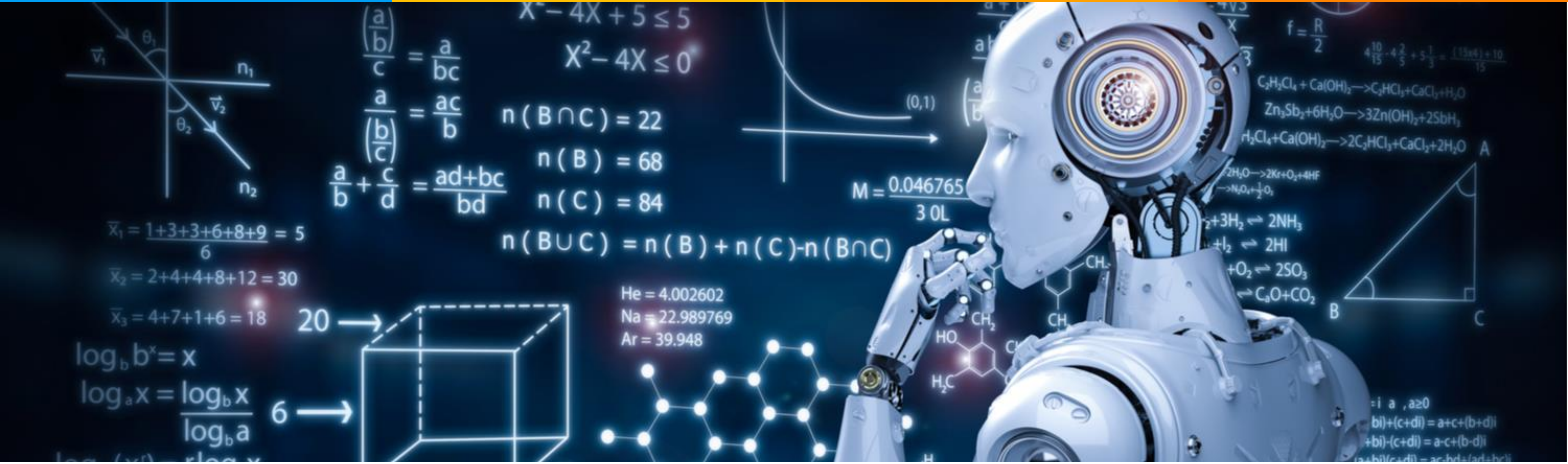
Duration: 60 min | Srikanth Shenoy | AML 5102 | M.E. AI & ML



Lecture 14: Beyond K Means Clustering

Recap

- Kmeans algorithm
- Expectation Maximization
- Centroid initialization with kmeans++
- Kmeans decision boundary
- Kmeans limitations with oblong data clusters
- Kmeans limitations with outliers
- Using Kmeans and silhouette analysis for outlier detection

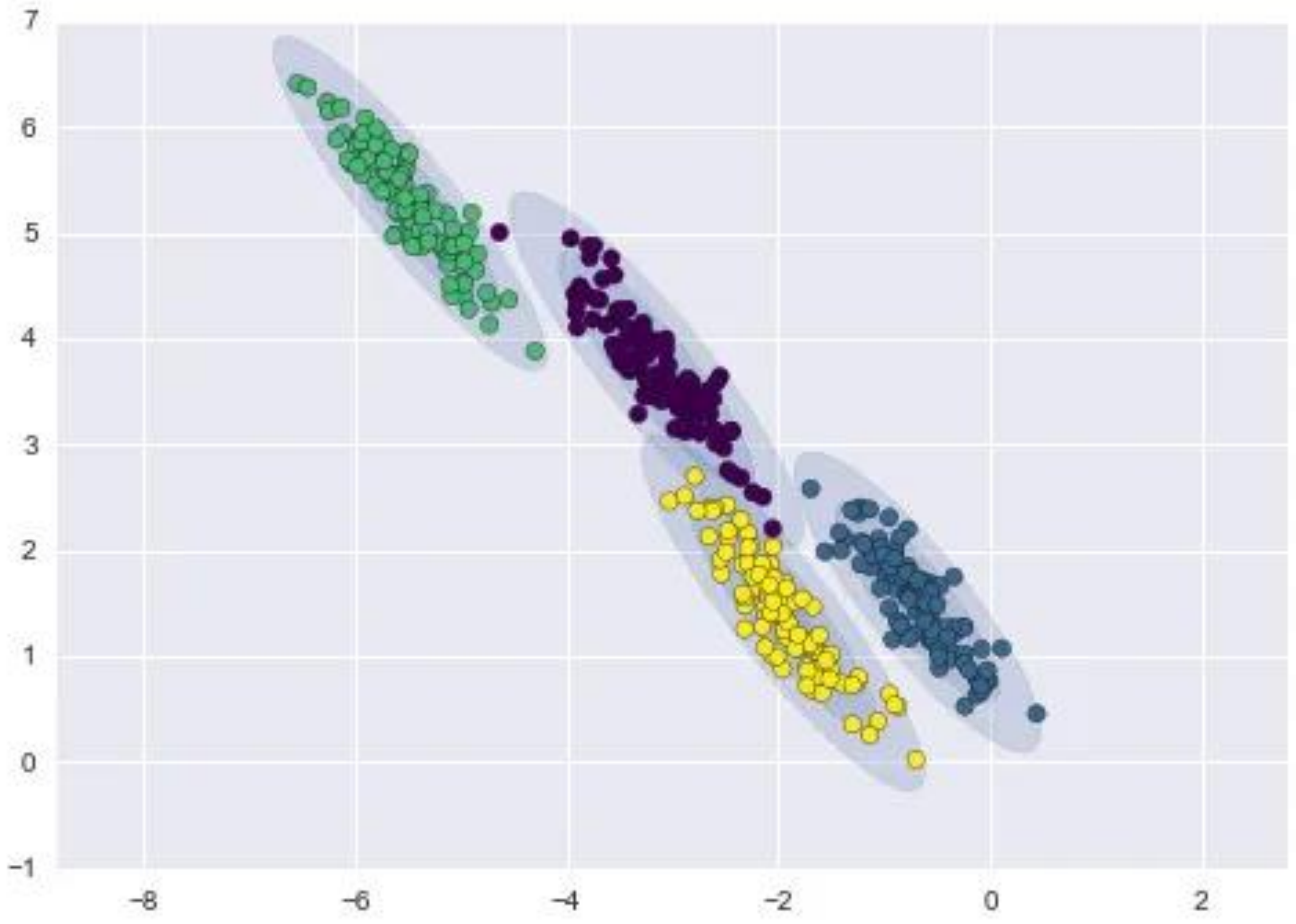
Mixture Models

Another way of looking at clusters

- Hard versus soft clustering
- Hard:
  - Clusters don’t overlap
  - Elements belong to a cluster or they don’t
  - E.g. K-Means
- Soft
  - Clusters may overlap
  - Strength of association between cluster and instances
  - 60% confidence of cluster1 membership, 40% cluster2
  - E.g. Gaussian Mixture Model Clustering

Mixture Model clustering

- Probabilistic way of doing soft clustering
  - Soft clustering - Cluster membership is not 0/1
  - Probability
- Each cluster is a generative model (probability distribution)
- But parameters (mean and covariance) are unknown
  - Discovered as part of clustering
- Parameters are discovered by EM
  - EM in GMM is EM in true sense ☺

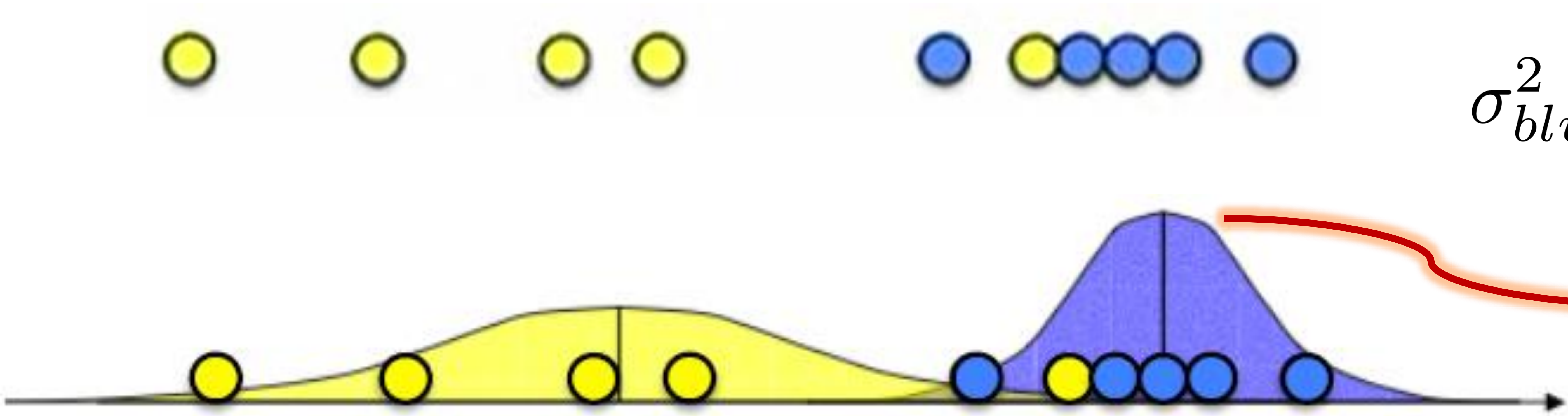


Recap: Estimate Mean & variance in generative ML

- We are given data x1 .. Xn
    - Mean and variance not known
    - Easy to find from labeled data

$$\mu_{blue} = \frac{x_1 + x_2 + ... + x_{n_b}}{n_b}$$

$$\sigma^2_{blue} = \frac{\Sigma(x_i - \mu_{blue})^2}{n_{blue}}$$



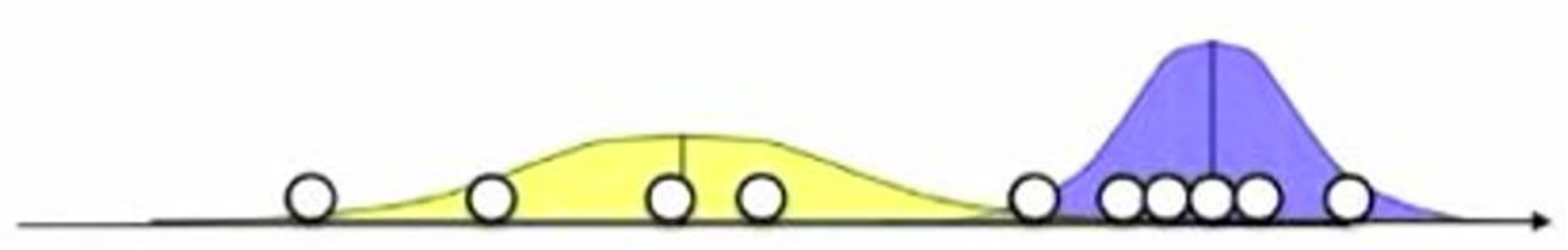
$$\frac{1}{\sqrt{2\pi\sigma^2}} e^{\frac{-1}{2}(\frac{x-\mu}{\sigma})^2}$$

- What if we didn't know which data came from which distribution? (unsupervised learning)

Gaussian Mixture Models

- Chicken & Egg
  - We need labels to determine mean, variance

  - We need mean, variance to predict labels



- If we knew mean/var, we could guess which point came from which Gaussian. But we don't know

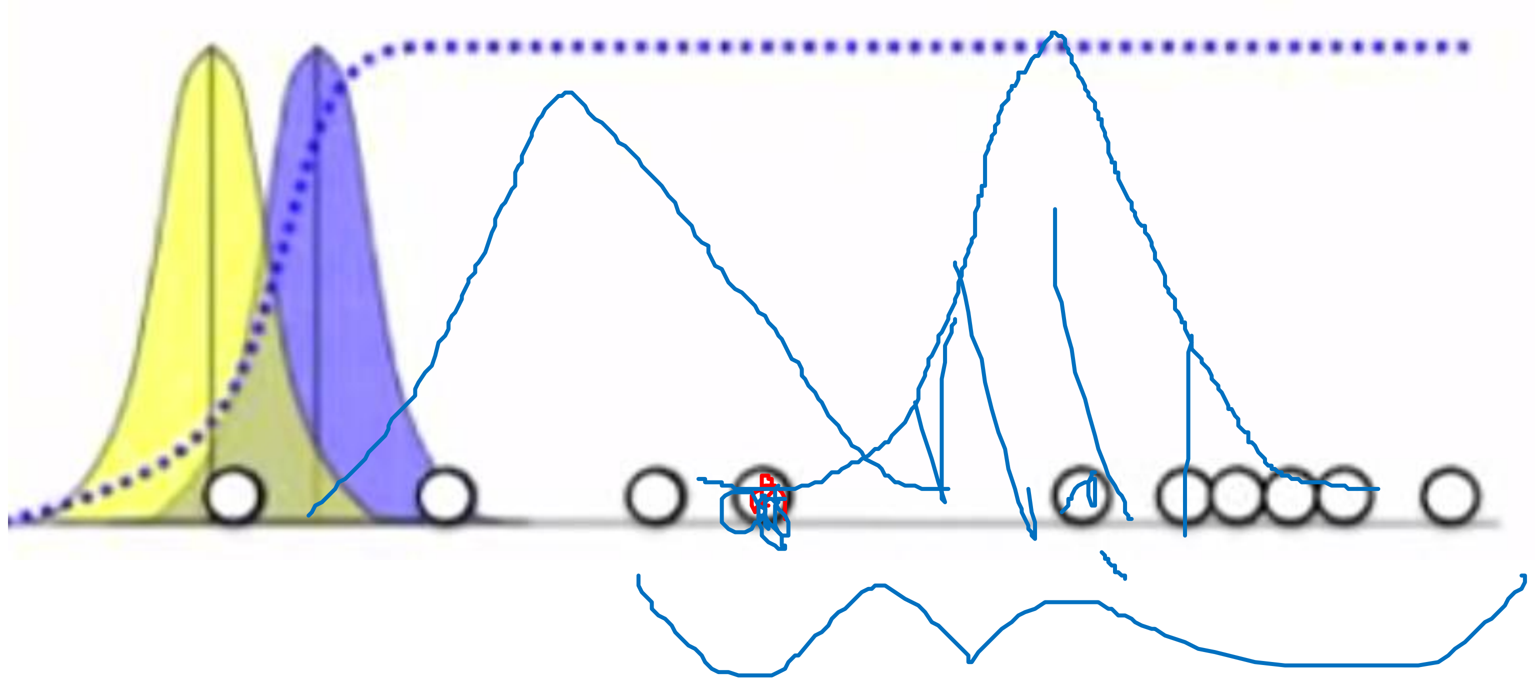
Gaussian Mixture Models Intuition

- We are given data points
- They came from k Gaussian distributions
- We don't know which point came from which Gaussian

- Solution: EM
- Start with two Gaussian with random mean and variances
  - Just like kmeans centroids

Gaussian Mixture Models EM

- 2 Gaussian with random mean and variances
- For each point xi, does this look like it came from a or b?



$$P(x^{(i)}|b) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x^{(i)}-\mu_b}{\sigma_b}\right)^2}$$

$$P(b|x^{(i)}) = \frac{P(x^{(i)}|b)P(b)}{P(x^{(i)}|b)P(b) + P(x^{(i)}|a)P(a)}$$

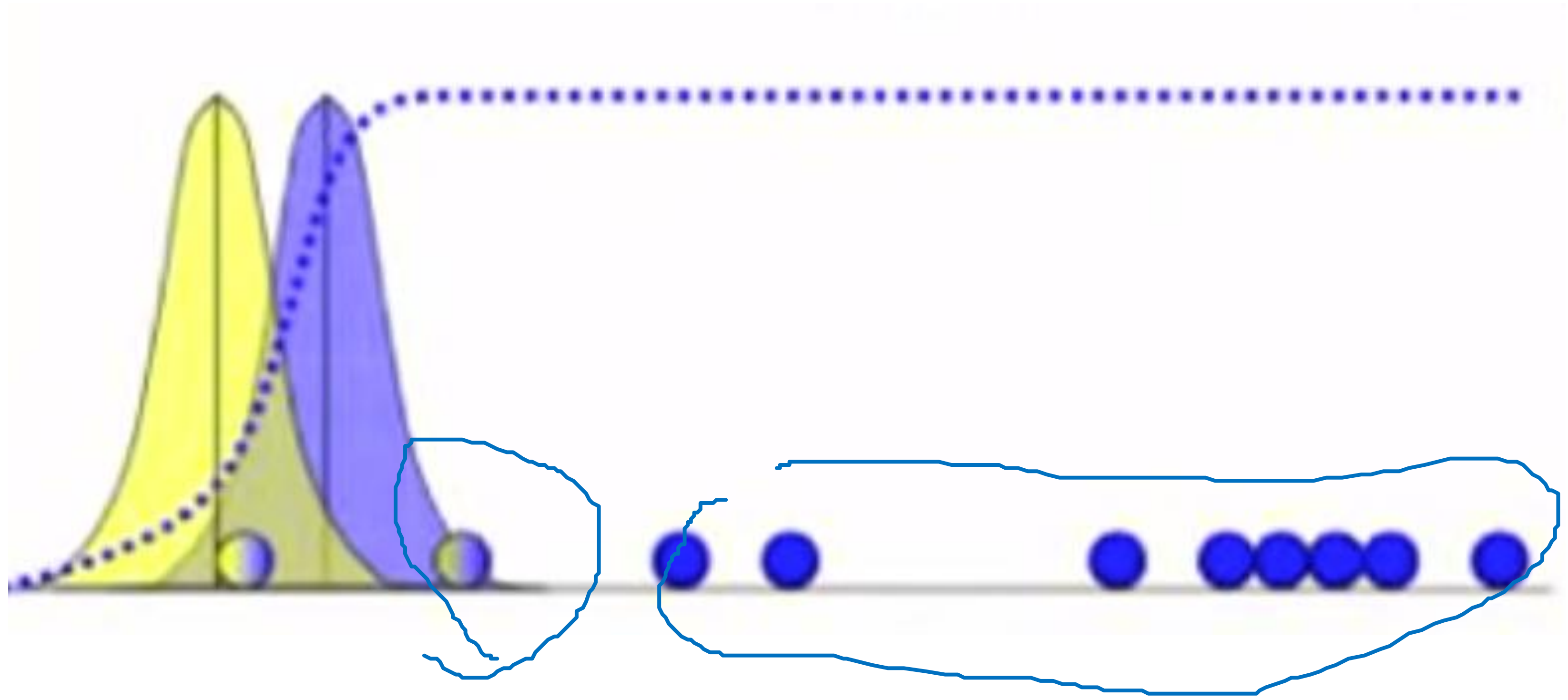
$$P(a|x^{(i)}) = \frac{P(x^{(i)}|a)P(a)}{P(x^{(i)}|b)P(b) + P(x^{(i)}|a)P(a)}$$

- Soft assignment
- No max P calc

Gaussian Mixture Models EM

$$p_{b_i} = P(b|x^{(i)}) = \frac{P(x^{(i)}|b)P(b)}{P(x^{(i)})}$$

$$p_{a_i} = P(a|x^{(i)}) = \frac{P(x^{(i)}|a)P(a)}{P(x^{(i)})}$$



- Calculate the new mean/var

$$\mu_b = \frac{p_{b_1}x^{(1)} + p_{b_2}x^{(2)} + ..p_{b_n}x^{(n)}}{p_{b_1} + p_{b_2} + ... + p_{b_n}}$$

$$\mu_a = \frac{p_{a_1}x^{(1)} + p_{a_2}x^{(2)} + ..p_{a_n}x^{(n)}}{p_{a_1} + p_{a_2} + ... + p_{a_n}}$$

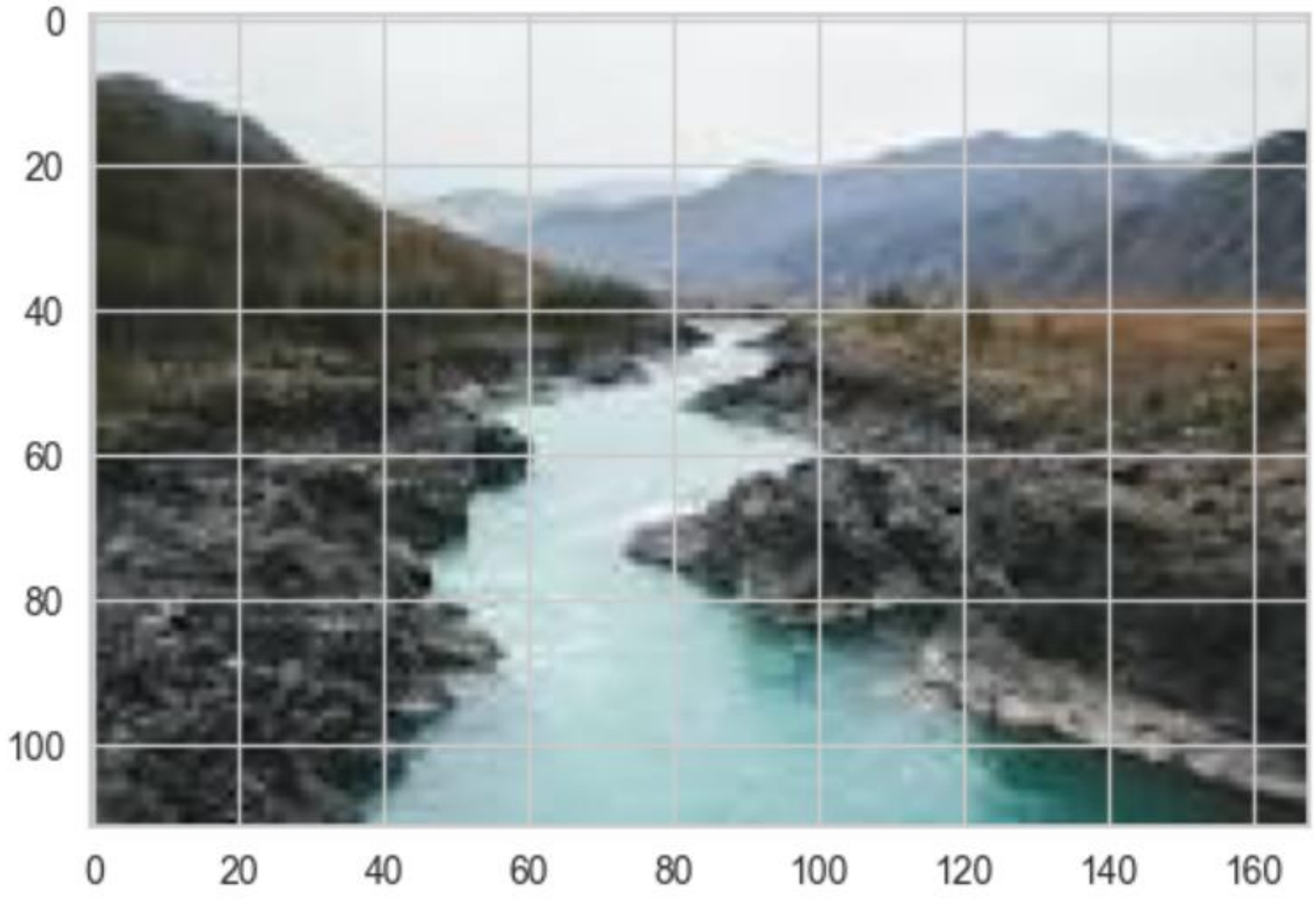
- Rinse and Repeat

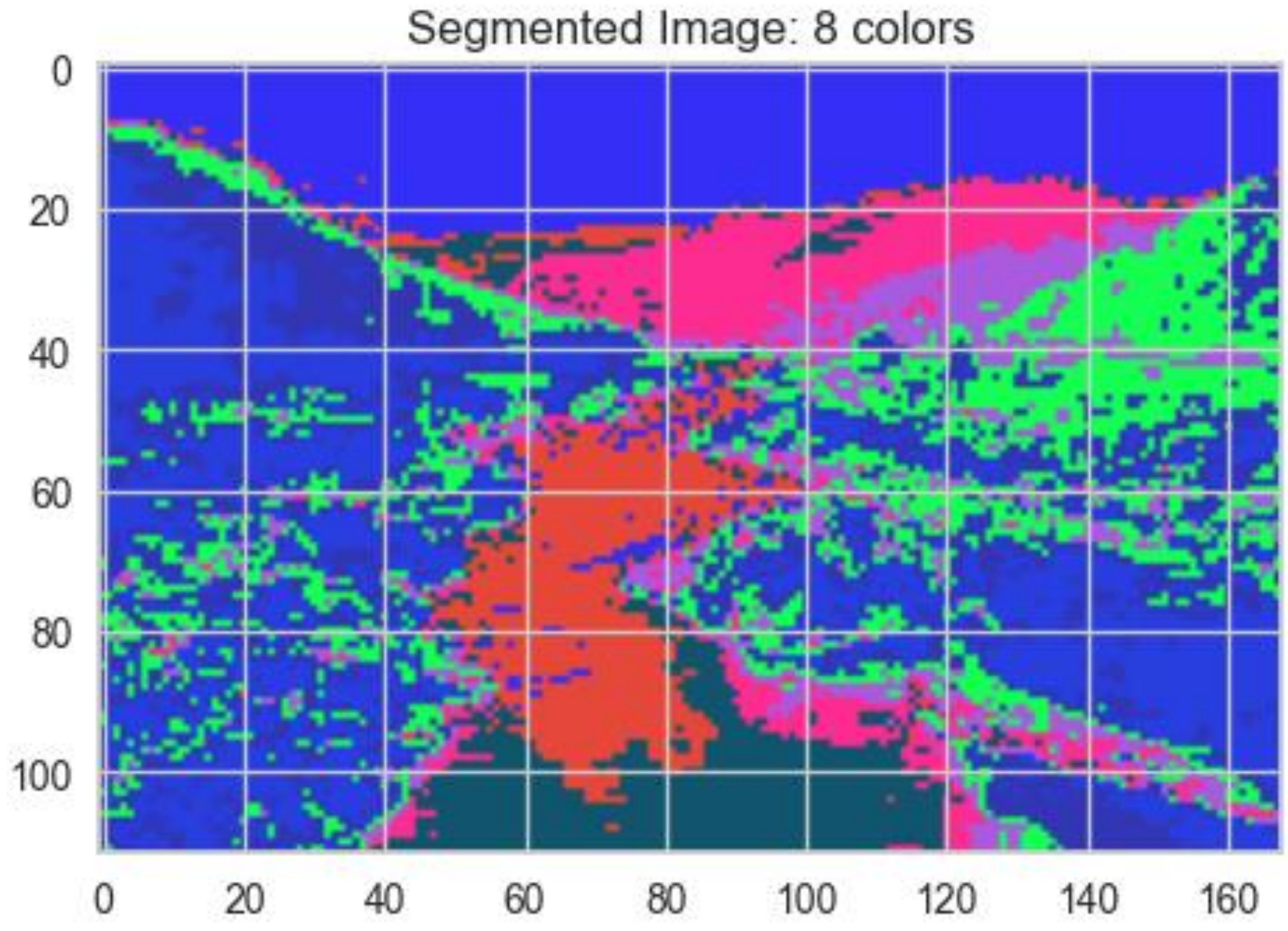
GMM clustering applications

- Real life scenarios are mixtures, never black and white
- Finance
  - Investment Portfolio construction
  - Identifying stocks for growth (outliers in a good way)

GMM clustering applications

- Image segmentation (less expensive way)
  - Split into patches & cluster based on image characteristics
  - Medical image – locate specific structures





GMM clustering applications

- One tool of many towards explainable solution
  - Population to 2 wheeler, 4 wheeler ratio
  - Accident stats, Poisson mixtures for pattern identification

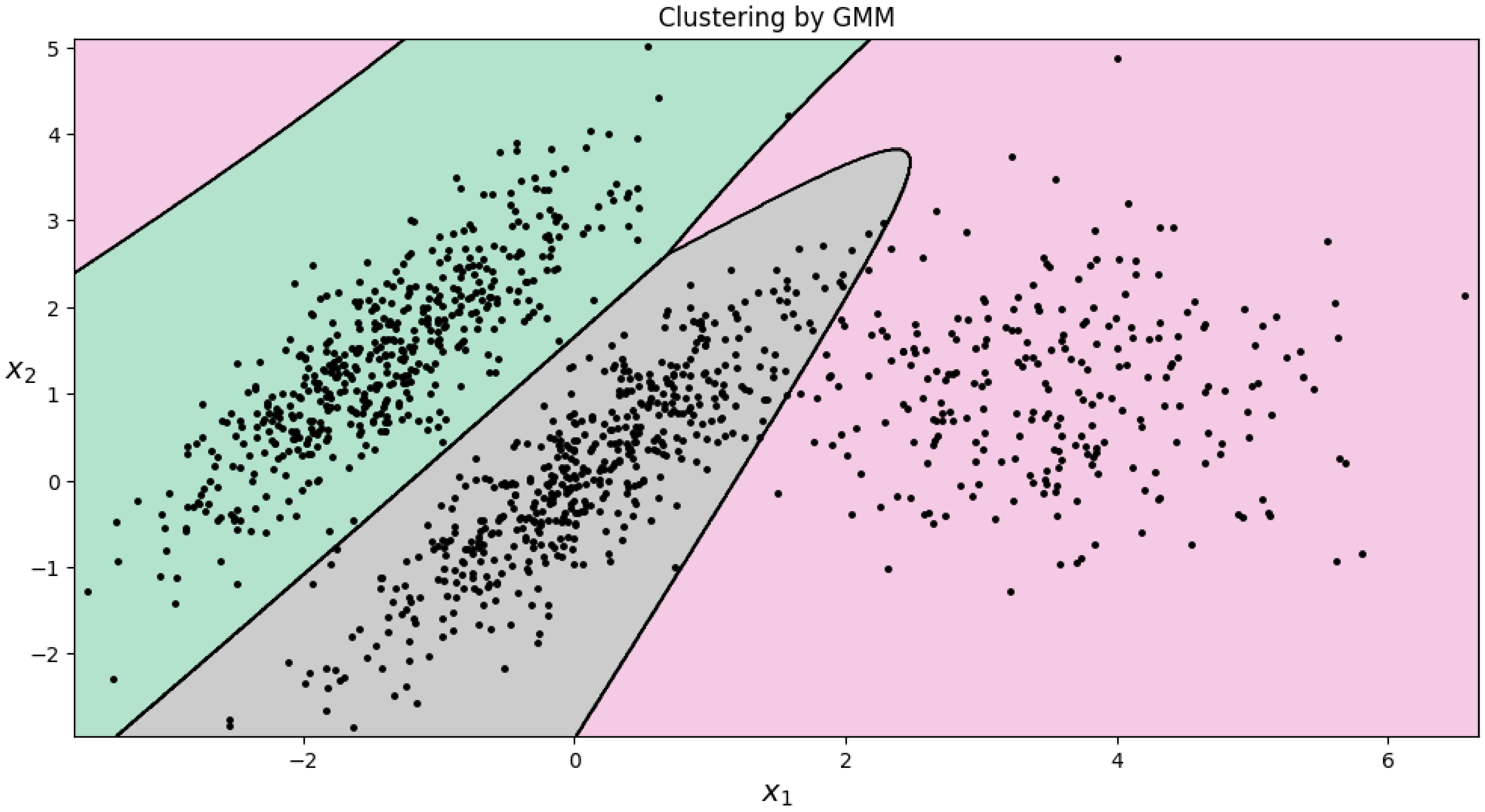
$$p_{b_i} = P(b|x^{(i)}) = \frac{P(x^{(i)}|b)P(b)}{P(x^{(i)})}$$

$$p_{a_i} = P(a|x^{(i)}) = \frac{P(x^{(i)}|a)P(a)}{P(x^{(i)})}$$

$$P(x^{(i)}|b) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{1}{2}\left(\frac{x^{(i)}-\mu_b}{\sigma_b}\right)^2}$$

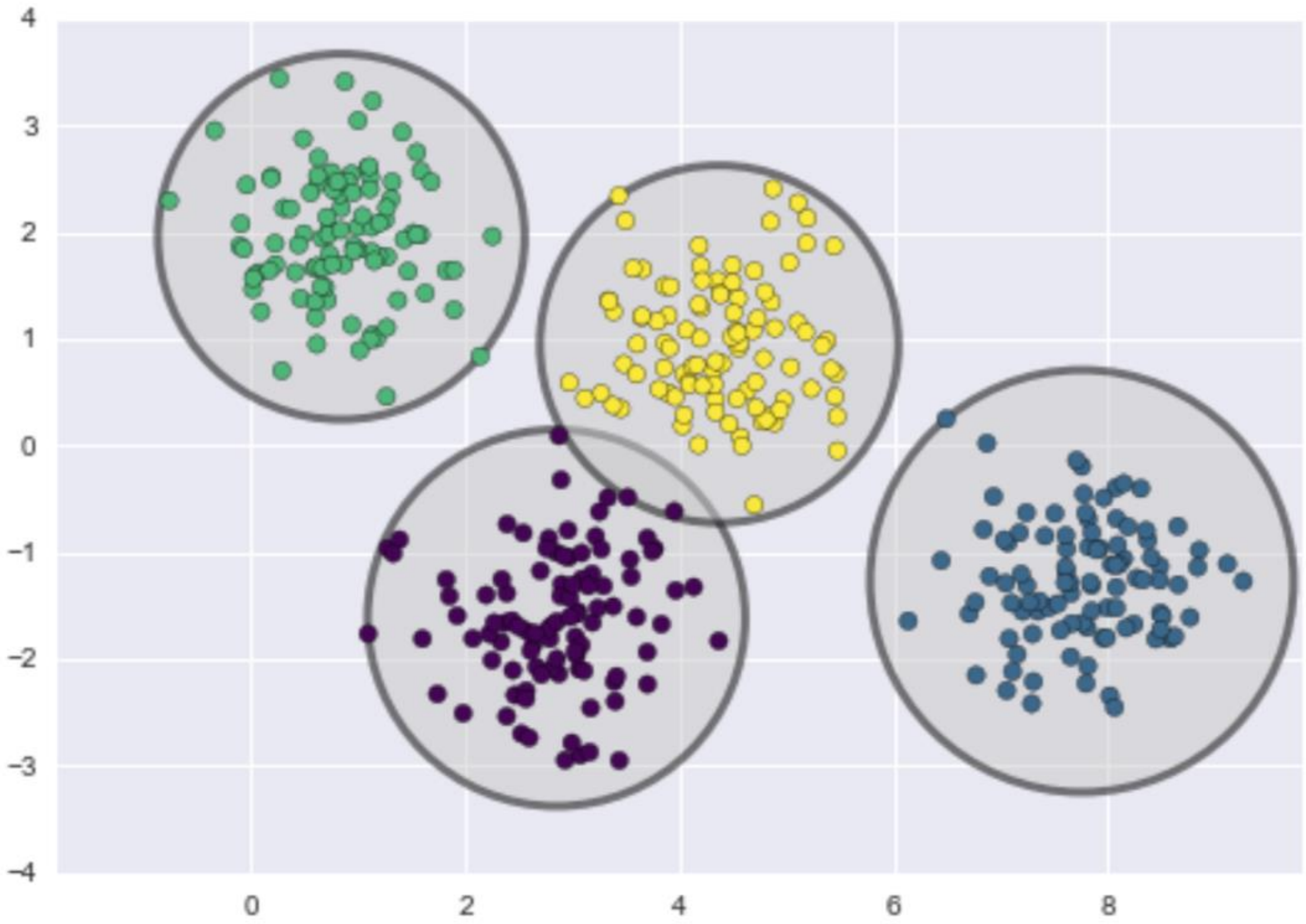
GMM decision boundary

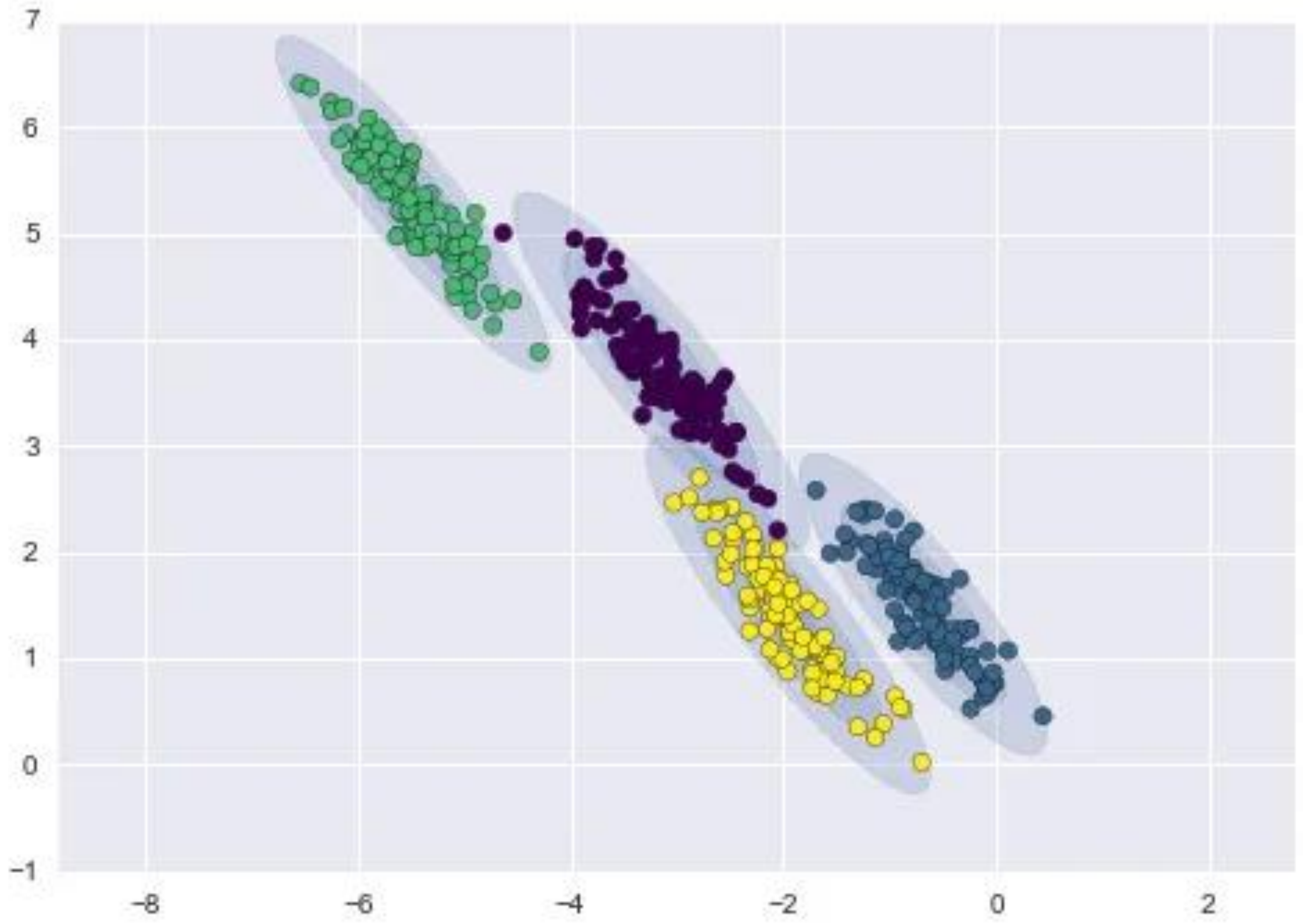
- Quadratic decision boundary



GMM model

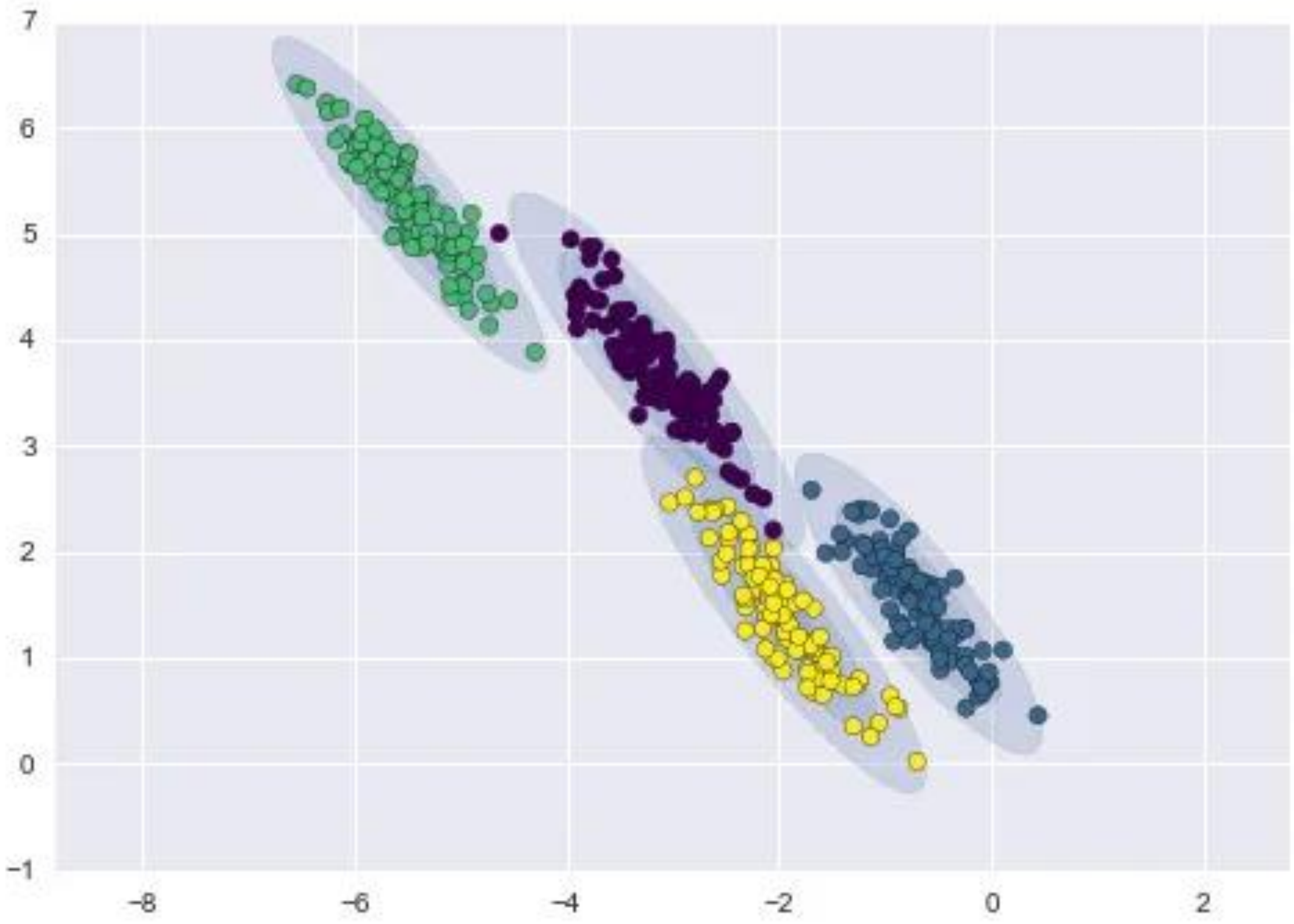
- Clustering every time some new data comes is expensive
- Could use extracted mean, variance, covariance as model
  - Multivariate Gaussian model from scratch!!





Handling outliers with GMM

- GMM is sensitive to outliers
- Can use multivariate Gaussian techniques (Mahalanobis distance) or silhouette analysis
- Can use Minimum Covariance Determinant also

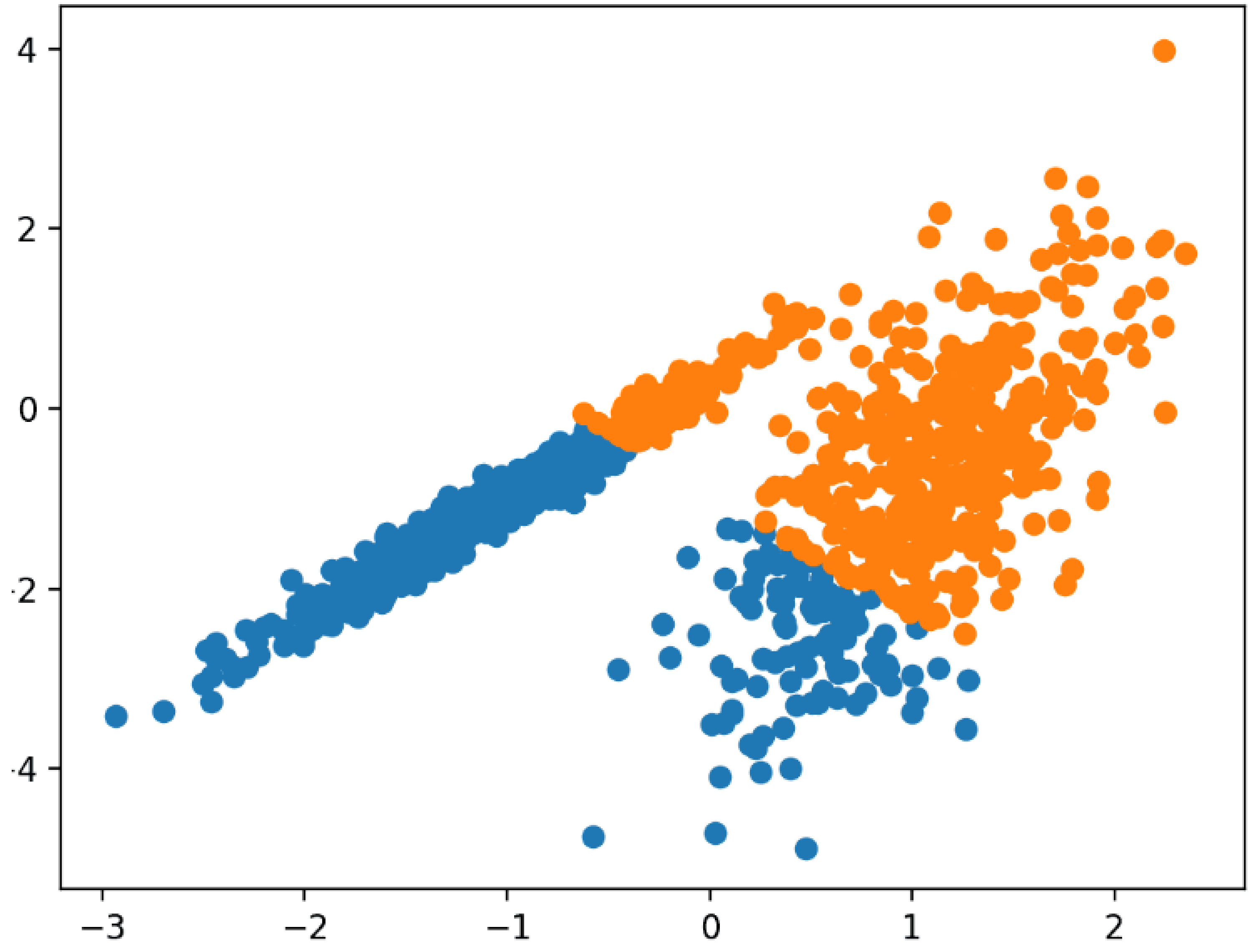


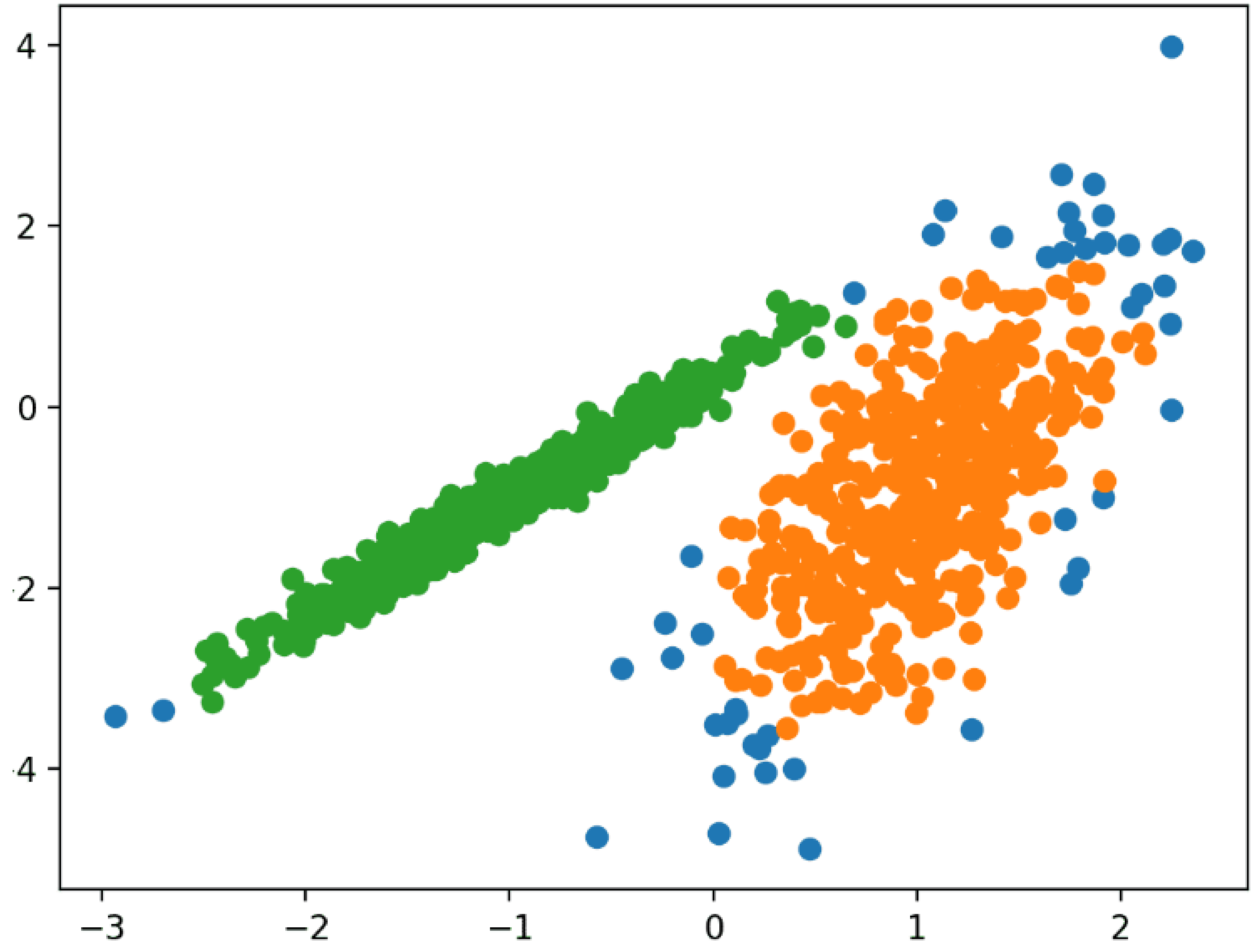
Beyond K-Means & GMM

Clustering for mixed data types

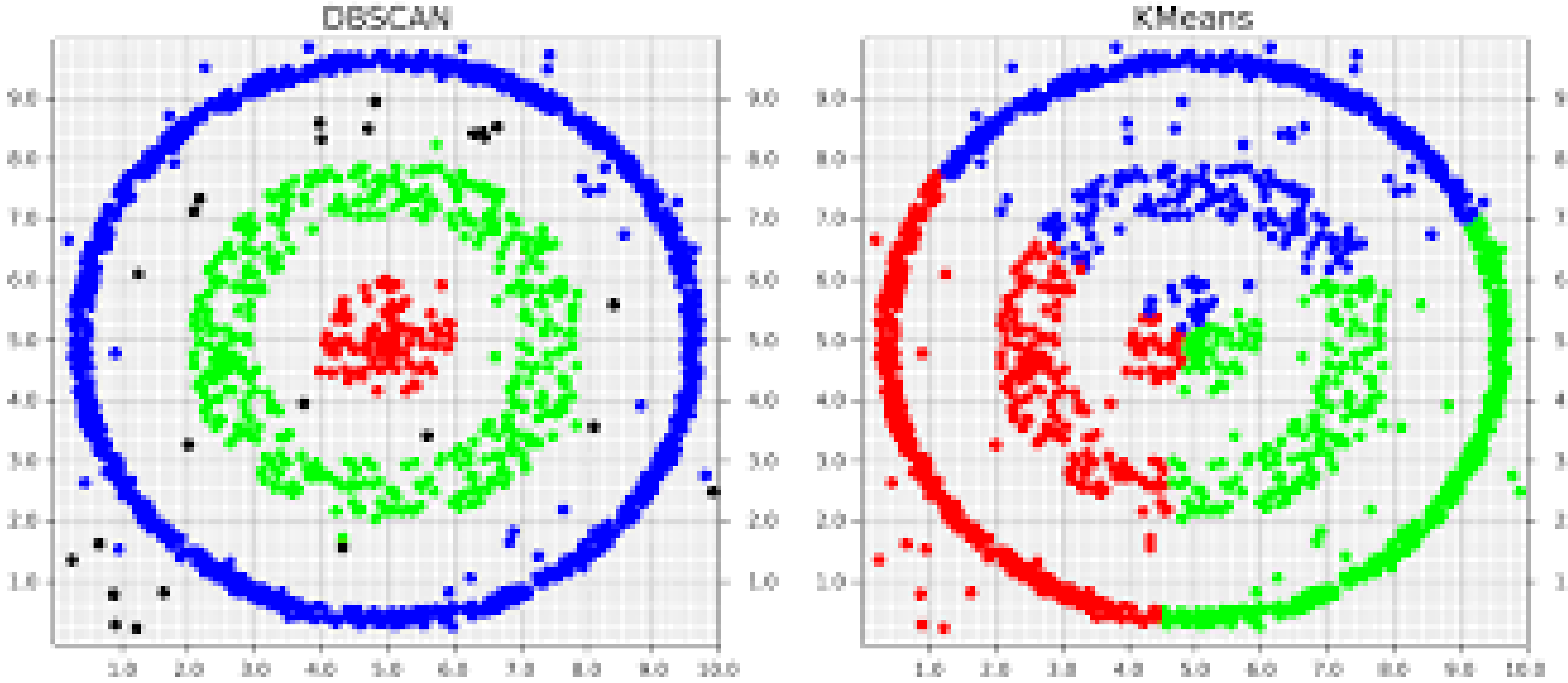
- K-Mode
- K-Prototypes
- K Medoids
  - Gowers distance
    - Manhattan for numeric, Dice for categorical

K-Means cannot handle asymmetric globular data

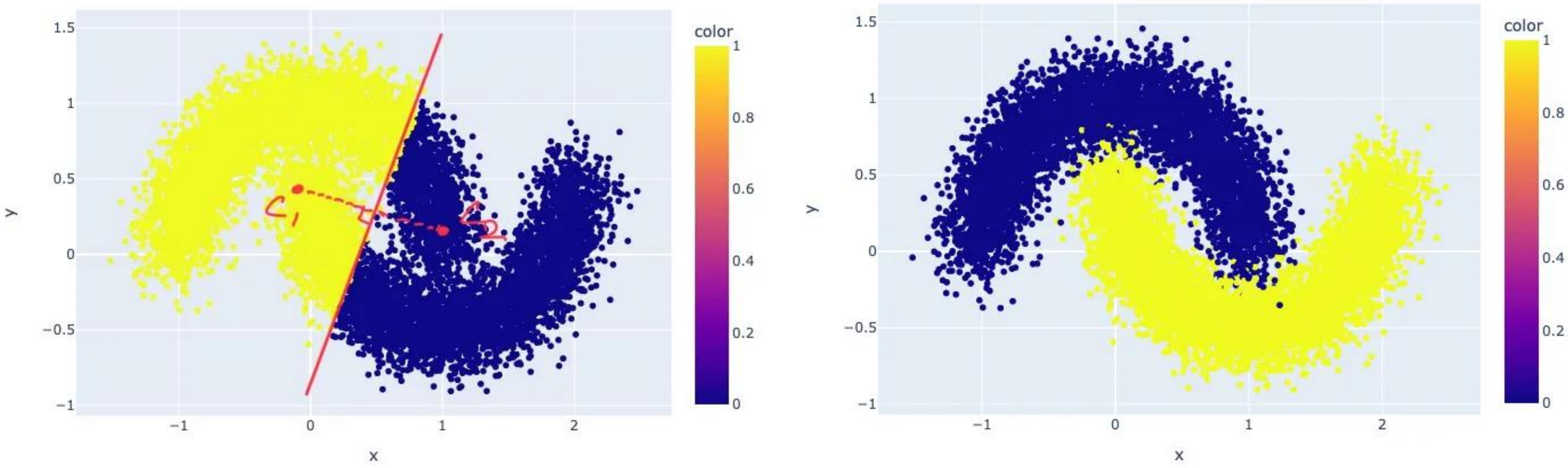




K-Means cannot handle non globular data



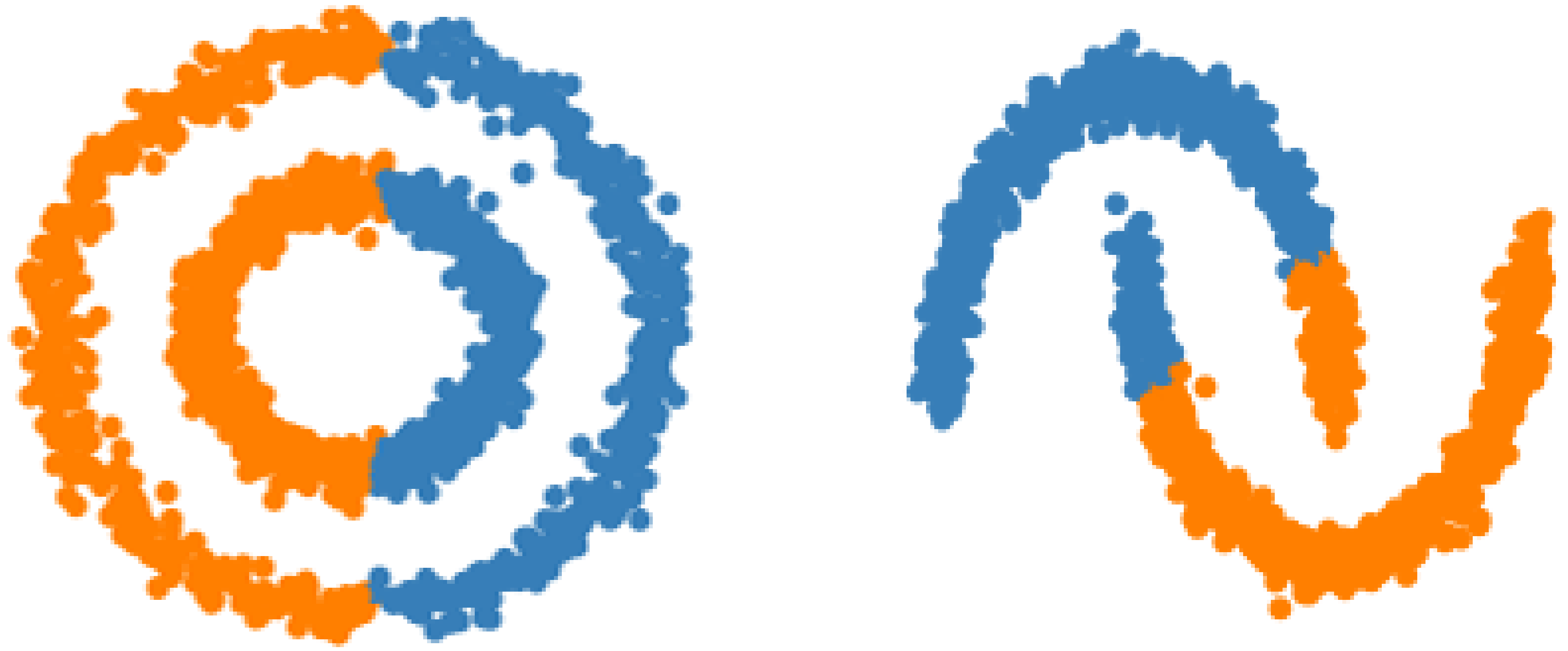
K-Means cannot handle non globular data



K-Means cannot handle non globular data

DBSCAN

k-means



Different types of clustering (optional)

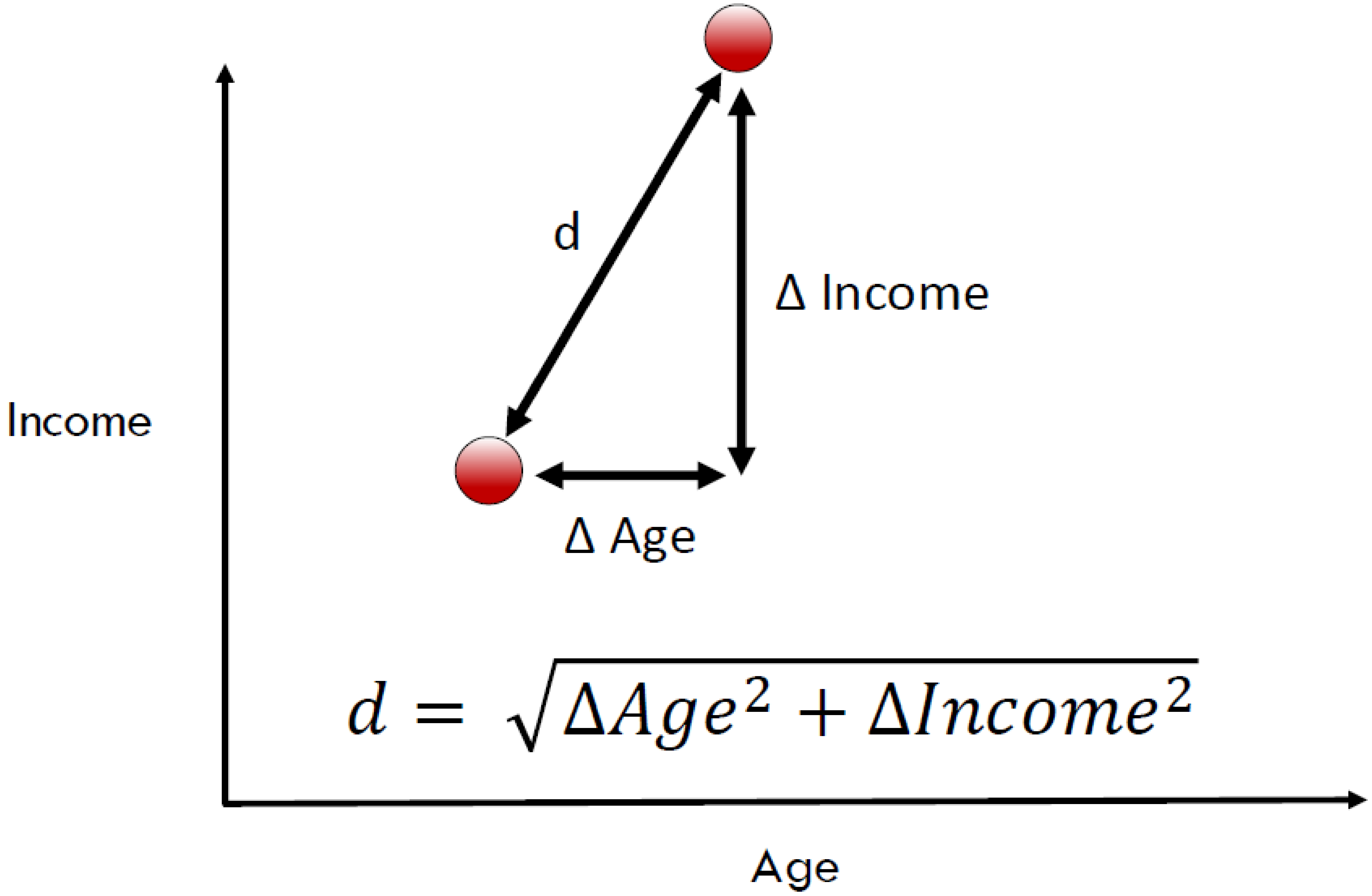
- DBSCAN
  - Some patterns of non globular data, diff metrics
  - NLP clustering, Cosine distance (1-cos theta)
  - DBSCAN Clearly explained Josh Stammer
    - https://www.youtube.com/watch?v=RDZUdRSDOok
  - Evaluation metric is also different (DBCV etc.)
- BIRCH clustering for large datasets
- Mean shift clustering
  - Finds use in unsupervised image segmentation

Case for Distance metrics

- Choice of distance metric is crucial for clustering success
- Also success in any distance based ML method
  - E.g. Nearest Centroid, KNN
- Each metric has strengths and appropriate use cases
  - For e.g. NLP and cosine distance
  - Linear Regression without outliers and Euclidean
- Sometimes metric is chosen by empirical eval (hyperparameter tuning)

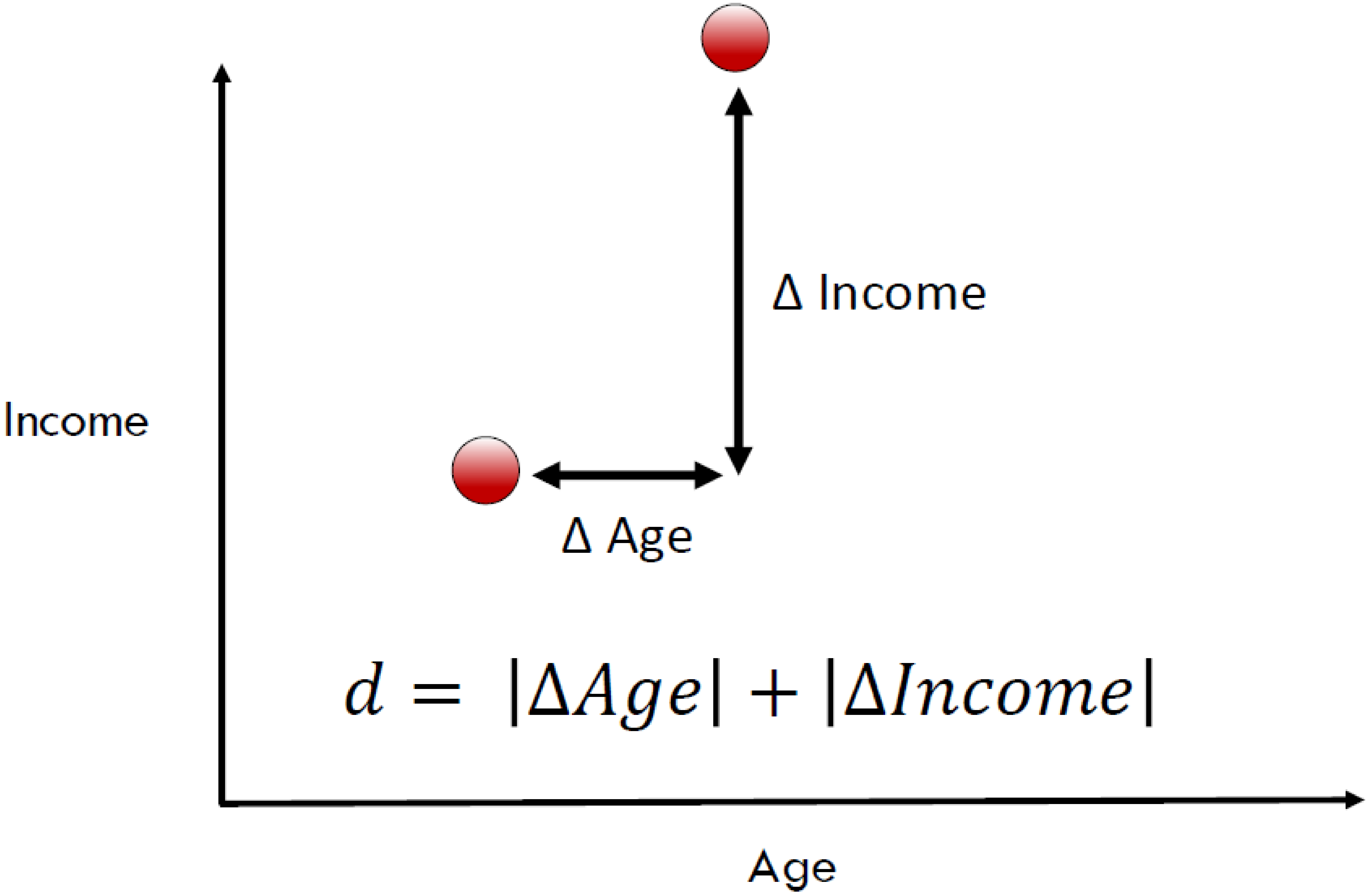
Distance Metric

Euclidean distance



$$d = \sqrt{\Delta Age^2 + \Delta Income^2}$$

Manhattan distance



$$d = |\Delta Age| + |\Delta Income|$$

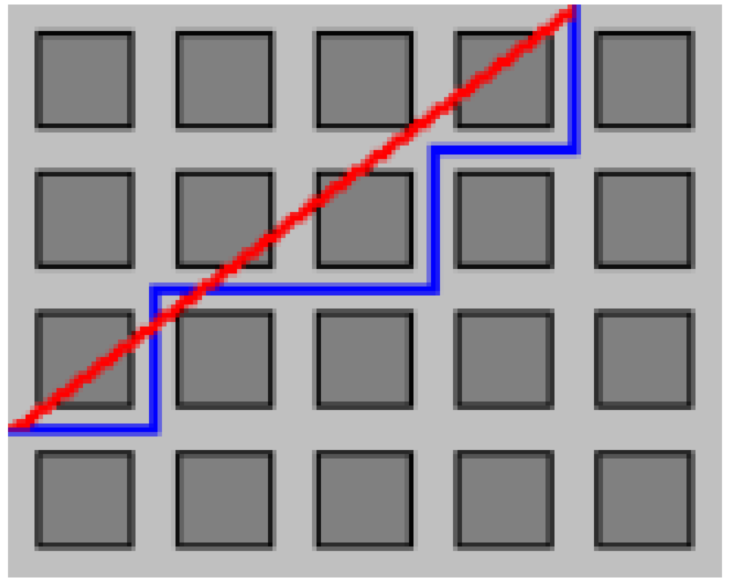
p norm as generalization of Euclidean

- Numerical attribute: Euclidean distance
  - Pros: Symmetrical, Spherical
  - Cons: Sensitive to extreme value of any single attribute

$$\mathcal{D}(x, x') = \sqrt{\sum_{i=1}^{d} (x_i - x'_i)^2}$$

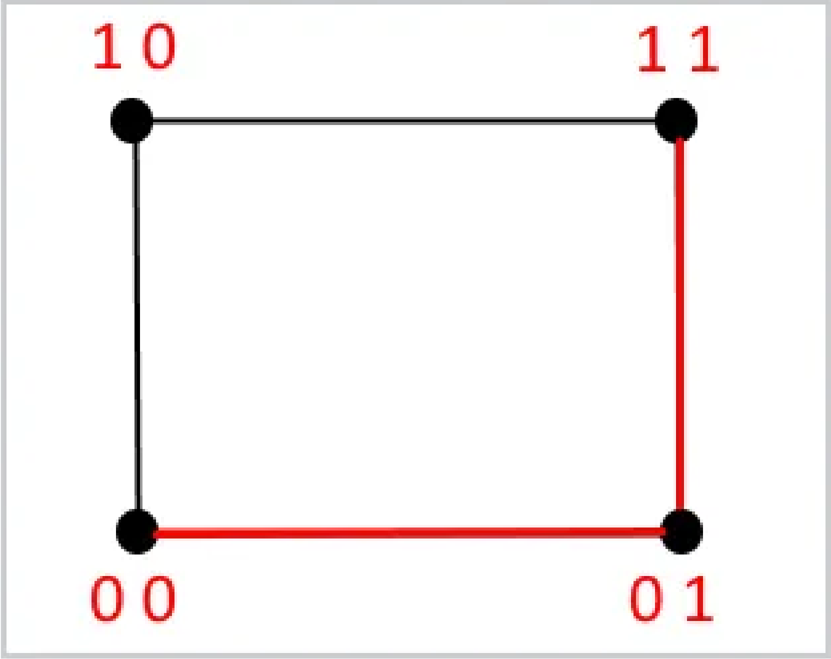
- Minkowski distance (p-norm)
  - P=1 Manhattan, p=2 Euclidean

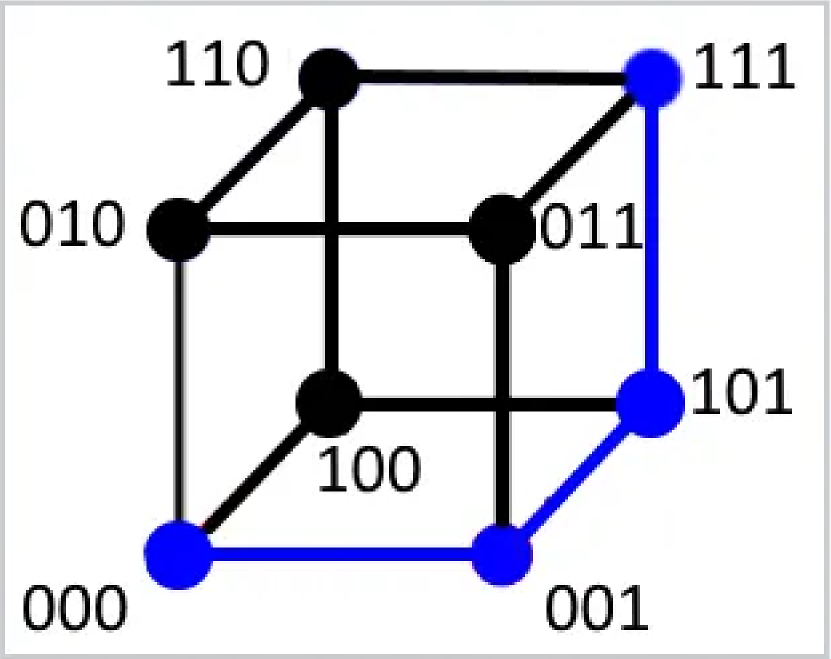
$$\mathcal{D}(x, x') = \sqrt[p]{\sum_{i=1}^{d} |x_i - x'_i|^p}$$



Default choice of distance

- Categorical attribute: Hamming distance
  - Number of attributes where x, x’ differ
  - Best for categorical attributes





$$\mathcal{D}(x, x') = \sum_{i=1}^{d} \mathbb{I}_{x_i = x'_i}$$

Special case of One Hot encoded feature

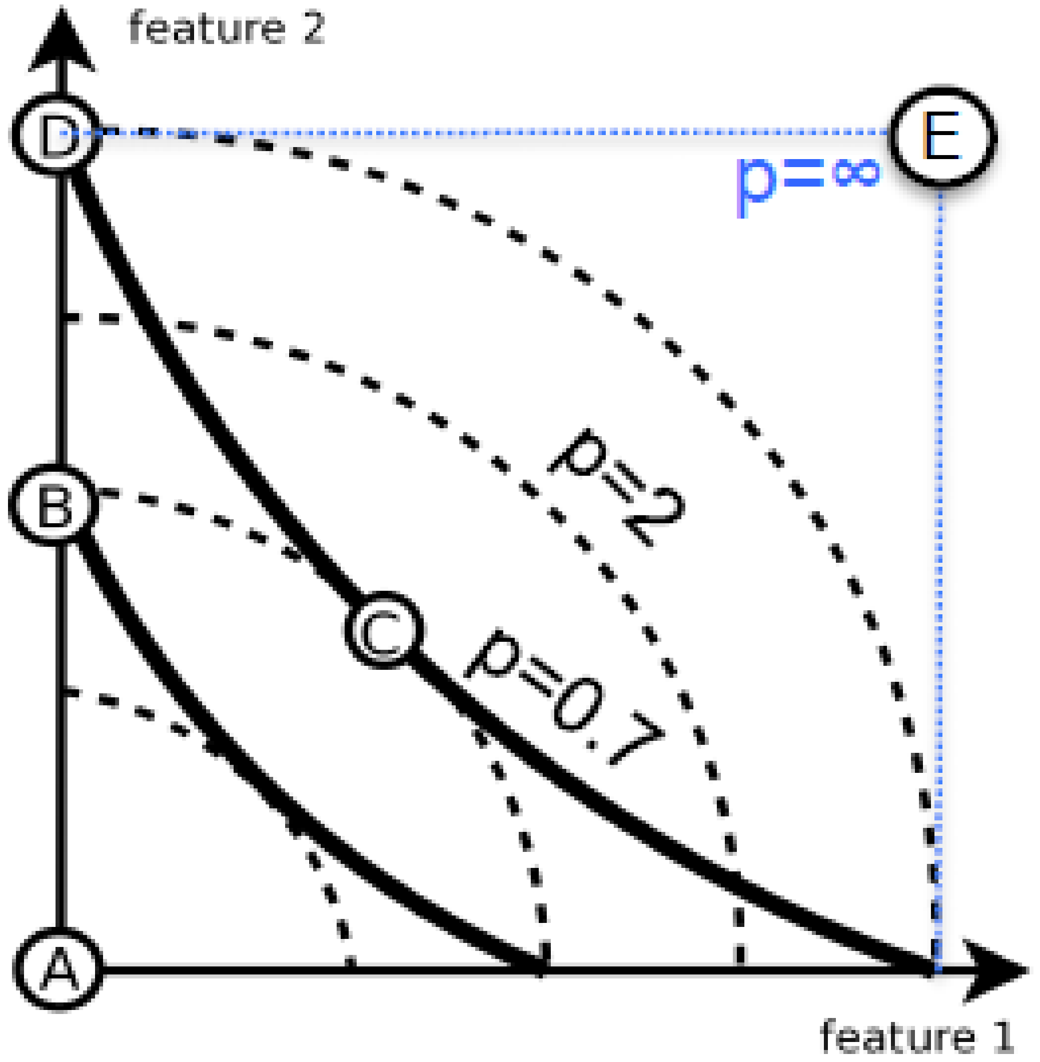
Category	F1	F2	F3
Low	0	0	1
Medium	0	1	0
High	1	0	0

$$\mathcal{D}(x, x') = \sum_{i=1}^{d} |x_i - x'_i|$$

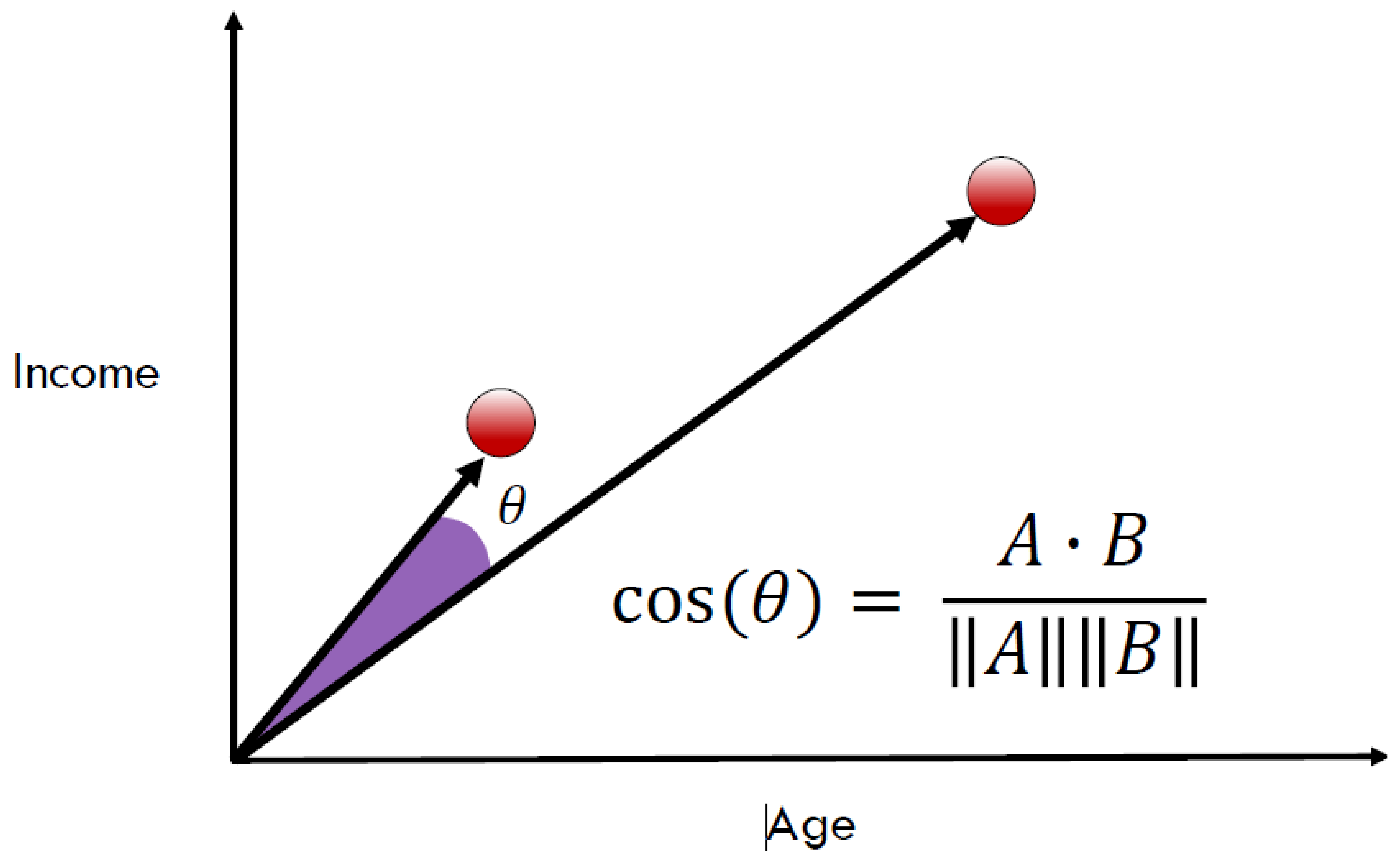
p norm for different p

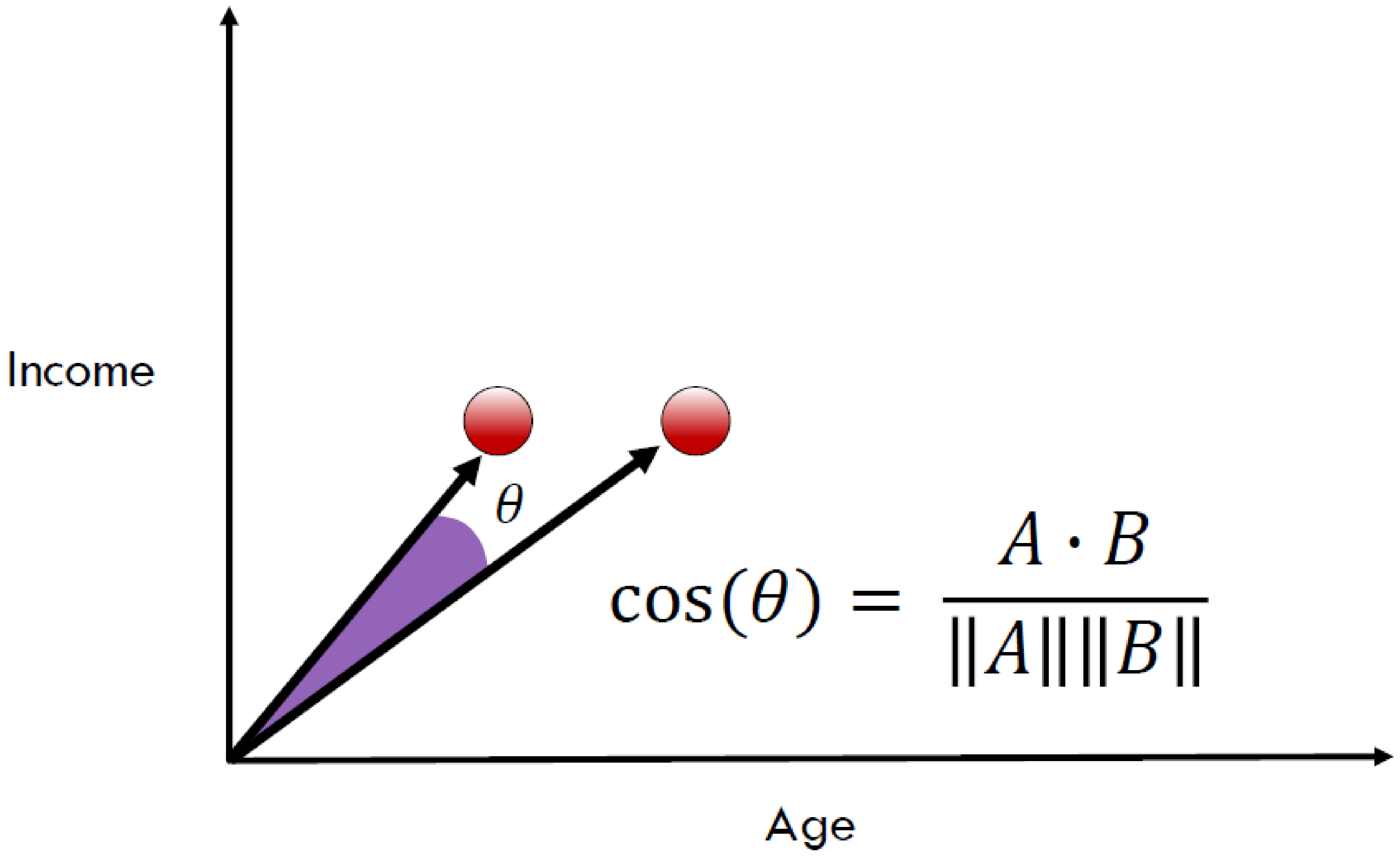
- Minkowski distance (p-norm) p=0
  - When x not equal to x'
  - When x equal to x'
  - Behaves like Hamming distance
- P=infinity $\mathcal{D}(x, x') = max_d |x_i - x'_i|$
- Different p

$$\mathcal{D}(x, x') = \sqrt[p]{\sum_{i=1}^{d} |x_i - x'_i|^p}$$



Cosine similarity & Cosine distance





- Euclidean distance does not matter
- Angular separation matters (e.g. NLP)
- A theta decreases Cosine similarity increases
- Cosine distance $= 1 - cos\theta$

Jaccard similarity & Jaccard distance

- Applies to set similarity, community similarity

Sentence A: "I like chocolate ice cream."

set A = {**I**, like, **chocolate**, ice, **cream**}

Sentence B: "Do I want chocolate cream or vanilla cream?"

set B = {Do, **I**, want, **chocolate**, **cream**, or, vanilla}

- Jaccard similarity $= \frac{A \cap B}{A \cup B} = \frac{3}{9}$

- Jaccard distance $= 1 - \frac{A \cap B}{A \cup B} = 1 - \frac{3}{9} = \frac{6}{9}$

Custom distance metrics

- Always non negative $\|x_1 - x_2\| >= 0$
- $\|x_1 - x_2\| = 0 \iff x_1 = x_2$
- $\|x_1 - x_2\| = \|x_2 - x_1\|$
- Triangle inequality $\|x + y\| <= \|x\| + \|y\|$

Intuitively true: Sides of triangle

- Should satisfy all of the above (generally speaking)

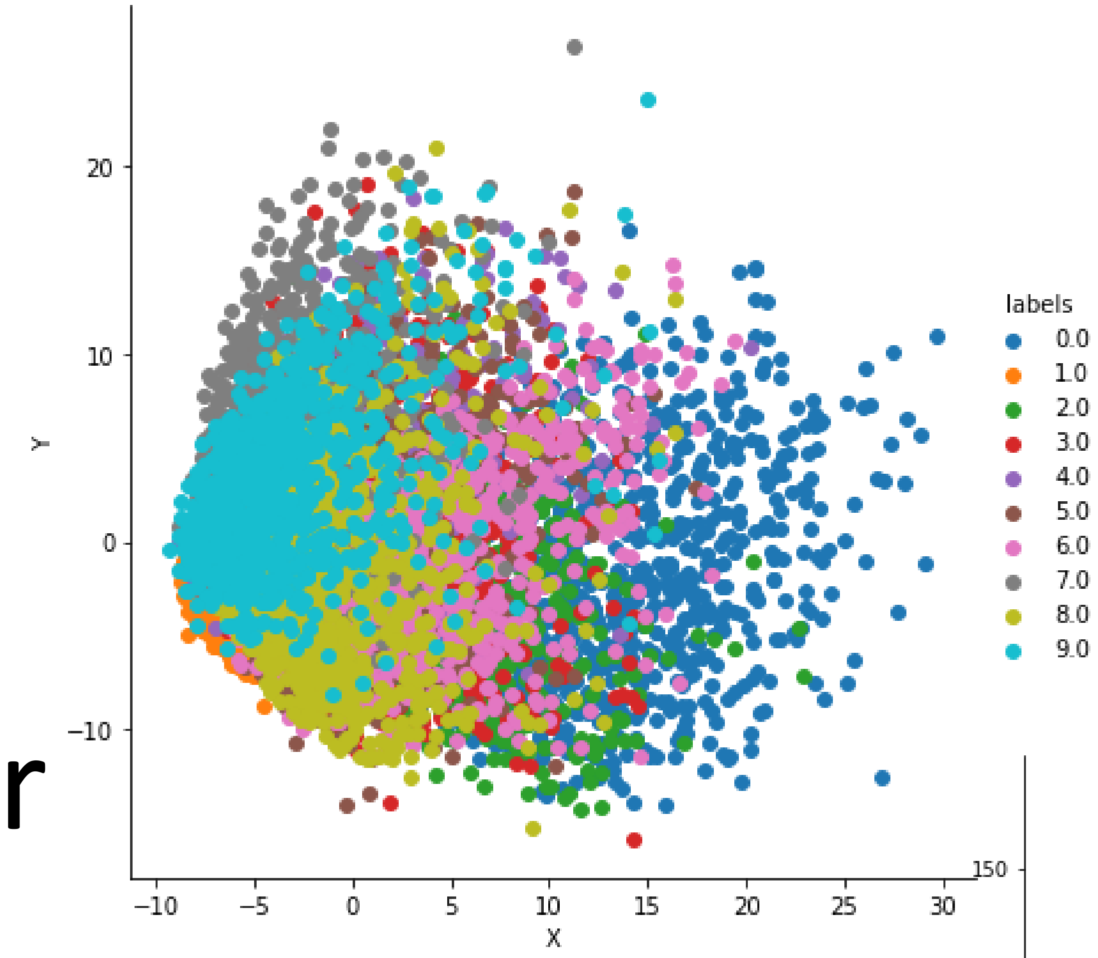
Distance metrics in sklearn

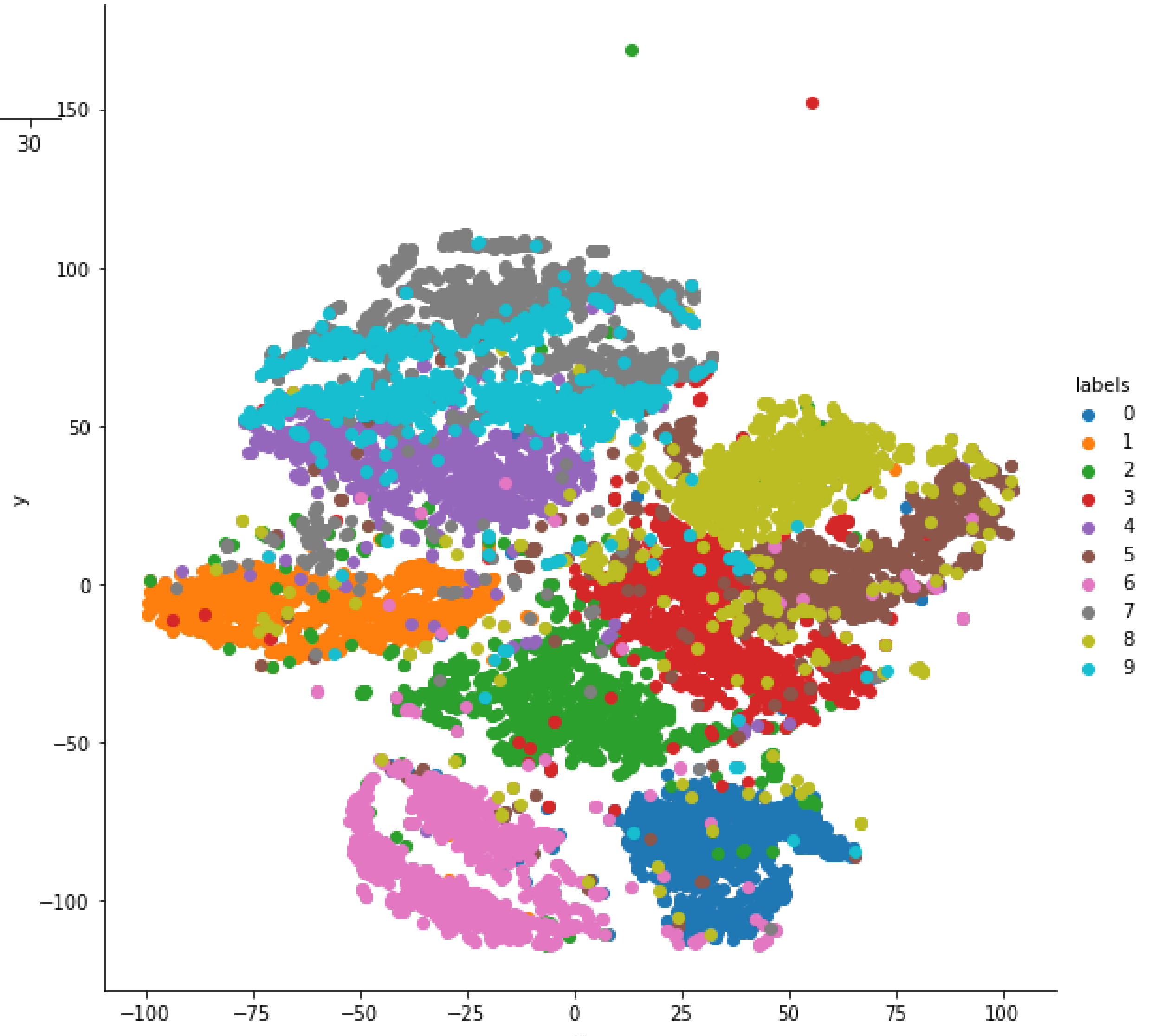
- from sklearn.metrics import pairwise_distances
- dist = pairwise_distances(X, X’, metric=“”)
- metric = euclidean, manhattan, cosine, jaccard

Dimensionality Reduction + Clustering for visualization (optional)

Dimensionality reduction

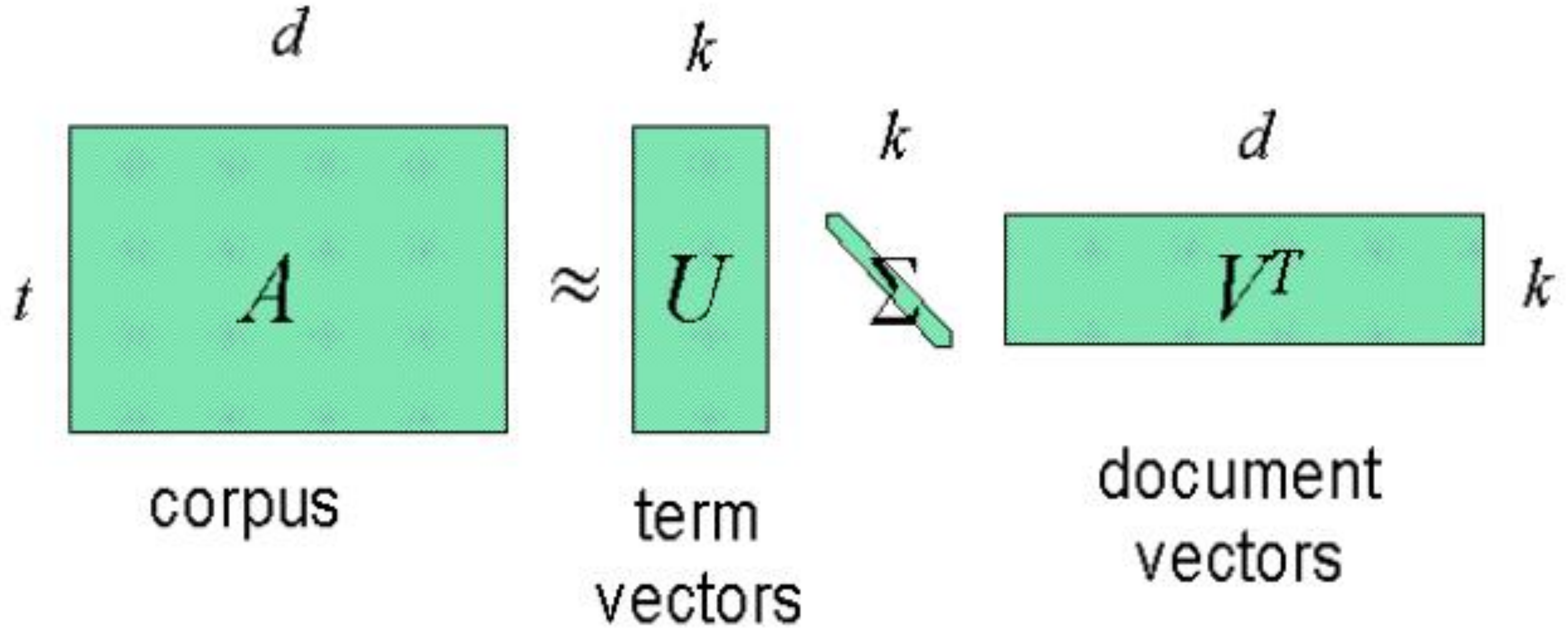
- Apply dimensionality reduction
  - PCA
  - T-SNE
- Then clustering in 2-D or 3-D
- E.g. PCA and t-SNE with MNIST for 2D clustering
  - Notice t-SNE gives better cluster separation





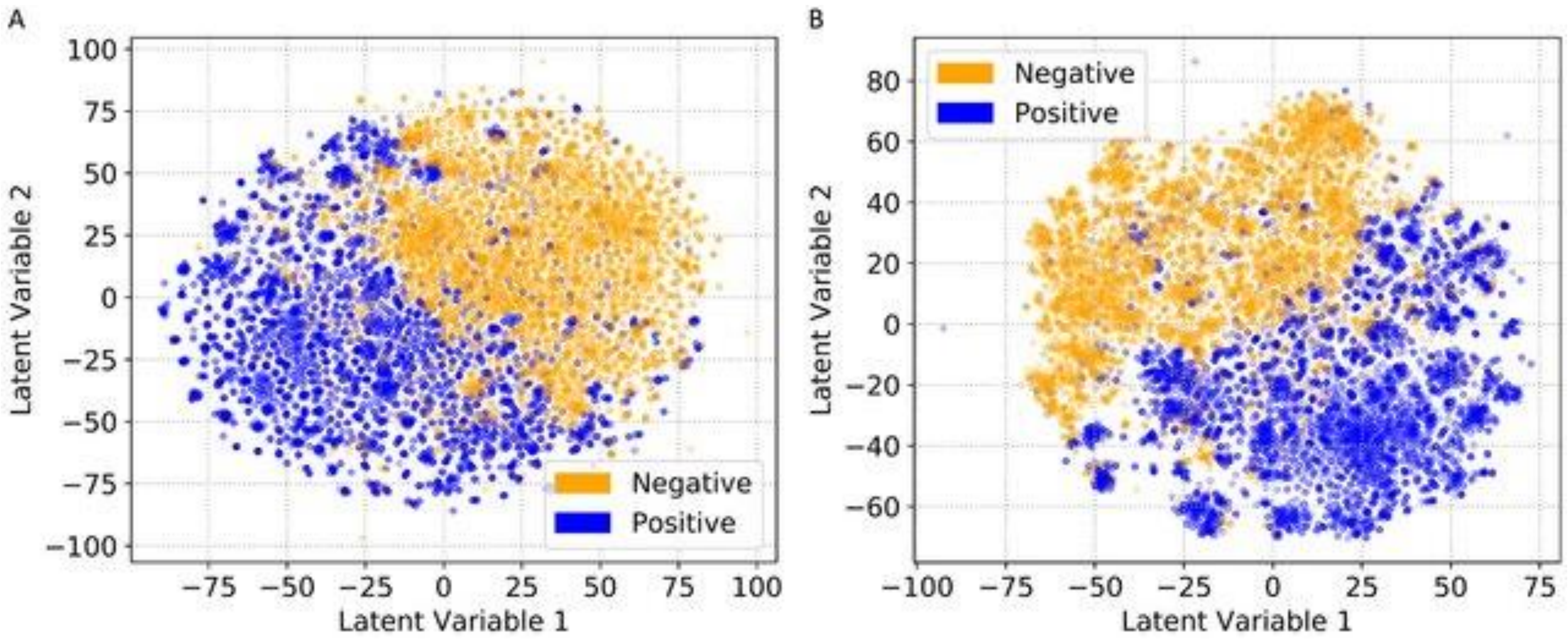
Dimensionality reduction

- Truncated SVD
  - Sparse Matrix cases (such as TF-IDF)



Clustering after dim reduction

- Truncated SVD
  - Sparse Matrix cases (such as TF-IDF)




QUESTIONS