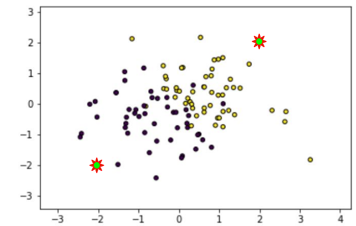
k Nearest Neighbors and Feature Scaling

Nearest Neighbors Algorithm

- Store all the training data as feature vectors
- Prediction for new, test data point: return the label of the closest training point

(you are the company you keep…)

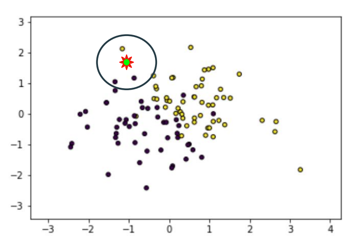
What is the predicted color for a new point (-2, -2)? Or for (2, 2)?



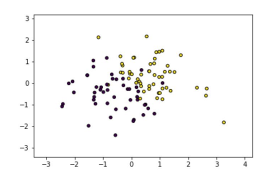
k Nearest Neighbors Algorithm

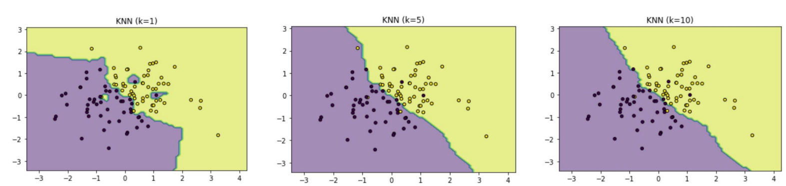
- Choose some integer value of *k* (say, 3)
- Compute the *k* closest training points to the test data point
- Return the majority label

What is the predicted color for a new point (-1.1, 1.7)?

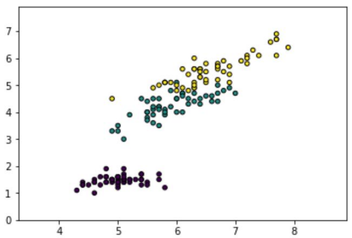


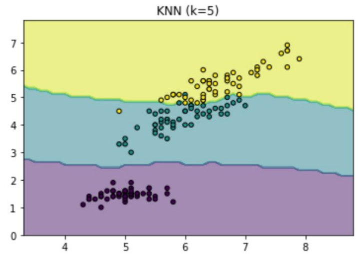
Effect of increasing *k*: smoother decision boundaries





Three Classes



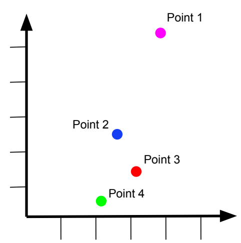


Choosing *k*

- *k* is a free "hyperparameter" of the algorithm. How do we choose it?
- ~~One option: try different values of *k* when evaluating on test data~~
- Rather than split data into two parts, training and test, we split data into three parts, training and validation and test.
  - Use the validation data as "pseudo-test data" to **tune** (choose best) *k*
  - Do final evaluation on the test data only once

Distance Measure in 2D

Point 1	3.8	5.4
Point 2	2.6	2.6
Point 3	3.1	1.5
Point 4	2.1	0.5



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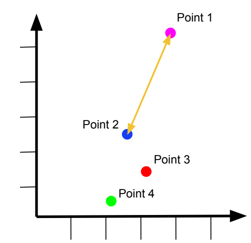
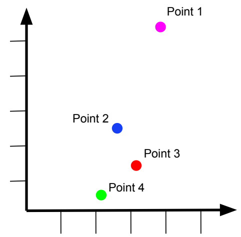


distance(Point 1, Point 2) = $\sqrt[2]{|3.8 - 2.6|^2 + |5.4 - 2.6|^2}$

Distance Measure in 2D - L^2 Norm

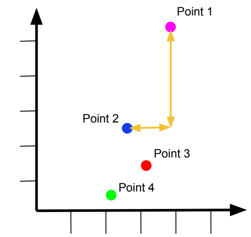
$$\begin{array}{l} \text{Point 1} \\ \text{Point 2} \\ \text{Point 3} \\ \text{Point 4} \end{array} \begin{bmatrix} 3.8 & 5.4 \\ 2.6 & 2.6 \\ 3.1 & 1.5 \\ 2.1 & 0.5 \end{bmatrix}$$



$$\textit{distance}(\text{Point } a, \text{Point } b) = \sqrt[2]{|a_1 - b_1|^2 + |a_2 - b_2|^2}$$

Distance Measure in 2D

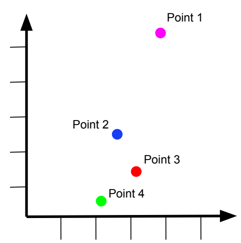
$$\begin{array}{l} \text{Point 1} \\ \text{Point 2} \\ \text{Point 3} \\ \text{Point 4} \end{array} \begin{bmatrix} 3.8 & 5.4 \\ 2.6 & 2.6 \\ 3.1 & 1.5 \\ 2.1 & 0.5 \end{bmatrix}$$



$$\textit{distance}(\text{Point 1}, \text{Point 2}) = \sqrt[1]{|3.8 - 2.6|^1 + |5.4 - 2.6|^1}$$

Distance Measure in 2D - L^1 Norm

$$\begin{array}{l} \text{Point 1} \\ \text{Point 2} \\ \text{Point 3} \\ \text{Point 4} \end{array} \begin{bmatrix} 3.8 & 5.4 \\ 2.6 & 2.6 \\ 3.1 & 1.5 \\ 2.1 & 0.5 \end{bmatrix}$$

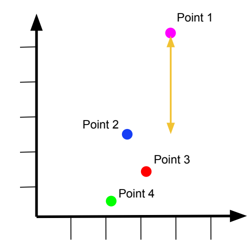


$$\textit{distance}(\text{Point } a, \text{Point } b) = \sqrt[1]{|a_1 - b_1|^1 + |a_2 - b_2|^1}$$

$$= |a_1 - b_1| + |a_2 - b_2|$$

Distance Measure in 2D

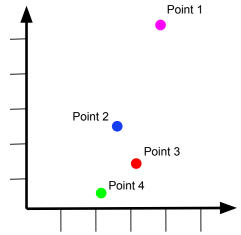
$$\begin{array}{l} \text{Point 1} \\ \text{Point 2} \\ \text{Point 3} \\ \text{Point 4} \end{array} \begin{bmatrix} 3.8 & 5.4 \\ 2.6 & 2.6 \\ 3.1 & 1.5 \\ 2.1 & 0.5 \end{bmatrix}$$



$$\textit{distance}(\text{Point 1}, \text{Point 2}) = \sqrt[\infty]{|3.8 - 2.6|^\infty + |5.4 - 2.6|^\infty}$$

Distance Measure in 2D - L^∞ Norm

Point 1	3.8	5.4
Point 2	2.6	2.6
Point 3	3.1	1.5
Point 4	2.1	0.5

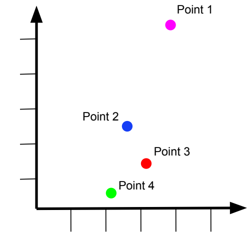


distance(Point a, Point b) = $\sqrt[\infty]{|a_1 - b_1|^\infty + |a_2 - b_2|^\infty}$

$= \max \{ |a_1 - b_1| , |a_2 - b_2| \}$

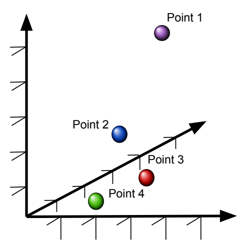
Distance Measure in 2D

Point 1	3.8	5.4
Point 2	2.6	2.6
Point 3	3.1	1.5
Point 4	2.1	0.5



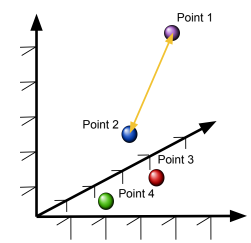
Distance Measure in 3D

Point 1	3.8	5.4	4.7
Point 2	2.6	2.6	2.6
Point 3	3.1	1.5	2.2
Point 4	2.1	0.5	1.2



Distance Measure in 3D

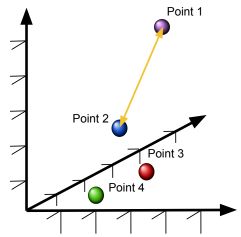
Point 1	3.8	5.4	4.7
Point 2	2.6	2.6	2.6
Point 3	3.1	1.5	2.2
Point 4	2.1	0.5	1.2



distance(Point 1, Point 2) = $\sqrt[2]{|3.8 - 2.6|^2 + |5.4 - 2.6|^2 + |4.7 - 2.6|^2}$

Distance Measure in 3D

$$
\begin{array}{l}
\text{Point 1} \\
\text{Point 2} \\
\text{Point 3} \\
\text{Point 4}
\end{array}
\begin{bmatrix}
3.8 & 5.4 & 4.7 \\
2.6 & 2.6 & 2.6 \\
3.1 & 1.5 & 2.2 \\
2.1 & 0.5 & 1.2
\end{bmatrix}
$$



$$\textit{distance}(\text{Point } a, \text{Point } b) = \sqrt[2]{|a_1 - b_1|^2 + |a_2 - b_2|^2 + |a_3 - b_3|^2}$$

Distance Measure in High Dimensions

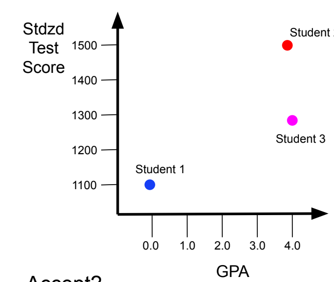
$$
\begin{array}{l}
\text{Point 1} \\
\text{Point 2} \\
\text{Point 3} \\
\text{Point 4}
\end{array}
\begin{bmatrix}
3.8 & 5.4 & 4.7 & 5.0 & \dots & 4.2 \\
2.6 & 2.6 & 2.6 & 2.6 & \dots & 2.6 \\
3.1 & 1.5 & 2.2 & 1.9 & \dots & 2.7 \\
2.1 & 0.5 & 1.2 & 0.9 & \dots & 1.7
\end{bmatrix}
$$

$$\textit{distance}(\text{Point } a, \text{Point } b) = \sqrt[2]{\sum_{i=1}^{d} |a_i - b_i|^2}$$

*k*NN Complexity

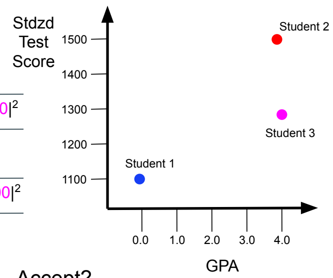
- Given *n* training examples and *d* features
- Training step
  - Time: approximately zero; just store the data points
  - Space: size of training data (*n* x *d*)
- Testing step (for each test example)
  - Time?

Feature Scaling



	GPA	Standardized Test Score	Accept?
Student 1	0.0	1110	0
Student 2	3.8	1500	1
Student 3	3.9	1300	?

Feature Scaling



distance(Student 1, Student 3) = $\sqrt[2]{|0.0 - 3.9|^2 + |1110 - 1300|^2}$

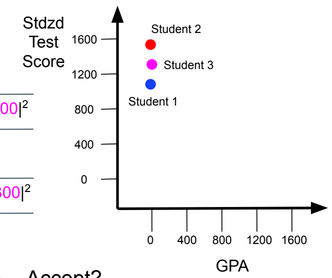
= $\sqrt[2]{15.21 \quad + \quad 36100}$

distance(Student 2, Student 3) = $\sqrt[2]{|3.8 - 3.9|^2 + |1500 - 1300|^2}$

= $\sqrt[2]{0.01 \quad + \quad 40000}$

	GPA	Standardized Test Score	Accept?
Student 1	0.0	1110	0
Student 2	3.8	1500	1
Student 3	3.9	1300	?

Feature Scaling



distance(Student 1, Student 3) = $\sqrt[2]{|0.0 - 3.9|^2 + |1110 - 1300|^2}$

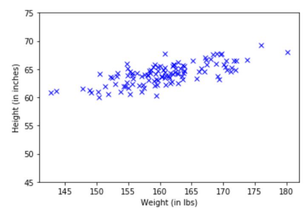
= $\sqrt[2]{15.21 \quad + \quad 36100}$

distance(Student 2, Student 3) = $\sqrt[2]{|3.8 - 3.9|^2 + |1500 - 1300|^2}$

= $\sqrt[2]{0.01 \quad + \quad 40000}$

	GPA	Standardized Test Score	Accept?
Student 1	0.0	1110	0
Student 2	3.8	1500	1
Student 3	3.9	1300	?

Feature Scaling



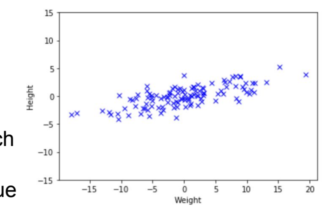
- Compute the mean (i.e., average) for each of the features in the training data and subtract this mean from each feature value

For each of the $1 \le i \le n$ training examples and $1 \le j \le d$ features, we subtract the mean: $x_{i,j} = x_{i,j} - \mu_j$

where the mean of the j^{th} feature is $\mu_j = \frac{1}{n} \sum_{1 \le i \le n} x_{i,j}$

- Data will then be centered around zero

Feature Scaling



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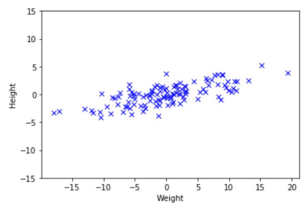
Feature Scaling



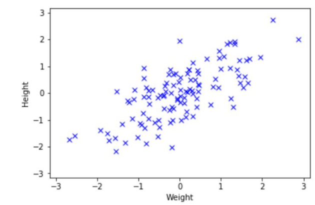
- Compute the standard deviation for each of the features in the training data and divide each feature value by this standard deviation

For each of the $1 \le i \le n$ training examples and $1 \le j \le d$ features, we divide by the standard deviation: $x_{i,j} = x_{i,j} \;/\; \sigma_j$

where the standard deviation of the j^{th} feature is $\sigma_j = \sqrt{\frac{1}{n} \sum_{1 \le i \le n} (x_{i,j} - \mu_j)^2}$

- Data will then have comparable scale

Feature Scaling



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- Data will then have comparable scale

Feature Scaling - Test Data

- When scaling the training data, we **store** the mean and standard deviation values that we compute for each feature as part of the scaling process
- When given a testing example, we need to make sure that it is on a comparable scale as the training data. Thus, we scale it using the stored mean and standard deviation values.

For the i^{th} testing example, we scale each of its $1 \le j \le d$ features by subtracting the j^{th} mean (μ_j) and dividing by the j^{th} standard deviation (σ_j):

$$x_{i,j} = (x_{i,j} - \mu_j)/\sigma_j$$

Pros and Cons of *k*NN

<u>Pros</u>

- Simple and intuitive
- Can be used with multiple classes (not just 2)
- Data do **not** have to be **linearly separable**

<u>Cons</u>

- Need to store large full training data
- Test time is SLOOOWW
    - Prefer to pay for expensive training in exchange for fast prediction

Looking ahead

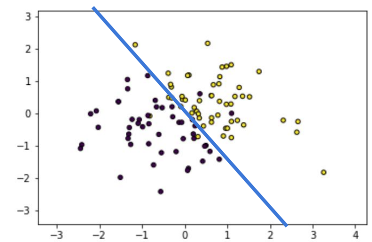
- *k*NN is an instance-based classifier: must carry around training data (waste of space)
- Training easy
- Testing hard

Future methods will be

- Parametric classifiers: compute a small "model" and then throw away training data
- Training hard
- Testing easy

Looking ahead: linear classifiers

- Training: find a dividing "hyperplane" between two classes
- Testing: check which side of hyperplane the new point falls in



Overview