Introduction to Clustering

CSCI 347

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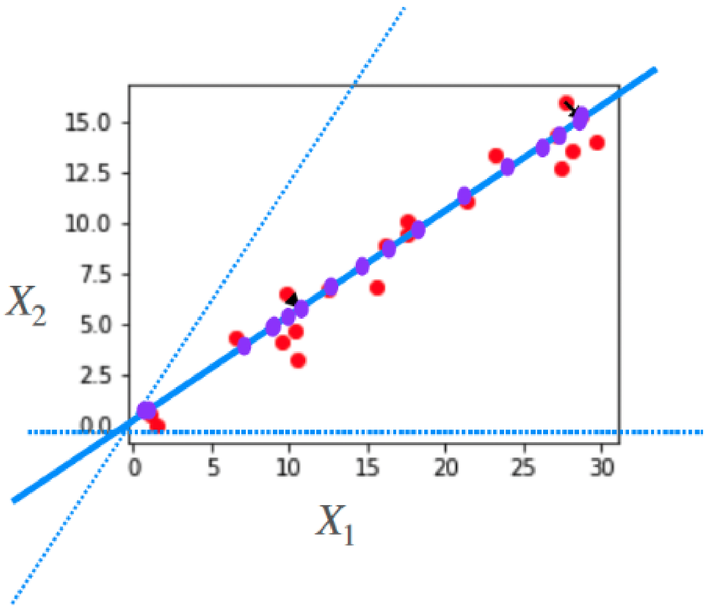
PCA summary

- A good “go-to” method for dimensionality reduction.
  - Advantages
    - Preserves a large fraction of the total variance.
    - Creates independent (uncorrelated) new attributes
    - Fast (very useful on large datasets)
  - Disadvantages
    - Not Interpretable (what does $0.8X_1 + 2X_2$ mean?)
    - Sensitive to scaling (need to do standardization or normalization)
    - Fails to capture nonlinear relationships.

Data often lies close to one dimensional linear space



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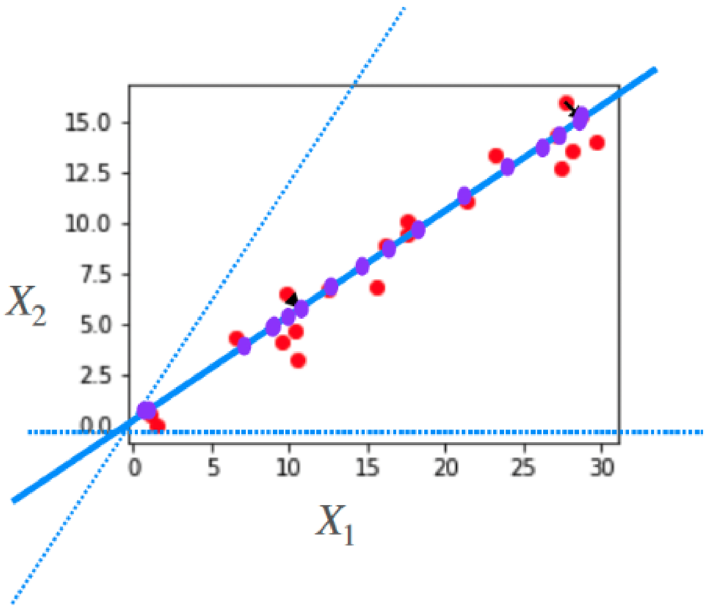

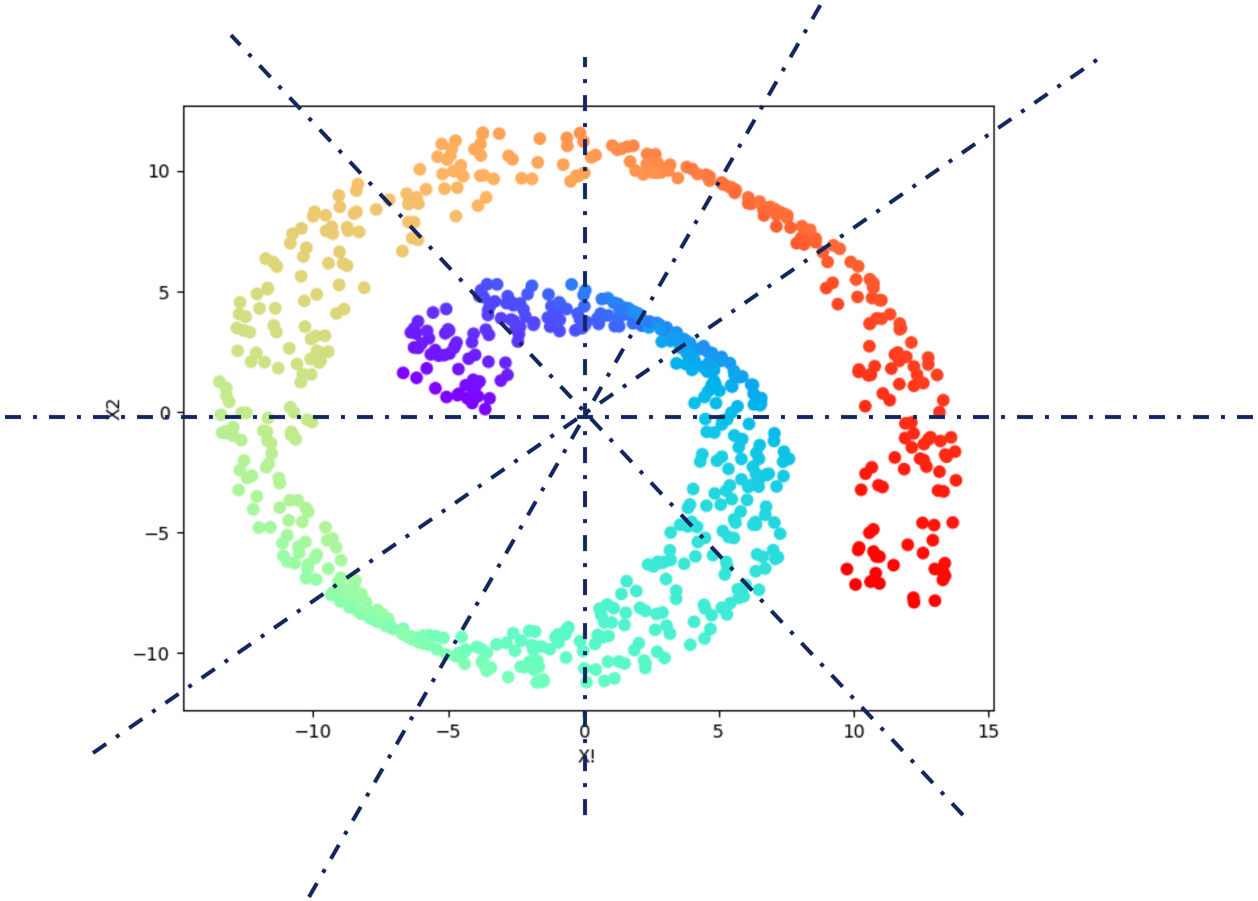

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What can we use for nonlinear dimensionality reduction?

- Kernel PCA
- Laplacian eigenmaps
- Locally linear embedding (*)
- T-SNE (t-distributed Stochastic Neighbor Embedding)
    - Looks at local structure
    - It converts the high-dimensional Euclidean distances between data points into conditional probabilities that represent similarities.
- UMAP (Uniform Manifold Approximation and Projection)
    - based on the idea that high-dimensional data often lies on or near a lower-dimensional manifold.
- ISOMAP (Isometric Mapping)
    - Aims to preserve the geodesic distances between data points.
    - Geodesic Distance: measures the shortest distance along the curved manifold.
    - ISOMAP assumes that the data lies on or near a lower-dimensional manifold embedded in a high-dimensional space. It tries to "unfold" this manifold to reveal its true structure.

Locally linear embedding

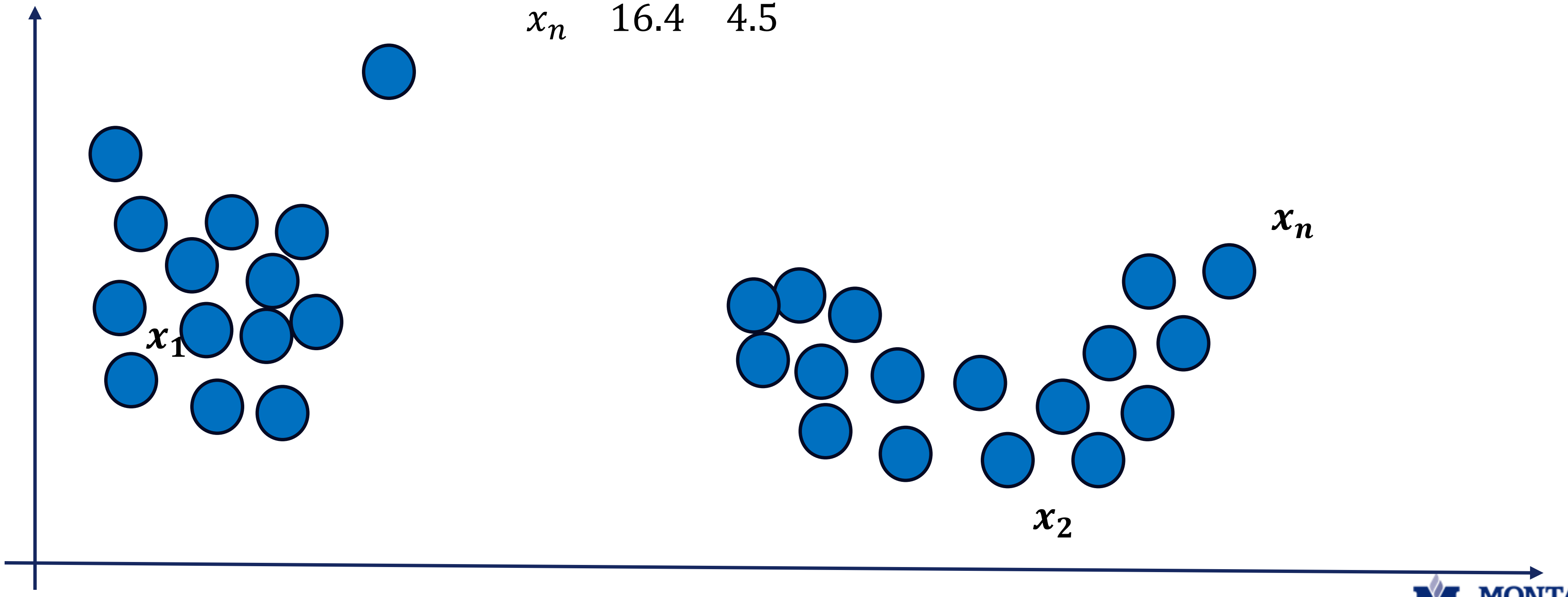
Key Concepts:

- Local Linearity: LLE assumes that the data is locally linear, meaning that each data point can be approximated as a linear combination of its neighbors.
- Neighborhood Preservation: The primary goal of LLE is to preserve the local neighborhood relationships in the low-dimensional embedding.
- Points that are close together in the high-dimensional space should remain close in the low-dimensional space.
- Weight Matrix: LLE constructs a weight matrix that captures the contribution of each neighbor in reconstructing a data point from its neighbors.
- Let’s look at an example for this.

What are clusters in a dataset

Data Matrix

	X_1	X_2
x_1	2	3.2
x_2	13.1	0.9
$\vdots$	$\vdots$	$\vdots$
x_n	16.4	4.5



Clustering

- Clustering is the task of partitioning the points into natural groups.
- These natural groups are called clusters.
- Points within these clusters are very similar, whereas points across clusters are dissimilar as possible.

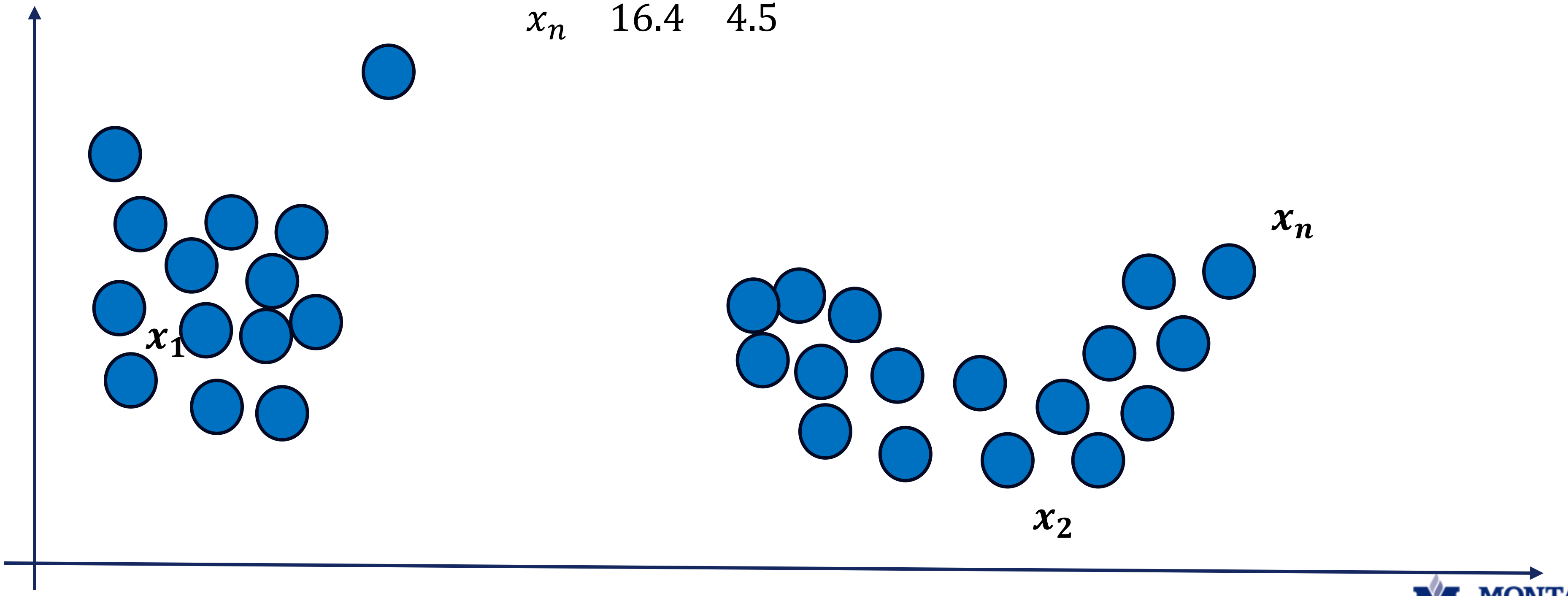
Applications of clustering

Movies

Data Matrix

People

$$\begin{array}{ccc} & X_1 & X_2 \\ x_1 & 2 & 3.2 \\ x_2 & 13.1 & 0.9 \\ \vdots & \vdots & \vdots \\ x_n & 16.4 & 4.5 \end{array}$$



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Applications of clustering

Samples

Data Matrix

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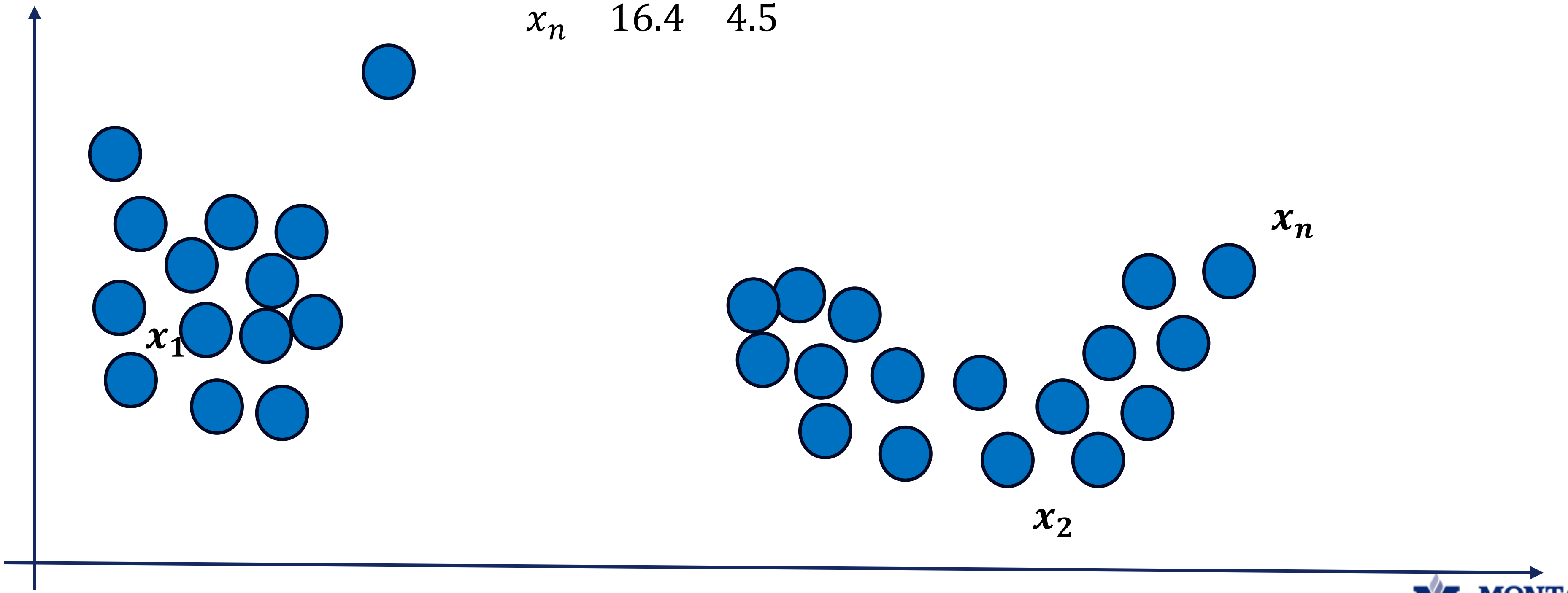

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Applications of clustering

Data Matrix

Words

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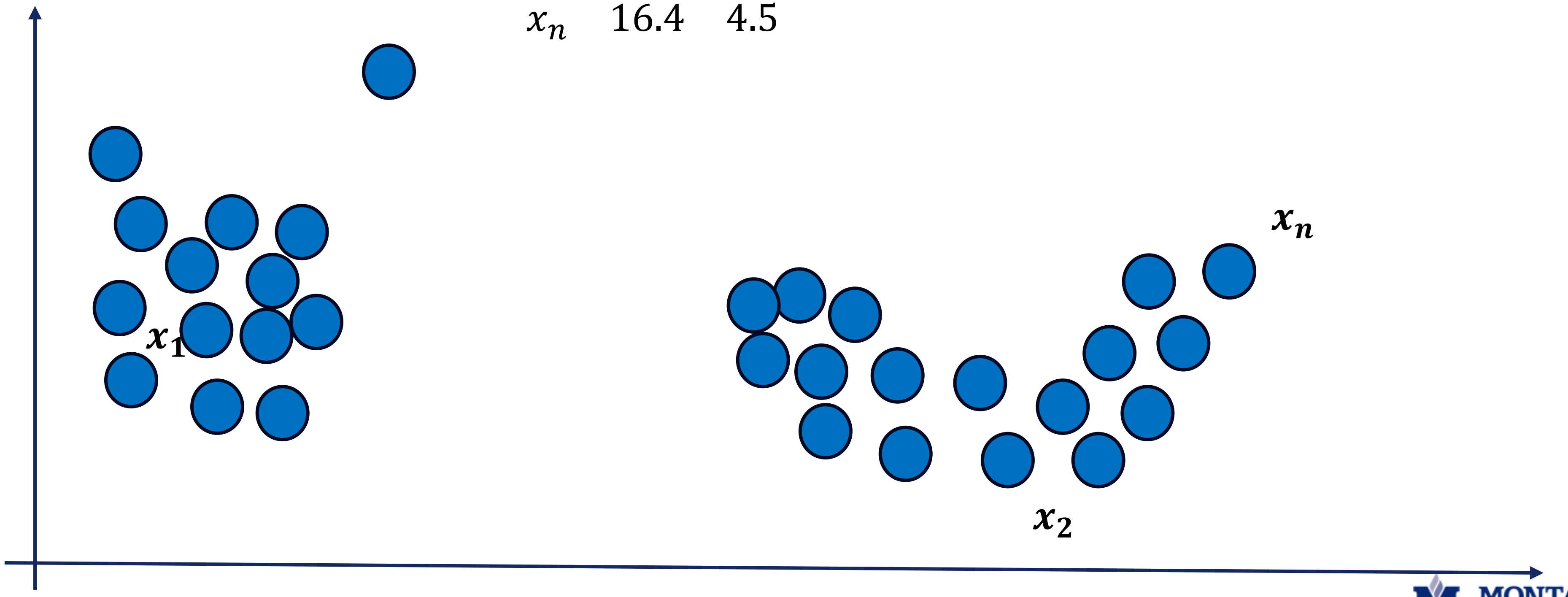

How do we find clusters in a dataset?

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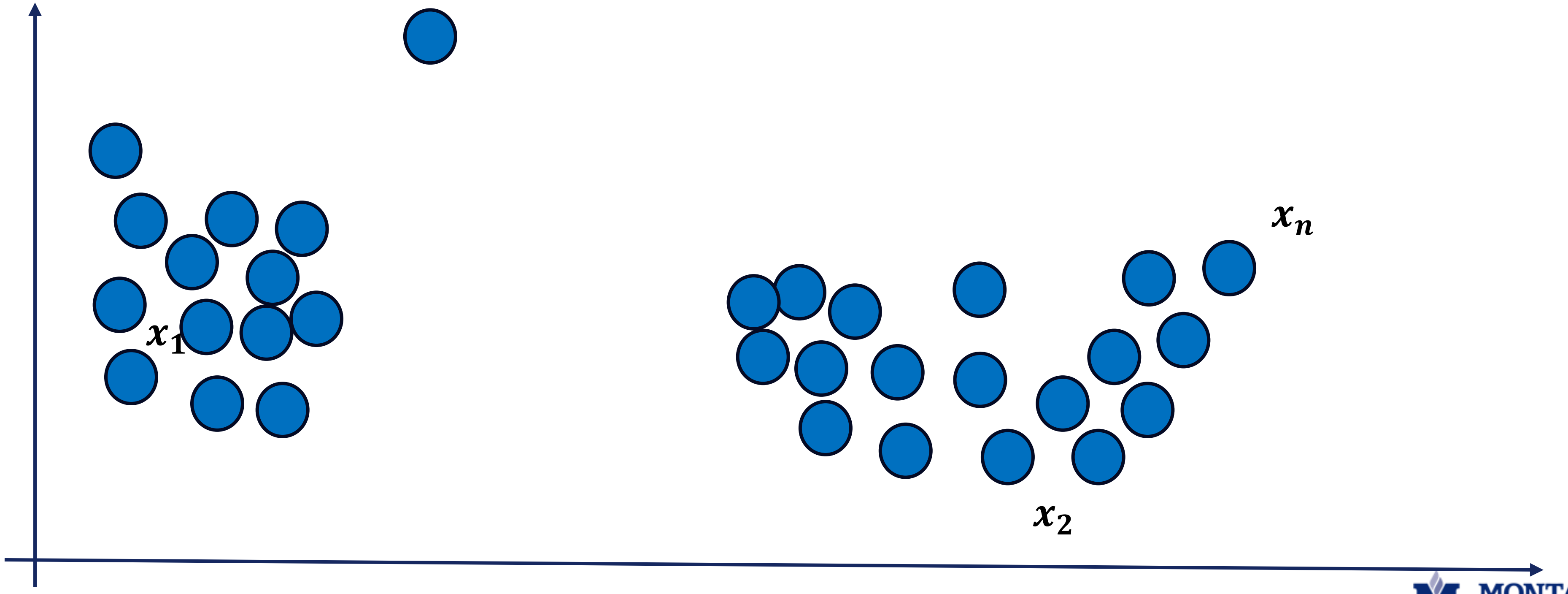
Our goal is to gather data instances into groups with high within-group similarity



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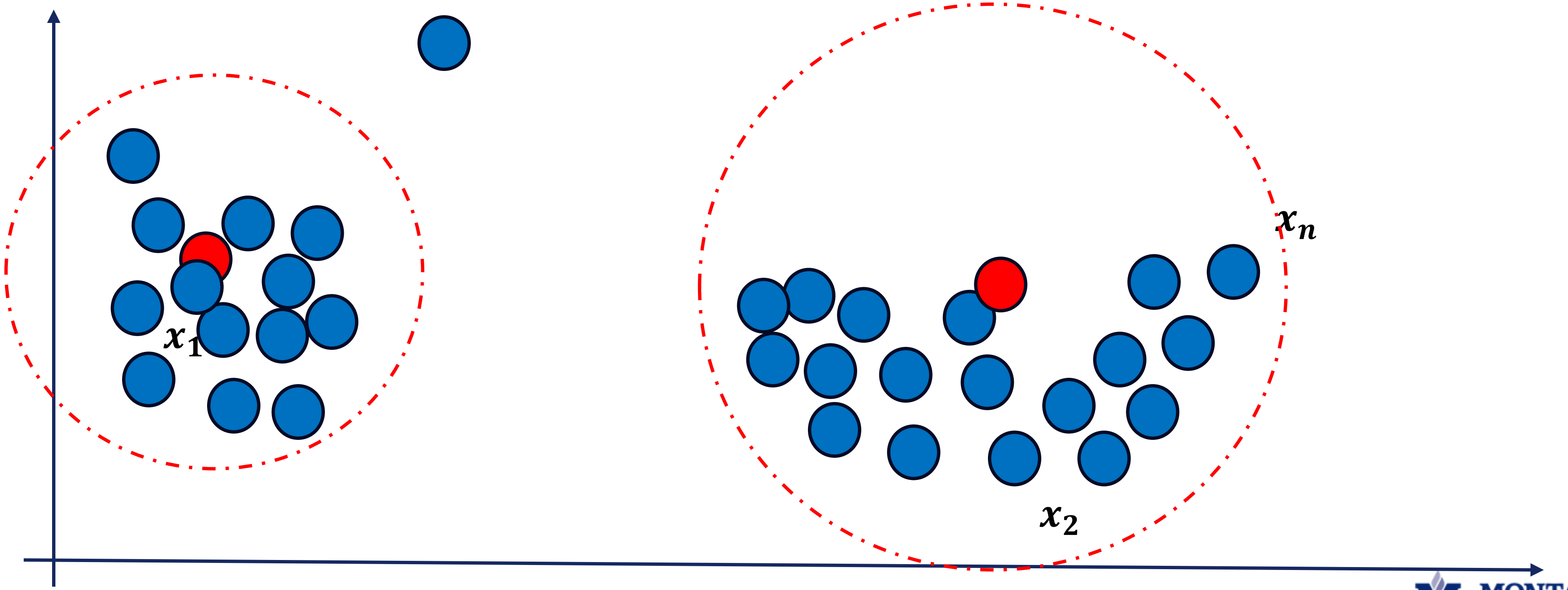
Representative-based methods

Find a representative that best represents each cluster, and group points based on their closest representative.



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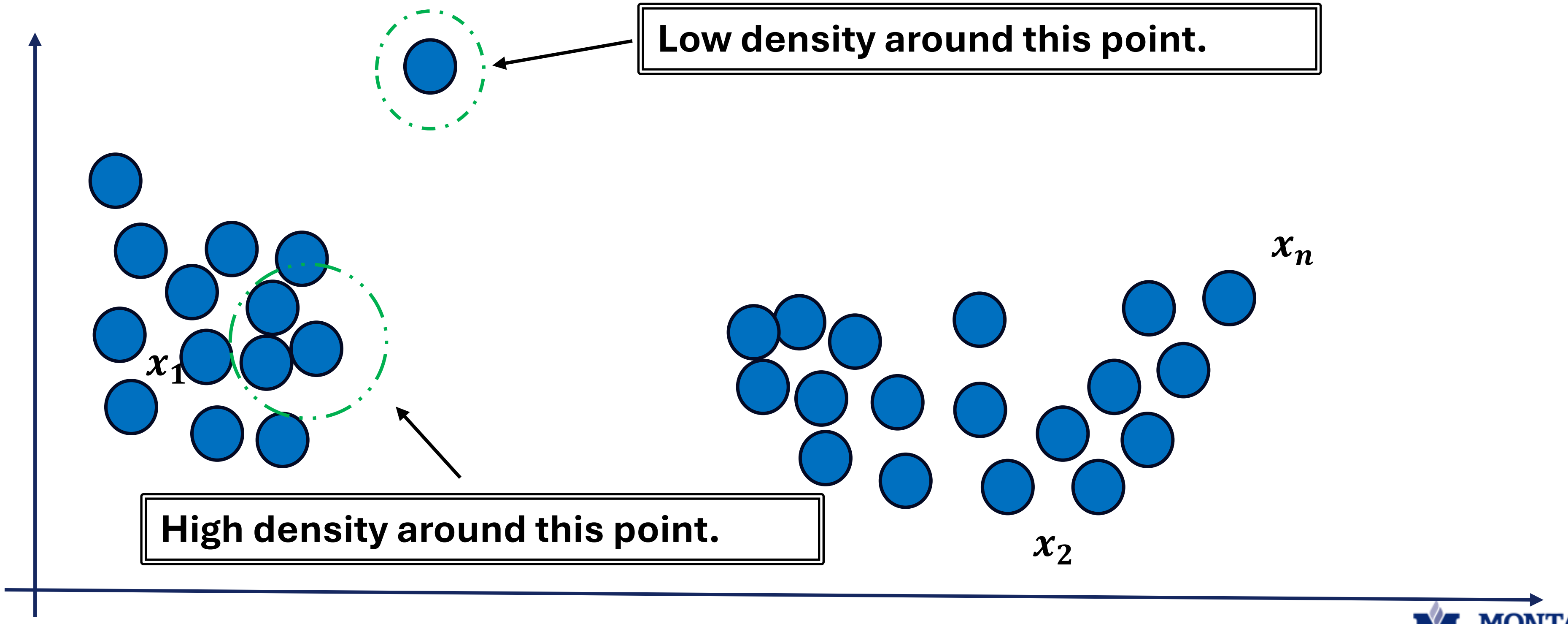
Density-based methods:

Find regions of high density (# points / some small volume)



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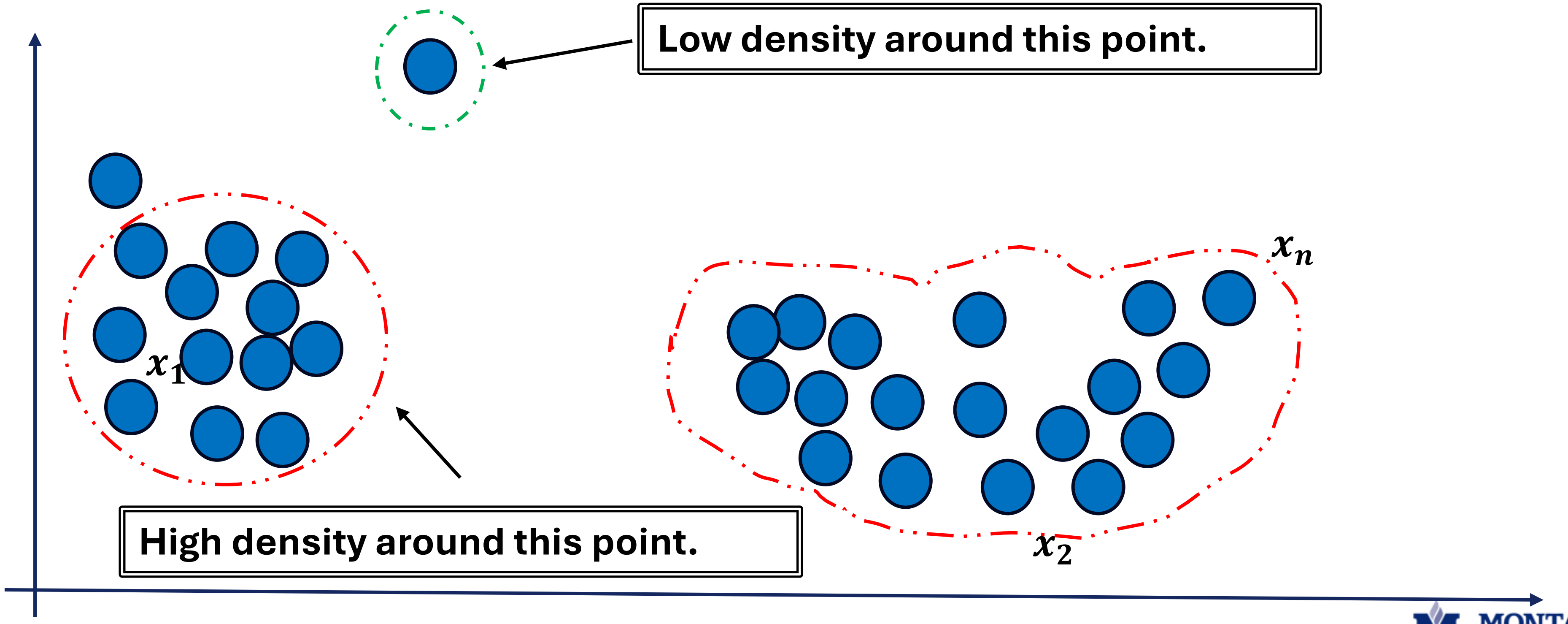

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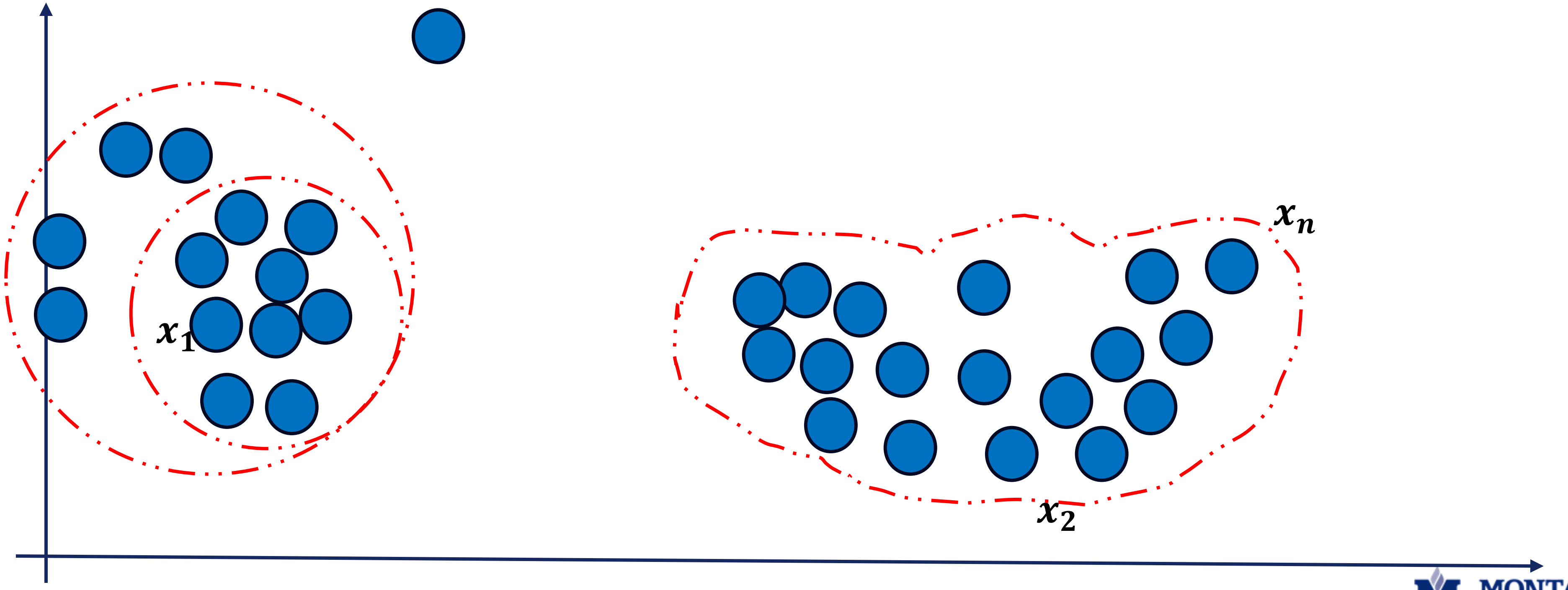
Hierarchical methods:

Clusters within clusters



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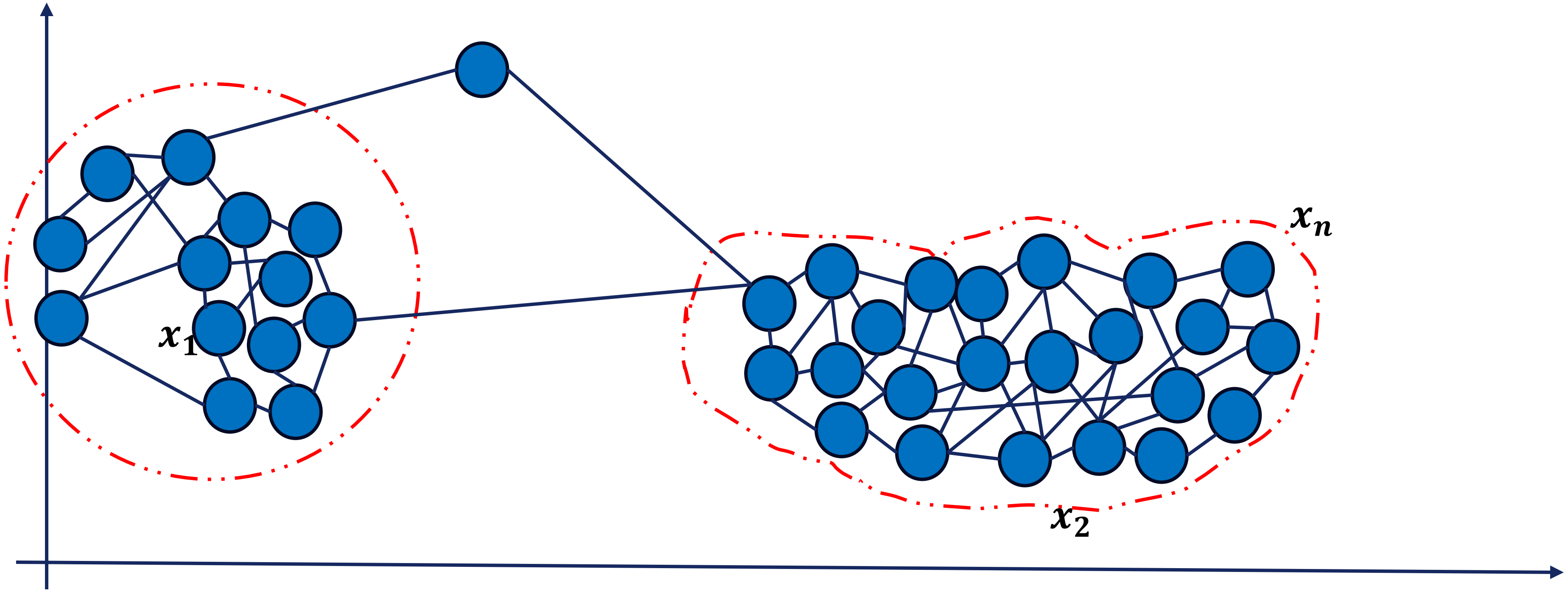
$\vdots$	$\vdots$	$\vdots$
x_n	16.4	4.5

$$\longrightarrow$$

$$\begin{array}{c|cccc} & x_1 & x_2 & \cdots & x_n \\ \hline x_1 & 0 & 0 & \cdots & 0 \\ x_2 & 0 & 0 & \cdots & 1 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_n & 0 & 0 & \cdots & 0 \end{array}$$

Graph based methods:

Find subgraphs with high edge connectivity



How do we find clusters in a dataset?

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⋮	⋮	⋮
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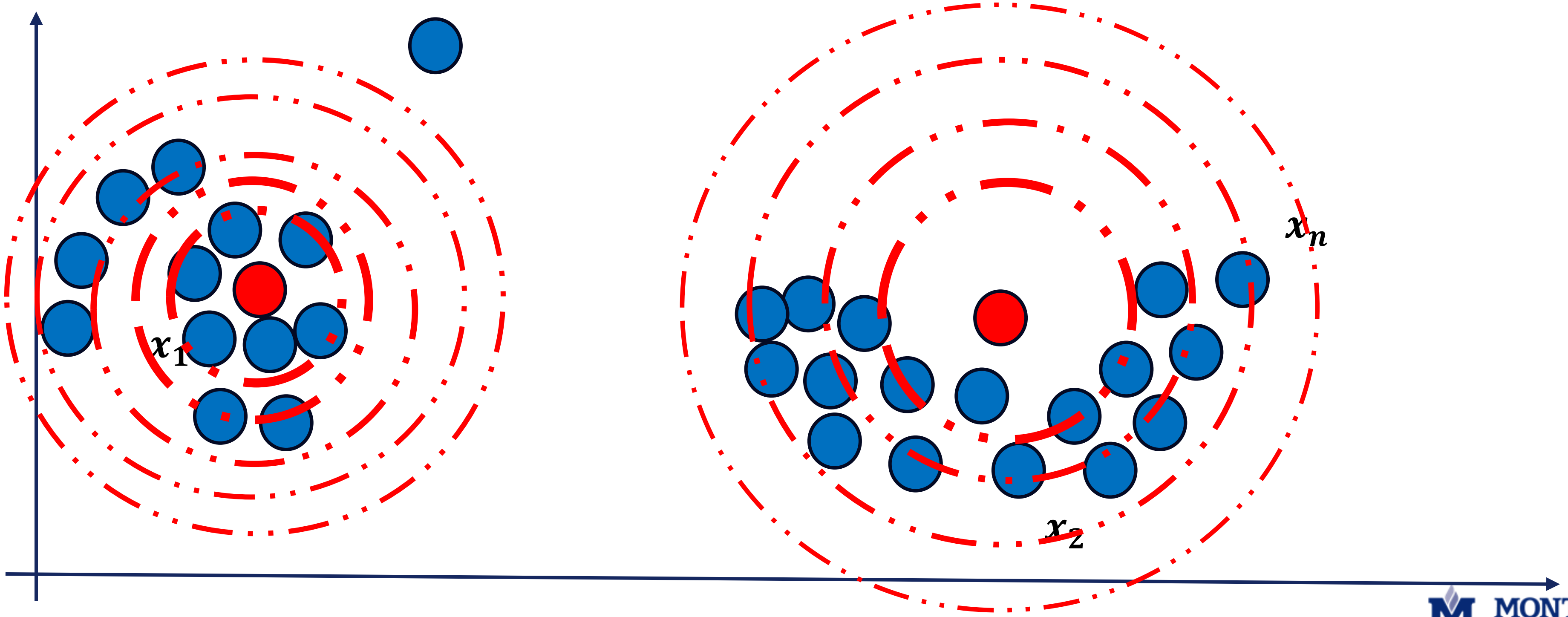
Soft clustering or probabilistic clustering

Estimate the probability distribution that the points come from



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	X_1
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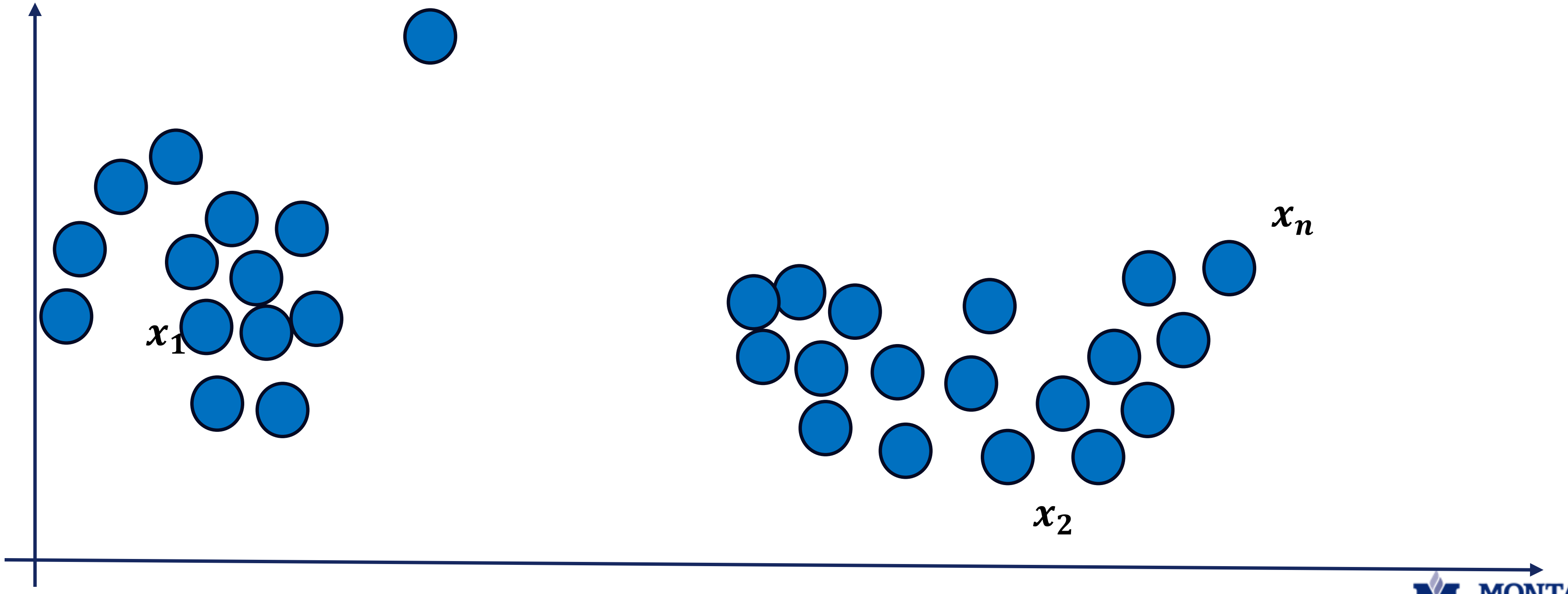
Spectral or subspace clustering methods:

Find a lower dimensional space that better represents the clusters



Clustering techniques

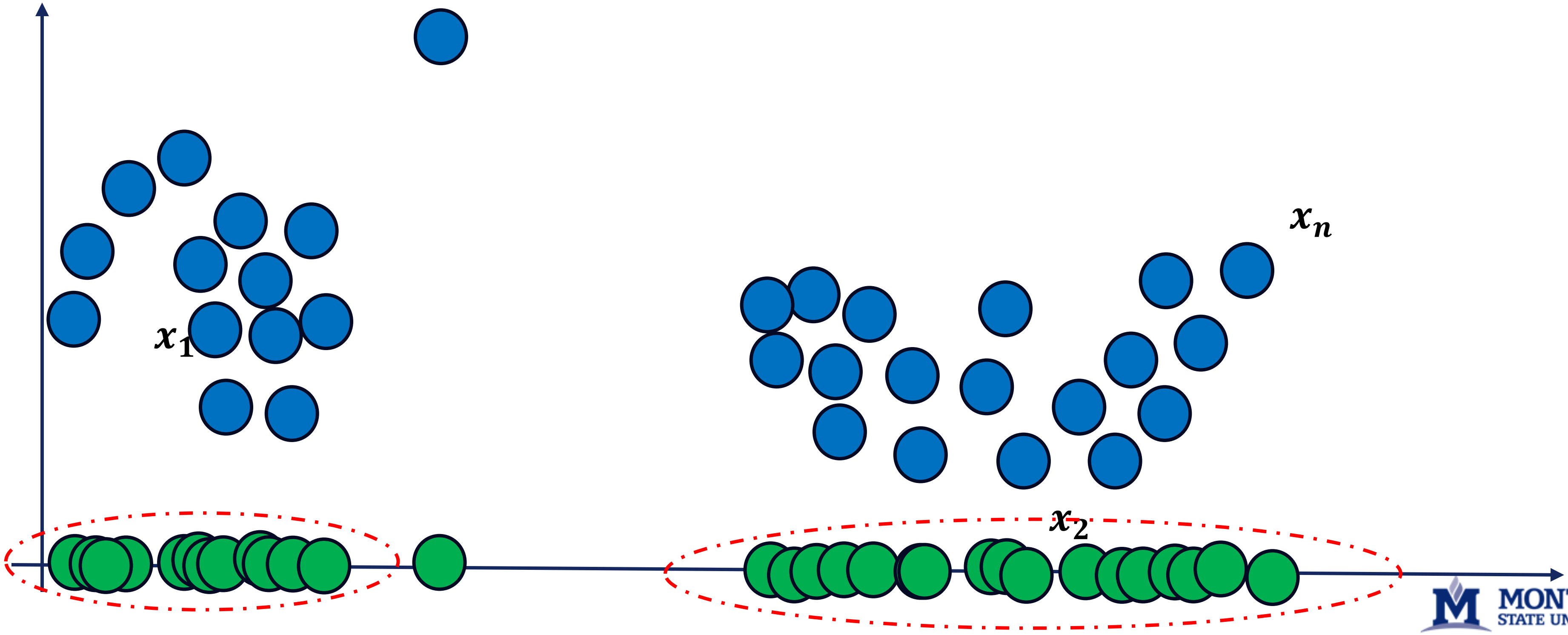
	X_1	X_2
x_1	2	3.2
x_2	13.1	0.9
$\vdots$	$\vdots$	$\vdots$
x_n	16.4	4.5

$\Rightarrow$

	X_1
x_1	2
x_2	13.1
$\vdots$	$\vdots$
x_n	16.4

Spectral or subspace clustering methods:

Find a lower dimensional space that better represents the clusters



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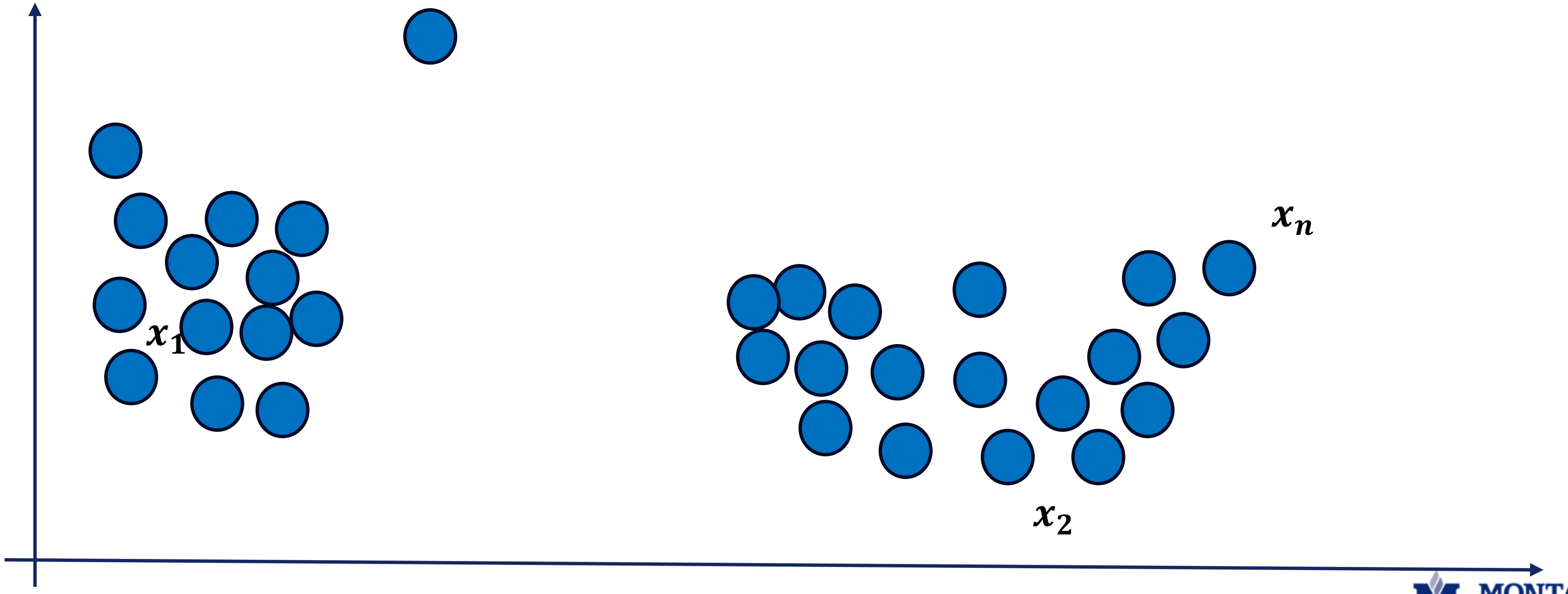
Clustering technique

Foundations
- Representative-based method
- Density-based methods
- Hierarchical methods
- Spectral methods
- Graph-based methods

Advanced topics and applications
- Subspace clustering
- Core sets
- Deep learning
- Document clustering
- Clustering for outlier detection



Clustering

- Clustering is broadly and vaguely defined as finding groups of similar entities in a dataset.
- In this class we will learn several clustering techniques and how to validate clustering that we do.
- K-means is a representative-based algorithm that finds a specified number of k of clustering.