L03: KNN & K-Means

Deep Dive: Mathematical Foundations and Implementation

Methods and Algorithms

MSc Data Science

Spring 2026

Outline

1. KNN Foundations
2. KNN Theory
3. K-Means Algorithm
4. K-Means Theory
5. Cluster Validation
6. Comparison and Applications
7. Implementation
8. Practice
9. Summary

How Machine Learning Really Works

XKCD #1838 by Randall Munroe (CC BY-NC 2.5)

Learning Objectives

By the end of this lecture, you will be able to:

1. **Analyze** the bias-variance tradeoff in KNN and derive its asymptotic error bounds
2. **Evaluate** clustering validity using statistical tests (Hopkins, Gap statistic, silhouette)
3. **Prove** K-Means convergence and analyze computational complexity
4. **Compare** distance metrics and assess their suitability for high-dimensional finance data

Finance Applications: Customer segmentation (RFM), fraud detection

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Bloom's Level 4–5: Analyze, Evaluate, Prove, Compare

KNN: The Lazy Learner

Key Insight

- No explicit model training – store all training data
- Classification by majority vote of K nearest neighbors
- "Lazy" because all computation happens at prediction time

The Algorithm in Words

1. Store all training examples $(\mathbf{x}_i, y_i)$
2. For new query $\mathbf{x}$: find K nearest training points
3. Return majority class among those K neighbors

Instance-based learning: the training data IS the model – no parameters to estimate

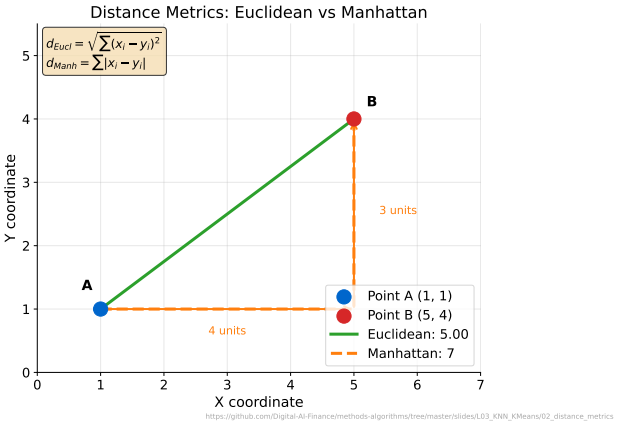
KNN Algorithm

Input: Training set $\mathcal{D}$, query point $\mathbf{x}$, number of neighbors K
Compute $d(\mathbf{x}, \mathbf{x}_i)$ for all $\mathbf{x}_i \in \mathcal{D}$
Select K points with smallest distances: $N_K(\mathbf{x})$
Count votes: $v_c = |\{i \in N_K(\mathbf{x}) : y_i = c\}|$ for each class c
if unique maximum class exists **then**
    $\hat{y} = \arg\max_c v_c$
else
    Tie-breaking: $\hat{y} = \arg\max_c \sum_{i:y_i=c} \frac{1}{d(\mathbf{x},\mathbf{x}_i)}$
end if
return $\hat{y}$

Complexity: $O(nd)$ per query (brute force over n samples, d features)

Tie-breaking via distance-weighted vote prevents non-determinism on decision boundaries

Distance Metrics: Visualization



Key Insight: Different metrics define different "neighborhoods" – the choice of metric shapes the decision boundary and determines which points count as nearest neighbors.

Euclidean (circular), Manhattan (diamond), Chebyshev (square) unit balls in 2D

Distance Metrics: Minkowski Family

Minkowski Distance

$$d_p(\mathbf{x}, \mathbf{y}) = \left(\sum_{i=1}^{d} |x_i - y_i|^p \right)^{1/p}$$

- $p = 1$: Manhattan (L1) – robust to outliers, sparse feature differences
- $p = 2$: Euclidean (L2) – default, geometrically intuitive
- $p = \infty$: Chebyshev – maximum absolute difference along any axis

Triangle Inequality: For $p \geq 1$, $d_p(\mathbf{x}, \mathbf{z}) \leq d_p(\mathbf{x}, \mathbf{y}) + d_p(\mathbf{y}, \mathbf{z})$

- Enables pruning in KD-Trees and Ball Trees
- For $p < 1$: violates triangle inequality (not a true metric)

Higher p amplifies large single-feature differences; $p = 2$ is the default for most applications

Beyond Minkowski: Cosine & Mahalanobis

Cosine Similarity (for text and embeddings)

$$\cos(\mathbf{x}, \mathbf{y}) = \frac{\mathbf{x} \cdot \mathbf{y}}{\|\mathbf{x}\|\|\mathbf{y}\|}, \quad \text{range: } [-1, 1]$$

- Measures angle, not magnitude – ideal for sparse, high-dimensional data
- Use for: document similarity, word embeddings, TF-IDF vectors

Mahalanobis Distance (accounts for correlation)

$$d_M(\mathbf{x}, \mathbf{y}) = \sqrt{(\mathbf{x} - \mathbf{y})^T \Sigma^{-1} (\mathbf{x} - \mathbf{y})}$$

- Uses feature covariance Σ – unit-less, scale-invariant
- Detects outliers accounting for correlation structure

Choose metric based on data type: Euclidean for dense, Cosine for sparse/text, Mahalanobis for correlated features

Choosing K: Bias-Variance Tradeoff

The Fundamental Tradeoff

- $K = 1$: High variance, low bias – very flexible, memorizes noise
- $K = n$: High bias, low variance – always predicts majority class

Practical Guidelines

- Start with $K = \sqrt{n}$ where n is training size
- Use odd K for binary classification (avoids ties)
- Always validate with cross-validation

Common Choices: $K \in \{3, 5, 7, 11\}$

Small K for complex patterns with clean data; larger K for noisy data requiring smoothing

Weighted KNN

Problem: All K neighbors have equal influence – a distant neighbor counts as much as the closest one.

Inverse-Distance Weighting

$$\hat{y} = \arg\max_c \sum_{i \in N_K(\mathbf{x})} w_i \cdot \mathbf{1}[y_i = c] \quad \text{where } w_i = \frac{1}{d(\mathbf{x}, \mathbf{x}_i)}$$

- Closer neighbors receive exponentially higher weight
- Reduces sensitivity to the choice of K
- For $d = 0$ (exact match): return that point's class directly

In scikit-learn: `weights='uniform'` (default) vs `weights='distance'`

Distance weighting often improves performance, especially when K is not perfectly tuned

K Selection via Cross-Validation

GridSearchCV for Optimal K

- `param_grid = {'n_neighbors': range(1, 21, 2)}`
- `grid = GridSearchCV(KNeighborsClassifier(), param_grid, cv=5)`
- `grid.fit(X_train, y_train)`
- `best_k = grid.best_params_['n_neighbors']`

Validation Curve Interpretation

- Plot accuracy vs K for both training and validation sets
- Choose K where validation accuracy peaks (before overfitting gap widens)
- Large gap between train/val curves signals overfitting

Cross-validation provides objective, data-driven K selection – never choose K by "eyeballing"

Feature Scaling for KNN

Why Scaling Matters – Without scaling:

- Income: ranges 20,000–200,000
- Age: ranges 20–80
- Distance dominated by income (180,000× larger scale!)

Scaling Methods

- **Standardization**: $z = \frac{x-\mu}{\sigma}$ (mean=0, std=1)
- **Min-Max**: $x' = \frac{x-x_{\min}}{x_{\max}-x_{\min}}$ (range [0,1])

Edge Cases

- If $\sigma = 0$ or $x_{\max} = x_{\min}$ (constant feature): drop feature or set to 0

Rule: ALWAYS scale features for distance-based methods. StandardScaler for Gaussian-like, MinMaxScaler for bounded.

Curse of Dimensionality

The Problem (Beyer et al., 1999)
In high dimensions, for any query point $\mathbf{x}$:

$$\lim_{d \to \infty} \frac{d_{\max} - d_{\min}}{d_{\min}} \to 0$$

- All points become approximately equidistant
- "Nearest neighbor" becomes meaningless
- Volume of unit hypersphere $\to 0$ as $d \to \infty$

Solutions

- **Dimensionality reduction**: PCA before KNN (see L05)
- **Feature selection**: keep only relevant features
- **Domain knowledge**: select meaningful features from subject matter

KNN works best with moderate dimensionality ($d < 15$–20, problem-dependent)

Cover & Hart (1967): Consistency Theorem

Theorem: As $n \to \infty$, the 1-NN error rate satisfies:

$$R^* \leq R_{\text{1-NN}} \leq 2R^*(1 - R^*)$$

where R^* is the Bayes optimal error rate.

Key Results

- 1-NN error is at most $2\times$ Bayes error – remarkably strong for such a simple method
- KNN is **universally consistent**: $R_{K\text{-NN}} \to R^*$ exactly
- Requires: $K \to \infty$ and $K/n \to 0$ simultaneously

Practical Implication: KNN is a strong baseline – if it performs badly, the features may be poor rather than the algorithm.

Universal consistency holds under mild conditions; see appendix for full proof

Cover & Hart: Proof Sketch

Proof idea (1-NN case, binary classification):

1. As $n \to \infty$, the nearest neighbor $\mathbf{x}_{(1)} \to \mathbf{x}$ (converges to query)
2. Let $\eta(\mathbf{x}) = P(Y = 1|\mathbf{x})$. The 1-NN error at $\mathbf{x}$:

$$R_{\text{1-NN}}(\mathbf{x}) = \eta(\mathbf{x})(1 - \eta(\mathbf{x})) + (1 - \eta(\mathbf{x}))\eta(\mathbf{x}) = 2\eta(\mathbf{x})(1 - \eta(\mathbf{x}))$$

Since $R^*(\mathbf{x}) = \min(\eta, 1 - \eta)$ and $2\eta(1 - \eta) \leq 2\min(\eta, 1 - \eta)$:

$$R^* \leq R_{\text{1-NN}} \leq 2R^*(1 - R^*)$$

For K-NN with $K \to \infty$, $K/n \to 0$: majority vote over K neighbors converges to $\mathbf{1}[\eta(\mathbf{x}) > 0.5]$, so $R_{K\text{-NN}} \to R^*$ exactly.

The $2\times$ bound is tight: equality when $\eta(\mathbf{x}) = 0.5$ everywhere (maximum ambiguity)

Bias-Variance Decomposition for KNN

For KNN regression, $\hat{f}_K(\mathbf{x}) = \frac{1}{K}\sum_{i \in N_K(\mathbf{x})} y_i$, the expected error decomposes as:

$$E[(\hat{f}_K(\mathbf{x}) - Y)^2] = \underbrace{\text{Bias}^2(\hat{f}_K(\mathbf{x}))}_{\text{increases with } K} + \underbrace{\text{Var}(\hat{f}_K(\mathbf{x}))}_{\text{decreases with } K} + \sigma^2$$

- **Variance**: $\text{Var}(\hat{f}_K) = \frac{\sigma^2}{K}$ (averaging K neighbors reduces variance)
- **Bias**: $\text{Bias}(\hat{f}_K) \approx f(\mathbf{x}) - \frac{1}{K}\sum_{i \in N_K} f(\mathbf{x}_i)$ (larger K = farther neighbors = more bias)
- **Optimal** K: balances this tradeoff; found via cross-validation

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$K = 1$: **zero bias, variance** $= \sigma^2$. $K = n$: **high bias (global mean), variance** $= \sigma^2/n$.

K-Means: The Idea

Goal: Partition n points into K clusters by minimizing within-cluster sum of squares (WCSS):

$$J = \sum_{k=1}^{K} \sum_{\mathbf{x}_i \in C_k} \|\mathbf{x}_i - \boldsymbol{\mu}_k\|^2$$

where $\boldsymbol{\mu}_k = \frac{1}{|C_k|} \sum_{\mathbf{x}_i \in C_k} \mathbf{x}_i$ is the centroid of cluster C_k.

Key Properties

- Each point assigned to its nearest centroid
- Iterative refinement: assign $\rightarrow$ update $\rightarrow$ repeat
- Converges to local (not global) optimum

Finding the globally optimal K-Means solution is NP-hard (Aloise et al., 2009)

K-Means Algorithm

1: **Input**: Data $\mathbf{X}$, number of clusters K
2: Initialize K centroids (K-Means++ or random)
3: **repeat**
4: **Assignment**: $C_k = \{\mathbf{x}_i : \|\mathbf{x}_i - \boldsymbol{\mu}_k\| \leq \|\mathbf{x}_i - \boldsymbol{\mu}_j\| \; \forall j\}$
5: **Update**: $\boldsymbol{\mu}_k = \frac{1}{|C_k|} \sum_{\mathbf{x}_i \in C_k} \mathbf{x}_i$
6: **Handle empty**: if $|C_k| = 0$, reinitialize $\boldsymbol{\mu}_k$ from farthest point
7: **until** centroid change $< \epsilon$ or max iterations reached
8: **return** cluster assignments, centroids

Convergence: Guaranteed – WCSS decreases monotonically each iteration. May converge to local optimum; run multiple restarts.

Each iteration costs $O(nKd)$ where n = samples, K = clusters, d = features

K-Means++: Smart Initialization

Problem: Random initialization is sensitive to starting positions and often converges to poor local optima.

K-Means++ Algorithm (Arthur & Vassilvitskii, 2007)

1. Choose first centroid uniformly at random from data
2. For each subsequent centroid: select point $\mathbf{x}$ with probability $\propto d(\mathbf{x})^2$ (squared distance to nearest existing centroid)
3. Repeat until K centroids chosen

Guarantee: Expected cost $\leq 8(\ln K + 2) \times$ optimal cost – an $O(\log K)$-competitive approximation.

K-Means++ is the default in scikit-learn (`init='k-means++'`); typically converges in fewer iterations

Silhouette Score

For each point i:

- $a(i)$: average distance to all other points in **same** cluster (cohesion)
- $b(i)$: average distance to points in **nearest other** cluster (separation)

Silhouette coefficient:

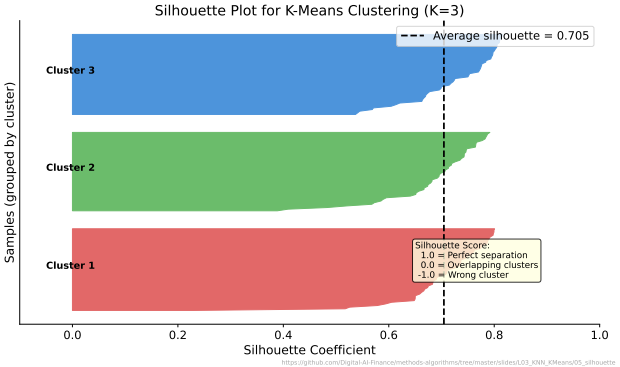
$$s(i) = \frac{b(i) - a(i)}{\max(a(i), b(i))}, \quad s(i) \in [-1, 1]$$

Interpretation:

- $s \approx 1$: point is well-clustered (far from neighboring clusters)
- $s \approx 0$: point lies on the boundary between clusters
- $s < 0$: point is likely assigned to the wrong cluster

Average silhouette score across all points summarizes overall clustering quality. Singleton: $s(i) = 0$ by convention.

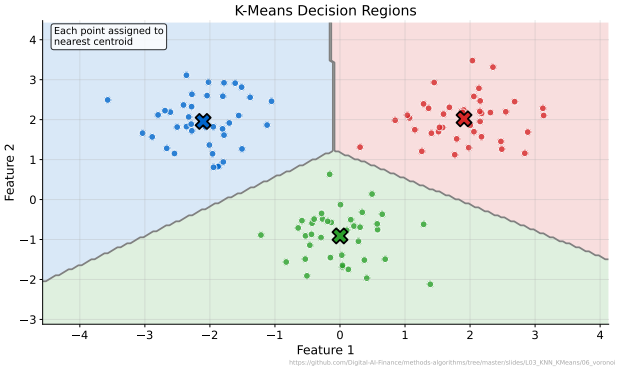
Silhouette Plot



Reading the Plot: Each cluster should have similar width (balanced sizes) and scores above the average line. Thin or negative clusters indicate poor assignments.

Compare silhouette plots across different K values to find the optimal number of clusters

K-Means Decision Regions



Voronoi Tessellation: K-Means partitions the feature space into convex polygonal regions. Every point within a region is closest to that region's centroid.

Voronoi cells are always convex – this is why K-Means cannot discover non-convex cluster shapes

K-Means Assumptions and Failure Cases

What K-Means Assumes

- Clusters are **spherical** (isotropic variance in all directions)
- Clusters have **similar sizes** (roughly equal number of points)
- Clusters have **similar densities**

When K-Means Fails

- Non-convex shapes (e.g., crescents, rings) – use DBSCAN
- Very different cluster sizes or densities – use GMM
- Strong outliers – use K-Medoids (centroids must be data points)

Always visualize clusters in 2D (via PCA/t-SNE) to check if assumptions hold

K-Means Convergence Proof

Theorem: Lloyd's algorithm converges in a finite number of iterations.

Proof (coordinate descent argument):
The WCSS objective $J = \sum_{k=1}^{K} \sum_{\mathbf{x}_i \in C_k} \|\mathbf{x}_i - \boldsymbol{\mu}_k\|^2$ satisfies:

1. **Assignment step** (fix $\boldsymbol{\mu}$, optimize C): Reassigning each point to its nearest centroid can only decrease J $\Rightarrow$ J non-increasing
2. **Update step** (fix C, optimize $\boldsymbol{\mu}$): The mean minimizes within-cluster SSE $\Rightarrow$ J non-increasing

Since $J \geq 0$ and non-increasing, and there are finitely many partitions of n points into K clusters: the algorithm must terminate. □

NP-hardness: Global optimum is NP-hard; K-Means++ provides $O(\log K)$ approximation.

Block coordinate descent: alternating optimization of two blocks (C and $\boldsymbol{\mu}$) on a bounded objective

K-Means as EM Special Case

Connection to Expectation-Maximization

- K-Means = "Hard EM" for Gaussian Mixture Models (GMM)
- Assumes: spherical Gaussians with equal variance $\sigma^2 I$
- **E-step**: assign points to nearest centroid (hard assignment, $\gamma_{ik} \in \{0, 1\}$)
- **M-step**: update centroids as cluster means

Why This Matters

- Explains WHY convergence is guaranteed (EM always converges)
- Explains WHY K-Means assumes spherical clusters
- Opens door to **soft clustering** via full GMM (probabilistic assignments)

Soft EM: $\gamma_{ik} \in [0, 1]$ **gives probability of membership – more flexible but computationally heavier**

K-Means Variants

Mini-Batch K-Means

- Uses random subsets (mini-batches) for centroid updates
- 10–100$\times$ faster for large datasets; slightly worse results

K-Medoids (PAM)

- Centroids must be actual data points (medoids)
- More robust to outliers; works with any distance metric

K-Modes / K-Prototypes

- K-Modes: for categorical data (uses mode instead of mean)
- K-Prototypes: mixed continuous and categorical features

Mini-Batch K-Means is recommended for $n > 10{,}000$ samples; K-Medoids for non-Euclidean distances

Computational Considerations

Method	Training	Prediction
KNN (brute force)	$O(1)$	$O(nd)$
KNN (KD-Tree)	$O(nd \log n)$	$O(d \log n)$
KNN (Ball Tree)	$O(nd \log n)$	$O(d \log n)$
K-Means (Lloyd's)	$O(nKdT)$	$O(Kd)$
Mini-Batch K-Means	$O(bKdT)$	$O(Kd)$

n = samples, d = features, K = neighbors/clusters, T = iterations, b = batch size.

- KD-Tree degrades to $O(nd)$ when $d > 15$–20
- For very large n: approximate nearest neighbors (LSH, FAISS)

scikit-learn `algorithm='auto'` selects the best method based on n and d

Hopkins Statistic: Should We Cluster?

Before Clustering: Test whether data has cluster tendency at all.

$$H = \frac{\sum_{i=1}^{m} u_i^d}{\sum_{i=1}^{m} u_i^d + \sum_{i=1}^{m} w_i^d}$$

- u_i = distance from random point (uniform in data range) to nearest data point
- w_i = distance from randomly sampled data point to its nearest neighbor

Interpretation:

- $H \approx 0.5$: uniform distribution (no clusters) – do not cluster
- $H > 0.75$: significant clustering tendency – proceed with clustering

Always run Hopkins test before K-Means – clustering uniform data produces meaningless results

Gap Statistic for K Selection

Gap Statistic (Tibshirani et al., 2001)

$$\text{Gap}_n(k) = E_n^*[\log W_k] - \log W_k$$

where $W_k = \sum_{r=1}^{k} \frac{1}{2|C_r|} \sum_{i,j \in C_r} \|x_i - x_j\|^2$ and E_n^* is the expectation under a reference (uniform) distribution.

Selection Rule: Choose smallest K such that:

$$\text{Gap}(k) \geq \text{Gap}(k+1) - s_{k+1}$$

where s_{k+1} is the standard error from B bootstrap reference samples.

Advantage over Elbow: Provides a statistical criterion rather than subjective visual inspection.

Tibshirani et al. recommend $B = 20$–50 bootstrap samples for stable estimates

Comparison of K Selection Methods

Method	Objectivity	Speed	Best For
Elbow (WCSS)	Low (subjective)	Fast	Quick exploration
Silhouette	High	Moderate	Cluster quality
Gap Statistic	High (statistical)	Slow	Rigorous analysis

Practical Recommendation:

- Start with elbow plot for quick overview
- Validate with silhouette score and silhouette plots
- Use Gap statistic when formal justification is needed (e.g., publications)

No single method is perfect – use multiple methods and check if they agree

KNN vs K-Means: Key Differences

Aspect	KNN	K-Means
Task	Classification / Regression	Clustering
Learning Type	Supervised (needs labels)	Unsupervised (no labels)
K meaning	Number of neighbors	Number of clusters
Training	None (lazy learner)	Iterative optimization
Prediction	Compute distances to all	Assign to nearest centroid
Output	Class label / value	Cluster assignment
Scalability	$O(nd)$ per query	$O(nKdT)$ total

The "K" in KNN and K-Means mean completely different things – a common source of confusion!

Finance: RFM Customer Segmentation

RFM Analysis (Industry Standard)

- **R**ecency: Days since last transaction
- **F**requency: Number of transactions in period
- **M**onetary: Total / average transaction value

Pipeline: Standardize RFM $\rightarrow$ K-Means (K=4–6) $\rightarrow$ Profile segments **Typical Segments**:

- "Champions" (high R, F, M) $\rightarrow$ loyalty rewards
- "At Risk" (low R, declining F) $\rightarrow$ retention campaigns
- "New Customers" (high R, low F) $\rightarrow$ onboarding programs

Business Value: Customer Lifetime Value (CLV) prediction per segment

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RFM segmentation is foundational for CRM, marketing analytics, and credit risk profiling

Finance: Fraud Detection with KNN

CRITICAL: Class Imbalance Problem

- Fraud is typically $<1\%$ of transactions (100:1 ratio)
- Naive KNN majority vote: ALWAYS predicts non-fraud (99% accuracy, zero fraud detected!)

Solutions for Imbalanced Data

- **SMOTE**: Synthetic Minority Oversampling TEchnique
- **Weighted KNN**: Higher weight for minority class neighbors
- **Anomaly score**: Use distance to K-th neighbor instead of majority vote

Evaluation: Use **Precision-Recall AUC**, NOT accuracy!

Always check class distribution before applying majority vote – accuracy is misleading for imbalanced data

Alternative Clustering: DBSCAN and Hierarchical

DBSCAN (Density-Based Spatial Clustering):

- **Core point**: $\geq$ minPts neighbors within radius ε
- **Border point**: within ε of a core point but not itself core
- **Noise**: neither core nor border $\Rightarrow$ automatic outlier detection
- Does not require K; discovers non-spherical clusters

Hierarchical (Agglomerative) Clustering:

- Bottom-up: each point starts as its own cluster, iteratively merge closest pairs
- Linkage: single (min), complete (max), Ward (minimize variance)
- **Dendrogram**: cut at desired height to get K clusters

DBSCAN for irregular shapes with outliers; hierarchical when exploring multiple K values via dendrogram

When to Use What

Use KNN When

- You have labeled training data (supervised)
- Local patterns matter (non-linear boundaries)
- Interpretability: "classified because similar to these examples"

Use K-Means When

- No labels available (unsupervised)
- Looking for natural groupings in data
- Clusters are roughly spherical and similar in size

Use Alternatives When

- Non-spherical clusters $\rightarrow$ DBSCAN or spectral clustering
- Soft assignments needed $\rightarrow$ Gaussian Mixture Models
- Very large $n \rightarrow$ Mini-Batch K-Means or approximate NN

K-Means is often used as preprocessing (cluster features) before supervised learning

KNN in scikit-learn

Classification

- `from sklearn.neighbors import KNeighborsClassifier`
- `knn = KNeighborsClassifier(n_neighbors=5, weights='distance')`
- `knn.fit(X_train, y_train)`
- `y_pred = knn.predict(X_test)`

Key Parameters

- `n_neighbors`: K value (default 5)
- `weights`: `'uniform'` or `'distance'`
- `metric`: `'euclidean'`, `'manhattan'`, `'minkowski'`
- `algorithm`: `'auto'`, `'ball_tree'`, `'kd_tree'`, `'brute'`

Also available: `KNeighborsRegressor` **for regression;** `RadiusNeighborsClassifier` **for radius-based**

K-Means in scikit-learn

Basic Usage

- `from sklearn.cluster import KMeans`
- `km = KMeans(n_clusters=3, init='k-means++', random_state=42)`
- `labels = km.fit_predict(X)`
- `centroids = km.cluster_centers_`

Key Parameters

- `n_clusters`: K (required, no default)
- `init`: `'k-means++'` (default) or `'random'`
- `n_init`: number of restarts (default 10; keeps best)
- `max_iter`: max iterations per run (default 300)

`km.inertia_` **gives WCSS after fitting;** `km.n_iter_` **gives iterations until convergence**

Pipeline: Scaling + Algorithm

Why Pipelines? Prevent data leakage – scaling must be fit on training data only.

- `from sklearn.pipeline import Pipeline`
- `from sklearn.preprocessing import StandardScaler`
- `pipe = Pipeline([('scaler', StandardScaler()),`
- `('knn', KNeighborsClassifier())])`
- `pipe.fit(X_train, y_train)`

GridSearchCV with Pipeline

- `params = {'knn__n_neighbors': [3,5,7,11],`
- `'knn__weights': ['uniform','distance']}`
- `grid = GridSearchCV(pipe, params, cv=5, scoring='f1')`

Pipelines ensure scaling is part of cross-validation – fitting scaler on full data before CV causes leakage

Hands-On Exercise

Open the Colab Notebook

- **Exercise 1**: Implement weighted KNN with distance weighting; compare uniform vs distance on fraud data
- **Exercise 2**: Compare Gap statistic vs Elbow vs Silhouette for K selection on customer data
- **Exercise 3**: Apply SMOTE + KNN pipeline for imbalanced fraud detection; evaluate with PR AUC

Link: See course materials for Colab notebook

All exercises use real-world-inspired financial datasets with class imbalance and mixed scales

Key Takeaways

K-Nearest Neighbors

- Instance-based lazy learner; Cover & Hart bound: $R_{\text{1-NN}} \leq 2R^*$
- Scale features, choose K via cross-validation, consider weighted voting

K-Means

- Iterative assign-update with guaranteed convergence (local optimum)
- K-Means++ for initialization; silhouette/Gap for K selection

Common Considerations

- Feature scaling is critical for both methods
- "K" means completely different things in each algorithm

Finance: RFM segmentation (K-Means), fraud detection with SMOTE (KNN)

Both are foundational algorithms: simple, interpretable, widely used across industries

Until Next Time...

"Even K-Means would struggle to cluster the ways students misuse K-Means."

With KNN and K-Means, you can now classify the known and discover the unknown.

Next Session: L04 – Random Forests (from distance-based to tree-based methods)

XKCD #2731 callback – clustering is easy, knowing when to cluster is the hard part

Appendix: Advanced Topics and Proofs

Distance Metric Properties: Triangle Inequality

Statement: For any metric d and points $\mathbf{x}, \mathbf{y}, \mathbf{z}$:

$$d(\mathbf{x}, \mathbf{z}) \leq d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z})$$

Proof for Euclidean (via Cauchy-Schwarz):

1. $\|\mathbf{x} - \mathbf{z}\| = \|(\mathbf{x} - \mathbf{y}) + (\mathbf{y} - \mathbf{z})\|$
2. $\leq \|\mathbf{x} - \mathbf{y}\| + \|\mathbf{y} - \mathbf{z}\|$ (by Minkowski inequality, itself a consequence of Cauchy-Schwarz)

Why It Enables KD-Tree Pruning:

- If current best distance is d^* and node center is $\mathbf{c}$:
- Prune subtree if $d(\mathbf{x}, \mathbf{c}) - r > d^*$ (where r = node radius)
- Triangle inequality guarantees no closer point can exist in that subtree

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Without triangle inequality ($p < 1$), spatial indexing structures cannot prune and brute force is required

K-Means Convergence: Formal Proof

Objective: $J(C, \boldsymbol{\mu}) = \sum_{k=1}^{K} \sum_{\mathbf{x}_i \in C_k} \|\mathbf{x}_i - \boldsymbol{\mu}_k\|^2$
Block Coordinate Descent:

1. **Fix $\boldsymbol{\mu}$, optimize C**: For each $\mathbf{x}_i$, $\frac{\partial J}{\partial C}$ is minimized by $C_k^* = \{\mathbf{x}_i : k = \arg\min_j \|\mathbf{x}_i - \boldsymbol{\mu}_j\|\}$ $\Rightarrow J^{(t+1)} \leq J^{(t)}$
2. **Fix C, optimize $\boldsymbol{\mu}$**: $\frac{\partial J}{\partial \boldsymbol{\mu}_k} = -2 \sum_{\mathbf{x}_i \in C_k} (\mathbf{x}_i - \boldsymbol{\mu}_k) = 0$ gives $\boldsymbol{\mu}_k^* = \frac{1}{|C_k|} \sum_{\mathbf{x}_i \in C_k} \mathbf{x}_i$ $\Rightarrow J^{(t+1)} \leq J^{(t)}$

Termination: $J \geq 0$ and strictly non-increasing. The number of distinct partitions of n points into K groups is $\leq K^n$ (finite). Each partition visited at most once $\Rightarrow$ convergence in $\leq K^n$ steps (in practice, much fewer).

Worst-case K^n iterations is exponential but never observed in practice; typical convergence in 10–50 iterations

Empty Cluster Handling Strategies

Problem: During K-Means iteration, a cluster may lose all its points.
Strategy 1: Farthest Point Reinitialization

- Find the point farthest from its assigned centroid
- Use it as the new centroid for the empty cluster
- Rationale: poorly fit points are good candidates for new clusters

Strategy 2: Split Largest Cluster

- Find cluster with highest WCSS, split it into two
- Maintains total number of clusters at K

Strategy 3: Random Reinitialization

- Randomly select a new data point as centroid
- Simplest but least principled approach

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scikit-learn uses a reassignment strategy; K-Means++ initialization makes empty clusters rare

Cover & Hart: Full Proof Details

Setup: Binary classification, $\eta(\mathbf{x}) = P(Y = 1|\mathbf{x})$, Bayes rule: $g^*(\mathbf{x}) = \mathbf{1}[\eta(\mathbf{x}) > 0.5]$.
1-NN Error Rate Derivation:

- As $n \to \infty$, nearest neighbor $\mathbf{x}_{(1)} \to \mathbf{x}$, so $\eta(\mathbf{x}_{(1)}) \to \eta(\mathbf{x})$
- $P(\text{error}|\mathbf{x}) = P(Y \neq Y_{(1)}|\mathbf{x})$
- $= \eta(\mathbf{x})(1 - \eta(\mathbf{x})) + (1 - \eta(\mathbf{x}))\eta(\mathbf{x}) = 2\eta(\mathbf{x})(1 - \eta(\mathbf{x}))$

Bounding:

$$R^*(\mathbf{x}) = \min(\eta, 1 - \eta) \leq 2\eta(1 - \eta) \leq 2\min(\eta, 1 - \eta) = 2R^*(\mathbf{x})$$

Integrating over $\mathbf{x}$: $R^* \leq R_{\text{1-NN}} \leq 2R^*(1 - R^*)$

K-NN Extension: With $K \to \infty$, $K/n \to 0$, majority vote converges to $\mathbf{1}[\eta > 0.5]$ by law of large numbers $\Rightarrow R_{K\text{-NN}} \to R^*$.

The tighter bound $2R^*(1 - R^*) \leq 2R^*$ shows 1-NN is at most $2\times$ suboptimal

KNN Computational Complexity

Algorithm	Build	Query (avg)	Query (worst)
Brute Force	$O(1)$	$O(nd)$	$O(nd)$
KD-Tree	$O(nd \log n)$	$O(d \log n)$	$O(nd)$
Ball Tree	$O(nd \log n)$	$O(d \log n)$	$O(nd)$
LSH (approx.)	$O(nd)$	$O(d)$	$O(nd)$

When Each Breaks Down:

- KD-Tree: degrades to brute force for $d > 15$–20 (curse of dimensionality)
- Ball Tree: better than KD-Tree in moderate-high d but still degrades
- LSH: approximate; tunable accuracy-speed tradeoff via hash functions

Locality-Sensitive Hashing (LSH) is used by FAISS, Annoy, and other large-scale NN libraries

Gap Statistic: Mathematical Details

Reference Distribution: Generate B datasets from uniform distribution over bounding box of data (or from PCA-aligned box for better null model).

Bootstrap Procedure:

1. For each $k = 1, \ldots, K_{\max}$: compute $\log W_k$ on real data
2. For $b = 1, \ldots, B$: generate reference data, compute $\log W_k^{*(b)}$
3. $\text{Gap}(k) = \frac{1}{B} \sum_{b=1}^{B} \log W_k^{*(b)} - \log W_k$
4. $s_k = \text{sd}(\log W_k^{*(b)}) \cdot \sqrt{1 + 1/B}$

Formal Selection Rule: Choose smallest k such that:

$$\text{Gap}(k) \geq \text{Gap}(k+1) - s_{k+1}$$

Intuition: Gap measures how much better the clustering is compared to clustering uniform (structureless) data.

Tibshirani et al. (2001) recommend $B = 20$–50; the $\sqrt{1 + 1/B}$ correction accounts for simulation error

References

Textbooks

- James et al. (2021). *ISLR*, Ch. 2 (KNN), Ch. 12 (Clustering)
- Hastie et al. (2009). *ESL*, Ch. 13 (Prototypes/NN), Ch. 14 (Unsupervised)

Key Papers

- Arthur & Vassilvitskii (2007). K-Means++: The Advantages of Careful Seeding
- Cover & Hart (1967). Nearest Neighbor Pattern Classification
- Tibshirani et al. (2001). Estimating the Number of Clusters via the Gap Statistic
- Beyer et al. (1999). When Is "Nearest Neighbor" Meaningful?

Next Lecture: L04 – Random Forests (from distance-based to tree-based ensemble methods)

All papers are available via university library access or open-access preprints