Lecture 8
Clustering with DBSCAN

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THE UNIVERSITY OF
TENNESSEE
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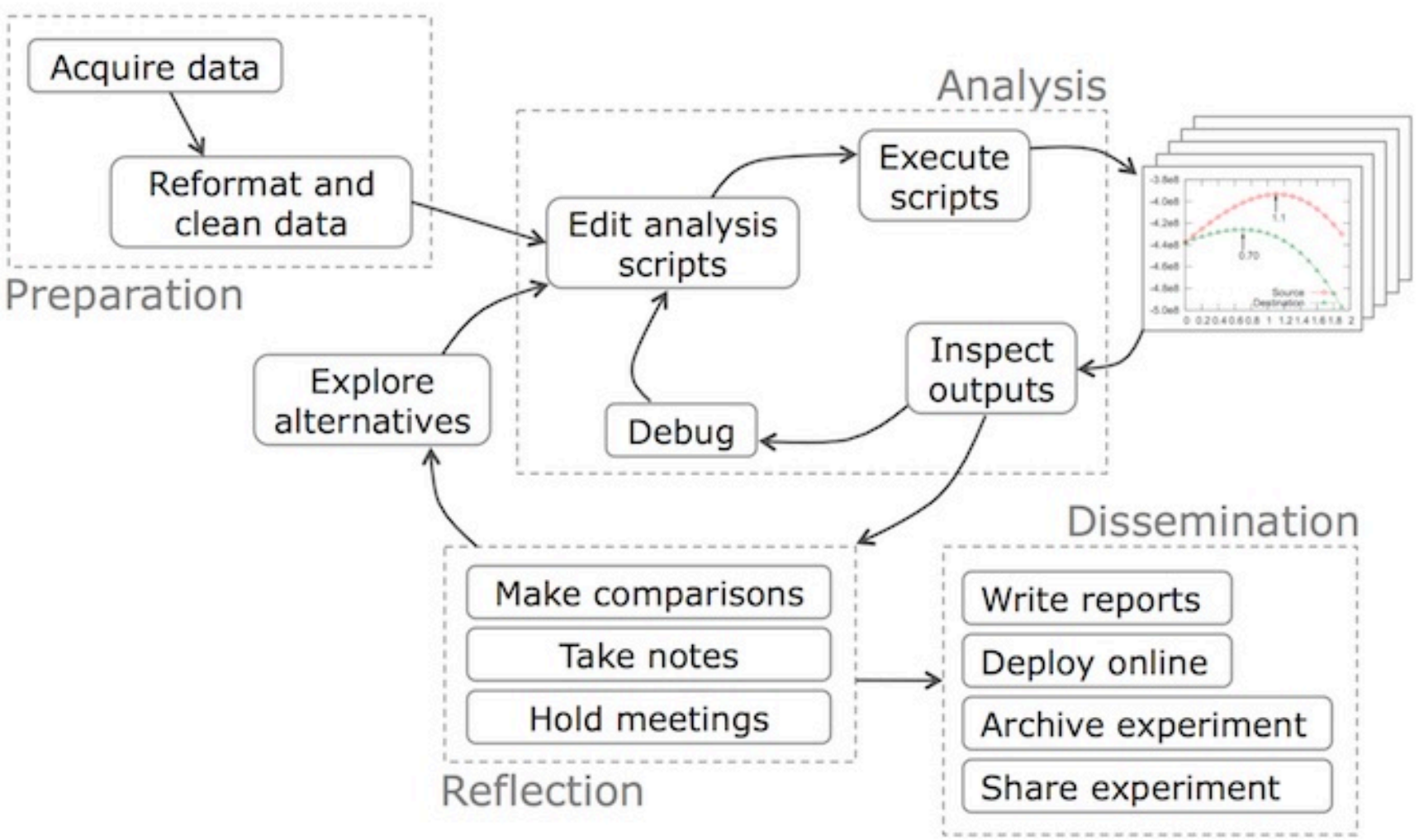
Lecture Outline

- Use work in paper "*Development of a Scalable Method for Creating Food Groups Using the NHANES Dataset and MapReduce"* to learn about:
  - Using a dataflow for tackling a data problem
  - Structuring a research project into a set of slides
    - Motivation, goals, background, methodology and results
  - Using a different clustering method than k-mean
    - How to cluster numerical data with the Density-based spatial clustering of applications with noise (DBSCAN)
    - How to set up the setting parameters of the DBSCAN
  - Using code from other scientists
    - Re-use rather than rewriting from scratch
    - Replicability of work as the first step for new research

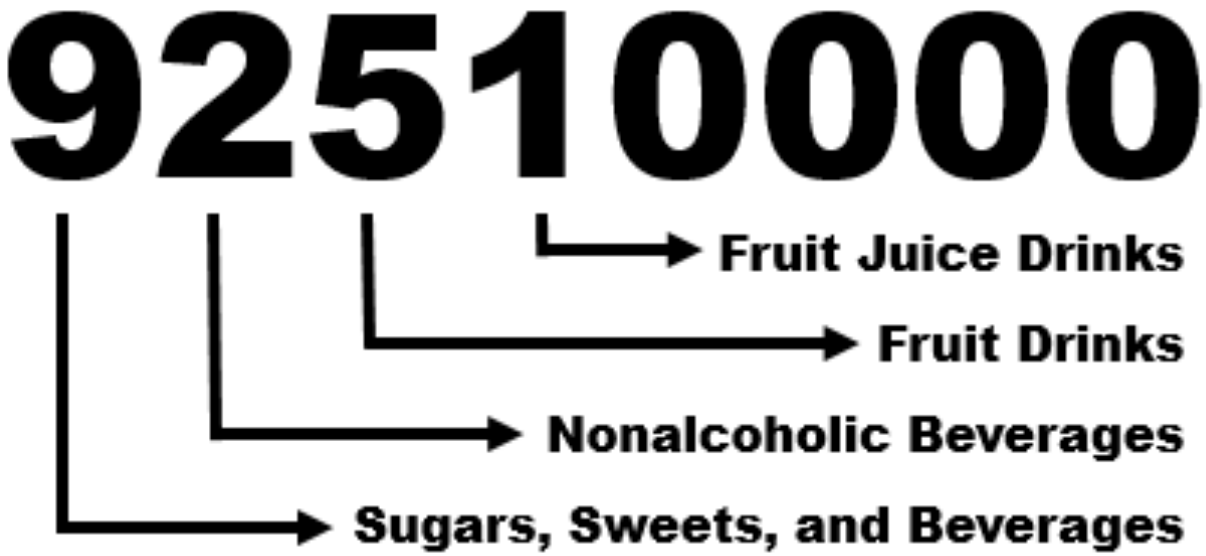
Data Workflow



Courtesy of Philip Guo: goo.gl/y42rp1

USDA Food Classification

- Used in dietary datasets to assign food items to groups
- Subjective and general
- Categorical, not nutrient-driven



What's Wrong with USDA Food Groups?

- Food Groups are **subjective**
  - Based on human expertise
  - Based on dietary trends
- Using **subjective** food groups for dietary studies give **bad results**
- Lack of standard food groups for use in dietary studies

How Do We Fix Food Groups?

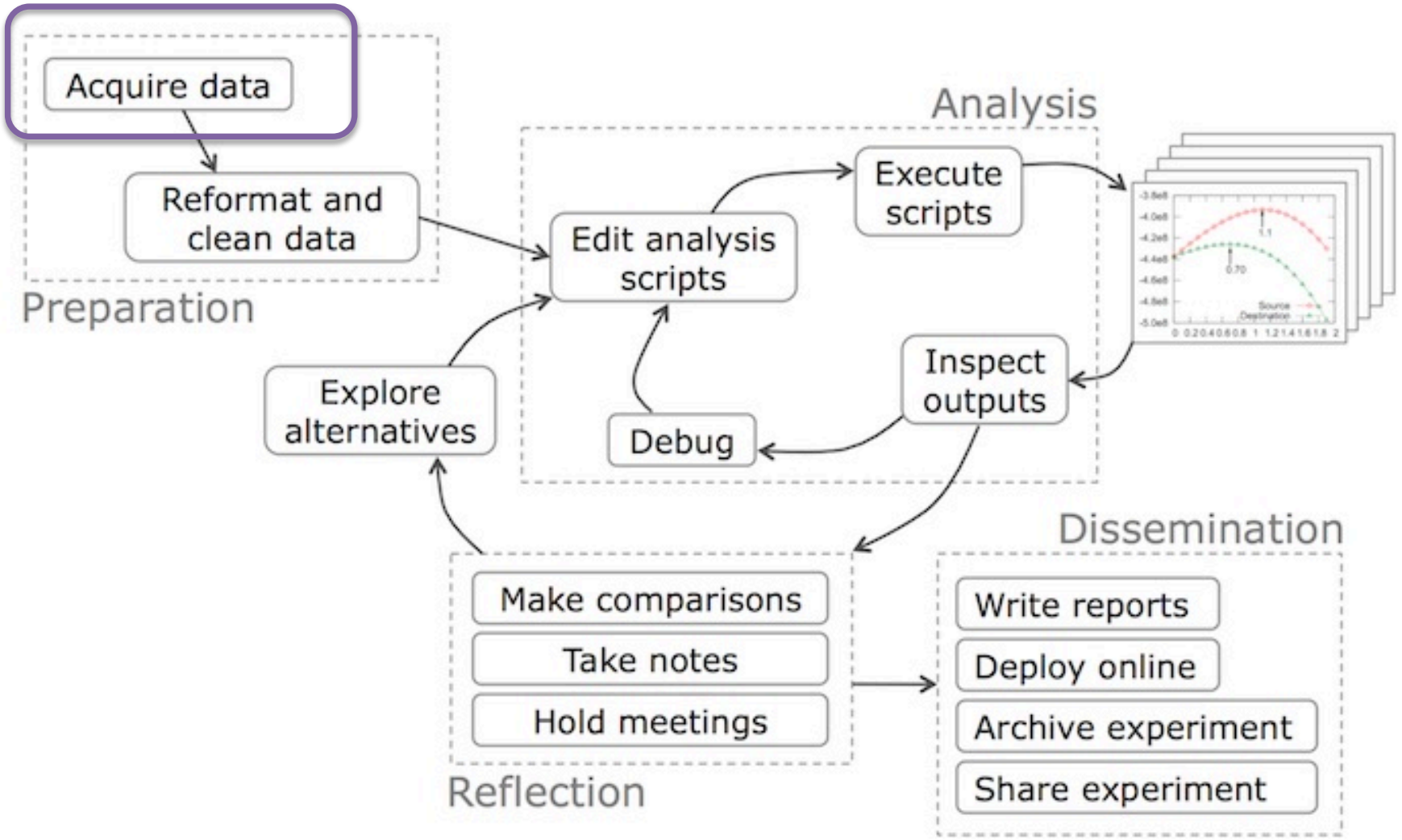
- Food Groups should be **objective**
  - Based on micro- and macro-nutrient content
- We need a standard set of food groups for dietary studies
- We need **scalable** methods for identifying food groups

"Define an objective methods to group food items in a dietary datasets based on the item micro- and macro-nutrient content"

Paper's Contributions

- Identify an **relevant, open-source dataset** with subjective classification of food item
- Define an objective method to classify food items into **nutrient-driven food groups**
- Parallelize our methods using a **scalable framework** such as Apache Spark's **based on MapReduce**
- Critically **compare and contrast** the subjective and our nutrient-driven food classification

Data Workflow



Courtesy of Philip Guo: goo.gl/y42rp1

Relevant Open-source Dataset

- Use a dataset with well-known and broadly used data format

NHANES: National Health and Nutrition Examination Survey

- Medical, demographic, and dietary records
- Available to the public for free
- *Contains subjective food groups provided by USDA*

Data available at: http://www.cdc.gov/nchs/nhanes/nhanes_questionnaires.htm

NHANES Dietary Data

- Dietary intake of 64,653 Americans
- 7,494 unique food items
- 1,587,750 food entries
- 46 nutrient features for each food item
  - Macronutrients (e.g., fats, carbohydrates)
  - Micronutrients (e.g., vitamins, minerals)

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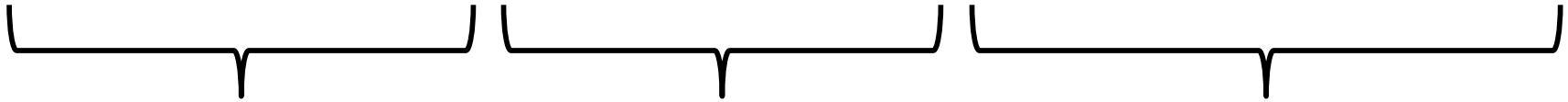
Structure of Dietary Data Item

<143672, 92510000, 3, 0, 8:15am, 7, 3, 10.1, 4, 3.45, 10, 178, …>

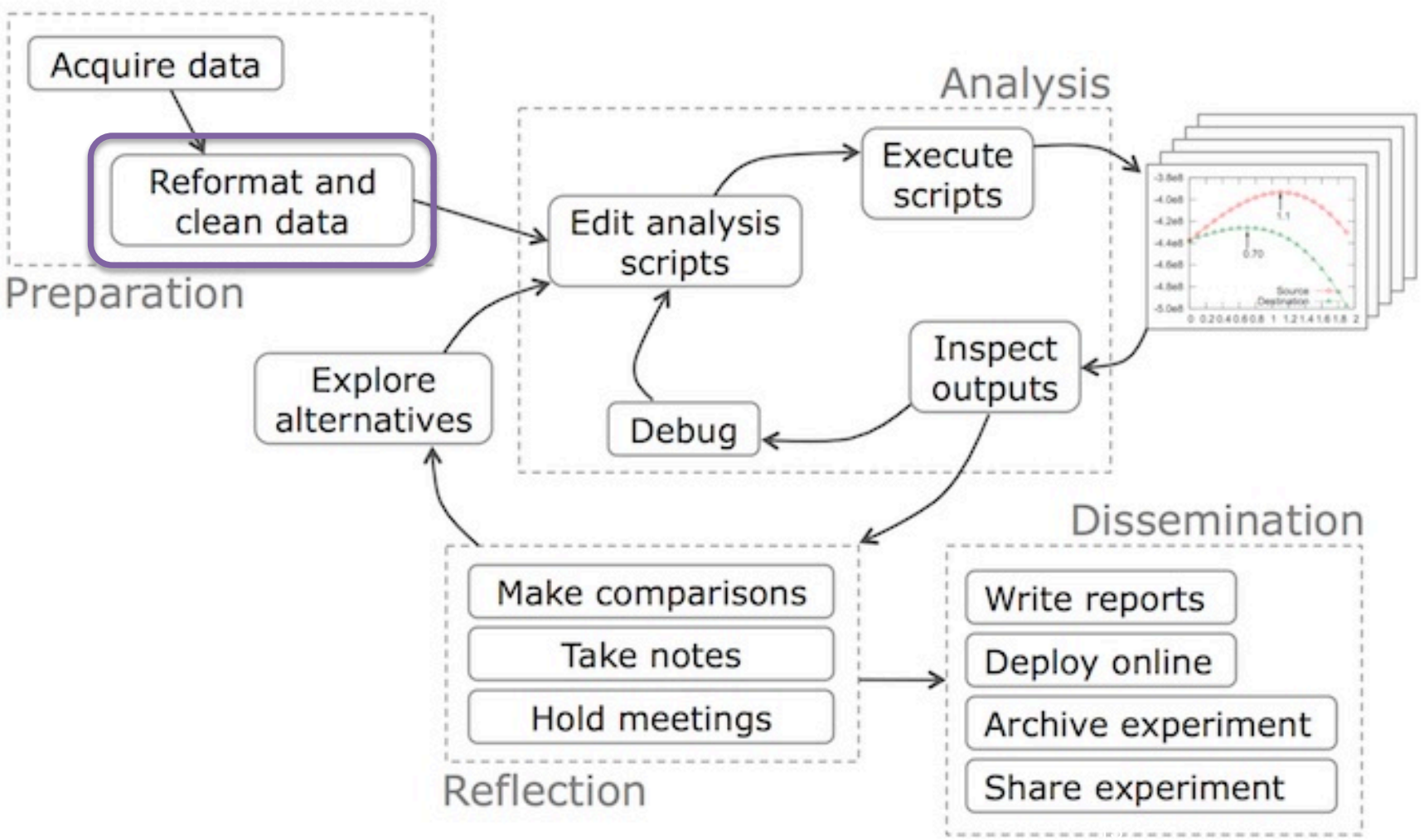


- Participant ID
- **USDA Food Code**

- Meta Data

- Macronutrients
- Micronutrients

Data Workflow



Courtesy of Philip Guo: goo.gl/y42rp1

NHANES Snapshot

Food	Mod Code	Weight (g)	Protein (g)	Sodium (mg)
Milk	*0*	244	8	107
Milk	*0*	122	4	54
Milk	*0*	100	3	44
Milk	*0*	300	10	132
Milk	*0*	10	0	4
Milk	*0*	93	3	41
Cereal	*0*	30	2	231
Cereal	*10*	60	6	462
Cereal	*0*	0	3	300
Cereal	*0*	10		77
Steak	*0*	256	62	146

Missing Values

Food	Mod Code	Weight (g)	Protein (g)	Sodium (mg)
Milk	*0*	244	8	107
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Weight-Based Nutrient Values

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Redundant Data

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Features on Different Scales

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Preprocessing: Missing Values

Food	Mod Code	Weight (g)	Protein (g)	Sodium (mg)
Cereal	*0*	10		77

- Standard Approach:
  - Fill in missing values e.g., median or zero
- Drawback:
  - Introduces artificial data which creates bias in the data
- Our Solution:
  - Redundant food entries allows us to discard entries with missing values
- Observations:
  - 9,586 of 1,587,750 entries removed
  - 0 unique foods lost

Preprocessing: Missing Values

Food	Mod Code	Weight (g)	Protein (g)	Sodium (mg)
Milk	*0*	244	8	107
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- Nutrient values are based on the weight of the food entry.
  - Unfair comparison between foods
  - Food entries of the same type do not match

Preprocessing: Weight-Based Values

Food	Mod Code	Weight (g)	Protein (g)	Sodium (mg)
Cereal	*0*	0	3	300

- Standard Approach:
  - Normalize with respect to weight – divide entry by weight
- Drawback:
  - Some entries have a weight of "0"
- Our Solution:
  - Redundant food entries allows us to discard entries with a weight of "0"
- Observations:
  - 10,983 of 1,587,750 entries removed
  - 0 unique foods lost

Preprocessing: Weight-Based Values

Food	Mod Code	Weight (g)	Protein (g)	Sodium (mg)
Milk	*0*	1 (244)	0.033	0.439
Milk	*0*	1 (122)	0.033	0.443
Milk	*0*	1 (100)	0.030	0.440
Milk	*0*	1 (300)	0.033	0.440
Milk	*0*	1 (10)	0	0.400
Milk	*0*	1 (93)	0.032	0.441
Cereal	*0*	1 (30)	0.067	7.70
Cereal	*10*	1 (60)	0.100	7.70
Cereal	*0*	0	3	300
Cereal	*0*	10		77
Steak	*0*	1 (256)	0.242	0.570

Preprocessing: Redundant Data

Food	Mod Code	Weight (g)	Protein (g)	Sodium (mg)
Milk	*0*	1 (244)	0.033	0.439
Milk	*0*	1 (10)	0	0.400
Cereal	*0*	1 (30)	0.067	7.70
Cereal	*10*	1 (60)	0.100	7.70

- Standard Approach:
  - Select one entry for each unique food item
- Drawback:
  - Nutrient densities don't always match for the same food item – How do we pick a representative entry?
    - Modification codes
    - Rounding error

Preprocessing: Redundant Data

Food	Mod Code	Weight (g)	Protein (g)	Sodium (mg)
Milk	*0*	1 (244)	0.033	0.439
Milk	*0*	1 (10)	0	0.400
Cereal	*0*	1 (30)	0.067	7.70
Cereal	*10*	1 (60)	0.100	7.70

- Our Solution:
  - Remove entries with a non-zero modification code
  - Average top 5 entries for each food when sorted by weight
- Observations:
  - 32 unique foods lost

Preprocessing: Redundant Data

Food	Mod Code	Weight (g)	Protein (g)	Sodium (mg)
Milk	*0*	1 (244)	0.033	0.439
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Preprocessing: Different Scales

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Steak	*0*	1	0.242	0.570

- Standard Approach:
  - Standardize – divide by largest value
- Drawback:
  - Removes effects of highly skewed feature distributions

Preprocessing: Different Scales

Food	Mod Code	Weight (g)	Protein (sd)	Sodium (sd)
Milk	*0*	1	-0.726	-0.593
Cereal	*0*	1	-0.416	1.16
Steak	*0*	1	1.13	-0.561

- Our Solution:
  - **Z-score standardization**: convert original values into values indicating how many standard deviations above or below a value is from the mean of the original distribution
- Observations:
  - Feature scales are similar, but not the same
  - Distributions are not dramatically altered

Preprocessing: Different Scales

Food	Mod Code	Weight (g)	Protein (g)	Sodium (mg)
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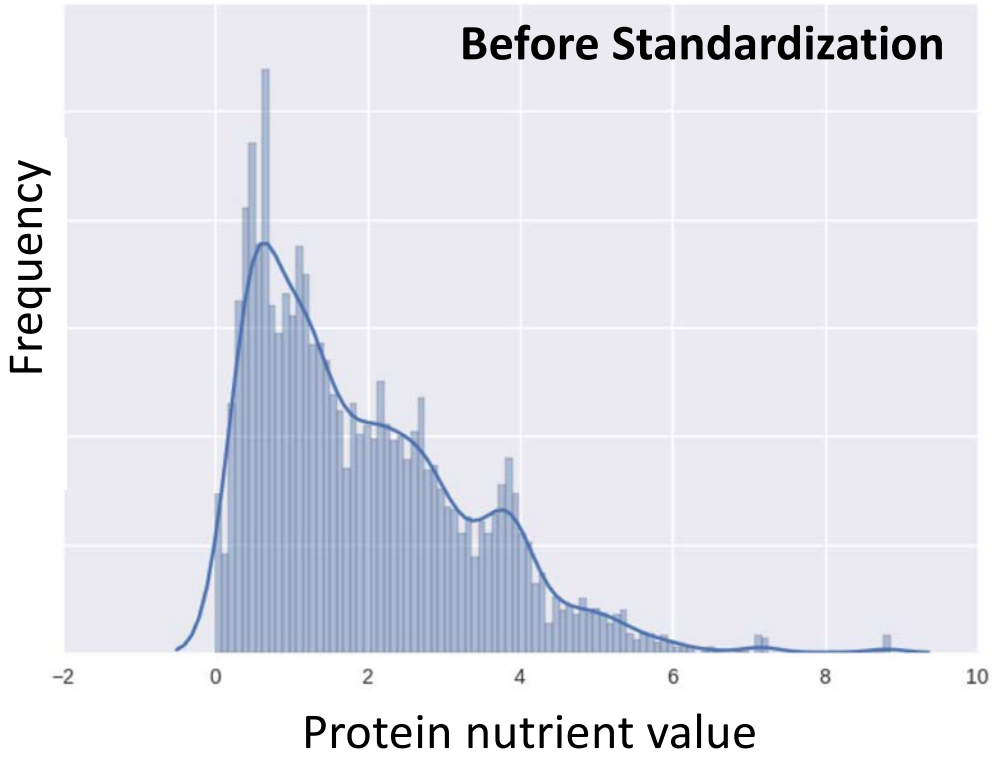
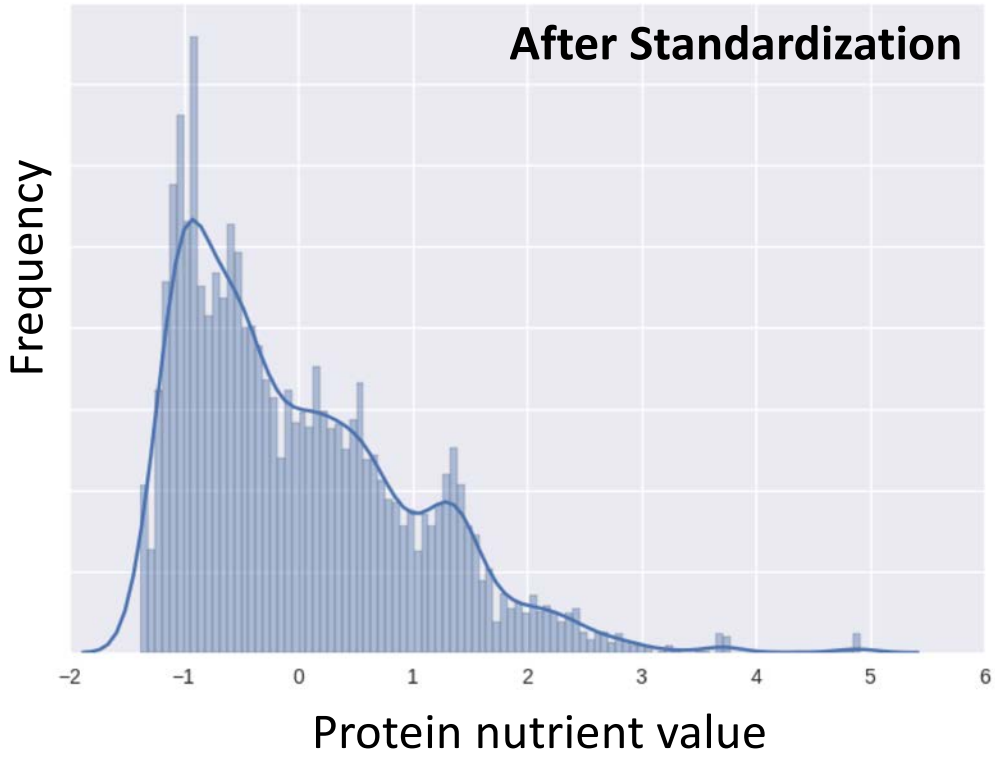
Example of Standardization

- Macro-nutrient, protein, with its content distribution before and after standardization





NHANSE Snapshot After Preparation

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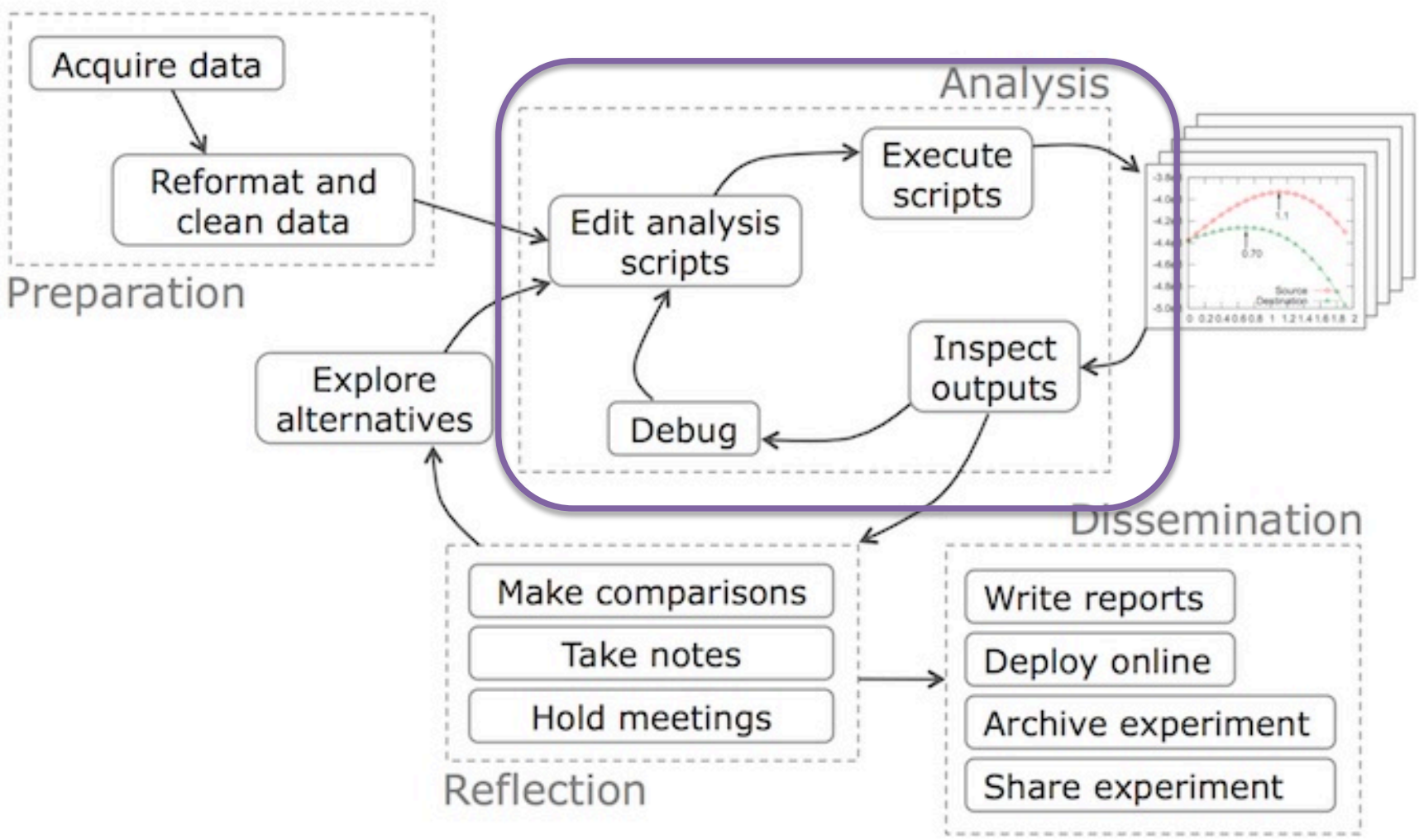
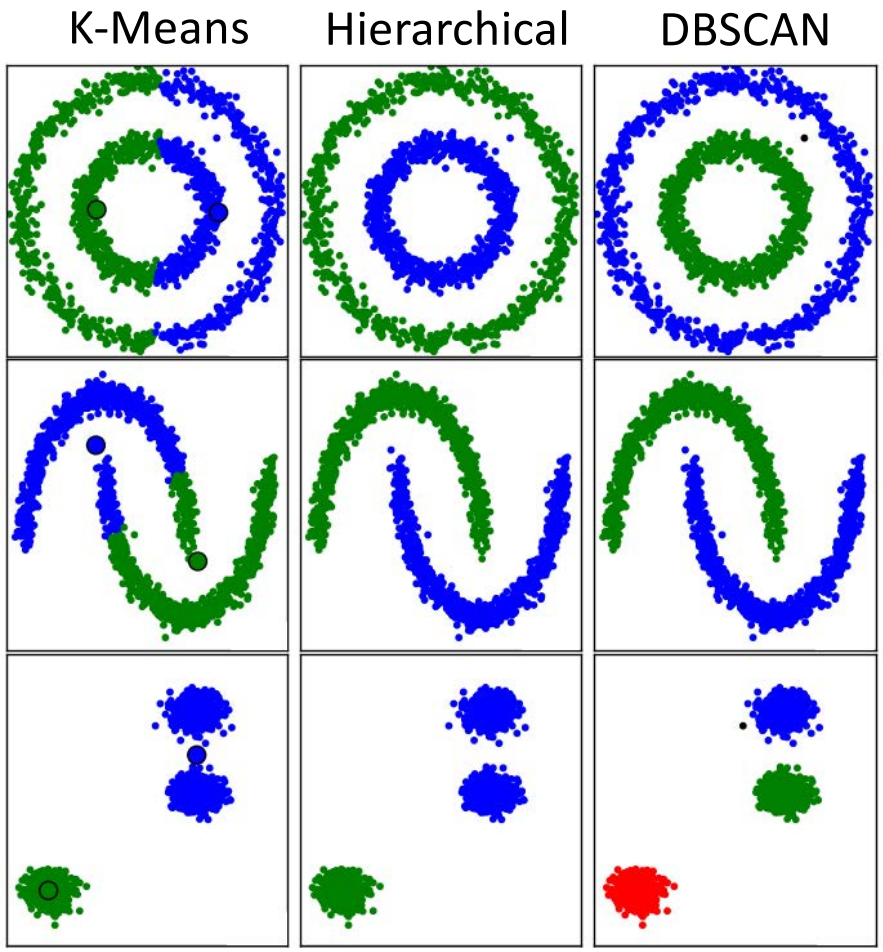
BEFORE: 7,494 unique food items
AFTER: 7,462 unique food items

Data Workflow



Courtesy of Philip Guo: goo.gl/y42rp1

Selecting a Good Clustering Algorithm

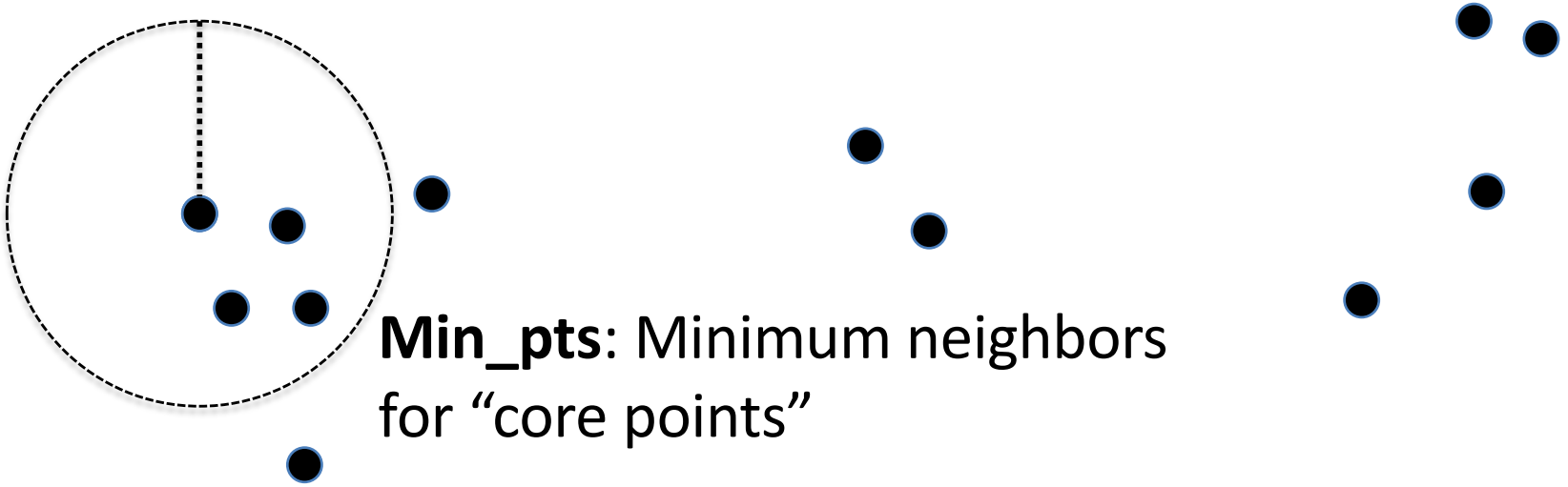


Feature	K-Means	Hierarchical	DBSCAN
Resource Efficient	Yes	No	Yes
Noise Insensitive	No	No	Yes
Outlier Detection	No	No	Yes
Spheroid Clusters	Yes	Yes	Yes
Non-Spheroid Clusters	No	Yes	Yes
Undefined Cluster Count	No	Yes	Yes

Image: http://scikit-learn.org/stable/modules/clustering.html

DBSCAN Algorithm

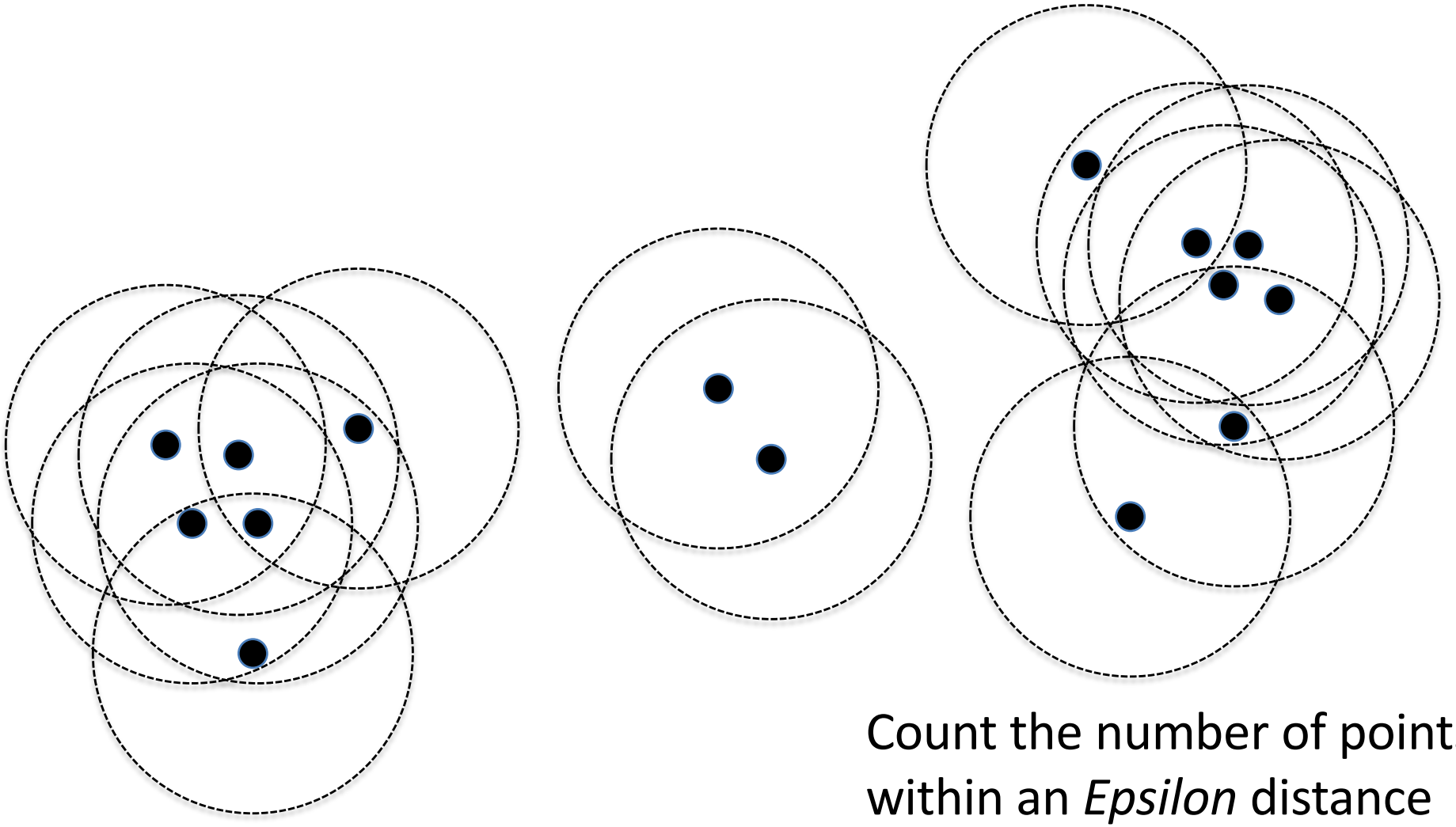
Epsilon: Distance around point for counting neighbors



Min_pts: Minimum neighbors for “core points”

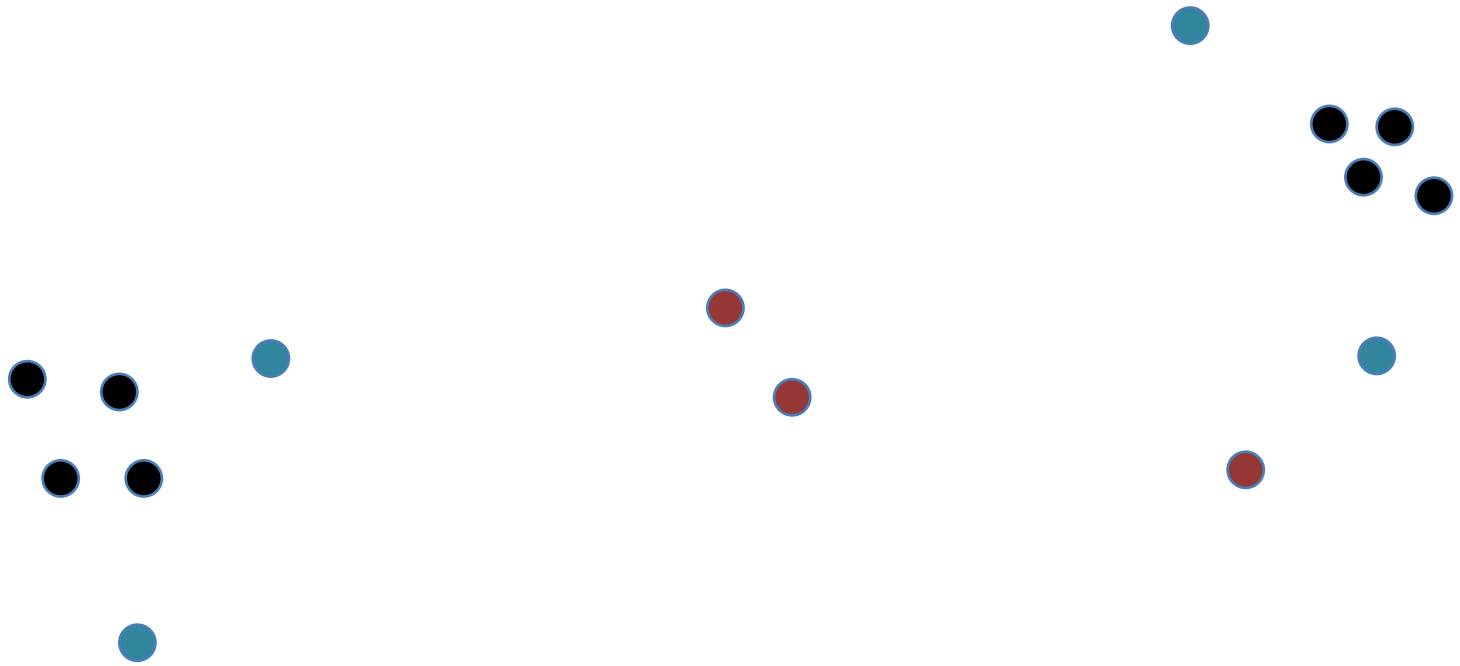
Together, these parameters define the minimum density for a cluster

DBSCAN Algorithm



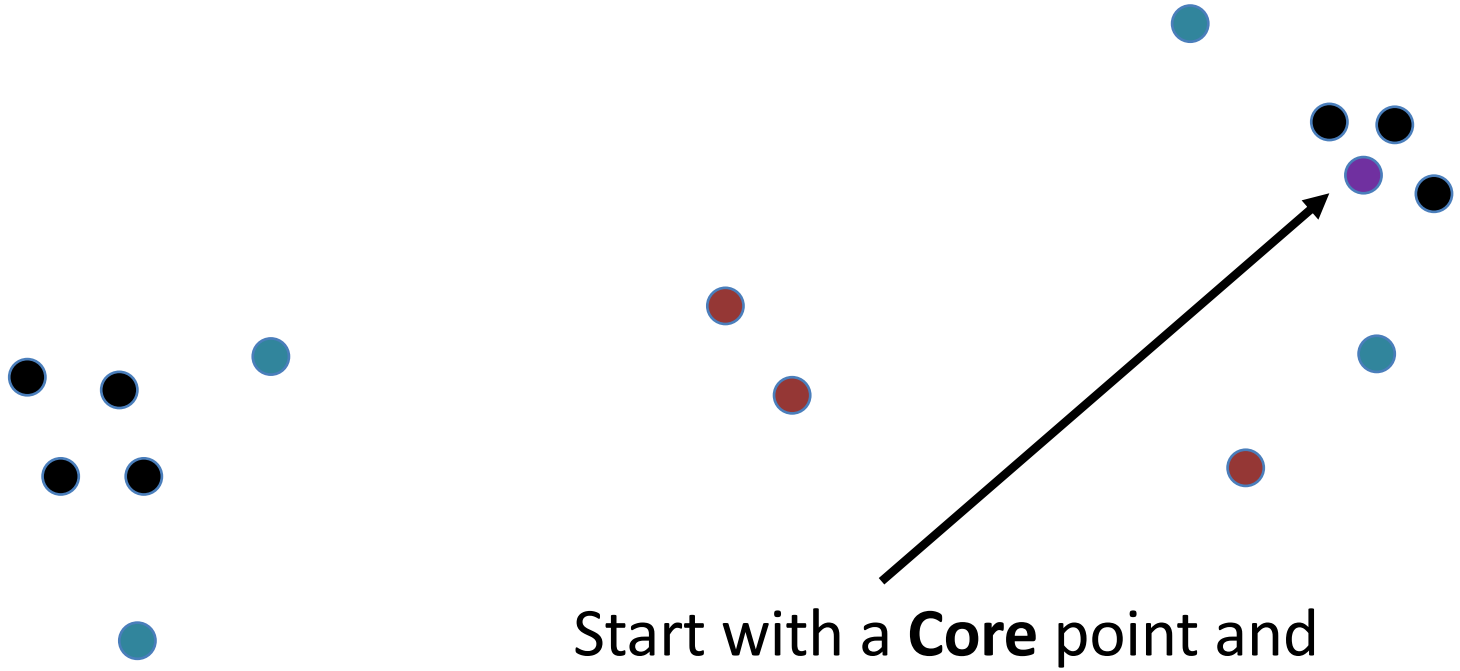
Count the number of points within an *Epsilon* distance

DBSCAN Algorithm



Identify **Core**, **Border**, and **Noise** points

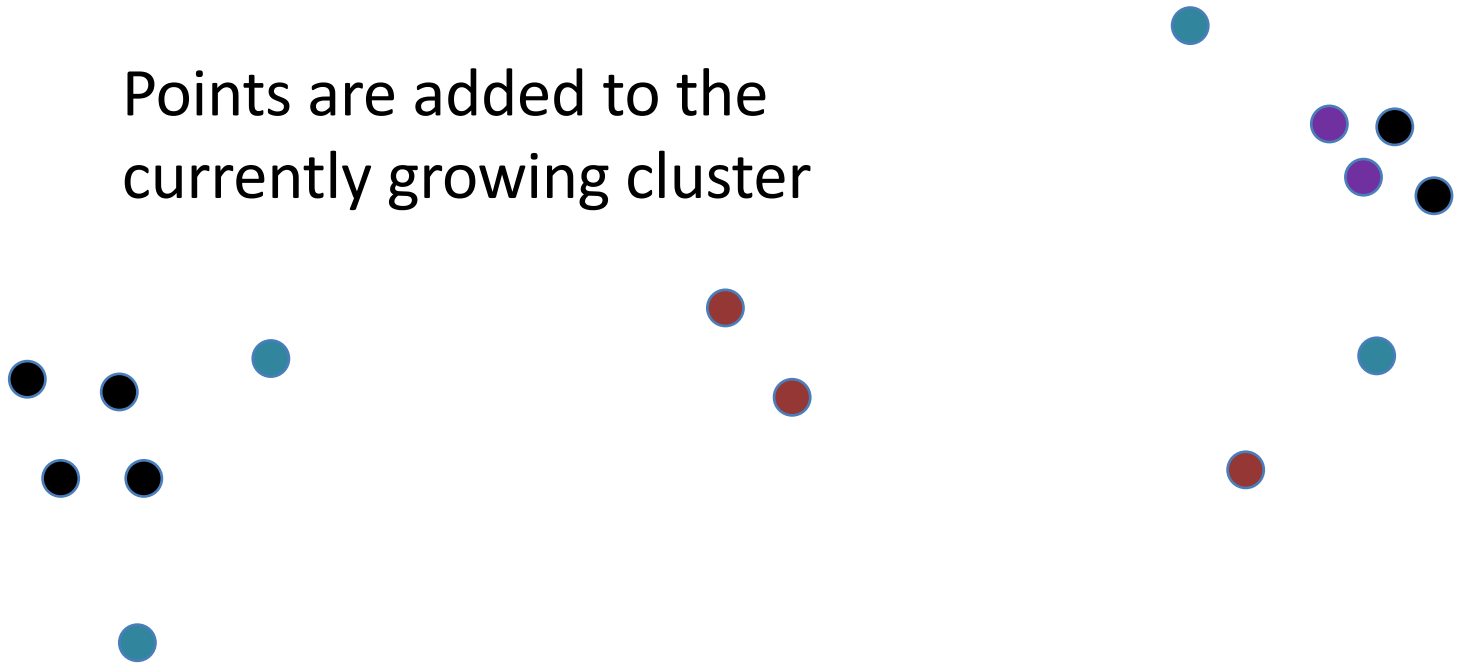
DBSCAN Algorithm



Start with a **Core** point and begin growing the clusters.

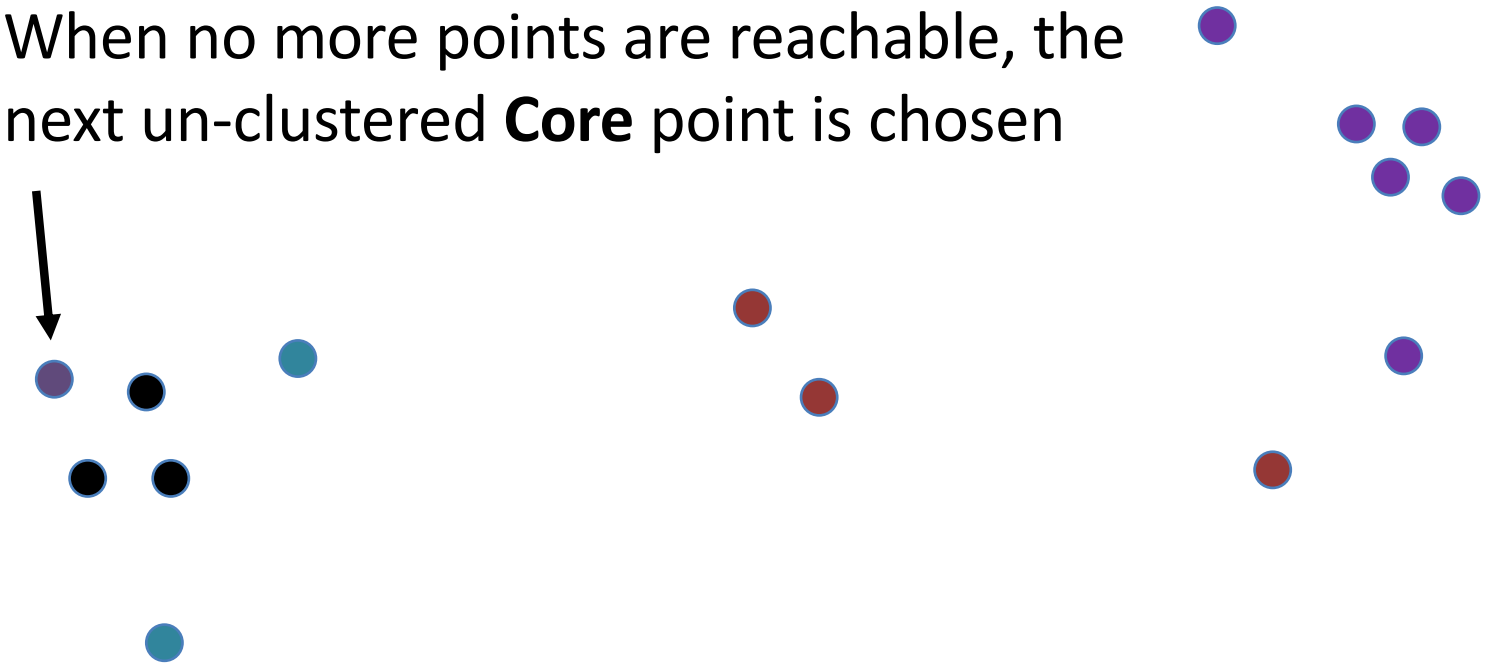
DBSCAN Algorithm

Points are added to the currently growing cluster

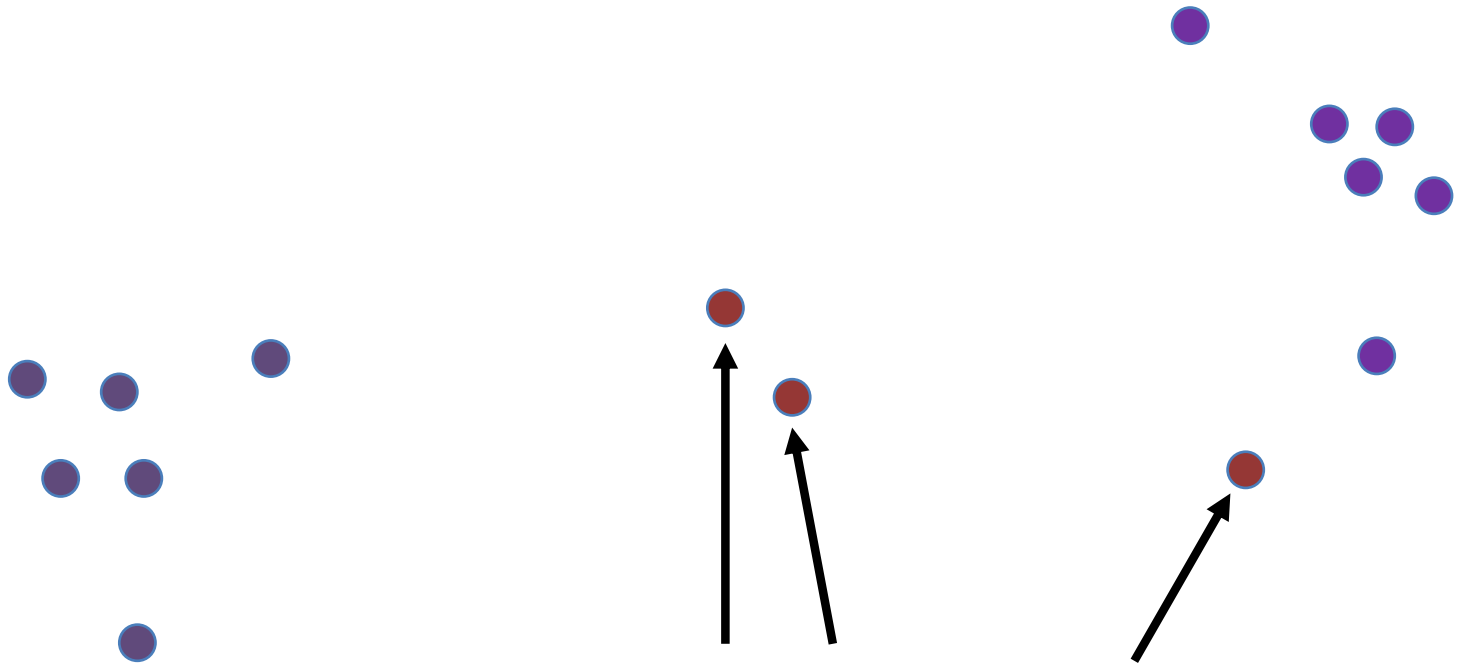


DBSCAN Algorithm

When no more points are reachable, the next un-clustered **Core** point is chosen



DBSCAN Algorithm



This pattern continues until only **Noise** points remain un-clustered.

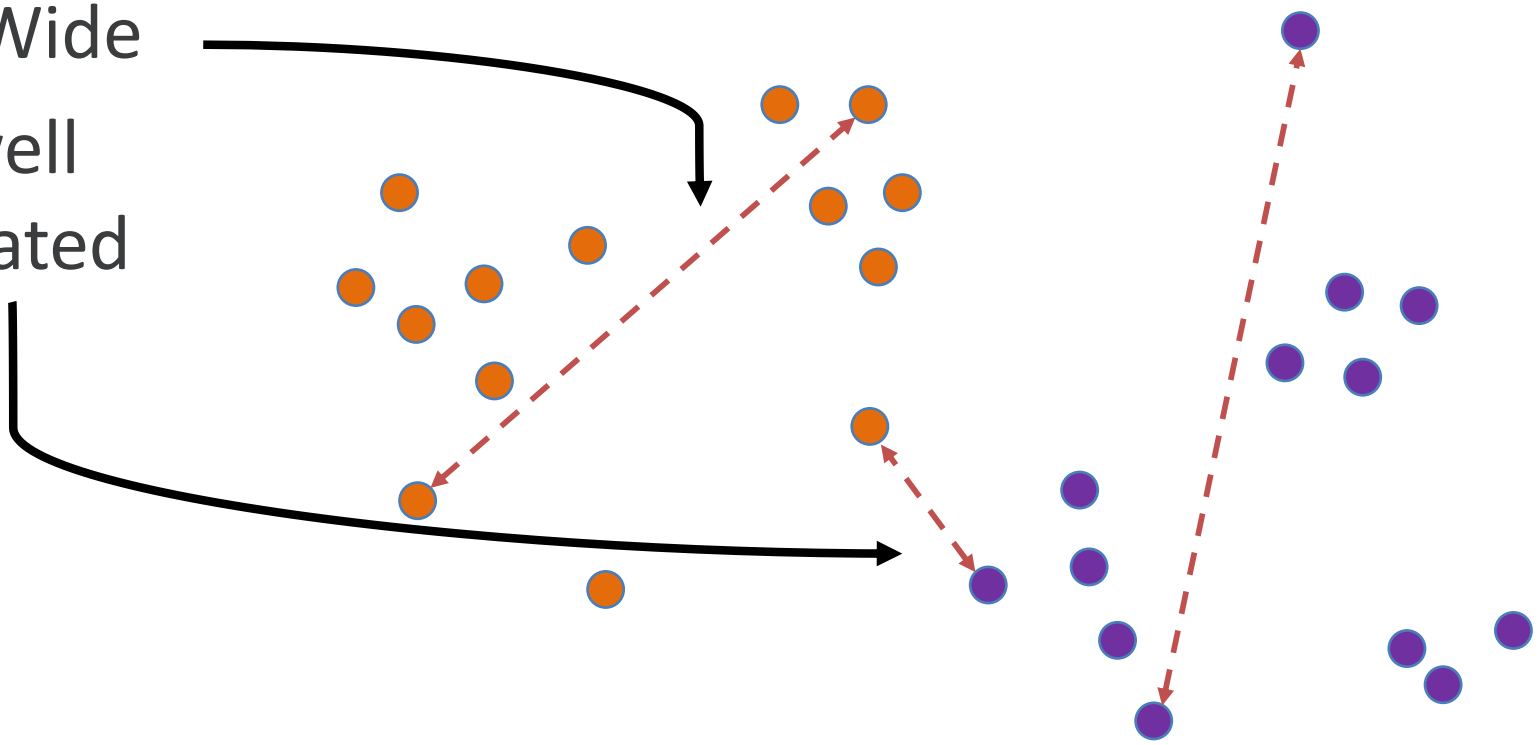
DBSCAN Algorithm

BDSCAN Demo

- Visualizing a DBSCAN clustering
  - Interactive interface at:
  - https://www.naftaliharris.com/blog/visualizing-dbscan-clustering/

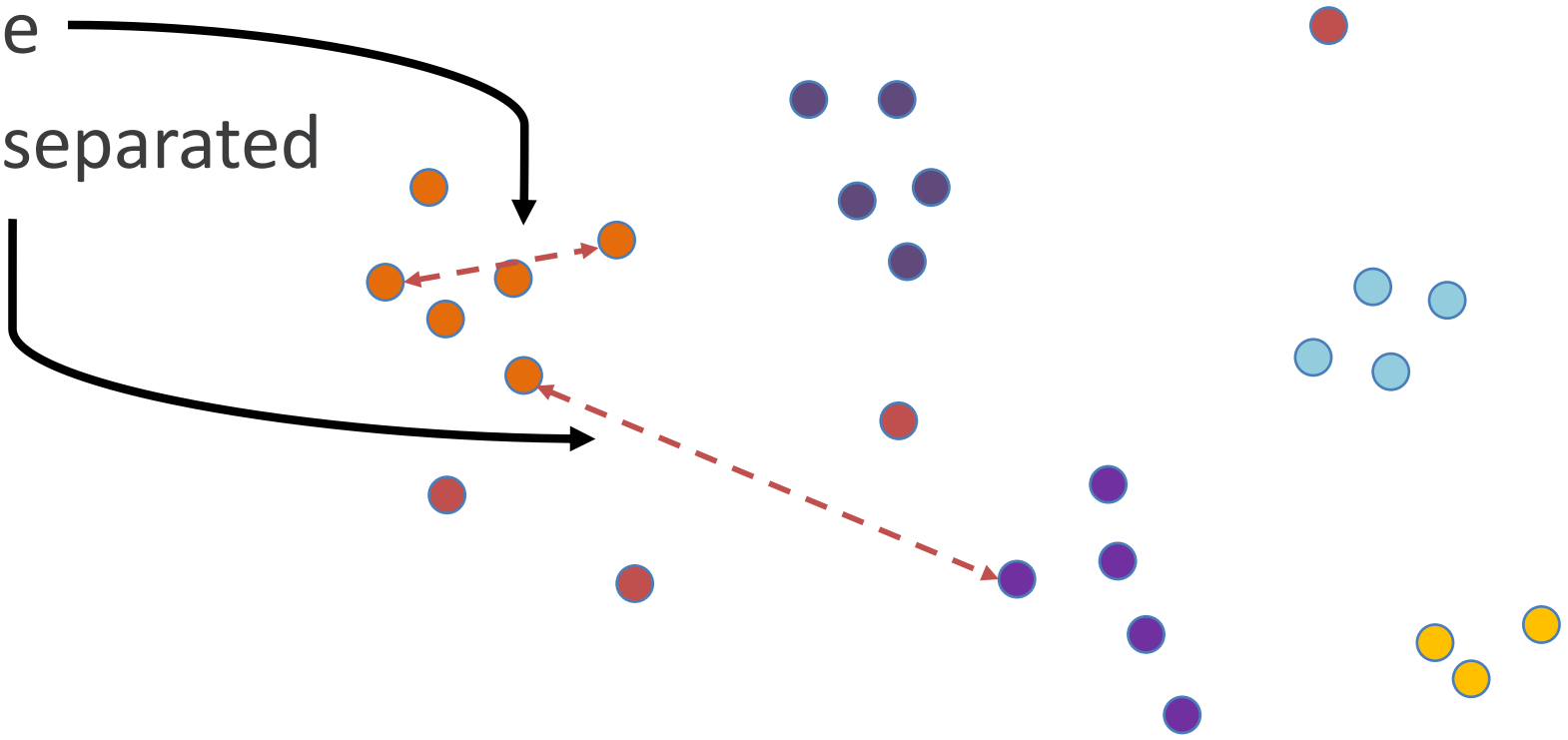
Bad Clustering

- Very Wide
- Not well separated



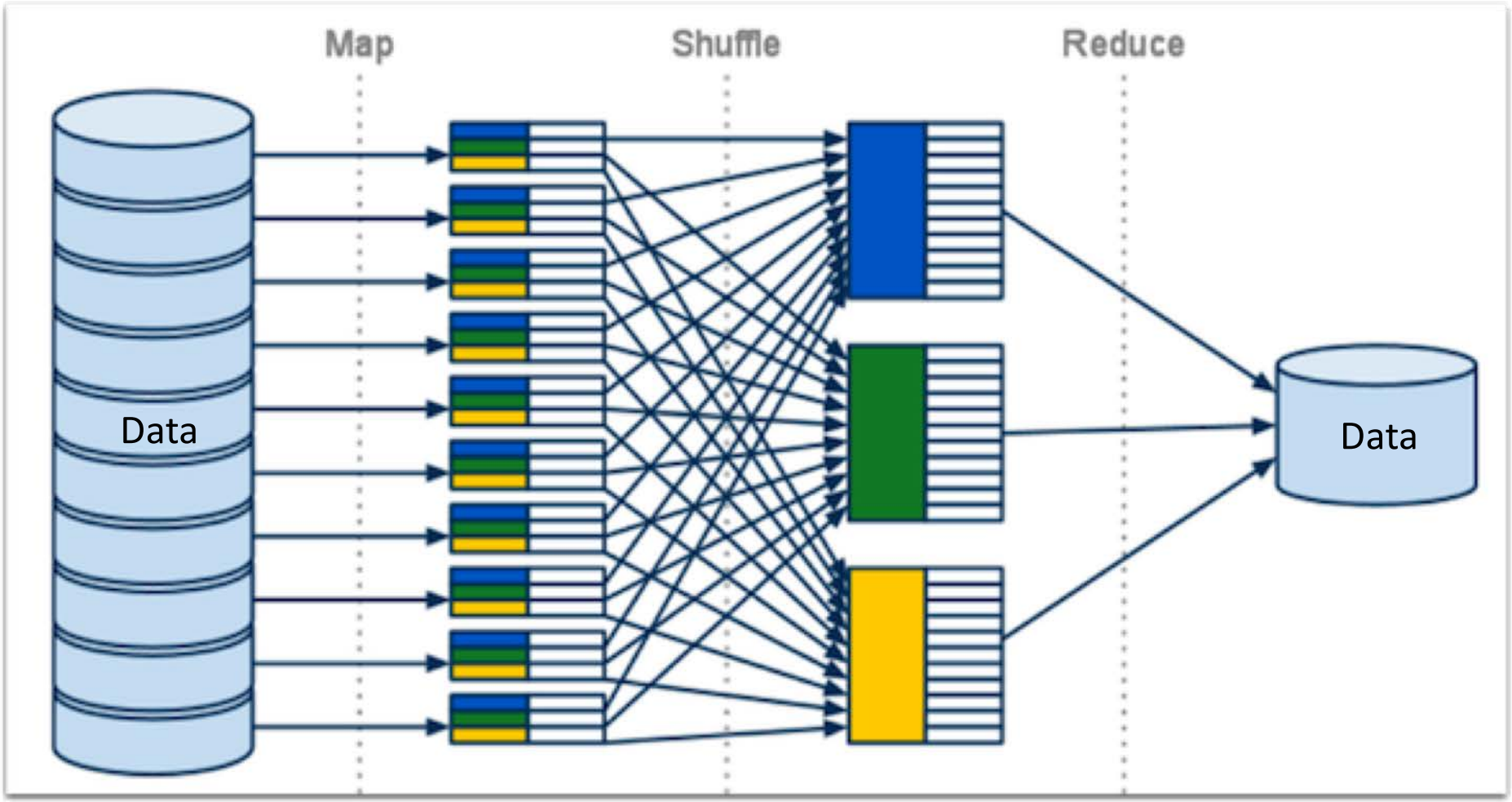
Good Clustering

- Dense
- Well separated

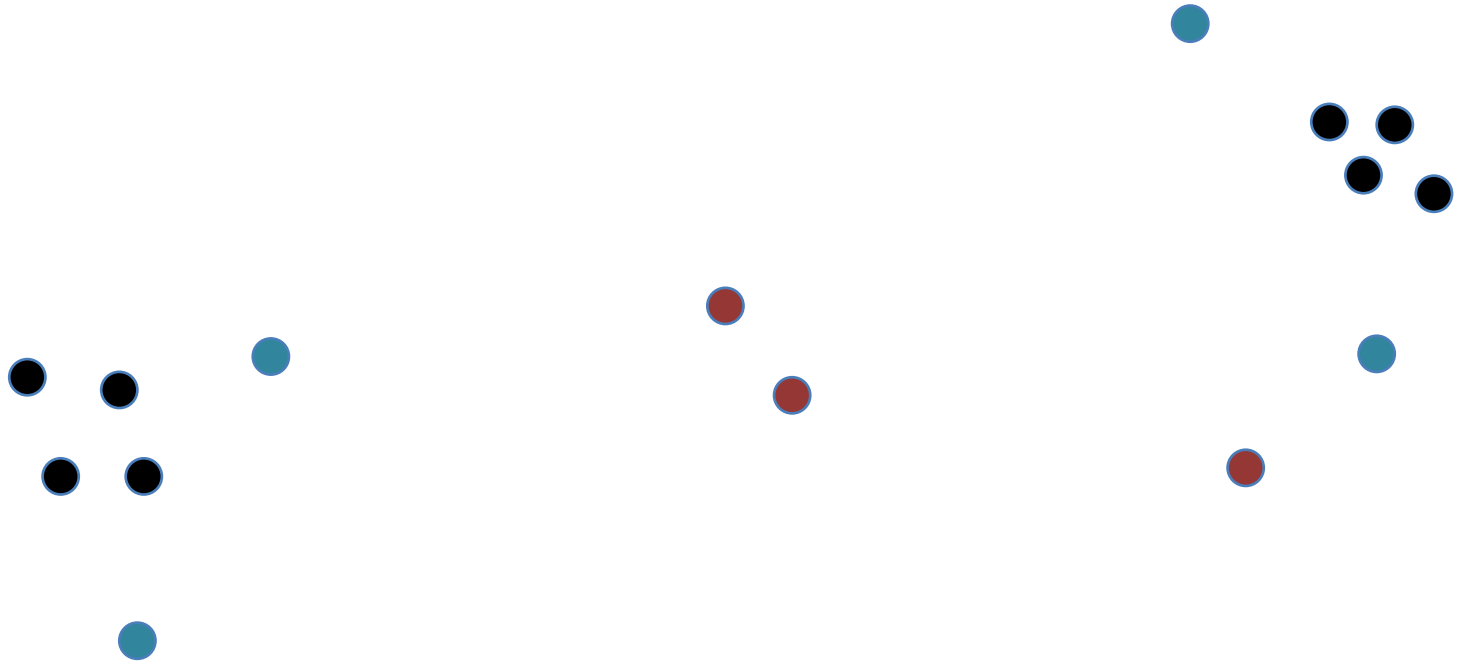


MapReduce Paradigm

Image: https://aimotion.blogspot.com/2012/08/introduction-to-recommendations-with.html

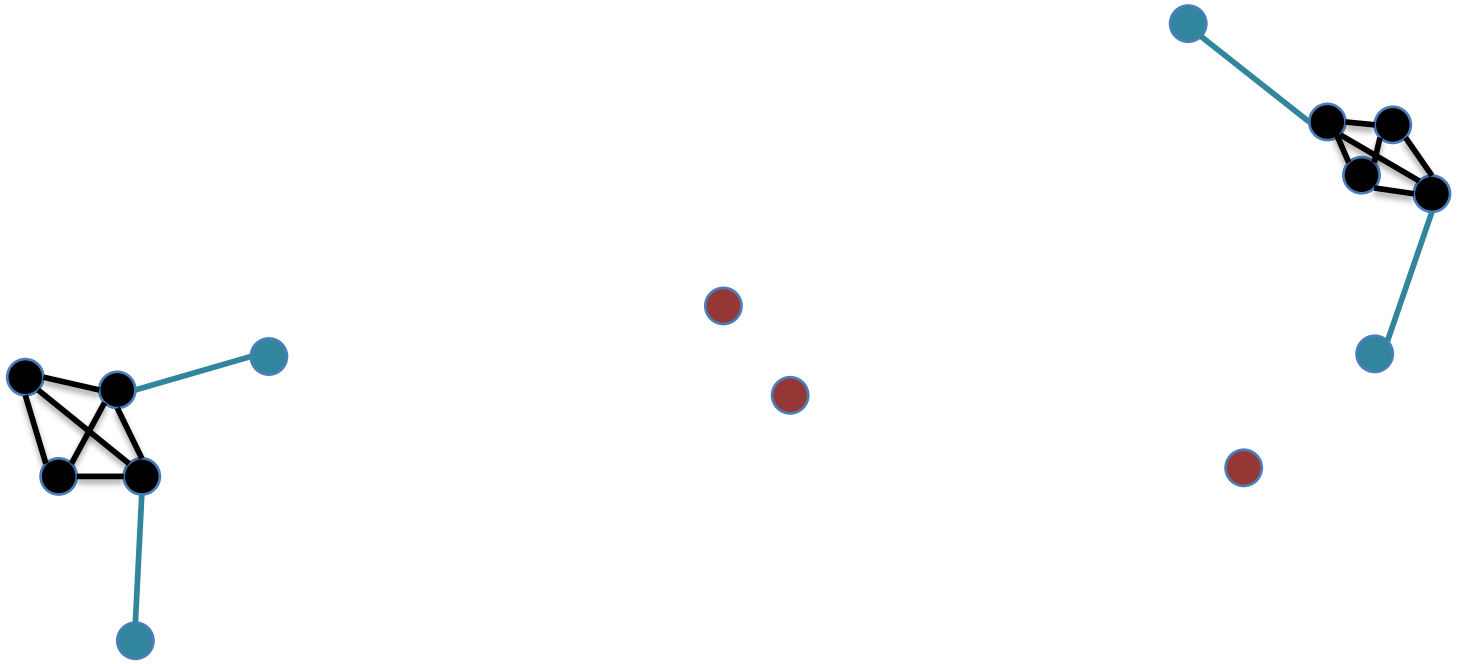


Parallel DBSCAN



Identify **Core**, **Border**, and **Noise** points.

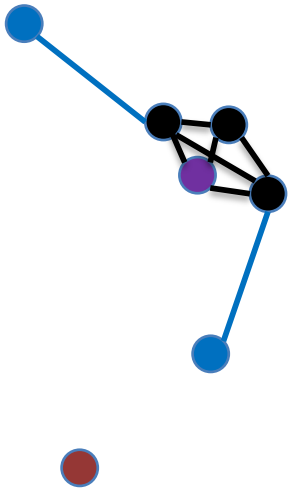
Parallel DBSCAN



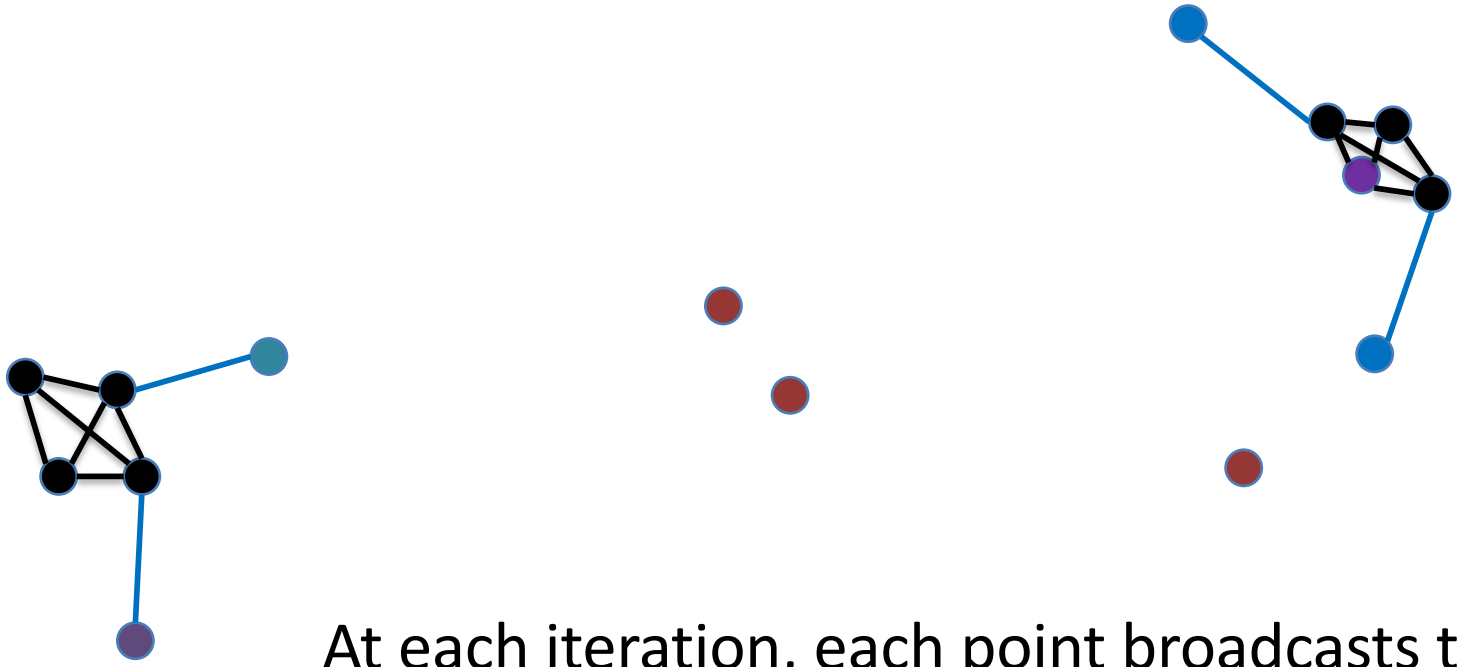
Connect **Core** and **Border** points.

Parallel DBSCAN

Each point is assigned a unique ID value and tracks the minimum ID value which it can “see”.

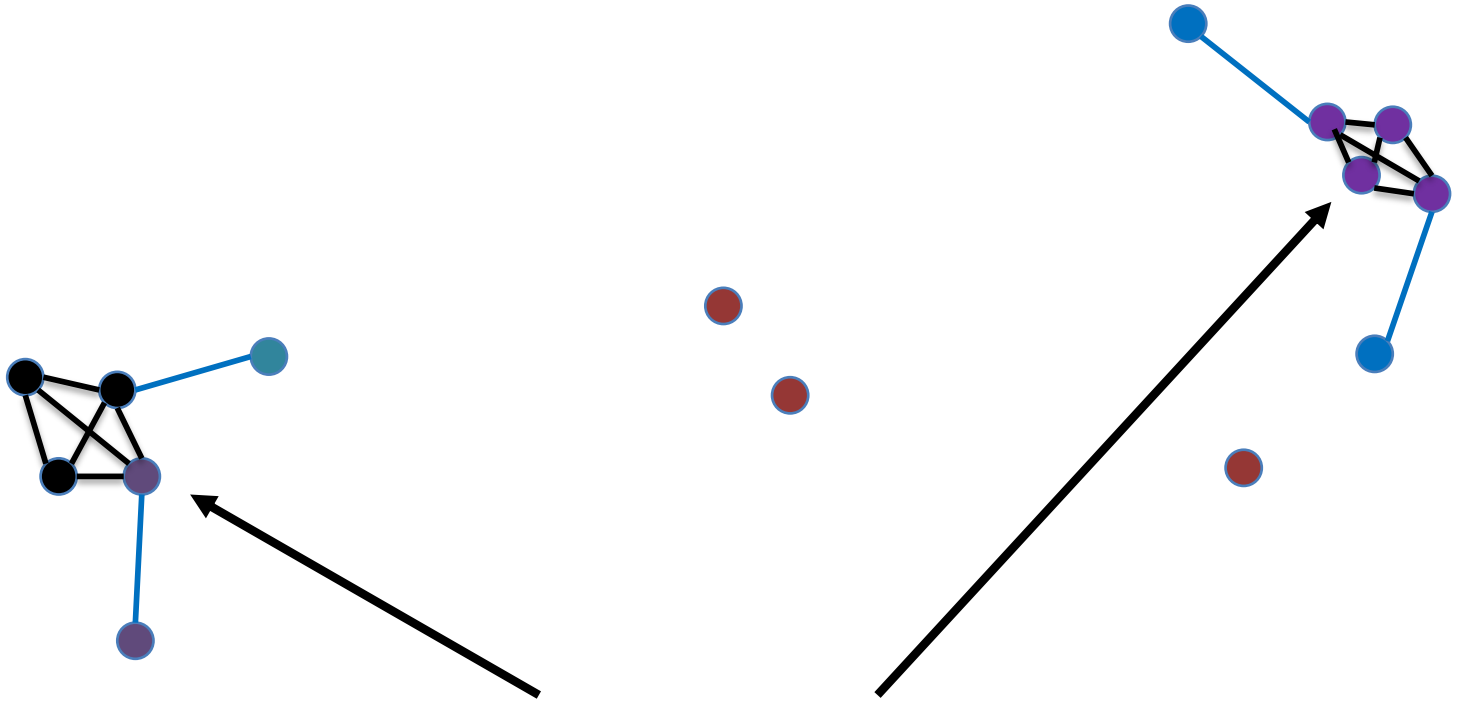


Parallel DBSCAN



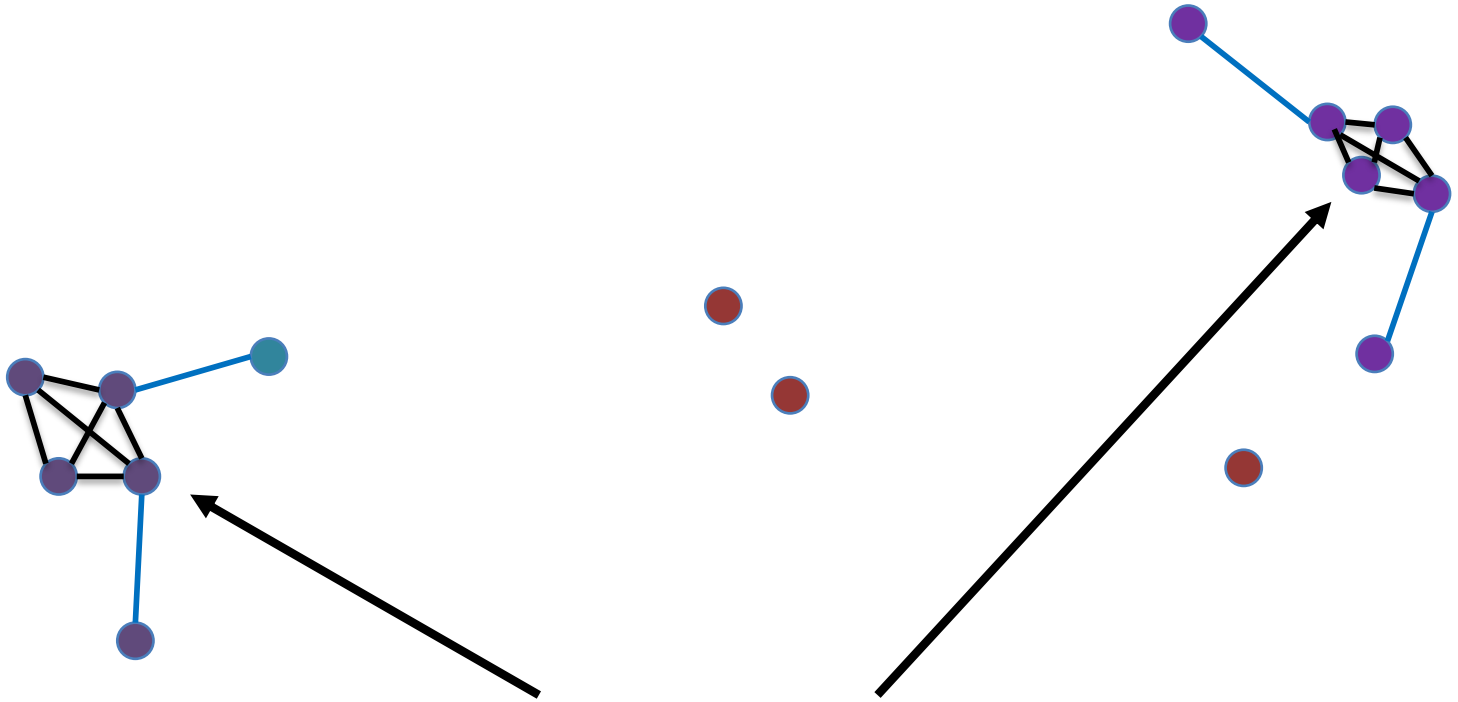
At each iteration, each point broadcasts the minimum ID value which they can “see” to all connected neighbors.

Parallel DBSCAN

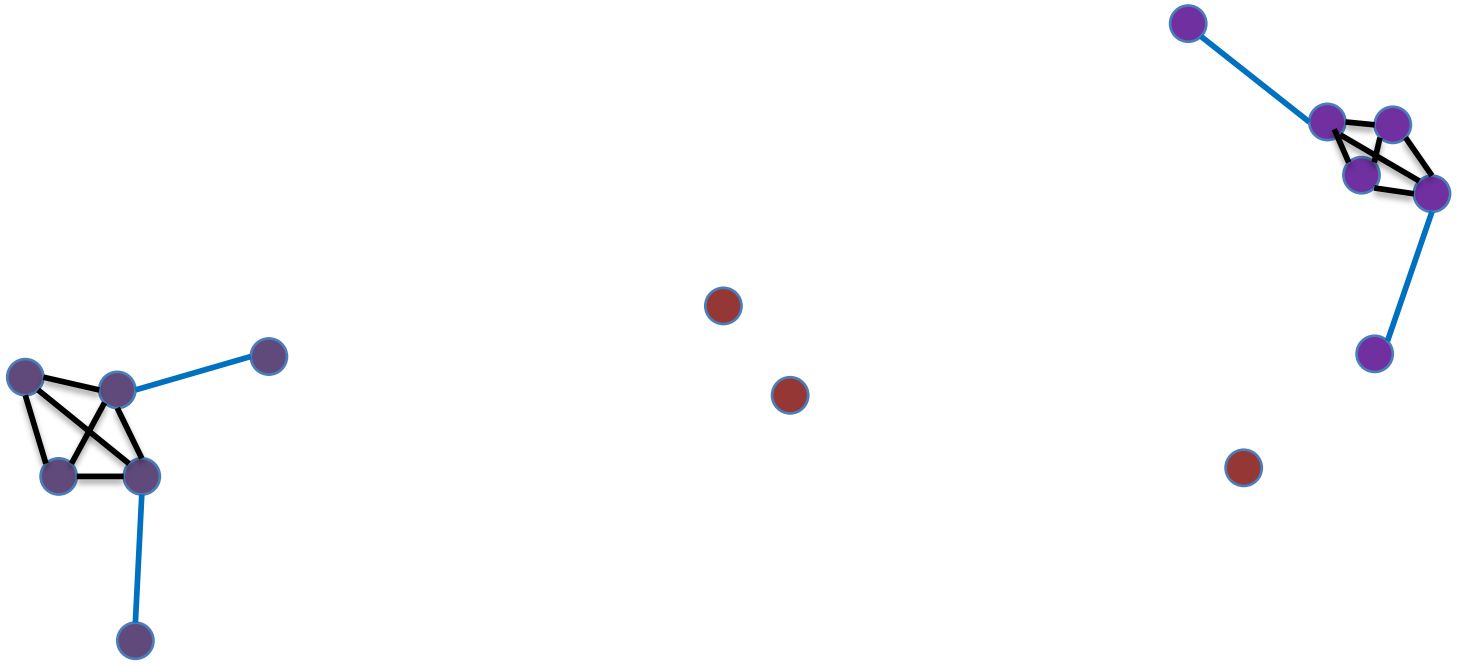


The minimum ID value for each cluster spreads across the graph.

Parallel DBSCAN

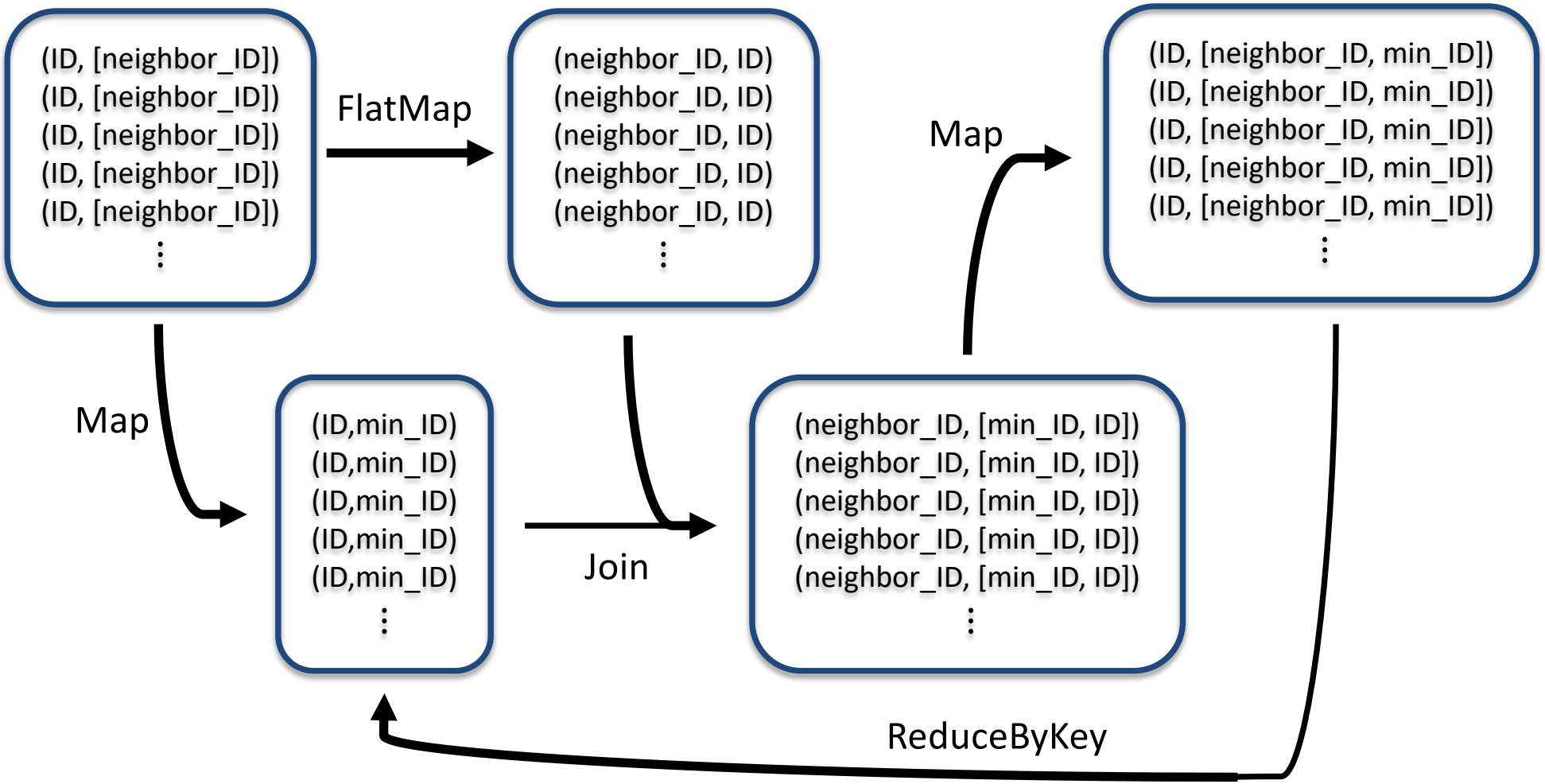


Parallel DBSCAN

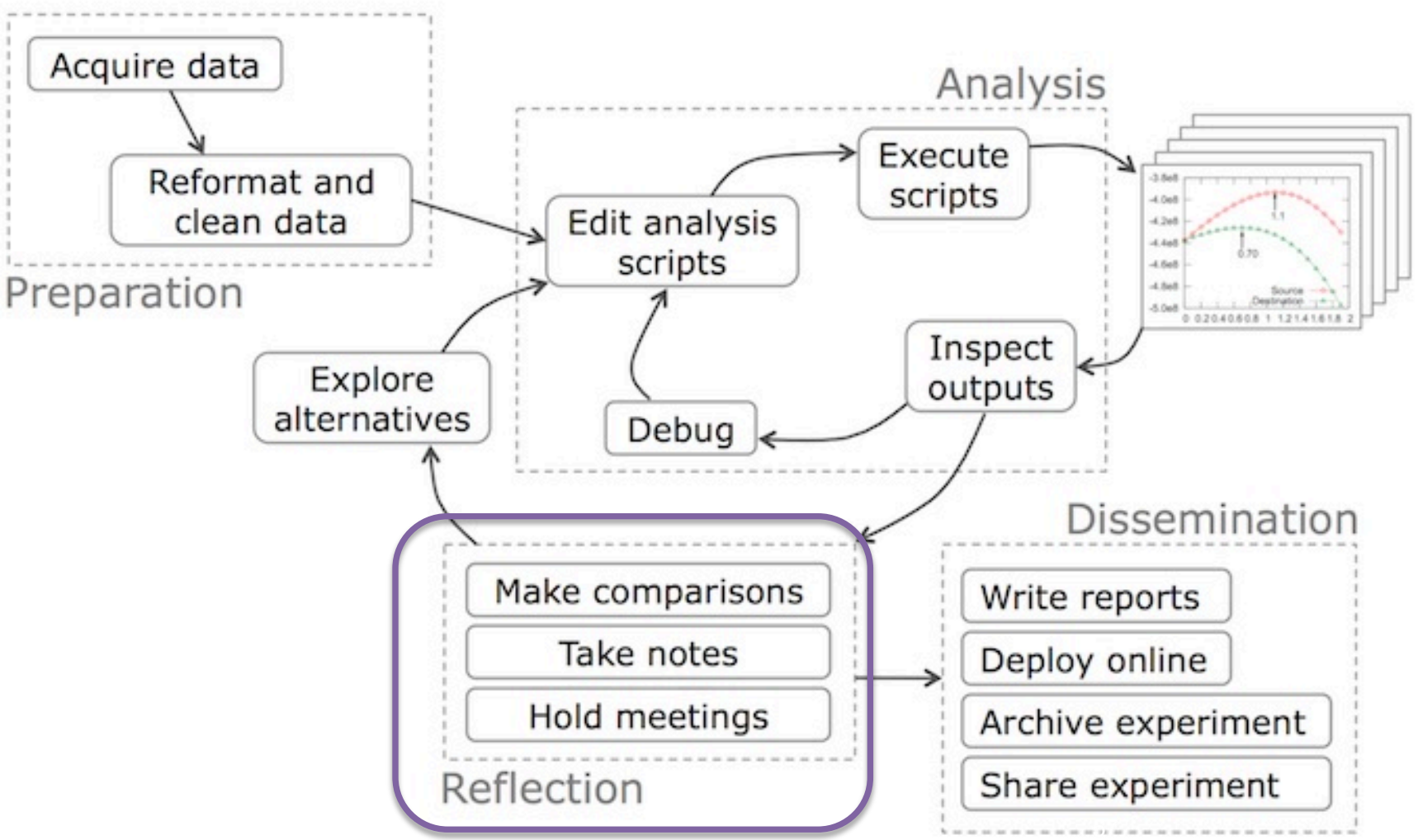


Parallel DBSCAN

Parallel DBSCAN with Spark



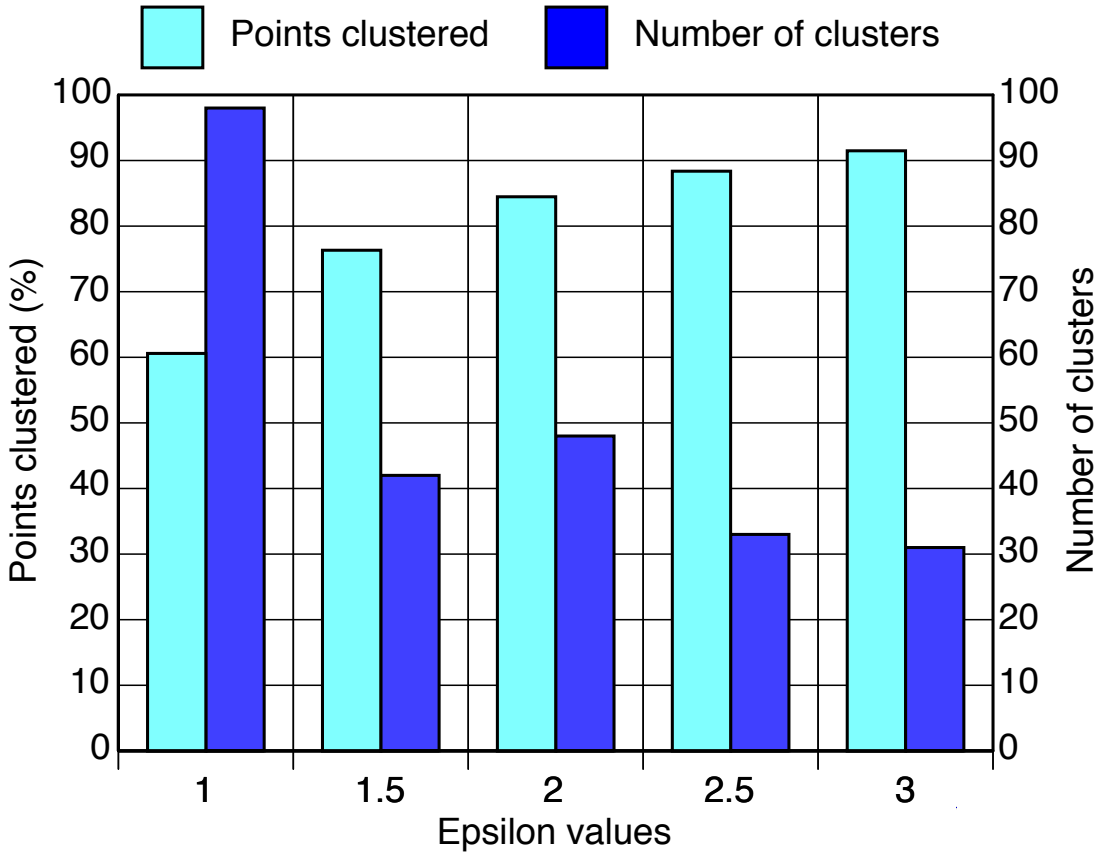
Data Workflow



Courtesy of Philip Guo: goo.gl/y42rp1

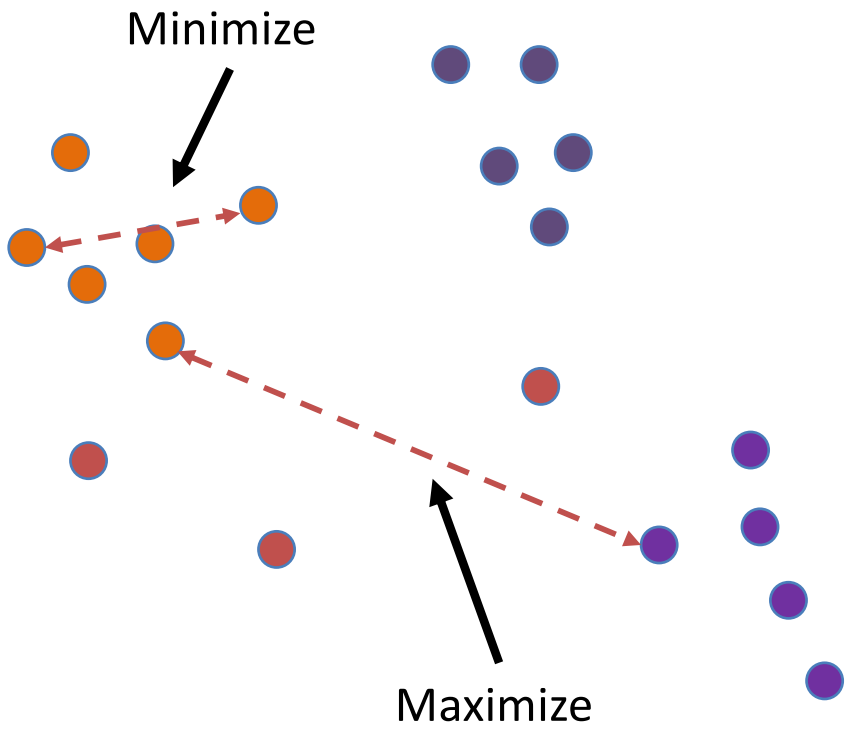
Experiment Setting and Metrics

- DBSCAN settings:
  - Epsilon = 1.0
  - Min_pts = 4
  - Euclidean distance



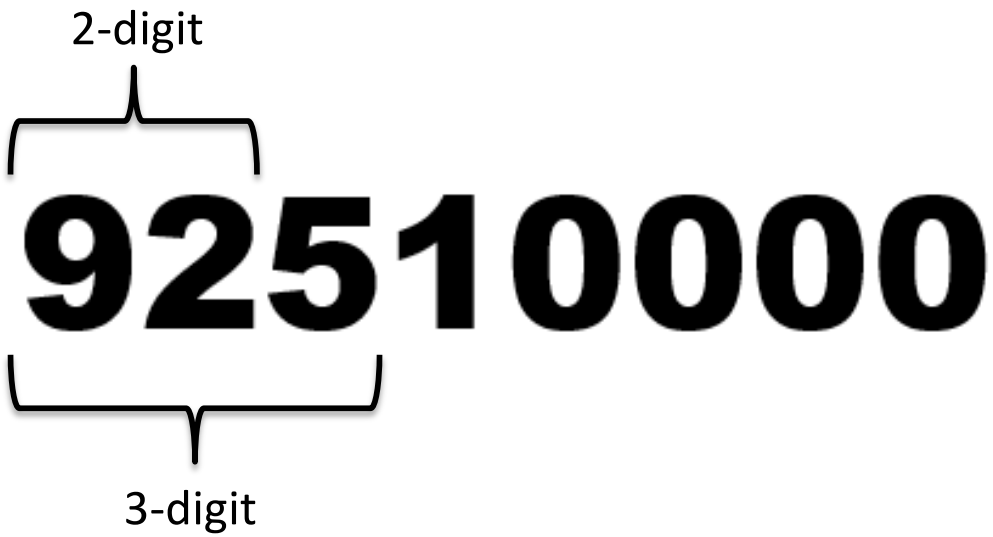
Experiment Setting and Metrics

- DBSCAN settings:
  - Epsilon = 1.0
  - Min_pts = 4
  - Euclidean distance
- Metrics of success:
  - Cluster diameter (min)
  - Cluster separation (max)

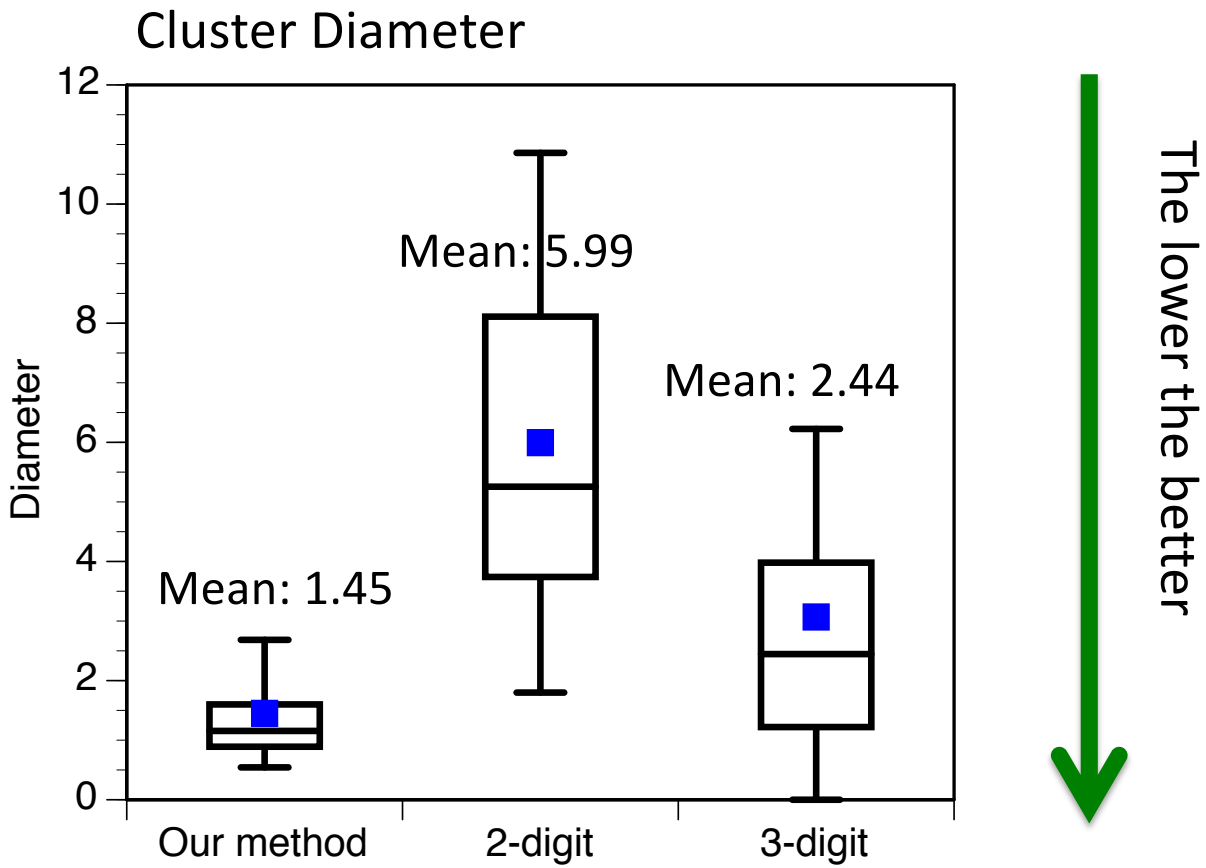


Experiment Setting and Metrics

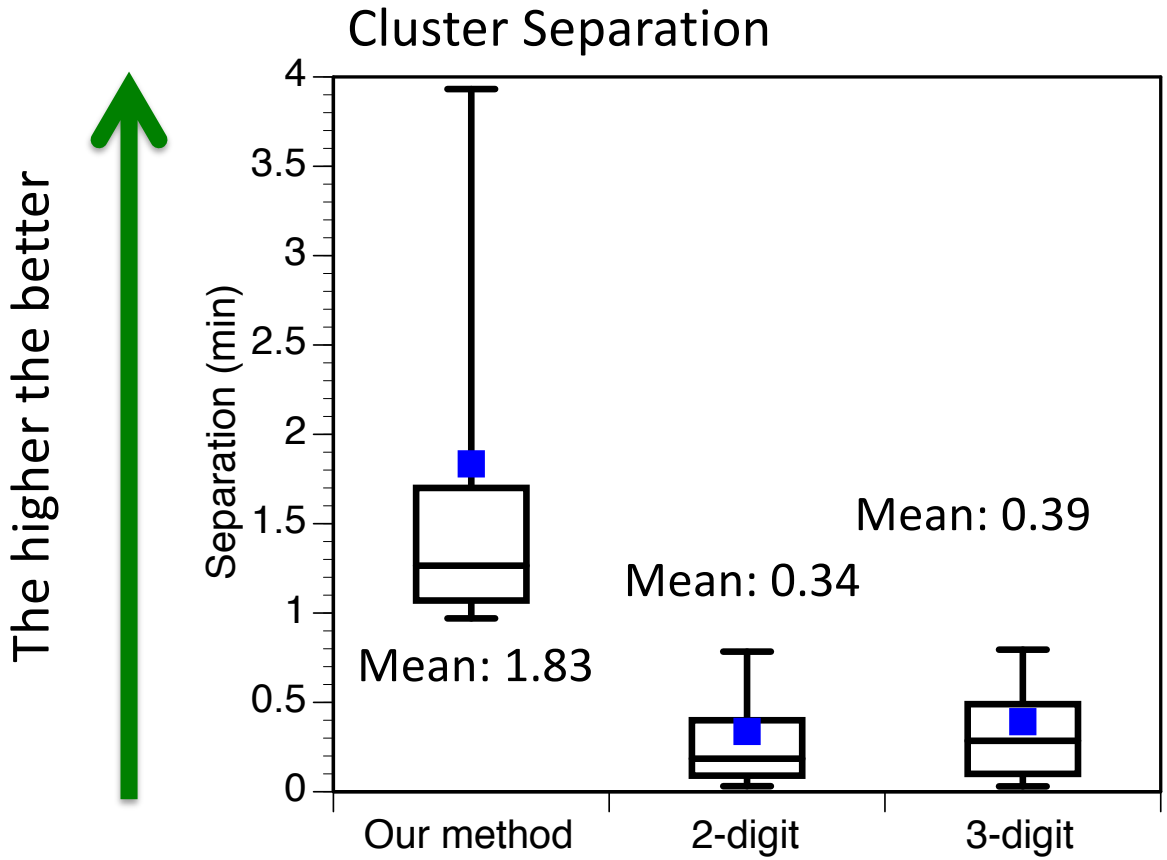
- DBSCAN settings:
  - Epsilon = 1.0
  - Min_pts = 4
  - Euclidean distance
- Metrics of success:
  - Cluster diameter (min)
  - Cluster separation (max)
- Comparisons:
  - **Our clustering**
  - **USDA code clustering with 2-digit code**
  - **USDA code clustering with 3-digit code**



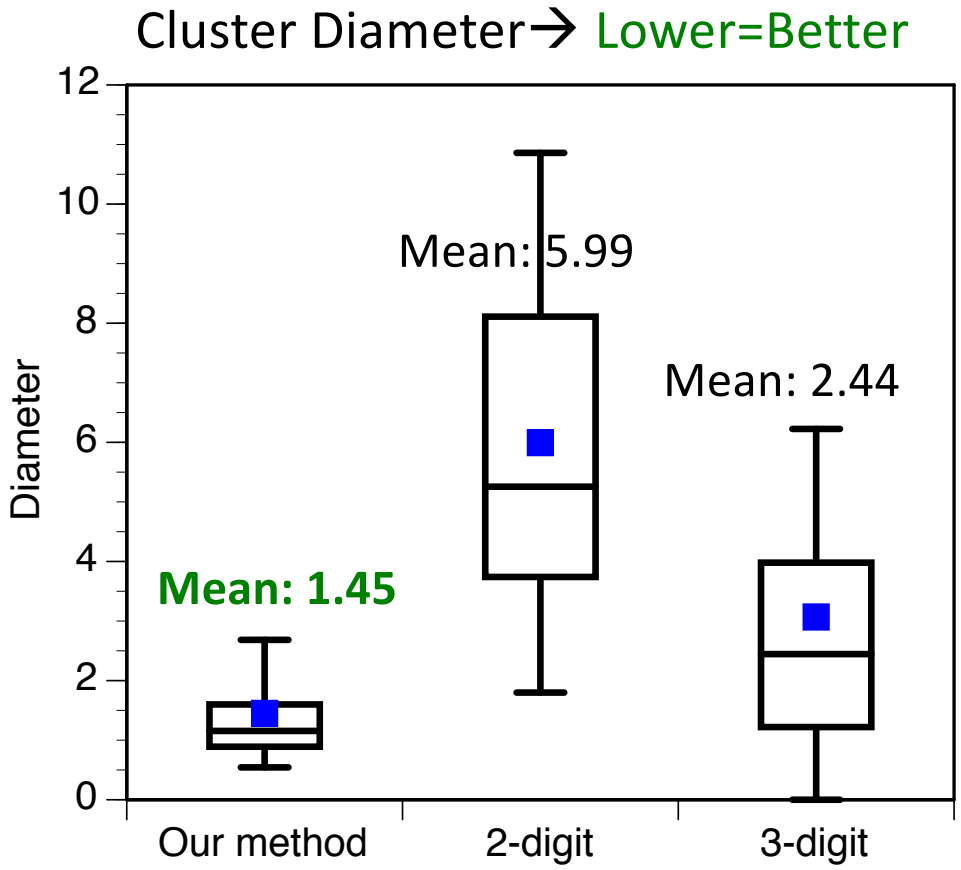
Clustering Results

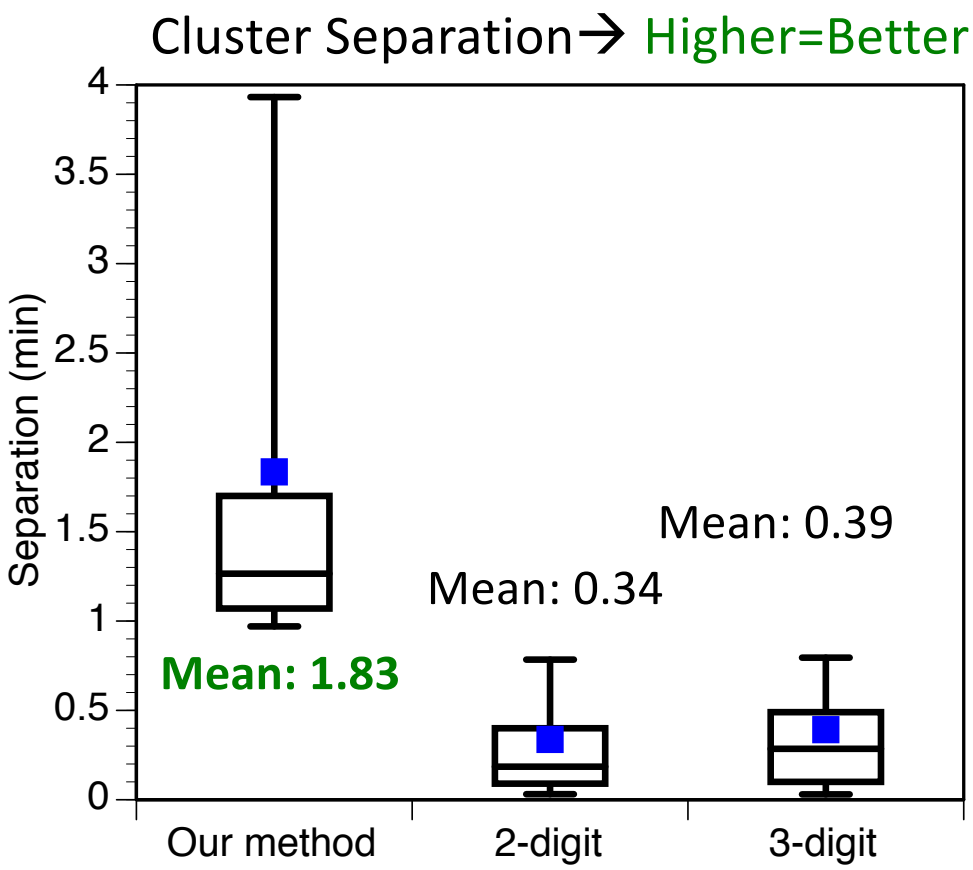


Clustering Results

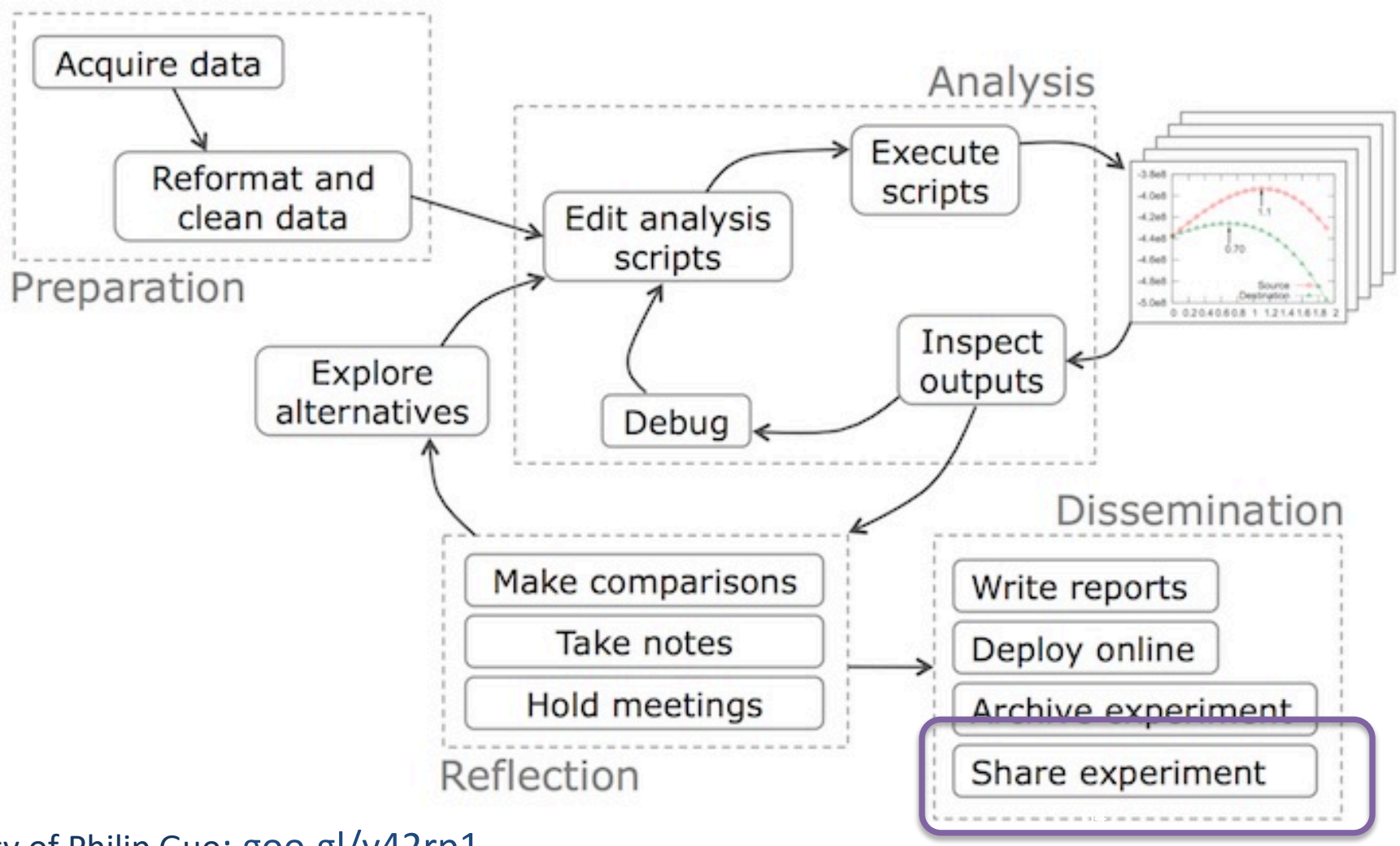


Clustering Results





Data Workflow



Courtesy of Philip Guo: goo.gl/y42rp1

Lessons Learned

- Using the traditional USDA classification of food items is misleading and can poorly advise patients with health issues

  "Eat less fat!" "but USDA codes aren't based on nutrient content!"
- We propose a comprehensive data analysis workflow for NHANES dietary data
- Our approach clusters food items based **EXCLUSIVELY** on their nutritional content (i.e., micro- and macro-nutrients)
- Our methods is **scalable** (based on MapReduce) and produces **denser** and **better separated** food groups than USDA
  - Denser cluster diameter: 1.45 vs. 5.99 and 3.07
  - Better separated cluster separation: 1.83 vs. 0.34 and 0.39
- Our approach can provide a better indication of food group quality when advising patients with dietary restrictions

Assignment 7

- Problem 1: Measure metrics to characterize clusters
  - *Define the functions that intake food clusters and returns percentage of food items clustered and number of food clusters found*
- Problem 2: Plot a heatmap
  - *Define the function that intakes a 2D array and plots a heatmap*
- Problem 3: Recreate Figure 6 from the paper
  - *Cluster food items with the **Euclidean distance metric** and epsilon and min_pts values in ranges [2,4] and [4,7], respectively*

Assignment 7 (II)

- Problem 4: Visualize n-dimension spaces
  - *Project the data down to 2 dimensions and visualize the clusters*
- Problem 5: Euclidian, or not Euclidian, “that is the question”
  - *Use the given code to examine the clusters found using DBSCAN and Cosine Similarity and compare with clusters found using the Euclidian distance*

DUE DATE: October 29, 2018 8AM ET

Project (I)

- What is your dataset?
- What are the scientific questions want to answer?
- What is the tentative methodology?
- What are the metrics of success?
- What are the milestones you want to meet from now until Dec 3 when you will present your poster at the poster showcase?

DUE DATE: October 29, 2018 8AM ET

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