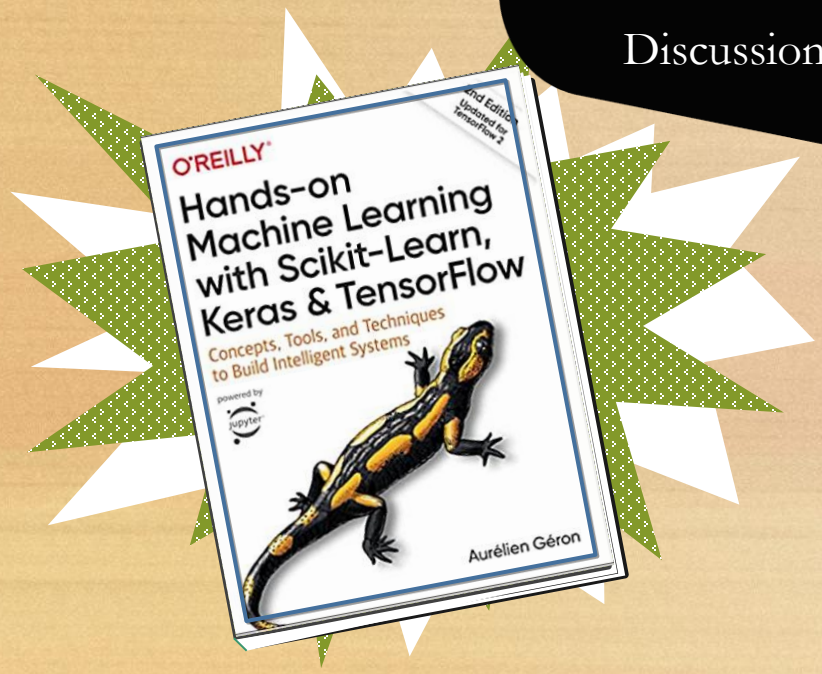
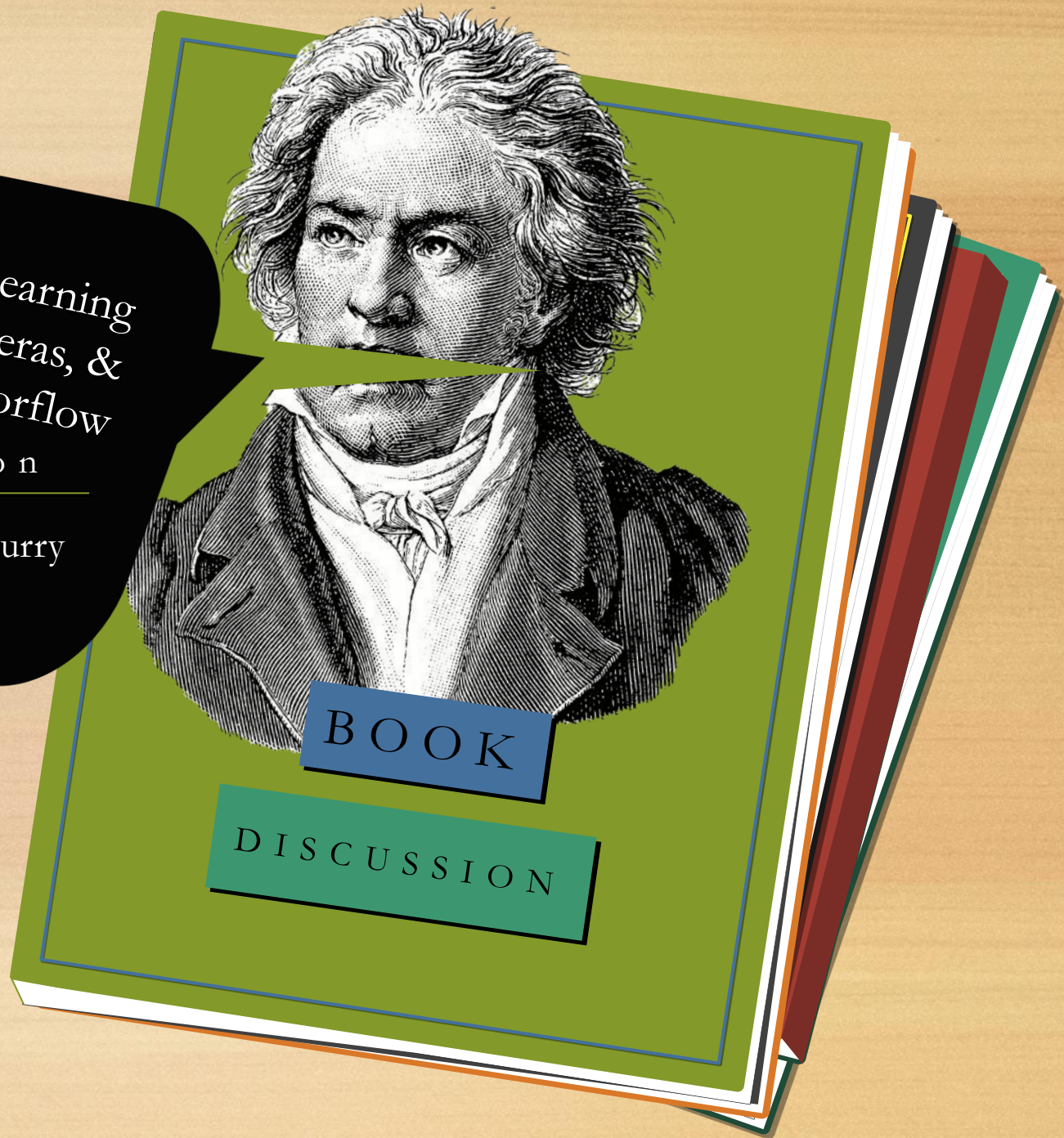
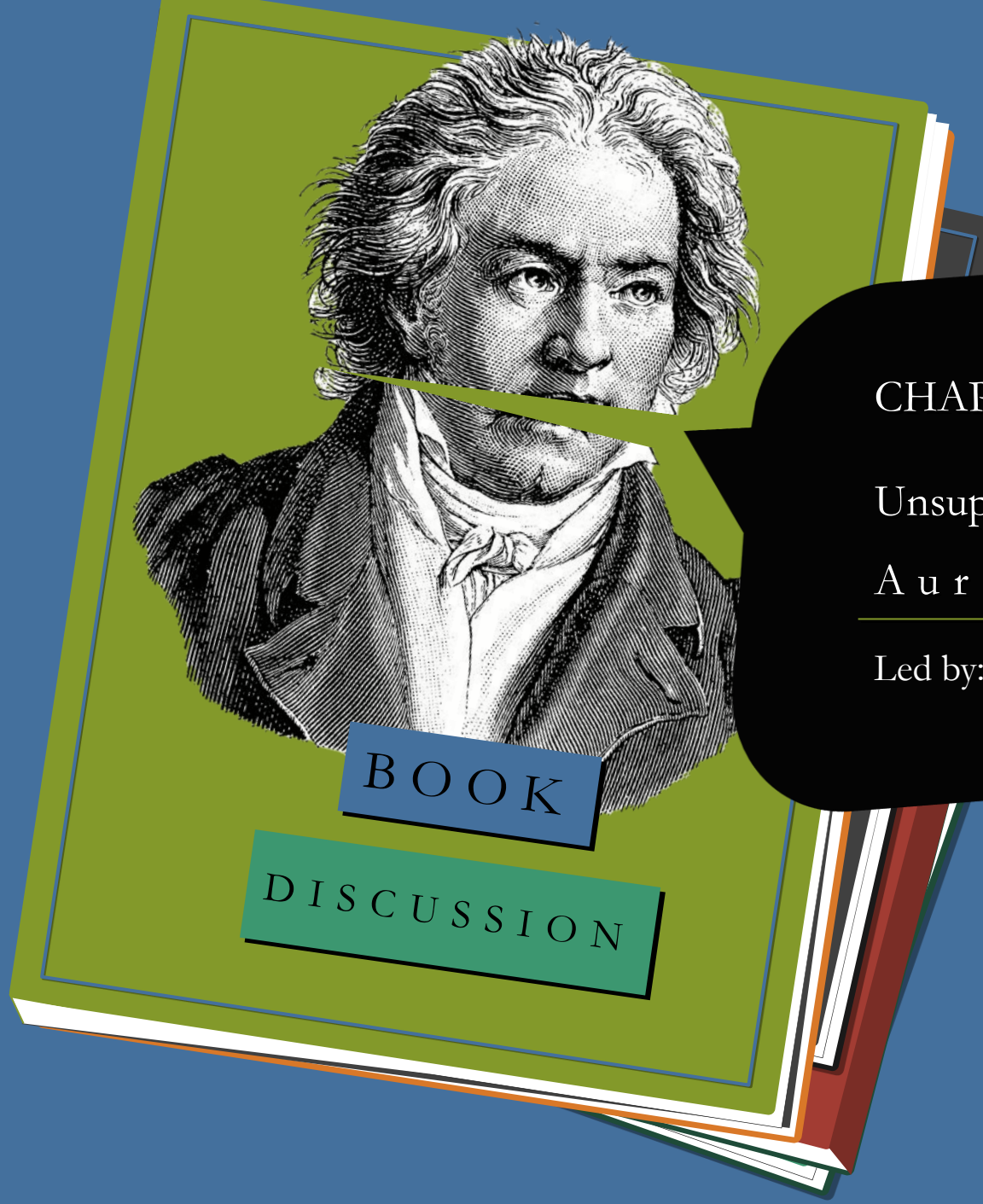
# Hands-on Machine Learning with Scitkit-Learn, Keras, & Tensorflow

Aurélien Géron

Discussion led by: Kalika Kay Curry






CHAPTER 9:

# Unsupervised Learning

Aurélien Géron

Led by: Kalika Kay Curry

# Unsupervised Learning

*Modeling Unlabeled Data*

Why Unsupervised Learning

- Unsupervised Learning – High Potential
- Works to cloister/compare unlabeled instances (*manufacturing example*).
- Dimensionality Reduction is the most common form of unsupervised learning method.

Types of Unsupervised Learning

- Clustering, objects are grouped together
- Anomaly Detection – learn what's normal to find what's abnormal.
- Density estimation – Probability density function (PDF) is estimated of the random process that generated the dataset. Used for anomaly detection, analysis, and visualization.

# Part I: Clustering

Focused on clustering unsupervised learning models

# Why Cluster

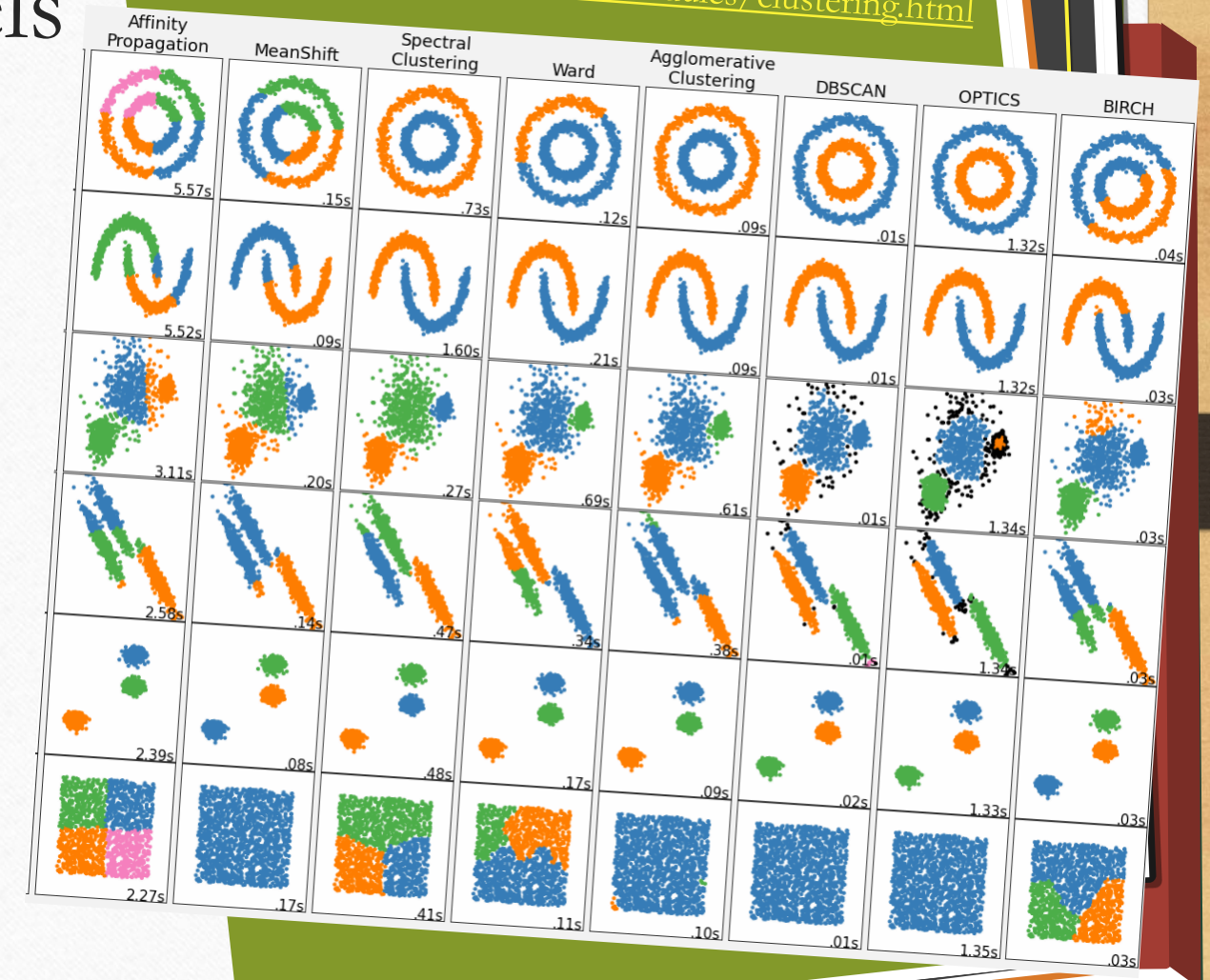
- Dimensionality reduction (Preprocessing)
  - Include cluster in the pipeline.
  - GridSearchCV for best k value
- Semi supervised learning
  - Train a dataset from labeled clusters
- Segment an image
  - Color segmentation

- Customer segmentation
- Data analysis
- Anomaly detection (outlier detection)
- Search engines

# Types of Clustering Models

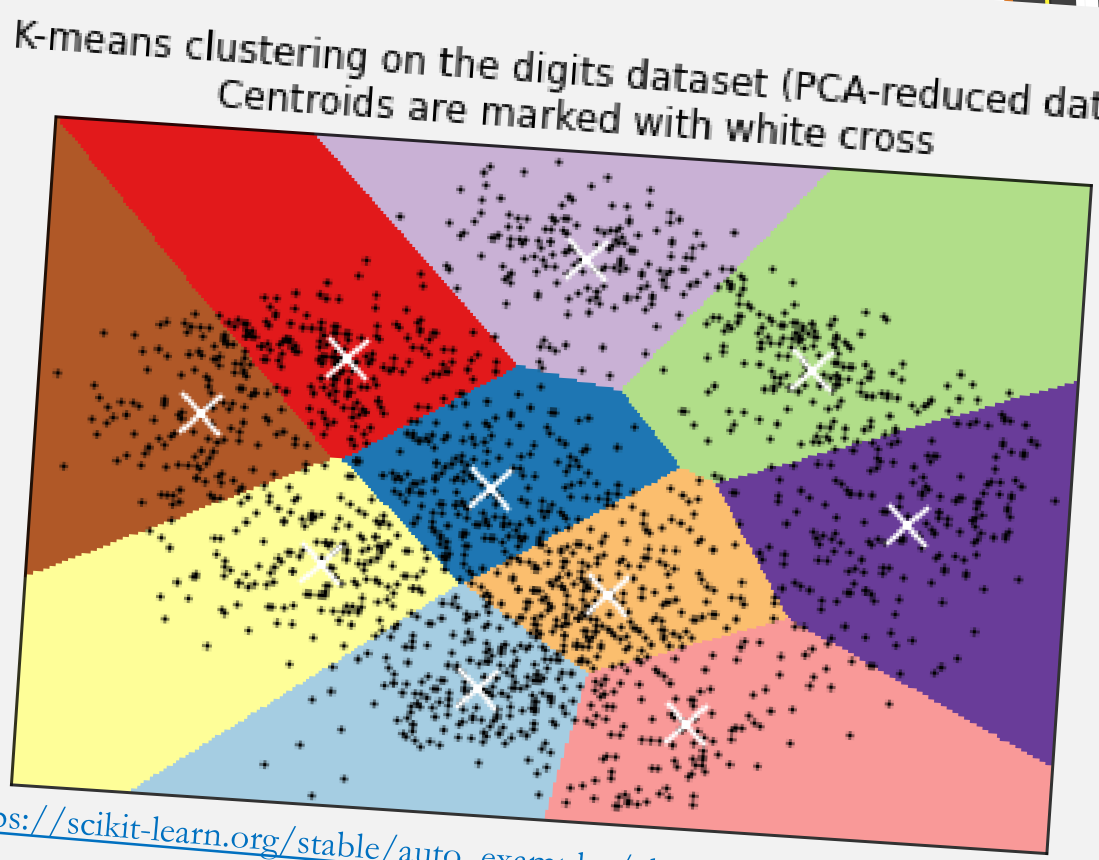
- K-Means
- DBScan
- Agglomerative – Hierarchical, matrix required for large datasets.
- BIRCH – Hierarchical, designed for large datasets.
- Mean-Shift – not suited for large datasets, similar to dbscan
- Affinity Propagation – not suited for large datasets. Uses a voting mechanism.
- Spectral – combo-unsupervised learning method. Combines an embedded dimensionality reduction with another unsupervised learning. Used for complex data structures and to cut graphs.

https://scikit-learn.org/stable/modules/clustering.html



# K-Means History

- Best described with a Voronoi diagram (right).
- AKA Lloyd-Forgy
  - Developed in 1957 by Lloyd (copyright)
  - Developed in 1965 by Forgy
- In 2006, Arthur and Vassilvitskii provided introduced a Kmeans++, faster way of identifying centroids and is the default.
- There are a couple of other varieties such as Mini-batch K-Means; is faster, but has more inertia.
- Requires the n_clusters parameter (k)




https://scikit-learn.org/stable/auto_examples/cluster/plot_kmeans_digits.html

# K-Means Usage

- Reminder: Scale the data
- Cluster amount
  - Inertia elbow chart
  - Silhouette line graph
  - Silhouette diagram
- Limited Solution
  - We're all a little limited.
  - Ladybug example from image segmentation.
  - Does not perform well with
    - Non spherical shapes (whatever that means)
    - Different densities
    - Varying sizes

- Inertia identifies the best solution (best centroid location).
  - Mean squared distance between each instance and its closest centroid
- Getting lucky: Centroid initialization methods *(Risk Mitigation)*
  - Random centroid initializations can produce suboptimal solutions as a convergence occurs at random.
  - Kmeans++ Algorithm
- n_init has a default setting and determines how many times the centroids should be selected for the optimal solution.
- If you know the initialization points for the clusters, you can set the init parameter manually. with an n_init parameter set to one.

# Types of Clustering

```
#function from chapter 5 (no plot)
def gaussian_rbf(x, landmark, gamma):
    return np.exp(-gamma * np.linalg.norm(x - landmark, axis=1)**2)
```

```
x1_example = X1D[3, 0]
for landmark in (-2, 1):
    k = gaussian_rbf(np.array([[x1_example]]), np.array([[landmark]]), gamma)
    print("Phi({}, {}) = {}".format(x1_example, landmark, k))
```

```
Phi(-1.0, -2) = [0.74081822]
Phi(-1.0, 1) = [0.30119421]
```

*Conversely to a distance transformation we can use a similarity function.*

## Hard Clustering and Soft Clustering

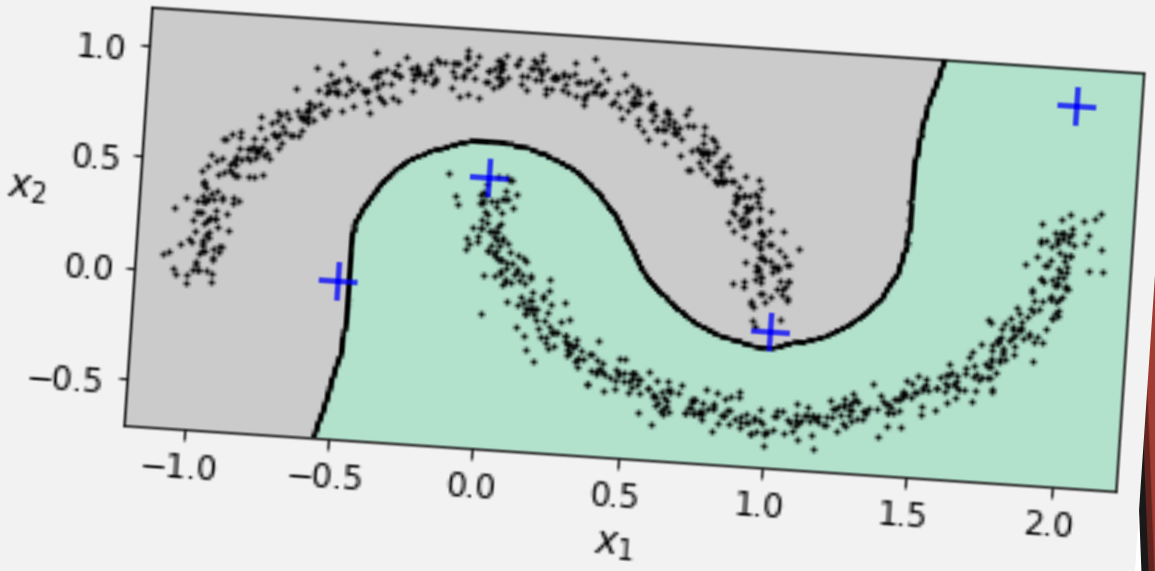
- Hard Clustering
  - is one instance is assigned to a cluster
- Soft Clustering
  - assigns each instance a score per cluster.
  - Can be the distance from the centroid, which can be found using the transform method; which represents the Euclidian distance of an instance form each centroid.
  - Can be the a similarity/affinity score such as the Gaussian Radial Basis Function. (chapter 5)
  - The transform method can be used to gather the distance between each instance to each centroid. It is in fact, the Euclidian distance.
- Note: the similarity/affinity function is not provided as an example in the github solutions/notebook provided to the author.
- The affinity function states that the number of features will increase, drastically with an extremely large training set. What does this mean for dimensionality reduction; when we're working with clustering? Can we expect to see that the similarity/affinity results would be overkill or over extensive?

# DBScan

https://scikit-learn.org/stable/modules/clustering.html#dbscan

https://github.com/alexhegit/handson-ml2/blob/master/09_unsupervised_learning.ipynb

- Continuous regions of high density.
- Epsilon neighborhood a count of the number of instances that are within a small distance from it.
- Min_samples: if it has at least these number of samples, it's a core instances.
- If you're in the same neighborhood; you belong to the same cluster. This can include many core instances, so if there is a long running instance; you're all one.
- If it's not a core instance and is not in the neighborhood, it's an outlier, represented with a -1.
- No predict method; a classifier is better at predicting the cluster the data may belong to (*knn example to the right*)

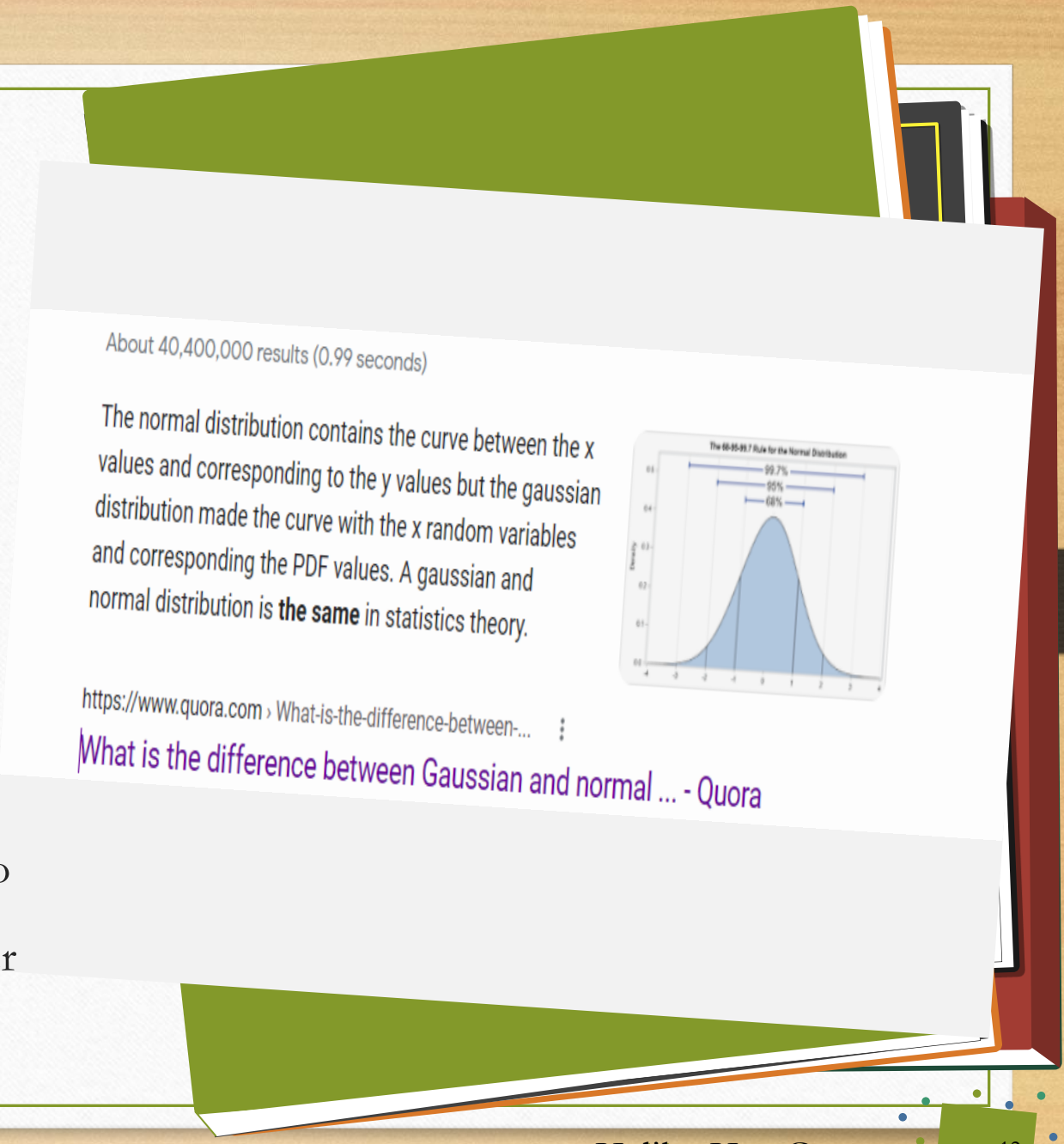


# Part II: Gaussian Mixture Modeling (GMM)

Focused on Gaussian Mixture Modeling (GMM).

# What is Gaussian Mixture Modeling?

- Model that uses soft clustering (returns a probability of an instance belonging to a cluster).
- Assumes that the instances are gaussian in type with unknown distributions.
- Ellipsoidal in shape, as opposed to the dense clusters seen with K-Means.
- Similar to K-Means algorithm, using the Expectation Maximization algorithm – which is where the soft cluster comes from.
- Also like K-Means, subject to poor convergence so several iterations are required to reach best solution. This is achieved with the n_init parameter whose default is 1; so be sure to check in on this one.



# Funny Pictures (Computational Complexity)

pages 261 and 271

- A couple of diagrams are available on both pages 261 (Gaussian) & 271 (Bayesian Gaussian) that provide a visual representation of what's going on with the model, for those interested.
- Covariance type hyper parameter to increase the chances of finding a optimal solution. Default is set to full, which means each cluster can take on any shape or size.
- Covariance hyper parameter impacts computation speeds – tied and full are the longest; spherical and diag are a bit faster.

# Anomaly Detection

- It can detect anomalies (outliers) or those that deviate from the norm.
- You do this by looking at the density of the clusters, which is returned as the score of the samples. The anomalies are those clusters that are below an agreed upon threshold.
- Gaussian is, by definition, an assumed normalized dataset so in cases where an extreme number of outliers are present; an EllipticEnvelope class exists as a more robust form of anomaly detection (??? Or does it do something else ???)

# AND > >> SCORE > > >

- Alkaike and Bayesian information criterion (AIC and BIC, respectively) scores are used to assist with cluster selection.
- The lower the score the greater better the choice, maybe.
- Another method is to search for the best value for the covariance_type hyperparameter. Spherical is faster but doesn't fit the data as well.
- Bayesian Gaussian Model Mixtures also help resolve the number of cluster conundrum by providing weights, but BGMM comes with many constraints one of which is a restriction to ellipsoidal shapes.

# Thank You

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