Lecture 18:

Advanced Unsupervised Learning

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Lecture Contents

Part 1/4:

Self-Supervised Learning

1. Lecture Overview and Recap
2. What is Self-Supervised Learning?
3. Contrastive Learning Principles
4. SimCLR Algorithm
5. MoCo and BYOL
6. Self-Supervised Pretraining
7. Hands-on: Image Representation Learning

Supervised Learning

Data: Labeled datasets

Requirement: Manual annotation

Cost: High (time + labor)

Unsupervised Learning

Data: Unlabeled data

Requirement: No labels needed

Goal: Find patterns

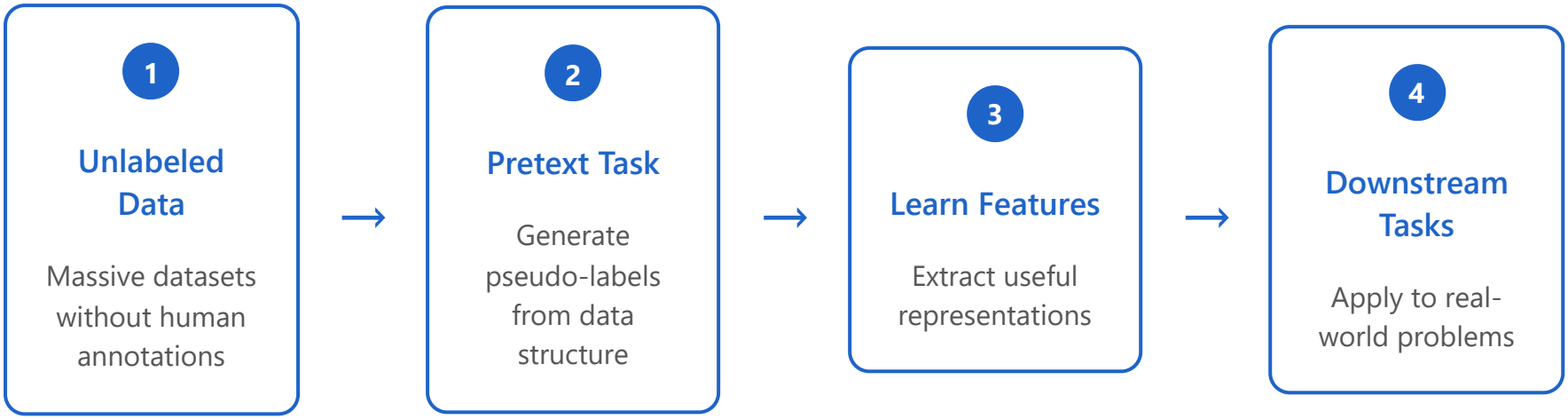
Self-Supervised Learning

Data: Unlabeled → Auto-labeled

Requirement: Labels from data itself

Advantage: Leverage abundant data

Traditional → *Pattern Discovery* → *Modern Bridge Approach*



Pretext Task Examples

Image Rotation
Predict rotation angle (0°, 90°, 180°, 270°)

Colorization
Predict colors from grayscale images

BERT (NLP)
Masked language modeling

GPT (NLP)
Next token prediction

✓ No human annotation required • Scales to massive datasets

🎯 **Core Idea:** Similar items close, dissimilar items far apart

✅ **Positive Pairs:** Augmented versions of same data

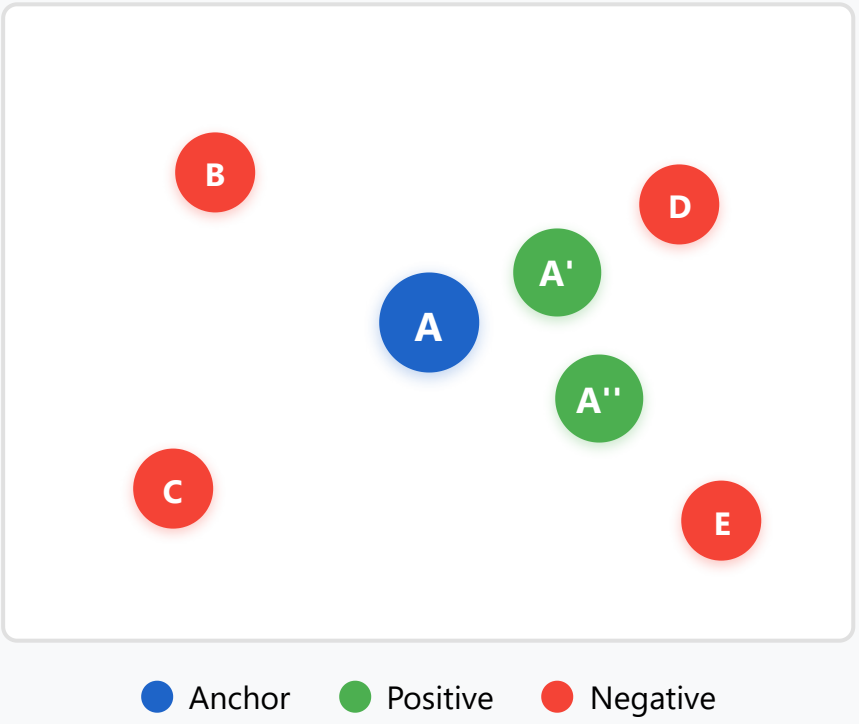
❌ **Negative Pairs:** Different data points

📊 **InfoNCE Loss:** Maximize agreement of positive pairs

🌡️ **Temperature (τ):** Controls distribution sharpness

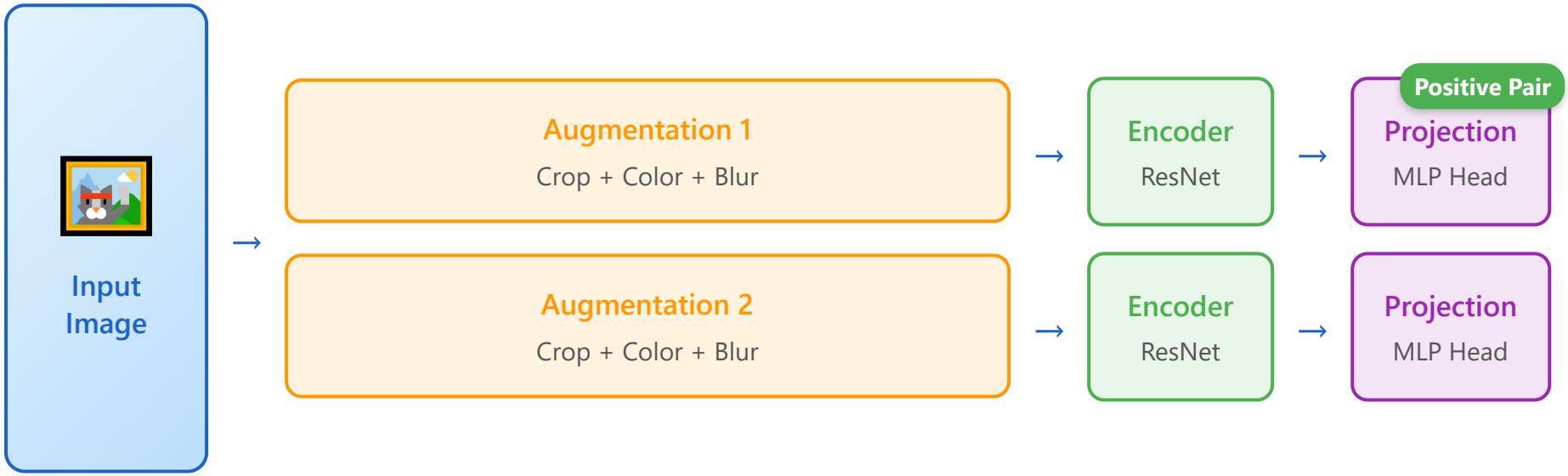
Pull positives close ⬅️ ➡️ Push negatives away

Embedding Space Visualization



SimCLR: Simple Framework for Contrastive Learning

Self-Supervised Visual Representation Learning



NT-Xent Loss — Maximize agreement between positive pairs with temperature scaling (τ)

- 🎯 Large batch size: 4096-8192
- 🔄 Strong data augmentation
- 🏆 SOTA on ImageNet (no labels)

Advanced Self-Supervised Methods

Architecture Comparison: MoCo vs BYOL

MoCo

Momentum Contrast

Query Encoder → Query

Momentum Encoder → Key

Queue of Negative Samples

Queue-based: Maintains large dictionary of negatives

Momentum update: Consistent representations over time

Contrastive: Uses negative pairs

BYOL

Bootstrap Your Own Latent

Online Network → Predictor

Target Network → Projection

Stop-Gradient

No negatives: Only positive pairs needed

Predictor network: Asymmetric architecture

Stop-gradient: Prevents collapse

✓ Excellent ImageNet Performance

✓ Excellent ImageNet Performance

1

Pretrain

Large unlabeled dataset

2

Fine-tune

Small labeled dataset

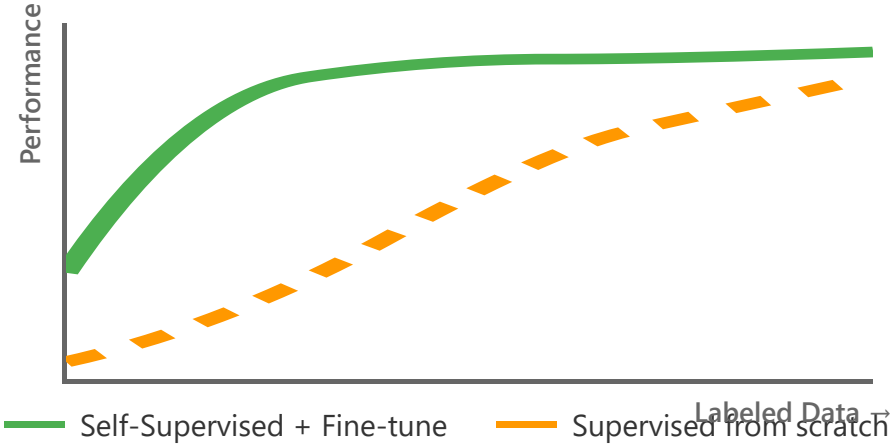
3

Deploy

Downstream task

- Cross-domain transfer learning
- Reduces labeled data needs
- Medical imaging applications
- Satellite imagery analysis
- Match pretraining & target domains

Performance vs Labeled Data Size



Text Images Audio Video

Hands-on: Image Representation Learning with SimCLR

PyTorch Implementation Workflow

CIFAR-10 / STL-10

1 Dataset Setup

Load unlabeled dataset for pretraining

2 Implement SimCLR

Build encoder & projection head

PyTorch

3 Data Augmentation

Setup augmentation pipeline

Crop + Color + Blur

4 Train Encoder

Optimize with contrastive loss

NT-Xent Loss

5 Linear Probe

Evaluate on labeled subset

Frozen Features

6 Visualize Embeddings

Plot learned representations

t-SNE

🎯 **Final Step:** Compare self-supervised results with supervised baseline performance

Example Data and Calculation Process

1. Input Images & Augmentation

Image	Size	Augmentation
Cat (Original)	32×32×3	-
Cat View 1	32×32×3	Random Crop + Flip
Cat View 2	32×32×3	Color Jitter + Blur

Key Point: Generate two different views from the same image to form a positive pair

2. Encoder & Projection Head

Architecture:
Input (3×32×32) → ResNet-18 → h (512-dim) → MLP → z (128-dim)

```
# Example embedding vectors
z1 = [0.23, -0.45, 0.67, ..., 0.12]  # 128-dim
z2 = [0.21, -0.43, 0.65, ..., 0.15]  # 128-dim (positive)
z3 = [-0.89, 0.34, -0.12, ..., 0.56] # 128-dim (negative)
```

Key Point: Calculate cosine similarity after L2 normalization

3. NT-Xent Loss Calculation (Batch Size N=4, Total 8 Samples)

NT-Xent Loss Formula:

$$\ell(i,j) = -\log\left[\exp(\text{sim}(z_i, z_j)/\tau) \;/\; \Sigma \exp(\text{sim}(z_i, z_k)/\tau) \right]$$

τ *(temperature)* $= 0.5$

Step 1: Calculate Similarity Matrix (8×8)

```
sim(z1, z2) = 0.92 // positive pair
sim(z1, z3) = 0.15 // negative
sim(z1, z4) = -0.23 // negative
sim(z1, z5) = 0.08 // negative
...
```

📋 Step 2: Temperature Scaling (τ=0.5)

```
sim(z1, z2)/τ = 0.92/0.5 = 1.84
sim(z1, z3)/τ = 0.15/0.5 = 0.30
sim(z1, z4)/τ = -0.23/0.5 = -0.46
...
```

📋 Step 3: Exponential Calculation

```
exp(1.84) = 6.297 // positive (numerator)
exp(0.30) = 1.350 // negative
exp(-0.46) = 0.631 // negative
exp(0.16) = 1.174 // negative
...
Denominator Sum = 6.297 + 1.350 + 0.631 + 1.174 + ... = 12.845
```

📋 Step 4: Loss Calculation

```
ℓ(z1, z2) = -log(6.297 / 12.845)
ℓ(z1, z2) = -log(0.490)
ℓ(z1, z2) = 0.713
```

Final Batch Loss (Average)

Loss = 0.713

🎯 **Interpretation:** Lower loss indicates that the model has learned good representations where positive pairs are close and negative pairs are far apart.

📈 Training Results Example

Self-Supervised Pretraining

Epoch	Loss	Time
1	2.456	8 min
50	1.234	-
100	0.876	-
200	0.623	26 hours

Settings: CIFAR-10 unlabeled, batch=256, ResNet-18

Linear Probe Evaluation (CIFAR-10 Test)

Method	Accuracy	Training Data
Random Init	23.4%	5,000 labels
SimCLR (ours)	78.6%	5,000 labels
Supervised	91.2%	50,000 labels

Self-Supervised Improvement

+55.2%

PyTorch Implementation (NT-Xent Loss)

```
# SimCLR NT-Xent Loss Implementation
def nt_xent_loss(z_i, z_j, temperature=0.5):
    """
    Args:
        z_i, z_j: [batch_size, embedding_dim] - positive pair
    Returns:
        loss: scalar tensor
    """
    batch_size = z_i.shape[0]

    # L2 normalization
    z_i = F.normalize(z_i, dim=1)
    z_j = F.normalize(z_j, dim=1)
```

```
    # Concatenate: [2*batch_size, embedding_dim]
    z = torch.cat([z_i, z_j], dim=0)

    # Similarity matrix: [2N, 2N]
    similarity_matrix = torch.mm(z, z.T) / temperature

    # Mask to exclude self-similarity
    mask = torch.eye(2 * batch_size, dtype=torch.bool)
    similarity_matrix = similarity_matrix.masked_fill(mask, -9e15)

    # Positive pairs: (i, N+i) and (N+i, i)
    positives = torch.cat([
        torch.diag(similarity_matrix, batch_size),
        torch.diag(similarity_matrix, -batch_size)
    ])

    # NT-Xent loss calculation
    nominator = torch.exp(positives)
    denominator = torch.sum(torch.exp(similarity_matrix), dim=1)
    loss = -torch.log(nominator / denominator)

    return loss.mean()
```

Key Insight: Self-supervised learning can learn powerful feature representations without labels, achieving high performance with only a small amount of labeled data.

Part 2/4:

Time Series Clustering

8. Characteristics of Time Series Data
9. DTW (Dynamic Time Warping) Principles
10. DTW-based Clustering
11. K-Shape Algorithm
12. Subsequence Clustering
13. Hands-on: Stock/Sensor Data Clustering

Time Series Data

Sequential data with temporal dependencies and ordering

Key Challenges

- **Variable lengths:** Different time durations
- **Sampling rates:** Inconsistent frequencies
- **Phase shifts:** Time warping between patterns
- **Noise:** Random fluctuations & outliers
- **Euclidean distance:** Inadequate for alignment

Time Series Characteristics

Trend & Seasonality

Phase Shift (Time Warping)

Noisy Signal

Different Lengths

Key Considerations


Finance
IoT Sensors
Healthcare
Seasonality
Trends
Outliers
Alignment-invariant metrics

Dynamic Time Warping

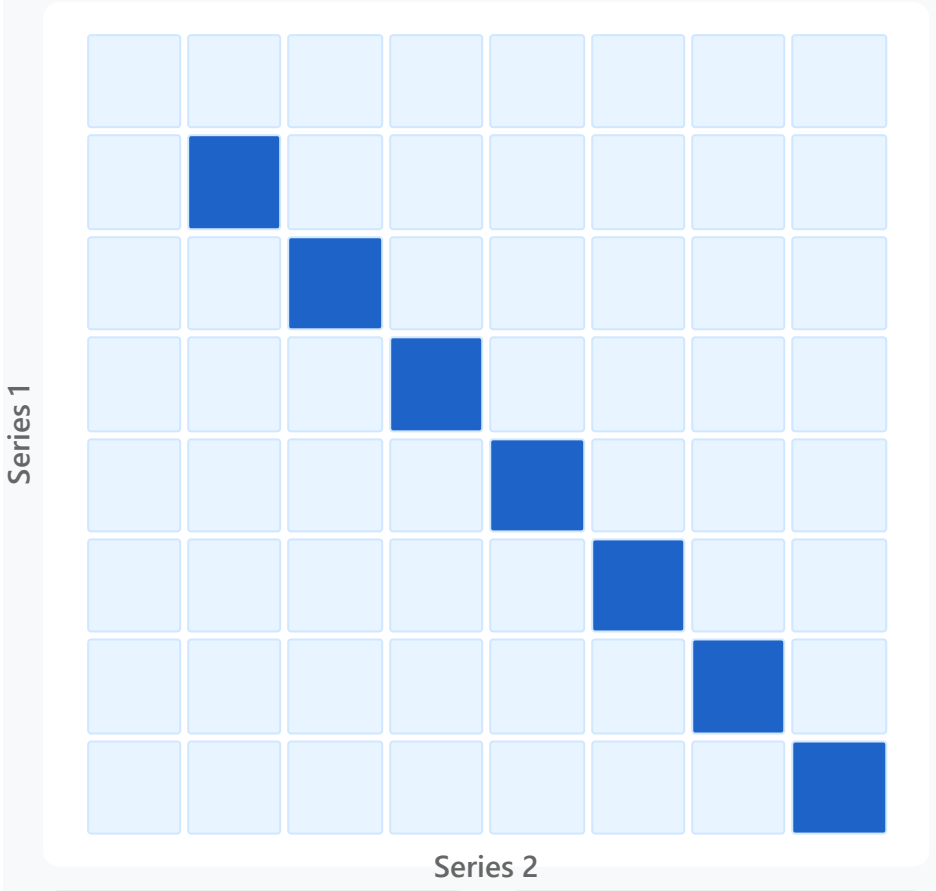
DTW Algorithm

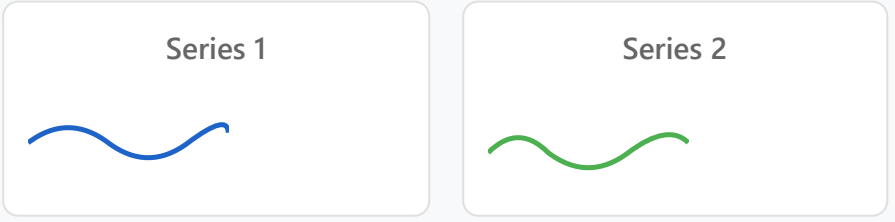
- **Warps time axis** to align sequences
- Finds **optimal alignment path**
- Allows **one-to-many** matching
- DTW distance = **sum of aligned distances**
- Handles **speed variations** & phase shifts

Time Complexity

$O(n^2)$

DTW Alignment Matrix & Warping Path





Alignment Constraints

- Sakoe-Chiba Band
- Itakura Parallelogram

DTW Calculation Example

Step-by-Step Computation

Sequence X

1	3	4	5

Sequence Y

2	3	5

DTW Matrix (Cumulative Cost)

	0	2	3	5
0	|1-2| 1	∞	∞	∞
1	|3-2| 2	|3-3| 2	∞	∞
3	|4-2| 4	|4-3| 3	|4-5| 4	∞
4	|5-2| 7	|5-3| 5	|5-5| 4	4

Calculation Steps

1. Initialize first cell with cost $|x_1-y_1|$

```
D(1,1) = |1-2| = 1
```

2. Fill remaining cells using:

```
D(i,j) = cost(i,j) + min(D(i-1,j),
      D(i,j-1), D(i-1,j-1))
```

3. Example: D(2,2)

```
|3-3| + min(1, 2, 1) = 0 + 2 = 2
```

4. Continue until reaching D(n,m)

5 Backtrack from end to find optimal path

Final DTW Distance

4

DTW-based Clustering

Time Series Clustering with DTW Distance Metric

Clustering Methods

K-medoids

Better than K-means (pairwise distances)

Hierarchical

DTW linkage for dendrogram

DBA

DTW Barycenter Averaging for centroids

Computational Cost

$$O(n^2m^2)$$

n series × length m

Speed Approximations

- FastDTW
- PrunedDTW

DTW Clustering Workflow

1. Compute DTW distance matrix for all pairs
2. Apply clustering algorithm (K-medoids/Hierarchical)
3. Compute cluster centroids using DBA
4. Iterate until convergence or max iterations
5. Evaluate clustering quality with silhouette score

Key Applications

- Gesture Recognition
- ECG Analysis
- Stock Patterns
- Speech Recognition

DTW Clustering: Calculation Example

Step-by-step computation with 3 time series

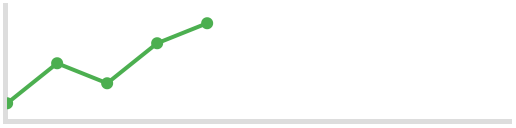
Input Time Series

Series A

[1, 2, 3, 4, 5]

Series B

[1, 3, 2, 4, 5]



Series C

[5, 4, 3, 2, 1]

Step 1: Compute DTW Distance Matrix

	A	B	C
A	0.0	2.4	8.9
B	2.4	0.0	9.2
C	8.9	9.2	0.0

DTW(A,B) = 2.4 < DTW(A,C) = 8.9

Step 2: Apply K-medoids (k=2)

Cluster 1

A B

Medoid: **Series A**

Cluster 2

C

Medoid: **Series C**

Step 3: DBA Centroid for Cluster 1

Average Alignment

Cluster 1 Centroid

[1.0, 2.5, 2.5, 4.0, 5.0]

K-Shape Algorithm

Shape-based Time Series Clustering

Key Features

- **Cross-correlation** for similarity
- **Scale & shift invariant** distance
- Efficient **shape-based centroid**
- **Iterative refinement** like K-means
- **Faster** than DTW-based methods

✓ Best For

Normalized time series data

Method Comparison

Feature	K-Shape	DTW
Speed	Fast	Slow
Scale Invariant	✓	✗
Shift Invariant	✓	✗
Time Warp	✗	✓
Complexity	O(nm)	$O(n^2m^2)$

K-Shape Algorithm Flow

1. Initialize k cluster centroids
2. Assign series to nearest centroid (cross-correlation)
3. Update centroids (shape extraction)
4. Repeat until convergence

K-Shape Algorithm Example

Step-by-Step Calculation with 2D Vectors

📌 Input Data: 4 Time Series (k=2 clusters)

$x_1 = [1, 2]$ $x_2 = [2, 3]$ $x_3 = [8, 9]$ $x_4 = [9, 10]$

🎯 Step 1: Normalization (z-score)

$$z = (x - \mu) / \sigma$$

$z_1 = [-1.0, 1.0]$ $z_2 = [-1.0, 1.0]$ $z_3 = [-1.0, 1.0]$ $z_4 = [-1.0, 1.0]$

💡 Example: Normalize $x_1 = [1, 2]$

$\mu = (1 + 2) / 2 = 1.5$

$\sigma = \sqrt{[((1-1.5)^2 + (2-1.5)^2) / 2]} = 0.5$

$z_1[0] = (1 - 1.5) / 0.5 = -1.0$

$z_1[1] = (2 - 1.5) / 0.5 = 1.0$

Result

$z_1 = [-1.0, 1.0]$

📝 Key Insight

All normalized vectors have the same shape pattern [-1.0, 1.0], showing they follow the same increasing trend!

This normalization makes K-Shape **scale-invariant** - it focuses on shape, not magnitude.

K-Shape Algorithm Example

Iteration 0: Initial Cluster Assignment

Iteration 0

Step 2: Initialize Centroids (Random)

$\mu_1 = [-1.0, 1.0]$ $\mu_2 = [-1.0, 1.0]$

Cross-Correlation Distance (SBD)

```
SBD(x, y) = 1 - max(CC(x, y)) / (||x|| × ||y||)
CC(x, y) = Σ x[i] × y[i] (Cross-Correlation)
```

Calculate distance for z_1 to μ_1:

$CC(z_1, \mu_1) = (-1.0)\times(-1.0) + (1.0)\times(1.0) = 2.0$

$||z_1|| = \sqrt{(1.0^2 + 1.0^2)} = 1.414$

$||\mu_1|| = 1.414$

$SBD(z_1, \mu_1) = 1 - 2.0/(1.414 \times 1.414) = 0.0$

Distance Result

$z_1 \rightarrow$ Cluster 1 (distance = 0.0)

Initial Cluster Assignment

Cluster 1

$z_1 = [-1.0, 1.0]$

Cluster 2

$z_3 = [-1.0, 1.0]$

z_2 = [-1.0, 1.0]

z_4 = [-1.0, 1.0]

K-Shape Algorithm Example

Iteration 1: Update Centroids

Iteration 1

🔄 Step 3: Update Cluster 1 Centroid

```
μ = argmax Σ CC(x_i, y) / ||y||²
Simplified: Average of cluster members
```

Members: z_1 , z_2 = [-1.0, 1.0]

μ_1 [0] = (-1.0 + -1.0) / 2 = -1.0

μ_1 [1] = (1.0 + 1.0) / 2 = 1.0

Updated Centroid

μ_1 = [-1.0, 1.0]

🔄 Step 3: Update Cluster 2 Centroid

Members: z_3 , z_4 = [-1.0, 1.0]

μ_2 [0] = (-1.0 + -1.0) / 2 = -1.0

μ_2 [1] = (1.0 + 1.0) / 2 = 1.0

Updated Centroid

μ_2 = [-1.0, 1.0]

⚠️ Convergence Check

Centroids unchanged!

$\mu_1 = \mu_2 = [-1.0, 1.0]$

✓ Algorithm converged!

💡 Why did it converge so quickly?

All normalized vectors have identical shape [-1.0, 1.0], so they all have perfect cross-correlation with any centroid of the same shape. The algorithm converged in just one iteration!

K-Shape Algorithm Example

Final Results & Analysis

Final Cluster Assignment

Cluster 1

$x_1 = [1, 2]$

$x_2 = [2, 3]$

Centroid: [-1.0, 1.0]

Cluster 2

$x_3 = [8, 9]$

$x_4 = [9, 10]$

Centroid: [-1.0, 1.0]

Key Observations

1. Shape-based clustering:

Groups series by pattern, not absolute values

2. Same normalized shape:

All series show increasing trend [-1, 1]

3. Scale invariance:

[1,2] and [8,9] treated similarly

Algorithm Insights

✓ **Fast convergence:**

Converged in 1 iteration

✓ **Cross-correlation:**

Measures shape similarity efficiently

✓ **Normalization effect:**

All vectors → same pattern

Complexity Analysis

For n=4 series, m=2 dimensions, k=2 clusters:

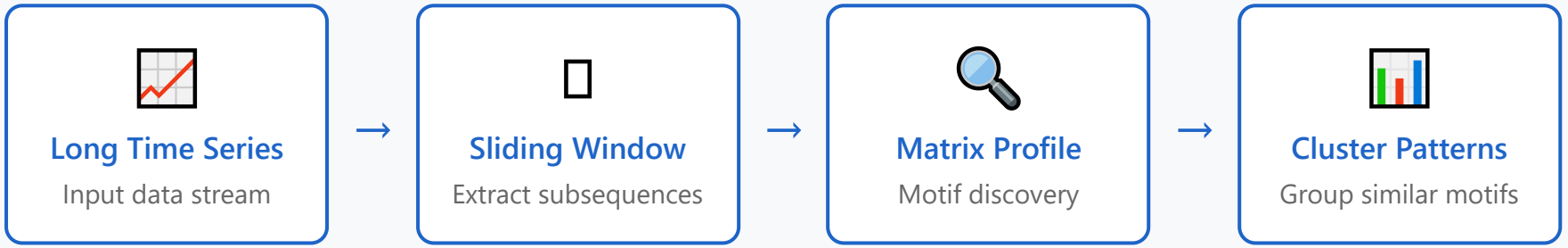
K-Shape	DTW
$O(4 \times 2) = O(8)$	$O(16 \times 4) = O(64)$

K-Shape is 8× faster! ⚡

Subsequence Clustering

Finding Recurring Patterns in Long Time Series

Subsequence Extraction & Clustering Pipeline



Key Challenges

⚠ **Trivial Matches**

Self-matches and near-duplicates

⚠ **Overlapping Patterns**

Adjacent subsequences too similar

Applications & Use Cases

🎯 **Key Applications**

Solutions

Matrix Profile

Efficient motif discovery technique

STOMP Algorithm

Scalable Time series Ordered-search Matrix Profile

- Anomaly Detection
- Pattern Mining
- Motif Discovery
- Sensor Analysis

Example Use Case

Identify repeated behaviors in IoT sensor data: recurring activity patterns, operational cycles, or anomalous sequences in manufacturing or healthcare monitoring systems.

Hands-on: Stock/Sensor Data Clustering

Time Series Clustering Implementation Workflow

1 Dataset Selection

Yahoo Finance or UCI sensor data

2 Preprocessing

Normalization & resampling

z-score

interpolate

3 DTW Distance

Implement distance function

Python/NumPy

4 Hierarchical Clustering

Apply DTW linkage

scipy.cluster

5 Compare K-Shape

Alternative algorithm comparison

tslearn

6 Visualization

Plot clusters & centroids

matplotlib

7 Interpret Results

Identify similar behaviors

Data Sources

Yahoo Finance (stocks) • UCI ML Repository (sensors)

Key Question

Which stocks/sensors behave similarly?

Part 3/4:

Graph Clustering

14. Introduction to Graph Data
15. Spectral Clustering
16. Community Detection (Louvain)
17. GNN Fundamentals
18. Clustering with GCN
19. Deep Graph Infomax
20. Hands-on: Social Network Analysis

Graph

Nodes (vertices) connected by Edges

Graph Types

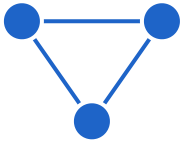
- Directed
- Undirected
- Weighted
- Attributed

Graph Properties

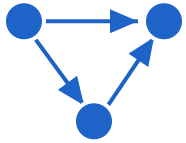
- **Degree:** # of connections
- **Density:** edge ratio
- **Clustering coeff:** local structure

⚠ Challenge

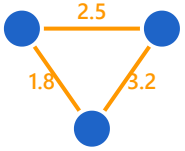
Undirected



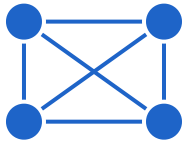
Directed



Weighted



Complete



Traditional ML assumes Euclidean space → Need

📋 Representations

- Adjacency Matrix
- Edge List

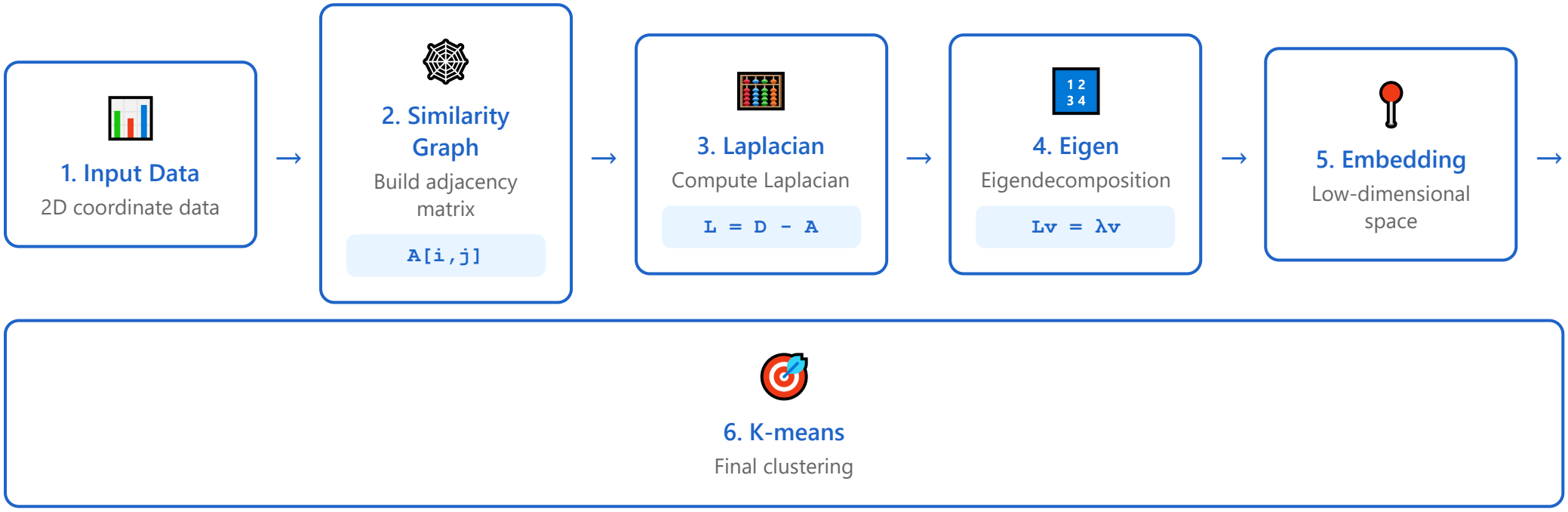
🎯 Applications

- Social Networks
- Molecules
- Knowledge Graphs

Spectral Clustering

Step-by-Step Calculation Example

Spectral Clustering Pipeline



Step-by-Step Calculation Example

1 Input Data

2 Adjacency Matrix

$p_1 = (1, 1)$ | $p_2 = (1, 2)$

$p_3 = (2, 1)$ | $p_4 = (5, 5)$

$p_5 = (5, 6)$ | $p_6 = (6, 5)$

Data Description

6 points in 2D space

- p_1, p_2, p_3: Lower-left cluster
- p_4, p_5, p_6: Upper-right cluster

$$A[i,j] = \exp(-||p_i - p_j||^2 / 2\sigma^2)$$

Using σ = 1.0, higher weight for closer points

Matrix A (6×6)

1.00	0.61	0.61	0.00	0.00	0.00
0.61	1.00	0.37	0.00	0.00	0.00
0.61	0.37	1.00	0.00	0.00	0.00
0.00	0.00	0.00	1.00	0.61	0.61
0.00	0.00	0.00	0.61	1.00	0.37
0.00	0.00	0.00	0.61	0.37	1.00

Block diagonal structure represents two clusters

3 Degree Matrix

$$D[i,i] = \Sigma_j A[i,j]$$

Sum of edge weights for each node

Matrix D (6×6 diagonal)

4 Laplacian Matrix

$$L = D - A$$

Matrix representing graph structure

Matrix L (6×6)

2.22	0	0	0	0	0
0	1.98	0	0	0	0
0	0	1.98	0	0	0
0	0	0	2.22	0	0
0	0	0	0	1.98	0
0	0	0	0	0	1.98

1.22	-0.61	-0.61	0	0	0
-0.61	0.98	-0.37	0	0	0
-0.61	-0.37	0.98	0	0	0
0	0	0	1.22	-0.61	-0.61
0	0	0	-0.61	0.98	-0.37
0	0	0	-0.61	-0.37	0.98

Block diagonal structure = two separated clusters

5 Eigendecomposition

$$Lv = \lambda v$$

Select eigenvectors corresponding to k smallest eigenvalues

Eigenvalues

$\lambda_1 = 0.00$ (first, connected graph)

$\lambda_2 = 0.00$ (second, 2 clusters!)

$\lambda_3 = 0.61$

$\lambda_4 = 1.59$

6 Spectral Embedding

$$X = [v_2 , v_3 , \ldots , v_{k+1}]$$

For k=2 clusters, use v_2 and v_3

Embedding Coordinates (6×2)

$\lambda_5 = 1.59$

$\lambda_6 = 1.83$

⚠ Key Observation

2 eigenvalues near zero → 2 clusters exist!
Number of eigenvalues = Number of connected components (clusters)

Second Eigenvector (v_2)

$v_2 = [0.58, 0.58, 0.58, -0.58, -0.58, -0.58]^T$

Positive values → Cluster 1 (p_1, p_2, p_3)
Negative values → Cluster 2 (p_4, p_5, p_6)

0.58	-0.12
0.58	0.45
0.58	-0.33
-0.58	-0.12
-0.58	0.45
-0.58	-0.33

First column (v_2) clearly separates clusters
Positive (0.58) vs Negative (-0.58)

7 K-means Clustering

`K-means(X, k=2)`

Perform K-means in embedding space

✅ Final Cluster Assignment

Cluster 1: {p_1 , p_2 , p_3 }
Cluster 2: {p_4 , p_5, p_6}

🎯 Why Does This Work?

1. Original space requires non-linear separation
2. Laplacian eigenvectors reflect graph structure
3. Embedding space allows linear separation
4. K-means easily discovers clusters

Key Insights

Advantages of Spectral Clustering

- ✅ Can find non-convex clusters
- ✅ Directly utilizes graph structure
- ✅ Can estimate number of clusters from eigenvalues
- ✅ Theoretical guarantees (minimizes normalized cut)

Complete Process Summary

Data → Similarity Graph → Laplacian → Eigenvectors → Low-dim Embedding → K-means

Community Detection - Louvain Algorithm

Finding Densely Connected Groups in Networks

Communities

Densely connected groups with sparse inter-group connections

Modularity Optimization

Measure of community structure quality

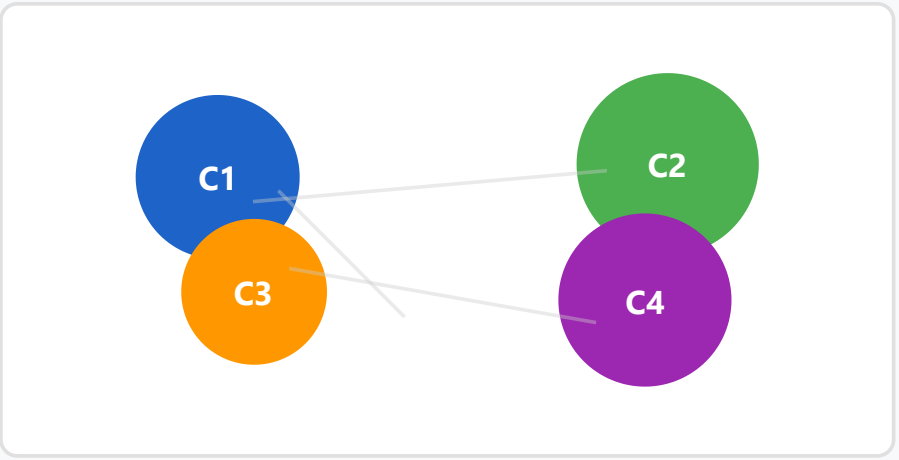
$$Q = \Sigma [e_{in} - (d_{tot}/2m)^2]$$

Two-Phase Iterative Approach

1 Local Phase

Move nodes to neighboring communities to maximize modularity gain

Community Structure Visualization



Key Advantages

- Fast & Scalable
- Hierarchical
- Large Networks
- High Quality

Applications

2

Global Phase

Aggregate communities into super-nodes, build new network

🔄 Iterate until modularity cannot be improved

Social Networks

Protein Interactions

Web Analysis

Citation Networks

Step 0: Initial State

2D Vector Input and Graph Construction

Input: 2D Vectors

```
v0:  (1.0, 1.5)
v1:  (1.2, 1.8)
v2:  (1.5, 1.3)
v3:  (5.0, 5.2)
v4:  (5.3, 5.5)
v5:  (5.1, 4.9)
```

Connection Criteria: Euclidean distance ≤ 1.0

Generated Edges:

• (v0, v1): 0.36 • (v0, v2): 0.54

• (v1, v2): 0.58 • (v3, v4): 0.42

• (v3, v5): 0.36 • (v4, v5): 0.63

Total Edges (m): 6

Initial State

Q = 0.000

Each node forms its own community.

Step 1: Move Node v0

v0 → C1 (ΔQ = +0.0833)

🔍 Node v0 Analysis

Neighbors: v1(C1), v2(C2)

Move Simulation:

• To C1: ΔQ = +0.0833 ✓

• To C2: ΔQ = +0.0694

Move v0 to C1

v0 → C1

Q = 0.083

C1={v0, v1}, C2={v2}, C3={v3}, C4={v4}, C5={v5}

Step 2: Check Node v1

v1 stays (already optimal)

🔍 Node v1 Analysis

Neighbors: v0(C1), v2(C2)

Move Simulation:

• To C2: ΔQ ≈ 0

Stay in current position

v1 stays

Q = 0.083

No change

Step 3: Move Node v2

v2 → C1 (ΔQ = +0.167)

🔍 Node v2 Analysis

Neighbors: v0(C1), v1(C1)

Move Simulation:

• To C1: ΔQ = +0.167 ✓

Move v2 to C1

Left cluster complete!

v2 → C1

Q = 0.250

C1={v0, v1, v2}, C3={v3}, C4={v4}, C5={v5}

Step 4: Move Node v3

v3 → C4 (ΔQ = +0.0833)

🔍 Node v3 Analysis

Neighbors: v4(C4), v5(C5)

Move Simulation:

• To C4: ΔQ = +0.0833 ✓

• To C5: ΔQ = +0.0694

Move v3 to C4

v3 → C4

Q = 0.333

C1={v0, v1, v2}, C4={v3, v4}, C5={v5}

Step 5: Check Node v4

v4 stays

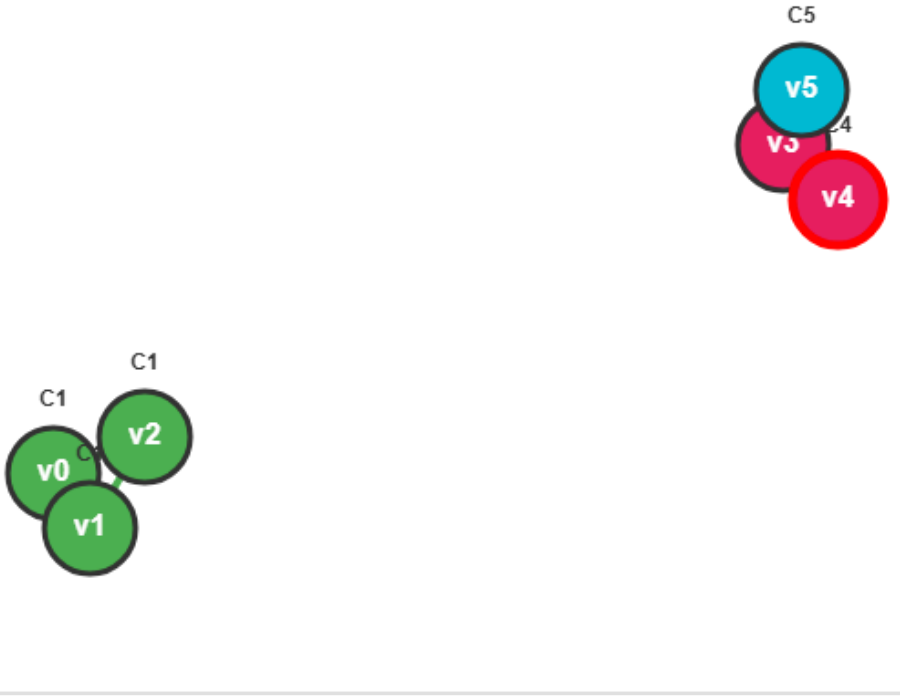
🔍 Node v4 Analysis

Neighbors: v3(C4), v5(C5)

Move Simulation:

• To C5: ΔQ ≈ 0

Stay in current position



v4 stays

Q = 0.333

No change

Step 6: Phase 1 Complete

v5 → C4 (ΔQ = +0.167)

🔍 Node v5 Analysis

Neighbors: v3(C4), v4(C4)

Move Simulation:

• To C4: ΔQ = +0.167 ✓

Move v5 to C4

Phase 1 Complete!

Phase 1 Complete

Q = 0.500

Final: C1={v0,v1,v2}, C4={v3,v4,v5}

Step 7: Phase 2 - Final Result

Super-node Creation and Algorithm Convergence

Super-nodes

S1 = {v0, v1, v2}

- Internal edges: 3
- Degree: 6

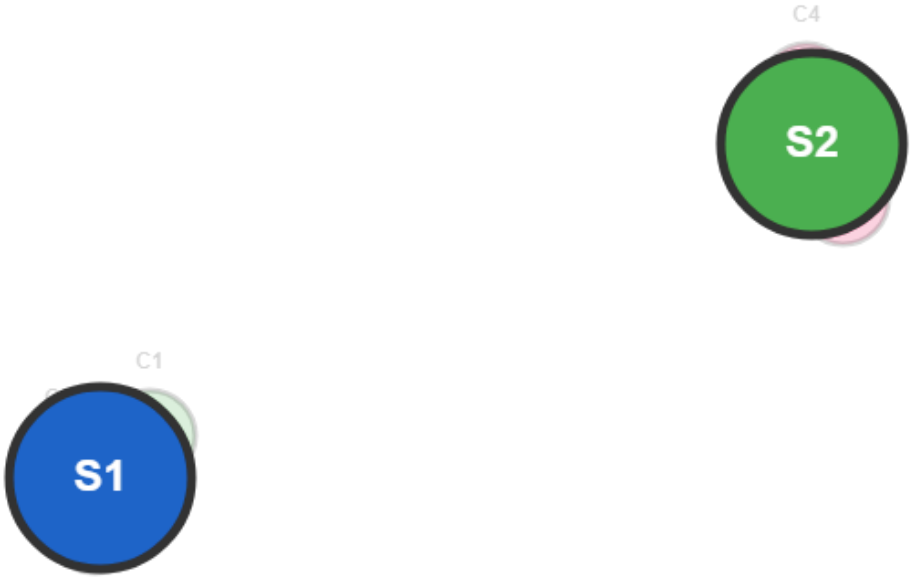
S2 = {v3, v4, v5}

- Internal edges: 3
- Degree: 6

New Graph:

- Nodes: 2
- Edges: 0

✓ Algorithm Terminated



Final Result

Q = 0.500

2 communities found!

No further improvement possible

📊 Algorithm Summary

Phase 1 Results

- Node moves: **4**
- Initial communities: **6**
- Final communities: **2**
- Modularity: **0.000** → **0.500**

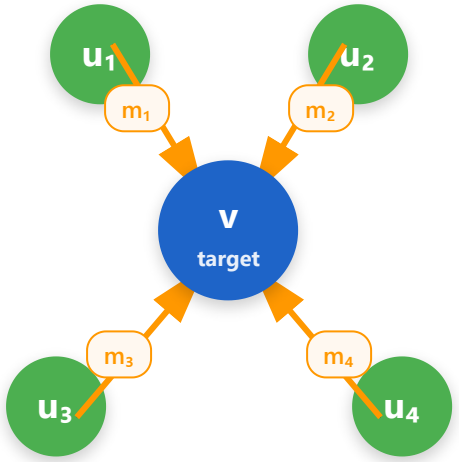
Phase 2 Results

- Super-nodes: **2**
- Hierarchy levels: **2**
- Inter-community edges: **0**
- Status: **Converged** ✓

Graph Neural Networks (GNN) Fundamentals

Deep Learning on Graph-Structured Data

Message Passing Mechanism



1 Aggregation
Collect neighbor messages

2 Transformation
Apply neural network

3 Update
Compute new representation

GNN Pipeline

Node Features

↓

Hidden Representations

↓

Predictions

✓ Key Properties

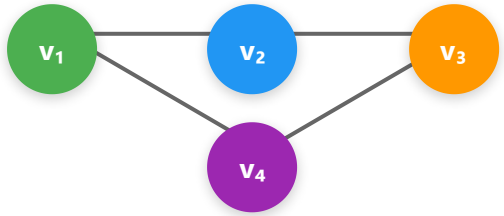
- Permutation invariant
- Learn node embeddings
- Preserve graph structure

Foundation

Basis for modern graph machine learning methods

How to Convert Graph to Convolution Input

📊 Example: Simple Graph



Adjacency Matrix (A)

$$\begin{bmatrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{bmatrix}$$

Feature Matrix (X)

$$\begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,a} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,a} \\ x_{3,1} & x_{3,2} & \cdots & x_{3,a} \\ x_{4,1} & x_{4,2} & \cdots & x_{4,a} \end{bmatrix}$$

⚙ Graph Convolution Operation

Step 1: Normalize Adjacency

$$\tilde{A} = D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$$

(Add self-loops & normalize)

↓

Step 2: Aggregate Features

$$H^{\sim} = \tilde{A} X$$

(Weighted sum of neighbors)

↓

Step 3: Apply Weights

$$H' = H^{\sim} W$$

(Linear transformation)

↓

Step 4: Non-linearity

$$H^{(l+1)} = \sigma(H')$$

(Apply activation function)

Complete Formula

$$H^{(l+1)} = \sigma(\tilde{D}^{-\frac{1}{2}}\tilde{A}\tilde{D}^{-\frac{1}{2}} H^{(l)} W^{(l)})$$

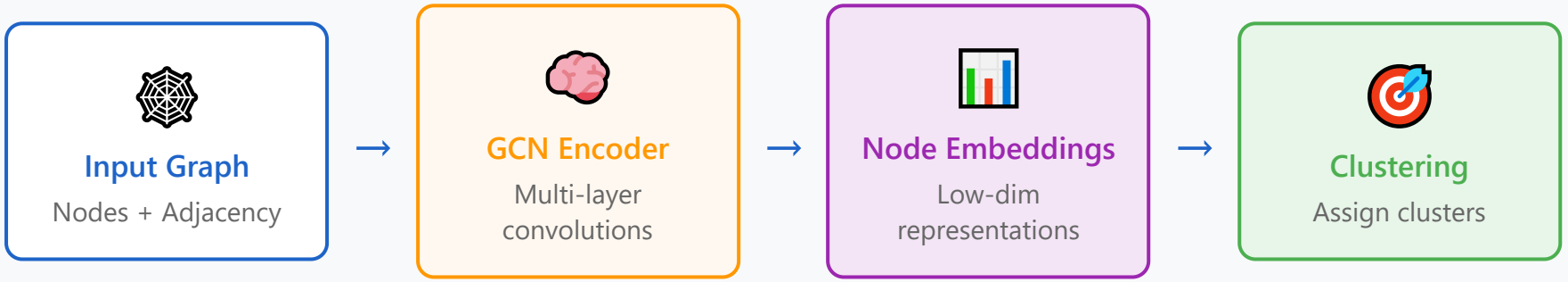
Key Points

- **Adjacency Matrix (A):** Encodes graph structure (who connects to whom)
- **Feature Matrix (X):** Node features (d-dimensional vectors for each node)
- **Degree Matrix (D):** Diagonal matrix with node degrees for normalization
- **Weight Matrix (W):** Learnable parameters (like CNN filters)
- **Output (H):** New node representations that incorporate neighborhood information

Clustering with Graph Convolutional Networks (GCN)

End-to-End Trainable Graph Clustering

GCN-based Clustering Architecture



Key Features

- ✓ Supervised or unsupervised learning
- ✓ Captures local & global structure

Advantages

- ✓ Outperforms spectral methods
- ✓ Better on benchmarks

✓ Joint optimization of encoder & clustering

✓ Learns rich node representations

Deep Graph Infomax (DGI)

Self-Supervised Graph Representation Learning

Contrastive Learning Architecture

✓ Positive Samples	✗ Negative Samples
Original Graph Real structure	**Corrupted Graph** Shuffled features
↓	↓
GNN Encoder Extract features	**GNN Encoder** Extract features
↓	↓
Local **Node Embeddings**	Global **Graph Summary**

Local representations

Global representation

🎯 Objective: Maximize Mutual Information

Maximize MI between local node embeddings and global graph summary

Self-Supervised

Learn from graph structure alone

No Labels Needed

Unsupervised training approach

Transfer Learning

Apply to downstream tasks

Hands-on: Social Network Analysis

Graph Clustering Implementation Workflow

1 Load Dataset

Karate Club or Facebook networks

NetworkX

2 Load Graph Data

Import and preprocess

NetworkX

Classical

3 Spectral Clustering

Eigendecomposition-based

scikit-learn

Classical

4 Louvain Method

Community detection

python-louvain

Deep Learning

5 Train GCN

Graph neural network

PyTorch Geometric

6 Visualize Communities

Plot detected clusters

matplotlib

Datasets

Zachary's Karate Club • Facebook Ego-networks

Step 7: Compare Results

Analyze Spectral vs Louvain vs GCN performance

Part 4/4:

Advanced Topics and Applications

21. Deep Clustering (DeepCluster, SwAV)
22. Multi-modal Clustering
23. Large-Scale Clustering
24. Real-world Applications (by Industry)

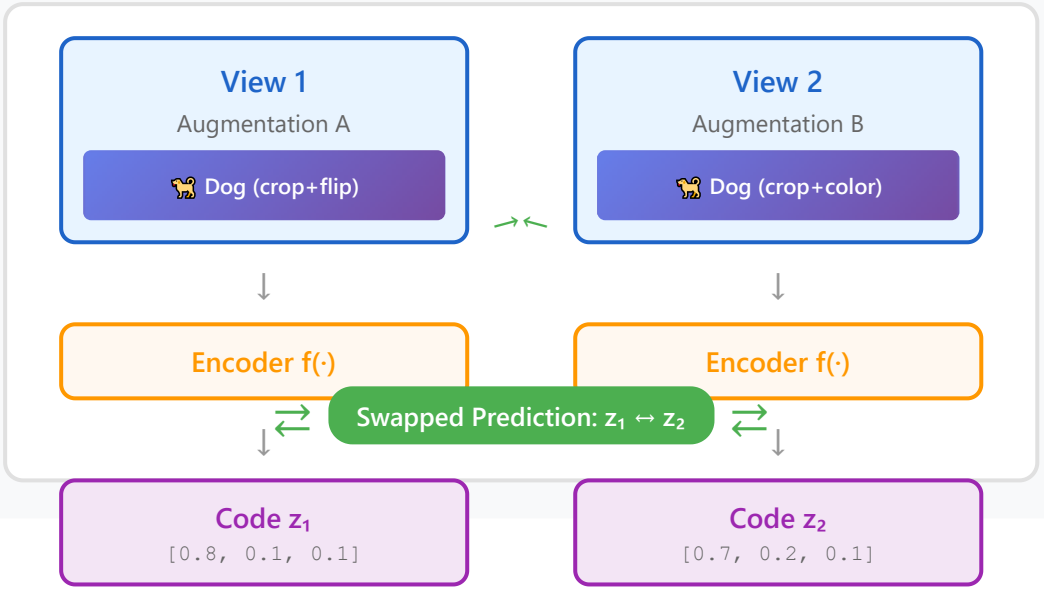
DeepCluster

- ✓ Alternates clustering and representation learning
- ✓ Cluster assignments as pseudo-labels
- ✓ Iterative refinement process

SwAV

- ✓ Swapping Assignments between Views
- ✓ Online clustering with prototypes
- ✓ Learnable cluster centroids
- ✓ No pairwise comparisons needed

SwAV Architecture & Training Process



Efficient
No pairwise comparisons

Online
Real-time clustering

Prototypes
Learnable centroids

Scalable
Large datasets

State-of-the-Art Self-Supervised Learning Results

DeepCluster Operating Principle

Algorithm Flow

1

Feature Extraction

Transform images into feature vectors using CNN

$$x \rightarrow f(x) \in \mathbb{R}^d$$

2

K-means Clustering

Group features into K clusters

$$\text{assign: } \arg\min \|f(x) - c_k\|^2$$

3

Pseudo-label Assignment

Use cluster ID as pseudo-label

```
y_pseudo = cluster_id
```

4

Network Update

Train CNN with pseudo-labels (classification)

$$L = -\log P(y_{pseudo} \mid x)$$

Problem: Trivial Solutions

All samples collapse into a single cluster

Solution: Empty Cluster Reassignment

Fill empty clusters with samples from the largest cluster

Iterate

SwAV Operating Principle

1. Multi-Crop Augmentation

224×224 (×2)

96×96 (×4)

Generate multiple views with various crop sizes

2. Prototype Assignment

$$q = \mathrm{softmax}(z \cdot C/\tau)$$

z: feature, C: prototypes, τ: temperature

Soft-assign each view to prototypes

3. Swapped Prediction

$$z_1 \rightarrow \text{predict } q_2$$

$$z_2 \rightarrow \text{predict } q_1$$

Predict View 2 from View 1's code (and vice versa)

4. Loss Computation

$$L = \ell(z_1, q_2) + \ell(z_2, q_1)$$

Cross-entropy between predictions

Online Clustering

Update prototypes every batch (no K-means needed)

Sinkhorn-Knopp

Ensures balanced cluster assignment (equipartition)

Memory Efficiency

No need to store negative pairs (vs SimCLR)

Multi-modal Clustering

Clustering Data with Multiple Modalities

⚠ Challenge

Different feature spaces and scales across modalities

Three Clustering Approaches

Early Fusion

Concatenate features from different modalities

Late Fusion

Cluster each modality separately, then combine results

Deep Multi-modal

Learn shared representation across modalities

Image

+

Text

→

Shared Space

Joint representation

🎯 Applications

🔥 Modern Approach

CLIP-style contrastive learning for multi-modal clustering

Video Analysis (visual + audio)

Medical Imaging with Reports

Contrastive Multi-modal Learning

Large-Scale Clustering

Scalable Techniques for Billions of Samples

Challenges: Billions of samples | High dimensionality

Scalability Techniques

Mini-batch K-means

Process streaming data in small batches

scikit-learn

Approximate NN

Fast nearest neighbor search

FAISS

Hierarchical

Multi-level clustering for scalability

scipy

Distributed

Parallel processing across clusters

MapReduce • Spark MLlib

GPU Acceleration

Fast distance computations

CUDA • cuML

Sampling

Representative subset selection

CoreSets

Critical Trade-off

Speed vs Accuracy

Real-world Applications by Industry

Clustering Applications Across Different Sectors

E-commerce

- Customer segmentation
- Product recommendations

Healthcare

- Patient stratification
- Disease subtyping

Finance

- Fraud detection
- Portfolio clustering

Manufacturing

- Anomaly detection
- Predictive maintenance

Social Media

- Community detection
- Content recommendation

Genomics

- Gene expression clustering
- Cell type discovery

Transportation

- Traffic pattern analysis
- Route optimization

Lecture18_31 Placeholder

콘텐츠 준비 중입니다.

Thank you

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