothness_worst  : num  0.139 0.121 0.137 0.137 0.113 ...
##  $ compactness_worst: num  0.127 0.252 0.148 0.182 0.174 ...
##  $ concavity_worst   : num  0.1242 0.1916 0.1067 0.0867 0.1362 ...
##  $ points_worst      : num  0.0939 0.0793 0.0743 0.0861 0.0818 ...
##  $ symmetry_worst    : num  0.283 0.294 0.3 0.21 0.249 ...
##  $ dimension_worst   : num  0.0677 0.0759 0.0788 0.0678 0.0677 ...
```

We drop the id variable.

```
dataset <- dataset[-1]
```

We check how many of the tumors are bening (B) and how many are malignant (M)

```
table(dataset$diagnosis)
```

```
##
##   B   M
## 357 212
```

We recode the variable of interest to a factor.

```r
if (is.factor(dataset[[variable_of_interest]])) {
  dataset[[variable_of_interest]] <- factor(dataset[[variable_of_interest]], levels = c("B", "M"), label
}
```

```r
round(prop.table(table(dataset[[variable_of_interest]])) * 100, digits = 1)
```

```
##
##    Benign Malignant
##      62.7      37.3
```

Min/max normalization

We normalize all features.

```r
dataset_normalized = as.data.frame(lapply(dataset[, -which(colnames(dataset) == variable_of_interest)],
                                          normalize))
```

We check everything worked out A-OK.

```r
summary(dataset_normalized$area_mean)
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
##  0.0000  0.1174  0.1729  0.2169  0.2711  1.0000
```

```r
get_splits_percentage <- function(n_dataset){
  if (n_dataset >= 500){
    n_test = 100
    n_train = n_dataset - 100
  }
  else {
    n_train = ceiling(n_dataset * 0.8) # random split decided by moi
    n_test = floor(n_dataset * 0.2)
  }
  return(c(n_train, n_test))
}
```

Fitting the model

We define the dataset to used for training and testing.

```r
splits_to_use=get_splits_percentage(nrow(dataset_normalized))
dataset_train = dataset_normalized[1:splits_to_use[1], ]
dataset_test = dataset_normalized[(splits_to_use[1]+1):nrow(dataset_normalized), ]
labels_train = dataset[[variable_of_interest]][1:splits_to_use[1]]
labels_test = dataset[[variable_of_interest]][(splits_to_use[1]+1):nrow(dataset_normalized)]
```

Now we'll use the `knn` function from the `class` package to fit the model.

```r
require(class)
```

```
## Loading required package: class
```

```r
test_pred = knn(train = dataset_train, test = dataset_test,
                cl = labels_train, k = 21)
```

```r
require(gmodels)
```

```
## Loading required package: gmodels
```

```
CrossTable(x = labels_test, y=test_pred, prop.chisq = F)
```

```
##
##
##    Cell Contents
## |-------------------------|
## |                       N |
## |           N / Row Total |
## |           N / Col Total |
## |         N / Table Total |
## |-------------------------|
##
##
## Total Observations in Table:  100
##
##
##              | test_pred
##  labels_test |    Benign | Malignant | Row Total |
## -------------|-----------|-----------|-----------|
##       Benign |        61 |         0 |        61 |
##              |     1.000 |     0.000 |     0.610 |
##              |     0.968 |     0.000 |           |
##              |     0.610 |     0.000 |           |
## -------------|-----------|-----------|-----------|
##    Malignant |         2 |        37 |        39 |
##              |     0.051 |     0.949 |     0.390 |
##              |     0.032 |     1.000 |           |
##              |     0.020 |     0.370 |           |
## -------------|-----------|-----------|-----------|
## Column Total |        63 |        37 |       100 |
##              |     0.630 |     0.370 |           |
## -------------|-----------|-----------|-----------|
##
##
```

Improving the model

Z-score Transformation

Now we try with z-score normalization.

```
dataset_zscored = as.data.frame(scale(dataset[, -which(colnames(dataset) == variable_of_interest)]))
summary(dataset_zscored$area_mean)
```

```
##    Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
## -1.4532 -0.6666 -0.2949  0.0000  0.3632  5.2459
```

We define the training and test set again.

```
train_zscore = dataset_zscored[1:splits_to_use[1], ]
test_zscore = dataset_zscored[(splits_to_use[1]+1):nrow(dataset_zscored), ]
```

We predict again the labels now using the zscore normalized dataset, and visualize the results using the CrossTable function.

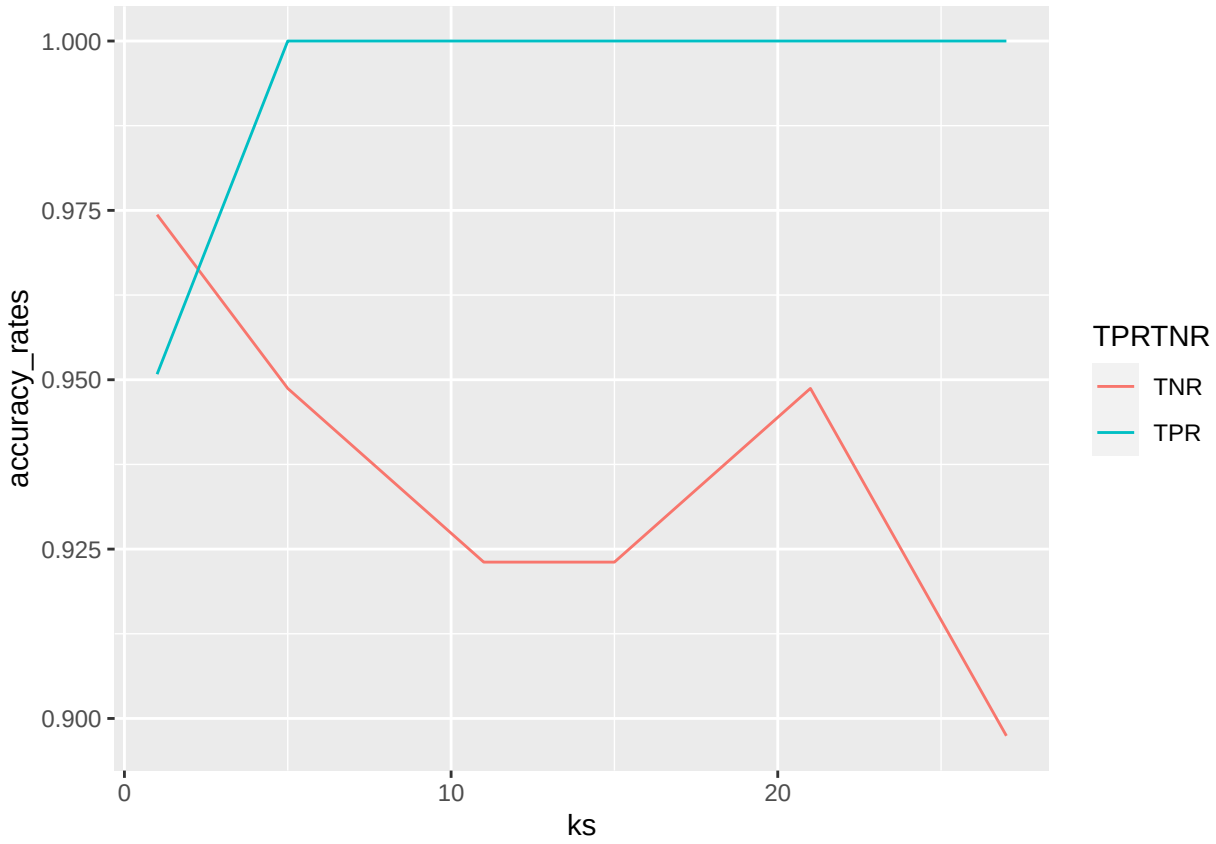
```
zscore_pred_test = knn(train=train_zscore, test=test_zscore,
                       cl=labels_train, k = ceiling(sqrt(nrow(train_zscore))))
```

```
CrossTable(x=labels_test, y=zscore_pred_test, prop.chisq=F)
```

```
##
##
##    Cell Contents
## |-------------------------|
## |                       N |
## |           N / Row Total |
## |           N / Col Total |
## |         N / Table Total |
## |-------------------------|
##
##
## Total Observations in Table:  100
##
##
##              | zscore_pred_test
##  labels_test |    Benign | Malignant | Row Total |
## -------------|-----------|-----------|-----------|
##       Benign |        61 |         0 |        61 |
##              |     1.000 |     0.000 |     0.610 |
##              |     0.924 |     0.000 |           |
##              |     0.610 |     0.000 |           |
## -------------|-----------|-----------|-----------|
##    Malignant |         5 |        34 |        39 |
##              |     0.128 |     0.872 |     0.390 |
##              |     0.076 |     1.000 |           |
##              |     0.050 |     0.340 |           |
## -------------|-----------|-----------|-----------|
## Column Total |        66 |        34 |       100 |
##              |     0.660 |     0.340 |           |
## -------------|-----------|-----------|-----------|
##
##
```

Alternative values of k

I'm not showing the code used to generate the data because it's ugly. If you wanna know my secrets open the Rmd file directly (please don't).



Appendix: "(Super-slow) Manual implementation of k-NN algorithm"

Just for fun I'm gonna implement the k-NN algorithm myself.

```
get_distance_obs <- function(vector1, vector2){
  return(sqrt(sum((vector1 - vector2)**2)))
}

compute_distance_y_to_train_observations <- function(y, train_obs){
  distances = c()
  for (row in 1:nrow(train_obs)){
    distances = append(distances, get_distance_obs(y, train_obs[row, ]))
  }
  return(distances)
}

subset_k_distances <- function(vector_distances, k){
  # Returns indices of values that minimize our distance function
  k_min_distances = which(vector_distances <= max(sort(vector_distances, decreasing = F)[1:k]))
  return(k_min_distances)
}

get_labels_corresponding_to_k_neighbors <- function(train_labels, indices){
  return(train_labels[indices])
}
```

```r
predict_one_observation <- function(y_obs, train_data, k, train_labels){
  distances_to_train_data <- compute_distance_y_to_train_observations(y_obs, train_data)
  k_distance_indices = subset_k_distances(distances_to_train_data, k=k)
  labels_sliced = get_labels_corresponding_to_k_neighbors(train_labels, k_distance_indices)
  return(names(sort(summary(labels_sliced), decreasing = T)[1]))
}

predict_all_observations <- function(dataset_with_ys, train_data, k, train_labels){
  predicted_labels_vec = c()
  if (is.data.frame(dataset_with_ys)){
    n_observations_to_predict = nrow(dataset_with_ys)
    for (obs in 1:n_observations_to_predict){
      predicted_label = predict_one_observation(y_obs=dataset_with_ys[obs, ],
                                                train_data = train_data,
                                                k=k, train_labels = train_labels)
      predicted_labels_vec = append(predicted_labels_vec, predicted_label)
    }
  }
  else if (is.vector(dataset_with_ys)){
    for (obs in dataset_with_ys){
      predicted_label = predict_one_observation(y_obs=obs,
                                                train_data = train_data,
                                                k=k, train_labels = train_labels)
      predicted_labels_vec = append(predicted_labels_vec, predicted_label)
    }
  }
  else {
    stop("Non supported data type")
  }
  return(predicted_labels_vec)
}
```

```r
labels_by_moi = predict_all_observations(dataset_with_ys = dataset_test, train_data = dataset_train,
                                         k=21, train_labels = labels_train)
using_knn_already_implemented = knn(train=dataset_train, test=dataset_test, cl=labels_train, k=21)

labels_by_moi == using_knn_already_implemented
```

```
##   [1] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
##  [16] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
##  [31] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
##  [46] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
##  [61] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
##  [76] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
##  [91] TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE TRUE
```

Com veiem, em dóna igual (aleluya). El meu codi és probablement 10000000 vegades més lent que la funció knn del paquet `class`, però ara mateix no tinc temps per a millorar-ho (i crec que tampoc és l'objectiu de l'activitat). Ho faria utilitzant apply enlloc de utilitzar `for loops`, i si fos en `Python` faria servir numpy i vectorització, no sé si a R hi ha algun equivalent.