Lecture 11: Unsupervised Learning

Yasuyuki Sawada, Yaolang Zhong

University of Tokyo
yaolang.zhong@e.u-tokyo.ac.jp

January 7, 2026

Lecture Overview

1. Recap: Classification
   - Logistic Regression
   - K-Nearest Neighbors (KNN)
2. Unsupervised Learning
   - Task 1: Clustering (K-Means)
   - Task 2: Dimensionality Reduction (PCA)
   - Task 3: Density Estimation (KDE)

Recap: Classification and Logistic Regression

- Setup: The response variable Y is categorical, taking values in $\mathcal{C} = \{1, 2, \ldots, K\}$.
- Goal: Estimate conditional class probabilities $\hat{p}_c(x) = \Pr(Y = c \mid X = x)$, and assign observations to the class with highest probability.
- Loss Function: Misclassification rate $\frac{1}{n}\sum_{i=1}^{n} \mathbf{1}(y_i \neq \hat{y}_i)$.
- Example (Logistic Regression): For binary classification ($Y \in \{0, 1\}$),

$$\Pr(Y = 1 \mid X) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}},$$

where β is estimated by maximum likelihood.

K - Nearest Neighbors (KNN)

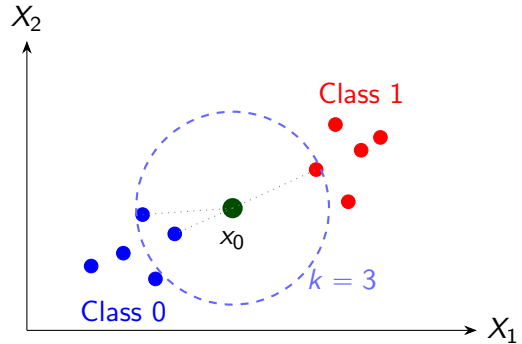
- Alternative Approach: Instead of a global parametric model for $\Pr(Y \mid X)$, KNN constructs a local, data-driven approximation.
- Local Similarity Principle:
  - For query point x_0, observations with covariates x_i close to x_0 are most informative.
  - Closeness is measured by a distance metric $d(x_i, x_0)$.
- Local Probability Estimation: Let $\mathcal{N}_k(x_0)$ be the k nearest neighbors of x_0.

$$\hat{p}_c(x_0) = \frac{1}{k} \sum_{i \in \mathcal{N}_k(x_0)} \mathbf{1}(y_i = c).$$

- Classification Rule:

$$\hat{Y}(x_0) = \arg\max_{c \in \mathcal{C}} \hat{p}_c(x_0).$$

KNN (Illustration)



Example with $k = 3$:

- 3 nearest neighbors: 2 from Class 0 (blue), 1 from Class 1 (red).
- Majority vote $\Rightarrow$ Predict Class 0. $\quad \hat{P}(\text{Class } 0) = 2/3.$

KNN: Algorithmic Implementation

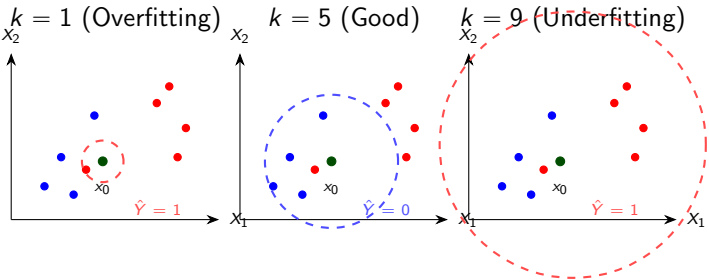
- Given the local probability estimator defined previously, KNN operationalizes it through the following steps. For a query point x_0:
  1. Choose the number of neighbors k.
  2. Compute distances $d(x_0, x_i)$ for all training observations.
  3. Identify the neighbor set $\mathcal{N}_k(x_0)$.
  4. Compute $\hat{p}_c(x_0)$ using neighbor frequencies.
  5. Assign class $\hat{Y}(x_0)$ by maximizing $\hat{p}_c(x_0)$.
- Remarks:
  - No parameters are estimated during training.
  - All computation occurs at prediction time ("lazy learning").
  - hyperparameters: k (number of neighbors), d (distance metric)

KNN: Choice of k and bias-variance trade-off

The hyperparameter k controls the bias-variance trade-off.

- Small k (e.g., $k = 1$):
  - Highly flexible, jagged boundary. Low bias, high variance.
  - Sensitive to noise and outliers. Risk of overfitting.
- Large k (e.g., $k = n$):
  - Smoother, more stable boundary. High bias, low variance.
  - Robust to noise. Risk of underfitting.
- Selecting k in Practice:
  - Use cross-validation to find optimal k.
  - Common starting point: $k = \sqrt{n}$. Odd k avoids ties in binary classification.

KNN: Effect of k (Illustration)



- $k = 1$: Only the red outlier $\Rightarrow$ misclassification.
- $k = 5$: 4 blue, 1 red $\Rightarrow$ correct (Class 0).
- $k = 9$: 4 blue, 5 red $\Rightarrow$ predicts global majority, ignores local structure.

KNN: Choice of d and curse of dimensionality

- The definition of "nearest" depends on the distance metric $d(x, x')$.
- Common choices:
  - Euclidean (L2): $d(x, x') = \sqrt{\sum_{j=1}^{p}(x_j - x'_j)^2}$ (most common)
  - Manhattan (L1): $d(x, x') = \sum_{j=1}^{p} |x_j - x'_j|$ (robust to outliers)
  - Cosine: $d(x, x') = 1 - \frac{x \cdot x'}{\|x\| \|x'\|}$ (text/high-dim sparse data)
- Critical preprocessing — Feature Scaling:
  - Features with larger scales dominate the distance calculation.
  - Standardization is essential: $\tilde{x}_j = \frac{x_j - \mu_j}{\sigma_j}$.

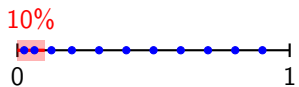
KNN: Dimensionality and Computation

- Curse of Dimensionality:
  - As the dimension p increases, observations become sparse in the feature space.
  - "Local" neighborhoods may no longer be meaningfully local.
  - To see this, note that to capture a fraction r of the data in p dimensions, a hypercube must have edge length $r^{1/p}$. Consider the example $r = 0.1$:
    - $p = 2 \Rightarrow 0.32$
    - $p = 10 \Rightarrow 0.80$
    - $p = 100 \Rightarrow 0.98$
- Computational Implications:
  - Training cost is negligible (data storage only).
  - Prediction requires distance computation to all n observations: $O(np)$ per query.
- Practical Responses:
  - Dimensionality reduction (feature selection, PCA).
  - Distance metrics adapted to high-dimensional data (e.g. cosine similarity).
  - Approximate nearest-neighbor methods for large datasets.

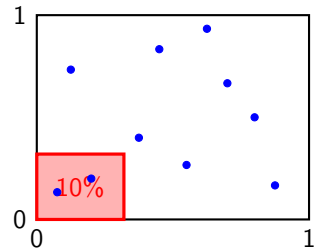
KNN: Curse of Dimensionality (Illustration)

To capture fraction r of data, neighborhood edge length $= r^{1/p}$.

$p = 1$: Edge $= 0.1$



$p = 2$: Edge $= \sqrt{0.1} \approx 0.32$



- In 1D, capturing 10% of data requires only 10% of the range.
- In 2D, capturing 10% of data requires 32% of each axis.
- As $p \to \infty$, "local" neighborhoods span nearly the entire space.

Unsupervised Learning: Overview

- Setup: We observe input vectors $X_1, \ldots, X_n$, but no response Y.

$$\mathcal{D} = \{x_1, x_2, \ldots, x_n\}.$$

- Challenge: Without an observed target, there is no explicit loss function to guide learning.
- Goal: Using only the joint distribution of X, we aim to:
  - Identify latent groupings or patterns among observations.
  - Construct low-dimensional representations preserving essential structure.
  - Characterize salient features of $P(X)$.

Task 1: Clustering (Definitions)

- Setup: We observe data $\{x_i\}_{i=1}^n$ drawn from a single, unknown distribution $P(X)$.
- Definition: Clustering partitions observations into groups using only information in X, without observing class labels or outcomes.
- Objective: Construct a partition $\{C_1, \ldots, C_K\}$ such that:
  - Observations within a cluster are similar according to a chosen metric.
  - Observations across clusters are dissimilar.
- Interpretation:
  - Clusters provide a discrete summary of structure in $P(X)$ (e.g. regions of high density or distinct geometric patterns).
  - In some models, clusters may be interpreted as latent components of a mixture distribution.

Task 1: Clustering (Example & Mechanism)

- Example: *Market Segmentation*. Given customer spending histories X, group customers with similar behavior.
- Mechanism: K-Means Clustering. Approximate the data distribution by K representative centers and solve

$$\min_{C_1,\dots,C_K} \sum_{k=1}^{K} \sum_{i \in C_k} \|x_i - \mu_k\|^2,$$

  where μ_k is the centroid of cluster k.
- Algorithm (Lloyd's Algorithm):
  - Initialize centroids $\{\mu_k^{(0)}\}_{k=1}^{K}$.
  - Assignment:

$$i \in C_k^{(t)} \iff \|x_i - \mu_k^{(t)}\| \leqslant \|x_i - \mu_j^{(t)}\| \ \ \forall j.$$

  - Update:

$$\mu_k^{(t+1)} = \frac{1}{|C_k^{(t)}|} \sum_{i \in C_k^{(t)}} x_i.$$

  - Iterate until assignments stabilize.

Task 2: Dimensionality Reduction (Definitions)

- Setup: Observations $\{x_i\}_{i=1}^n$ lie in a high-dimensional space $\mathbb{R}^p$.
- Definition: Dimensionality reduction constructs a low-dimensional representation of X using only information in X.
- Objective: Find a mapping

$$x_i \in \mathbb{R}^p \longmapsto z_i \in \mathbb{R}^q, \quad q \ll p,$$

  such that essential structure in the data is preserved.
- Interpretation:
  - The low-dimensional representation captures dominant patterns in $P(X)$.
  - Reduces noise and redundancy while retaining informative variation.

Task 2: Dimensionality Reduction (Example & Mechanism)

- Example: *Visualizing Genetic Data*. Gene expression levels for $p = 10{,}000$ genes observed across $n = 50$ patients; direct visualization in $\mathbb{R}^p$ is infeasible.
- Mechanism: Principal Component Analysis (PCA)

  PCA seeks low-dimensional projections of the form $Z_j = \phi_j^\top X$, where directions $\{\phi_j\}$ are chosen sequentially.
- First Principal Component:
  - Choose ϕ_1 to maximize variance:

$$\phi_1 = \arg\max_{\|\phi\|=1} \mathrm{Var}(\phi^\top X).$$

- Subsequent Components:
  - For $j \geqslant 2$, choose

$$\phi_j = \arg\max_{\|\phi\|=1} \mathrm{Var}(\phi^\top X) \quad \text{s.t. } \phi^\top \phi_\ell = 0 \ \ \forall \ell < j.$$

  - This enforces orthogonality and ensures components are uncorrelated.

Task 3: Density Estimation (Definitions)

- Setup: Observations $\{x_i\}_{i=1}^n$ are drawn from an unknown distribution $P(X)$.
- Definition: Density estimation aims to estimate the probability distribution $P(X)$ itself.
- Objective: Construct an estimator $\hat{p}(x)$ of the data density $p(x)$ using only the observed sample.
- Interpretation:
  - Provides a global, probabilistic description of $P(X)$.
  - Serves as a foundation for anomaly detection, simulation, and likelihood-based analysis.

Task 3: Density Estimation (Example & Mechanism)

- Example: Estimate the distribution of income, asset returns, or firm productivity using only observed data $\{x_i\}_{i=1}^n$.
- Mechanism: Kernel Density Estimation (KDE)

  KDE estimates the density at a point x by locally averaging nearby observations:

$$\hat{p}(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right),$$

  where $K(\cdot)$ is a kernel function and $h > 0$ is a bandwidth.
- Algorithmic Interpretation:
  - Center a kernel K at each observation x_i.
  - Evaluate proximity using the scaled distance $(x - x_i)/h$.
  - Average the contributions across all observations.
- Bandwidth Choice:
  - Small h: highly local averaging (low bias, high variance).
  - Large h: strong smoothing (high bias, low variance).

References

James, G., Witten, D., Hastie, T., Tibshirani, R. (2021).

An Introduction to Statistical Learning with Applications in Python.

Springer.

https://www.statlearning.com/