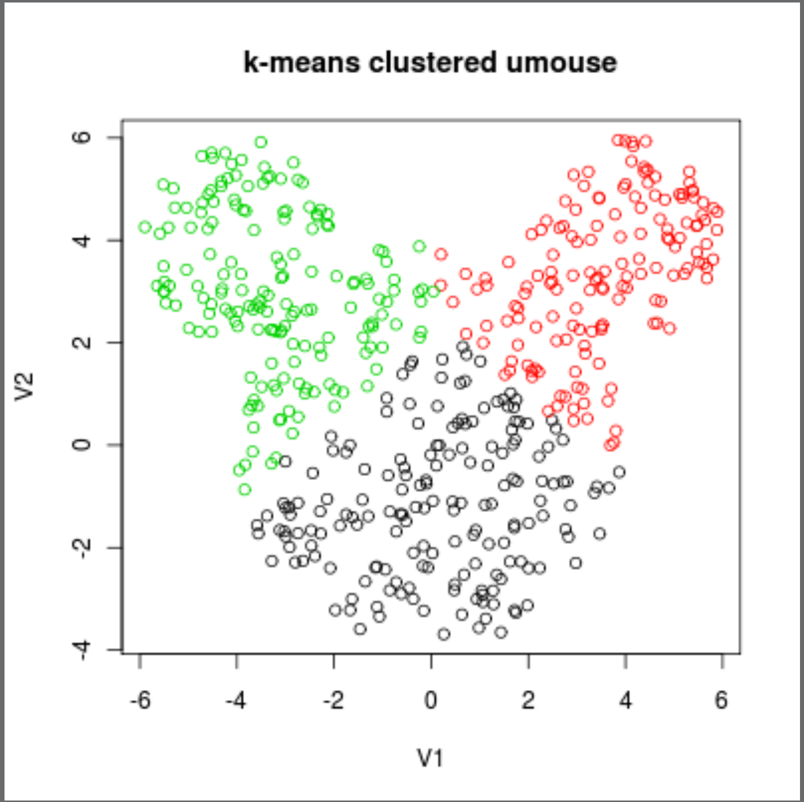
# K-Means Clustering





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Morning Lecture - Dec. 6, 2017

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# Learning Objectives

- Introduce unsupervised learning, compare to supervised
- Introduce clustering concept
- Enumerate clustering use-cases
- Define K-means algorithm:
  - How to code
  - Centroid initialization
  - Stopping Criteria
  - Evaluating the algorithm (metrics)
  - How to choose k

# Review: Queue the Questionator

- What does supervised learning mean? Give an example
- Describe the difference between parametric and non-parametric learners, and give an example of each
- How do we measure the "success" of a supervised learning algorithm? Give examples for classification and regression
- Describe the euclidean distance metric. Name two additional distance metrics we have discussed and describe.
- What is the curse of dimensionality?

# Supervised vs. Unsupervised Learning

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### Supervised

- Have a target/label that we model
- Models look like functions that take in features (X) and predict a label (y)
- Have an error metric that we can use to compare models
- Used to predict future unlabeled data

### Unsupervised

- No target/label to predict
- Goal is to find underlying structure, patterns, or organization in data
- No stark error metric to compare models - determining if you have the optimal solution is very challenging. Cross validation often not applicable.

# Where We've Been - Supervised Learning

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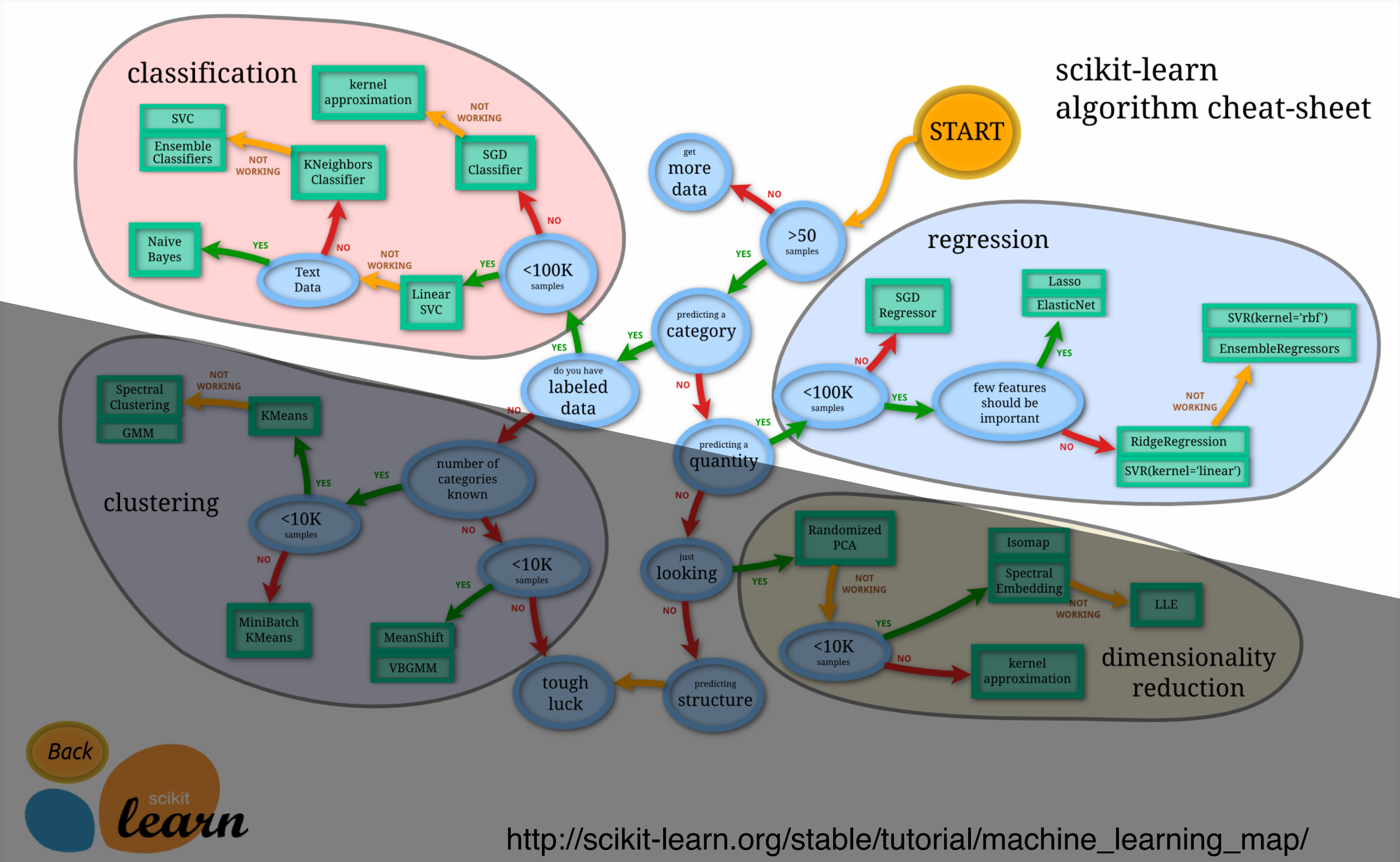
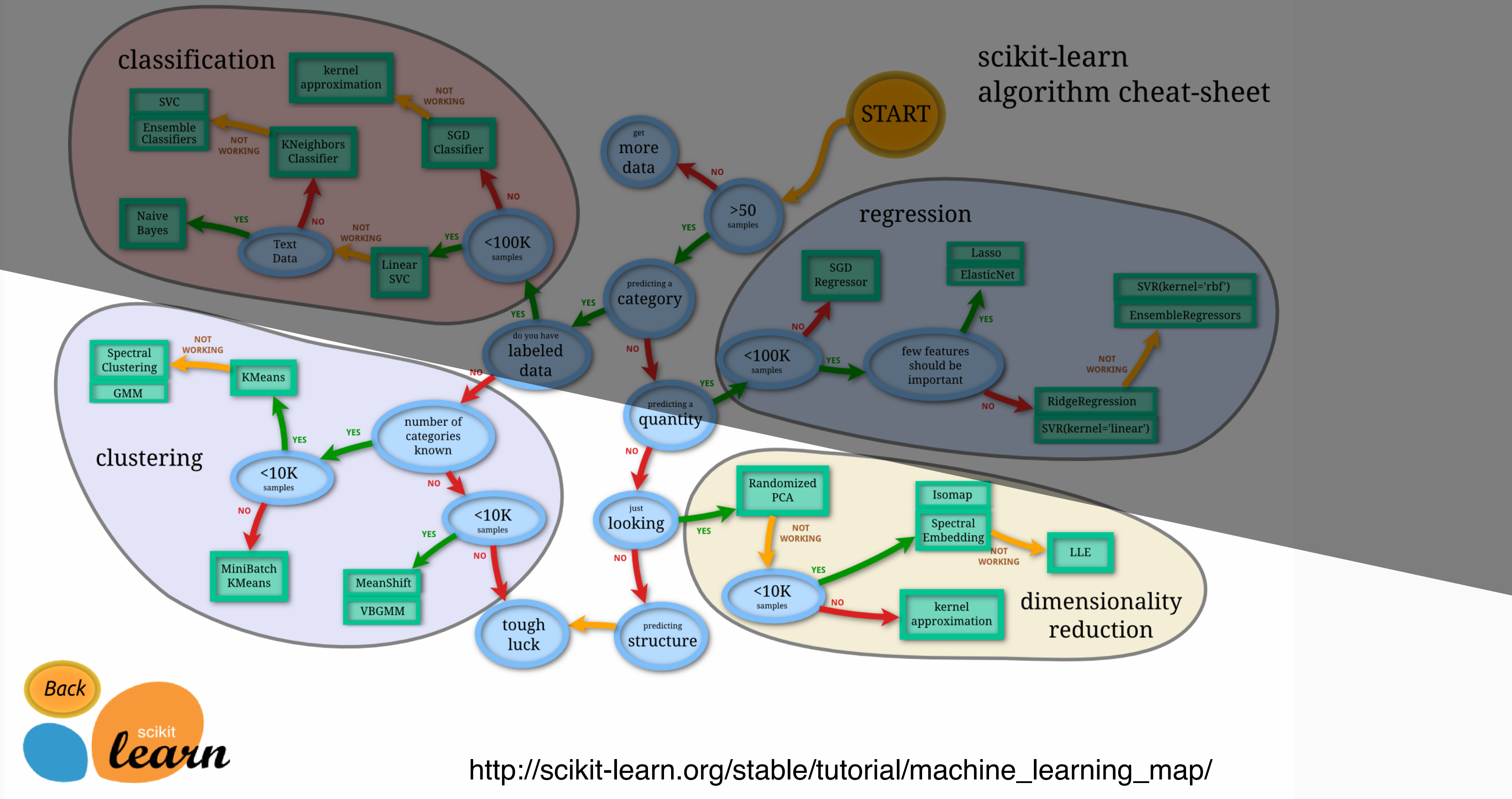



http://scikit-learn.org/stable/tutorial/machine_learning_map/

# Unsupervised Learning - Where We are Going!




http://scikit-learn.org/stable/tutorial/machine_learning_map/

# Basic K-Means Algorithm

Initialize k centroids*

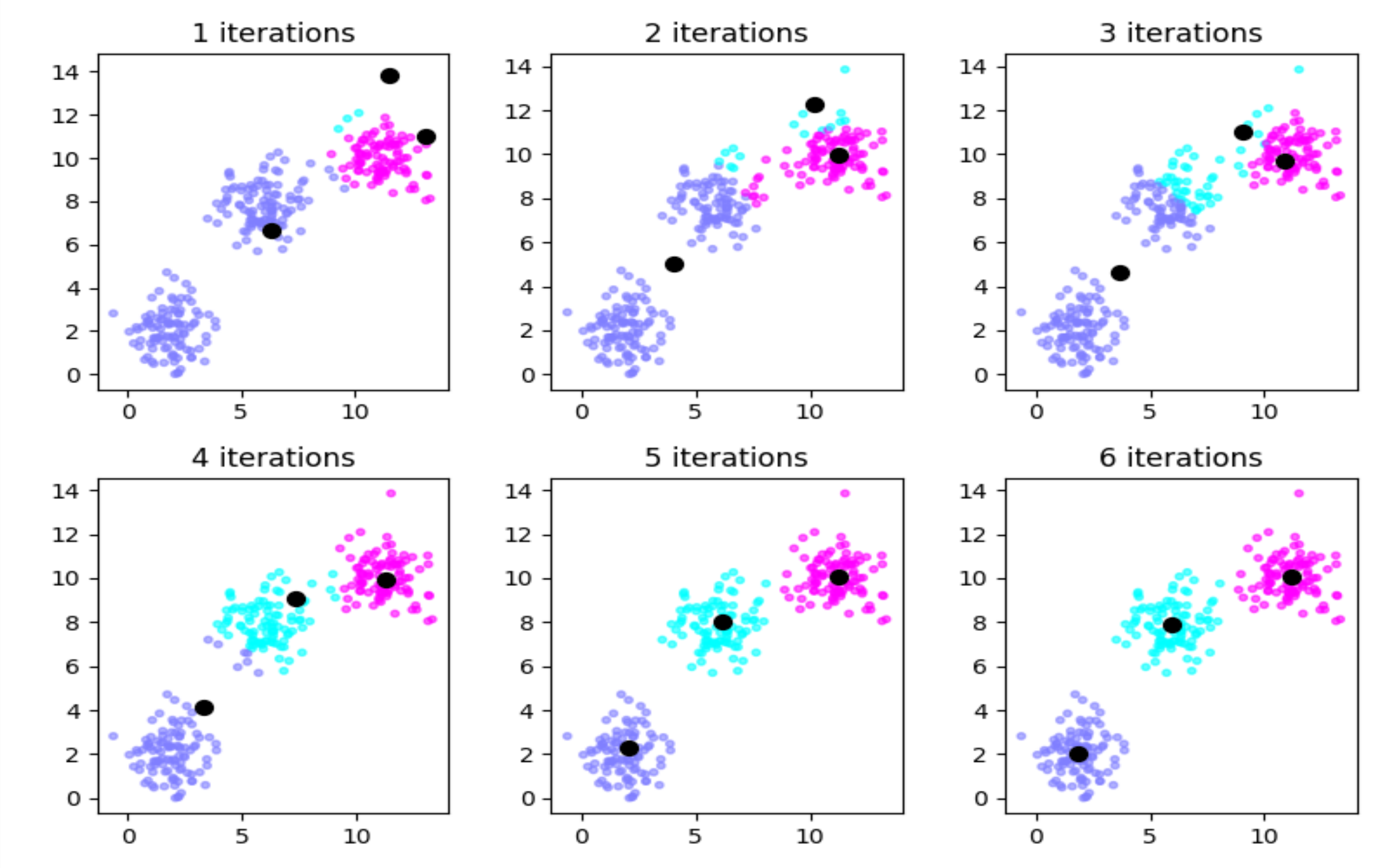
Until convergence**:

- assign each data point to the nearest centroid

- recompute the centroids as the mean of the data points

```
# psuedocode
initialize_centroids
while not converged:
  assign_data_to_centroids
  compute_new_centoid_means
```

# K-Means - What it looks like



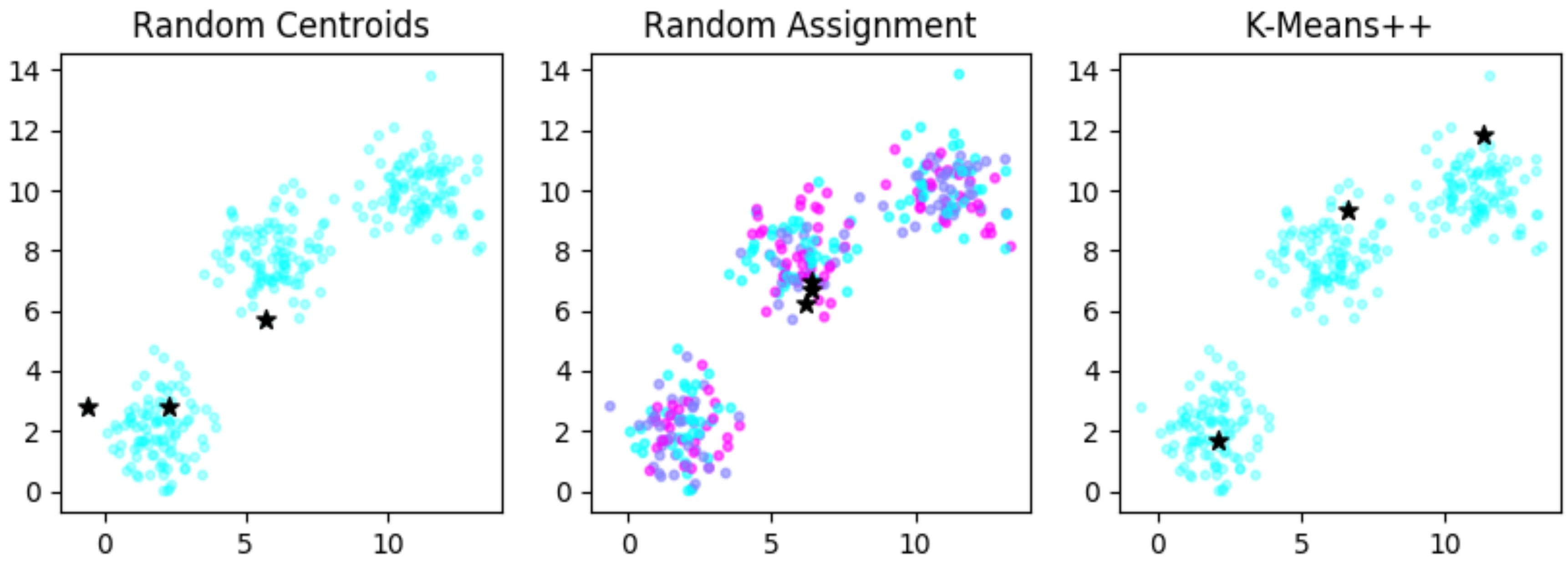
# Centroid Initialization Methods

1) Randomly choose k points from your data and make those your initial centroids (simplest)

2) Randomly assign each data point to a number 1-k and initialize the kth centroid to the average of the points with the kth label (what happens as N becomes large?)

3) **k-means++** chooses well spread initial centroids. First centroid is chosen at random, with subsequent centroids chosen with probability proportional to the squared distance to the closest existing centroid. *(default initialization in sklearn).*

# Centroid Initialization Methods



# Stopping Criteria

We can update for:

1) A specified number of iterations (*sklearn default : max_iter= 1000*)

2) Until the centroids don't change at all

3) Until the centroids don't move by very much (*sklearn default : tol= .0001*)

# Quick Review

Goal of unsupervised learning?

Describe the 2 steps in each k-means fitting iteration

Name 3 ways to choose centroids

Name 3 stopping criteria

Is K-Means deterministic?

Should we standardize features?

# Breakout (numpy practice)

Use these arrays:

```
features = np.array([[ 3,  4],
                     [ 2,  2],
                     [ 5,  4],
                     [ 6,  9],
                     [-1,  0]])

labels = np.array([1, 0, 1, 0, 1])
```

1. Use masking to grab the rows of features that correspond to the label of 1
2. Find the column-wise mean of that subset of features
3. Compute the euclidean distance from each data point in features to this mean. Try to do this in one line with broadcasting!

# Breakout (numpy practice)

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                     [-1,  0]])

labels = np.array([1, 0, 1, 0, 1])
```

1. `subset = features[labels == 1]`
2. `mean = subset.mean(axis = 0)`
3. `np.linalg.norm(features - mean, axis = 1)`

# Evaluating K-Means

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How do we measure clustering performance / effectiveness?

Quantify how similar items are within a cluster

Minimize Intra-Cluster Variance or Within Cluster Variance (WCV)

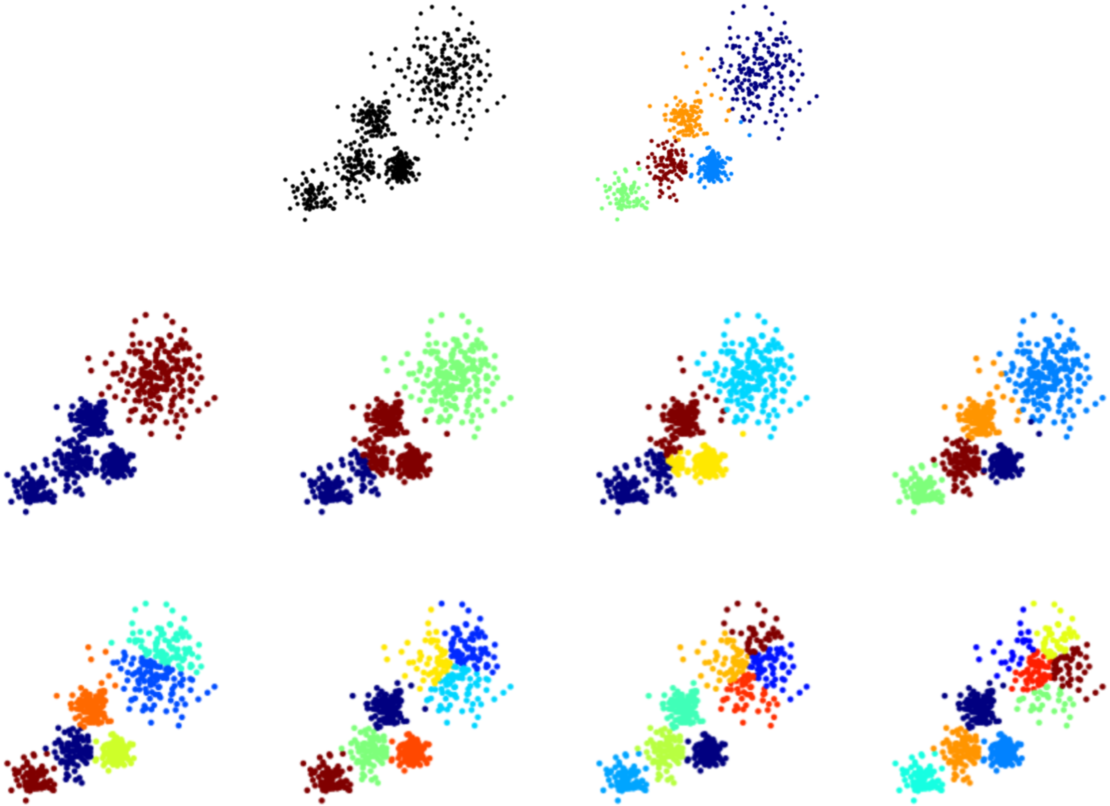
$$\min \left\{ \sum_{k=1}^{K} WCV(C_k) \right\}$$

Where WCV for the kth cluster is the sum of all the pairwise Euclidean distances

$$WCV(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$

Centroid of cluster $C_k$

# K?



# Choosing k

Choosing k requires *a-priori* information:

- business logic (e.g. identify low, medium and high propensity customers)

- domain knowledge (e.g. there are k equilibrium states resultant from the phenomena)

Or a *heuristic*:

- Elbow plot

- Silhouette score

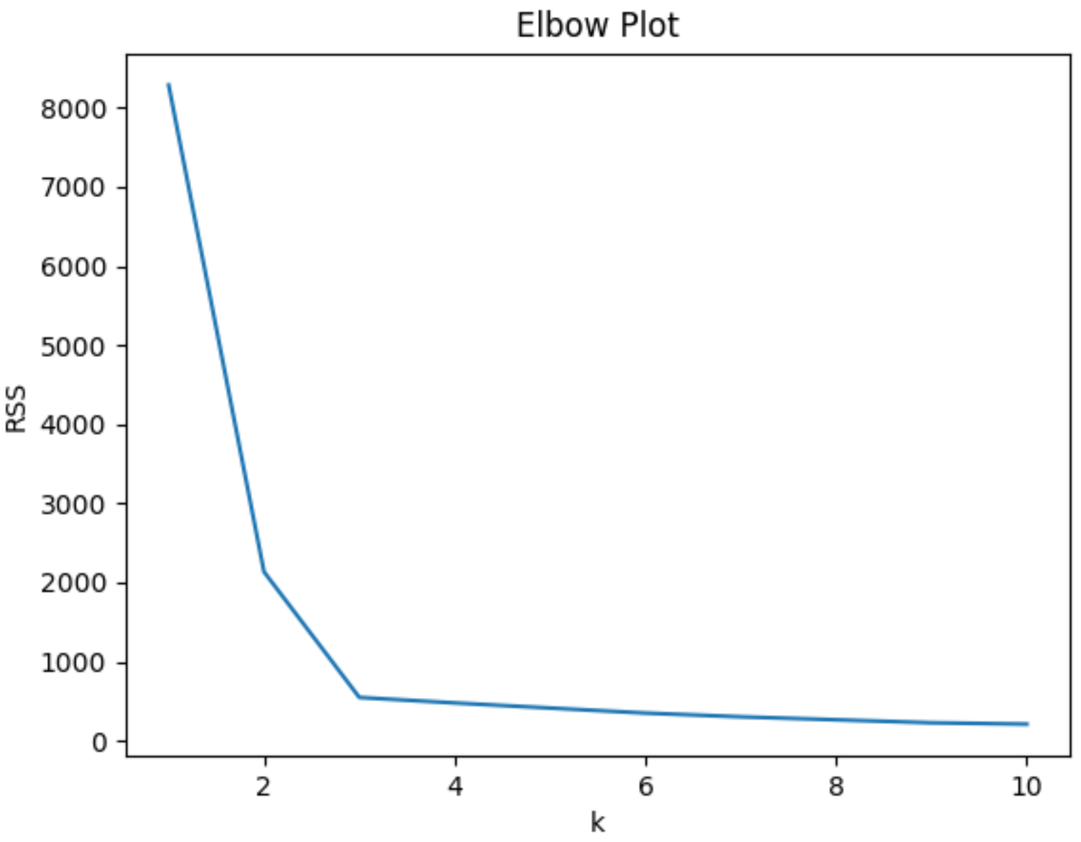
- GAP statistic and other methods that you don't need to know today

# Elbow Plot

Elbow method - look for value of k that drastically reduces the residual sum of squares within the clusters

$$RSS = \sum_{k=1}^{K} \sum_{(i)=k} \left\| x_i - \bar{x}_k \right\|^2$$

Look for inflection point or value of k where improvement diminishes



# Silhouette Score

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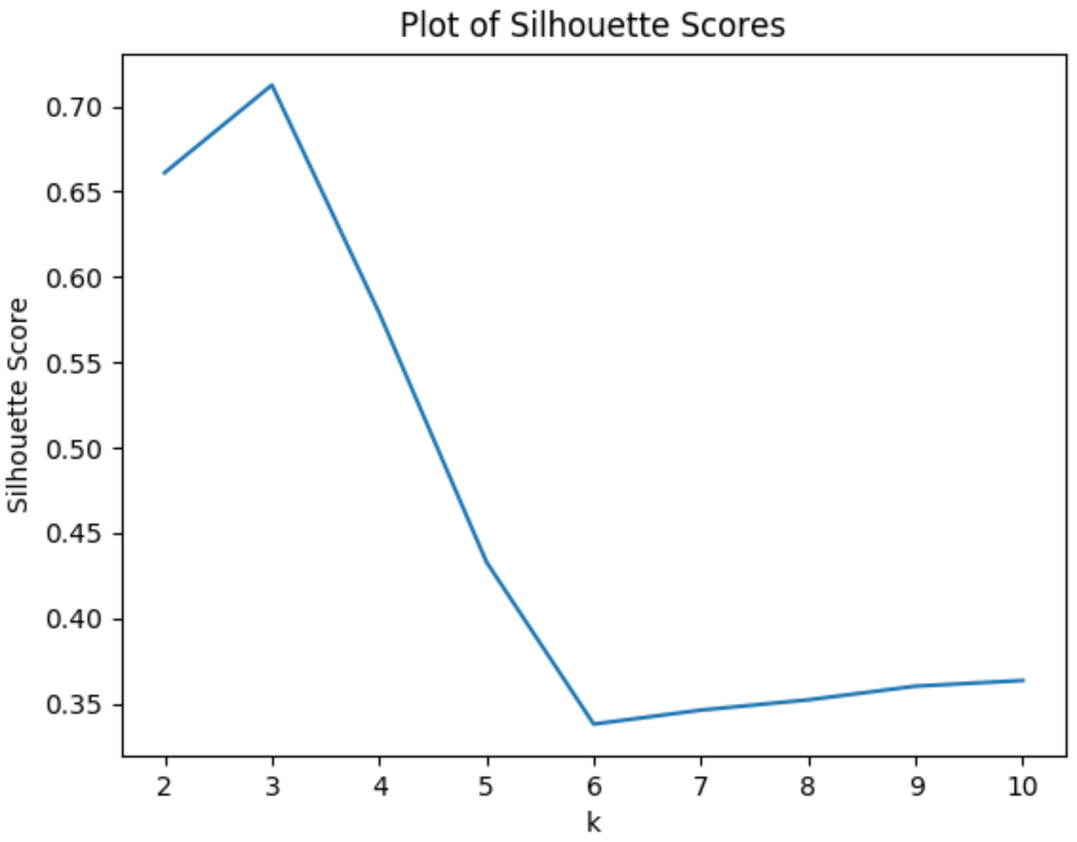
The Silhouette Coefficient is calculated using the mean intra-cluster distance (a) and the mean nearest-cluster distance (b) for each sample

***(b - a) / max(a, b)***

*only defined for 2 <= k < n

Values range from -1 to 1, with 1 being optimal and -1 being the worst

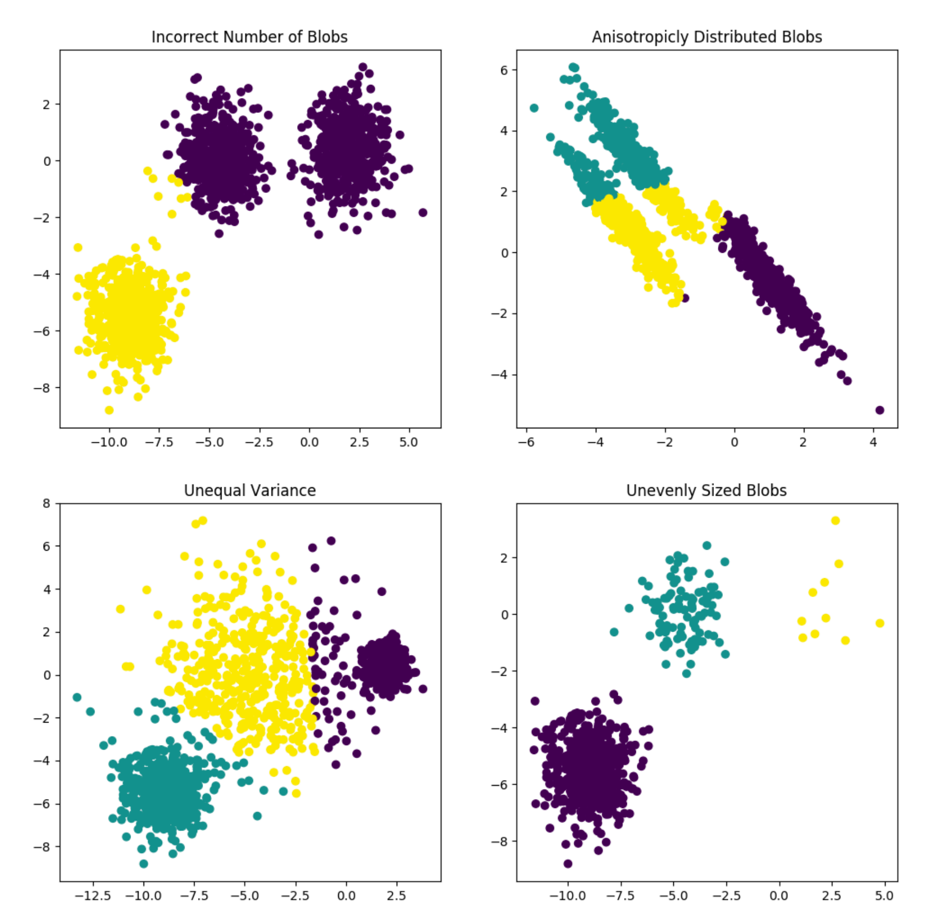
http://scikit-learn.org/stable/modules/generated/sklearn.metrics.silhouette_score.html#sklearn.metrics.silhouette_score



# K-Means Assumptions

- Picked the "correct" k
- Clusters have equal variance
- Clusters are isotropic (variance spherical)
- Clusters do NOT have to contain the same number of observations

http://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_assumptions.html



# Practical Considerations

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- K-means is not deterministic -- falls into local minima. Remedy by reinitializing multiple times and take the version with the lowest within-cluster variance (sklearn does multiple initializations by default)
- Susceptible to curse of dimensionality
- One hot encoded categorical can overwhelm - look into k-modes (https://pypi.python.org/pypi/kmodes/)
- Try MiniBatchKMeans for large datasets (finds local minima, so be careful)

# DBScan Algorithm

- Also computes clusters using distance metric, but decides the number of clusters for you

- With K-Means, you choose k - this is your **main** hyper-parameter

- With DBScan, your main hyper-parameter is **eps,** which is the maximum distance between two points that are allowed to be in the same ‘neighborhood’

# Real world use cases

- Customer segmentation
- Product segmentation
- Image segmentation
- Anomaly detection
- Social network analysis
- and many more…

# Learning Objectives: Recap

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- **Define K-means algorithm:**
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# Questions?

For your morning assignment, you will be coding the KMeans algorithm from scratch, and testing it on the iris dataset. I have included some (optional) starter code with the notes. You should be using numpy and vectorizing your calculations - there should only be one for loop, in the ‘fit’ method.