CS167: Machine Learning

Normalization Code
Weighted k-Nearest Neighbor (k-NN)

Monday, September 23rd, 2024

Drake
UNIVERSITY

Announcements

- Notebook #2: kNN and Normalization
  - to submit, download the `.ipynb` file from Colab
  - directly upload to CodePost
  - due Today — Tuesday 09/23 by 11:59pm

CS 167 (Reza) | Fall 2024

Assignment	Code	Grade	Upload
Notebook #1	Assignment not yet published		Due: 11:59 pm on Sep 16 CDT Upload assignment
Notebook #2	Assignment not yet published		Due: 11:59 pm on Sep 23 CDT Upload assignment

Announcements

- Heads up that Quiz #1
  - will be released today (09/23) at 10:00 pm
  - will be due next Monday 09/30 by 11:59pm
  - contains some question which will be covered this week eg, evaluation metric, confusion matrix, cross validation, etc
  - Types of questions:
    - MCQ
    - True/False
    - Fill in the blanks (may or may not require calculations)

Quick Review: Missing Data

- Most datasets you will work with will not be in perfect shape
  - you'll need to clean the data before you can run any machine learning algorithms on it

- Missing data is a pretty common thing — so much so that there's a special value for missing data:
  - `NaN`, or not a number

Quick Review: Missing Data

- The steps of cleaning data normally include:
  - Step 1: Identifying which columns have missing data `df.isna().any()`
  - Step 2: Determining how much data is missing in each column
    - `df.col_missing_data.value_counts(dropna=False)`
  - Step 3: Deciding what to do with the missing data:
    - drop it: `dropna()`
      - remember to either save the returned result
        - `result = df.whatever_column.dropna()`, or use `df.whatever_column.dropna(inplace=True)`
    - fill it: `fillna()`
    - let it be

Quick Review: Identifying Missing Data

```
titanic.loc[0:4]
```

	survived	pclass	sex	age	sibsp	parch	fare	embarked	class	who	adult_male	deck	embark_town
0	0	3	male	22.0	1	0	7.2500	S	Third	man	True	NaN	Southampton
1	1	1	female	38.0	1	0	71.2833	C	First	woman	False	C	Cherbourg
2	1	3	female	26.0	0	0	7.9250	S	Third	woman	False	NaN	Southampton
3	1	1	female	35.0	1	0	53.1000	S	First	woman	False	C	Southampton
4	0	3	male	35.0	0	0	8.0500	S	Third	man	True	NaN	Southampton

- Now, let's call `isna()`, and see what we get as an output

```
titanic.loc[:4].isna()
#look at the 'deck' column...
```

	survived	pclass	sex	age	sibsp	parch	fare	embarked	class	who	adult_male	deck	embark_town
0	False	False	False	False	False	False	False	False	False	False	False	True	False
1	False	False	False	False	False	False	False	False	False	False	False	False	False
2	False	False	False	False	False	False	False	False	False	False	False	True	False
3	False	False	False	False	False	False	False	False	False	False	False	False	False
4	False	False	False	False	False	False	False	False	False	False	False	True	False

Quick Review: How much data is missing?

- Let's apply **`value_counts()`** on the various columns (eg, `deck`) of Titanic dataset

If you don't do this, it won't show the NaN counts

```
titanic.deck.value_counts(dropna=False)
#688 missing values
```

```
NaN    688
C       59
B       47
D       33
E       32
A       15
F       13
G        4
Name: deck, dtype: int64
```

https://pandas.pydata.org/docs/reference/api/pandas.Series.value_counts.html

Quick Review: Fill it using fillna()

- What do you think we should use to fill in the missing data in the age column?
  - we probably don't want to throw off our statistics...

```
print("before: ", titanic['age'].isna().any())
age_mean = titanic['age'].mean()
titanic['age'].fillna(age_mean, inplace=True)
print("after: ", titanic['age'].isna().any())
titanic.head(7)
```

	survived	pclass	sex	age	sibsp	parch	fare	embarked	class	who	adult_male	deck	embark_town	alive	alone
0	0	3	male	22.000000	1	0	7.2500	S	Third	man	True	NaN	Southampton	no	False
1	1	1	female	38.000000	1	0	71.2833	C	First	woman	False	C	Cherbourg	yes	False
2	1	3	female	26.000000	0	0	7.9250	S	Third	woman	False	NaN	Southampton	yes	True
3	1	1	female	35.000000	1	0	53.1000	S	First	woman	False	C	Southampton	yes	False
4	0	3	male	35.000000	0	0	8.0500	S	Third	man	True	NaN	Southampton	no	True
5	0	3	male	29.699118	0	0	8.4583	Q	Third	man	True	NaN	Queenstown	no	True
6	0	1	male	54.000000	0	0	51.8625	S	First	man	True	E	Southampton	no	True

Quick Review: Missing Data Functions

- `isna()`: returns True for any missing data
- `notna()`: returns True for any data that is **not** `NaN`
- `any()`: returns true if any of the elements in a Series is True
- `value_counts()`: returns a list of the values in a Series, use `dropna=False` to see `NaN` values
- `dropna()`: drops rows or columns (specify which axis, 1 or 0) that have missing data. Don't forget to either save the result of the call or add `inplace=True` as a parameter
- `fillna(new_val, inplace=True)`: replaces missing data with a given value (generally 0 or the mean)

Quick Review: Normalization Motivation

- In datasets that have numeric data, the columns that have the largest magnitude will have a greater 'say' in the decision of what to predict

- In the penguin dataset, `body_mass_g` will have a much bigger say in the prediction than the other options

```
penguins.head()
```

	species	island	culmen_length_mm	culmen_depth_mm	flipper_length_mm	body_mass_g
0	Adelie	Torgersen	39.1	18.7	181.0	3750.0
1	Adelie	Torgersen	39.5	17.4	186.0	3800.0
2	Adelie	Torgersen	40.3	18.0	195.0	3250.0
3	Adelie	Torgersen	NaN	NaN	NaN	NaN
4	Adelie	Torgersen	36.7	19.3	193.0	3450.0

Quick Review: Normalization

- Normalizing data:
  - rescale attribute values so they're about the same
  - adjusting values measured on different scales to a common scale

Quick Review: A Simple Normalization

- One simple method of normalizing data is to replace each value with a proportion relative to the max value.

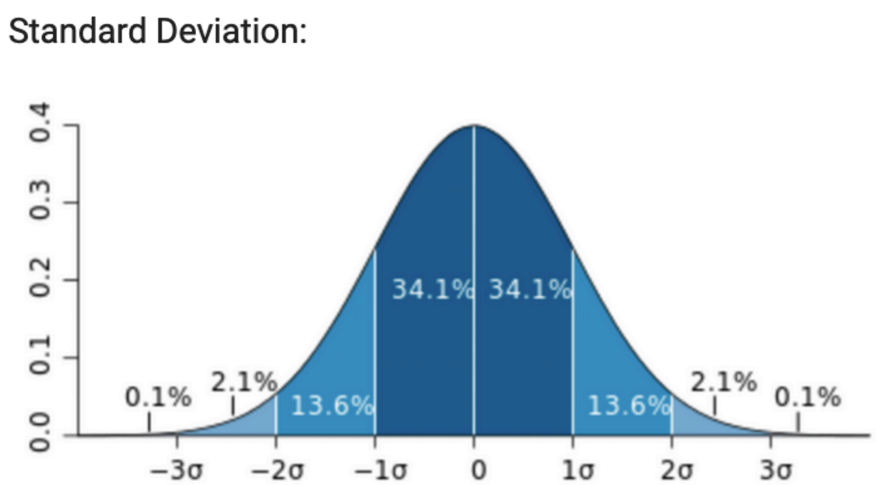
- For example, the oldest person on the Titanic dataset was 80, so:

age	replaced by
80	80/80 = 1
50	50/80 = 0.625
48	48/80 = 0.6
25	25/80 = 0.3125
4	4/80 = 0.05

Z-Score: Another Normalization Method

- **Idea:** rather than normalize to proportion of max, normalize based on how many standard deviations they are away from the mean

- **Standard Deviation:** usually represented as σ(sigma), a kind of **`average`** distance from the mean value
  - a low standard deviation indicates that the values tend to be close to the mean
  - a high standard deviation indicates that the values are spread out over a wider range



Quick Review: Computing the Z-Score

- After computing the corrected sample standard deviation, to normalize, replace each value x_i with it's **z-score** based on the mean (μ) and standard deviation (σ) of it's column.

$$\boxed{Z - score : \frac{x_i - \mu}{\sigma}}$$

Quick Review: Computing the Z-Score

- For example: on the Titanic:
  - sex mean(0:male, 1:female): 0.35
  - sex standard deviation: 0.48
  - age mean: 29.7
  - age standard deviation: 13

$$Z - score : \frac{x_i - \mu}{\sigma}$$

	sex	age
example 1	1	50
example 2	0	48
example 3	1	25

Z-Score for male: $(0 - 0.35)/0.48 \approx -0.73$
Z-Score for female: $(1 - 0.35)/0.48 \approx 1.35$

Z-Score for age 50: $(50 - 29.7)/13 \approx 1.56$
Z-Score for age 48: $(48 - 29.7)/13 \approx 1.41$
Z-Score for age 25: $(25 - 29.7)/13 \approx -0.36$

Quick Review: Distance Computation Before Normalization

	sex	age
example 1	1	50
example 2	0	48

distance: $\sqrt{(1-0)^2 + (50-48)^2} \approx 2.24$

	sex	age
example 1	1	50
example 3	1	25

distance: $\sqrt{(1-1)^2 + (50-25)^2} = 25$

age is overemphasized here in the distance calculation

Quick Review: Distance Computation After Normalization

	sex	age
example 1	1.35	1.56
example 2	-0.73	1.41

distance:

$$\sqrt{(1.35 - -0.73)^2 + (1.56 - 1.41)^2}$$
$$\approx 2.09$$

	sex	age
example 1	1.35	1.56
example 3	1.35	-0.36

distance:

$$\sqrt{(1.35 - 1.35)^2 + (1.56 - -0.36)^2}$$
$$= 1.92$$

Neither **sex** nor **age** is overemphasized here in the distance calculation

Quick Review: Computing the Z-Score on Titanic

- Called on a DataFrame, will replace values given in `to_replace` with `value`. Let's use this to make the `sex` column of the dataset numeric.

```
titanic['sex'] = titanic['sex'].replace(to_replace='female', value=1)
titanic['sex'] = titanic['sex'].replace(to_replace='male', value=0)
titanic.head()
```

	survived	pclass	sex	age	sibsp	parch	fare	embarked	class	who	adult_male	deck	embark_town	alive	alone
0	0	3	0	22.0	1	0	7.2500	S	Third	man	True	NaN	Southampton	no	False
1	1	1	1	38.0	1	0	71.2833	C	First	woman	False	C	Cherbourg	yes	False
2	1	3	1	26.0	0	0	7.9250	S	Third	woman	False	NaN	Southampton	yes	True
3	1	1	1	35.0	1	0	53.1000	S	First	woman	False	C	Southampton	yes	False
4	0	3	0	35.0	0	0	8.0500	S	Third	man	True	NaN	Southampton	no	True

Programming Exercise #1

- Normalize each of the predictor columns in the iris dataset
  - Write a function called `z_score()` that will take in a list of the names of the columns that you want to normalize, and the DataFrame, and will return a DataFrame where those columns have been z-score normalized.

```
def z_score(columns, data):
    """
    takes in a list of columns to normalize using the z-score method
    Params:
        columns, a list of columns to normalize
        data, the dataframe, preferably a copy
    Return:
        a copy of the dataframe with the specified columns normalized
    """
    normalized_data = data.copy()

    mean_list = []
    std_list  = []

    for col in columns:

        # get the mean and std

        # keep appending the mean, std into the lists initilized above

        # z score

        # replace the column with the z-score


    return normalized_data, mean_list, std_list
```

Programming Exercise #1

- Normalize each of the predictor columns in the iris dataset
  - Note: you need a way to transform the new reading (the specimen) that you will make the prediction on so that the new one and the training data will all be on the same scale. How can you do that?

```
column_names = ['sepal length', 'sepal width', 'petal width', 'petal length']

iris_norm, mean_list, std_list = z_score(column_names, iris)

iris_norm.head()
```

	sepal length	sepal width	petal length	petal width	species
0	-0.897674	1.028611	-1.336794	-1.308593	Iris-setosa
1	-1.139200	-0.124540	-1.336794	-1.308593	Iris-setosa
2	-1.380727	0.336720	-1.393470	-1.308593	Iris-setosa
3	-1.501490	0.106090	-1.280118	-1.308593	Iris-setosa
4	-1.018437	1.259242	-1.336794	-1.308593	Iris-setosa

Today's Agenda

- Topics:
  - Normalization
  - Weighted k-NN

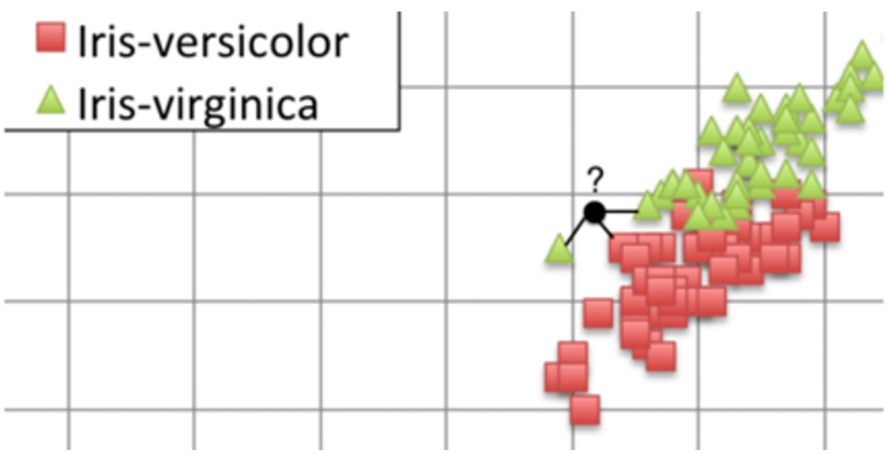
Quick Review: 3-Nearest Neighbor (3-NN)

- **3-Nearest-Neighbor Algorithm:** predict the *most commonly appearing* class among the 3 closest training examples
  - In other words, k=3
- Let's assume this subset of Iris has only 2 classes (even number):

  `Iris-versicolor`

  `Iris-virginica`

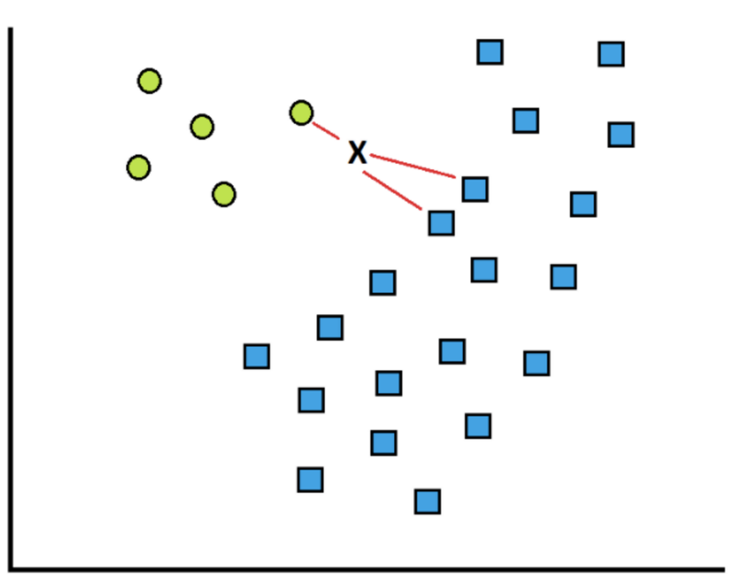
- What class will a **3NN** algorithm predict?



k-Nearest Neighbor (k-NN)

- The way we've learned **k-Nearest-Neighbor (k-NN)** so far, each neighbor gets an equal vote in the decision of what to predict.

- Do we see any problems with this? If so, what?

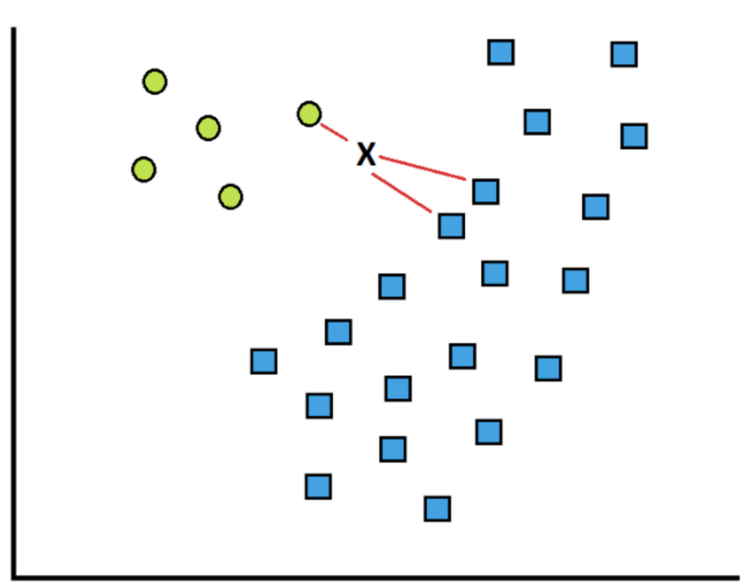


- Should neighbors that are closer to the new instance get a larger share of the vote?

Weighted k-NN Intuition

- In weighted kNN, the nearest k points are given a weight, and the weights are grouped by the target variable. The class with the largest sum of weights will be the class that is predicted

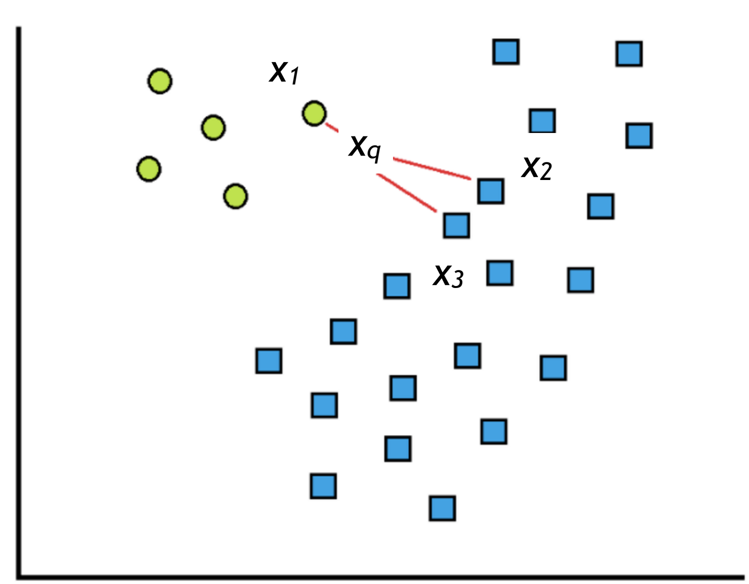
- The intuition is to give more weight to the points that are nearby and less weight to the points that are farther away.
  - distance-weighted voting



Weighted k-NN Intuition

- In **w-kNN**, we want to predict the target variable with the most weight, where the weight is defined by the inverse distance function

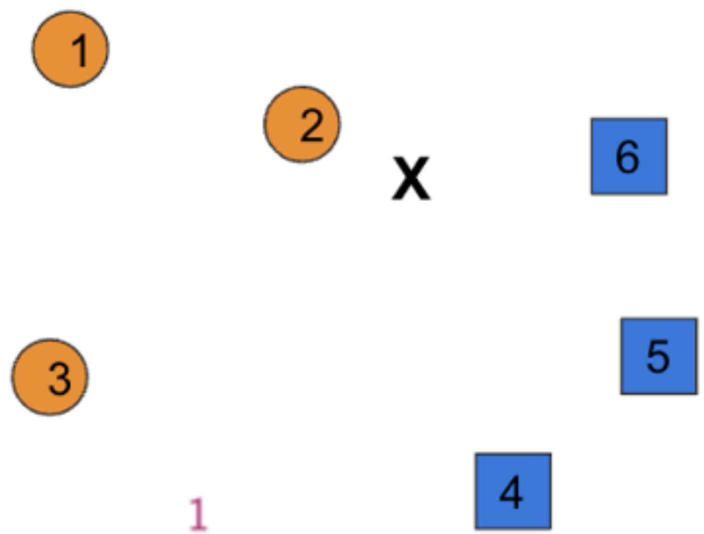
$$w_{q,i} = \frac{1}{d(x_q, x_i)^2}$$



- In English, you can read that as the **weight** of a training example is equal to 1 divided by the distance between the new instance and the training example squared

Weighted k-NN Example: Step 1

- Start by calculating the distance between the new example ***X***, and each of the other training examples:

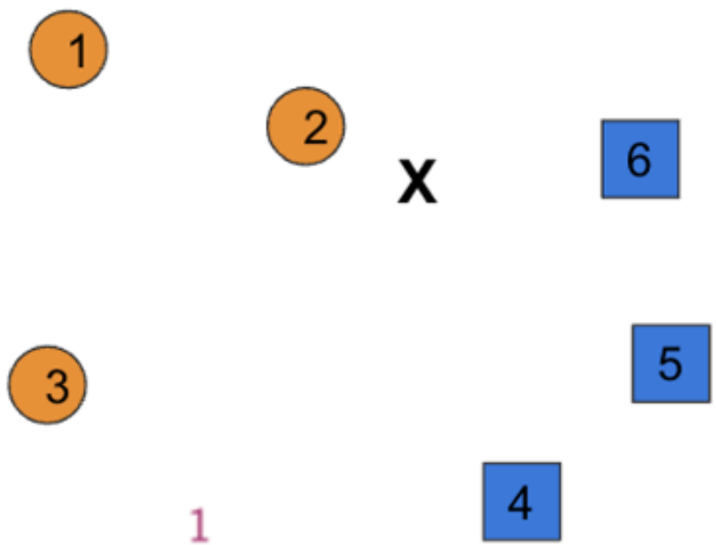


$$w_{q,i} = \frac{1}{d(x_q, x_i)^2}$$

Example #	Distance	Weight
1	5	
2	1	
3	7	
4	5	
5	4	
6	3	

Weighted k-NN Example: Step 2

- Then, **calculate the weight** of each training example using the inverse distance squared.

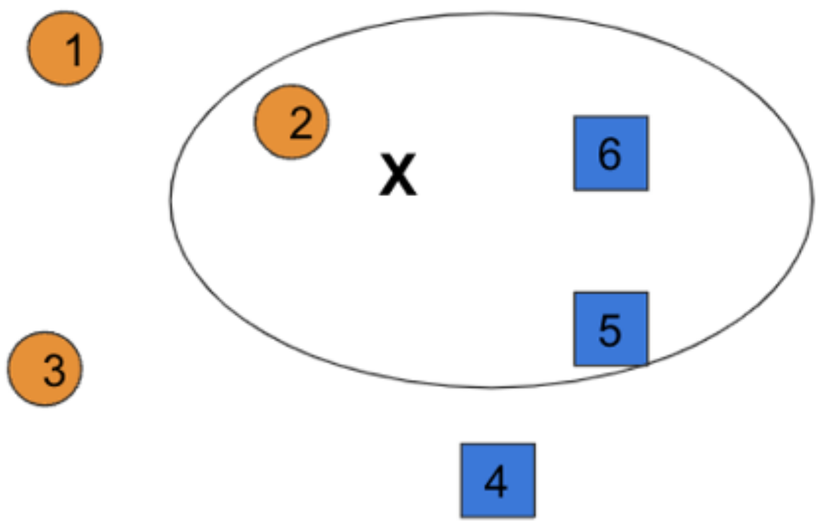


$$w_{q,i} = \frac{1}{d(x_q, x_i)^2}$$

Example #	Distance	Weight
1	5	1/25
2	1	1
3	7	1/49
4	5	1/25
5	4	1/16
6	3	1/9

Weighted k-NN Example: Step 3

- Find the k closest neighbors – let's assume **k=3** for this example:



Example #	Distance	Weight
1	5	1/25
2	**1**	**1**
3	7	1/49
4	5	1/25
5	**4**	**1/16**
6	**3**	**1/9**

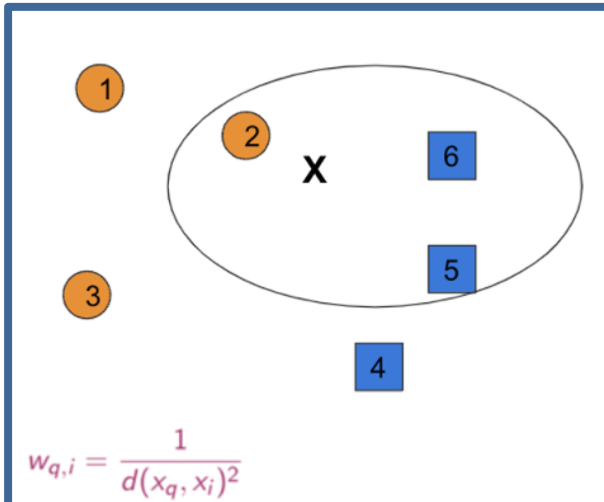
$$w_{q,i} = \frac{1}{d(x_q, x_i)^2}$$

Weighted k-NN Example: Step 4

- Then, sum the weights for each possible class:

  - Orange: 1
  - Blue: 1/16 + 1/9 = 0.115

- What would a **normal 3NN** predict?
- What would a **Weighted 3NN** predict?



Example #	Distance	Weight
1	5	1/25
2	**1**	**1**
3	7	1/49
4	5	1/25
5	**4**	**1/16**
6	**3**	**1/9**

Code: weighted inn

- Write a new function `weighted_knn()`
- Pass the iris measurements (specimen), data frame, and k as parameters and return the predicted class

```
import numpy as np

def weighted_knn(specimen, data, k):

  # step 1: calculate the distances from 'specimen' to all other samples in 'data'
  data['distances'] = np.sqrt( (specimen['petal length'] - data['petal length'])**2 +
                               (specimen['sepal length'] - data['sepal length'])**2 +
                               (specimen['petal width']  - data['petal width'])**2 +
                               (specimen['sepal width']  - data['sepal width'])**2 )

  # step 2: calculate the weights for each sample (remember, weights are 1/d^2)
  # data['weights']    = ... (TBD)

  # step 3: find the k closest neighbors as follows
  # first: sort the data and take the first k samples as neighbors
  sorted_data         = data.sort_values(['distances'])
  print('Nearest k samples in the training data:')
  neighbors           = sorted_data.iloc[0:k]
  # second: use groupby to sum the weights of each species in the closest k
  # TBD


  # third: return the class that has the largest sum of weight.
  # TBD
```

Recall: Some Handy Functions

- `unique()`, `groupby()`

```
#get the unique values of the Deck column
titanic.deck.unique()

array([nan, 'C', 'E', 'G', 'D', 'A', 'B', 'F'], dtype=object)
```

```
titanic.groupby(['survived'])['age'].mean()

survived
0    30.626179
1    28.343690
Name: age, dtype: float64
```

```
[19] condition = titanic['survived'] == 0
     survivor_0 = titanic[condition]['age']
     survivor_0.mean()

     30.62617924528302

[20] condition = titanic['survived'] == 1
     survivor_1 = titanic[condition]['age']
     survivor_1.mean()

     28.343689655172415

titanic.groupby('survived')['age'].mean()

survived
0    30.626179
1    28.343690
Name: age, dtype: float64
```

Programming Exercise #2

- Normalize each of the predictor columns in the iris dataset, or just use `iris_norm` which we created earlier (ie, Programming Exercise#1)
  - **Note**: you need a way to transform the new reading (the specimen) that you will make the prediction on so that the new one and the training data will all be on the same scale. How can you do that?
  - **Hint**: modify the z_score() method to save the <mean, std> for each column, then utilize that later

Programming Exercise #4

- Repeat your k-NN prediction code for the normalized data.
  - Does the value of k change the predictions?
  - compare using `k=3`, and `k=5` on each method (normalized and non-normalized), (weighted and unweighted)

Use these tables to keep track of your predictions:

k=3

	not normalized	normalized
unweighted kNN		
weighted kNN		

k=5

	not normalized	normalized
unweighted kNN		
weighted kNN		

Discussion Question

- What do we do if the features aren't numbers?
  - like Titanic `embark_town`... how can we calculate a distance between `Southampton` and `Queenstown`?

```
[ ] titanic.embark_town.unique()

array(['Southampton', 'Cherbourg', 'Queenstown', nan],
```

```
pd.get_dummies(titanic.embark_town)
```

	Cherbourg	Queenstown	Southampton
0	0	0	1
1	1	0	0
2	0	0	1
3	0	0	1
4	0	0	1
...	...	...	...
886	0	0	1
887	0	0	1
888	0	0	1
889	1	0	0
890	0	1	0

891 rows × 3 columns

Discussion Question

- What if our **target variable** is continuous rather than categorical? How would we make a prediction using kNN?
    - Can we do regression with kNN? If so, how?

- Example of regression problems
    - predict tomorrow's temperature
    - predict the fuel efficiency of a vehicle
    - predict how much someone will like a show on Netflix