

# **Machine Learning & Artificial Intelligence for Data Scientists: Classification (Part1)**

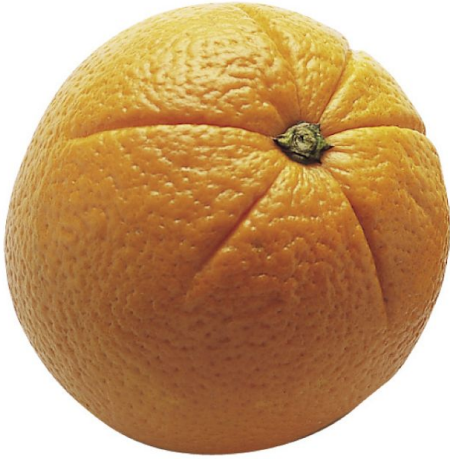
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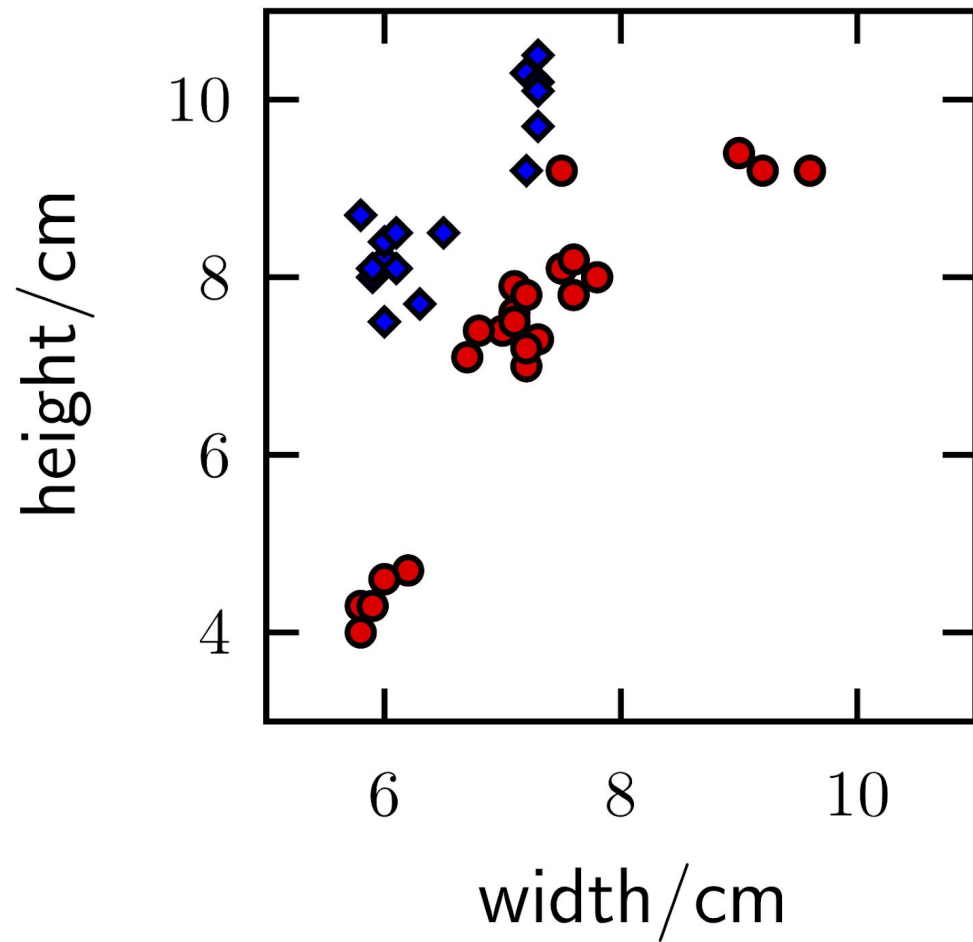
**School of Computing Science**

# Again some data, and a problem

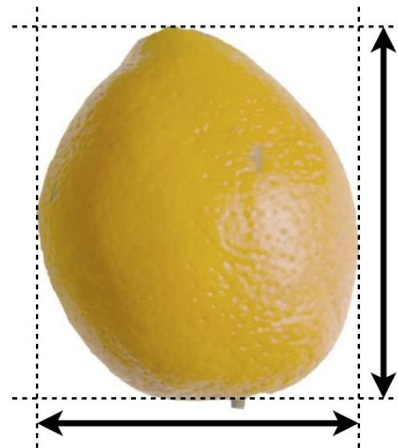
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Source: [https://homepages.inf.ed.ac.uk/imurray2/teaching/oranges\\_and lemons/](https://homepages.inf.ed.ac.uk/imurray2/teaching/oranges_and_lemons/)

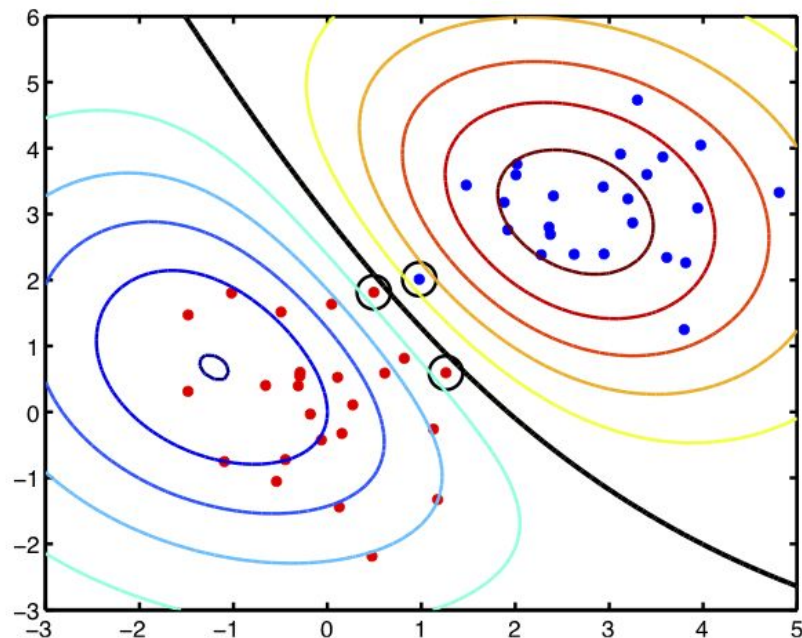


Oranges: ●  
Lemons: ◆



# Classification

— — —



- ▶ A set of  $N$  objects with attributes (usually vector)  $\mathbf{x}_n$ .
- ▶ Each object has an associated response (or label)  $t_n$ .
- ▶ Binary classification:  $t_n = \{0, 1\}$  or  $t_n = \{-1, 1\}$ ,
  - ▶ (depends on algorithm).
- ▶ Multi-class classification:  $t_n = \{1, 2, \dots, K\}$ .

# Probabilistic v non-probabilistic classifiers

— — — Classifier is trained on  $\mathbf{x}_1, \dots, \mathbf{x}_N$  and  $t_1, \dots, t_N$  and then used to classify  $\mathbf{x}_{\text{new}}$ .

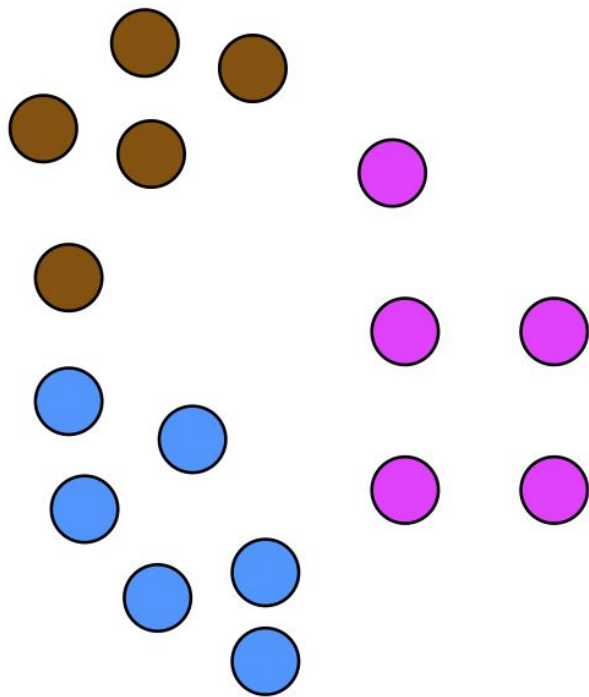
- ▶ Probabilistic classifiers produce a probability of class membership  $P(t_{\text{new}} = k | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t})$ 
  - ▶ e.g. binary classification:  $P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t})$  and  $P(t_{\text{new}} = 0 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t})$ .
- ▶ Non-probabilistic classifiers produce a hard assignment
  - ▶ e.g.  $t_{\text{new}} = 1$  or  $t_{\text{new}} = 0$ .
- ▶ Which to choose depends on application....

# Probabilistic v non-probabilistic classifiers

- ▶ Probabilities provide us with more information –  $P(t_{\text{new}} = 1) = 0.6$  is more useful than  $t_{\text{new}} = 1$ .
  - ▶ Tells us how **sure** the algorithm is.
- ▶ Particularly important where cost of misclassification is high and imbalanced.
  - ▶ e.g. Diagnosis: telling a diseased person they are healthy is much worse than telling a healthy person they are diseased.
- ▶ Extra information (probability) often comes at a cost.

# Algorithm 1: K-Nearest Neighbours (KNN)

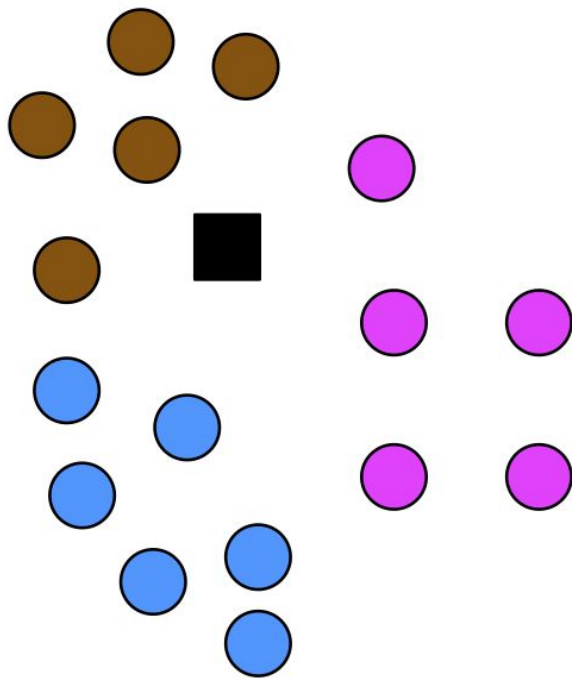
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Training data from 3 classes.

# KNN

— — —

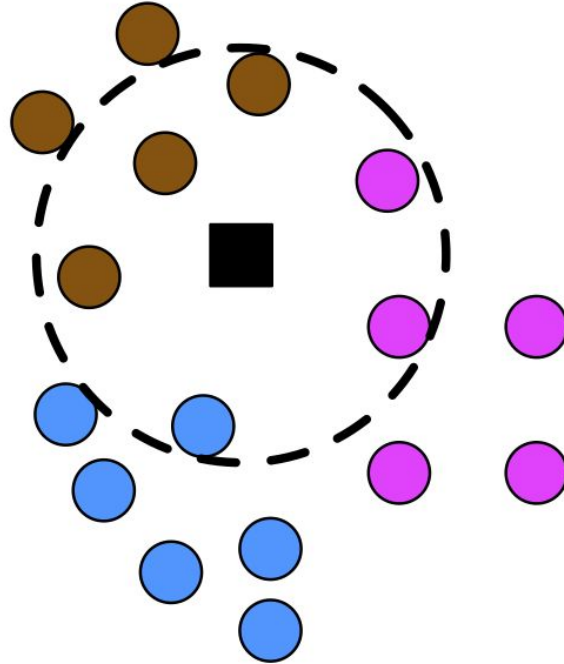


Test point.



# KNN

— — —



Find  $K = 6$  nearest neighbours.

# KNN

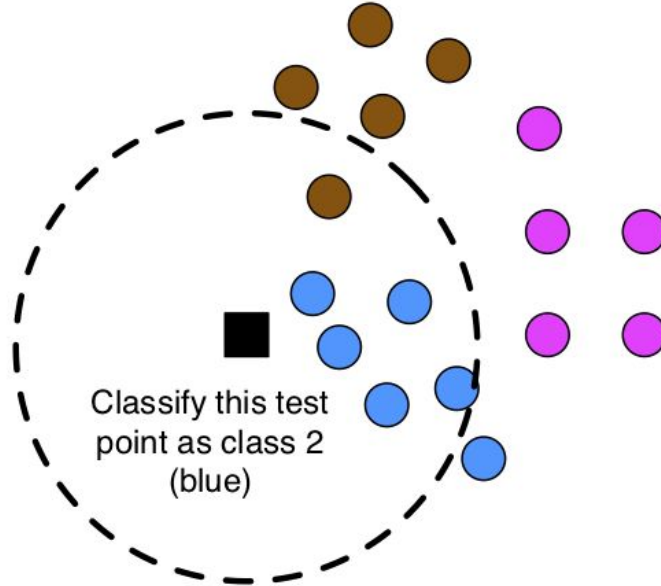
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Class one has most votes – classify  $\mathbf{x}_{\text{new}}$  as belonging to class 1.

# KNN

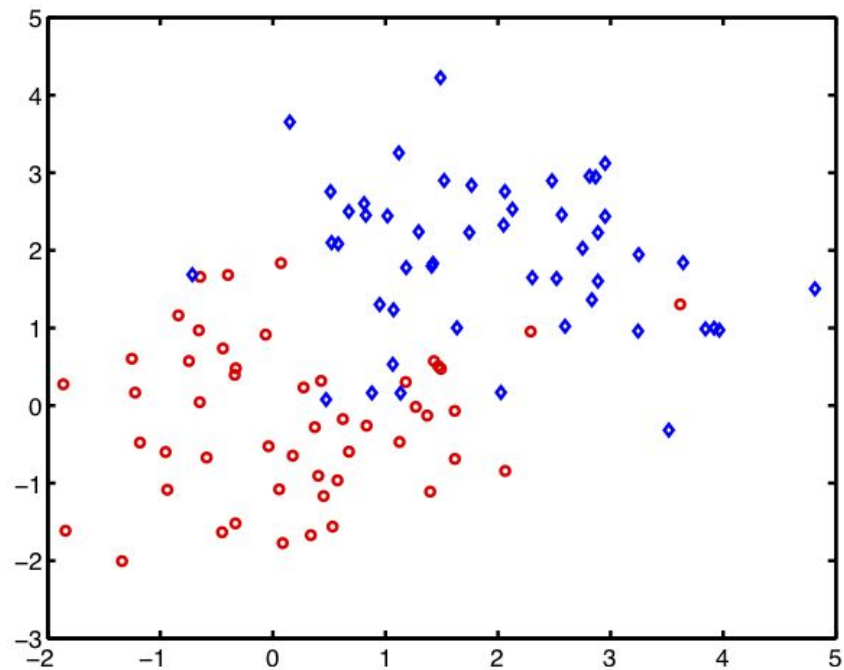
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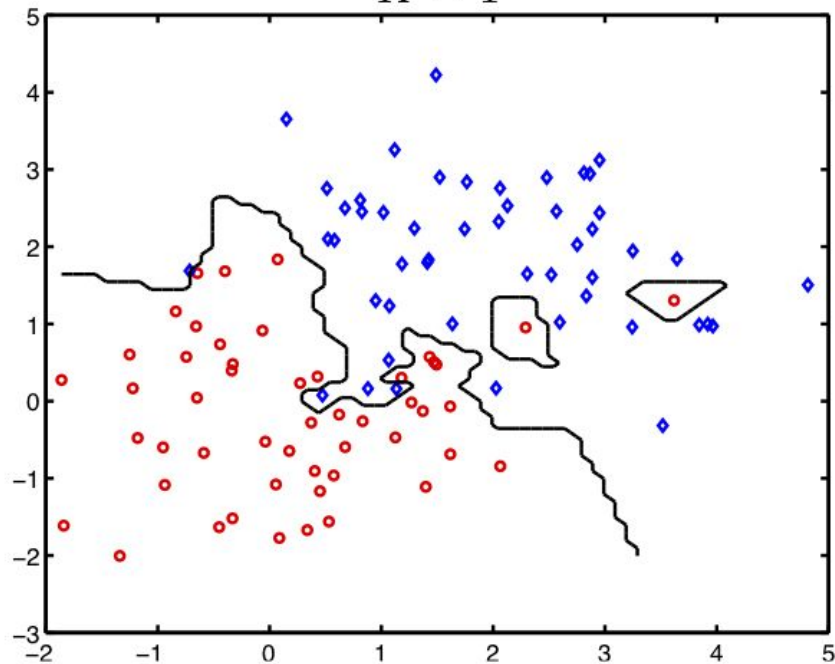
Second example – class 2 has most votes.

# KNN: Binary data

— — —

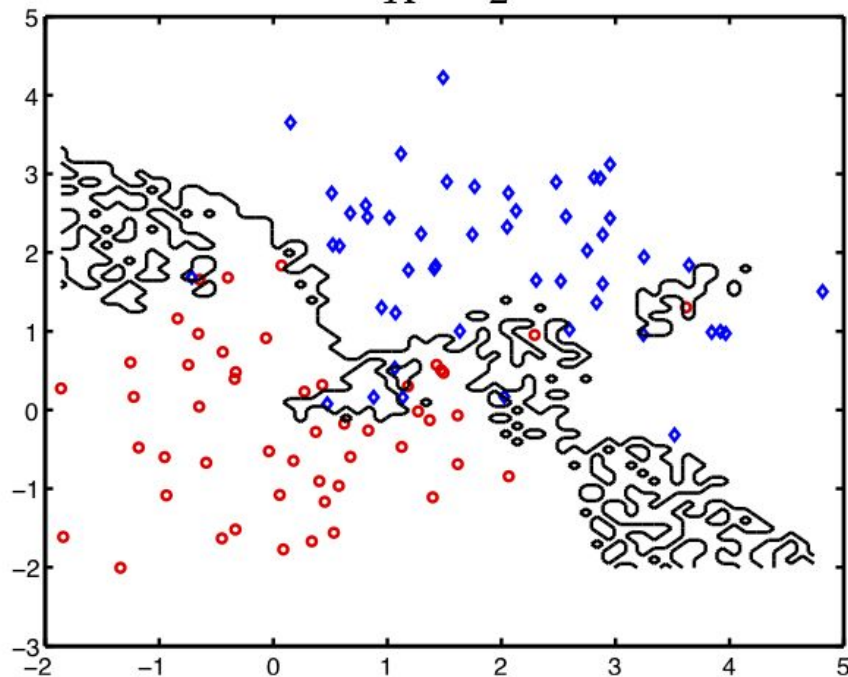


$K = 1$



- ▶ 1-Nearest Neighbour.
- ▶ Line shows decision boundary.
- ▶ Too complex – should the islands exist?

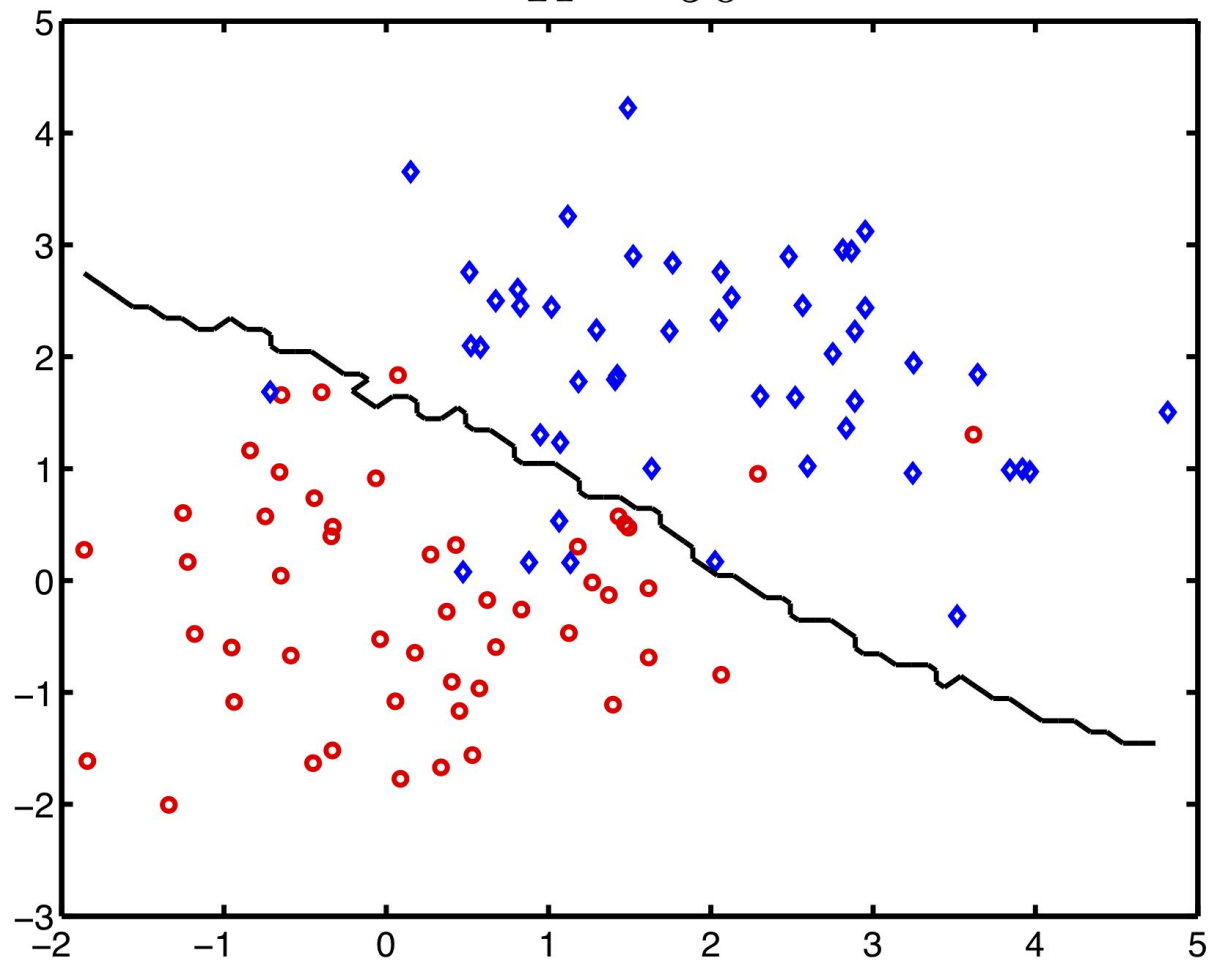
$$K = 2$$



- ▶ 2-Nearest Neighbour.
- ▶ What's going on?
- ▶ Lots of ties – random guessing.

$K = 50$

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# Problem with KNN

- ▶ Class imbalance
  - ▶ As  $K$  increases, small classes will disappear!
  - ▶ Imagine we had only 5 training objects for class 1 and 100 for class 2.
  - ▶ For  $K \geq 11$ , class 2 will **always** win!
- ▶ How do we choose  $K$ ?
  - ▶ Right value of  $K$  will depend on data.
  - ▶ Cross-validation!

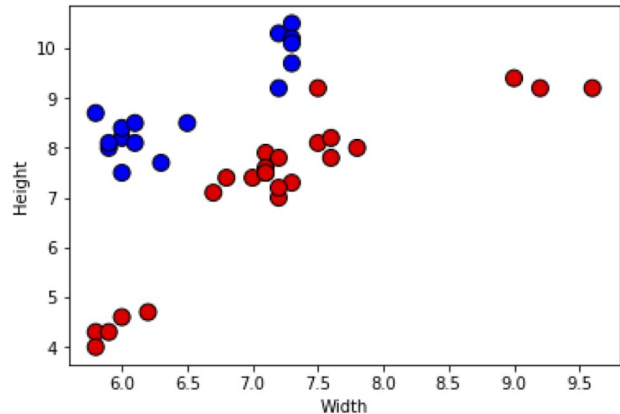


```
In [2]: import numpy as np
%matplotlib inline
import pylab as plt
from matplotlib.colors import ListedColormap

# Create color maps
cmap_light = ListedColormap(['#FFAAAA', '#AAFFAA', '#AAAAFF'])
cmap_bold = ListedColormap(['#FF0000', '#00FF00', '#0000FF'])

data = np.loadtxt('orange_lemon.txt', delimiter=',') # load fruit data
X = data[:,1:3]
t = data[:,0]
plt.scatter(X[:, 0], X[:, 1], c=t, cmap=cmap_bold, edgecolor='k', s=100)
plt.xlabel('Width')
plt.ylabel('Height')
```

Out[2]: Text(0, 0.5, 'Height')

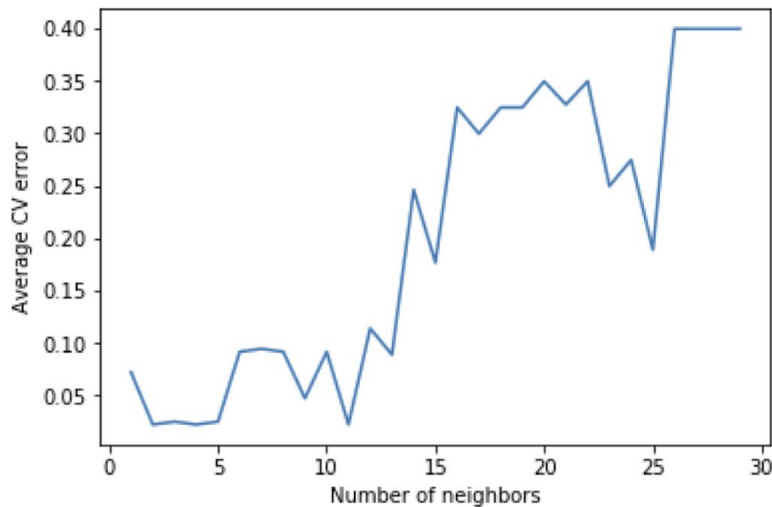


We can see it with oranges and lemons

```
In [17]: cv_scores = []
for i in range(1,30,1):
    knn_cv = KNeighborsClassifier(n_neighbors=i)
    cv_scores.append(1-np.mean(cross_val_score(knn_cv, X, t, cv=5)))

plt.plot(np.arange(1,30,1),cv_scores)
plt.xlabel('Number of neighbors')
plt.ylabel('Average CV error')
print(np.min(cv_scores))
```

0.022222222222222143

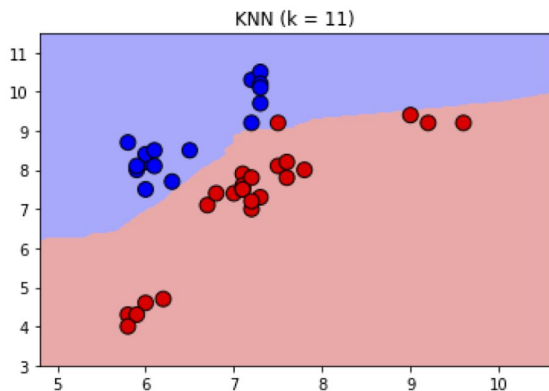


**5-fold CV to select  
K**

```
In [4]: from sklearn.neighbors import KNeighborsClassifier
        from sklearn.model_selection import cross_val_score
```

```
n_neighbors = 11
clf = KNeighborsClassifier(n_neighbors)
clf.fit(X, t)
Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
# Put the result into a color plot
Z = Z.reshape(xx.shape)
plt.pcolormesh(xx, yy, Z, cmap=cmap_light)
# Plot also the training points
plt.scatter(X[:, 0], X[:, 1], c=t, cmap=cmap_bold,
            edgecolor='k', s=100)
plt.xlim(xx.min(), xx.max())
plt.ylim(yy.min(), yy.max())
plt.title("KNN (k = %i)"
         % (n_neighbors))
```

```
Out[4]: Text(0.5, 1.0, 'KNN (k = 11)')
```

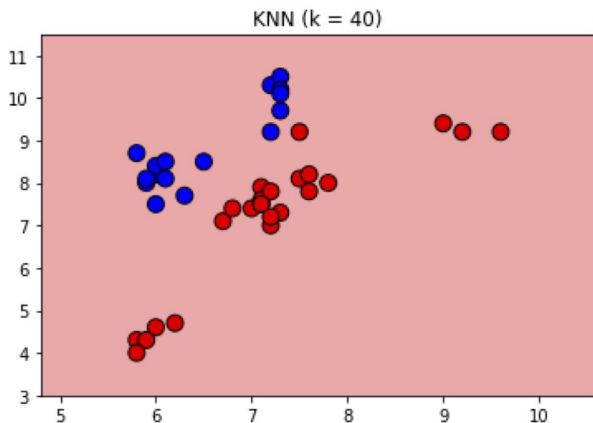


```
In [3]: # Plot the decision boundary. For that, we will assign a color to each
        # point in the mesh [x_min, x_max]x[y_min, y_max].
        h = .02
        x_min, x_max = X[:, 0].min() - 1, X[:, 0].max() + 1
        y_min, y_max = X[:, 1].min() - 1, X[:, 1].max() + 1
        xx, yy = np.meshgrid(np.arange(x_min, x_max, h),
                              np.arange(y_min, y_max, h))
```

**K = 11**

```
In [6]: n_neighbors = 40
clf = KNeighborsClassifier(n_neighbors)
clf.fit(X, t)
Z = clf.predict(np.c_[xx.ravel(), yy.ravel()])
# Put the result into a color plot
Z = Z.reshape(xx.shape)
plt.pcolormesh(xx, yy, Z, cmap=cmap_light)
# Plot also the training points
plt.scatter(X[:, 0], X[:, 1], c=t, cmap=cmap_bold,
            edgecolor='k', s=100)
plt.xlim(xx.min(), xx.max())
plt.ylim(yy.min(), yy.max())
plt.title("KNN (k = %i)"
          % (n_neighbors))
```

```
Out[6]: Text(0.5, 1.0, 'KNN (k = 40)')
```



**K = 40**

# KNN summary

— — —

- ▶ Non-probabilistic.
- ▶ Fast.
- ▶ Only one parameter to tune ( $K$ ).
- ▶ Important to tune it well....
- ▶ ...can use CV.
- ▶ There is a probabilistic version.
  - ▶ Not covered in this course.
- ▶ Now onto a (different) probabilistic classifier...