Clustering Algorithms and High Dimensional Data

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December 4th, 2019

Outline

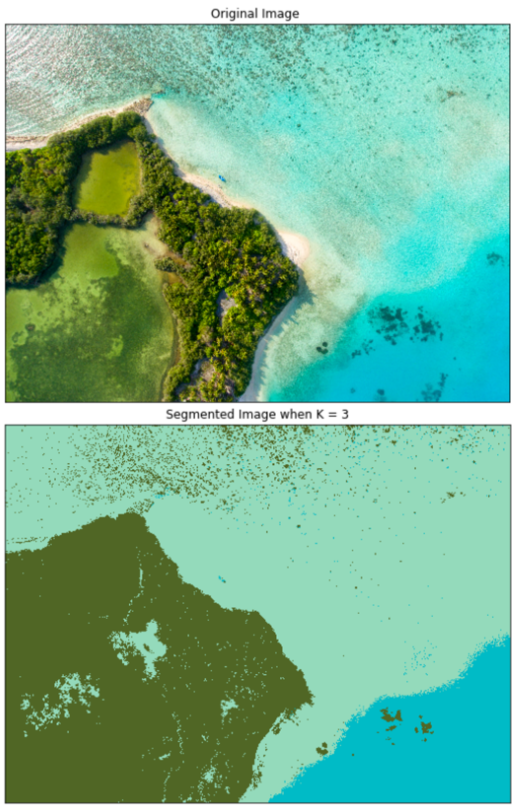
Introduction

Given a set of data-points, the goal of clustering is to group similar points together and have a high dissimilarity between the groups.

A data-point is characterized by a feature vector $X = \{x_1, x_2, ..., x_d\}$, where d is its dimension.

Various notions of similarity:

- Distance between objects
- Density around a given point
- Distribution of features



[1]

[1] https://towardsdatascience.com/introduction-to-image-segmentation-with-k-means-clustering-83fd0a9e2fc3

K-Means

Goal: Partition the data into k sets, so as to minimize the squared distances between points within a cluster.

K-Means

Parameters: *num_clusters*

```
Initialize num_clusters cluster centers
assign points to cluster based on nearest center
while not centres converged do
    Recalculate centers
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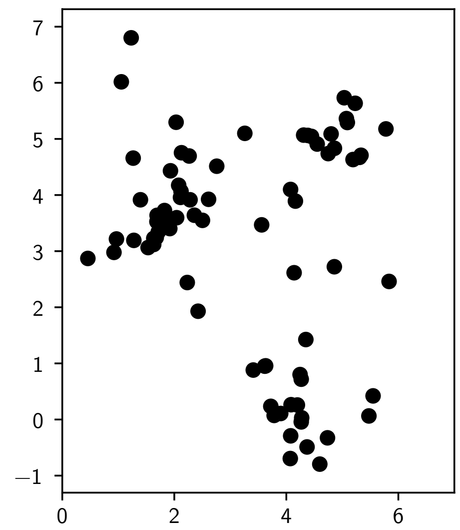

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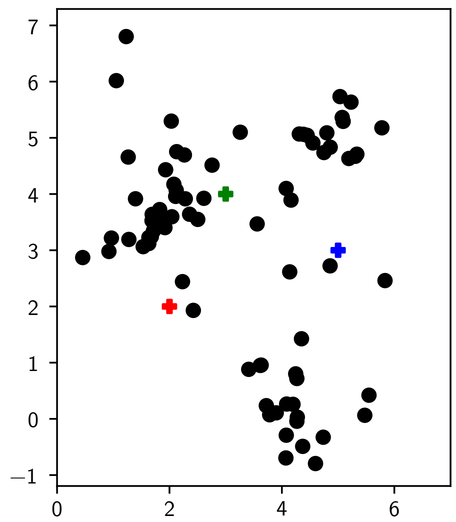

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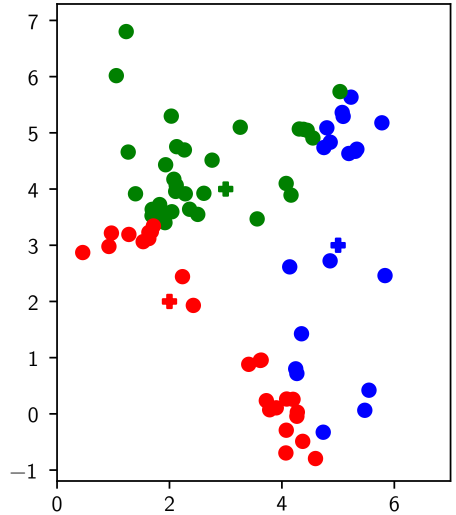

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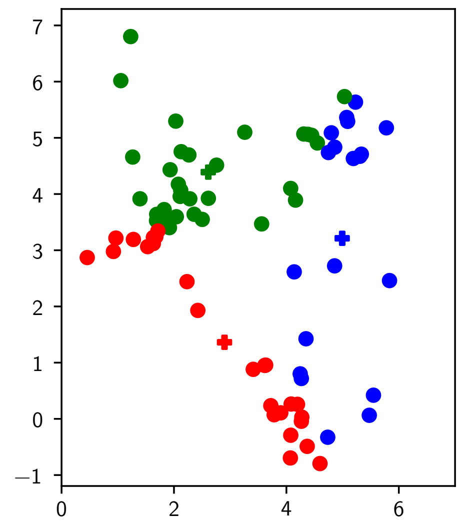

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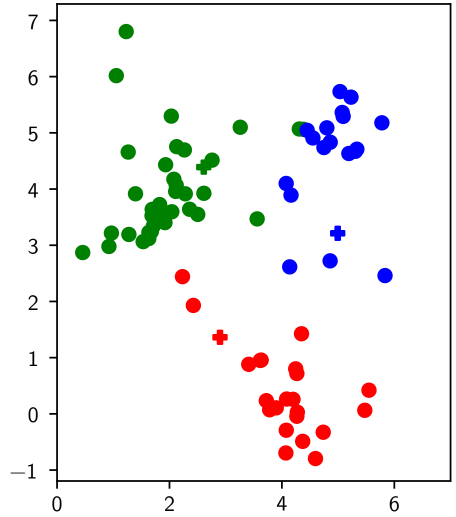

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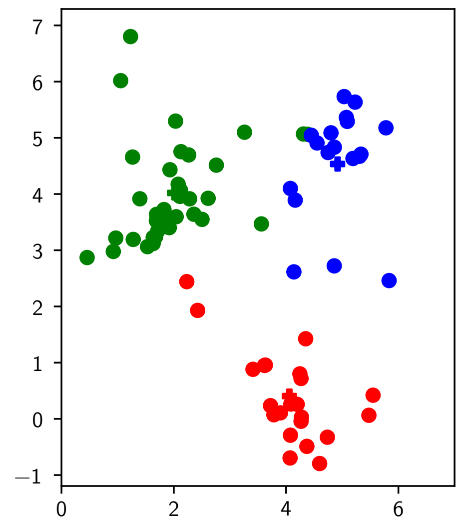

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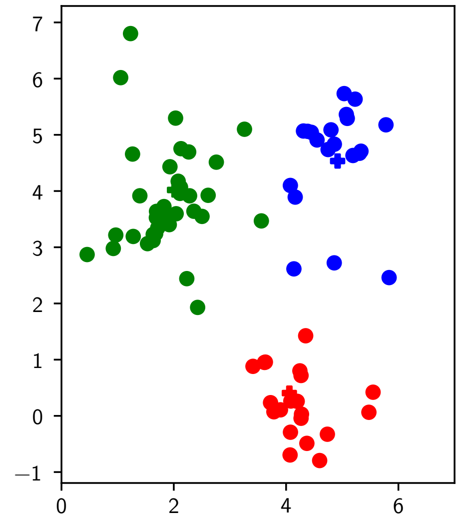

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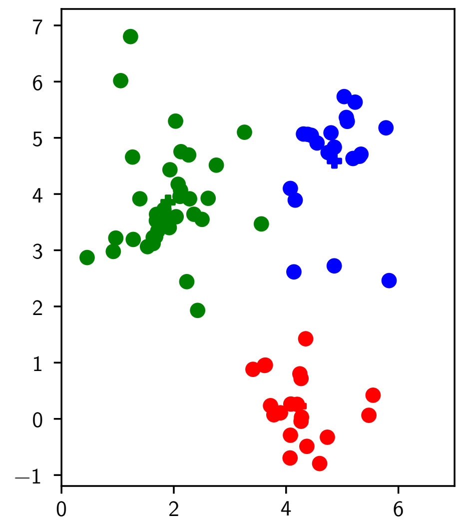

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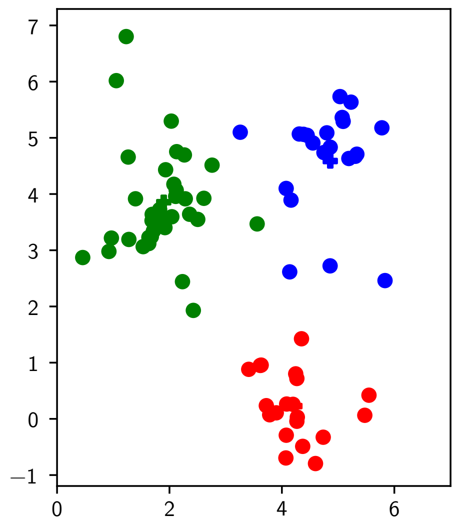

K-Means

- Number of clusters is an input parameter
- Based on a notion of distance
- Tends to find spherical clusters of the same size
- Unstable with respect to initial starting points

DBScan

Goal: Find connected regions in space that are highly populated.

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[a] Chire, CC BY-SA 3.0,
https://commons.wikimedia.org/w/index.php?curid=17045963

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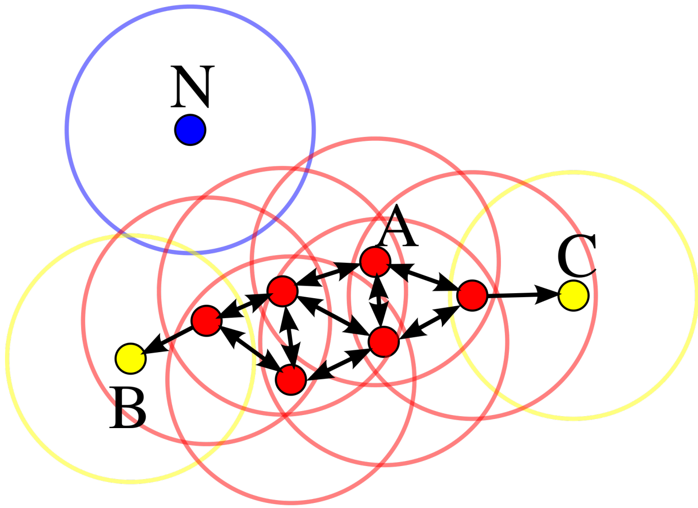
- Core points: Have at least *minPts* neighbors within distance *eps*
- Directly reachable points: At least one core point within distance *eps*



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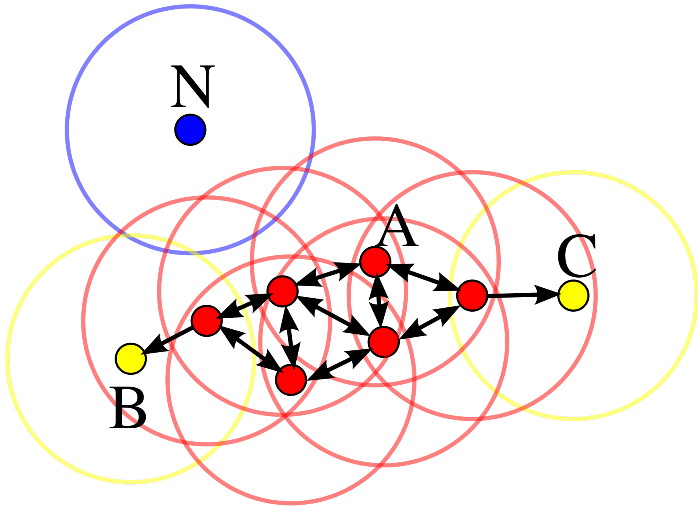

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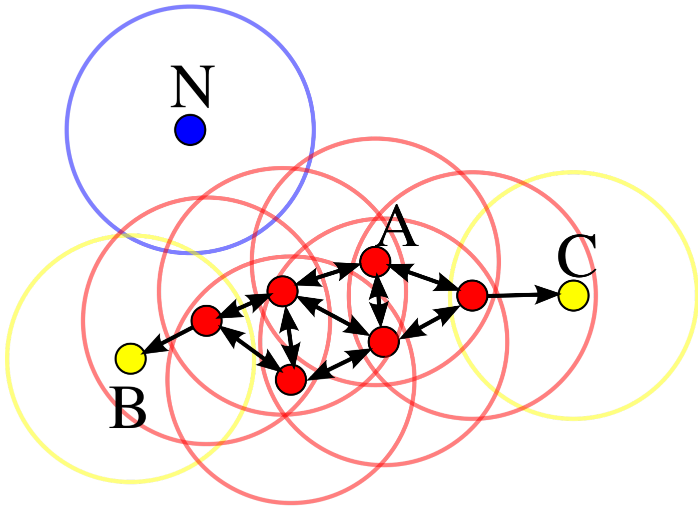

B is reachable from A, if there exists a path of following directly reachable points.
B and C are density connected if, they are reachable from a common point A.

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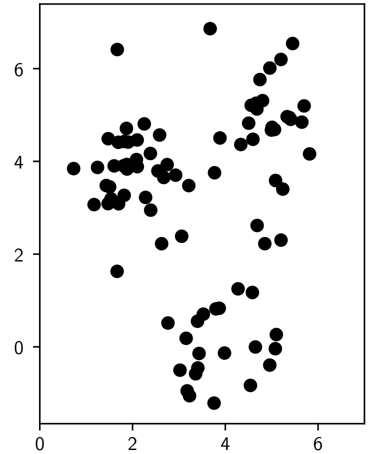
DBScan

Parameters: *minPts*, *eps*

1. Find all neighbors closer than *eps* of every point
2. Identify core points with more than *minPts* neighbors
3. Create clusters of neighboring core points
4. Assign the remaining points to a nearby cluster or noise



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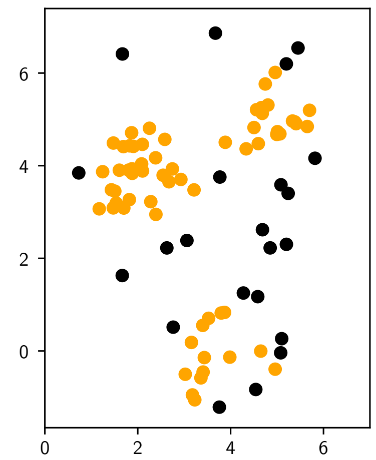

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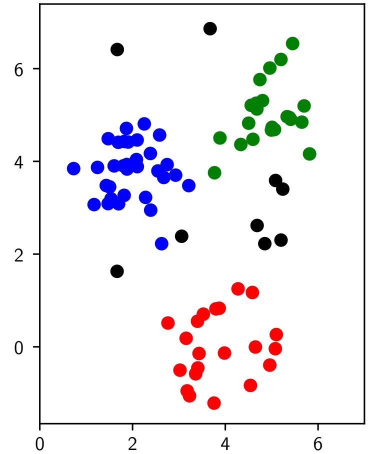

DBScan

- Groups by point density in a neighborhood that is controlled using input parameters
- Finds arbitrarily shaped clusters
- Has a notion of noise
- Generally stable between runs
- Parameters require knowledge of the data

The Curse of Dimensionality

Data quickly becomes sparse in high dimensions:

- Consider a problem with 50 dimensions of binary features and 10^{12} observations.
- Then we still only have examples for $\frac{10^{12}}{2^{50}} \approx 0.089\%$ of categories.

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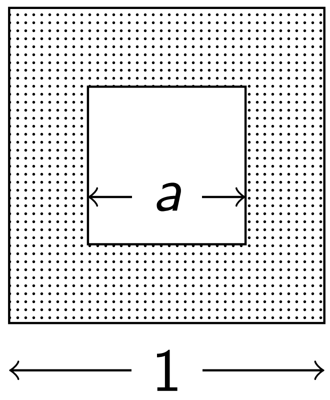
Problem 1: It becomes impossible to correctly estimate distributions.

The Curse of Dimensionality

Our intuition fails in higher dimensions:

- Consider uniformly distributed data on a cube in d dimensions with side length 1.
- How big can we make a so that more than 95% of the probability mass lies inside the dotted region?



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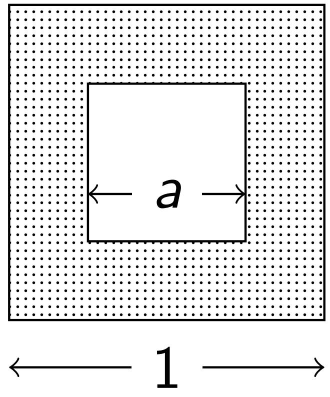

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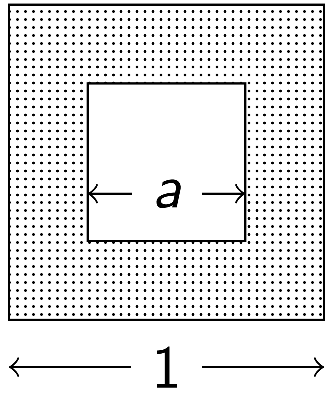

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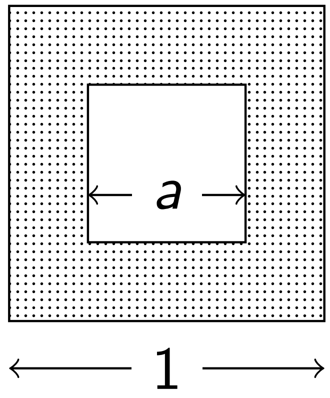

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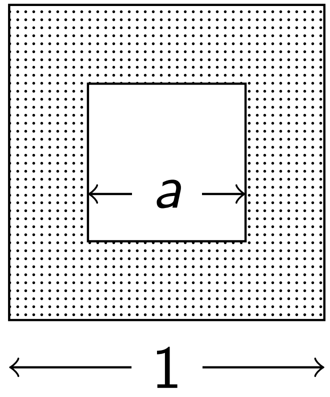

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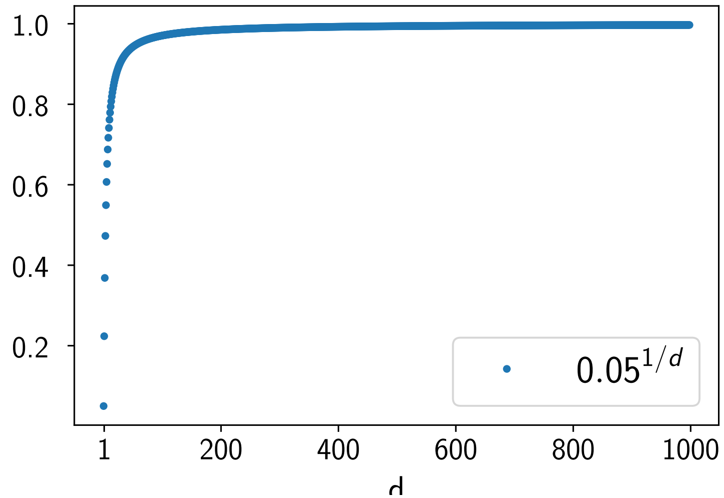

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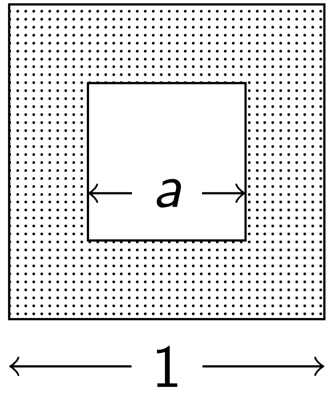

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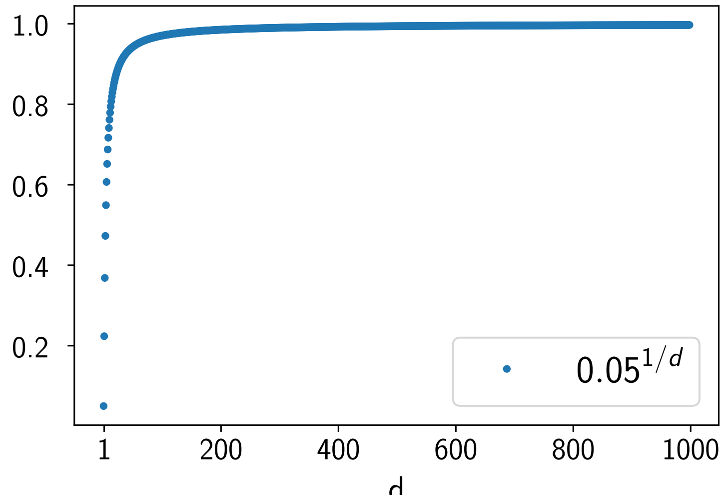

Problem 2: Regions with a high density can be empty.

Optigrid

A grid based approach to overcome the problems of distance and density in high dimensional spaces.

Hinneburg and Keim, *Optimal Grid-Clustering: Towards Breaking the Curse of Dimensionality in High-Dimensional Clustering*

Goal: Partition the space into grid-cells such that dense regions do not get cut in half.

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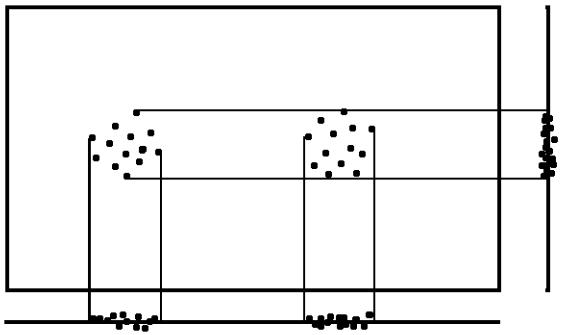
Key Observation: If the density at a point in one coordinate is low, it is low at all points in the high dimensional space that get projected onto that point.



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Calculate Projections to lower dimensional space
Approx. Densities and find peaks above *noiseLevel*
Find q best cutting planes with score $\leq$ *maxCutScore*
if *cutting planes were found* **then**
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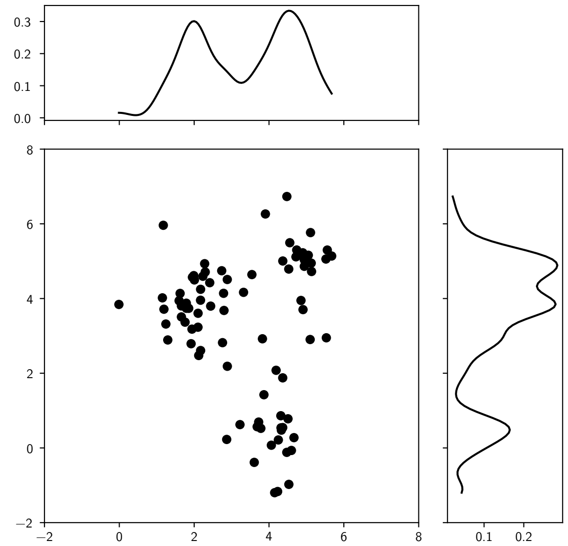

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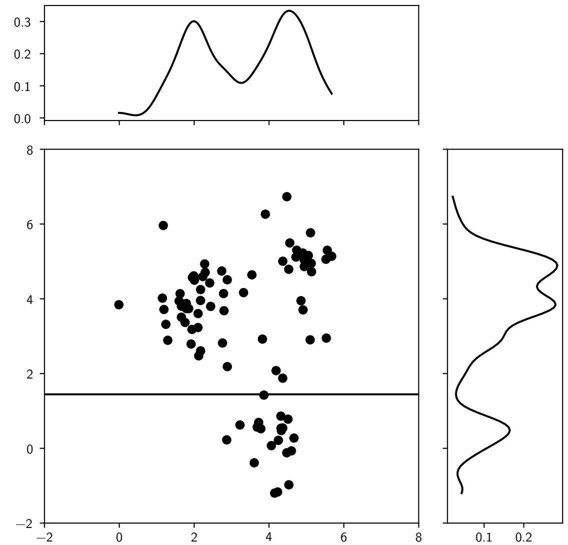

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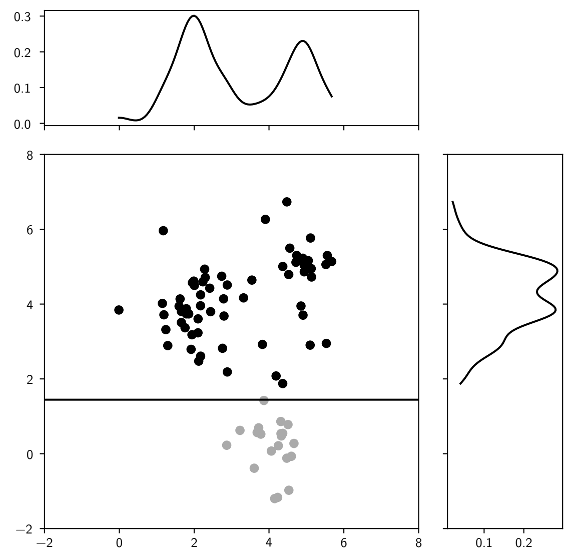

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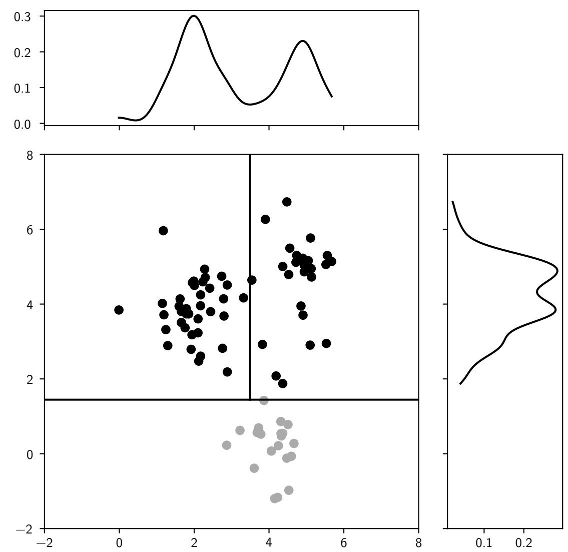

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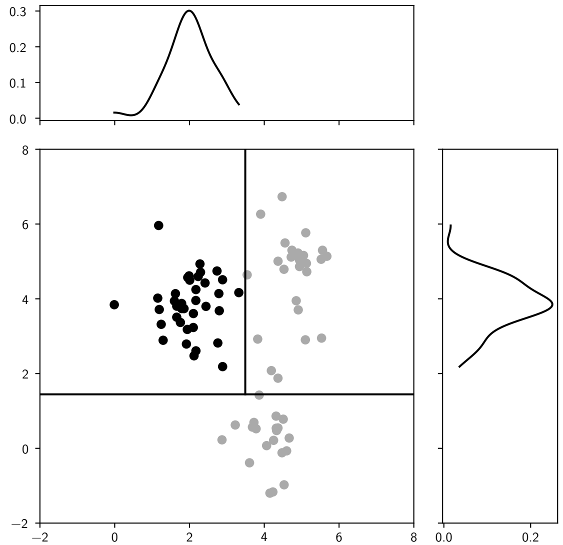

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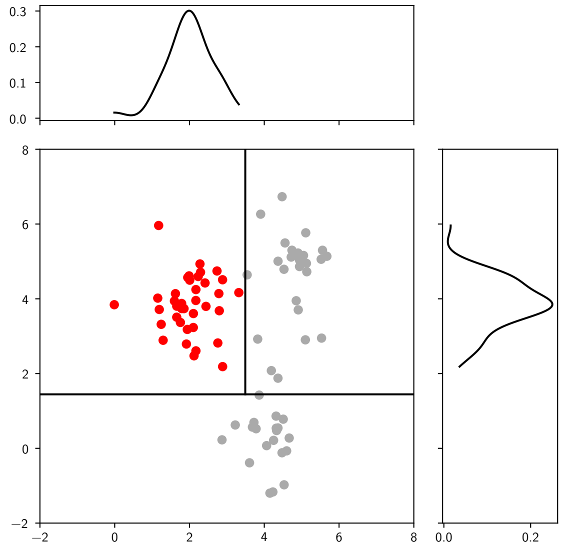

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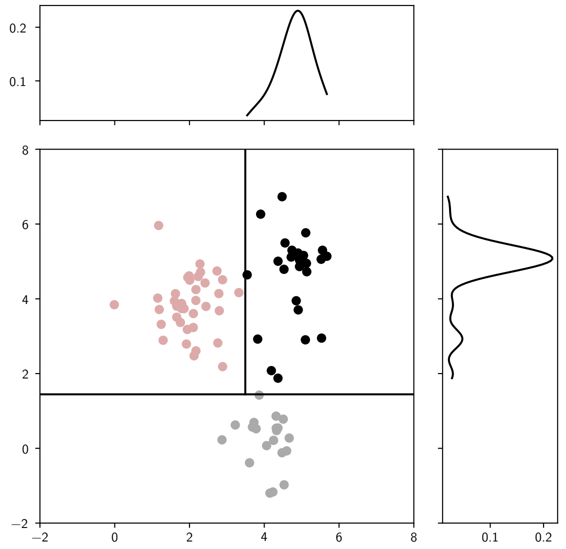

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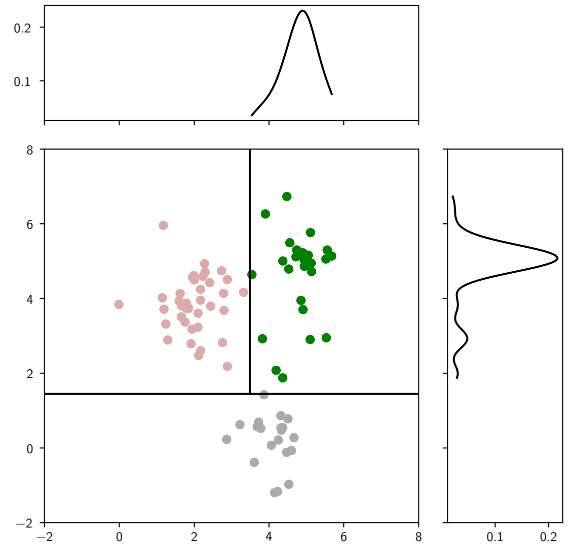

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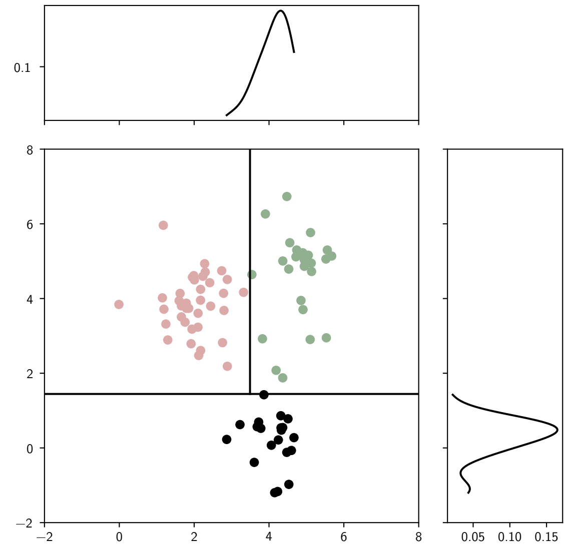

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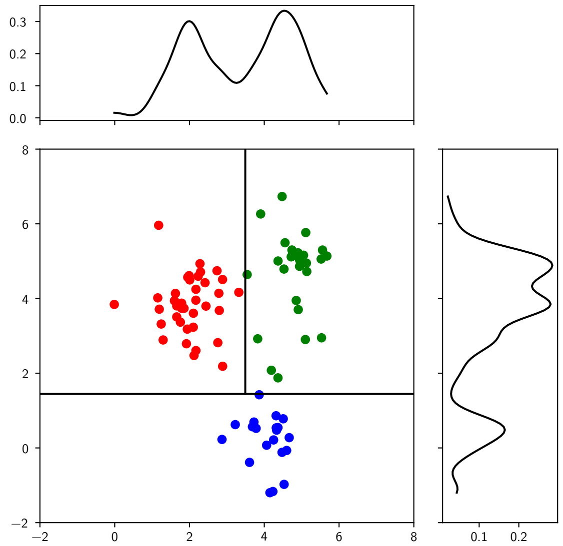

Optigrid

- Divides the input space into an irregular grid
- Calculations happen in low dimensions
- Finds clusters that can be enclosed in a rectangle
- Parameters can be chosen by analyzing the density distributions

Outlook

Can we find any clusters in the parameter settings of the Linac3 ion source?