

# K-Nearest Neighbors

Applied Machine Learning for Educational Data Science

true

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## 1. Distance Between Two Vectors

Measuring distance between two data points is at the core of K Nearest Neighbors (KNN) algorithm, and it is important to understand the concept of distance between two vectors.

Imagine that each observation in a dataset lives in an  $P$ -dimensional space, where  $P$  is the number of predictors.

- Observation 1:  $\mathbf{A} = (A_1, A_2, A_3, \dots, A_P)$
- Observation 2:  $\mathbf{B} = (B_1, B_2, B_3, \dots, B_P)$

A general definition of distance between two vectors is the **Minkowski Distance**. The Minkowski Distance can be defined as

$$\left( \sum_{i=1}^P |A_i - B_i|^q \right)^{\frac{1}{q}},$$

where  $q$  can take any positive value.

For the sake of simplicity, suppose that we have two observations and three predictors, and we observe the following values for the two observations on these three predictors.

- Observation 1: (20,25,30)
- Observation 2: (80,90,75)

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If we assume that the  $q = 1$  for the Minkowski equation above, then we can calculate the distance as the following:

```
A <- c(20,25,30)
B <- c(80,90,75)

sum(abs(A - B))
```

```
[1] 170
```

When  $q$  is equal to 1 for the Minkowski equation, it becomes a special case and is known as **Manhattan Distance**. Manhattan Distance between these two data points is visualized below.

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If we assume that the  $q = 2$  for the Minkowski equation above, then we can calculate the distance as the following:

```
A <- c(20,25,30)
B <- c(80,90,75)
```

```
(sum(abs(A - B)^2))^(1/2)
```

```
[1] 99.24717
```

When  $q$  is equal to 2 for the Minkowski equation, it is also a special case and is known as **Euclidian Distance**. Euclidian Distance between these two data points is visualized below.

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## 2. K-Nearest Neighbors

Given  $N$  observations in a dataset, a distance between any observation and  $N - 1$  remaining observations using Minkowski distance (with a user-defined choice of  $q$  value). Then, for any given observation, we can rank order the remaining observations based on how close they are to the given observation and then decide the  $K$  nearest neighbors ( $K = 1, 2, 3, \dots, N - 1$ ),  $K$  observations closest to the given observation based on their distance.

Suppose that there are 10 observations measured on three predictor variables (X1, X2, and X3) with the following values.

```
d <- data.frame(x1 =c(20,25,30,42,10,60,65,55,80,90),  
                x2 =c(10,15,12,20,45,75,70,80,85,90),  
                x3 =c(25,30,35,20,40,80,85,90,92,95),  
                label= c('A','B','C','D','E','F','G','H','I','J'))
```

d

	x1	x2	x3	label
1	20	10	25	A
2	25	15	30	B
3	30	12	35	C
4	42	20	20	D
5	10	45	40	E
6	60	75	80	F
7	65	70	85	G
8	55	80	90	H

9	80	85	92	I
10	90	90	95	J

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Given that there 10 observations, we can calculate the distance between all 45 pairs of observations (e.g., Euclidian distance).

```
dist <- as.data.frame(t(combn(1:10,2)))
dist$euclidian <- NA

for(i in 1:nrow(dist)){

  a <- d[dist[i,1],1:3]
  b <- d[dist[i,2],1:3]
  dist[i,]$euclidian <- sqrt(sum((a-b)^2))

}

dist
```

	V1	V2	euclidian
1	1	2	8.660254
2	1	3	14.282857
3	1	4	24.677925
4	1	5	39.370039
5	1	6	94.074439
6	1	7	96.046864
7	1	8	101.734950

```

8  1  9 117.106789
9  1 10 127.279221
10 2  3  7.681146
11 2  4 20.346990
12 2  5 35.000000
13 2  6 85.586214
14 2  7 87.464278
15 2  8 93.407708
16 2  9 108.485022
17 2 10 118.638105
18 3  4 20.808652
19 3  5 38.910153
20 3  6 83.030115
21 3  7 84.196199
22 3  8 90.961530
23 3  9 105.252078
24 3 10 115.256236
25 4  5 45.265881
26 4  6 83.360662
27 4  7 85.170417
28 4  8 93.107465
29 4  9 104.177733
30 4 10 113.265176
31 5  6 70.710678
32 5  7 75.332596
33 5  8 75.828754
34 5  9 95.937480
35 5 10 107.004673
36 6  7  8.660254
37 6  8 12.247449
38 6  9 25.377155
39 6 10 36.742346
40 7  8 15.000000
41 7  9 22.338308
42 7 10 33.541020
43 8  9 25.573424
44 8 10 36.742346
45 9 10 11.575837

```

Now, for instance, we can find the three closest observation to **Point E** (3-Nearest Neighbors). As seen below, the 3-Nearest Neighbors for **Point E** in this dataset would be **Point B**, **Point C**, and **Point A**.

```

# Point E is the fifth observation in the dataset

loc <- which(dist[,1]==5 | dist[,2]==5)

tmp <- dist[loc,]

tmp[order(tmp$euclidian),]

```

```

      V1 V2 euclidian
12    2  5 35.00000
19    3  5 38.91015

```

4	1	5	39.37004
25	4	5	45.26588
31	5	6	70.71068
32	5	7	75.33260
33	5	8	75.82875
34	5	9	95.93748
35	5	10	107.00467

---

#### NOTE 1

The  $q$  in the Minkowski distance equation and  $K$  in the K-nearest neighbor are user-defined hyperparameters in the KNN algorithm. As a researcher and model builder, you can pick any values for  $q$  and  $K$ . They can be tuned using a similar approach applied in earlier classes for regularized regression models. One can pick a set of values for these hyperparameters and apply a grid search to find the combination that provides the best predictive performance.

It is typical to observe overfitting (high model variance, low model bias) for small values of  $K$  and underfitting (low model variance, high model bias) for large values of  $K$ . In general practice, people tend to focus their grid search for  $K$  around  $\sqrt{N}$ .

---



---

#### NOTE 2

It is important to keep in mind that the distance calculation between two observations is highly dependent on the scale of measurement for the predictor variables. If predictors are on different scales, the distance metric formula will favor the differences in predictors with larger scale. This is not an ideal situation. Therefore, it is important to center and scale all predictors prior to the KNN algorithm so each predictor contributes to the distance metric calculation in the same way.

---

### 3. Prediction with K-Nearest Neighbors

Given that we learn about distance calculation and how to identify K-nearest neighbors based on a distance metric, the prediction in KNN is very simple and straightforward.

Below is a list of steps for predicting an outcome for a given observation.

1. Calculate the distance between the observation and remaining  $N - 1$  observations in the data (with a user choice of  $q$  in Minkowski distance).
2. Rank order the observations based on the calculated distance, and choose the K-nearest neighbor. (with a user choice of  $K$ )
3. Calculate the mean of observed outcome in the smaller set of K-nearest neighbors as your prediction.

Note that, Step 3 applies regardless of the type of outcome. If the outcome variable is continuous, we take the average outcome for the K-nearest neighbors as our prediction. If the outcome variable is binary variable (e.g., 0 vs. 1), then the proportion of observing each class among the K-nearest neighbors yield predicted probabilities for each class.

Below, I provide an example for both types of outcome using the Readability and Recidivism datasets.

### 3.1. Predicting a continuous outcome with the KNN algorithm

The code below is identical to the code we used in earlier classes for data preparation of the Readability datasets. Note that this is only to demonstrate the logic of model predictions in the context of K-nearest neighbors. So, we are using the whole dataset. In the next section, we will demonstrate the full workflow of model training and tuning with 10-fold cross-validation using the `caret::train()` function.

1. Import the data
2. Remove variables with more than 80% missingness
3. Write a recipe for processing variables
4. Apply the recipe to the dataset

```
# Import the dataset

readability <- read.csv('https://raw.githubusercontent.com/uo-datasci-specialization/c4-ml-fall-2021/main/readability.csv')

# Remove the variables with more than 80% missingness

require(finalfit)

missing_      <- ff_glimpse(readability)$Continuous
flag_na       <- which(as.numeric(missing_$missing_percent) > 80)
readability   <- readability[,-flag_na]

# Write the recipe

require(recipes)

blueprint_readability <- recipe(x      = readability,
                                vars    = colnames(readability),
                                roles   = c(rep('predictor', 990), 'outcome')) %>%

  step_zv(all_numeric()) %>%
  step_nzv(all_numeric()) %>%
  step_impute_mean(all_numeric()) %>%
  step_normalize(all_numeric_predictors()) %>%
  step_corr(all_numeric(), threshold=0.9)

# Apply the recipe

baked_read <- blueprint_readability %>%
  prep(training = readability) %>%
  bake(new_data = readability)
```

Our final dataset (`baked_read`) has 2834 observations and 888 columns (887 predictors, and the last column is target outcome). Now, suppose that we would like to predict the readability score for the first observation. The code below will calculate the Minkowski distance (with  $q = 2$ ) between the first observation and each of the remaining 2833 observations by using the first 887 columns of the dataset (predictors).

```
dist <- data.frame(obs = 2:2834, dist = NA, target=NA)

for(i in 1:2833){

  a <- as.matrix(baked_read[1,1:887])
```



```

b <- as.matrix(baked_read[dist[i+1,1],1:887])
dist[i,]$dist <- sqrt(sum((a-b)^2))
dist[i,]$target <- baked_read[dist[i,1,],]$target

# print(i)
}

```

We now rank order the observations from closest to the most distant, and then choose the 20-nearest observations ( $K=20$ ). Finally, we can calculate the average of the observed outcome for the 20-nearest neighbors, this will become our prediction of the readability score for the first observation.

```

# Rank order the observations from closest to the most distant

dist <- dist[order(dist$dist),]

# Check the 20-nearest neighbors

dist[1:20,]

```

	obs	dist	target
2440	2441	23.39269	0.55897492
2418	2419	25.35221	-0.21279072
2312	2313	25.90366	-0.25321371
2348	2349	26.15836	-0.15932546
2484	2485	26.28408	-0.92538206
2016	2017	26.54107	0.13989288
2319	2320	26.72020	-1.48029561
1570	1571	26.87505	-1.13367793
44	45	26.92854	-0.58635946
14	15	26.97686	0.24580571
2263	2264	27.27469	-0.90345299
118	119	27.28308	-0.20640822
2530	2531	27.31948	-0.32031046
1133	1134	27.54420	0.38387363
124	125	27.69614	-0.09360404
2153	2154	27.70797	-1.11412508
125	126	27.82294	-0.36537882
2268	2269	27.83390	-0.23113845
2521	2522	27.85822	-0.63588777
1244	1245	27.86323	0.70560033

```

# Mean target for the 20-nearest observations

mean(dist[1:20,]$target)

```

```
[1] -0.3293602
```

```

# Check the actual observed value of reability for the first observation

readability[1,]$target

```

```
[1] -0.3402591
```

### 3.2. Predicting a binary outcome with the KNN algorithm

We can follow the same procedures to predict the recidivism in the second year after the initial release from prison for an individual.

```
# Import data

recidivism <- read.csv('https://raw.githubusercontent.com/uo-datasci-specialization/c4-ml-fall-2021/main/recidivism.csv')

# Write the recipe

# List of variable types

outcome <- c('Recidivism_Arrest_Year2')

categorical <- c('Residence_PUMA',
  'Prison_Offense',
  'Age_at_Release',
  'Supervision_Level_First',
  'Education_Level',
  'Prison_Years',
  'Gender',
  'Race',
  'Gang_Affiliated',
  'Prior_Arrest_Episodes_DVCharges',
  'Prior_Arrest_Episodes_GunCharges',
  'Prior_Conviction_Episodes_Viol',
  'Prior_Conviction_Episodes_PPViolationCharges',
  'Prior_Conviction_Episodes_DomesticViolenceCharges',
  'Prior_Conviction_Episodes_GunCharges',
  'Prior_Revocations_Parole',
  'Prior_Revocations_Probation',
  'Condition_MH_SA',
  'Condition_Cog_Ed',
  'Condition_Other',
  'Violations_ElectronicMonitoring',
  'Violations_Instruction',
  'Violations_FailToReport',
  'Violations_MoveWithoutPermission',
  'Employment_Exempt')

numeric <- c('Supervision_Risk_Score_First',
  'Dependents',
  'Prior_Arrest_Episodes_Felony',
  'Prior_Arrest_Episodes_Misd',
  'Prior_Arrest_Episodes_Violent',
  'Prior_Arrest_Episodes_Property',
  'Prior_Arrest_Episodes_Drug',
  'Prior_Arrest_Episodes_PPViolationCharges',
  'Prior_Conviction_Episodes_Felony',
  'Prior_Conviction_Episodes_Misd',
  'Prior_Conviction_Episodes_Prop',
  'Prior_Conviction_Episodes_Drug',
```

```

      'Delinquency_Reports',
      'Program_Attendances',
      'Program_UnexcusedAbsences',
      'Residence_Changes',
      'Avg_Days_per_DrugTest',
      'Jobs_Per_Year')

props      <- c('DrugTests_THC_Positive',
               'DrugTests_Cocaine_Positive',
               'DrugTests_Meth_Positive',
               'DrugTests_Other_Positive',
               'Percent_Days_Employed')

# Convert all nominal, ordinal, and binary variables to factors
# Leave the rest as is

for(i in categorical){

  recidivism[,i] <- as.factor(recidivism[,i])

}

# For variables that represent proportions, add/subtract a small number
# to 0s/1s for logit transformation

for(i in props){
  recidivism[,i] <- ifelse(recidivism[,i]==0,.0001,recidivism[,i])
  recidivism[,i] <- ifelse(recidivism[,i]==1,.9999,recidivism[,i])
}

# Blueprint for processing variables

require(recipes)

blueprint_recidivism <- recipe(x = recidivism,
                              vars = c(categorical,numeric,props,outcome),
                              roles = c(rep('predictor',48),'outcome')) %>%
  step_indicate_na(all_of(categorical),all_of(numeric),all_of(props)) %>%
  step_zv(all_numeric()) %>%
  step_impute_mean(all_of(numeric),all_of(props)) %>%
  step_impute_mode(all_of(categorical)) %>%
  step_logit(all_of(props)) %>%
  step_ns(all_of(numeric),all_of(props),deg_free=3) %>%
  step_normalize(paste0(numeric,'_ns_1'),
                paste0(numeric,'_ns_2'),
                paste0(numeric,'_ns_3'),
                paste0(props,'_ns_1'),
                paste0(props,'_ns_2'),
                paste0(props,'_ns_3')) %>%
  step_dummy(all_of(categorical),one_hot=TRUE) %>%
  step_num2factor(Recidivism_Arrest_Year2,
                 transform = function(x) x + 1,
                 levels=c('No','Yes'))

```

```
# Apply the recipe

baked_recidivism <- blueprint_recidivism %>%
  prep(training = recidivism) %>%
  bake(new_data = recidivism)
```

The final dataset (`baked_recidivism`) has 18111 observations and 166 columns (165 predictors, and the first column is the outcome variable). Now, suppose that we would like to predict the probability of Recidivism for the first individual. The code below will calculate the Minkowski distance (with  $q = 2$ ) between the first individual and each of the remaining 18,110 individuals by using values of the 166 predictors in this dataset.

```
dist2 <- data.frame(obs = 2:18111, dist = NA, target=NA)

for(i in 1:18110){

  a <- as.matrix(baked_recidivism[1,2:165])
  b <- as.matrix(baked_recidivism[dist2[i+1,1],2:165])
  dist2[i,]$dist <- sqrt(sum((a-b)^2))
  dist2[i,]$target <- as.character(baked_recidivism[dist2[i,1],]$Recidivism_Arrest_Year2)

  #print(i)
}
```

We now rank order the individuals from closest to the most distant, and then choose the 100-nearest observations ( $K=100$ ). Then, we calculate proportion of individuals who were recidivated (YES) and not recidivated (NO) among these 100-nearest neighbors. These proportions are the predictions for the probability of being recidivated or not recidivated for the first individual.

```
# Rank order the observations from closest to the most distant

dist2 <- dist2[order(dist2$dist),]

# Check the 100-nearest neighbors

dist2[1:100,]
```

	obs	dist	target
7069	7070	7.659967	No
4526	4527	7.755362	No
8445	8446	7.859353	No
11531	11532	8.081124	Yes
9731	9732	8.090887	No
6663	6664	8.480201	No
4042	4043	8.484186	No
596	597	8.538511	No
646	647	8.558983	Yes
9112	9113	8.663452	No
1697	1698	8.687675	No
1771	1772	8.697517	No
2159	2160	8.742357	No
1028	1029	8.765372	Yes
5117	5118	8.775667	No

3690	3691	8.806331	No
830	831	8.821060	No
8140	8141	8.839652	Yes
385	386	8.856510	Yes
8468	8469	8.861272	No
7314	7315	8.874215	No
8767	8768	8.890606	No
4094	4095	8.927379	No
11386	11387	8.942428	Yes
2714	2715	8.949004	No
4423	4424	8.956050	Yes
1516	1517	8.963143	Yes
13841	13842	9.022972	No
1575	1576	9.051930	No
14384	14385	9.055670	No
8187	8188	9.067094	No
13021	13022	9.068971	No
9071	9072	9.073520	No
6356	6357	9.097278	No
3967	3968	9.108941	Yes
13821	13822	9.109367	No
2948	2949	9.109936	No
895	896	9.116890	No
11092	11093	9.117779	No
14203	14204	9.122793	No
6023	6024	9.135977	No
3435	3436	9.141237	Yes
11016	11017	9.153111	Yes
9947	9948	9.166294	No
12474	12475	9.174083	No
564	565	9.179573	Yes
1573	1574	9.187760	No
7786	7787	9.188086	No
808	809	9.199478	Yes
14784	14785	9.205327	Yes
15153	15154	9.205441	No
10817	10818	9.206677	Yes
3030	3031	9.221680	No
987	988	9.224630	No
2947	2948	9.231919	No
14506	14507	9.241374	No
13911	13912	9.250168	No
5307	5308	9.254097	Yes
4871	4872	9.278566	Yes
14527	14528	9.278633	Yes
4795	4796	9.282708	No
1562	1563	9.287491	No
9026	9027	9.287869	Yes
10168	10169	9.289060	No
3	4	9.305465	No
289	290	9.307759	Yes
600	601	9.336480	No
4779	4780	9.353857	No
4167	4168	9.367567	No

7298	7299	9.371710	No
4645	4646	9.374108	No
2300	2301	9.375541	No
1448	1449	9.386387	No
9677	9678	9.399002	Yes
9135	9136	9.412505	No
4584	4585	9.420181	Yes
7959	7960	9.425067	No
10762	10763	9.425995	Yes
7202	7203	9.437474	No
5315	5316	9.445364	No
1918	1919	9.448661	Yes
15126	15127	9.455830	Yes
3171	3172	9.460053	No
1389	1390	9.461795	Yes
9287	9288	9.465960	No
616	617	9.468258	No
549	550	9.469860	No
4230	4231	9.475141	No
4744	4745	9.476835	No
3642	3643	9.481367	No
4875	4876	9.481934	Yes
9728	9729	9.485522	No
15327	15328	9.486961	No
9382	9383	9.489079	Yes
3363	3364	9.489238	Yes
8642	8643	9.490666	Yes
2746	2747	9.491828	No
5742	5743	9.493817	No
1579	1580	9.496209	No
8964	8965	9.515531	No

```
# Mean target for the 100-nearest observations
```

```
table(dist2[1:100,]$target)
```

```
No Yes
70  30
```

```
# This indicates that the predicted probability of being recidivated is 0.30
# for the first individual given the observed data for 100 most similar
# observations
```

```
# Check the actual observed outcome for the first individual
```

```
recidivism[1,]$Recidivism_Arrest_Year2
```

```
[1] 0
```

## 4. Kernels to Weight the Neighbors

In the previous section, we tried to understand how KNN predicts a target outcome by simply averaging the observed value for the target outcome from K-nearest neighbors. This was a simple average by equally

weighting each neighbor.

Another way of averaging the target outcome from K-nearest neighbors would be to weight each neighbor according to its distance, and calculate a weighted average. A simple way to weight each neighbor is to use the inverse of distance. For instance, consider the earlier example where we find the 20-nearest neighbor for the first observation in the readability dataset.

```
dist <- dist[order(dist$dist),]

k_neighbors <- dist[1:20,]

k_neighbors
```

	obs	dist	target
2440	2441	23.39269	0.55897492
2418	2419	25.35221	-0.21279072
2312	2313	25.90366	-0.25321371
2348	2349	26.15836	-0.15932546
2484	2485	26.28408	-0.92538206
2016	2017	26.54107	0.13989288
2319	2320	26.72020	-1.48029561
1570	1571	26.87505	-1.13367793
44	45	26.92854	-0.58635946
14	15	26.97686	0.24580571
2263	2264	27.27469	-0.90345299
118	119	27.28308	-0.20640822
2530	2531	27.31948	-0.32031046
1133	1134	27.54420	0.38387363
124	125	27.69614	-0.09360404
2153	2154	27.70797	-1.11412508
125	126	27.82294	-0.36537882
2268	2269	27.83390	-0.23113845
2521	2522	27.85822	-0.63588777
1244	1245	27.86323	0.70560033

We can assign a weight to each neighbor by taking the inverse of their distance and rescaling them such that the sum of the weights are equal to 1.

```
k_neighbors$weight <- 1/k_neighbors$dist
k_neighbors$weight <- k_neighbors$weight/sum(k_neighbors$weight)

k_neighbors
```

	obs	dist	target	weight
2440	2441	23.39269	0.55897492	0.05732923
2418	2419	25.35221	-0.21279072	0.05289814
2312	2313	25.90366	-0.25321371	0.05177203
2348	2349	26.15836	-0.15932546	0.05126793
2484	2485	26.28408	-0.92538206	0.05102271
2016	2017	26.54107	0.13989288	0.05052867
2319	2320	26.72020	-1.48029561	0.05018993
1570	1571	26.87505	-1.13367793	0.04990073

```

44      45 26.92854 -0.58635946 0.04980163
14      15 26.97686  0.24580571 0.04971241
2263   2264 27.27469 -0.90345299 0.04916958
118     119 27.28308 -0.20640822 0.04915446
2530   2531 27.31948 -0.32031046 0.04908897
1133   1134 27.54420  0.38387363 0.04868847
124     125 27.69614 -0.09360404 0.04842137
2153   2154 27.70797 -1.11412508 0.04840069
125     126 27.82294 -0.36537882 0.04820069
2268   2269 27.83390 -0.23113845 0.04818172
2521   2522 27.85822 -0.63588777 0.04813964
1244   1245 27.86323  0.70560033 0.04813100

```

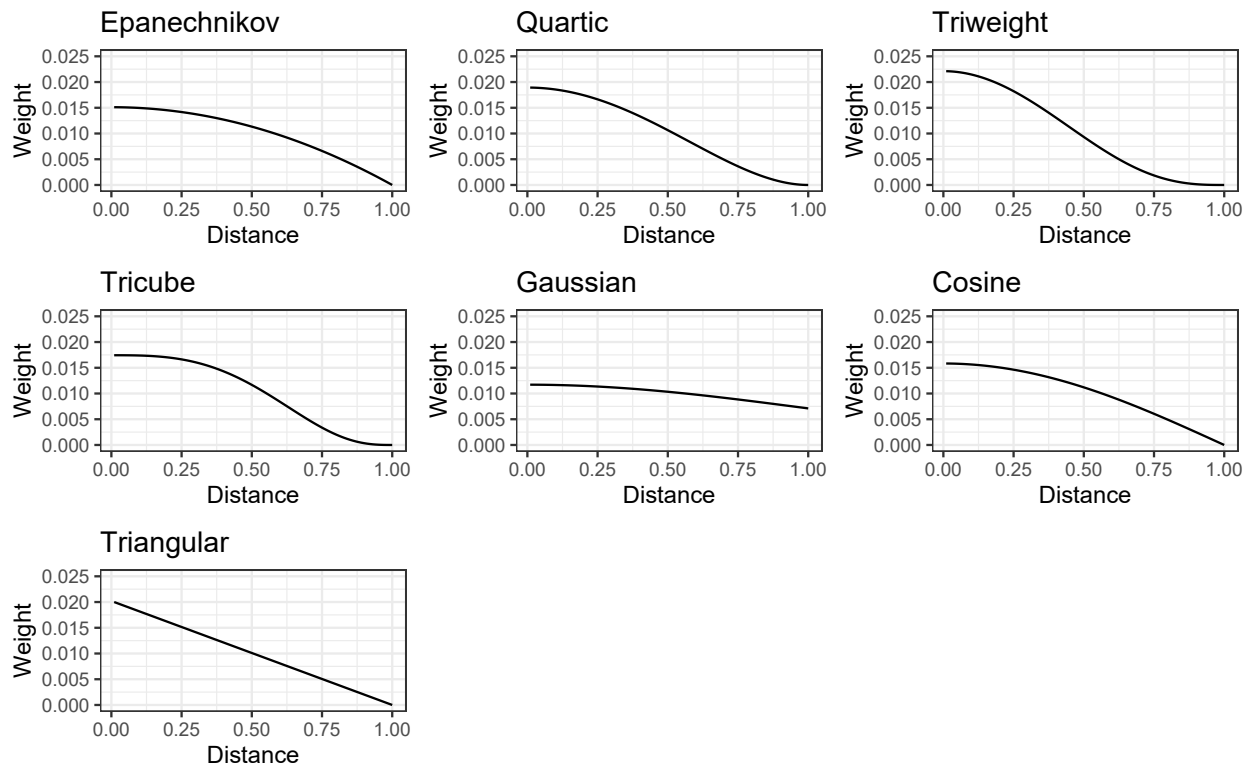
Then, we can compute a weighted average of the target scores instead of a simple average.

```
# Weighted Mean target for the 20-nearest observations
```

```
sum(k_neighbors$target*k_neighbors$weight)
```

```
[1] -0.3239415
```

There are a number of different kernel function to assign weight to K-nearest neighbors (e.g., epanechnikov, quartic, triweight, tricube, gaussian, cosine). For all of them, closest neighbors are assigned higher weights while the weight gets smaller as the distance increases. They slightly differ the way they assign the weight. Below is a demonstration how assigned weight changes as a function of distance for different kernel functions.





### NOTE 3

Which kernel function should we use for weighting the distance? The type of kernel function can also be considered as a hyperparameter to tune.

---

## 5. Parallel Processing with the `caret::train()` function

The KNN algorithm can become computationally quite intensive and grid search with so many combinations may take days particularly when you have a very large sample size. One way to reduce the computational time and make it reasonable is to use parallel processing when you have access to multiple core computers (or computing clusters).

The `caret` package is designed in a way to take advantage of multiple cores in a computer via another package `doParallel`. If you are worried about the computation time for fitting any model using the `caret::train` function, you can run the following lines of code to use as many cores as available in your computing device.

```
require(doParallel)

ncores <- 15      # depends on the number of cores available in your computer

cl <- makePSOCKcluster(ncores)

registerDoParallel(cl)
```

Once you run these lines of code, anytime you run the `caret::train` function to train any model, it will use all registered cores to do the computations. This could significantly reduce the computational time from days to hours or from hours to minutes.

After you are done with training the model, you can run the following line of code to stop the computational cluster registered for the use of your current R session.

```
stopCluster(cl)
```

You can find more information about parallel processing with the `caret` package at [this link](#).

## 6. K-Nearest Neighbors Algorithm to Predict Readability Scores

In this section, we implement the KNN algorithm to build a prediction model for the readability score. The first part of the code is identical to the code we use in earlier classes for the following steps:

1. Split the data into train and test sets
2. Create the list of row indices for 10-fold cross validation
3. Set the object for cross validation settings.

```
# Train and Test Split

set.seed(10152021) # for reproducibility

loc <- sample(1:nrow(readability), round(nrow(readability) * 0.9))
```

```

read_tr <- readability[loc, ]
read_te <- readability[-loc, ]

# Create the row indices for 10-folds

# Randomly shuffle the training data

read_tr = read_tr[sample(nrow(read_tr)),]

# Create 10 folds with equal size

folds = cut(seq(1,nrow(read_tr)),breaks=10,labels=FALSE)

# Create the list for each fold

my.indices <- vector('list',10)
for(i in 1:10){
  my.indices[[i]] <- which(folds!=i)
}

# Cross-validation settings

cv <- trainControl(method = "cv",
                   index = my.indices)

```

We will use the `kkn` package to implement the KNN algorithm, and this method is available through the `caret::train()` function. First, let's check which hyperparameters are available to tune for this method.

```

# install.package('kkn')

require(caret)
require(kkn)

getModelInfo()$kkn$parameters

```

	parameter	class	label
1	kmax	numeric	Max. #Neighbors
2	distance	numeric	Distance
3	kernel	character	Kernel

There are three hyperparameters available to optimize for the `kkn` method. These are the same parameters discussed earlier:

- **kmax**: the choice of K for the K-nearest neighbors (numeric).
- **distance**: the choice of power value ( $q$ ) for the Minkowski distance (numeric)
- **kernel**: the choice of kernel function for weighted predictions (character)

The possible kernel functions available are “rectangular”, “triangular”, “epanechnikov”, “biweight”, “triweight”, “cos”, “inv”, and “gaussian”. The “rectangular” indicates a simple average with no weight applied (equally weighted).

The next step is to create a matrix for hyperparameter grid search. Let's consider the following values for these three hyperparameters:

- kmax: 2, 3, 4, ..., 25
- distance: 1, 2, 3
- kernel: rectangular, epanechnikov

#### *# Hyperparameter Tuning Grid*

```
grid <- expand.grid(kmax = 3:25,
                  distance = c(1,2,3),
                  kernel = c('epanechnikov','rectangular'))
grid
```

	kmax	distance	kernel
1	3	1	epanechnikov
2	4	1	epanechnikov
3	5	1	epanechnikov
4	6	1	epanechnikov
5	7	1	epanechnikov
6	8	1	epanechnikov
7	9	1	epanechnikov
8	10	1	epanechnikov
9	11	1	epanechnikov
10	12	1	epanechnikov
11	13	1	epanechnikov
12	14	1	epanechnikov
13	15	1	epanechnikov
14	16	1	epanechnikov
15	17	1	epanechnikov
16	18	1	epanechnikov
17	19	1	epanechnikov
18	20	1	epanechnikov
19	21	1	epanechnikov
20	22	1	epanechnikov
21	23	1	epanechnikov
22	24	1	epanechnikov
23	25	1	epanechnikov
24	3	2	epanechnikov
25	4	2	epanechnikov
26	5	2	epanechnikov
27	6	2	epanechnikov
28	7	2	epanechnikov
29	8	2	epanechnikov
30	9	2	epanechnikov
31	10	2	epanechnikov
32	11	2	epanechnikov
33	12	2	epanechnikov
34	13	2	epanechnikov
35	14	2	epanechnikov
36	15	2	epanechnikov
37	16	2	epanechnikov
38	17	2	epanechnikov
39	18	2	epanechnikov
40	19	2	epanechnikov
41	20	2	epanechnikov
42	21	2	epanechnikov

43	22	2 epanechnikov
44	23	2 epanechnikov
45	24	2 epanechnikov
46	25	2 epanechnikov
47	3	3 epanechnikov
48	4	3 epanechnikov
49	5	3 epanechnikov
50	6	3 epanechnikov
51	7	3 epanechnikov
52	8	3 epanechnikov
53	9	3 epanechnikov
54	10	3 epanechnikov
55	11	3 epanechnikov
56	12	3 epanechnikov
57	13	3 epanechnikov
58	14	3 epanechnikov
59	15	3 epanechnikov
60	16	3 epanechnikov
61	17	3 epanechnikov
62	18	3 epanechnikov
63	19	3 epanechnikov
64	20	3 epanechnikov
65	21	3 epanechnikov
66	22	3 epanechnikov
67	23	3 epanechnikov
68	24	3 epanechnikov
69	25	3 epanechnikov
70	3	1 rectangular
71	4	1 rectangular
72	5	1 rectangular
73	6	1 rectangular
74	7	1 rectangular
75	8	1 rectangular
76	9	1 rectangular
77	10	1 rectangular
78	11	1 rectangular
79	12	1 rectangular
80	13	1 rectangular
81	14	1 rectangular
82	15	1 rectangular
83	16	1 rectangular
84	17	1 rectangular
85	18	1 rectangular
86	19	1 rectangular
87	20	1 rectangular
88	21	1 rectangular
89	22	1 rectangular
90	23	1 rectangular
91	24	1 rectangular
92	25	1 rectangular
93	3	2 rectangular
94	4	2 rectangular
95	5	2 rectangular
96	6	2 rectangular

97	7	2	rectangular
98	8	2	rectangular
99	9	2	rectangular
100	10	2	rectangular
101	11	2	rectangular
102	12	2	rectangular
103	13	2	rectangular
104	14	2	rectangular
105	15	2	rectangular
106	16	2	rectangular
107	17	2	rectangular
108	18	2	rectangular
109	19	2	rectangular
110	20	2	rectangular
111	21	2	rectangular
112	22	2	rectangular
113	23	2	rectangular
114	24	2	rectangular
115	25	2	rectangular
116	3	3	rectangular
117	4	3	rectangular
118	5	3	rectangular
119	6	3	rectangular
120	7	3	rectangular
121	8	3	rectangular
122	9	3	rectangular
123	10	3	rectangular
124	11	3	rectangular
125	12	3	rectangular
126	13	3	rectangular
127	14	3	rectangular
128	15	3	rectangular
129	16	3	rectangular
130	17	3	rectangular
131	18	3	rectangular
132	19	3	rectangular
133	20	3	rectangular
134	21	3	rectangular
135	22	3	rectangular
136	23	3	rectangular
137	24	3	rectangular
138	25	3	rectangular

There are a total of 138 combinations we would like to search. Note that, this means a total of 1380 model fitted with 10-fold cross validation for each combination. Also, the KNN algorithm is very slow to fit (because you have to calculate  $N*(N-1)/2$  distances). This may take very long. Therefore, I will also use parallel processing with 15 cores.

```
require(doParallel)

ncores <- 15      # depends on the number of cores available in your computer

cl <- makePSOCKcluster(ncores)
```

```
registerDoParallel(cl)
```

Now, we can fit the model with these settings.

```
# Train the model
```

```
caret_knn_readability <- caret::train(blueprint_readability,  
                                     data      = read_tr,  
                                     method   = "knn",  
                                     trControl = cv,  
                                     tuneGrid = grid)
```

```
caret_knn_readability$times
```

```
$everything
```

```
   user  system elapsed  
208.17    5.86 11534.15
```

```
$final
```

```
   user  system elapsed  
186.16    0.50  186.25
```

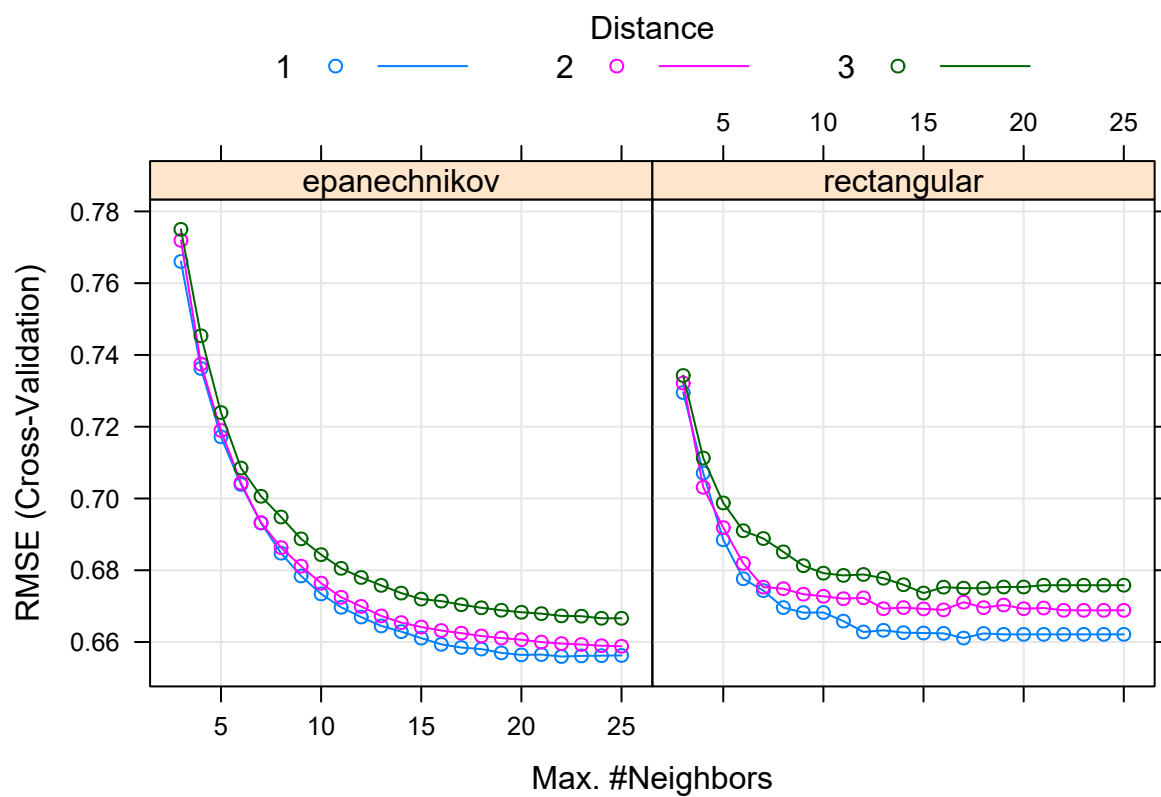
```
$prediction
```

```
[1] NA NA NA
```

The training took 11534.15 seconds (~ 3 hours 12 minutes) with 15 cores running at the same time (!).

Let's check the best combination of hyperparameters that optimizes the 10-fold cross validated performance metric (RMSE).

```
plot(caret_knn_readability)
```



```
caret_knn_readability$bestTune
```

```
      kmax distance      kernel
115    22         1 epanechnikov
```

Now, we can check the performance of the KNN algorithm on the test dataset.

```
predicted_te <- predict(caret_knn_readability,read_te)
```

```
# R-square
```

```
cor(read_te$target,predicted_te)^2
```

```
[1] 0.6226773
```

```
# RMSE
```

```
sqrt(mean((read_te$target - predicted_te)^2))
```

```
[1] 0.6297403
```

```
# MAE  
mean(abs(read_te$target - predicted_te))
```

```
[1] 0.4998969
```

The table below provides a comparison to the models we discussed earlier.

	R-square	MAE	RMSE
Linear Regression	0.644	0.522	0.644
Ridge Regression	0.727	0.435	0.536
Lasso Regression	0.725	0.434	0.538
KNN	0.623	0.500	0.629

## Variable Importance

You can ask for the variable importance plot from the KNN algorithm similar to other models (although I am not sure how they calculate the variable importance in the context of KNN).

```
require(vip)  
  
vip(caret_knn_readability,  
    num_features = 10,  
    geom = "point") +  
    theme_bw()
```



