Unsupervised learning & Mixture models

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The Machine Learning Landscape

scikit-learn

Machine Learning in Python

- Simple and efficient tools for data mining and data analysis
- Accessible to everybody, and reusable in various contexts
- Built on NumPy, SciPy, and matplotlib
- Open source, commercially usable - BSD license

Classification

Identifying to which category an object belongs to.

Applications: Spam detection, Image recognition.
Algorithms: *SVM*, *nearest neighbors*, *random forest*, ... — *Examples*

Regression

Predicting a continuous-valued attribute associated with an object.

Applications: Drug response, Stock prices.
Algorithms: *SVR*, *ridge regression*, *Lasso*, ... — *Examples*

Clustering

Automatic grouping of similar objects into sets.

Applications: Customer segmentation, Grouping experiment outcomes
Algorithms: *k-Means*, *spectral clustering*, *mean-shift*, ... — *Examples*

Dimensionality reduction

Reducing the number of random variables to consider.

Applications: Visualization, Increased efficiency
Algorithms: *PCA*, *feature selection*, *non-negative matrix factorization*. — *Examples*

Model selection

Comparing, validating and choosing parameters and models.

Goal: Improved accuracy via parameter tuning
Modules: *grid search*, *cross validation*, *metrics*. — *Examples*

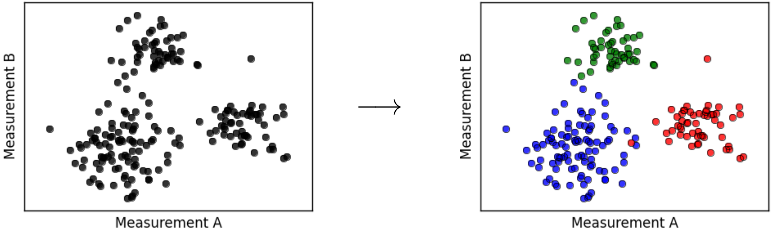
Preprocessing

Feature extraction and normalization.

Application: Transforming input data such as text for use with machine learning algorithms.
Modules: *preprocessing*, *feature extraction*. — *Examples*

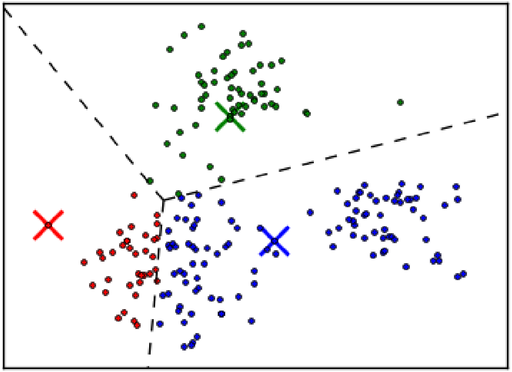
Unsupervised learning

- No labels / no truth: We are not given a target value we want to reconstruct
- Just given the data (usually assumed: low-dimensional measurements with equal noise)
- Main task: Clustering



Clustering: the K-means algorithm

- Assume K clusters, each characterized by a centroid
- Start by randomly choosing K data points as centroids
- Iteratively:
  - Assign each data point to the nearest cluster
  - Compute new cluster center based on assigned data points



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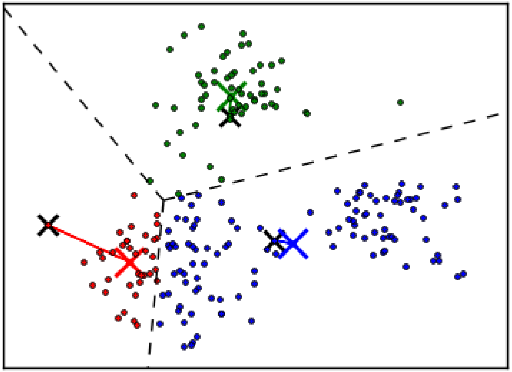

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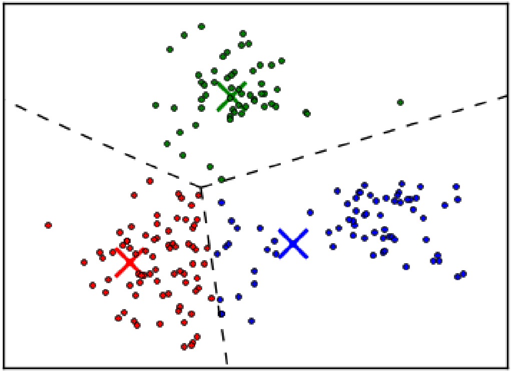

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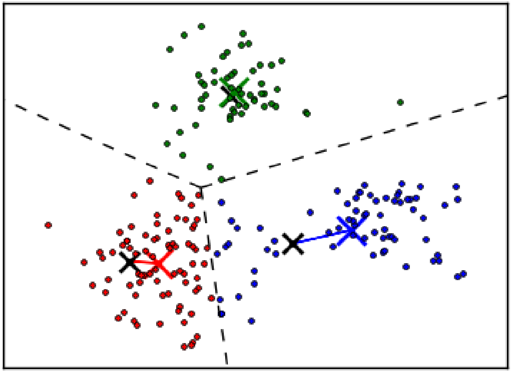

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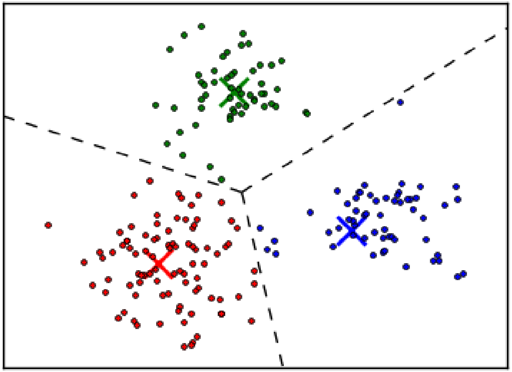

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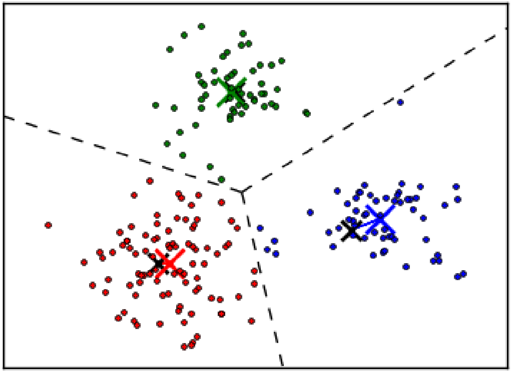

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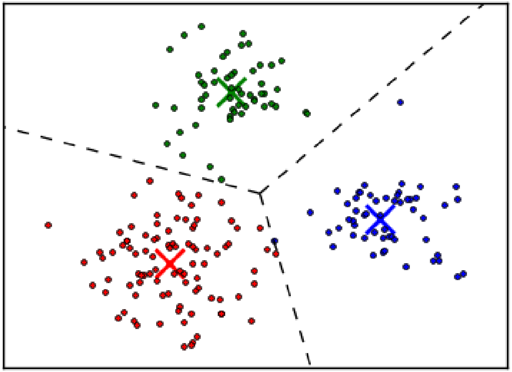

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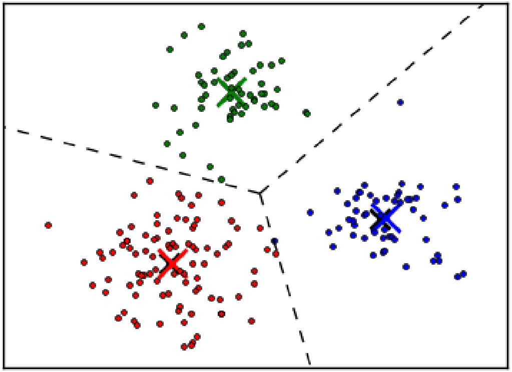

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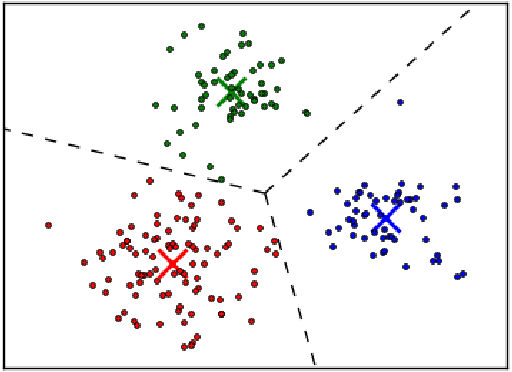

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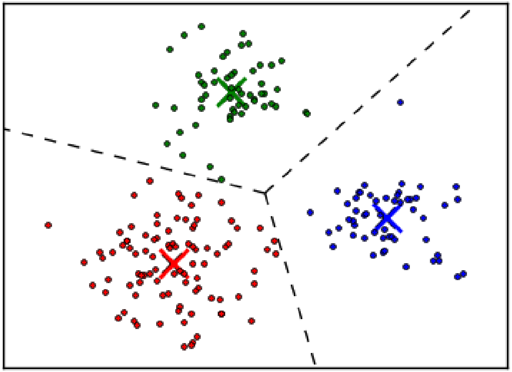

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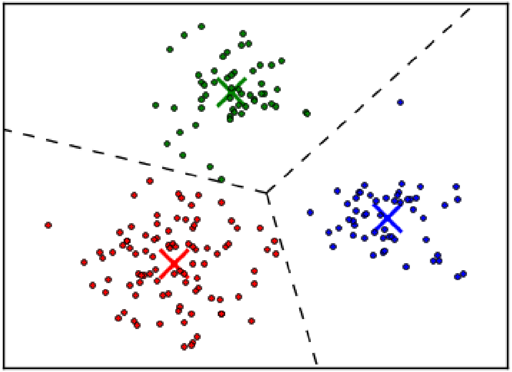

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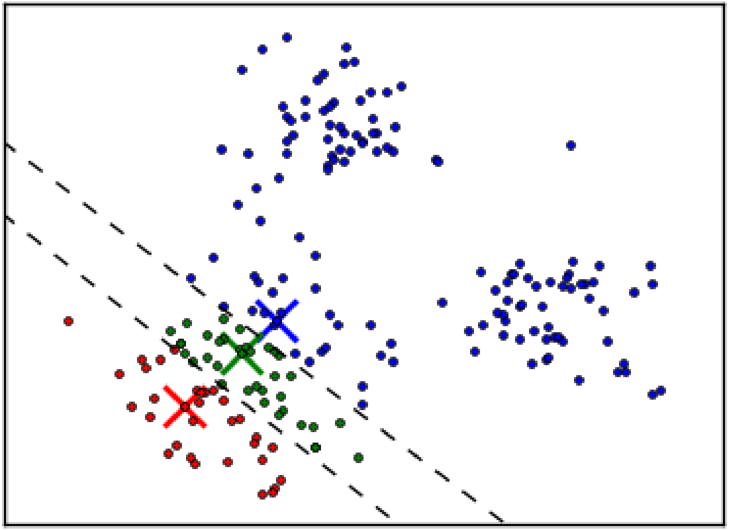
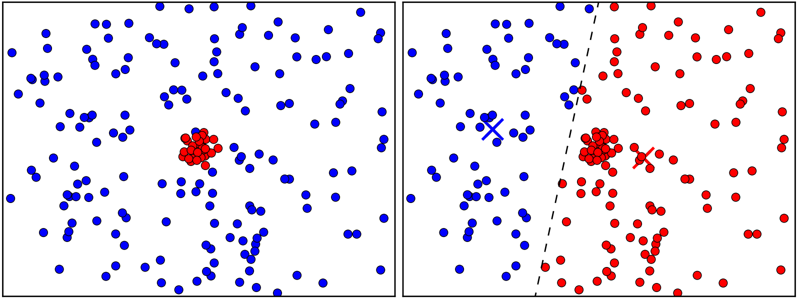


Problems with K-means

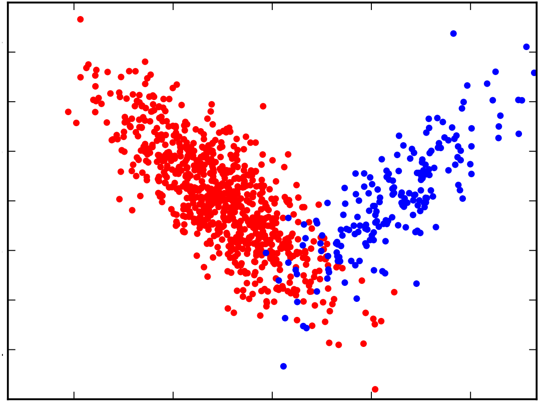
Clusters are defined by centroids alone

- clusters are separated by hyper-planes
- no covariances in the clusters
- no weights for clusters
- data points are hard-assigned to clusters
- noisy measurements not considered
- local optimization (multiple random initializations)



Gaussian Mixture Models

- Instead of finding just centroids, we want to find weights and Gaussians means and covariances of clusters
- Can be optimized efficiently using the Expectation-Maximization (EM) algorithm



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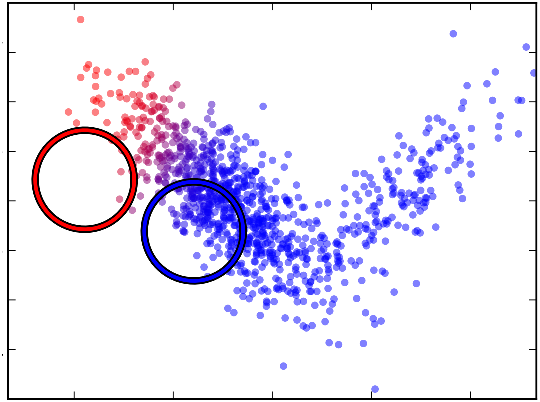

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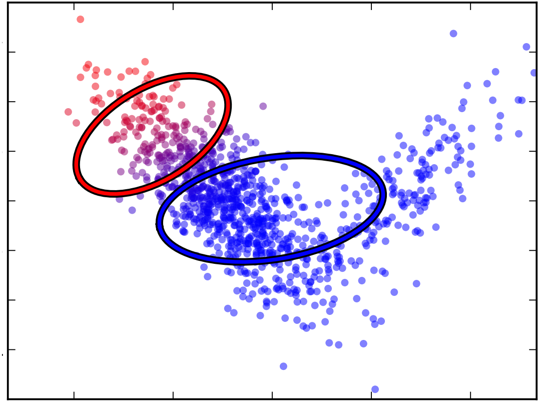

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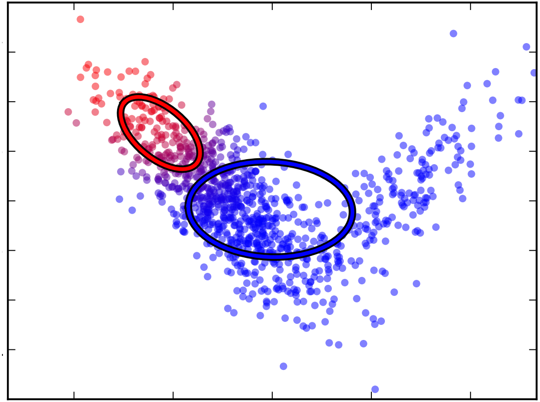

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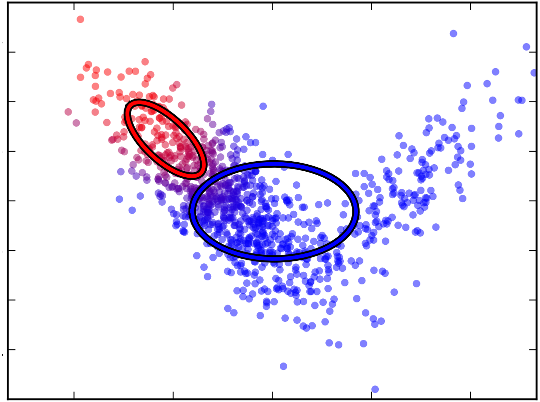

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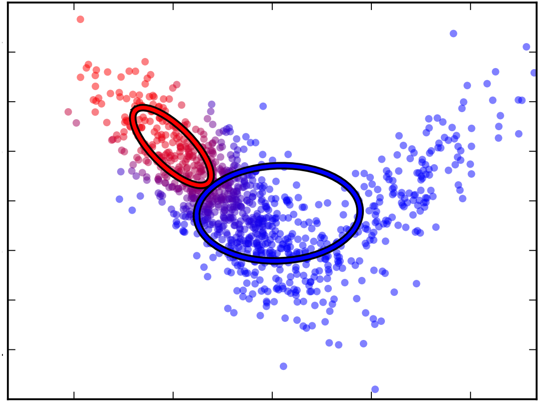

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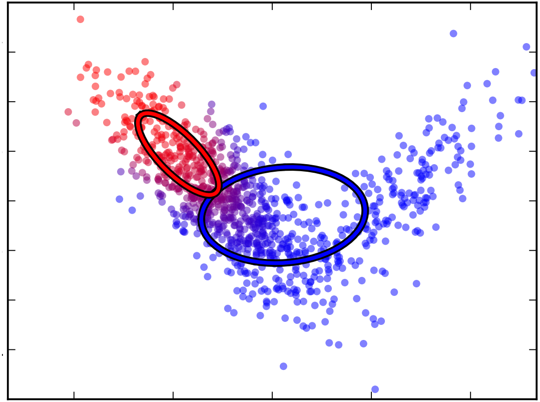

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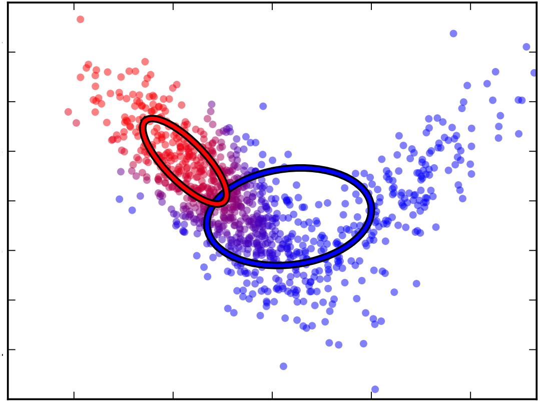

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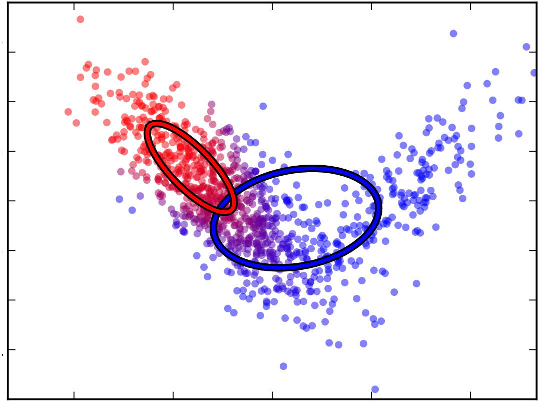

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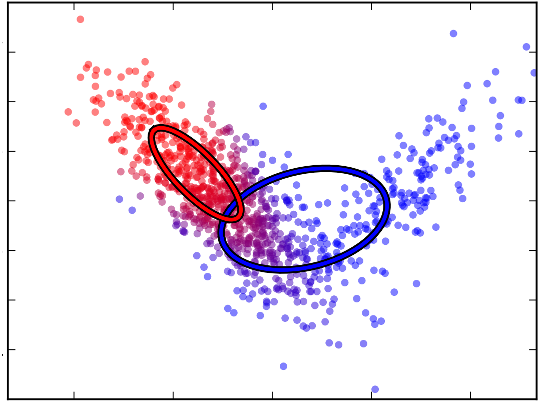

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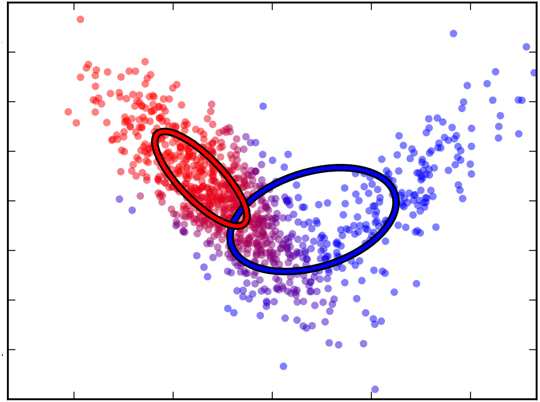

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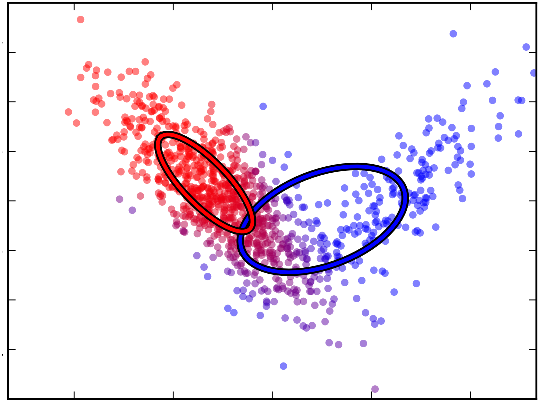

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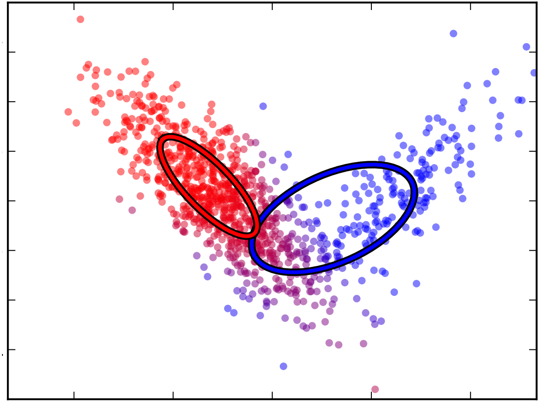

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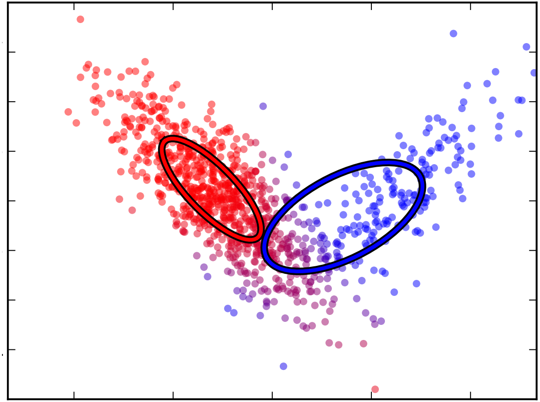

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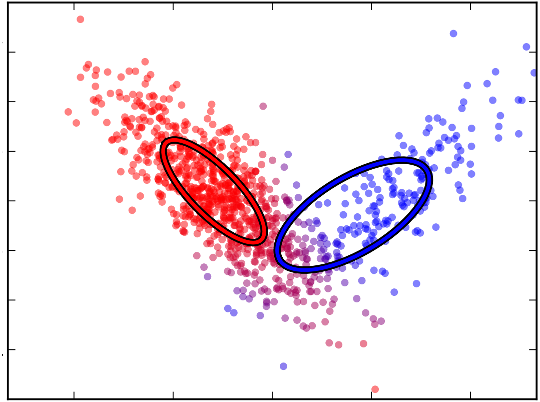

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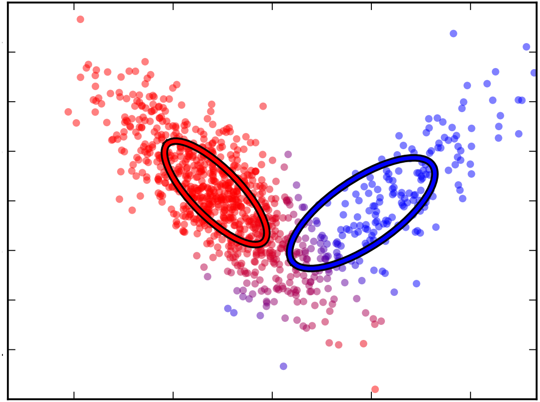

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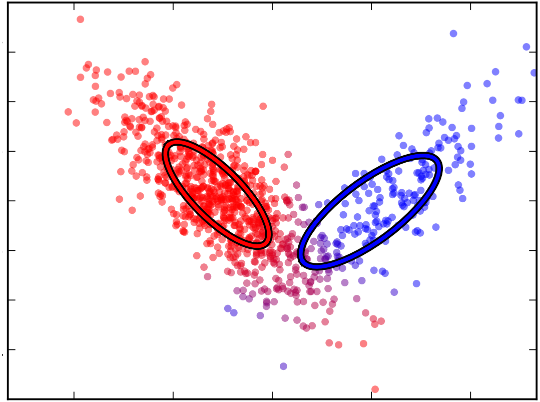

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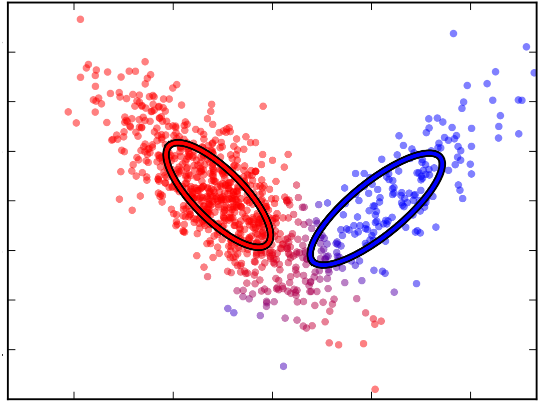

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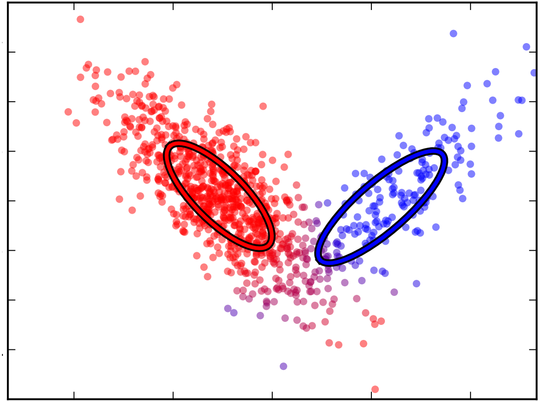

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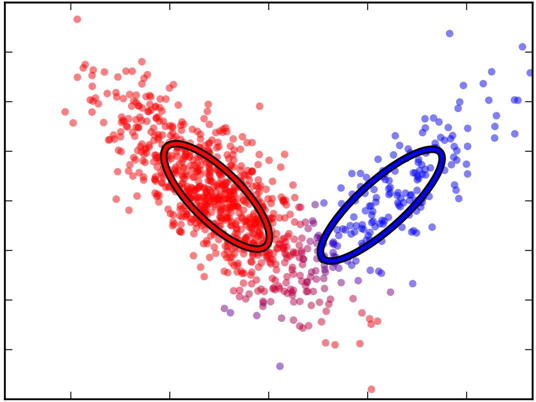

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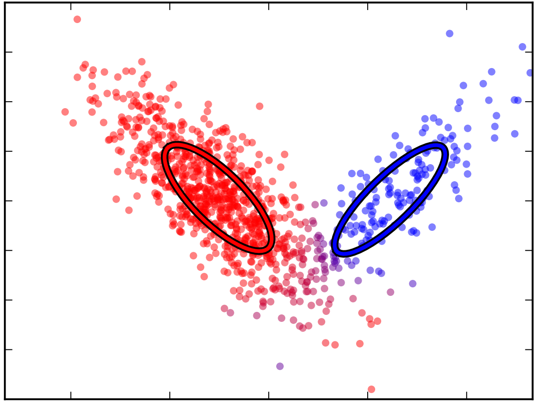

Gaussian Mixture Models / Expectation-Maximization

E-M proceeds by:

- E: compute probability of drawing each data point i from each cluster or component k:

  $$z_{i,k} = a_k \, \mathcal{N}(x_i \,|\, \mu_k, \Sigma_k)$$

  where a_k is the cluster weight, and μ_k,Σ_k are its mean and covariance.
- M: compute new component weights and parameters, weighting by *relative* component-weights

Gaussian Mixture Models / Expectation-Maximization

- E-M "update equations" (M step) for Gaussian mixtures:

$$z'_{i,k} = \frac{z_{i,k}}{\sum_k z_{i,k}} \tag{1}$$

$$a'_k = \sum_k z'_{i,k} \tag{2}$$

$$\mu'_{i,k} = \frac{1}{a'_k} z'_{i,k} x_i \tag{3}$$

$$\Sigma'_{i,k} = \frac{1}{a'_k} z'_{i,k} (x_i - \mu_k)(x_i - \mu_k)^T \tag{4}$$

Mixture Models / Foreground-Background Models

- Often, junk or interlopers can get into your sample (of galaxies, stars, etc)
- If not dealt with, can strongly skew results (outliers)
- Model the objects you don't care about (background) as well as the ones you do care about (foreground)
- Background model can be a regular Gaussian component, or a flat (uniform) probability distribution

Problems with Gaussian Mixture Models

- Choosing the number of components
- Measurement noise not considered
- Local optimization