Lecture 17:

Clustering and Unsupervised Learning Fundamentals

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Lecture Contents

Part 1/4:

Unsupervised Learning Overview

1. What is Unsupervised Learning?
2. Supervised vs Unsupervised vs Semi-supervised
3. Applications of Unsupervised Learning
4. Key Challenges and Evaluation Methods
5. Data Preprocessing and Scaling

Supervised Learning

- Labeled training data
- Explicit target variables
- Learning from examples
- Ground truth labels

Unsupervised Learning

- Unlabeled data only
- No target variables
- Discover hidden patterns
- Self-directed insights

Three Main Categories of Unsupervised Learning

Clustering

Group similar data points together

Dimensionality Reduction

Reduce feature space complexity

Anomaly Detection

Identify unusual patterns

Supervised Learning

DATA TYPE

Labeled data (X, y)

GOAL

Predict y from X

- ✓ Requires labeled data
- ✓ High accuracy
- ✓ Expensive labeling
- ✓ Domain expertise needed

Labeling Cost

Unsupervised Learning

DATA TYPE

Only X (unlabeled)

GOAL

Find structure in X

- ✓ No labels needed
- ✓ Discover patterns
- ✓ Highly scalable
- ✓ Cost-effective

Labeling Cost

Semi-supervised Learning

DATA TYPE

Small labeled + Large unlabeled

GOAL

Leverage both data types

- ✓ Best of both worlds
- ✓ Balanced approach
- ✓ Practical solution
- ✓ Often best results

Labeling Cost

Unsupervised Learning Applications

Customer Segmentation
Group customers by behavior patterns

Anomaly Detection
Fraud detection, intrusion detection

Recommendation Systems
Find similar items without ratings

Image Compression
Reduce dimensionality efficiently

Market Basket Analysis
Discover product associations

Document Clustering
Organize articles and papers

Biological Analysis
Gene expression patterns

Feature Engineering
Create better features for models

Evaluation Framework for Unsupervised Learning

Key Challenge

No ground truth available
Cannot compute accuracy

Evaluation Question

What makes a 'good' clustering?

Internal Metrics

- Silhouette Score
- Davies-Bouldin Index
- Inertia

External Metrics

When labels available:

- ARI (Adjusted Rand Index)
- NMI (Normalized Mutual Info)
- Purity

Visual Inspection

Plot clusters in 2D/3D space

Domain Validation

Do clusters make business sense?

Stability Analysis

Consistent results across runs?

Interpretability

Can we explain patterns?

Data Preprocessing and Scaling

⚠ **Feature scaling is critical: Distance-based algorithms are sensitive to scale**

Scaling Methods

StandardScaler

```
z = (x - μ) / σ
```

- ✓ Zero mean
- ✓ Unit variance
- ✓ Assumes Gaussian

MinMaxScaler

```
x' = (x - min) / (max - min)
```

- ✓ Scale to [0, 1]
- ✓ Preserves zero
- ✓ Bounded range

RobustScaler

```
x' = (x - median) / IQR
```

- ✓ Uses median
- ✓ Uses IQR
- ✓ Robust to outliers

Preprocessing Pipeline

1. **Missing Values**
   Imputation before clustering
2. **Outlier Treatment**
   Remove or cap extremes
3. **Feature Selection**
   Remove irrelevant features
4. **Dimensionality**
   Handle curse of dimensions

Calculation Examples

StandardScaler Example

Data: [10, 20, 30, 40, 50]

μ = 30
σ = 14.14
For x = 10:
z = (10 - 30) / 14.14
z = -1.41

Result: [-1.41, -0.71, 0, 0.71, 1.41]

MinMaxScaler Example

Data: [10, 20, 30, 40, 50]

min = 10, max = 50
range = 50 - 10 = 40
For x = 20:
x' = (20 - 10) / 40
x' = 0.25

Result: [0, 0.25, 0.5, 0.75, 1.0]

RobustScaler Example

Data: [10, 20, 30, 40, 100]

median = 30
Q1 = 20, Q3 = 40
IQR = 40 - 20 = 20
For x = 100:
x' = (100 - 30) / 20 = 3.5

Result: [-1.0, -0.5, 0, 0.5, 3.5]

Part 2/4:

Clustering Algorithms

6. Clustering Problem Definition
7. K-Means Algorithm
8. K-Means++ Initialization
9. Hierarchical Clustering
10. DBSCAN - Density-Based
11. Mean Shift
12. Gaussian Mixture Models
13. Cluster Evaluation Metrics

Clustering Problem Definition

Core Objective

🎯 Partition n observations into k groups

⚖️ Maximize intra-cluster similarity
Minimize inter-cluster similarity

Distance Metrics: Euclidean • Manhattan • Cosine • Mahalanobis

Types of Clustering Approaches

Hard Clustering

Each point belongs to exactly one cluster

Binary membership

Soft Clustering

Points have probability distribution over clusters

Fuzzy membership

Hierarchical

Nested clusters forming tree structure

Dendrogram output

Density-Based

Clusters as high-density regions

Arbitrary shapes

Model-Based Approach

Data generated from mixture of probability distributions

K-Means Algorithm

1 Initialize

Randomly select k centroids

↓

2 Assignment Step

Assign each point to nearest centroid

↓

3 Update Step

Recompute centroids as cluster means

↓

4 Check Convergence

Stop when centroids don't move

Time Complexity

$O(n \cdot k \cdot i \cdot d)$

linear in samples and features

Strengths

- ✓ Simple to understand
- ✓ Fast computation
- ✓ Scalable to large datasets

Weaknesses

- ✗ Assumes spherical clusters
- ✗ Sensitive to initialization
- ✗ Requires pre-specified k

Finding optimal k: Use elbow method or silhouette analysis

📊 Detailed Computational Example (k=3)

0 Initial Dataset

🔢 Given 6 points in 2D space:

$P_1 = (2, 3)$ $P_2 = (3, 3)$ $P_3 = (8, 7)$ $P_4 = (9, 6)$ $P_5 = (5, 2)$

$P_6 = (6, 3)$

🎯 **Goal:** Partition these 6 points into k=3 clusters

1 Initialize Centroids

🎲 Randomly selected initial centroids:

$C_1 = (2, 3)$ $C_2 = (8, 7)$ $C_3 = (5, 2)$

In practice, we randomly select k points from the dataset as initial centroids

2 Iteration 1 - Assignment Step

Calculate Euclidean distances from each point to all centroids:

For P_1 = (2, 3):

$d(P_1, C_1) = \sqrt{[(2-2)^2 + (3-3)^2]} = \sqrt{[0 + 0]} = 0.00$

$d(P_1, C_2) = \sqrt{[(2-8)^2 + (3-7)^2]} = \sqrt{[36 + 16]} = 7.21$

$d(P_1, C_3) = \sqrt{[(2-5)^2 + (3-2)^2]} = \sqrt{[9 + 1]} = 3.16$

→ **Assign P_1 to Cluster 1 (minimum distance: 0.00)**

For P_2 = (3, 3):

$d(P_2, C_1) = \sqrt{[(3-2)^2 + (3-3)^2]} = \sqrt{[1 + 0]} = 1.00$

$d(P_2, C_2) = \sqrt{[(3-8)^2 + (3-7)^2]} = \sqrt{[25 + 16]} = 6.40$

$d(P_2, C_3) = \sqrt{[(3-5)^2 + (3-2)^2]} = \sqrt{[4 + 1]} = 2.24$

→ **Assign P_2 to Cluster 1 (minimum distance: 1.00)**

For P_3 = (8, 7):

$d(P_3, C_1) = \sqrt{[(8-2)^2 + (7-3)^2]} = \sqrt{[36 + 16]} = 7.21$

$d(P_3, C_2) = \sqrt{[(8-8)^2 + (7-7)^2]} = \sqrt{[0 + 0]} = 0.00$

$d(P_3 , C_3) = \sqrt{[(8-5)^2 + (7-2)^2]} = \sqrt{[9 + 25]} = 5.83$

→ **Assign P_3 to Cluster 2 (minimum distance: 0.00)**

For P_4 = (9, 6):

$d(P_4 , C_1) = \sqrt{[(9-2)^2 + (6-3)^2]} = \sqrt{[49 + 9]} = 7.62$

$d(P_4 , C_2) = \sqrt{[(9-8)^2 + (6-7)^2]} = \sqrt{[1 + 1]} = 1.41$

$d(P_4 , C_3) = \sqrt{[(9-5)^2 + (6-2)^2]} = \sqrt{[16 + 16]} = 5.66$

→ **Assign P_4 to Cluster 2 (minimum distance: 1.41)**

For P_5 = (5, 2):

$d(P_5, C_1) = \sqrt{[(5-2)^2 + (2-3)^2]} = \sqrt{[9 + 1]} = 3.16$

$d(P_5, C_2) = \sqrt{[(5-8)^2 + (2-7)^2]} = \sqrt{[9 + 25]} = 5.83$

$d(P_5, C_3) = \sqrt{[(5-5)^2 + (2-2)^2]} = \sqrt{[0 + 0]} = 0.00$

→ **Assign P_5 to Cluster 3 (minimum distance: 0.00)**

For P_6 = (6, 3):

$d(P_6, C_1) = \sqrt{[(6-2)^2 + (3-3)^2]} = \sqrt{[16 + 0]} = 4.00$

$d(P_6, C_2) = \sqrt{[(6-8)^2 + (3-7)^2]} = \sqrt{[4 + 16]} = 4.47$

$d(P_6, C_3) = \sqrt{[(6-5)^2 + (3-2)^2]} = \sqrt{[1 + 1]} = 1.41$

→ **Assign P_6 to Cluster 3 (minimum distance: 1.41)**

Cluster 1

$P_1 = (2, 3)$

$P_2 = (3, 3)$

Cluster 2

$P_3 = (8, 7)$

$P_4 = (9, 6)$

Cluster 3

$P_5 = (5, 2)$

$P_6 = (6, 3)$

3 Iteration 1 - Update Centroids

🔄 Calculate new centroids as the mean of assigned points:

New C_1 :

Points in Cluster 1: P_1 (2,3), P_2 (3,3)

C_1 _new = ((2+3)/2, (3+3)/2) = (2.5, 3.0)

C_1 : (2, 3) → (2.5, 3.0) ✓ Changed

New C_2 :

Points in Cluster 2: P_3 (8,7), P_4 (9,6)

C_2 _new = ((8+9)/2, (7+6)/2) = (8.5, 6.5)

C_2 : (8, 7) → (8.5, 6.5) ✓ Changed

New C_3 :

Points in Cluster 3: P_5(5,2), P_6(6,3)

C_3 _new = ((5+6)/2, (2+3)/2) = (5.5, 2.5)

C_3 : (5, 2) → (5.5, 2.5) ✓ Changed

📍 Updated centroids for Iteration 2:

C_1 = (2.5, 3.0) | C_2 = (8.5, 6.5) | C_3 = (5.5, 2.5)

🔁 Centroids have moved! Continue to Iteration 2...

2 Iteration 2 - Assignment Step

📏 Recalculate distances with new centroids:

For P_1 = (2, 3):

$d(P_1, C_1) = \sqrt{[(2-2.5)^2 + (3-3)^2]} = 0.50$ ✓ min

$d(P_1, C_2) = \sqrt{[(2-8.5)^2 + (3-6.5)^2]} = 7.27$

$d(P_1, C_3) = \sqrt{[(2-5.5)^2 + (3-2.5)^2]} = 3.54$

→ Remains in Cluster 1

... (similar calculations for P_2, P_3, P_4, P_5, P_6) ...

Cluster 1

$P_1 = (2, 3)$

$P_2 = (3, 3)$

Cluster 2

$P_3 = (8, 7)$

$P_4 = (9, 6)$

Cluster 3

$P_5 = (5, 2)$

$P_6 = (6, 3)$

Result: No points changed clusters! (same as Iteration 1)

3 Iteration 2 - Update Centroids

Recalculate centroids:

$C_1\_new = ((2+3)/2, (3+3)/2) = (2.5, 3.0)$

$C_2\_new = ((8+9)/2, (7+6)/2) = (8.5, 6.5)$

$C_3\_new = ((5+6)/2, (2+3)/2) = (5.5, 2.5)$

Centroids after Iteration 2:

$C_1 = (2.5, 3.0)$ - No change

$C_2 = (8.5, 6.5)$ - No change

$C_3 = (5.5, 2.5)$ - No change

4 Check Convergence

✅ Algorithm Converged!

Condition met: Centroids did not move between iterations

- C_1: (2.5, 3.0) → (2.5, 3.0) - Movement: 0.00
- C_2: (8.5, 6.5) → (8.5, 6.5) - Movement: 0.00
- C_3: (5.5, 2.5) → (5.5, 2.5) - Movement: 0.00

🎉 Final Clustering Result:

🔴 Cluster 1

- P_1 = (2, 3)
- P_2 = (3, 3)
- Centroid: (2.5, 3.0)

🔵 Cluster 2

- P_3 = (8, 7)
- P_4 = (9, 6)
- Centroid: (8.5, 6.5)

🟡 Cluster 3

- P_5 = (5, 2)
- P_6 = (6, 3)
- Centroid: (5.5, 2.5)

📊 **Summary:** The algorithm converged in 2 iterations. Total distance calculations: 6 points × 3 centroids × 2 iterations = 36 distance computations

K-Means++ Initialization

Improved initialization strategy for K-Means

Algorithm Steps

1. **First centroid:** Choose randomly from data points
2. **Subsequent centroids:** Probability proportional to squared distance
3. **Result:** Spreads initial centroids far apart in data space

Selection Probability

$$P(x) \propto D(x)^2$$

D(x) = distance to nearest centroid

Faster Convergence

Significantly reduces iterations to convergence

Better Quality

Large gains in clustering quality

Provable Guarantee

O(log k) approximation to optimal solution

Widely Adopted

Default in scikit-learn and other libraries

Trade-off Analysis

Small overhead in initialization → Large gains in quality and speed

Hierarchical Clustering

Builds hierarchy of clusters (dendrogram)

Agglomerative
Bottom-Up

Start with n clusters (each point)
Merge iteratively

Divisive
Top-Down

Start with 1 cluster (all points)
Split iteratively

Linkage Criteria

Single
Minimum distance

Complete
Maximum distance

Average
Mean distance

Ward ★
Minimizes variance

✓

No k Required
Cut dendrogram at desired level

$O(n^3)$ Complexity
Not scalable to large datasets

Exploratory Analysis
Understanding data structure

Agglomerative Clustering Algorithm

1. **Initialize**
   Start with n clusters (each data point as individual cluster)

2. **Compute Distance Matrix**
   Calculate distances between all pairs of clusters to create distance matrix

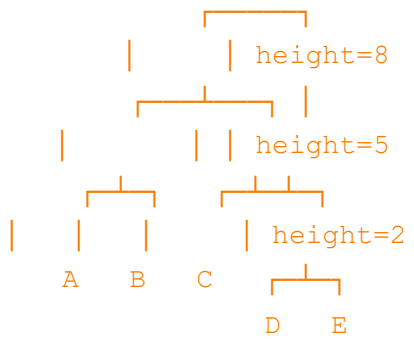
3. **Find Closest Pair**
   Find the two closest clusters from the distance matrix

4. **Merge Clusters**
   Merge the two closest clusters into one and record the merge distance

5. **Update Distance Matrix**
   Recalculate distances between the newly formed cluster and other clusters

6. **Repeat**
   Repeat steps 3-5 until all points form a single cluster

Dendrogram Structure



Y-axis (Height)

Represents the distance at which clusters merge. Higher values indicate merging of more dissimilar clusters

Horizontal Lines

Represent the merging of two clusters. The height of the line indicates the distance at merge

Cutting Dendrogram

Visualizes the height (distance) at which merges occur

Cutting horizontally at a desired height determines the number of clusters at that level

🎯 Optimal Cut Point

Cutting where there are large height differences reveals natural cluster boundaries

Phylogenetics

Essential for constructing phylogenetic trees representing evolutionary relationships among species

Data Exploration

Visually understand natural groupings and hierarchical structure of data through dendrograms

Intuitive Interpretation

Easy to understand cluster similarity by viewing merge order and distances at a glance

Flexible Clustering

More flexible than k-means as you can choose the desired number of clusters after analysis

DBSCAN - Density-Based Clustering

Density-Based Spatial Clustering of Applications with Noise

Parameters

ε (epsilon)
Neighborhood radius

minPts
Minimum density threshold

Core Points

≥ minPts neighbors within ε

Border Points

In neighborhood of core, but not core

Noise Points

Neither core nor border (outliers)

🎯 **Discovers clusters of arbitrary shape**

💪 Advantages

- ✓ Finds outliers automatically
- ✓ No need to specify k
- ✓ Handles arbitrary shapes
- ✓ Works with non-spherical clusters

⚠ Challenges

- ⚠ Sensitive to parameters (ε, minPts)
- ⚠ Struggles with varying densities
- ⚠ Difficulty in high dimensions

DBSCAN Step-by-Step Calculation Example

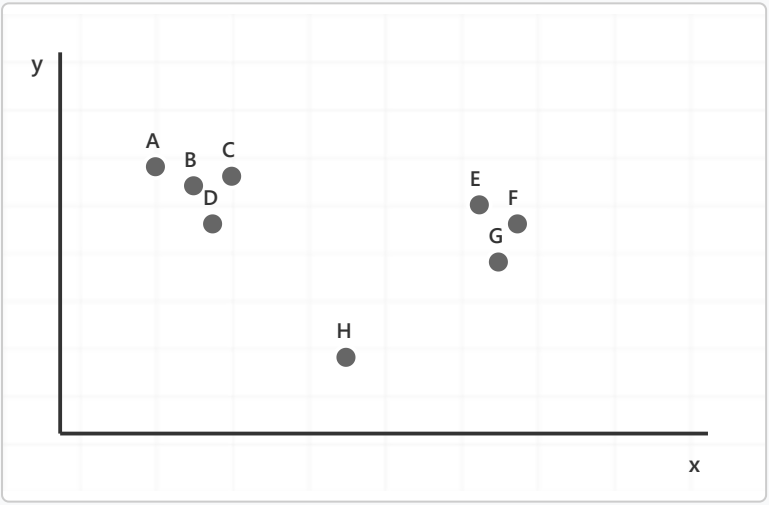
Detailed Process Using 2D Coordinate Data

Radius (Epsilon) **ε = 1.5**

Minimum Points **minPts = 3**

1

Dataset Definition



Point	x coord	y coord
A	2.0	3.0
B	2.5	2.5
C	3.0	2.7
D	2.8	1.8
E	6.5	2.5
F	7.0	2.0
G	6.8	1.5
H	5.0	0.5

Total 8 points

Data distributed on 2D plane

2

Distance Calculation - Euclidean Distance

Finding neighbors of Point A (2.0, 3.0)

$$d(A,B) = \sqrt{[(2.5-2.0)^2 + (2.5-3.0)^2]} = \sqrt{[0.25 + 0.25]} = 0.71 < 1.5 \checkmark$$

$$d(A,C) = \sqrt{[(3.0-2.0)^2 + (2.7-3.0)^2]} = \sqrt{[1.0 + 0.09]} = 1.04 < 1.5 \checkmark$$

$$d(A,D) = \sqrt{[(2.8-2.0)^2 + (1.8-3.0)^2]} = \sqrt{[0.64 + 1.44]} = 1.44 < 1.5 \checkmark$$

$$d(A,E) = \sqrt{[(6.5-2.0)^2 + (2.5-3.0)^2]} = \sqrt{[20.25 + 0.25]} = 4.53 > 1.5 \times$$

Neighbors of A: {B, C, D} → 3 points ≥ minPts(3) → Core Point

3

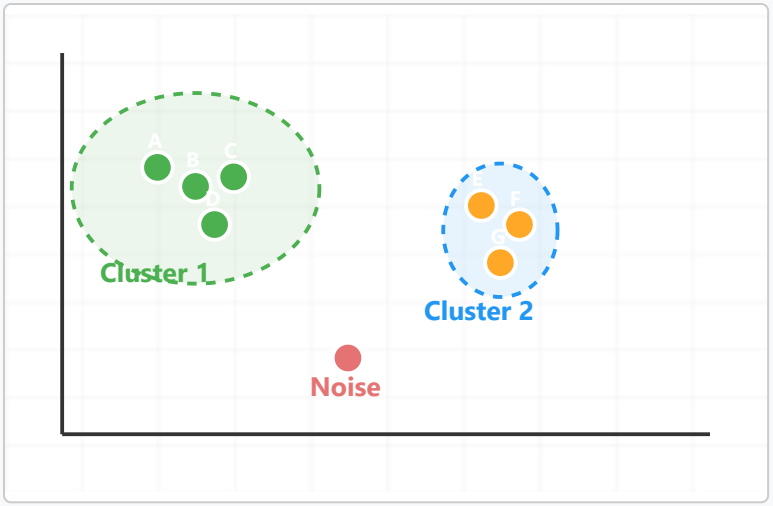
Finding Neighbors for All Points

Point	Neighbors (within ε=1.5)	# Neighbors	Type
A	{B, C, D}	3	Core
B	{A, C, D}	3	Core
C	{A, B, D}	3	Core
D	{A, B, C}	3	Core
E	{F, G}	2	Non-Core
F	{E, G}	2	Non-Core
G	{E, F}	2	Non-Core
H	{}	0	Noise

Core Points: A, B, C, D
Non-Core Points: E, F, G (neighbors < minPts)
Isolated Point: H (no neighbors)

4

Cluster Formation - Connectivity Check



Cluster 1 Formation:

- A is Core Point (starting point)
- Add neighbors B, C, D of A
- B, C, D are all Core Points
- Connected together to form one cluster

Cluster 2 Check:

- E, F, G are Non-Core Points
- Neighbors of each other but < minPts
- E, F, G are connected but
- No Core Point, needs special handling

H is not a neighbor of any Core Point → Noise

5

Final Classification Results

Point	Final Classification	Cluster	Description
A	Core Point	Cluster 1	Meets density condition, cluster center
B	Core Point	Cluster 1	Meets density condition, cluster center
C	Core Point	Cluster 1	Meets density condition, cluster center
D	Core Point	Cluster 1	Meets density condition, cluster center
E	Border Point	Cluster 2	Insufficient neighbors, connected to other Borders
F	Border Point	Cluster 2	Insufficient neighbors, connected to other Borders
G	Border Point	Cluster 2	Insufficient neighbors, connected to other Borders

Point	Final Classification	Cluster	Description

🎯 Clustering Results Summary

Cluster 1	Cluster 2	Noise
4 points	**3 points**	**1 point**
A, B, C, D (All Core)	E, F, G (All Border)	H (Outlier)

Mean Shift

Non-parametric clustering using kernel density estimation

Algorithm Process

Key Features

- ✓ Automatically determines number of clusters
- ✓ Finds clusters of arbitrary shape
- ✓ Robust to outliers
- ✓ No assumption on cluster shape

Detailed Calculation Example (2D Data)

Input Data Points

x_1	x_2	x_3	x_4	x_5
(1, 2)	(2, 3)	(2, 2)	(8, 7)	(9, 8)

Goal

Starting from point $x_1 = (1, 2)$, we'll calculate its mean shift and update its position iteratively until convergence. We'll use Gaussian kernel with bandwidth $h = 3$.

Step 1: Estimate Density using Gaussian Kernel

Gaussian Kernel Formula

$$K(x) = (1 / (2\pi h^2)) \cdot \exp(-||x||^2 / (2h^2))$$

$$\text{For } h = 3: K(x) = (1 / 56.55) \cdot \exp(-||x||^2 / 18)$$

Calculate distances from $x_1 = (1, 2)$ to all points

Distance to x_1:

$$d_1 = ||(1,2) - (1,2)|| = 0$$

Distance to x_2:

$$d_2 = ||(1,2) - (2,3)|| = \sqrt{((1-2)^2 + (2-3)^2)} = \sqrt{2} \approx 1.414$$

Distance to x_3:

$$d_3 = ||(1,2) - (2,2)|| = \sqrt{((1-2)^2 + (2-2)^2)} = 1$$

Distance to x_4:

$$d_4 = ||(1,2) - (8,7)|| = \sqrt{((1-8)^2 + (2-7)^2)} = \sqrt{74} \approx 8.602$$

Distance to x_5:

$$d_5 = ||(1,2) - (9,8)|| = \sqrt{((1-9)^2 + (2-8)^2)} = \sqrt{100} = 10$$

🔢 Step 2: Calculate Kernel Weights

Apply Gaussian kernel to each distance

$K(d_1)$:

$$K(0) = \exp(-0^2/18) = 1.000$$

$K(d_2)$:

$$K(1.414) = \exp(-2/18) \approx 0.895$$

$K(d_3)$:

$$K(1) = \exp(-1/18) \approx 0.946$$

$K(d_4)$:

$$K(8.602) = \exp(-74/18) \approx 0.015$$

$K(d_5)$:

$$K(10) = \exp(-100/18) \approx 0.004$$

Observation

Notice that points x_1, x_2, x_3 (which are close) have high weights (≈ 0.9-1.0), while distant points x_4, x_5 have very low weights (< 0.02). This ensures local density estimation.

🔢 Step 3: Compute Mean Shift Vector

Mean Shift Formula

$$m(x) = [\Sigma_i \, x_i \cdot K(||x_i - x||)] / [\Sigma_i \, K(||x_i - x||)] - x$$

Calculate weighted sum of points

Numerator (weighted sum):

$$\Sigma_i \, x_i \cdot K(d_i) = (1,2) \cdot 1.000 + (2,3) \cdot 0.895 + (2,2) \cdot 0.946 + (8,7) \cdot 0.015 + (9,8) \cdot 0.004$$
$$= (1.000, 2.000) + (1.790, 2.685) + (1.892, 1.892) + (0.120, 0.105) + (0.036, 0.032)$$
$$= (4.838, 6.714)$$

Denominator (sum of weights):

$$\Sigma_i \, K(d_i) = 1.000 + 0.895 + 0.946 + 0.015 + 0.004 = 2.860$$

Weighted mean:

$$\bar{x} = (4.838, 6.714) / 2.860 = (1.691, 2.347)$$

Mean shift vector:

$m(x_1) = (1.691, 2.347) - (1, 2) = (0.691, 0.347)$

🔢 Step 4: Update Position

Iteration 1 Update

New position:

$x_1^{(1)} = x_1^{(0)} + m(x_1^{(0)}) = (1, 2) + (0.691, 0.347) = (1.691, 2.347)$

🔄 Iteration 2

Starting from $x_1^{(1)} = (1.691, 2.347)$:

- Recalculate distances to all points
- Compute new kernel weights
- Calculate new mean shift vector
- Update position: $x_1^{(2)} \approx (1.85, 2.50)$

🔄 Iteration 3 and beyond

Continue iterations until $||m(x)|| < \varepsilon$ (convergence threshold)
Typically converges to a local mode around (1.9, 2.5) after 5-10 iterations

🔢 Step 5: Cluster Assignment

🎯 Final Result

After running mean shift for all points:

- Points x_1, x_2, x_3 converge to mode ≈ (1.9, 2.5) → **Cluster 1**
- Points x_4, x_5 converge to mode ≈ (8.5, 7.5) → **Cluster 2**

Points that converge to the same mode are assigned to the same cluster.

✅ Convergence Criterion

The algorithm stops when the mean shift vector magnitude falls below a threshold:
$||m(x)|| < \varepsilon$, where ε is typically set to 0.01 or 0.001

Gaussian Mixture Models (GMM)

Model-based soft clustering approach

📊 Model Components

Data generated from mixture of k Gaussian distributions

μ	Σ	π
Mean	Covariance	Weight

🔄 EM Algorithm

E — Expectation Step
Assign probabilities to clusters

M — Maximization Step
Update parameters (μ, Σ, π)

↻ Iterate
Repeat until convergence

⚖️ K-means vs GMM

K-means	GMM
Hard assignment	Soft assignment
Spherical clusters	Elliptical clusters

💪 Advantages

- ✓ Probability distribution over clusters
- ✓ Models elliptical clusters
- ✓ Soft assignment flexibility
- ✓ Captures uncertainty

📈 Model Selection

`BIC • AIC`

Choose optimal k

⚠ **Assumes Gaussian distribution**

Cluster Evaluation Metrics

📊 Internal Metrics

🎯 Silhouette Score

`Range: [-1, 1]`

Measures separation and cohesion

Higher is better

📉 Davies-Bouldin Index

`Range: [0, ∞)`

Ratio of within to between cluster distances

Lower is better

📈 Calinski-Harabasz Index

`Range: [0, ∞)`

Ratio of between to within variance

Higher is better

🎲 Inertia (WCSS)

`Range: [0, ∞)`

Within-cluster sum of squares

🏷️ External Metrics

When ground truth labels are available

🖇️ Adjusted Rand Index (ARI)

`Range: [-1, 1]`

Similarity between two clusterings

Closer to 1 is better

ℹ️ Normalized Mutual Info (NMI)

`Range: [0, 1]`

Mutual information between clusterings

Closer to 1 is better

📊 Fowlkes-Mallows Index

`Range: [0, 1]`

Geometric mean of precision and recall

Closer to 1 is better

Minimize for K-means

Visual Methods

Silhouette plots, cluster distributions

Domain Validation

Do clusters make business sense?

Domain validation is the most important!

Try Interactive Clustering Visualization

Test K-means, DBSCAN, Hierarchical, and MeanShift clustering algorithms

Open Clustering Visualizer →

Part 3/4:

Dimensionality Reduction

14. Curse of Dimensionality
15. PCA Principles and Implementation
16. Kernel PCA
17. t-SNE Algorithm
18. UMAP
19. Autoencoder Dimensionality Reduction
20. VAE Basics

⚠ Curse of Dimensionality

High dimensions create counterintuitive geometric properties

Distance Concentration

All points become equidistant in high dimensions

Volume Concentration

Data occupies tiny fraction of space

Exponential Growth

Required samples grow exponentially with features

↓

Nearest Neighbors
Become meaningless

Visualization
Impossible beyond 3D

Computational Cost
Memory & time increase

↓

Solution: Dimensionality Reduction

Preserve structure in lower dimensions while maintaining essential information and relationships

PCA: Principal Component Analysis

Linear dimensionality reduction technique

Core Concepts

- **Goal:** Find directions of maximum variance
- **Principal Components:** Orthogonal eigenvectors of covariance matrix
- **Eigenvalues:** Variance explained by each component

Implementation Steps

1. Center data (subtract mean)
2. Compute covariance matrix
3. Eigen decomposition

Component Selection

Use scree plot to choose k components

Example: Select k explaining 95% variance

Limitations

- Linear transformation only
- Sensitive to feature scaling
- May lose interpretability

Applications

- Data compression
- Noise reduction
- Visualization

4 Project onto top k components

📐 PCA Step-by-Step Numerical Example

2D to 1D Dimension Reduction

🔢 Sample Dataset

Sample	X_1	X_2
1	2	1
2	3	5
3	4	3
4	5	6
5	6	7
6	7	8

Step 1: Calculate Mean Vector (μ)

$$\mu_1 = (2+3+4+5+6+7)/6 = 4.5$$
$$\mu_2 = (1+5+3+6+7+8)/6 = 5.0$$

Mean Vector: μ = [4.5, 5.0]

Step 2: Center the Data (Subtract Mean)

```
X_centered = X - μ [-2.5, -4.0] [-1.5, 0.0] [-0.5, -2.0] [ 0.5, 1.0] [ 1.5, 2.0] [ 2.5, 3.0]
```

Step 3: Compute Covariance Matrix

$$Cov(X) = (1/(n-1)) \times X\_centered^T \times X\_centered$$

```
Covariance Matrix: [ 3.5 3.75 ] [ 3.75 10.0 ]
```

💡 **Interpretation:** The diagonal elements (3.5, 10.0) represent variances of X_1 and X_2. Off-diagonal elements (3.75) show positive correlation between variables.

🔍 Eigendecomposition & Component Selection

⚙️ Computing Eigenvectors and Eigenvalues

Step 4: Solve Characteristic Equation

$$det(Cov(X) - \lambda I) = 0$$

```
| 3.5-λ 3.75 | | 3.75 10.0-λ | = 0 (3.5-λ)(10.0-λ) - (3.75)² = 0 λ² - 13.5λ + 20.94 = 0
```

Eigenvalues:
λ_1 = 11.93 (88.4% variance explained)

λ_2 = 1.57 (11.6% variance explained)

Step 5: Calculate Eigenvectors

```
For λ₁ = 11.93: Eigenvector v₁ = [0.478, 0.878] (normalized) For λ₂ = 1.57: Eigenvector v₂ = [-0.878, 0.478] (normalized)
```

🎯 **Principal Component 1 (PC1):** Direction of maximum variance, pointing towards [0.478, 0.878]

Step 6: Variance Explained

Component	Eigenvalue	% Variance	Cumulative %
PC1	11.93	88.4%	88.4%
PC2	1.57	11.6%	100.0%

Step 7: Project Data onto PC1

$$Z = X\_centered \times v_1$$

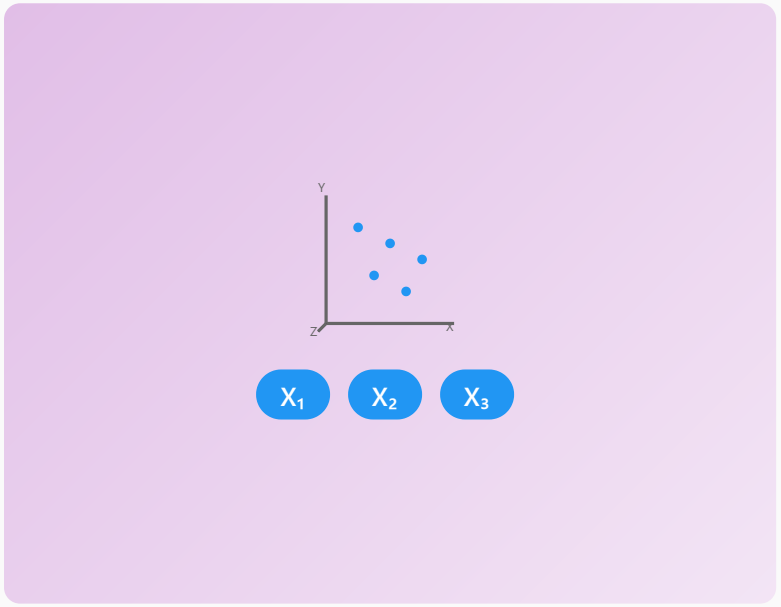
```
Transformed Data (1D): z₁ = [-2.5, -4.0] · [0.478, 0.878] = -4.71 z₂ = [-1.5, 0.0] · [0.478, 0.878] = -0.72 z₃ = [-0.5, -2.0] · [0.478, 0.878] = -1.99 z₄ = [ 0.5, 1.0] · [0.478, 0.878] = 1.12 z5 = [ 1.5, 2.0] · [0.478, 0.878] = 2.47 z6 = [ 2.5, 3.0] · [0.478, 0.878] = 3.83
```

📊 PCA Visualization: 3D to 2D Example

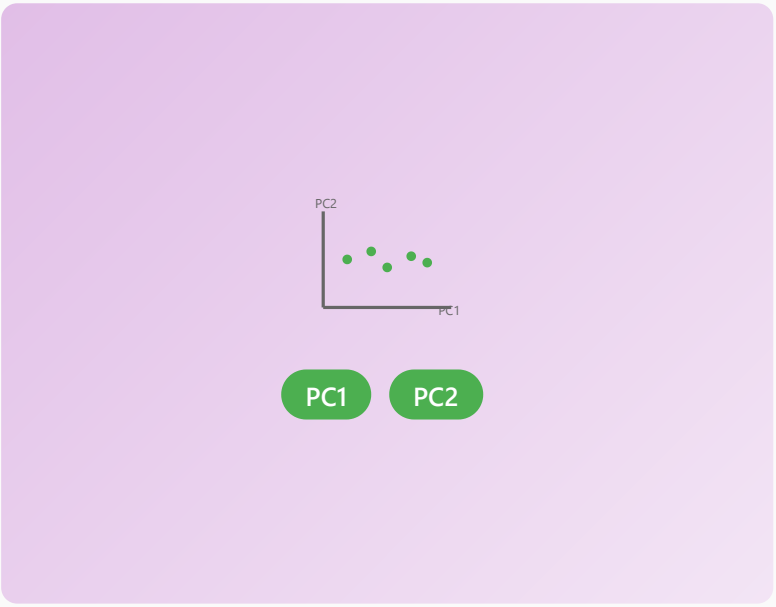
Understanding dimensionality reduction visually

🎨 3D Data Visualization

Original 3D Data Space



Reduced 2D Space (PC1 & PC2)



📉 **Dimension Reduction:** From 3D (X_1, X_2, X_3) → 2D (PC1, PC2) while preserving 95%+ of variance

🔍 Visual Interpretation Guide

🎯 **PC1 Direction:** Points along the direction of maximum spread (variance) in the data. This is where the data varies the most.

📐 **PC2 Direction:** Orthogonal to PC1, captures the second largest variance. Always perpendicular to all previous components.

🔄 **Data Projection:** Each data point is projected onto the new PC axes. Distance from origin indicates the component score.

📊 **Information Loss:** The reduction from 3D to 2D means discarding PC3. The eigenvalue of PC3 tells us how much information is lost.

💻 Python Implementation Example

Using NumPy and scikit-learn

🐍 Method 1: NumPy (From Scratch)

```
# Import libraries
import numpy as np

# Sample data
X = np.array([[2, 1], [3, 5], [4, 3],
              [5, 6], [6, 7], [7, 8]])
```

```
# Step 1: Center the data
X_mean = np.mean(X, axis=0)
X_centered = X - X_mean

# Step 2: Compute covariance matrix
cov_matrix = np.cov(X_centered.T)

# Step 3: Eigendecomposition
eigenvalues, eigenvectors = np.linalg.eig(cov_matrix)

# Step 4: Sort by eigenvalues
idx = eigenvalues.argsort()[::-1]
eigenvalues = eigenvalues[idx]
eigenvectors = eigenvectors[:, idx]

# Step 5: Project data onto PC1
PC1 = eigenvectors[:, 0]
X_pca = X_centered @ PC1

print("Eigenvalues:", eigenvalues)
print("PC1:", PC1)
print("Transformed data:", X_pca)
```

⚡ Method 2: scikit-learn (Production Ready)

```
# Import PCA from scikit-learn
from sklearn.decomposition import PCA
import numpy as np

# Sample data
```

```
X = np.array([[2, 1], [3, 5], [4, 3],
              [5, 6], [6, 7], [7, 8]])

# Create PCA object (reduce to 1 component)
pca = PCA(n_components=1)

# Fit and transform
X_pca = pca.fit_transform(X)

# Access results
print("Explained variance ratio:",
      pca.explained_variance_ratio_)
print("Principal components:",
      pca.components_)
print("Transformed data:", X_pca)

# For 3D to 2D reduction
pca_3d = PCA(n_components=2)
X_3d_to_2d = pca_3d.fit_transform(X_3d_data)
```

📈 Before PCA

✓ Original dimensions: 3D or more
✓ All features present
✓ Full information retained
✗ Computational cost high
✗ Difficult to visualize
✗ Possible multicollinearity

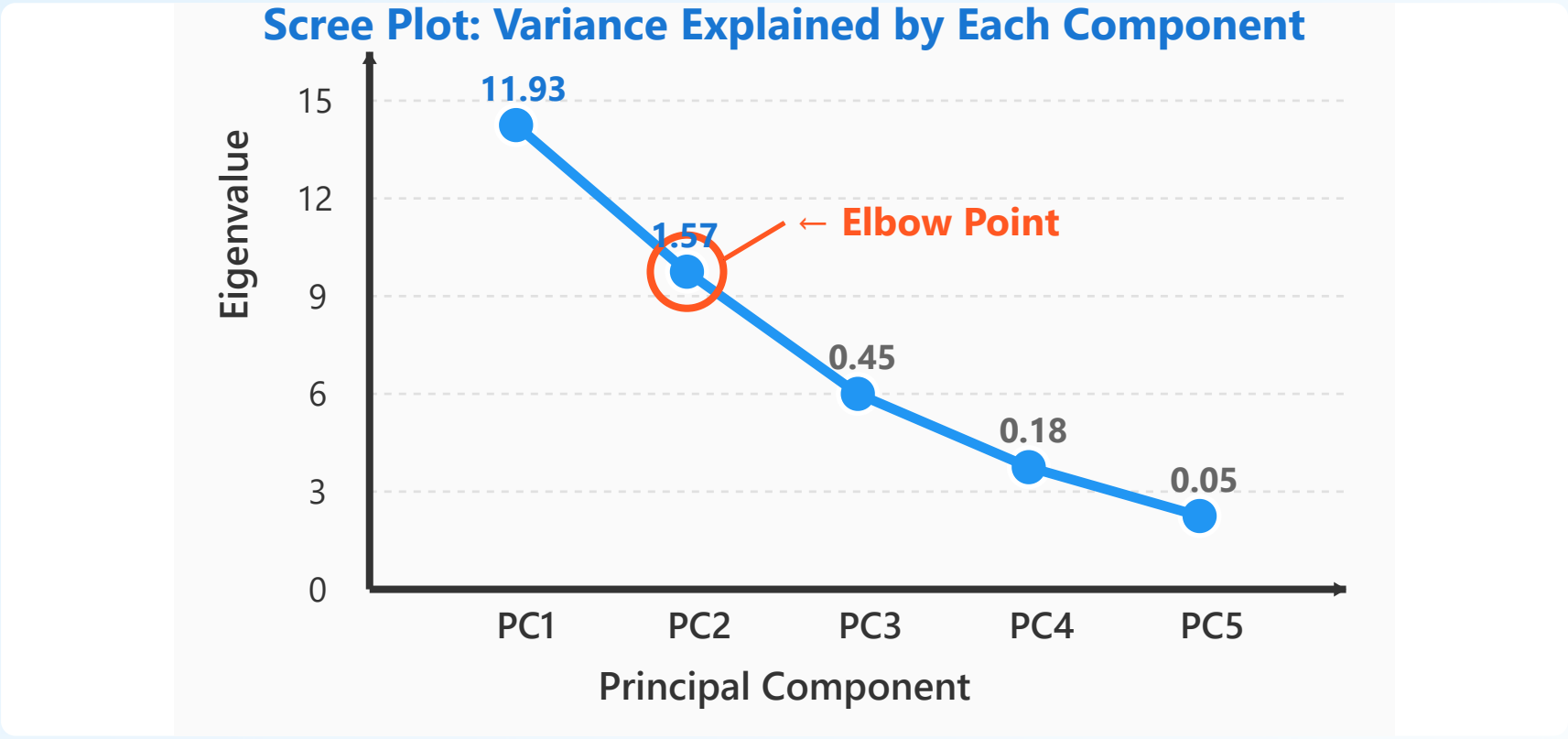
📉 After PCA

✓ Reduced dimensions: 2D or 1D
✓ Uncorrelated components
✓ 95%+ variance retained
✓ Faster computation
✓ Easy visualization
✗ Interpretability reduced

📈 Component Selection & Scree Plot

How many components should we keep?

📊 Scree Plot Analysis



🎯 **Elbow Method:** Choose the number of components at the "elbow" point where the eigenvalue curve flattens out. In this example, keeping 2 components is optimal.

Decision Criteria for Component Selection

Method	Rule	Example
Variance Threshold	Keep components explaining 95% variance	If PC1+PC2 = 96%, keep 2 components
Kaiser Rule	Keep eigenvalues > 1	If λ_1=11.93, λ_2=1.57, keep both
Elbow Method	Visual inspection of scree plot	Choose point where curve bends
Fixed Dimension	Reduce to 2D or 3D for visualization	Always keep exactly 2 or 3 PCs

🎓 Practical Guidelines

✅ When to Use PCA:

- High-dimensional data (p > 50 features)
- Features are highly correlated
- Need for data visualization
- Computational efficiency required
- Noise reduction in signal processing

❌ When NOT to Use PCA:

- Need to maintain feature interpretability
- Features have different scales (standardize first!)
- Non-linear relationships in data (use Kernel PCA)
- Small sample size (n < p)
- Sparse data (many zeros)

🌍 Real-World PCA Applications

From theory to practice

🔬 Case Study 1: Image Compression

Problem: A 100×100 grayscale image has 10,000 pixels (dimensions)

PCA Solution

Step 1: Treat each image as a 10,000-dimensional vector

Step 2: Apply PCA to find principal components

Step 3: Keep top 100 components (99% variance)

Step 4: Reconstruct image using only 100 components

Result: 100× compression ratio with minimal quality loss!
Storage: 10,000 → 100 coefficients per image

📊 Case Study 2: Stock Market Analysis

Problem: Analyzing 500 stocks (S&P 500) with daily returns

PCA Insights

```
# Stock returns data: 252 days × 500 stocks
from sklearn.decomposition import PCA
import pandas as pd

# Apply PCA
pca = PCA(n_components=10)
pc_scores = pca.fit_transform(stock_returns)

# Analyze variance explained
variance_explained = pca.explained_variance_ratio_
cumulative_variance = variance_explained.cumsum()

print("PC1 explains:", variance_explained[0])
# Output: PC1 explains: 0.42 (42% of market movement!)
```

Interpretation: PC1 often represents "the market" - overall market movement. PC2-PC3 capture sector-specific effects.

🧬 Case Study 3: Gene Expression Analysis

Problem: 20,000 genes measured across 100 patients

Bioinformatics Application

Original	After PCA	Benefit
20,000 dimensions	50 dimensions	400× reduction
Impossible to visualize	2D/3D plot	Pattern discovery
High noise	Filtered signal	Better classification

PCA revealed hidden patient subgroups that weren't visible in original data!

Reference

Interactive 3D Visualization Tutorial:
LearnPCA - Visualizing PCA in 3D

Kernel PCA

Non-linear extension of PCA using kernel trick

Linear PCA

- Linear transformations only
- Works in original space
- Fast computation
- Limited to linear patterns

Kernel PCA

- Captures non-linear patterns
- Projects to high-dim space
- No explicit computation
- More expressive power

Common Kernel Functions

RBF (Gaussian)

Most popular choice

Polynomial

For polynomial features

Sigmoid

Neural network-like

Key Advantages

- ✓ Handles non-linear relationships
- ✓ No explicit feature mapping
- ✓ Works with complex data structures

Trade-off

More powerful but computationally expensive. Requires careful hyperparameter tuning.

🎯 The Kernel Trick

✨ How It Works

❌ Without Kernel Trick

Explicitly map data to high-dimensional space → Computationally expensive for very high dimensions

✅ With Kernel Trick

Compute inner products in high-dimensional space without explicit mapping → Much more efficient!

💡 Key Insight

Kernel function K(x, y) computes the dot product in feature space without ever computing the coordinates in that space

🔑 Mathematical Beauty

Instead of computing $\varphi(x)\cdot\varphi(y)$ explicitly, we directly compute $K(x, y) = \varphi(x)\cdot\varphi(y)$

🔄 Kernel PCA Process

📋 Step-by-Step Algorithm

1

2

Choose Kernel

Select appropriate kernel function (RBF, polynomial, etc.) and set hyperparameters

Compute Kernel Matrix

Calculate pairwise similarities between all data points using kernel function

3

Center the Matrix

Center the kernel matrix in feature space to ensure zero mean

4

Find Eigenvectors

Compute eigenvalues and eigenvectors of the centered kernel matrix

5

Sort Components

Sort eigenvectors by eigenvalues in descending order

6

Project Data

Project original data onto top k principal components for dimensionality reduction

📊 Visual Example

🎨 Donut-Shaped Data Separation

🔴 Problem: Non-Linearly Separable Data

Imagine red points forming a circle in the center, surrounded by blue points in a donut shape. In 2D, no straight line can separate these classes.

⚙️ Solution: Transform to Higher Dimension

Apply transformation: $f(x, y) = (x, y, 2x^2 + 2y^2)$ to map 2D → 3D

$$f((x, y)) = (x, y, 2x^2 + 2y^2)$$

✨ Result: Linear Separation

In 3D space, the classes become linearly separable. Kernel PCA can now find principal components that effectively separate red and blue points!

🌍 Real-World Applications

🚀 Where Kernel PCA Shines

Facial Recognition

Captures complex non-linear facial features for identity verification and security systems

NLP & Text Analysis

Reduces dimensionality of text data for sentiment analysis, document clustering, and classification tasks

Genomics

Analyzes gene expression data and DNA sequences where non-linear biological relationships exist

Financial Modeling

Captures complex patterns in stock prices and market data for prediction and risk analysis

Image Processing

Speech Recognition

Object detection and recognition by extracting non-linear visual features from image data

Processes audio signals to identify non-linear patterns in speech for better transcription accuracy

🎯 Kernel Selection Guide

🔍 Detailed Kernel Comparison

⭕ RBF (Radial Basis Function) Kernel

Best for: Most general-purpose applications, unknown data patterns

$$K(u, v) = \exp(-\gamma ||u - v||^2)$$

Hyperparameter γ: Controls influence radius. Larger γ = more local influence

📈 Polynomial Kernel

Best for: Data with polynomial relationships, specific degree interactions

$$K(u, v) = (\gamma u \cdot v + c)^d$$

Hyperparameters: degree d, coefficient γ, constant c

〰️ Sigmoid Kernel

Best for: Neural network-like transformations

$$K(u, v) = \tanh(\gamma u \cdot v + c)$$

Note: Similar to neural network activation functions

Selection Strategy

Use cross-validation to test different kernels and hyperparameters. Start with RBF as default, then experiment with polynomial if domain knowledge suggests polynomial relationships.

t-SNE Algorithm

t-Distributed Stochastic Neighbor Embedding

Non-linear dimensionality reduction for visualization

Two-Step Process

1. Compute pairwise similarities in high-dimensional space

↓

2. Optimize low-dimensional embedding to match similarities

Key Parameter

Perplexity

`Range: 5 - 50`

Balances local vs global structure

Primary Use

- 2D/3D visualization
- ✗ NOT for general dim reduction

Key Features

- **Preserves local structure:** Similar points stay close
- **Student t-distribution:** Avoids crowding problem
- **Stochastic:** Different runs produce different results

Limitations

- ⚠ Computationally expensive: $O(n^2)$
- ⚠ Best with <10k samples
- ⚠ Non-deterministic results
- ⚠ Sensitive to hyperparameters

Step-by-Step Example: MNIST Digits

3D → 2D Visualization Process

1 Input: High-Dimensional Data

Data Preparation

MNIST handwritten digit data (simplified example)

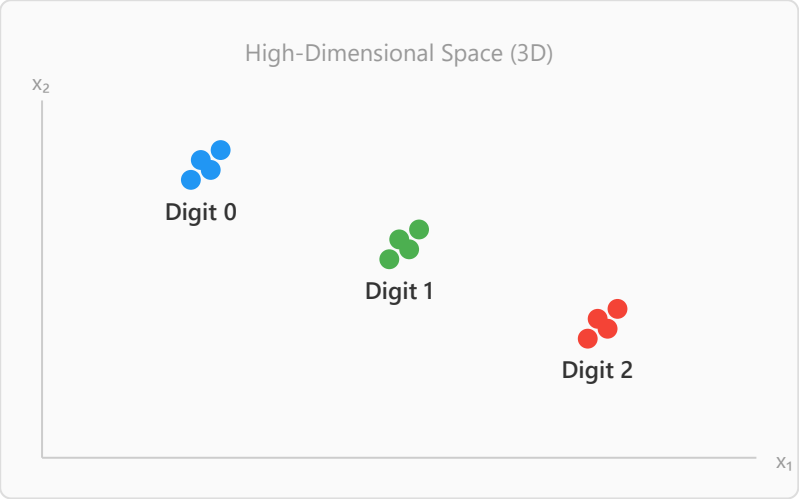
Original dimensions: 784D (28×28 pixels) → simplified to 3D

Number of samples: 12 (4 samples each for digits 0, 1, 2)

$$X = [x_1, x_2, \ldots, x_{12}]$$
$$x_i \in \mathbb{R}^3$$

Sample	Label	x_1	x_2	x_3
1	0	2.1	3.4	1.2
2	0	2.3	3.1	1.5
3	0	1.9	3.6	1.0
4	0	2.4	3.3	1.3
...	...	...	...	...

3D Space Visualization



2 Compute High-Dimensional Similarities

Similarity Calculation (Gaussian Distribution)

Compute conditional probabilities between each pair of points

$$p(j|i) = \exp(-||x_i - x_j||^2 / 2\sigma_i^2) / \Sigma_k \exp(-||x_i - x_k||^2 / 2\sigma_i^2)$$

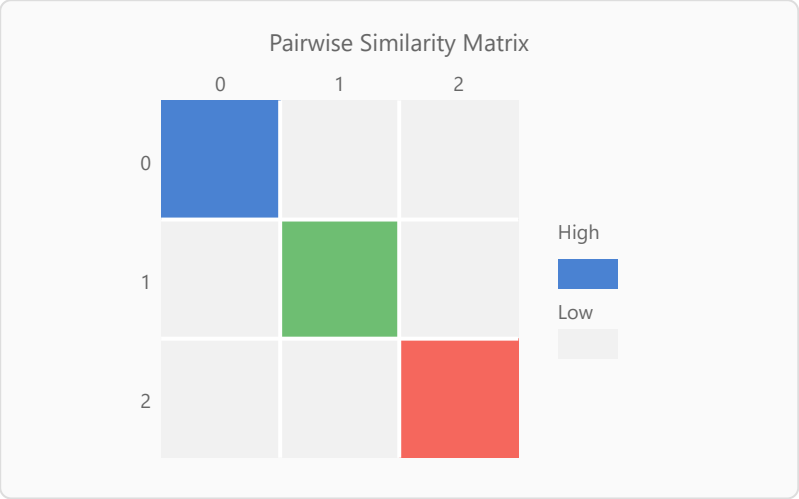
$$p_{ij} = (p(j|i) + p(i|j)) / 2n$$

Perplexity = 5 (determines number of neighbors)

Intermediate result: 12×12 similarity matrix P generated
- Same class: $p_{ij} \approx 0.08 \sim 0.12$
- Different class: $p_{ij} \approx 0.001 \sim 0.005$

	S1	S2	S5	S9
S1(0)	-	0.095	0.003	0.001
S2(0)	0.095	-	0.002	0.001
S5(1)	0.003	0.002	-	0.089
S9(2)	0.001	0.001	0.089	-

Similarity Matrix Heatmap



3 Initialize Low-Dimensional Embedding

Random Initialization in 2D Space

Randomly place points in the target dimension (2D)

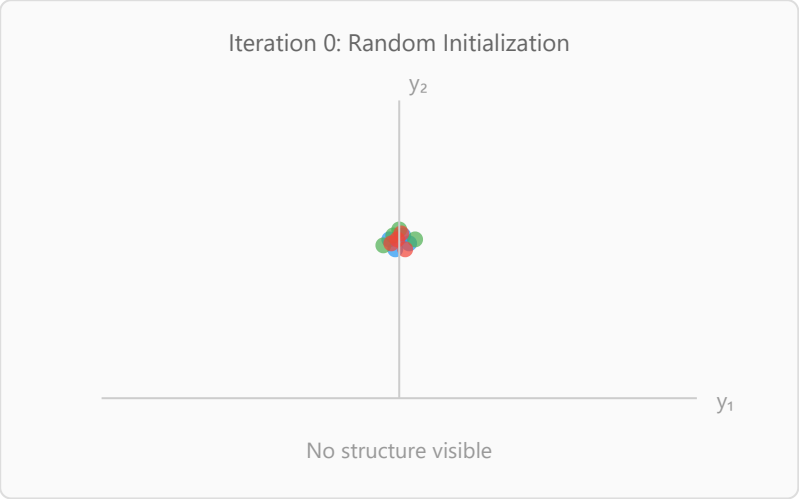
$$Y^{(0)} = [y_1^{(0)}, y_2^{(0)}, \ldots, y_{12}^{(0)}]$$
$$y_i^{(0)} \sim N(0, 0.0001 \cdot I)$$

Initial state:

- All points clustered near the origin
- No class structure
- No meaningful patterns yet

Iteration 0: Completely random placement
Cost = Very high (≈ 8.5)

Initial Random Embedding



↓

4 Iterative Optimization (Gradient Descent)

Matching Similarities in Low-Dimensional Space

Compute low-dimensional similarities using Student t-distribution

$$q_{ij} = (1 + ||y_i - y_j||^2)^{-1} / \Sigma_{kl}(1 + ||y_k - y_l||^2)^{-1}$$

$$Cost = KL(P||Q) = \Sigma_{ij}\ p_{ij}\ \log(p_{ij}/q_{ij})$$

Gradient:

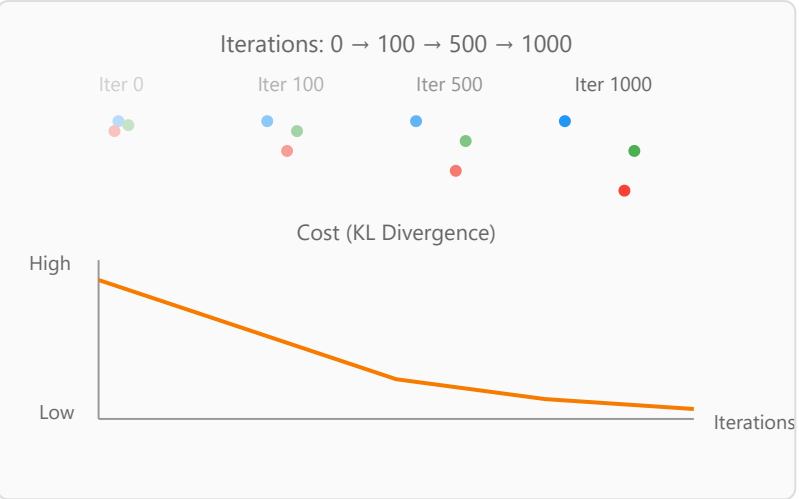
$$\partial C/\partial y_i = 4\Sigma_j\ (p_{ij} - q_{ij})(y_i - y_j)(1 + ||y_i - y_j||^2)^{-1}$$

Progress:

Iteration	Cost (KL)	Status
0	8.523	Random
100	3.214	Clusters forming
500	0.892	Well separated
1000	0.435	Converged

Learning rate: Early exaggeration (η=200) → Fine-tuning (η=50)

Optimization Progress



5 Final 2D Embedding

Final Visualization Result

Low-dimensional embedding after convergence

Result Analysis:
✓ Same classes clustered together
✓ Different classes clearly separated
✓ Local structure preserved
✓ Visually interpretable

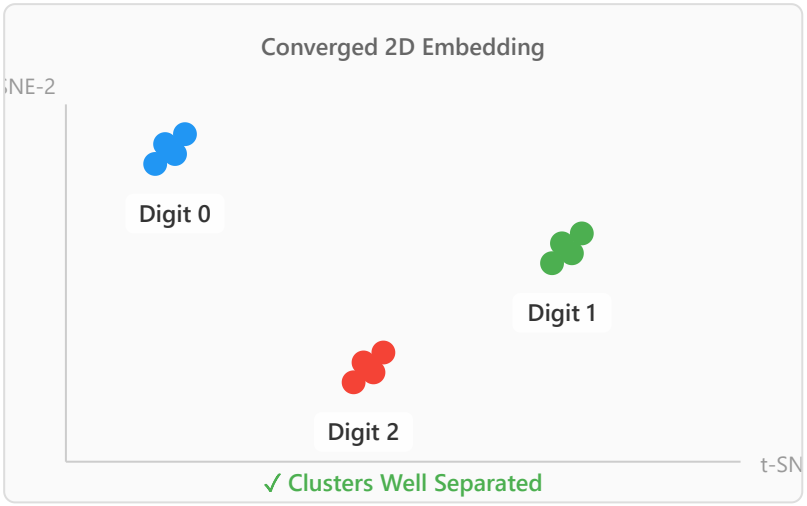
Performance Metrics:

- Final Cost: 0.435
- Convergence time: ~15s
- Total Iterations: 1000

Key Characteristics:

- Inter-cluster distances are meaningless
- Cluster sizes are also meaningless
- Only local structure is reliable
- Different results on re-runs possible

Final t-SNE Visualization



Key Takeaways

✅ What t-SNE Preserves

- Close neighbor relationships

❌ What t-SNE Does NOT Preserve

- Absolute distances

- Local cluster structure
- Density within same class

- Relative distances between clusters
- Cluster sizes/densities

Practical Tips:

- Adjust Perplexity: Small values (5-10) emphasize local structure, large values (30-50) consider global structure
- Run multiple times to verify stable patterns
- For >10,000 samples, first reduce to 50D with PCA, then apply t-SNE
- Use only for visualization purposes, not suitable for classification/regression preprocessing

UMAP

Uniform Manifold Approximation and Projection

⭐ State-of-the-art for visualization and dimensionality reduction

t-SNE

- Slower computation
- Local structure focus
- Limited scalability
- Mainly for visualization

UMAP

- Faster computation
- Local + global structure
- Better scalability
- Visualization + reduction

Mathematical Foundation

Riemannian geometry & topological data analysis

Scalability

Handles larger datasets than t-SNE

Structure Preservation

Both local and global structure

Supervised Mode

Supports dimensionality reduction with labels

Key Parameters

n_neighbors

min_dist

Controls local structure preservation

Controls embedding tightness

UMAP Computation Principles

1 High-dimensional Graph Construction

Find k-nearest neighbors (k-NN) to create a weighted graph. Calculate distances from each data point to its neighbors to determine probabilistic connection strengths.

$$w(i,j) = \exp(-(d(i,j) - \rho_i) / \sigma_i)$$

2 Fuzzy Simplicial Complex

Transform the weighted graph into a fuzzy topological structure. This is a mathematical representation that preserves the topological properties of the data.

$$P(i \leftrightarrow j) = w(i,j) + w(j,i) - w(i,j) \times w(j,i)$$

3 Low-dimensional Optimization

Optimize the low-dimensional embedding using Stochastic Gradient Descent (SGD). Minimize cross-entropy to reduce the difference between high-dimensional and low-dimensional structures.

$$Loss = \Sigma\ P(i,j)\ \log(P(i,j)/Q(i,j)) + (1-P(i,j))\ \log((1-P(i,j))/(1-Q(i,j)))$$

High-dimensional Space

- Local metric estimation
- k-NN graph construction
- Topological structure representation

Low-dimensional Space

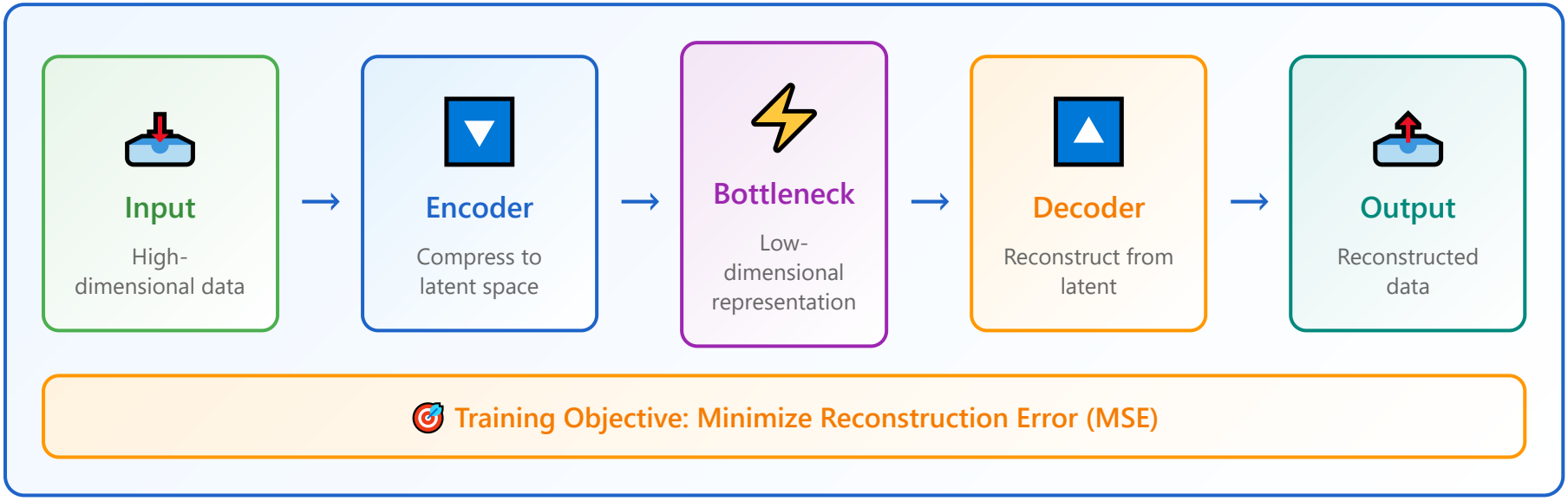
- Initial embedding generation
- Iterative optimization
- Structure preservation verification

🎮 Interactive UMAP Explorer

Try UMAP Explorer →

Autoencoder for Dimensionality Reduction

Neural network approach with encoder-bottleneck-decoder architecture



Variants

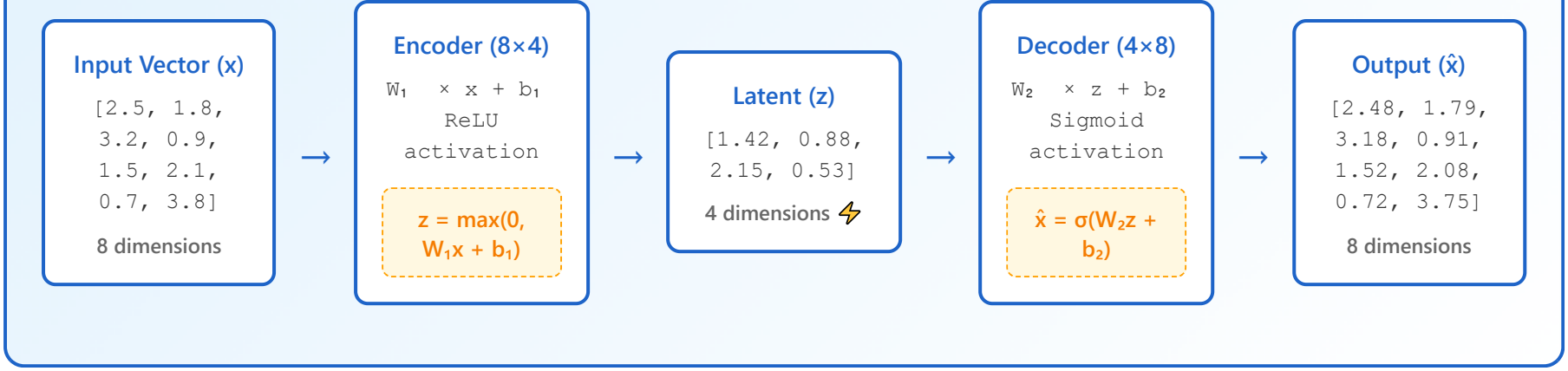
- Denoising
- Sparse
- Contractive

Non-linear transformation can learn complex manifolds

Applications

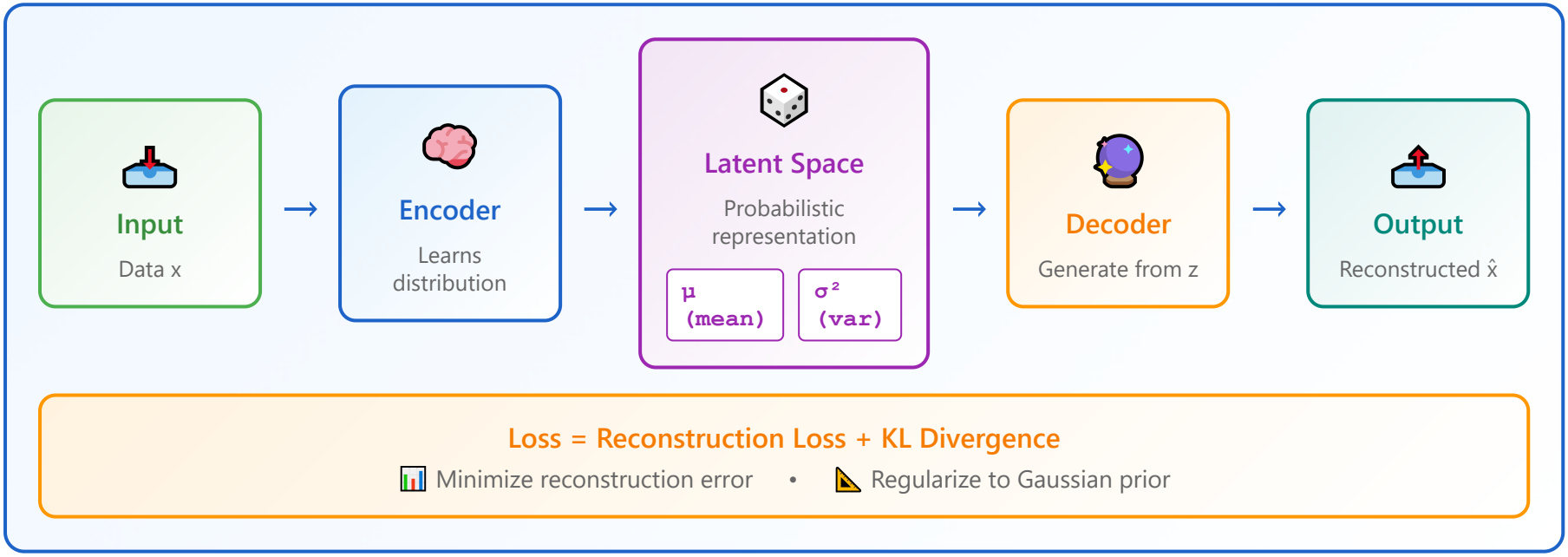
- Image compression
- Feature learning
- Anomaly detection

Calculation Example: 8D → 4D Compression


Input Vector (x)
[2.5, 1.8, 3.2, 0.9, 1.5, 2.1, 0.7, 3.8]
8 dimensions
Encoder (8×4)
W₁ × x + b₁
ReLU activation
z = max(0, W₁x + b₁)
Latent (z)
[1.42, 0.88, 2.15, 0.53]
4 dimensions
Decoder (4×8)
W₂ × z + b₂
Sigmoid activation
x̂ = σ(W₂z + b₂)
Output (x̂)
[2.48, 1.79, 3.18, 0.91, 1.52, 2.08, 0.72, 3.75]
8 dimensions

VAE: Variational Autoencoder

Probabilistic generative model with latent distribution



Key Concepts

- **Probabilistic:** Distribution over latent space
- **Reparameterization:** Enables backpropagation
- **Generation:** Sample latent → new data

Applications

- Image generation
- Data augmentation

Semi-supervised learning

Part 4/4:

Basic Anomaly Detection

21. Anomaly Detection Overview
22. Statistical Methods
23. Isolation Forest
24. Hands-on: Implementation with scikit-learn
25. Summary and Next Lecture Preview

Anomaly Detection Overview

Identify rare items/events that differ from normal patterns

🎯 Types of Anomalies

Detection Approaches

Popular Anomaly Detection Algorithms

Key methods for identifying outliers and anomalies

📊 Statistical Methods

- **Z-Score**
  Measures standard deviations from mean. Points beyond 3σ are anomalies.
- **IQR (Interquartile Range)**
  Uses quartiles Q1 and Q3. Outliers beyond Q1-1.5×IQR or Q3+1.5×IQR.
- **Gaussian Distribution**
  Models normal data, identifies points in low-probability regions.

🎯 Density-based Methods

- **LOF (Local Outlier Factor)**
  Measures local density deviation. Fast training, effective for local anomalies.
- **DBSCAN**
  Clustering algorithm that identifies points not belonging to any cluster.
- **K-Means Clustering**
  Points far from cluster centers are considered anomalies.

📏 Distance-based Methods

- **K-Nearest Neighbors (KNN)**
  Detects anomalies based on distance to k-nearest neighbors.
- **Mahalanobis Distance**
  Accounts for correlation between features in multivariate data.

🌲 Ensemble Methods

- **Isolation Forest**
  Isolates anomalies using decision trees. Works well on most datasets.
- **Random Forest**
  Can be adapted for anomaly detection in classification tasks.

⚠ Imbalanced data distribution

⚠ Defining normal behavior

⚠ Lack of labeled anomalies

⚠ Evolving patterns over time

🚀 Advanced Methods & Learning Approaches

Modern techniques and learning paradigms for anomaly detection

🧠 Machine Learning Methods

- **One-Class SVM**
  Creates hypersphere around normal data, separating anomalies.
- **Autoencoders**
  Neural networks that reconstruct data. High reconstruction error indicates anomalies.
- **LSTM Networks**
  Captures temporal patterns in time-series data for sequence anomaly detection.

📐 Dimensionality Reduction

- **PCA (Principal Component Analysis)**
  Reduces dimensions, highlights influential features and outliers.
- **t-SNE**
  Non-linear technique for visualizing high-dimensional data and clusters.
- **UMAP**
  Fast dimensionality reduction preserving global structure.

🎓 Learning Paradigms

Supervised

Requires labeled data with normal and anomalous examples

SVM, Neural Networks, Random Forest

Unsupervised

No labels needed. Most common approach in practice

Isolation Forest, LOF, K-Means, Autoencoders

Semi-supervised

Trained on normal data only, detects deviations

One-Class SVM, Novelty Detection

💡 Key Insight

Algorithm choice depends on data characteristics, computational resources, and whether labels are available. Isolation Forest and LOF are popular starting points due to their effectiveness and ease of use.

Implementation & Popular Tools

Python libraries and practical considerations

Python Libraries

Scikit-learn

Isolation Forest, One-Class SVM, LOF, DBSCAN

PyOD

Python Outlier Detection - 40+ algorithms specialized for anomaly detection

TensorFlow/PyTorch

Deep learning models: Autoencoders, LSTM, Variational Autoencoders

PyCaret

Low-code ML library with built-in anomaly detection module

Implementation Tips

Data Preprocessing
Normalize/standardize features for distance-based methods

Feature Engineering
Create relevant features that capture domain knowledge

Threshold Tuning
Adjust contamination rate based on expected anomaly percentage

Model Comparison
Test multiple algorithms to find best fit for your data

Interpretability
Use explainable methods when stakeholder understanding is critical

Performance Considerations

Speed
LOF: Fast training
Isolation Forest: Moderate

Accuracy
Depends on data characteristics & tuning

Scalability
Consider distributed algorithms for big data

Adaptability
Retrain models for evolving patterns

Best Practice

Start with simple statistical methods (Z-score, IQR) for baseline performance, then progress to more sophisticated algorithms (Isolation Forest, One-Class SVM) if needed. Always validate results with domain experts.

Statistical Methods for Anomaly Detection

Assume data follows a known distribution (usually Gaussian)

Z-Score Method

$$|z| > \text{threshold}$$
$$(e.g., \pm 3\sigma)$$

Points beyond threshold are anomalies

Box Plot Method

$$Q1 - 1.5 \times IQR$$
$$Q3 + 1.5 \times IQR$$

Points beyond 1.5×IQR from quartiles

Mahalanobis Distance

$$D^2 = (x-\mu)^T \Sigma^{-1} (x-\mu)$$

For multi-feature data

Strengths

- ✓ Simple and interpretable
- ✓ Fast computation
- ✓ Well-understood theory
- ✓ Easy to implement

Limitations

- ✗ Assumes specific distribution
- ✗ Sensitive to outliers in training
- ✗ May not work for complex patterns
- ✗ Requires distribution knowledge

Works Well For

Low-dimensional data with known distribution

Preprocessing Tip

Remove known anomalies before fitting distribution

Z-Score Example

Student Test Score Analysis

Box Plot Example

Employee Salary Data Analysis

Mahalanobis Example

Customer Purchase Pattern (Amount,

Scores: 85, 90, 88, 92, 87, 89, 150 Mean(μ): 94.4 Std Dev(σ): 22.9 Z-score(150) = 2.43

150 detected as outlier (|z| > 2)

Salary($10k): 300, 320, 310, 330, 340, 325, 800 Q1 = 310, Q3 = 340 IQR = 30 Upper Fence = 340 + 1.5×30 = 385

$8M detected as outlier

Frequency)

Normal: ($500k, 10 times) Suspicious: ($2M, 2 times) Mahalanobis Distance considering correlation = 5.8

Abnormal pattern detected ($D^2 > 4$)

Isolation Forest

Tree-based anomaly detection algorithm

Key Principle: Anomalies are easier to isolate (require fewer splits)

Algorithm Process

1. Build ensemble of random trees
2. Use random feature splits
3. Compute average path length
4. Calculate anomaly score

Anomaly Scoring

Anomalies

Normal Points

Key Parameters

n_estimators
Number of trees in the ensemble

contamination
Expected ratio of anomalies in dataset

Advantages

- ✓ No distribution assumptions
- ✓ Handles high dimensions
- ✓ Efficient and scalable
- ✓ Works on large datasets

Time Complexity

`O(n log n)`

Shorter paths
Easy to isolate

Longer paths
Hard to isolate

Scales to large datasets

Isolation Process: Path Length Comparison

Why anomalies are easier to isolate

Normal Data Point

Dense data around the point

Split 1

Split 2

Split 3

Split 4

Split 5

Split 6

Path Length
6

Anomaly Point

Few data points nearby

Split 1

Split 2

Path Length
2

Key Insight

Anomalies are isolated with **fewer node splits** → Shorter path length → **Higher anomaly score**

📐 Anomaly Score Formula

Normalizing path length to 0~1 range

Formula

$$s(x, n) = 2^{-E(h(x))/c(n)}$$

$$c(n) = 2H(n-1) - 2(n-1)/n$$

$$H(i) = \ln(i) + 0.5772 \text{ (Euler's constant)}$$

x
Specific data point

n
Total number of data points

h(x)
Path length of data point x

E[h(x)]
Average of h(x) across all trees

c(n)
Average path length of all data (normalization constant)

📊 Score Interpretation

⚠ Anomaly

$E[h(x)] \rightarrow 0$

✓ Normal Data

$E[h(x)] \rightarrow n-1$

$s(x, n) \to 2^{0}$

≈ 1.0

$s(x, n) \to 2^{-(n-1)}$

≈ 0.0

💡 **Note:** Score near 0.5 indicates ambiguous cases ($E[h(x)] \approx c(n)$)

💻 Hands-on: Implementation with scikit-learn

Practical implementation guide for unsupervised learning algorithms

📦 Key Imports

```
from sklearn.cluster import KMeans
from sklearn.cluster import DBSCAN
from sklearn.decomposition import PCA
from sklearn.ensemble import IsolationForest
```

🔄 ML Pipeline

1. StandardScaler
2. Dimensionality Reduction
3. Clustering Algorithm

📊 Evaluation Metrics

- `silhouette_score`
- `davies_bouldin_score`
- `calinski_harabasz_score`

📈 Visualization Tools

matplotlib | **seaborn**

For plotting results and analysis

✨ Best Practices

- ✓ Cross-validation for robustness
- ✓ Careful parameter tuning
- ✓ Domain knowledge validation
- ✓ Iterative experimentation

Clustering / Anomaly Detection

Summary and Next Lecture Preview

Today's Lecture: Unsupervised Learning

Discovering patterns without labels

Clustering

K-Means, DBSCAN, Hierarchical, GMM - each has trade-offs

Dimensionality Reduction

PCA, t-SNE, UMAP - visualization and compression

Anomaly Detection

Statistical methods, Isolation Forest - identify outliers

Key Considerations

Scaling, evaluation metrics, interpretability

Next Lecture

Advanced Topics in Deep Learning

- Deep Autoencoders
- Generative Adversarial Networks (GANs)
- Self-Supervised Learning

Practice Assignment

Apply these algorithms to real-world datasets

Thank you

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