Data Engineering Notes

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Disclaimer

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Contents

1 Introduction and Basic Data Types

We call the data **Tabular** when there are no modelled dependencies between attributes, for example, demographic attributes such as age, gender, ZIP code, etc. (also called *Nondependency-Oriented Data*). Otherwise it is **Non-Tabular**, e.g. social networks, time series, etc.

Matrix Representation of Data

A set $X = \{X_i \mid i \in \{1 \dots n\}\}$, with n records (samples) is a d-dimensional dataset iff each sample X_i is a set of $\{x_j \mid j \in \{1 \dots d\}\}$ attributes (features). X is tabular if it is invariant w.r.t shuffling of samples and features. Each feature x_j has its own domain $\mathcal{D}_j$

Quantitative vs. Categorical: A variable x is quantitative (numeric) if its domain $\mathcal{D}_x$ is numeric. Otherwise, Categorical. *Examples (Q):* age, weight, height, BMI, Date of Birth. *Examples (C):* name, gender, country, ZIP Code, weather, ID, day.

Nominal vs. Ordinal: A categorical variable x is ordinal if its domain $\mathcal{D}_x$ has a natural ordering. Otherwise, Nominal. *Examples (N):* weather, name, gender, country, ZIP, ID, day *Examples (O):* heat level, textual gpa.

Finite vs. Infinite: A variable x has a finite domain iff $|\mathcal{D}_x| = N, N \in \mathbb{N}$. Otherwise, Infinite. *Examples (F):* age (years), country, ZIP, ID, gender, day. *Examples (I):* BMI, height, Date of Birth.

> Note
>
> All categorical variables have finite domains, not the other way around.

Discrete vs. Cont.: A Quantitative variable x is continuous iff $\forall z, y \in \mathcal{D}_x \exists w \in \mathcal{D}_x, z < w < y$. Otherwise, Discrete. *Examples (D):* age (years, months, days, hours, etc). *Examples (C):* age (unitless, number), Date of Birth (point in cont. time), BMI.

> Note
>
> By **rounding** quantitative data, we can transform cont. domains into discrete ones.

> Note
>
> Age is quantitative finite discrete if it is computed as whole years, months, days, hours. However, it is quantitative infinite continuous it is computed as precise value including fractions

> Note
>
> Date of Birth is quantitative infinite continuous since it is a point in a continuous endless time

Binary: We call a variable x binary iff $|\mathcal{D}_x| = 2$

Temporal: We call a variable x temporal iff $\mathcal{D}_x$ represents time points or intervals. *Examples:* day, month, Date of Birth

Encoding: Data Encoding refers to the technique of converting data into a form that allows it to be properly used by different systems.

Binning: Binning is an encoding technique that is a function $f : \mathcal{D} \to \{1 \dots K\}$

Example: Equal-Width Binning: Size (width) of each bin is calculated as $W = \frac{\text{Max}(x) - \text{Min}(x)}{K}$ where K is the number of bins.

One-Hot Encoding

To mitigate the problem of label encoding for nominal variables.
How? Create a fixed-size vector with size = |unique(x)|, where each position corresponds to a unique category value. Assign a `1` to the position representing the category and `0`s elsewhere.

Example: Suppose unique(x) = {Red, Green, Blue}

- Red → [1, 0, 0]
- Green → [0, 1, 0]
- Blue → [0, 0, 1]

Note

One-hot encoding avoids the problem of implying ordinal relationships. However, it increases dimensionality significantly, especially when the number of categories is large (curse of dimensionality).

Cyclic Encoding

Some categorical variables are *ordinal* and have a natural *cyclic* structure. A classic example is the months of the year:

$$\mathcal{D}_x = \{\text{Jan}, \text{Feb}, \ldots, \text{Dec}\}$$

This variable has both an order (Jan < Feb < ... < Dec) and a cyclic relationship (Dec is followed by Jan).

To encode this properly, we use the index i of each category in the ordered list, where $i = 1, 2, \ldots, k$, and k is the total number of categories.

Encoding Function:

$$\text{enc}(c_i) = (x_i, y_i)$$

$$x_i = \cos\left(\frac{2\pi(i-1)}{k}\right), \quad y_i = \sin\left(\frac{2\pi(i-1)}{k}\right)$$

This maps each category to a unique point on the unit circle, preserving both order and cyclicity.

Note

Cyclic encoding is useful when the first and last categories are conceptually adjacent (e.g., December and January). This is not possible with standard label or one-hot encoding.

Optional: Normalize to Unit Square

$$\text{enc}(c_i) = \left(\frac{x_i + 1}{2}, \frac{y_i + 1}{2}\right)$$

This scaled version maps points to the square $[0, 1] \times [0, 1]$, which can be useful when input normalization is required for machine learning models. Note that this transformation alters the original unit circle geometry.

Note

Use raw unit circle encoding when preserving angular distance is important. Use the normalized version when the model expects features in the range $[0, 1]$.

Non-Tabular Data

Such as Spatial data, images, time series, string, graphs.

A set $X = \{x_i \mid i \in \{1 \ldots n\}\}$ is a d-dimensional **spatial** dataset with n samples if each sample x_i contains a set of $\{x_j \mid j \in \{1 \ldots d\}\}$ features AND each data point x_{ij} is associated with a specific spatial location l.

A spatial location l can be a point $(l_x, l_y) \in \mathbb{R}^2$ (2D spatial data) or $(l_x, l_y, l_z) \in \mathbb{R}^3$ (3D spatial data), etc.

Tokenization (Character-Level)

Tokenization is the process of converting raw text into smaller units called tokens. In character-level tokenization, each unique character from the corpus is treated as a token.

Example: Consider the corpus consisting of a single sentence: `"hi ai"`

- Unique characters: {`h, i,  , a`}
- Assign token IDs: `h:0, i:1, :2, a:3`
- Tokenized sentence: `"hi ai"` → `[0, 1, 2, 3, 1]`

Each character in the sentence is replaced by its corresponding token ID.

Graphs

A graph is a mathematical structure used to model pairwise relations between objects.

- A graph G is defined as $G = (V, E)$, where:
  - V is a set of *vertices* (or *nodes*).
  - $E \subseteq V \times V$ is a set of *edges*.

Types of Graphs:

- **Undirected Graph:** An edge $(u, v) \in E$ implies a bidirectional connection:

  $$(u, v) \in E \Rightarrow (v, u) \in E$$

- **Directed Graph (Digraph):** Edges have direction:

  $$(u, v) \in E \not\Rightarrow (v, u) \in E$$

Graph Representations

Adjacency Matrix:

A $|V| \times |V|$ matrix A, where:

$$A[u][v] = \begin{cases} 1 & \text{if } (u, v) \in E \\ 0 & \text{otherwise} \end{cases}$$

- **Space consumption:** $\mathcal{O}(|V|^2)$
- **Edge access:** $\mathcal{O}(1)$
- **Neighbor iteration:** $\mathcal{O}(|V|)$

Adjacency List:

Each vertex $u \in V$ maintains a list of its neighbors.

- **Space consumption:** $\mathcal{O}(|V| + |E|)$
- **Edge access:** $\mathcal{O}(|V|)$ (worst-case search)
- **Neighbor iteration:** $\mathcal{O}(\deg(u))$, where $\deg(u)$ is the degree of vertex u

Weighted Graphs:

In some graphs, each edge $(u, v) \in E$ is associated with a numerical value called a *weight*, often representing cost, distance, capacity, etc.

- For weighted graphs, the edge set becomes:

  $$E \subseteq V \times V \times \mathbb{R}$$

  or we define a weight function:

  $$w : E \to \mathbb{R}$$

- In the adjacency matrix, $A[u][v]$ stores the weight instead of a binary 0 or 1.
- In the adjacency list, each neighbor can be stored along with its edge weight as a tuple: $(v, w(u, v))$.

2 Conceptual Modeling

ER Model: Entity-Relationship Model is a high-level, conceptual framework to describe entities, their attributes, and the relationships between them.

Entity: Basic concept of the Entity-Relationship (ER) model. It is an object in the real world. E.g. e1 (some employee).

Attribute: Entities have attributes that are the properties that describe them.

Entity Type: All entities that have the same entity type share the same attributes. E.g. EMPLOYEE (type), e1 (Entity).

Attribute Value: A particular entity has a specific value for each of its attributes.

Composite: An attribute is composite if it is described in terms of its smaller parts. E.g. Name, some databases consider name as a composite attribute consisting of two **atomic** attributes First Name and Last Name.

Atomic/Simple: Cannot be divided into smaller parts.

Note

These days, we store **date** as a single value attribute of the type *DATE*. Earlier, date was considered as a composite attribute consisting of atomic attributes *day, month, year*.

Derived: An attribute is derived if its value is calculated using other **stored** attributes, e.g. age.

Stored: An attribute is stored if it cannot be derived from other attributes.

Note

Age is both derived and atomic. DateOfBirth is both composite and stored.

Single-Valued: An attribute is single-valued if it can have only one value. E.g. DateOfBirth is single-valued composite. Biological sex is single-valued atomic.

Multi-Valued: An attribute is multivalued if it can have several values. E.g. college degrees is multivalued atomic and can have BSc, MSc, BEng, etc.

Note

Affiliation of an entity type RESEARCHER is multivalued (because one can have different affiliations) and composite because an affiliation could be represented as (Org. Name, Dept., Address, Role, Start Date, End Date).

Entity Set: Collection of entities of a particular entity type in a database in a given time point.

Entity Type	Blueprint/Description
Entity Set	Actual set of entities (entity instances) at a point in time

Note

In ancient logic and philosophy we refer to the definition or conceptual content of a term as an *intension*. However, the set of actual things that satisfy a concept is called *extension*. Hence, Entity Type is called intension, Entity Set is called extension.

Candidate Key (Key Attribute): A candidate key is an attribute (or set of attributes) that **uniquely** and **minimally** identifies each entity in an entity set. E.g. StudentID, studentEmail.

Primary Key: A primary key is the chosen candidate key that will be used to uniquely identify entities in the database.

Foreign Key: A foreign key is an attribute in one table/entity that references the primary key of another table/entity. It expresses a relationship between two entity sets.

Composite Primary Key: A composite primary key is a primary key that consists of two or more attributes combined together to uniquely identify a record in a table. Neither attribute alone is sufficient to guarantee uniqueness — but together, they do.

This is common in relationship tables, for example: enrollment relationship between students and courses (M:M):

StudentID	CourseID	Grade
101	CS101	A
101	MATH201	B
102	CS101	B+

Weak Entity Types: Entity types without key attributes.

Strong Entity Types: Entity types with key attributes.

Relations

If we want to model 1:M or M:1 relations, we use the idea of foreign key (modeling the relation with single value attribute). Examples:

PersonID	PersonName
1	Alice
2	Bob

categoryID	categoryName
1	Sport
2	Science

catID	catName	ownerID
1	Daisy	1
2	Smart	2
3	Sweet	1

articleID	title	categoryID
1	title	1
2	title	2
3	title	1

We model M:M Relations by creating an entity representing that relation (usually with composite primary key).

Relationship Type: The definition / template / blueprint of the relationship

Relationship Instance: A single actual link between entities.

Relationship Set: The collection of all relationship instances at a given time.

Participation: We say that entity types $E_1 \dots E_n$ participate in the **relationship type** R.

Relationship Degree: Number of participating entity types in the relation. E.g. consider a relation SUPPLY that models which suppliers supply which projects and what parts are supplied, the degree here is 3 due the three entity types (SUPPLIER, PROJECT, PART).

Role Name: The name describing the part an entity plays in a relationship.

Recursive Relationship: A relationship where the same entity type participates more than once with different roles. E.g. SUPERVISION.

Cardinality Ratio: Specifies the maximum number of entities of one type that can be associated with an entity of another type in a relationship. Examples (E_1 BINARY_RELATION E_2):

Let E_1 and E_2 be the sets of entities of type E_1 and E_2, respectively. Let $R \subseteq E_1 \times E_2$ be the binary relation between them: $R = \{(e_1, e_2) \mid e_1 \in E_1,\ e_2 \in E_2\}$

- **1:1** each entity of type E_1 can be related to at most one entity of type E_2 and vice versa

  $$\forall e_1 \in E_1, \quad |\{e_2 \in E_2 \mid (e_1, e_2) \in R\}| \leq 1$$

  $$\forall e_2 \in E_2, \quad |\{e_1 \in E_1 \mid (e_1, e_2) \in R\}| \leq 1$$

- **1:M** one entity of type E_1 can be related to many entities of type E_2. Each entity of type E_2 can be related to at most one entity of type E_1

  $$\forall e_1 \in E_1, \quad |\{e_2 \in E_2 \mid (e_1, e_2) \in R\}| \geq 0$$

  $$\forall e_2 \in E_2, \quad |\{e_1 \in E_1 \mid (e_1, e_2) \in R\}| \leq 1$$

- **M:1** Inverse of **1:M**

  $$\forall e_1 \in E_1, \quad |\{e_2 \in E_2 \mid (e_1, e_2) \in R\}| \leq 1$$

  $$\forall e_2 \in E_2, \quad |\{e_1 \in E_1 \mid (e_1, e_2) \in R\}| \geq 0$$

- **M:M** many entities of type E_1 can be related to many entities of type E_2 and vice versa

  $$\forall e_1 \in E_1, \quad |\{e_2 \in E_2 \mid (e_1, e_2) \in R\}| \geq 0$$

  $$\forall e_2 \in E_2, \quad |\{e_1 \in E_1 \mid (e_1, e_2) \in R\}| \geq 0$$

Total vs. Partial Participation

- **Total Participation of** E_1 in R
  $\forall e_1 \in E_1,\ \exists e_2 \in E_2 : (e_1, e_2) \in R$ (Every entity of E_1 is related to at least one entity of E_2.)
- **Partial Participation of** E_1 in R
  $\exists e_1 \in E_1 : \forall e_2 \in E_2, (e_1, e_2) \notin R$ (There exists an entity in E_1 that does not participate in R.)

Migrating attributes from relations to entities:

- 1:1 relationship types: Attributes can be migrated to either participating entity. (e.g. EMP MANAGES DEPT, start_date)
- 1:N or N:1 relationship types: Attributes should be migrated to the entity that participates at most once. (e.g. EMP WORKS_FOR DEPT, start_date)
- M:N relationship types: Attributes cannot be migrated to the participating entities and must remain on the relationship itself.

Identifying Relationships: a special relationship where a weak entity is identified by its relationship with a strong entity. The weak entity cannot exist without the strong entity, and the relationship plays a crucial role in providing the weak entity with a composite key.

Existence Dependency: A weak entity depends on the strong entity for its existence. It cannot exist without being related to a strong entity.

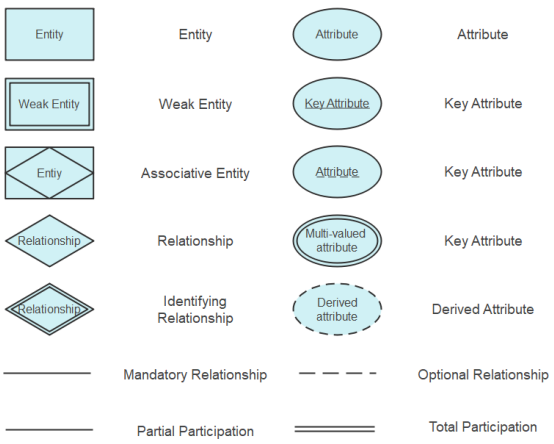
> **Note**
>
> A weak entity type has total participation in its identifying relationship. This means that every instance of the weak entity must be associated with at least one instance of the strong entity. If it doesn't, the weak entity doesn't exist ("existence dependency").

Example:

- Consider we have the following strong entities, customer, product.
- To manage orders, we have two entities, order, orderItem.
- Order is a strong entity since each order has its ID
- However, OrderItem entity can have OrderID, LineNumber, ProductID, quantity, price, discount, etc.
- In this case, OrderItem entity is a weak one, it cannot exist unless an order exists, therefore, the primary key is composite (OrderID, LineNumber)

Min-Max Modeling: Given an entity E participating in Relation R. If at least min and at most max instances of E must participate in R with $min >= 0, max >= 1, max >= min$, then we say E respects min-max constraint (min, max) w.r.t R.

ER Diagram



3 The Relational Data Model

Set: A set is a well-defined collection of distinct objects, considered as an object in its own right. The objects in a set are called elements or members. Sets are usually denoted by capital letters like A, B, or S, and elements are listed within curly braces. For example, $A = \{1, 2, 3\}$ is a set containing the numbers 1, 2, and 3.

Element of a Set: If x is an element of set A, we write $x \in A$. If x is not in A, we write $x \notin A$.

Set-builder Notation: Set-builder notation is a shorthand used to describe a set by stating the properties that its elements must satisfy. For example: $\{x \in \mathbb{N} \mid x \text{ is even}\}$ describes the set of even natural numbers.

Cardinality: The cardinality of a set is the number of elements in the set, denoted $|A|$. For example, if $A = \{1, 2, 3\}$, then $|A| = 3$.

Cartesian Product: Let A and B be sets, then $A \times B = \{(a, b) \mid a \in A, b \in B\}$, e.g. $A = \{1, 2\}, B = \{x, y\}, A \times B = \{(1, x), (1, y), (2, x), (2, y)\}$

Subset: $A \subseteq B \Leftrightarrow \forall X.X \in A \Rightarrow X \in B$

Proper Subset: $A \subset B \Leftrightarrow A \subseteq B \wedge A \neq B$

Relation: $R \subseteq A \times B$. If $(a, b) \in R$, we say that a is related to b via R

Left Total Relation: A relation $R \subseteq A \times B$ is left total (total on A) iff each element in A is related to at least on element in B. $\forall a \in A.\exists b \in B.(a, b) \in R$

Right Unique Relation: A relation $R \subseteq A \times B$ is right unique iff each element in A is related to at most one element in B. $\forall a \in A, \forall b1, b2 \in B, ((a, b1) \in R, (a, b2) \in R) \Rightarrow b1 = b2$

Function: A function is left total and right unique relation. $f : A \to B$

Partial Function: A partial function is a right unique relation, **not** necessarily left total. $f \rightharpoonup B$

Set Union: $x \in A \cup B \Leftrightarrow x \in A$ or $x \in B$

Set Intersection: $x \in A \cap B \Leftrightarrow x \in A$ and $x \in B$

Disjoint: We say two sets A, B are disjoint iff $A \cap B = \phi$

Relation Schema: A declaration $R\big(A_1{:}D_1, \ldots, A_n{:}D_n\big)$ consisting of a name R, a finite, non-empty attribute set $\{A_i\}$ and, for each attribute, its domain $\text{dom}(A_i) = D_i$.

Schema Satisfaction: A *tuple* $t = (v_1, \ldots, v_n)$ *satisfies* the schema if $v_i \in D_i \ \forall i$.

Types: *Classes* of atomic values that share representation and operations, e.g. `Int`, `Real`, or `String`.

Domain: A *set* of atomic values with application-specific semantics whose underlying implementation type is fixed. Domains may define default values. Example: $\mathit{EmployeeAge} = \texttt{Int}[18, 65]$.

> Note
>
> Domain declaration examples: `Name = String(20)`, `DollarPrice = Decimal(5,2)`.

Instance: A *finite set* of tuples that all satisfy a given relation schema. While the schema is comparatively stable (static), its instance is *dynamic*: it evolves through insertions, deletions, and updates.

Two Equivalent Views on Tuples

- **Positional (Cartesian-product) view:** t is an *ordered list* $\big(v_1, \ldots, v_n\big)$. Column order carries meaning; attribute names are implicit.
- **Functional view:** Fix $A = \{A_1, \ldots, A_n\}$ and $D = \bigcup_i D_i$. Then a tuple is a *function* $t : A \to D$ with $t(A_i) \in D_i$. Here, order is irrelevant and attribute names are explicit.

Domain Constraint: Each attribute value must lie in its declared domain D_i. Usually enforced by the DBMS type checker.

Functional Dependency (FD): For attribute sets $X, Y \subseteq A$, the notation $X \to Y$ states: for any two tuples t_1, t_2, equality of X-values implies equality of Y-values. Written out: $t_1[X] = t_2[X] \Rightarrow t_1[Y] = t_2[Y]$.

Superkey: An attribute set K with $K \to A$ (it functionally determines the whole tuple).

Candidate Key: A *minimal* superkey — removing any attribute from it destroys the functional determination of A.

Primary Key: The candidate key chosen by the database designer to serve as the principal identifier of tuples in a relation. Remaining candidate keys are called *alternate keys*.

Example

- Relation schema *Employee*(*EmpID*, *SSN*, *Email*, *Name*, *Dept*).
- *Superkeys* include any attribute set that uniquely identifies tuples, e.g $\{EmpID\}$, $\{SSN\}$, $\{EmpID, Name\}$. The third set still determines the whole tuple but is *not* minimal.
- *Candidate keys*: the minimal superkeys $\{EmpID\}$ and $\{SSN\}$. Each is irreducible.
- *Primary key*: suppose we designate *EmpID* as the primary key. The other candidate becomes an *alternate key* available for unique look-ups.

Foreign Key: Attribute(s) in relation R whose values must also appear as the primary-key values of another relation S (ensuring referential integrity).

Note

When an insertion, deletion or modification would break any constraint, the DBMS may (i) reject the change or (ii) repair it automatically ("cascade", insert default/null, etc.). The exact behaviour is part of the schema definition.

A word on modeling different cardinalities

Relational databases use foreign keys (FKs) to represent associations between entities. The modeling depends on the cardinality:

One-to-One (1:1)

A FK is placed in one of the tables.

Person	ID (PK)	Name	PassportID (FK)
	1	Alice	101

Passport	ID (PK)	Number	DateOfIssue
	101	X1234	2020-01-01

One-to-Many (1:M) or Many-to-One (M:1)

The FK is placed in the table on the "many" side, referencing the "one" side.

Department	ID (PK)	Name
	1	Human Resources

Employee	ID (PK)	Name	DepartmentID (FK)
	101	John	1

Many-to-Many (M:M)

Modeled via a relation table with two FKs, each referencing one of the related tables. The combination of FKs often serves as the primary key.

StdID	StdName
1	Jane
2	Mark
3	Sara

CourseID	CourseTitle
10	Database Systems
11	Operating Systems
12	Algorithms

StdID	**CourseID**
1	10
1	12
2	10
2	11
3	11

4 Functional Dependencies

Prime Attribute: An attribute that is part of any candidate key.

Nonprime Attribute: An attribute that is not part of any candidate key.

Example: consider the simple relation `STUDENT(ID, Email, Name, Phone, CourseID)`. Possible super keys:

$$\{\texttt{ID}\}, \{\texttt{Email}\}, \{\texttt{ID}, \texttt{Name}\}, \{\texttt{ID}, \texttt{Email}, \texttt{Phone}\}$$

Only $\{\texttt{ID}\}$ and $\{\texttt{Email}\}$ are prime attributes.

Trivial FD: We say that a functional dependency $X \to Y$ is **trivial** iff $Y \subseteq X$.

Full FD: A functional dependency $X \to Y$ is full iff for any $A \in X$, $(X - \{A\}) \to Y$ does not hold, i.e. you cannot remove any attribute from X without breaking the dependency. Example: {studentID, CourseID} → Grade.

Partial FD: A functional dependency $X \to Y$ is partial iff $\exists A \in X.\ (X - \{A\}) \to Y$ holds.

Transitive FD: A functional dependency $X \to Y$ is transitive in a relation R iff $\exists$ **Nonprime set of attributes** $Z \in R$ and both $X \to Z$ and $Z \to Y$ hold.

Inference: A functional dependency $X \to Y$ is **inferred** from a set of functional dependencies F on a relation R iff $X \to Y$ holds in every instance of R that satisfies all dependencies in F

Armstrong's Inference Rules for Functional Dependencies

- **IR1**: $(Y \subseteq X) \Rightarrow (X \to Y)$ (reflexive)
- **IR2**: $(X \to Y) \Rightarrow (X \cup Z \to Y \cup Z)$ (augmentation)
- **IR3**: $((X \to Y) \wedge (Y \to Z)) \Rightarrow X \to Z$ (transitive)

Closure: The closure of attribute set X under a set of functional dependencies F, denoted as X_F^+ is the set of all attributes that X can determine using FDs in F. $X_F^+ = \{A \mid X \to A \in F \text{ or can be inferred from it}\}$

Closure Algorithm

- input: a set F of FDs on a relation R, and a set of attributes X contained in R
- initialization: $X_F^+ = X$
- changed = True
- while changed:
  1. changed = False
  2. for each FD $Y \to Z \in F$:
     (a) If $(Y \subseteq X_F^+) \wedge (Z \notin X_F^+)$:
        i. $X_F^+ = X_F^+ \cup \{Z\}$
        ii. changed = True
- Output: X_F^+

FDs Verification: F implies $X \to Y$ *iff* $Y \subseteq X_F^+$

Superkeys Verification: X is a super key for R with attribute set U *iff* $X_F^+ = U$

Finding Candidate Keys

```
Input: Relation (R) over set of attributes (U), set of FDs (F)
initialization: K:= U
minimal = False
while not minimal
    minimal = True
    for each attribute A in K
        compute closure of (K-A) under F
            if the closure = U
                set K := K - {A}
                minimal = False
Return: K
```

Coverage: For any two sets of functional dependencies F_1, F_2, we say that F_1 covers F_2, *iff* $\forall X \to Y \in F_2.Y \subseteq X^+_{F_1}$.

Equivalence: For any two sets of functional dependencies F_1, F_2, we say they are equivalent, *iff* they cover each other. Example: verify whether the following FDs are equivalent.

- $F_1 = \{A \to C, AC \to D, E \to AD, E \to H\}$ and
- $F_2 = \{A \to CD, E \to AH\}$

We check first if F_1 covers F_2

- considering $A \to \{C, D\}$ $\quad \{C, D\} \in A^+_{F_1} = \{A, C, D\}$
- considering $E \to \{A, H\}$ $\quad \{A, H\} \in E^+_{F_1} = \{E, A, D, H, C\}$
- Hence F_1 covers F_2

Next, we check first if F_2 covers F_1

- considering $A \to C$ $\quad C \in A^+_{F_2} = \{C, D\}$
- considering $\{A, C\} \to D$ $\quad D \in \{A, C\}^+_{F_2} = \{A, C, D\}$
- considering $E \to \{A, D\}$ $\quad \{A, D\} \in E^+_{F_2} = \{A, H, C, D\}$
- considering $E \to H$ $\quad H \in E^+_{F_2} = \{A, H, C, D\}$
- Hence F_2 covers F_1

Therefore, they are equivalent

Redundancy: A functional dependency $f = X \to A$ is redundant in FDs set F *iff* $A \subseteq X^+_G$ where $G = F - \{X \to A\}$, i.e. $F - \{f\}$ implies f.

Extraneous: Given a set F of FDs and one $f = AX \to B \in F$, then A is extraneous if $B \subseteq X^+_F$

Minimal cover: A set of FDs F is a minimal cover of a set of FDs E iff F covers E and there is no $f \in F$. $\quad F - \{f\}$ covers E

Canonical: A functional dependency $f = X \to Y$ is in a canonical form iff $|Y| = 1$

Minimal set of FDs: A set F of FDs is minimal iff it satisfies the following conditions: (i) All FDs in a canonical form. (ii) No extraneous attributes. (iii) No redundant FDs.

Steps to Obtain a Minimal Set of Functional Dependencies

1. Transform to Canonical form
2. Remove Extraneous Attributes
3. Remove Redundant FDs

5 Relational Algebra and SQL

Data Model: In relational databases, the data model specifies how data is structured and how it can be manipulated. i.e. it says that data is organized into tables (called relations) with columns (attributes) and rows (tuples).

Relational model: In relational databases, the relational model represent data as relations (tables). Each relation has constraints, such as keys or data types, to ensure data integrity.

Relational Algebra: The formal system for manipulating relations. It provides a theoretical foundation for **Query** operations used in relational databases

Algebra: A formal system in which expressions are constructed using operators and atomic operands. These expressions can be evaluated, and two expressions are considered equivalent if they yield the same result for all possible values of their operands.

Relational Algebra: A type of algebra where the operands are relations (tables), and the operators are defined for any instance of those relations. Operations can be combined to form complex expressions, and evaluating an expression produces a result schema (the structure of the output) and a result instance (the actual data produced).

SQL: The Standard Query Language (SQL) is the language used to interact with relational databases. It is a **declarative** language, meaning that when you write a query, you describe what result you want, not how the database should compute it. This contrasts with procedural languages, where you must specify every step.

SQL Structure

SQL is organized into several sub-languages, each serving a distinct purpose:

- Data Definition Language (DDL): used to define or alter the structure of database objects. Commands used such as: `CREATE, ALTER, DROP`
- Data Manipulation Language (DML): used to retrieve and manipulate data. Command used such as: `SELECT, UPDATE, INSERT, DELETE`
- Data Control Language (DCL): manages user permissions and access control. Commands used such as: `GRANT, REVOKE`
- Transaction Control Language (TCL): manages database transactions. Commands used such as: `COMMIT ROLLBACK`

Example DML Queries:

```
SELECT name, age FROM Student WHERE age >= 18 ORDER BY name ASC;

INSERT INTO Student (stdId, name, age) VALUES (101, "Alice", 20);

UPDATE Student SET age = age + 1 WHERE stdId = 101;

DELETE FROM Student WHERE stdId = 101;
```

Examples on `COUNT, DISTINCT, EXIST, IN`

```
SELECT COUNT(*) FROM Student;

SELECT COUNT(DISTINCT stdID) FROM Student;

SELECT * FROM employees e
WHERE EXISTS (
    SELECT 1
    FROM bonus b
    WHERE b.employee_id = e.employee_id
);

SELECT * FROM employees WHERE department_id IN (1, 2, 5);
```

Example DDL Queries:

```
    CREATE TABLE Course (courceID INT PRIMARY KEY,
                         title    VARCHAR(100)
                        );

    ALTER TABLE Course ADD COLUMN credits INT;

    DROP TABLE Course;
```

Example DCL Queries:

```
    GRANT SELECT, INSERT ON Student TO user1;

    REVOKE INSERT ON Student FROM user1;
```

Example TCL Queries:

```
    BEGIN;
    UPDATE Account SET balance = balance - 100 WHERE id = 1;
    COMMIT;
```

Example Primary Key and Foreign Key:

```
CREATE TABLE Department (
    deptID INT PRIMARY KEY,
    deptName VARCHAR(100)
);

CREATE TABLE Employee (
    empID INT PRIMARY KEY,
    empName VARCHAR(100),
    deptID INT,
    FOREIGN KEY (deptID) REFERENCES Department(deptID)
);
```

Example Composite Primary Key:

```
    CREATE TABLE Student (
    stdID INT PRIMARY KEY,
    stdName VARCHAR(100)
);

CREATE TABLE Course (
    crsID INT PRIMARY KEY,
    crsName VARCHAR(100)
);

CREATE TABLE Enrollment (
    stdID INT,
    crsID INT,
    grade CHAR(2),
    PRIMARY KEY (stdID, crsID),
    FOREIGN KEY (stdID) REFERENCES Student(stdID),
    FOREIGN KEY (crsID) REFERENCES Course(crsID)
);
```

Example Domain Constraints:

```
CREATE TABLE Product (
    id INT PRIMARY KEY,
    price DECIMAL(10,2) CHECK (price >= 0),
    category VARCHAR(50) NOT NULL
);
```

Set Operators

Arity / Degree: let $R(A_1, \cdots, A_n)$ be a relation schema, the arity of R is $\text{arity}(R) = n$

Union Compatible: We say that relations $R(A_1, \cdots, A_n)$ and $S(B_1, \cdots, B_n)$ are union compatible if $\text{artiy}(R) = \text{arity}(S)$ and $\text{dom}(A_i) = \text{dom}(B_i) \quad \forall i \in \{1, \cdots, n\}$

Relation Union: $R_1 \cup R_2 = \{t \mid t \in R_1 \vee t \in R_2\}$. SQL Equiv.: `SELECT * FROM R UNION SELECT * FROM S`

Relation Intersection: $R_1 \cap R_2 = \{t \mid t \in R_1 \wedge t \in R_2\}$. SQL: `SELECT * FROM R INTERSECT SELECT * FROM S`

Relation Difference: $R_1 - R_2 = \{t \mid t \in R_1 \wedge t \notin R_2\}$. SQL: `SELECT * FROM R EXCEPT SELECT * FROM S`

Relation Cartesian Product: $R_1 \times R_2 = \{t_1 \circ t_2 \mid t_1 \in R_1,\ t_2 \in R_2\}$. SQL: `SELECT * FROM R CROSS JOIN S`

Relation Operators (Unary)

Rename: Changes the schema of the relation R by renaming attribute A_1 to B_1 and so on. $\rho_{(B1,\cdots,B_n \leftarrow A_1,\cdots,A_n)}(R)$. SQL: `SELECT a AS b FROM R AS R1`

Selection: $\sigma_C(R) = \{t \in R \mid C(t)\}$ is the set of all tuples in R that satisfy the condition C.
The condition C is a Boolean expression composed of predicates:

$$C = P_1\ op_1\ P_2\ op_2\ \cdots\ op_{n-1}\ P_n$$

where each operator $op_i \in \{\text{AND},\ \text{OR},\ \text{NOT}\}$, and each predicate P_i has the form:

$$P_i ::= A\ \theta\ B \quad \text{or} \quad A\ \theta\ c$$

with attributes A, B, constant c, and comparison operator $\theta \in \{=,\ <,\ \leq,\ >,\ \geq,\ \neq\}$.

SQL Equiv. : `SELECT * FROM R WHERE C`

Projection: $\Pi_Y(R) = \{t[Y] \mid t \in R\}$. SQL: `SELECT Y FROM R`

Idempotent: An operator $\mathcal{O}$ is called *idempotent* if applying it multiple times has the same effect as applying it once: $\mathcal{O}(\mathcal{O}(x)) = \mathcal{O}(x) \quad \forall x$. **Projection** is *Idempotent*

Relation Operators (Binary)

Theta Join: $R_1 \bowtie_C R_2 = \{t_1 \circ t_2 \mid t_1 \in R_1 \wedge t_2 \in R_2 \wedge C(t_1 \circ t_2)\} = \sigma_C(R_1 \times R_2)$

Example: `SELECT * FROM Employee JOIN Bonus ON Employee.salary > Bonus.threshold`

id	salary
1	50000
2	30000

threshold
20000
40000

id	salary	threshold
1	50000	20000
1	50000	40000
2	30000	20000

Equi-Join: Theta Join with C consists only of equality comparison.

Example: `SELECT * FROM Orders JOIN Customers ON Orders.cust_id = Customers.id`

order_id	cust_id
101	1
102	2
103	4

id	name
1	Alice
2	Bob
3	Carol

order_id	cust_id	id	name
101	1	1	Alice
102	2	2	Bob

Natural Join: Equi-Join where C is quality on common attributes and duplicate common attributes are removed from the result.

Example: `SELECT * FROM Employee NATURAL JOIN Department`

emp_id	dept_id
1	10
2	20
3	10
4	40
5	50

dept_id	name
10	HR
20	IT
30	Sales
60	Legal

emp_id	dept_id	name
1	10	HR
2	20	IT
3	10	HR

Outer Join: Natural Join but preserves unmatched tuples by padding them with NULL values. That can be done on the relation on the left, right or both.

Left Outer Join: Includes all tuples from the left relation, padding unmatched right-side tuples with NULLS.

Example: `SELECT * FROM Orders LEFT OUTER JOIN Customers ON Orders.cust_id = Customers.id`

order_id	cust_id
101	1
102	2
103	4

id	name
1	Alice
2	Bob
3	Carol

order_id	cust_id	id	name
101	1	1	Alice
102	2	2	Bob
103	4	NULL	NULL

Right Outer Join: Includes all tuples from the right relation, padding unmatched left-side tuples with NULLS.

Example: `SELECT * FROM Orders RIGHT OUTER JOIN Customers ON Orders.cust_id = Customers.id`

order_id	cust_id
101	1
102	2
103	4

id	name
1	Alice
2	Bob
3	Carol

order_id	cust_id	id	name
101	1	1	Alice
102	2	2	Bob
NULL	NULL	3	Carol

Full Outer Join: Includes all tuples from both relations, padding unmatched tuples from either side with NULLS.
Example: `SELECT * FROM Orders FULL OUTER JOIN Customers ON Orders.cust_id = Customers.id`

order_id	cust_id
101	1
102	2
103	4

id	name
1	Alice
2	Bob
3	Carol

order_id	cust_id	id	name
101	1	1	Alice
102	2	2	Bob
103	4	NULL	NULL
NULL	NULL	3	Carol

Operators Properties

Operator	**Result Schema**	**Result Size**	**Comm.**	**Assoc.**	**Idem.**	**Duplicates**
Union	Same as inputs	$\leq \lvert R\rvert + \lvert S\rvert$	Yes	Yes	No	No
Intersection	Same as inputs	$\leq \min(\lvert R\rvert, \lvert S\rvert)$	Yes	Yes	Yes	No
Difference	Same as R	$\leq \lvert R\rvert$	No	No	No	No
Cartesian Product	$R \cup S$	$\lvert R\rvert \cdot \lvert S\rvert$	Yes	Yes	No	Yes
Rename	Same	$\lvert R\rvert$	N/A	N/A	N/A	N/A
Selection	Same as R	$\leq \lvert R\rvert$	Yes	Yes	No	Yes
Projection	Subset of R	$\leq \lvert R\rvert$	No	No	Yes	No
Theta Join	$R \cup S$	$[0,\ \lvert R\rvert \cdot \lvert S\rvert]$	No	No	No	Yes
Equi-Join	$R \cup S$	$[0,\ \lvert R\rvert \cdot \lvert S\rvert]$	No	No	No	Yes
Natural Join	$R \cup S \setminus C$	$[0,\ \lvert R\rvert \cdot \lvert S\rvert]$	Yes	Yes	No	Yes
Left Outer Join	$R \cup S$	$\geq \lvert R\rvert$	No	No	No	Yes
Right Outer Join	$R \cup S$	$\geq \lvert S\rvert$	No	No	No	Yes
Full Outer Join	$R \cup S$	$\geq \max(\lvert R\rvert, \lvert S\rvert)$	No	No	No	Yes

Common Datatypes

Category	**Common Data Types**
Numeric	INT, BIGINT, DECIMAL(p,s), FLOAT, DOUBLE
Character	CHAR(n), VARCHAR(n), TEXT
Date/Time	DATE, TIME, TIMESTAMP, DATETIME
Boolean	BOOLEAN / BOOL

Algebra to SQL Example

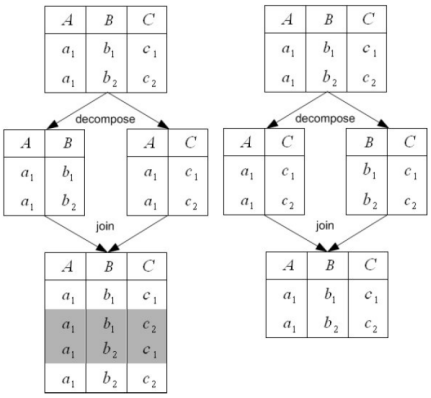
$$\pi_{\text{supplier\_name},\ \text{product\_name}}\left(\sigma_{\text{price}>50}\left((\text{Suppliers} \bowtie_{\text{supplier\_id}} \text{Products}) \bowtie_{\text{category\_id}} \text{Categories}\right)\right)$$

```
WITH SupplierProducts AS (
    SELECT
        s.supplier_name,
        p.product_name,
        p.price,
        p.category_id
    FROM Suppliers s
    JOIN Products p ON s.supplier_id = p.supplier_id
),
Filtered AS (
    SELECT * FROM SupplierProducts WHERE price > 50
)
SELECT f.supplier_name, f.product_name
FROM Filtered f
JOIN Categories c ON f.category_id = c.category_id;
```

6 Normal Forms

Normalization: Decomposing a large schema $R(A)$ into smaller schemata $R_i(A_i)$ with $A_i \subset A$ to minimize redundancy, avoid information loss and preserve functional dependencies.

Spurious Tuples: Decomposing a relation into multiple relations as part of normalization can lead to spurious tuples when these relations are rejoined (tuples that did not exist in the original relation). **Example**



Lossless-Join Decomposition: We call a decomposition of $R(A, B, C)$ into $R_1(A, B)$ and $R_2(B, C)$ lossless-join iff, for all instances r of R that respect the FDs, the following identity holds: $r = \Pi_{A,B}(r) \bowtie \Pi_{B,C}(r)$

Example (Lossless): Consider the relation: `empDept(empID, name, deptID, deptName)` with FDs:

`empID` $\rightarrow$ `name`
`empID` $\rightarrow$ `deptID`
`deptID` $\rightarrow$ `deptName`

We decompose the relation into:

- `emp(empID, name, deptID)`
- `dept(deptID, deptName)`

Consider legal instances r:

empID	name	deptID	deptName
1	Alice	10	CS
2	Bob	10	CS
3	Carol	20	Math

$\Pi_{\text{empID, name, deptID}}(r)$

empID	name	deptID
1	Alice	10
2	Bob	10
3	Carol	20

$\Pi_{\text{deptID, deptName}}(r)$

deptID	deptName
10	CS
20	Math

$\Pi_{\text{deptID, deptName}}(r) \bowtie \Pi_{\text{deptID, deptName}}(r)$

empID	name	deptID	deptName
1	Alice	10	CS
2	Bob	10	CS
3	Carol	20	Math

$= r$

Example (Lossy): Consider the relation: `R(empName, empLevel, empSalary)` with FDs:

`empName` $\rightarrow$ `empLevel`
`empName` $\rightarrow$ `empSalary`
`empLevel` $\rightarrow$ `empSalary`

Consider legal instances r:

empName	empLevel	empSalary
Alice	Junior	50K
Bob	Junior	50K
Carol	Senior	50K

$\Pi_{\text{empName, empSalary}}(r)$

empName	empSalary
Alice	50K
Bob	50K
Carol	50K

$\Pi_{\text{empLevel, empSalary}}(r)$

Level	Salary
Junior	50K
Senior	50K

$\Pi_{\text{empName, empSalary}}(r) \bowtie \Pi_{\text{empLevel, empSalary}}(r)$

empName	empLevel	empSalary
Alice	Junior	50K
Alice	Senior	50K
Bob	Junior	50K
Bob	Senior	50K
Carol	Junior	50K
Carol	Senior	50K

$\neq r$

> Note
>
> A decomposition of $R(A, B, C)$ into $R_1(A, B)$ and $R_2(B, C)$ is lossless-join iff B is a **superkey** in R_1 *or* R_2

Dependency-Preserving: We call a decomposition dependency preserving if the *union* of FDs from decomposed relations yields all FDs in the original relation.

Example: If we decompose `R(empName, empLevel, empSalary)` into `R1(empName, empLevel)`, `R2(empName, empSalary)`. This is a **lossless-join** decomposition:

$\Pi_{\text{empName, empLevel}}(r)$

empName	empLevel
Alice	Junior
Bob	Junior
Carol	Senior

$\Pi_{\text{empName, empSalary}}(r)$

empName	Salary
Alice	50K
Bob	50K
Carol	50K

$\Pi_{\text{empName, empLevel}}(r) \bowtie \Pi_{\text{empName, empSalary}}(r)$

empName	empLevel	empSalary
Alice	Junior	50K
Bob	Junior	50K
Carol	Senior	50K

$= r$

However, This is not *dependency preserving*. Proof:

FDs of $R_1 = \{\texttt{empName} \rightarrow \texttt{empLevel}\}$

FDs of $R_2 = \{\texttt{empName} \rightarrow \texttt{empSalary}\}$

The union of both is $\{\texttt{empName} \rightarrow \texttt{empLevel}, \texttt{empName} \rightarrow \texttt{empSalary}\}$ which is not equal to $\{\texttt{empName} \rightarrow \texttt{empLevel}, \texttt{empName} \rightarrow \texttt{empSalary}, \texttt{empLevel} \rightarrow \texttt{empSalary}\}$ i.e. the FD `empLevel` $\rightarrow$ `empSalary` is **lost**!

Example (Lossless-join and Dependency Preserving Decomposition)

$R_1(empName, empLevel), R_2(empLevel, empSalary)$

- Lossless-join becasue `empLevel` is superkey in R_2
- Dependency Preserving becasue $F_1 \cup F_2 = \{empName \to \texttt{empLevel}, \texttt{empLevel} \to \texttt{empSalary}\}$ and *through transitivity* we get $\{empName \to \texttt{empSalary}\}$

The Chase Test to Check the Lossless-Join Property

Input:

- A relation schema $R = \{A_1, A_2, \ldots, A_n\}$
- A set of functional dependencies F
- A decomposition $\mathcal{D} = \{R_1, R_2, \ldots, R_k\}$

Goal: Determine whether the decomposition is **lossless-join** with respect to F.

Procedure:

Step 1. Initialize a Chase Table:

- Create a table with one row per sub-relation $R_i \in \mathcal{D}$, and one column per attribute $A_j \in R$.
- For each row i and attribute A_j:
  - If $A_j \in R_i$, set the cell to α_{A_j}
  - If $A_j \notin R_i$, set the cell to a unique symbol β_{iA_j}

Step 2. Apply Functional Dependencies:

- For each FD $X \to Y \in F$, and for each row:
  - If all attributes in X have the same symbol in the row (e.g., all equal to σ),
  - Then set each attribute in Y to that same symbol σ
- Repeat until no further changes occur in the table.

Step 3. Check for Losslessness:

- If any row contains only the original α_{A_j} symbols across all attributes, the decomposition is **lossless**.
- Otherwise, it is **lossy**.

Example (Lossless)

Let $R(A, B, C)$, with FDs $F = \{A \to B\}$, and decomposition:

$$R_1(A, B), \quad R_2(A, C)$$

Initial Chase Table:

A	B	C
α_A	α_B	β_{1C}
α_A	β_{2B}	α_C

Apply $A \to B$:

A	B	C
α_A	α_B	β_{1C}
α_A	α_B	α_C

Since row 2 contains only α-symbols, the decomposition is **lossless**.

Example (Lossy)

Let $R(A, B, C)$, with FDs $F = \{A \to B\}$, and decomposition:

$$R_1(A, B), \quad R_2(B, C)$$

Initial Chase Table:

A	B	C
α_A	α_B	β_{1C}
β_{2A}	α_B	α_C

Apply $A \to B$: Only row 1 has $A = \alpha_A$, but $B = \alpha_B$ already $\to$ no changes.

No row becomes all-α, so the decomposition is **lossy**.

1NF: A relation is in First Normal Form (1NF) iff the domain contains only atmoic single values.

2NF

A relation is in Second Normal Form iff:

- It is in 1NF
- There is no *non-prime* attribute A such that $Y \to A \in F$, where Y is a proper subset of a candidate key K ($Y \subsetneq K$)

In other words, if all *candidate* keys consist of a single attribute, 2NF is guaranteed.

Example: Consider the relation `EMP_PROJ(EmpID, EmpName, ProjId, ProjName, ProjLocation, Hours)` With Candidate Key `(EmpID, ProjId)` and set of FDs:
{(`EmpID, ProjId` $\to$ `Hours`),
(`EmpID` $\to$ `EmpName`),
(`ProjId` $\to$ `ProjName, ProjLocation`)}

`EmpName` is a *non-prime* attribute that is determined by `EmpID` $\subsetneq$ {`EmpID, ProjId`} Hence 2NF is violated. (the same applies for `ProjName, ProjLocation`)

Normalization This relation can be normalized to 2NF by decomposing it in a way so we do not have these *partial* dependencies on the primary key: `EMP(EmpID, EmpName)`, `PROJ(ProjID, ProjName, ProjLocation)`, `EMP_PROJ(EmpID, ProjID, Hours)`

3NF

A relation is in Third Normal Form iff it is in 2NF and for each FD $X \to Y$, one of the following statements holds:

- $X \to Y$ is trivial ($Y \subseteq X$)
- X is a **superkey**
- Every attribute $A \in Y - X$ is a *prime* attribute

Example: Consider the relation `EMP_DEPT(EmpID, EmpName, EmpBD, EmpAddress, DeptID, DeptName, DeptMgrId)` With FDs:

- `EmpID` $\to$ `EmpName`, `EmpAddress`, `EmpBD`, `DeptID`
- `DeptID` $\to$ `DeptName`, `DeptMgrId`

For FD1, `EmpID` is superkey (we are safe). For FD2 it is not trivial, `DeptID` is not superkey, and none of `DeptName` or `DeptMgrId` is prime. So this violates 3NF.

Normalization

We must remove transitive dependencies to normalize to 3NF.

- `EMP(EmpID, EmpName, EmpBD, EmpAddress, DeptID )`
- `DEPT(DeptID, DeptName, DeptMgrId)`

BCNF

A relation R is Boyce-Codd Normal Form (BCNF) iff for each FD $X \to Y$, one the following statements holds:

- $Y \subseteq X$ (trivial)
- X is a *superkey*

Note: Relations that violate BCNF are rare and hard to find in practice. In real projects, normalizing to 3NF usually guarantee BCNF except for some rare cases.

Example: Assume we are building a system to manage land properties across different districts. Each property is assigned a globally unique property ID.

Locally, properties are identified by the lot number, which is only unique within a district. A property is uniquely identified by district and lot number.

Additionally, each property belongs to one area (each district has multiple areas)

Condider we model this relation as `LOTS(PropertyID, District, LotNum, Area)` with FDs:

- `PropertyID` → `District, LotNum, Area`
- `District, LotNum` → `PropertyID, Area`
- `Area` → `District`

We have the following candidate keys:

- `PropertyID`
- `District, LotNum`

The relation is in 3NF because, for each FD:

- `PropertyID` is a super key (candidate means minimal super key)
- `District, LotNum` is a super key (same reasoning)
- `District` is *prime* since it is part of `District, LotNum`

The relation is not in BCNF because FD3 violates that (`Area` is not a super key)

Normalization

To normalize to BCNF, we decompose in a way that `Area` is a super key in one of the relations. Because Area determines district, we make a separate relation for that with `Area` as our primary: `AREA_DISTRICT(Area, District)`

The relation have to be: `LOTS(PropertyID, LotNum, Area)`

Disadvantage: We lost `District, LotNum` → `PropertyID, Area`

7 Graph Databases and Cypher Queries

Graph Data Model

A graph database represents data as a property graph $G = (V, E, \lambda_V, \lambda_E)$, where:

- V: set of nodes (entities)
- E: set of edges (relationships)
- λ_V: node properties
- λ_E: edge properties

Example Node and Edge

- Node: `(a:Person {name: 'Alice', age: 30})`
- Edge: `(a)-[:FRIEND_OF {since: 2015}]->(b)`

Graph DBs favor connected data and avoid joins by treating relationships as first-class citizens.

Advantages of Graph Databases

- Efficient Traversals: Constant time access to related nodes.
- Schema Flexibility: Easily adapt to changing requirements.
- Natural Modeling: Direct mapping of real-world relationships.
- Performance: Particularly efficient for deep, multi-hop queries.

Graph DB Instances and Schemata

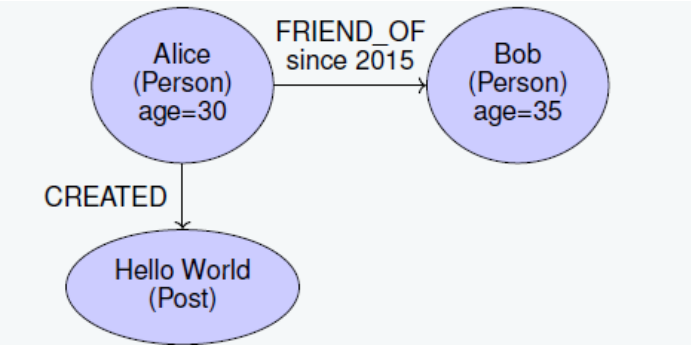


Figure 1: Instance

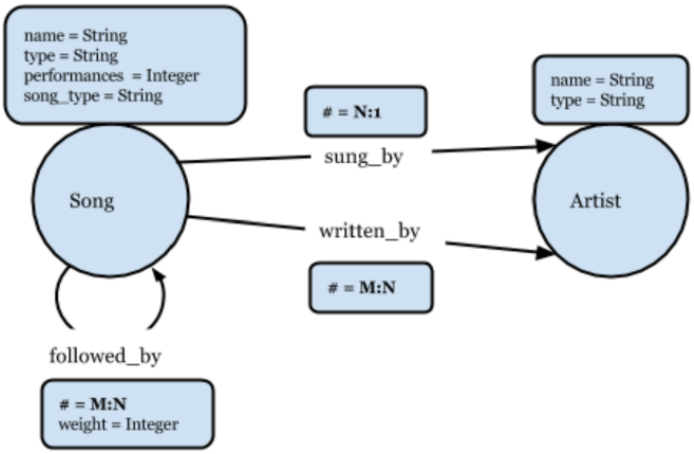


Figure 2: Schema

Note

Unlike relational databases, graph databases can be populated without prior specification of the schema!

Native vs Non-Native Storage

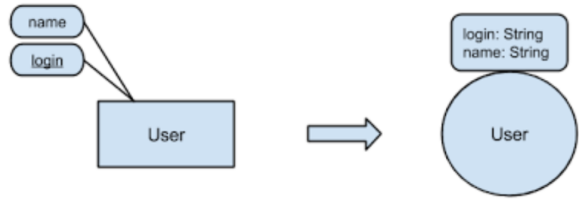
- **Native**: Index-free adjacency, fast for traversal
- **Non-Native**: Graph overlay on relational backend

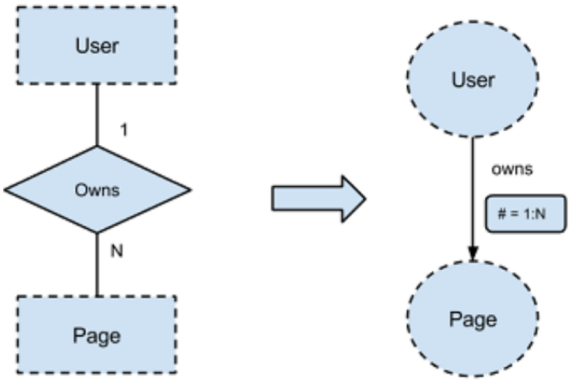
ER to Graph Schema Transformation

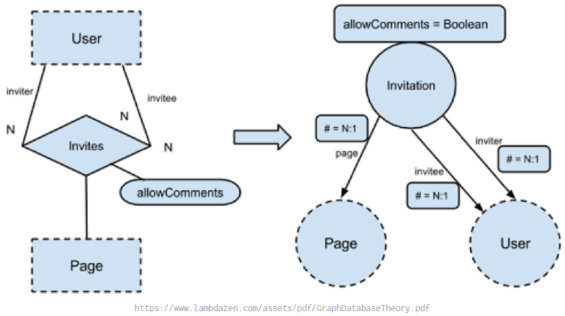
- Entities → Nodes
- Binary relations → Edges

- N-ary relations → Nodes with role-labeled edges

Examples:







https://www.lambdazen.com/assets/pdf/GraphDatabaseTheory.pdf

Graph Schema Equivalence

Graph Universe: The graph universe $U(S)$ of a graph schema S is the infinite set of all graph instances of S

Equivalent: Two graph schemata S and $\hat{S}$ are equivalent iff $\exists f. f : U(S) \to U(\hat{S})$

Graph Schema Transformation Rules

- **Renaming**: Change label/property names *(schema-preserving)*
- **Reverse Edges**: Invert direction if no conflict exists
- **Property Displacement**: Move edge prop to node if look-across is 1
- **Specialization/Generalization**: Split or merge types by property predicates
- **Edge Promotion**: Turn edge into node with two new edges
- **Property Promotion**: Factor property set into a separate node
- **Multivalued Expansion**: Turn list-valued property into connected nodes

Derived Vertex Types, Edge Types, and Properties

Let S be a graph schema and $U(S)$ the corresponding graph universe.

- A vertex type T is *derived* in S iff, for all graphs $G \in U(S)$, the graph G can be uniquely reconstructed from $G - V_T$, where V_T is the set of all vertices in G with type T.
- An edge type T is *derived* in S iff, for all graphs $G \in U(S)$, the graph G can be uniquely reconstructed from $G - E_T$, where E_T is the set of all edges in G with type T.
- A vertex or edge property P is *derived* in S iff, for all graphs $G \in U(S)$, the graph G can be uniquely reconstructed from a graph G' where the property P has been deleted from all vertices and edges.

General Rule To Simplify Graph Schemas

Given a graph schema S, deleting a derived property or vertex/edge type yields an equivalent graph schema $\hat{S}$

General Rule To Make Graph Schemas More Complex

Given a graph schema S, adding a vertex type, edge type, or property T such that T is derived in $\hat{S} = S + T$ yields an equivalent graph schema $\hat{S}$

Cypher Query Language

Cypher: Declarative graph query language used in Neo4j. Pattern-based, ASCII-art style.

Pattern Matching

```
MATCH (a:Person)-[:KNOWS]->(b) RETURN b.name
```

Core Constructs

- Node: `(p:Person {name: 'Anna'})`
- Edge: `[:KNOWS {since: 2019}]`
- Path: `(a)-[:KNOWS*1..3]-(b)` (1–3 undirected hops)
- Undirected Edge: `(a)-[:KNOWS]-(b)`

Modifying Data

CREATE

- `CREATE (a:Person {name: 'Bob'})` – new node
- `CREATE (a)-[:KNOWS]->(b)` – new edge

DELETE

- `DELETE a` – only if a has no edges
- `DETACH DELETE a` – delete node and connected edges

SET

- `SET a.surname = 'Smith'` – add or update property
- `SET a = {name: 'X', age: 42}` – overwrite all properties

Schema Constraints in Cypher

- **Uniqueness**: `REQUIRE (n.p1, n.p2) IS UNIQUE`
- **Existence**: `REQUIRE n.prop IS NOT NULL`
- **Type**: `REQUIRE n.prop IS :: STRING`
- **Key**: `REQUIRE (n.p1, n.p2) IS NODE KEY`

Example: Key Constraint: Ensure each Actor has a unique name combination:
`CREATE CONSTRAINT actor_id FOR (a:Actor) REQUIRE (a.firstname, a.surname) IS NODE KEY`

8 Descriptive Statistics and Data Normalization

Measures of Central Tendency

Mean: $\mu = \frac{1}{n}\sum_{i=1}^{n} x_i$

> Note
>
> Mean is best for symmetrical distributions without outliers

Optimization-Based Median

In the context of Optimization, the median for n numbers is a *set-valued function* when n is even and a *single-valued function* when n is odd. The function gives us the value or the set of values that minimizes the distance to all elements.

$$\text{Median} = \min_x \sum_{i=1}^{n} |x - x_i|$$

Examples (odd): data: $\{1, 2, 3, 6, 10\}$ we want to minimize $f(x) = \sum |x - x_i|$

- $f(1) = |1-1| + |1-2| + |1-3| + |1-6| + |1-10| = 0 + 1 + 2 + 5 + 9 = 17$
- $f(2) = |2-1| + |2-2| + |2-3| + |2-6| + |2-10| = 1 + 0 + 1 + 4 + 8 = 14$
- $f(3) = |3-1| + |3-2| + |3-3| + |3-6| + |3-10| = 2 + 1 + 0 + 3 + 7 = 13$
- $f(6) = |6-1| + |6-2| + |6-3| + |6-6| + |6-10| = 5 + 4 + 3 + 0 + 4 = 16$
- $f(10) = |10-1| + |10-2| + |10-3| + |10-6| + |10-10| = 9 + 8 + 7 + 4 + 0 = 28$

Hence, the minimum occurs at $x = 3$ with $f(3) = 13$. Since the number of data points is odd, the optimization-based median is **unique** and equal to the middle value in the sorted list: $\boxed{3}$.

Examples (even): data: $\{1, 2, 3, 6\}$ we want to minimize $f(x) = \sum |x - x_i|$

- $f(1) = |1-1| + |1-2| + |1-3| + |1-6| = 0 + 1 + 2 + 5 = 8$
- $f(2) = |2-1| + |2-2| + |2-3| + |2-6| = 1 + 0 + 1 + 4 = 6$
- $f(3) = |3-1| + |3-2| + |3-3| + |3-6| = 2 + 1 + 0 + 3 = 6$
- $f(6) = |6-1| + |6-2| + |6-3| + |6-6| = 5 + 4 + 3 + 0 = 12$

We observe that $f(x)$ attains its minimum value of 6 for any $x \in [2, 3]$. Since the number of data points is even, the optimization-based median is **set-valued**, and any value in the interval $\boxed{[2, 3]}$ minimizes the total absolute deviation.

> Note
>
> The Optimization-Based Median can be computed using simple rules when the data is sorted in ascending order and indexed as $x_1, x_2, \ldots, x_n$. If n is odd, the median is the single value at index $i = \frac{n+1}{2}$ (i.e., the middle element). If n is even, the median is any value in the interval $[x_{n/2},\, x_{\frac{n}{2}+1}]$.

Statistical Median

Conventually in statistics, the median is always one single value, therefore when n is even, the median is calculated as $\frac{x_{\frac{n}{2}} + x_{\frac{n}{2}+1}}{2}$. and for odd we just use the middle value formula $(x_{\frac{n+1}{2}})$

Example: Data: $\{1, 4, 7, 9\}$

Here, $n = 4$ is even, so we compute:

$$\text{median} = \frac{x_2 + x_3}{2} = \frac{4+7}{2} = \boxed{5.5}$$

> Note
>
> Median is preferred for skewed distributions or when outliers are present

Mode: The most frequent value(s) in the dataset. $\text{mode} = \arg\max_x |\{i \in \{1, \ldots, n\} \mid x_i = x\}|$ **Example:**

Data: $\{2, 3, 5, 3, 8, 3, 2\}$

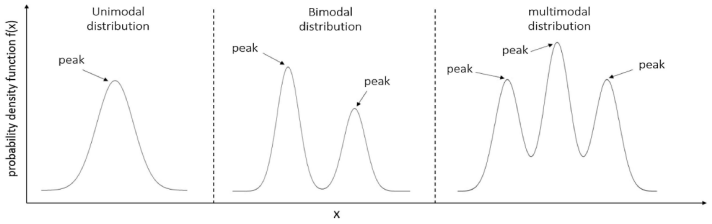
We compute the size of each set:

$$|\{i \mid x_i = 2\}| = 2 \quad \text{(indices 1 and 7)}$$
$$|\{i \mid x_i = 3\}| = 3 \quad \text{(indices 2, 4, and 6)}$$
$$|\{i \mid x_i = 5\}| = 1 \quad \text{(index 3)}$$
$$|\{i \mid x_i = 8\}| = 1 \quad \text{(index 5)}$$

The maximum count is 3, which occurs at $x = 3$.

> Note
>
> Mode is useful for categorical data or to identify the most frequent value

Unimodal vs. Multimodal



Measures of Dispersion

Range: The difference between the maximum and minimum values ($\max_i X_i - \min_i X_i$)

> Note
>
> Range is best for a quick estimate of variability. However it is sensitive to outliers since it only considers extreme values

IQR: Interquartile Range (IQR) is the difference between the third quartile (Q3) and first quartile (Q1), measuring the spread of the middle 50% of data ($Q_3 - Q_1$)

> Note
>
> IQR is a robust measure of spread. It is useful when dealing with skewed distributions or outliers since it ignores extreme values

Variance σ^2: The average squared deviation from the mean. Calculated as $\sigma^2 = \frac{1}{n}\sum_{i=1}^{n}(X_i - \mu_X)^2$

Unnormalized Variance (Total Variability): The raw sum of squares, called total sum of squares. $\text{TSS} = \sum_{i=1}^{n}(X_i - \mu_X)^2 = n\sigma_X^2$

> Note
>
> Variance measures overall data dispersion. However, squaring emphasizes larger deviations, making it more sensitive to extreme values

Standard Deviation σ: The square root of variance ($\sqrt{\sigma^2}$), indicating the average deviation from the mean

Unnormalized Standard Deviation: $\hat{\sigma}_X = \sqrt{\text{TSS}} = \sqrt{\sum_{i=1}^{n}(X_i - \mu_X)^2} = \sqrt{n\sigma_X^2} = \sqrt{n}\sigma_X$

> Note
>
> Standard Deviation is measured in the same unit as the data (more intuitive). It is used in many statistical methods like confidence intervals and hypothesis testing

Covariance: $\text{Cov}(X,Y) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu_X)(y_i - \mu_Y)$

Unnormalized Covariance: $\text{Cov}_{unnormalized}(X,Y) = \sum_{i=1}^{n}(x_i - \mu_X)(y_i - \mu_Y) = n\text{Cov}(X,Y)$

Coefficient of Variation (CV): relative measure of dispersion, calculated as the standard deviation divided by the mean ($\text{CV} = \frac{\sigma}{\mu} \times 100\%$)

> **Note**
>
> CV is useful for comparing variability across datasets with different units or scales. Low CV indicates less relative variability and more consistency. High CV suggests greater dispersion relative to the mean

Side Note: Only use CV for data measured on a ratio scale, where quantity ratios and zeros are meaningful.

Skewness: Measures data asymmetry by relating the average cubed distances from the mean to the standard deviation. It is calculated as $\frac{\frac{1}{n}\sum_{i=1}^{n}(X_i-\mu)^3}{\sigma^3}$.

The Cubed distances from the mean preserve sign of distances, tend to cancel out for symmetric distributions.

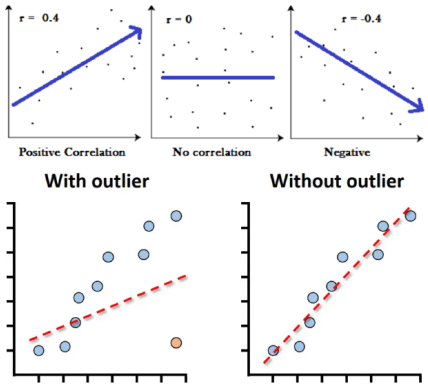
> **Note**
>
> Skewness close to zero: indicates a symmetric distribution (mean, median and mode are close). Positive skewness: suggests a longer right tail (mode $\leq$ median $\leq$ mean). Negative skewness: indicates a longer left tail (mode $\geq$ median $\geq$ mean)

Measures of Correlation

Pearson's Correlation Coefficient

Assume we have quantitative data points $X = \{x_i \mid i \in [1 \dots n]\}$ and $Y = \{y_i \mid i \in [1 \dots n]\}$. Pearson's Correlation Coefficient (r) is defined as the covariance of X and Y divided by the product of their standard deviations:

$$r = \frac{\frac{1}{n}\sum_{i=1}^{n}(x_i - \mu_X)(y_i - \mu_Y)}{\sigma_X \sigma_Y} = \frac{\text{Cov}(X,Y)}{\sqrt{\sigma_X^2}\sqrt{\sigma_Y^2}} = \frac{\frac{1}{n}\sum_{i=1}^{n}(x_i - \mu_X)(y_i - \mu_Y)}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(X_i - \mu_X)^2}\sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \mu_Y)^2}} \qquad \boxed{r(X,Y) \in [-1,1]}$$



Unnormalized r:

$$\hat{r} = \frac{\text{Cov}_{unnormalized}(X,Y)}{\sqrt{\text{TSS}_X}\sqrt{\text{TSS}_Y}} = \frac{\sum_{i=1}^{n}(x_i - \mu_X)(y_i - \mu_Y)}{\sqrt{\sum_{i=1}^{n}(x_i - \mu_X)^2}\sqrt{\sum_{i=1}^{n}(y_i - \mu_Y)^2}}$$

OLS Regression: To find the line that best fits our data and explain how our Y is linearly dependent on X, we find model parametes α and β that minimize the sum of squared errors $\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$ where $\hat{y}_i = \alpha x_i + \beta + \epsilon_i$ There is a *closed-form* solution for this optimization problem and that is:

$$\alpha = \frac{\text{Cov}_{unnormalized}(X,Y)}{\text{TSS}_X} = \frac{\sum_{i=1}^{n}(x_i - \mu_X)(y_i - \mu_Y)}{\sum_{i=1}^{n}(x_i - \mu_X)^2}$$

$$= \frac{n\text{Cov}(X,Y)}{n\sigma_X^2} = \frac{\text{Cov}(X,Y)}{\sigma_X^2}$$

Remember: $r = \frac{\text{Cov}(X,Y)}{\sigma_X \sigma_Y}$. Meaning: $\text{Cov}(X,Y) = r\sigma_X\sigma_Y$

$$\alpha = \frac{r\sigma_X\sigma_Y}{\sigma_X^2} = r\frac{\sigma_Y}{\sigma_X}$$

$$\beta = \mu_Y - \alpha\mu_X$$

Explained Variability: Once we fit a line $\hat{y}_i = \alpha x_i + \beta + \epsilon$ we can calculate the explained variability. $\sum_{i=1}^n (\hat{y}_i - \mu_Y)^2$

Coefficient of Determination (R^2): What fraction of the total variability in Y is explained by our linear model.

$$R^2 = \frac{\text{Explained Variability}}{\text{Total Variability}} = \frac{\sum_{i=1}^n (\hat{y}_i - \mu_Y)^2}{\sum_{i=1}^n (y_i - \mu_Y)^2} \qquad R^2 = 1 \rightarrow \text{perfect prediction}$$

Remember: $\hat{y}_i = \alpha x_i + \beta$ and $\mu_Y = \alpha\mu_X + \beta$

$$R^2 = \frac{\sum_{i=1}^n (\alpha x_i + \beta - (\alpha\mu_X + \beta))^2}{\sum_{i=1}^n (y_i - \mu_Y)^2}$$

$$R^2 = \frac{\sum_{i=1}^n (\alpha x_i + \beta - \alpha\mu_X - \beta)^2}{\sum_{i=1}^n (y_i - \mu_Y)^2}$$

$$R^2 = \frac{\sum_{i=1}^n (\alpha x_i - \alpha\mu_X)^2}{\sum_{i=1}^n (y_i - \mu_Y)^2}$$

$$R^2 = \frac{\sum_{i=1}^n (\alpha(x_i - \mu_X))^2}{\sum_{i=1}^n (y_i - \mu_Y)^2}$$

$$R^2 = \frac{\alpha^2 \sum_{i=1}^n (x_i - \mu_X)^2}{\sum_{i=1}^n (y_i - \mu_Y)^2} = \frac{\alpha^2 \text{TSS}_X}{\text{TSS}_Y} = \alpha^2 \frac{n\sigma_X^2}{n\sigma_Y^2} = \frac{\alpha^2\sigma_X^2}{\sigma_Y^2}$$

Remember: $\alpha = r\frac{\sigma_Y}{\sigma_X}$ Hence $\alpha^2 = r^2\frac{\sigma_Y^2}{\sigma_X^2}$

$$R^2 = \alpha^2 \frac{\sigma_X^2}{\sigma_Y^2}$$
$$= r^2 \frac{\sigma_Y^2}{\sigma_X^2}\frac{\sigma_X^2}{\sigma_Y^2}$$
$$R^2 = r^2$$

Spearman's Rank Correlation Coefficient

Because r is sensitive to outliers and only suitable for linear relationships. We apply the Rank-Transformation trick to the data by the following steps:

1. Transform data $X = \{x_i \mid i \in [1 \dots n]\}$ and $Y = \{y_i \mid i \in [1 \dots n]\}$ into fractional ranks $X^R = \{x_i^R \mid i \in [1 \dots n]\}$ and $Y^R = \{y_i^R \mid i \in [1 \dots n]\}$
   (a) For each x_i collect set $J_i = \{j \in [1 \dots n] \mid x_i = x_j\}$ of indices j of data points identical to x_i
   (b) Sort the data in ascending order and store position π_i of x_i in sorted array (ordinal ranking)
   (c) Compute fractional ranks as *mean* of ordinal ranks of identical values:

$$X_i^R = \frac{\sum_{i \in J_i} \pi_i}{|J_i|} = \frac{\min_{j \in J_i} \pi_i + \max_{j \in J_i} \pi_i}{2}$$

2. Compute Spearman's rank correlation coefficient as Pearson's correlation coefficient (r) of rank-transformed data X^R and Y^R

$$\rho = r(X^R, Y^R) = \frac{\sum_{i=1}^{n}(x_i^R - \mu_X^R)(y_i^R - \mu_Y^R)}{\sqrt{\sum_{i=1}^{n}(x_i^R - \mu_X^R)^2}\sqrt{\sum_{i=1}^{n}(y_i^R - \mu_Y^R)^2}}$$

> Note
>
> The mean of the ordinal ranks of elements in J_i is equal to the mean of the minimum and maximum of these ordinal ranks

Assume we have data $[1, 2, 2, 2, 3]$ and their ordinal ranks $[1, 2, 3, 4, 5]$. We have $k = 3$ tied elements starting from $r = 2$, their ordinal ranks are $2, 3, 4$ which is $r, r+1, r+2$ and their mean is $\frac{r+(r+1)+(r+2)}{k}$. The general formula for the mean is:

$$\frac{(r) + (r+1) + (r+2) + \cdots + (r+k-1)}{k}$$

And the mean of the first and last ordinal ranks is $\frac{r+(r+k-1)}{2} = \frac{2r+k-1}{2} = \frac{2r}{2} + \frac{k-1}{2} = r(\frac{2}{2}) + \frac{k-1}{2} = r + \frac{k-1}{2}$

We want to prove the following equality:

$$\frac{(r) + (r+1) + (r+2) + \cdots + (r+k-1)}{k} = r + \frac{k-1}{2}$$

$$\frac{(r) + (r+1) + (r+2) + \cdots + (r+k-1)}{k} = \frac{\sum_{i=0}^{k-1} r + i}{k} = \frac{1}{k}\sum_{i=0}^{k-1} r + i$$

$$\frac{1}{k}\sum_{i=0}^{k-1} r + i = \frac{1}{k}(\sum_{i=0}^{k-1} r + \sum_{i=0}^{k-1} i) \qquad \sum_{i=0}^{k-1} r \quad \text{evaluates to } kr$$

$$\sum_{i=0}^{k-1} i = \frac{k(k-1)}{2} \qquad \text{triangular numbers } (\sum_{i=1}^{n} i = 1 + 2 + 3 + \cdots + n = \frac{n(n+1)}{2})$$

$$\frac{1}{k}(\sum_{i=0}^{k-1} r + \sum_{i=0}^{k-1} i) = \frac{1}{k}(kr + \frac{k(k-1)}{2}) = \frac{kr}{k} + \frac{k(k-1)}{2k} = r + \frac{k-1}{2}$$

Example:

Let:

$$X = [1,\ 1,\ 3,\ 5,\ 5,\ 5,\ 7], \quad Y = [2,\ 2,\ 4,\ 6,\ 7,\ 6,\ 9]$$

1. **Rank-transform both X and Y**

   Step 1: Ordinal Ranks

   - Sorted X: $[1, 1, 3, 5, 5, 5, 7] \rightarrow$ Ordinal ranks: $[1, 2, 3, 4, 5, 6, 7]$
   - Sorted Y: $[2, 2, 4, 6, 6, 7, 9] \rightarrow$ Ordinal ranks: $[1, 2, 3, 4, 5, 6, 7]$

   Step 2: Fractional Ranks

   - For X:

$$\begin{aligned} x_1 = x_2 = 1 &\Rightarrow x_1^R = x_2^R = \frac{1+2}{2} = 1.5 \\ x_3 = 3 &\Rightarrow x_3^R = 3 \\ x_4 = x_5 = x_6 = 5 &\Rightarrow x_{4..6}^R = \frac{4+6}{2} = 5 \\ x_7 = 7 &\Rightarrow x_7^R = 7 \end{aligned}$$

   - For Y:

$$\begin{aligned} y_1 = y_2 = 2 &\Rightarrow y_1^R = y_2^R = \frac{1+2}{2} = 1.5 \\ y_3 = 4 &\Rightarrow y_3^R = 3 \\ y_4 = y_6 = 6 &\Rightarrow y_4^R = y_6^R = \frac{4+5}{2} = 4.5 \\ y_5 = 7 &\Rightarrow y_5^R = 6 \\ y_7 = 9 &\Rightarrow y_7^R = 7 \end{aligned}$$

   Fractional Ranks:

$$X^R = [1.5,\ 1.5,\ 3,\ 5,\ 5,\ 5,\ 7] \quad Y^R = [1.5,\ 1.5,\ 3,\ 4.5,\ 6,\ 4.5,\ 7]$$

2. **Compute Pearson r on ranks**

   - Mean ranks:

$$\mu_X^R = \frac{1}{7}(1.5 + 1.5 + 3 + 5 + 5 + 5 + 7) = \frac{28}{7} = 4$$

$$\mu_Y^R = \frac{1}{7}(1.5 + 1.5 + 3 + 4.5 + 6 + 4.5 + 7) = \frac{28}{7} = 4$$

   - Numerator

$$\sum (x_i^R - \mu_X^R)(y_i^R - \mu_Y^R) \approx 22.25$$

   - Denominator

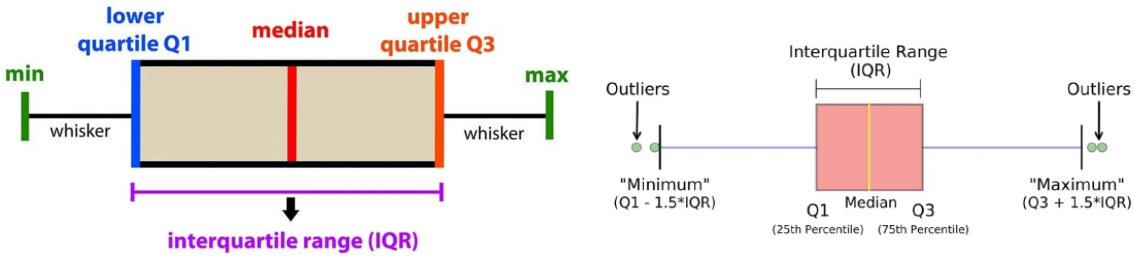
$$\sqrt{\sum_{i=1}^{n} (x_i^R - \mu_X^R)^2} \sqrt{\sum_{i=1}^{n} (y_i^R - \mu_Y^R)^2} = \sqrt{25.5}\sqrt{27}$$

   - Then:

$$\rho = \frac{22.25}{\sqrt{25.5} \cdot \sqrt{27}} = \frac{22.25}{\sqrt{688.5}} \approx \frac{22.25}{26.24} \approx 0.848$$

Visualization

Box Plots



Use Case (Detecting Outliers): Given the sorted dataset:

$$\text{data} = [10, 20, 30, 40, 50, 60, 70, 80, 90, 500], \quad n = 10$$

To compute the 25th percentile using linear interpolation, we use the formula:

$$\text{Position} = \frac{p}{100} \cdot (n - 1)$$

Substituting $p = 25$, we get:

$$\text{Position} = \frac{25}{100} \cdot (10 - 1) = 0.25 \cdot 9 = 2.25$$

This indicates that the 25th percentile lies 25% of the way between the values at positions 2 and 3 (using zero-based indexing), which are:

$$\text{data}[2] = 30, \quad \text{data}[3] = 40$$

We linearly interpolate between these values:

$$25\text{th percentile} = 30 + 0.25 \cdot (40 - 30) = 30 + 2.5 = 32.5$$

Therefore, the 25th percentile of the dataset is:

$$\boxed{Q1 = 32.5}$$

For the 75th percentile: Substituting $p = 75$, we get:

$$\text{Position} = \frac{75}{100} \cdot (10 - 1) = 0.75 \cdot 9 = 6.75$$

This indicates that the 75th percentile lies 75% of the way between the values at positions 6 and 7, which are:

$$\text{data}[6] = 70, \quad \text{data}[7] = 80$$

We linearly interpolate between these values:

$$75\text{th percentile} = 70 + 0.75 \cdot (80 - 70) = 70 + 7.5 = 77.5$$

Therefore, the 75th percentile of the dataset is:

$$\boxed{Q3 = 77.5}$$

Using Q1 and Q3, we can calculate IQR $= Q3 - Q1 = 77.5 - 32.5 = 45$

From that, we can calculate lower and upper bounds to detect outliers:

$$\text{Lower Fence} = Q_1 - 1.5 \cdot \text{IQR} = 32.5 - 67.5 = -35$$

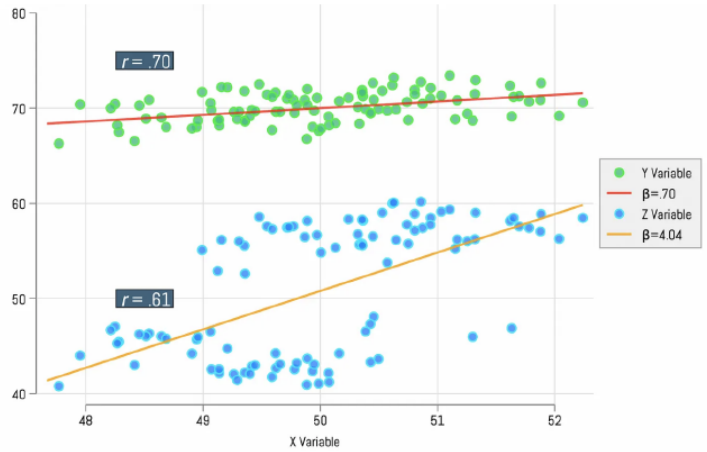
$$\text{Upper Fence} = Q_3 + 1.5 \cdot \text{IQR} = 77.5 + 67.5 = 145$$

Min and Max (excluding outliers):

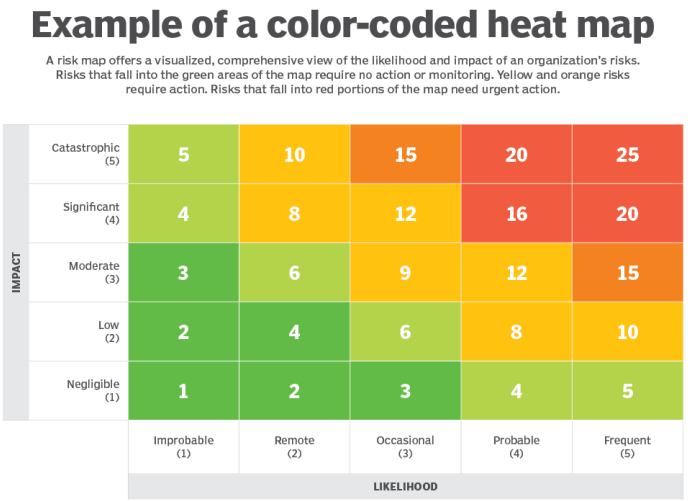
$$\text{Min} = 10, \quad \text{Max} = 90$$

Outlier: The value 500 exceeds the upper fence and is therefore an outlier.

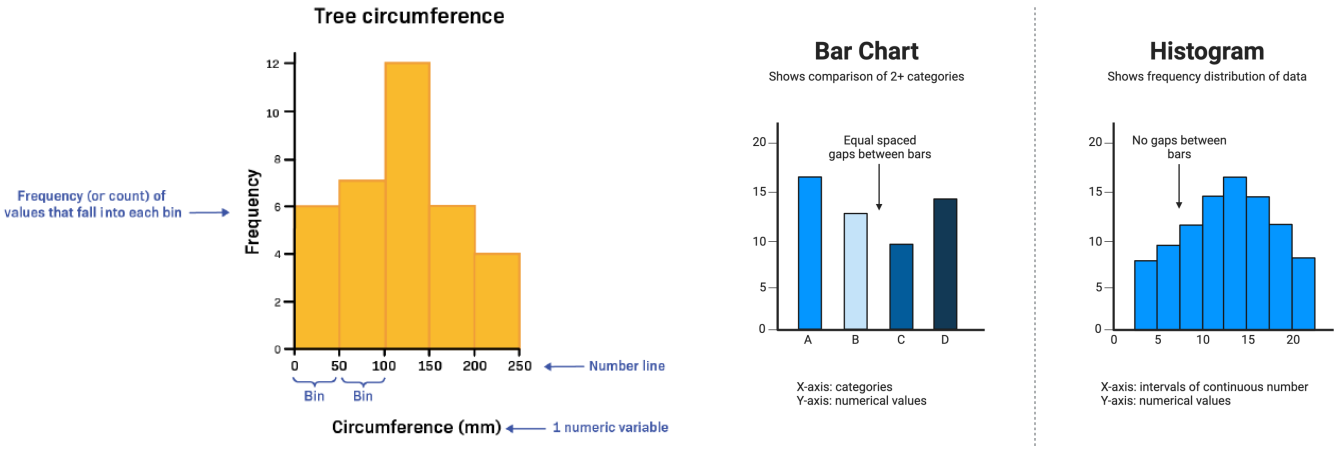
Scatter Plots



Heat Maps



Histograms and Bar Charts



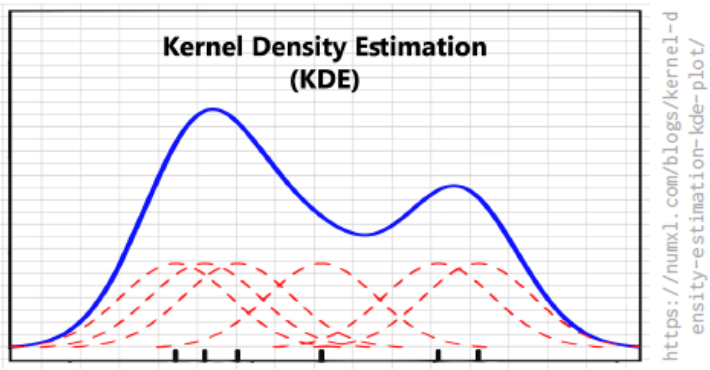
KDE Plots

- Provides smooth estimate of the probability density function (PDF) from data, as a continuous alternative to a histogram.

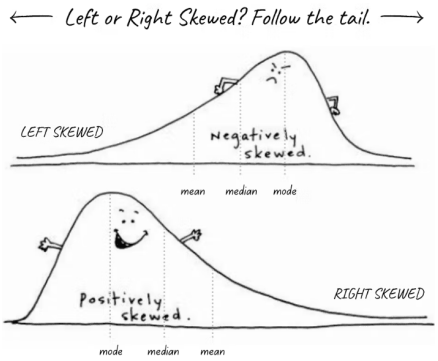
- Each data point x_i contributes a Gaussian $\mathcal{N}(x_i, h^2)$ to the total density. These are averaged to get an estimate of the full density

$$f(x) = \frac{1}{nh} \sum_{i=1}^{n} \frac{1}{\sqrt{2\pi}} e^{-\frac{(x-x_i)^2}{2h^2}}$$

- too small $h \rightarrow$ under-smoothed plot
- too high $h \rightarrow$ over-smoothed plot

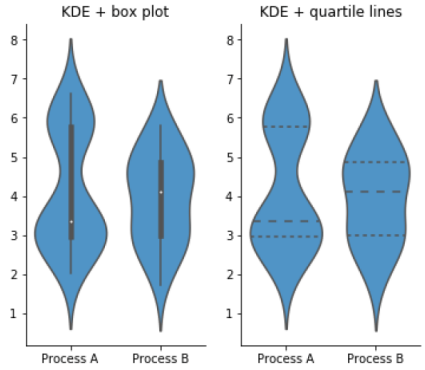


Detect skewness from density plots:



Violin Plots

A violin plot shows **summary statistics** *(box plot)* and **full distribution** *(KDE)*



Normalization

Min-Max

- Preserves orders and scaling. Fixed range $[0, 1]$ (Good for bounded data)
- Sensitive to outliers and does not generalize well

$$\hat{x} = \frac{x - \min}{\max - \min}$$

Z-Score

Useful when data is not bounded. Handles outliers well. Normalized data have zero mean and standard deviation of one. Handles varying distributions.

$$\hat{x} = \frac{x - \mu_X}{\sigma_X}$$

Robust Scaling

More resistant to outliers (best for handling outliers). Works well with skewed and non-Gaussian data

$$\hat{x} = \frac{x - \text{median}_X}{\text{IQR}_X}$$

Decimal Scaling

Used when you want to avoid using min-max but still need a fixed range (Quick and dirty)

$\hat{x} = \frac{x}{10^k}$ where k is the smallest natural number such that $\frac{x}{10^k} \in [-1, 1] \forall x$

Log Transformation

- Reduces skewness and improves normality. Stabilizes variance and Preserves order.
- Best for reducing skewness in rightskewed data.
- Not defined for negative values and can distort small values

  $\hat{x} = \log(x + 1)$

What to choose?

- No one-size-fits-all solution: choose based on data properties and requirement analysis
- Consider preprocessing techniques before normalization
- Always visualize data before and after transformation

Consider the Data Distribution

- If your data is *right-skewed*, use log transformation
- If it is with outliers, use robust scaling
- If transformed data needed in fixed range, then min-max or decimal
- If your data is normality distributed, then use Z-scores

9 Distance and Similarity Measures

Matrix Multiplication $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \qquad B = \begin{bmatrix} e & f \\ g & h \end{bmatrix} \qquad AB = \begin{bmatrix} ae+bg & af+bh \\ ce+dg & cf+dh \end{bmatrix}$

Symmetric: A matrix A is symmetric iff $A = A^T$. Or iff $A_{ij} = A_{ji} \quad \forall\, i, j$. **Example:** $A = \begin{bmatrix} 2 & 5 \\ 5 & 3 \end{bmatrix}$

Positive Definite (PD): A **symmetric matrix** A is **positive definite** if, for every **nonzero** vector x, $x^T Ax > 0$. Example: Let $A = \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix}$ For any vector $x = \begin{bmatrix} a \\ b \end{bmatrix}$,

$$x^T Ax = \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} 2a \\ 3b \end{bmatrix} = 2a^2 + 3b^2$$

For any $x \neq 0$, $2a^2 + 3b^2 > 0$, so A is positive definite.

Positive Semi-Definite (PSD): A **symmetric matrix** A is **positive semi-definite** if, for every vector x, $x^T Ax \geq 0$. Example:

Let $A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$ For any $x = \begin{bmatrix} a \\ b \end{bmatrix}$,

$$x^T Ax = \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} a \\ 0 \end{bmatrix} = a^2$$

$a^2 \geq 0$ always. So A is positive semi-definite, but not positive definite.

Gram Matrix: Given vectors $x_1, x_2, \ldots, x_n$ in $\mathbb{R}^d$, the **Gram matrix** G is the $n \times n$ matrix whose entries are all possible dot products: $G_{ij} = x_i^T x_j$ for $i, j = 1, \ldots, n$. Example:

Let $x_1 = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \quad x_2 = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$

Compute all dot products:

$$x_1^T x_1 = 1 \times 1 + 2 \times 2 = 1 + 4 = 5$$
$$x_1^T x_2 = 1 \times 3 + 2 \times 4 = 3 + 8 = 11$$
$$x_2^T x_1 = 3 \times 1 + 4 \times 2 = 3 + 8 = 11$$
$$x_2^T x_2 = 3 \times 3 + 4 \times 4 = 9 + 16 = 25$$

Thus, the Gram matrix is

$$G = \begin{bmatrix} x_1^T x_1 & x_1^T x_2 \\ x_2^T x_1 & x_2^T x_2 \end{bmatrix} = \begin{bmatrix} 5 & 11 \\ 11 & 25 \end{bmatrix}$$

Note that, considering the vectors matrix $X = \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix}$. The Gram matrix is $X^T X$

$$X^T = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \qquad X^T X = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} = \begin{bmatrix} 5 & 11 \\ 11 & 25 \end{bmatrix}$$

Properties of the Gram Matrix:

- Symmetric: $G_{ij} = G_{ji}$.
- Positive semi-definite (PSD): For any vector c, $c^T Gc \geq 0$

Distance Measures: Quantify how far apart two objects are. *Properties:* symmetrical, non-negative, triangle inequality (direct path is at least as short as any detour), etc.

Similarity Measures: Quantify how similar or alike two objects are. *Properties:* symmetrical and ranges from 0 (completely different) to 1 (completely alike)

Metrics: Let X be a set of data objects, $x, y, z \in X$. A **metric** is a distance function $d : X \times X \to \mathbb{R}$ that satisfies:

1. Non-negativity: $d(x, y) \geq 0 \quad \forall x, y \in X$
2. Identity of indiscernibles: $d(x, y) = 0 \Leftrightarrow x = y$
3. Symmetry: $d(x, y) = d(y, x)$
4. Triangle inequality: $d(x, z) \leq d(x, y) + d(y, z)$

Pseudometrics: Same as **metrics** but allow zero distance between different objects

1. Non-negativity: $d(x, y) \geq 0 \quad \forall x, y \in X$
2. $d(x, x) = 0$ and it is possible that $d(x, y) = 0 \quad x \neq y$
3. Symmetry: $d(x, y) = d(y, x)$
4. Triangle inequality: $d(x, z) \leq d(x, y) + d(y, z)$

Example (Pseudometrics):

$$d(x, y) = \begin{cases} 0 & \text{if lowercase}(x) = \text{lowercase}(y) \\ 1 & \text{otherwise} \end{cases} \qquad d(\text{Apple}, \text{apple}) = 0$$

Quasimetrics: A quasimetric is a distance function that *relaxes* the symmetry requirement of a **metric**

1. Non-negativity: $d(x, y) \geq 0 \quad \forall x, y \in X$
2. Identity of indiscernibles: $d(x, y) = 0 \Leftrightarrow x = y$
3. Triangle inequality: $d(x, z) \leq d(x, y) + d(y, z)$

From Distance to Similarity and Vice Versa

Linear Scaling: $d(x, y) = 1 - \frac{s(x,y)}{s_{\max}} \qquad s(x, y) = 1 - \frac{d(x,y)}{d_{\max}}$ Example: $d(\text{cat}, \text{cat}) = 0 \qquad s(\text{cat}, \text{cat}) = 1$

Note

Preserves relative differences in distances. Requires normalization of distances. Not suitable for unbounded distances.

Reciprocal transformation: $s(x, y) = \frac{1}{1+d(x,y)}$ Example: $d(\text{cat}, \text{dog}) = 2 \qquad s(\text{cat}, \text{dog}) = 0.33$

Note

Keeps values bounded between 0 and 1. Works well when small distances should lead to high similarity. Sensitive to large distances, as similarity first decays quickly and then slowly.

Exponential decay: $s(x, y) = e^{-\lambda d(x,y)} \quad \lambda = \frac{1}{\mu_d}$ Example:

- $d(\text{cat}, \text{cat}) = 0$
- $d(\text{cat}, \text{dog}) = 2$
- $d(\text{cat}, \text{lion}) = 4$
- $\mu_d = 2 \qquad \lambda = 0.5$
- $s(\text{cat}, \text{cat}) = e^{-\lambda d(x,y)} = e^0 = 1$
- $s(\text{cat}, \text{dog}) = e^{-\lambda d(x,y)} = e^{-1} = 0.368$
- $s(\text{cat}, \text{lion}) = e^{-\lambda d(x,y)} = e^{-2} = 0.135$

Note

Smoothly decreases similarity with increasing distance. Handles large distances better than reciprocal transformation. Requires tuning λ and can be unintuitive when distances vary widely.

Dot Product: For vectors $x, y \in \mathbb{R}^n \quad |x| = |y|$ their dot product is given by $x.y = \sum_{i=1}^{n} x_i y_i$

- Dot product between two vectors measure their **alignment**

- It ranges from $-\infty$ to $+\infty$
- If x and y point in the same direction, then $x.y > 0$
- If x and y point in opposite directions, then $x.y < 0$
- If they are **orthogonal (perpendicular)**, then $x.y = 0$

Remember (The Norms):

A norm on a vector space is a function $\|\cdot\|$ that satisfies:

- Positive Definiteness: $\|x\| \geq 0$ with equality iff $x = 0$
- Homogeneity: $\|\lambda x\| = |\lambda|\|x\|$
- Triangle Inequality: $\|x + y\| \leq \|x\| + \|y\|$

Most Common Norms: L_1, L_2, L_p, L_∞

$\|x\|_1 = \sum_{i=1}^{n} |x_i|$ $\|x\|_2 = \left(\sum_{i=1}^{n} |x_i|^2\right)^{1/2}$ $\|x\|_p = (\sum_{i=1}^{n} |x_i|^p)^{1/p}$ $\|x\|_\infty = \max_i |x_i|$

Note: a norm *induces* a **metric** $d(x, y) = \|x - y\|$ which satisfies:

- $d(x, y) \leq 0$ and $d(x, y) = 0$ iff $x = y$
- $d(x, y) = d(y, x)$
- $d(x, y) \leq d(x, y) + d(y, z)$

Cosine Similarity: A normalized version of the **dot product**. It measures the angle between two vectors regardless their magnitude. $s_C(x, y) = cos(\theta_{x,y}) = \frac{x.y}{\|x\|_2 \|y\|_2}$

> Note
>
> Cosine similarity ranges from -1 (opposite direction) to 1 (same direction), if they are orthogonal then 0

Cosine Distance: $d_{\text{cosine}}(x, y) = 1 - s_C(x, y)$. Range is $[0, 2]$ (unintuitive)

> Note
>
> Cosine Distance does not satisfy the triangle inequality

Angular Distance: $d_{\text{angular}}(x, y) = \frac{\theta_{x,y}}{\pi} = \frac{\cos^{-1}(s_C(x,y))}{\pi}$. Range is $[0, 1]$

> Note
>
> Angular Distance satisfies the triangle inequality

> Note
>
> When comparing vectors of different magnitudes, neither cosine nor angular distance always respect the "identity of indiscernibles" axiom, meaning two different vectors can sometimes have zero distance under these measures if one is a scaled version of the other (colinear).

Example: Cosine Distance Does Not Satisfy Identity of Indiscernibles

Let $x = [1, 2]$ and $y = [2, 4]$ (note $y = 2x$):

$$\|x\|_2 = \sqrt{1^2 + 2^2} = \sqrt{5}$$

$$\|y\|_2 = \sqrt{2^2 + 4^2} = \sqrt{20}$$

$$x \cdot y = 1 \cdot 2 + 2 \cdot 4 = 10$$

$$s_C(x, y) = \frac{10}{\sqrt{5}\sqrt{20}} = \frac{10}{10} = 1$$

$$d_{\text{cosine}}(x, y) = 1 - 1 = 0$$

But $x \neq y$, so the identity of indiscernibles is not satisfied.

Example: Cosine Distance Violates the Triangle Inequality

Let $x = [1, 0]$, $y = [0, 1]$, and $z = [1, 1]$:

$$d_{\text{cosine}}(x, y) = 1 - 0 = 1$$

$$x \cdot z = 1 \cdot 1 + 0 \cdot 1 = 1$$
$$\|z\|_2 = \sqrt{1^2 + 1^2} = \sqrt{2}$$
$$s_C(x, z) = \frac{1}{1 \cdot \sqrt{2}} = \frac{1}{\sqrt{2}} \approx 0.707$$
$$d_{\text{cosine}}(x, z) = 1 - 0.707 = 0.293$$

Similarly, $d_{\text{cosine}}(y, z) \approx 0.293$

But:

$$1 \nleq 0.293 + 0.293 = 0.586$$

So the triangle inequality is violated.

Example: Angular Distance Does Not Satisfy Identity of Indiscernibles

Let $x = [1, 2]$ and $y = [2, 4]$:

$$s_C(x, y) = 1$$
$$d_{\text{angular}}(x, y) = \frac{\arccos(1)}{\pi} = \frac{0}{\pi} = 0$$

But $x \neq y$, so the identity of indiscernibles is not satisfied.

Euclidean (L2) Distance: $d_{\text{Euclidean}}(x, y) = \sqrt{\sum_{i=1}^{n}(x_i - y_i)^2}$ (L2 Norm of the difference vector)

It is the most commonly used distance measure in vector spaces. It represents the straight-line (geometric) distance between two points in Euclidean space.

Note

Euclidean Distances satisfies all four metric properties. It is widely used in machine learning, clustering, nearest-neighbor search, etc., due to its intuitive geometric interpretation.

Manhattan (L1) Distance (taxicab): $d_{\text{Manhattan}}(x, y) = \sum_{i=1}^{n} |x_i - y_i|$ (L1 Norm of the difference vector)

It measures the shortest path between points if movement is restricted to axis-aligned steps (like navigating city blocks in a grid). It satisfies all four metric properties. It is often used in ML and clustering when axis-aligned movement makes sense.

Minkowski (L_p) Distance: $d_p(x, y) = \left(\sum_{i=1}^{n} |x_i - y_i|^p\right)^{1/p}$

Note

The larger p, the bigger the impact of the dimensions with the larger differences on the overall distance. The Minkowski distance satisfies all metric properties $\forall p \geq 1$

Chebyshev (L_∞) Distance: $d_\infty(x, y) = \max_i |x_i - y_i|$

- Measures the greatest absolute difference between any coordinate of two vectors
- It is the limit case of the Minkowski distance as $p \to \infty$
- Useful for scenarios where only the largest coordinate difference matters
- The unit ball (set of points at distance 1) under Chebyshev distance is a square in 2D

Remember: Unit Ball

For a given norm (distance function) $\|\cdot\|$, the unit ball is the set of all points (vectors) whose distance from the origin is less than or equal to one. Formally, in $\mathbb{R}^n$: $B = \{x \in \mathbb{R}^n \mid \|x\| \leq 1\}$. For example, consider $\mathbb{R}^2$ and L2 Norm, B is the set of points (x_1, x_2) such that $\sqrt{(x_1)^2 + (x_2)^2} \leq 1$, i.e. $x_1^2 + x_2^2 \leq 1$.

Remember, the circle of radius r is the set of points (x_1, x_2) such that $x_1^2 + x_2^2 = r^2$. Hence, unit ball of L2 norm is a circle.

For a point (x_1, x_2) the Chebyshev norm is $\max(|x_1|, |x_2|)$. The unit ball for Chebyshev norm are the points (x_1, x_2) where $\max(|x_1|, |x_2|) \leq 1$. Hence, unit ball of L_∞ is a square.

For $L1$, the unit ball is all points (x_1, x_2) such that $|x_1| + |x_2| \leq 1$. Hence, the unit ball is a diamond for $L1$.

Excursion

Let's pick a vector and compute two different norms:

Let $x = (3, 4)$ in $\mathbb{R}^2$.

$$\|x\|_1 = |3| + |4| = 7$$

$$\|x\|_2 = \sqrt{3^2 + 4^2} = \sqrt{9 + 16} = \sqrt{25} = 5$$

Let's try another two vectors:

Let $y = (1, 0)$:

$$\|y\|_1 = |1| + |0| = 1$$

$$\|y\|_2 = \sqrt{1^2 + 0^2} = 1$$

Let $z = (1, 1)$:

$$\|z\|_1 = |1| + |1| = 2$$

$$\|z\|_2 = \sqrt{1^2 + 1^2} = \sqrt{2} \approx 1.414$$

Compare the Norms:

Vector	$\|x\|_1$	$\|x\|_2$	$\|x\|_2 \leq \|x\|_1$	$\|x\|_1 \leq \sqrt{2}\|x\|_2$
$(3, 4)$	7	5	$5 \leq 7$	$7 \leq 7.07$
$(1, 0)$	1	1	$1 \leq 1$	$1 \leq 1.41$
$(1, 1)$	2	1.414	$1.414 \leq 2$	$2 \leq 2$

In all cases,

$$\|x\|_2 \leq \|x\|_1 \leq \sqrt{2}\|x\|_2$$

The General Pattern: For any vector x in $\mathbb{R}^2$, $\|x\|_2 \leq \|x\|_1 \leq \sqrt{2}\|x\|_2$. For x in $\mathbb{R}^n$, $\|x\|_2 \leq \|x\|_1 \leq \sqrt{n}\|x\|_2$

In the general equivalence of norms, C_1 and C_2 are the constants making the inequalities true for all vectors:

$$C_1\|x\|_2 \leq \|x\|_1 \leq C_2\|x\|_2$$

For L_1 and L_2 in $\mathbb{R}^2$, these are $C_1 = 1$ and $C_2 = \sqrt{2}$:

$$1 \cdot \|x\|_2 \leq \|x\|_1 \leq \sqrt{2} \cdot \|x\|_2$$

Theorem: For any two norms $\|\cdot\|_a$ and $\|\cdot\|_b$ on a finite-dimensional vector space, there exist constants $C_1, C_2 > 0$ such that, for all vectors x:

$$C_1\|x\|_a \leq \|x\|_b \leq C_2\|x\|_a$$

Correlation-Based Similarity

- Pearson r quantities similarity as degree of linear correlation
- Spearman ρ quantities similarity as monotonicity of x w.r.t y
- $\text{corr}(x, y) \in [-1, 1]$

Kernel Function: A function $k(x, \bar{x})$ that computes the similarity between two input vectors x and $\bar{x}$ and satisfies the following properties

1. Symmetry: $k(x, \bar{x}) = k(\bar{x}, x)$
2. Positive semi-definiteness: For any finite set $\{x_1, \cdots, x_n\}$ of vectors, the Gram matrix $K = (K_{ij}) \in \mathbb{R}^{n \times n}$ with entries $K_{ij} = k(x_i, x_j)$ is positive semi-definite (PSD), i.e. satisfies

$$c^T K c = \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k(x_i, x_j) \leq 0$$

for all vectors of coefficients $c = (c_i) \in \mathbb{R}^n$

> Note
>
> The definition of a kernel does not require that k is non-negative.

Linear Kernel: The simplest form of kernel (dot product similarity). $k(x, \bar{x}) = x \cdot \bar{x} = x^T \bar{x}$

Example: consider $x = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$, $\bar{x} = \begin{bmatrix} 3 \\ 4 \end{bmatrix}$ Then $k(x, \bar{x}) = x^T \bar{x} = 1 \cdot 3 + 2 \cdot 4 = 3 + 8 = 11$

Proof that linear kernel is PSD:

For input vectors $x_1, x_2, \cdots, x_n$ our vectors matrix is $X = [x_1, x_2, \cdots, x_n]$ and the Gram matrix $K = X^T X$ (as shown previously)

For any vector c, we have $c^T K c = c^T X^T X c = (Xc)^T (Xc) = \|Xc\|_2^2 \geq 0 \quad \forall c$

Gaussian (RBF) Kernel: The Gaussian (radial basis function) kernel is the most widely used kernel in the ML field. $k(x, \bar{x}) = exp(-\frac{\|x - \bar{x}\|_2^2}{2\sigma^2})$

- small $\sigma \rightarrow$ kernel is more sensitive to distance between vectors
- large $\sigma \rightarrow$ kernel is less sensitive to distance between vectors

Polynomial Kernel: $k(x, \bar{x}) = (x^T \bar{x} + c)^d$. Where $d \geq 1$ is the degree. If $d = 1$, the kernel captures linear relationships between the variables, if $d = 2$, the kernel captures quadratic relationships, and so on.

> Note
>
> The larger the constant $c \geq 0$ the smoother the similarity landscape (small differences get swallowed by c)

Example: let $c = 1$ and $d = 2$, and assume we have 1D data $x, y \in \mathbb{R}$ then $k(x, y) = (xy + 1)^2 = x^2 y^2 + 2xy + 1$

Notice that $x^2 y^2 + 2xy + 1$ is the result of dot product between two feature vectors $\phi(x) = [x^2, \sqrt{2}x, 1]$ and $\phi(y) = [y^2, \sqrt{2}y, 1]$

Which means that the kernel is *implicitly* mapping our original 1D data (x, y) into a 3D space. i.e., we can instead of transforming all data into higher dimensions, we just use the kernel function which gives us inner product result as if we had transformed.

- A linear kernel only detects linear alignment between data points
- A Polynomial kernel defines similarity in a much richer way: it says two inputs are similar if their higher-order features are similar, not just their values.

Mercer's Theorem: if k is a symmetric and PSD kernel function, then there exists a feature map ϕ into a higher-dimensional space D (possibly ∞) such that $k(x, y) = \phi(x) \cdot \phi(y)$

Note

In these higher-dimensional spaces, patterns may be detectable that are impossible or difficult to individuate in the original feature spaces.

Kernel Trick: A method in machine learning that enables algorithms which depend only on inner products between data points to be generalized to nonlinear feature spaces.

Note

The kernel trick allows algorithms to operate in high- or infinite-dimensional feature spaces at the computational cost of operating in the original space, thereby enabling them to learn nonlinear patterns while remaining scalable.

Applications of the Kernel Trick in Machine Learning:

- Support vector machines (SVMs): Supervised ML approach that implicitly fits separating hyperplanes in the higher-dimensional spaces.
- Kernelized perceptron: Another supervised ML approach that uses the kernel trick to learn non-linear decision boundaries.
- Kernel principal component analysis (kernel PCA): An extension of PCA that uses kernel functions to perform non-linear dimensionality reduction. It implicitly maps the data to a higher-dimensional space and then performs PCA in that space, allowing for the extraction of non-linear principal components.
- Kernelized clustering (e.g., k-means): Clustering methods that use the kernel trick to implicitly compute distances in the higher-dimensional space, allowing for the identification of non-linear clusters in the original data space.

Edit Distances: Ways to measure how different two structured objects are, typically strings, trees, or graphs.

- You define a set of basic operations that can "edit" one object into another. *Examples for strings:* insert a character, delete a character, substitute one character for another.
- Each operation has a cost (often 1 for each, but could be different).
- The edit distance between two objects S and T is the minimum total cost needed to turn S into T by a sequence of allowed operations.

Edit distances always respect the triangle inequality. If you know a way to turn A into B with cost $d(A, B)$, and a way to turn B into C with $d(B, C)$, then you could do both sequences of edits to turn A into C at a total cost $d(A, B) + d(B, C)$

Edit distances are generally not symmetric (Quasimetrics). The cost to edit A into B is not always the same as the cost to edit B into A.

Levenshtein Distance (metric): An edit distance for strings, defined as minimum number of single-character insertions, deletions, or substitutions needed to transform a source string a into a target string b.

Base Cases:
$\text{lev}(a, "") = |a|$
$\text{lev}("", b) = |b|$

Recursive Cases:

$$\text{lev}(a, b) = \begin{cases} \text{lev}(\text{tail}(a), \text{tail}(b)) & \text{if head}(a) = \text{head}(b) \\ 1 + \min \begin{cases} \text{lev}(\text{tail}(a), b) \\ \text{lev}(a, \text{tail}(b)) \\ \text{lev}(\text{tail}(a), \text{tail}(b)) \end{cases} & \text{if head}(a) \neq \text{head}(b) \end{cases}$$

Example:

$$\text{lev}(\text{"kit"},\text{"cat"}) = \text{lev}(\text{"ki"},\text{"ca"}) \qquad \text{(heads: 't' = 't')}$$

$$\text{lev}(\text{"ki"},\text{"ca"}) = 1 + \min \begin{cases} \text{lev}(\text{"k"},\text{"ca"}) \\ \text{lev}(\text{"ki"},\text{"c"}) \\ \text{lev}(\text{"k"},\text{"c"}) \end{cases} \qquad \text{(heads: 'i' } \neq \text{ 'a')}$$

$$\text{lev}(\text{"k"},\text{"ca"}) = 1 + \min \begin{cases} \text{lev}(\text{""},\text{"ca"}) = 2 \\ \text{lev}(\text{"k"},\text{"c"}) = 1 \quad (1 + \min\{1,1,0\}) \\ \text{lev}(\text{""},\text{"c"}) = 1 \end{cases}$$

$$\text{lev}(\text{"ki"},\text{"c"}) = 1 + \min \begin{cases} \text{lev}(\text{"k"},\text{"c"}) = 1 \\ \text{lev}(\text{"ki"},\text{""}) = 2 \\ \text{lev}(\text{"k"},\text{""}) = 1 \end{cases}$$

$$\text{lev}(\text{"k"},\text{"c"}) = 1 + \min \begin{cases} \text{lev}(\text{""},\text{"c"}) = 1 \\ \text{lev}(\text{"k"},\text{""}) = 1 \\ \text{lev}(\text{""},\text{""}) = 0 \end{cases}$$

Finally,

$$\text{lev}(\text{"ki"},\text{"ca"}) = 1 + \min\{2,2,1\} = 1 + 1 = 2$$

$$\text{lev}(\text{"kit"},\text{"cat"}) = \text{lev}(\text{"ki"},\text{"ca"}) = 2$$

Graph Edit Distance (GED): Given two graphs G_1 and G_2, $\text{GED}(G_1, G_2)$ is minimum cost of a sequence of edit operations that transform G_1 into a graph $\bar{G}_2$ that is **isomorphic** to G_2

GED Edit Operations: There are six elementary edit operations: Insertions of isolated nodes, deletions of isolated nodes, attribute substitutions for nodes, deletions of edges, insertions of edges between existing nodes, attribute substitutions for edges.

Note

If "identity" means "isomorphism", then GED satisfies all pseudometric axioms. If "identity" means exact equality, then GED would be a metric.

Shortest-Path Distance: Let $G = \langle V, E \rangle$ be a graph, and let $w : E \to \mathbb{R}_{\geq 0}$ assign a non-negative weight (cost) to each edge. The shortest-path distance from node u to $v \in V$ is: $d_G(u, v) = \min_P \sum_{e \in P} w(e)$

In other words: The shortest-path distance between two nodes is the smallest possible total cost to travel from u to v along the edges of the graph.

Note

In undirected graphs with symmetric edge costs, Shortest-path distance is a metric. In directed graphs or graphs with asymmetric edge costs, Shortest-path distance is a quasimetric.

Linkage Distances for Clusters of Data Objects

Consider we have a set of data objects V that are grouped into n clusters $\{C_i, \cdots, C_n\}$. And we also have a distance measure between individual objects $u, v \in V$ defined as $d_V : V \times V \to \mathbb{R}$.

We want to define a distance measure between **clusters** ($d(C_i, C_j)$)

Linkage Distances: Ways to aggregate (combine) the distances between all pairs of points in two clusters, in order to get a single distance value between the clusters themselves.

Single Linkage: $d_{SL}(C_i, C_j) = \min\{d_V(u, v) \mid (u, v) \in C_i \times C_j\}$

For all possible pairs of points (u, v) where $u \in C_i$ and $v \in C_j$ compute the distance $d_V(u, v)$ and take the smallest of these values. This is the minimum distance between the two clusters.

Complete Linkage: $d_{CL}(C_i, C_j) = \max\{d_V(u, v) \mid (u, v) \in C_i \times C_j\}$ (maximum distance)

Average Linkage: $d_{AL}(C_i, C_j) = (|C_i| \cdot |C_j|)^{-1} \sum_{u \in C_i} \sum_{v \in C_j} d_V(u, v)$ (mean distance) i.e. for all possible pairs (u, v), sum all the distance and divide by number of all possible pairs.

Sets Similarity and Distance

Jaccard Similarity: For sets A, B, the Jaccard similarity is given by $J(A, B) = \frac{|A \cap B|}{|A \cup B|}$ range $\to [0, 1]$

Jaccard Distance (metric): $d_J(A, B) = 1 - \frac{|A \cap B|}{|A \cup B|}$

Sørensen-Dice Similarity: $S(A, B) = \frac{2|A \cap B|}{|A| + |B|}$. It is never smaller than the Jaccard index, $S(A, B) \geq J(A, B)$

Sørensen-Dice Distance: $d_S(A, B) = 1 - \frac{2|A \cap B|}{|A| + |B|}$

> Note
>
> The Sørensen-Dice "distance" fails the triangle inequality, so it is not a metric.

Proof by example:

Let:

$$A = \{1\}, \quad B = \{1, 2\}, \quad C = \{2\}$$

Compute the Sørensen-Dice similarity for each pair:

$$S(A, B) = \frac{2|A \cap B|}{|A| + |B|} = \frac{2 \cdot 1}{1 + 2} = \frac{2}{3}$$

$$S(B, C) = \frac{2|B \cap C|}{|B| + |C|} = \frac{2 \cdot 1}{2 + 1} = \frac{2}{3}$$

$$S(A, C) = \frac{2|A \cap C|}{|A| + |C|} = \frac{2 \cdot 0}{1 + 1} = 0$$

Compute the corresponding distances:

$$d_S(A, B) = 1 - S(A, B) = 1 - \frac{2}{3} = \frac{1}{3}$$

$$d_S(B, C) = 1 - S(B, C) = 1 - \frac{2}{3} = \frac{1}{3}$$

$$d_S(A, C) = 1 - S(A, C) = 1 - 0 = 1$$

Sum the distances for the triangle inequality:

$$d_S(A, B) + d_S(B, C) = \frac{1}{3} + \frac{1}{3} = \frac{2}{3}$$

But:

$$d_S(A, C) = 1 > \frac{2}{3} = d_S(A, B) + d_S(B, C)$$

Binary Data

Iverson bracket: [True] $= 1$ and [False] $= 0$

Hamming Distance (metric): Quantifies the bit-wise difference between two binary arrays of the same size. For two binary arrays $A, B \in \{0, 1\}^n$ it is defined as $\mathrm{HD}(A, B) = \frac{1}{n} \sum_{i=1}^{n} [A_i \neq B_i]$

10 Data Bias

Data Bias: Systematic distortion in the data that arises from how data is collected, measured, labeled, or represented.

Algorithmic Bias: Bias that arises from how an algorithm processes data, sometimes amplifying or introducing new bias even if the data is fair.

> Note
>
> Data bias often leads to algorithmic bias

Examples:

- A survey about workplace satisfaction is only distributed to office workers, not to remote workers. The data is biased because it misses the opinions of remote staff. (Data)
- A job matching algorithm only looks at education level and ignores years of experience, unfairly filtering out skilled candidates with less formal education. (Algorithmic)

Data Bias Modalities: Structural Bias, Measurement Bias, Representational Bias.

Structural Bias: Systematic distortion in data that originates from social, institutional, or historical structures; it is embedded in the design of systems, policies, or practices and is often invisible or normalized within the processes that generate data.

Examples:

- If police spend more time working in certain neighborhoods, the crime data will show more crimes in those areas, even if crime happens elsewhere too. The data is biased because of where police focus their efforts, not necessarily where crime actually happens.
- If a health survey only collects responses from people who have internet access, it leaves out people without internet. This means the data doesn't represent everyone's health needs.
- If school performance data is mostly collected from wealthy schools with more resources, the results won't reflect what's happening in underfunded schools. The data is biased because it misses less privileged students.
- If a fitness tracker is only tested on young athletes, it may not work as well for older people or people with disabilities. The product's data and performance are biased towards the group it was tested on.

Sampling Bias: Occurs when the data collection process leads to a dataset that is not representative of the full population. Often influenced by experimental design, logistical, historical, or institutional constraints.

Examples:

- Medical research relying heavily on data from urban hospitals, underrepresenting rural populations.
- Overrepresentation of university students in behavior studies.
- Surveys conducted during work hours, missing responses from people with full-time jobs.

Historical Bias: Distortion in data that results from reflecting past social norms, policies, or practices, so even if current data collection is fair, the data remains biased because it captures and preserves the unfairness of the past.

Examples:

- Employment records reflecting past gender discrimination in hiring.
- Loan approval data influenced by decades of financial redlining.
- Historical crime data shaped by over-policing of certain neighborhoods.

Label Imbalance: One group or category in the data is much bigger than the others. For example, if a fraud detection dataset has way more "not fraud" examples than "fraud" examples, a model trained on it might miss most fraud cases.

Missing Annotations: When some data points don't have labels or extra information (like demographic details). This can cause the model to miss hidden patterns or be biased, especially if the missing information isn't random.

Availability Bias: When you only collect data from sources that are easy to reach, so your dataset is not representative. For instance, if you analyze opinions on Twitter, you might miss people who don't post much or have private accounts.

Survivorship Bias: When you only look at the "winners" or those who made it through a process, and ignore the "losers" or those who dropped out. This leads to false conclusions, like thinking all startups are successful if you only study the ones that survived.

Measurement Bias: Stems from how data is captured or labeled. Can result from specifics of measurement instruments or inconsistent labelling. Example: Imaging data generated with different scanners can have systematic differences.

Experimental and technical bias: Occurs when the way data is created or measured introduces systematic error. This can be due to the design of the experiment, the equipment used, or how the data is processed. For instance, in pathology, the way tissue samples are fixed (preserved) before analysis can change the results. This means:

- The analysis might not reflect real tissue properties ("misrepresentation").
- Data from different labs might not be comparable ("inconsistency"), because they use different fixation methods.

Human Labeling (Annotation) Bias: Bias introduced during manual labeling or annotation of data, often due to human subjectivity, inconsistency, or lack of context.

Sources of annotation bias: lack of clear guidelines or ambiguous labeling criteria, inattention during the annotation process, or annotators' cultural background, personal beliefs, or implicit biases.

Note: There is almost no manually labeled dataset that is entirely free of labeling bias!

Examples:

- Medical image annotations varying between radiologists with different training.
- Toxicity labeling in online comments differing across cultures and languages.

Impact:

- If there is a strong annotation bias in the data, it can lead to inconsistent ground truth and unreliable model training and evaluation.
- When benchmarking AI models on manually annotated data, it does not make sense to compare model accuracy beyond the expected error in the manual annotation process.

Proxy Variables: Indirect measure used as a substitute for a concept that is difficult to observe or quantify directly. E.g. $BMI \rightarrow$ metabolic health $= \frac{\text{Body Mass (kg)}}{(\text{Body Height (m)})^2}$

Proxies may carry hidden biases or assumptions. They may correlate with sensitive attributes (e.g., socio-cultural background, gender) even if unintentionally. The relationship between the proxy and the true target can vary across contexts.

Temporal Bias: Occurs when data collected at one point in time no longer reflects current patterns, leading to degraded model performance or flawed conclusions.

There are different sources of temporal bias, for example: changes in population behavior / environment / technology, shifts in clinical practices / diagnostic criteria / coding standards, or introduction of new policies / medications / treatments.

Examples:

- Consumer behavior data: Gradual shifts in online shopping habits, as more users adopt mobile shopping over desktop, unnoticed by models trained on older data.
- Financial predictions: Gradual changes in credit risk due to evolving economic conditions, where the same factors no longer predict creditworthiness as reliably.

Representational Bias: Occurs when some demographic groups are underrepresented in the data. Can lead to poor generalizability of model or result to underrepresented populations.

Demographic imbalance: Data often reflects the demographics of its source, leading to overrepresentation of majority or dominant groups. E.g., Facial recognition datasets overrepresent lighter-skinned individuals.

Aggregation Bias: Occurs when a model is trained on pooled data without accounting for group-specific differences. It assumes one-size-fits-all and fails to capture group-driven variability. E.g., A medical diagnostic model performs well for adults but poorly for children due to physiological differences.

Large language models (LLMs) and other foundation models use language data to learn patterns, but this language data already contains societal norms, stereotypes, and power structures. These biases are embedded in the model's core representations, which rely on breaking language into tokens (sub-words) and mapping those tokens into numerical vectors, called embeddings.

The process starts with tokenization, where a dictionary of tokens is created and input text is split into these tokens. Then, each token is mapped to a numeric vector through token embeddings. Biases can enter and be reinforced at multiple points in this process. For instance, tokenization can favor words from languages that are more prevalent in the training data, making those languages easier to represent and disadvantaging less common ones.

Embeddings themselves can also reflect societal biases. For example:

- In the tokenization stage, words from dominant languages are often represented more efficiently than those from underrepresented languages.
- In the embedding stage, word associations can reinforce stereotypes, such as linking "doctor" with "he" and "nurse" with "she."

These biases mean that the models may perform better for dominant languages and groups, and they can propagate stereotyped or unfair associations. Similar problems also affect foundation models in domains beyond language, wherever the training data carries built-in biases.

Metrics for Measuring Bias of Predictive Models

We want to assess if a predictive model that outputs a prediction $\hat{Y}$ is biased by a potential confounder A. For simplicity, assume that both the target variable Y and the confounder A are binary. Common metrics exist for such purpose, examples:

- Demographic Parity (Statistical Parity): Outcome should be independent of protected attribute.

$$P(\hat{Y} = 1 \mid A = a) = P(\hat{Y} = 1 \mid A = b)$$

- Equal Opportunity: True positive rates should be equal across groups.

$$P(\hat{Y} = 1 \mid Y = 1, A = a) = P(\hat{Y} = 1 \mid Y = 1, A = b)$$

- Equalized Odds: Both True positive rates and False positive rates should be equal across groups.

$$P(\hat{Y} = y \mid Y = y, A = a) = P(\hat{Y} = y \mid Y = y, A = b) \quad \forall y$$

- Predictive Parity: Positive predictive value (precision) should be equal across groups.

$$P(Y = 1 \mid \hat{Y} = 1, A = a) = P(Y = 1 \mid \hat{Y} = 1, A = b)$$

Bias Detection in Different Types of Data

Text Data

- Analyze word embeddings for stereotype associations, e.g., via WEAT ("Word Embedding Association Test").
- Compute similarity (e.g., cosine similarity) between embeddings of two sets of target words (e.g., male vs. female names) and two sets of attribute words (e.g., career vs. family words).
- Bias score: If one target group (e.g., male) is systematically closer to one attribute group (e.g., career) than the other (e.g., female), the embedding is said to exhibit bias.

Image Data

- Check for over/under-representation of demographic groups.
- Use saliency maps and other explainable AI techniques to reveal model attention biases.

Tabular Data

- Audit feature correlations with potential sources of data bias.
- Apply fairness metrics (e.g., demographic parity, equal opportunity).
- Use feature attribution techniques and other explainable AI methods to explain biased outcomes.

Mitigation Strategies

Data Preprocessing Techniques

Principal Component Analysis (PCA): A method that transforms the data into key directions capturing most of the variance. If you find that some of these directions are highly correlated with sources of bias (like gender or which lab the data came from), you can remove those, so the model is less likely to use biased information.

Normalization and Transformation: Standardizing or normalizing features prevents models from favoring attributes with larger scales. Techniques such as log-transformations can help reduce skewness tied to group disparities.

Reweighing

Reweighing is a bias mitigation strategy that doesn't alter the data but changes how much each data point "counts" during training.

- You assign higher weights to underrepresented groups or outcomes, so the model learns more from them.
- This can help equalize group representation in model predictions.

The method keeps the original data unchanged and is easy to use if your modeling approach supports weights. However, you need to know which groups are underrepresented, and if the data is extremely imbalanced, this method might not be enough.

Resampling

Resampling is a way to deal with imbalanced datasets by either increasing the number of samples from underrepresented groups (oversampling) or decreasing samples from overrepresented groups (undersampling)

Oversampling can be done by simply duplicating samples or by creating new, synthetic ones. Synthetic data can be generated by altering existing data (e.g. rotate images) or by interpolating between samples (e.g. SMOTE). These methods help the model learn from all groups more equally.

The approach is straightforward, but oversampling can cause the model to memorize data (overfitting), and undersampling might throw away useful information.

What is SMOTE? Synthetic Minority Oversampling Technique (SMOTE) is a method used to balance class distribution in imbalanced datasets by creating new, synthetic samples for the minority class. It generates these synthetic samples by interpolating between existing minority class examples, rather than simply duplicating them, which helps models learn from a more diverse set of data points.

The general steps (simplified) are as follows:

1. For each minority-class sample x, compute the k nearest minority-class neighbors, using some appropriate distance measure.
2. Randomly select a nearest neighbor $\bar{x}$ of x.
3. Randomly select a number $r \in [0, 1]$.
4. Add point at position r on line between x and $\bar{x}$ as a new synthetic sample for the minority class.
5. Repeat this process until enough synthetic samples have been generated.

> **Note**
>
> The most crucial step in dealing with data bias is being aware that bias might exist, especially hidden or subtle bias. Most mitigation techniques only work if you already know where the bias could come from, so it's essential to understand how the data was generated. If you build models without this understanding, you risk making serious mistakes. Talking to domain experts helps to really know what your data represents and how it was collected.

Bias Mitigation Measures in ChatGPT

- Data curation: Filtering and deduplication of pretraining data to reduce harmful and overrepresented content.
- Reinforcement learning from human feedback (RLHF): Fine-tuning using human preferences that reward helpful, harmless, and unbiased responses.
- Content moderation: Safety layers detect and block harmful or biased inputs and outputs in real time.
- Bias testing: Evaluation with benchmarks to detect and measure bias over time.

- Instruction tuning and guardrails: Post-training interventions help reduce overconfidence and encourage responsible language use.
- User feedback: Reports and ratings from users inform continuous improvements and fine-tuning.

11 Outlier Detection

Outlier Detection: The process of identifying data points that deviate from the normal data. The challenge is in defining what normal means.

Notions of Outlierness:

- Deviation from Center: Classic idea of being far from the mean or median.
- Deviation from Trend: A point may follow a different pattern even if it is not far from the center in a geometric sense.

> Note
>
> Normality is contextual: The appropriate notion of normality depends on the nature and distribution of the data.

Sources of Outliers:

- Errors: Mistakes during data entry or sensor failures.
- Rare but significant events: For example, fraudulent transactions or hardware failures.
- Emerging patterns: Genuinely novel behaviors or trends not seen in training or historical data.

Why Does Outlier Detection Matter?

We might detect outliers to **remove noise** from data because outliers caused by noise or technical errors can skew our results. Hence, removing them improves data quality and the robustness of any downstream analysis.

On the other hand, we might want to **detect critical issues** early, for example:

- Fraud Detection: Spot irregular financial activity.
- Quality Control: Detect anomalies in manufacturing that could indicate defects.
- Cybersecurity: Flag abnormal system or network activity.
- Healthcare: Identify rare or abnormal clinical measurements that may signal serious conditions.
- Finance: Catch unusual market behavior or trading patterns early.

Types of Outliers: Point, Contextual, and Collective Outliers.

Point Outliers: A single data point deviates significantly from all others. Example: A sudden temperature spike in a weather dataset.

Contextual Outliers: A value that is only abnormal in a given context or condition. Example: A warm winter day may be abnormal for the season, even if the temperature itself isn't extreme.

Collective Outliers: A group of data points that together behave unusually. Example: A sequence of failed login attempts from a single IP address.

Global vs. Local Outliers: An outlier can be **global** if it is relative to the entire dataset. If it is within its local neighborhood or cluster, then it is **local**. Example: A data point might blend into the dataset globally but still stand out when compared to nearby points.

Challenges in Outlier Detection

- High Dimensionality: In high dimensions, distances become less meaningful (curse of dimensionality).
- Scale and Variability: Features may have different scales (e.g. age in years vs. income in dollars). Data needs normalization or standardization to avoid misleading distances. High within-class variability can mask outliers.
- Noise and Data Quality: Noisy data can falsely appear as outliers. Missing or inconsistent data complicates both detection and evaluation.
- Defining "Normal": There's no universal definition of normal. Behavior considered normal today might become anomalous tomorrow (concept drift).

Outlier Detection Techniques (Overview)

- **Statistical Methods**
  - Assume a known distribution (e.g., Gaussian).
  - Outliers are data points in low-probability regions.
  - Example: Z-score thresholding.
- **Distance-Based Methods**
  - Outliers are far from most other points.
  - Based on distances to k nearest neighbors.
  - Example: k-NN outlier detection.
- **Density-Based Methods**
  - Compare local density of a point with its neighbors.
  - Outliers reside in lower-density regions.
  - Example: Local Outlier Factor (LOF).
- **Model-Based Methods**
  - Build a model of normal data behavior.
  - Points poorly explained by the model are outliers.
  - Examples: Isolation Forests, Autoencoders, Regression residuals.

Evaluating Outlier Detection Methods: Precision at k (P@k) and Average Precision (AP)

Precision at k (P@k)

Consider a dataset X with n data points, and a subset $O \subsetneq X$ with m true outliers (ground truth). And consider we have an outlier detection method that ranks all data points from most to least suspicious $x_1, \cdots, x_n$.

Using Precision at k (P@k) we can know out of the top k ranked data points, how many are actually true outliers.

$$P@k = \frac{1}{k} \cdot |x \in O \mid \text{rank}(x) \leq k| \qquad \text{where rank}(x) = i \text{ if } x = x_i \text{ in the model output ranking}$$

Example: suppose $n = 10$ data points and the true outliers are $O = \{x_3, x_7\}, m = 2$. Assume an outlier detection method ranks the points as $[x_5, x_3, x_1, x_9, x_2, x_7, x_4, x_6, x_8, x_{10}]$

Let's compute $P@k$ for a few values of k:

$P@1 = \frac{1}{1} \cdot |\{x \in \{x_3, x_7\} \mid \text{rank}(x) \leq 1\}| = \frac{1}{1} \cdot 0 = 0$

$P@2 = \frac{1}{2} \cdot |\{x \in \{x_3, x_7\} \mid \text{rank}(x) \leq 2\}| = \frac{1}{2} \cdot 1 = 0.5$

$P@3 = \frac{1}{3} \cdot |\{x \in \{x_3, x_7\} \mid \text{rank}(x) \leq 3\}| = \frac{1}{3} \cdot 1 \approx 0.33$

$P@6 = \frac{1}{6} \cdot |\{x \in \{x_3, x_7\} \mid \text{rank}(x) \leq 6\}| = \frac{1}{6} \cdot 2 \approx 0.33$

Maximum possible value of $P@k$: $\max P@k = \min\{1, \frac{m}{k}\}$, i.e. if we select k points and all true outliers are in the top k, then the most we can get is either 1 if $m \geq k$ (perfect precision) or $\frac{m}{k}$ if $m \lneq k$.

Example:

- Total data points: $n = 5$
- True outliers: $O = \{x_2, x_4\}$, so $m = 2$
- Model ranking: $[x_3, x_2, x_1, x_4, x_5]$

Compute $P@k$ and max $P@k$ for $k = 1$ to 5:

k	Top-k Ranked Points	$P@k$ (Actual)	Max $P@k = \min\left\{1, \frac{m}{k}\right\}$
1	$[x_3]$	$\frac{0}{1} = 0$	1
2	$[x_3, x_2]$	$\frac{1}{2} = 0.5$	1
3	$[x_3, x_2, x_1]$	$\frac{1}{3} \approx 0.33$	$\frac{2}{3} \approx 0.67$
4	$[x_3, x_2, x_1, x_4]$	$\frac{2}{4} = 0.5$	$\frac{2}{4} = 0.5$
5	$[x_3, x_2, x_1, x_4, x_5]$	$\frac{2}{5} = 0.4$	$\frac{2}{5} = 0.4$

Note

- Max $P@k$ is the best possible precision achievable at each k if all outliers are ranked at the top.
- Actual $P@k$ depends on your model's output. It can match max $P@k$ if your model ranks perfectly.

Expected Value under random ordering: The expected value of P@k under random ordering is what we expect just by chance, i.e. if the ranking is random:

$$\mathbb{E}[P@k] = \frac{1}{k} \sum_{x \in O} \mathbb{P}[\text{rank}(x) \leq k]$$

Where $\mathbb{P}[\text{rank}(x) \leq k]$ is the probability that the data point x is ranked among the top k positions. Since each point is equally likely to appear anywhere in a random order, we have:

$$\mathbb{P}[\text{rank}(x) \leq k] = \frac{k}{n}$$

So:

$$\mathbb{E}[P@k] = \frac{1}{k} \sum_{x \in O} \frac{k}{n} = \frac{1}{k} \cdot m \cdot \frac{k}{n} = \frac{m}{n} \qquad \text{For the previous example, we have } \frac{2}{5} = 0.4$$

Adjusted P@k: It tells us how much better our model's ranking is compared to random guessing, scaled relative to the best possible performance.

$$\text{Adjusted P@k } = \frac{P@k - \mathbb{E}[P@k]}{\max P@k - \mathbb{E}[P@k]}$$

- $1 \rightarrow$ model is perfect (P@k = max P@k)
- $0 \rightarrow$ model is as good as random (P@k = expected P@k)
- $< 0 \rightarrow$ model is worse than random (P@k < expected P@k)

In the previous example case, assume we picked $k = 2$, then the Adjusted P@2 is $\frac{0.5-0.4}{1-0.4} \approx 0.167$ That means our model is only slightly better than random (0.167 out of 1)

In a nutshell, for $k = 2$, we have:

- Max precision we can get: 1 (by ranking both outliers in top 2)
- Precision: 0.5 (we got one of them, we are closer to random)
- Average under random ordering: 0.4
- Adjusted Precision: 0.167

Problem with P@k Lets say we have $n = 10,000$ and $m = 10$ (only 10 true outliers) and the model ranks all outliers between positions 11 and 20 (the top 10 ranked are not outliers), then P@10 = 0.

Solution: Average Precision (AP): Instead of fixing one k, look at the models ranking of the actual outliers, and average the precision at each of their positions.

$$\text{AP} = \frac{1}{m} \sum_{x \in O} P@(\text{rank}(x))$$

Where $\text{rank}(x)$ is the position of true outlier x in the models ranked list and $P@(\text{rank}(x))$ is the precision at that position.

So we compute the precision only at the ranks where true outliers appear, and average that.

Example, $n = 5, O = \{x_2, x_4\}$, model output: $[x_1, x_3, x_2, x_4, x_5]$

$$\text{AP} = \frac{1}{2} P@(\text{rank}(x_2)) + P@(\text{rank}(x_4)) = \frac{1}{2}(P@3 + P@4) = \frac{0.33 + 0.5}{2} = 0.415$$

This tells us that, on average, when our model hits a true outlier, the precision at that point in the ranking is about 41.5%.

Note: Max possible AP is 1.

Expected Value of AP under random ranking

$$\mathbb{E}[\text{AP}] = \frac{1}{m}\sum_{x\in O}\mathbb{E}[P@\text{rank}(x)] = \frac{1}{m}\sum_{x\in O}\frac{m}{n} = \frac{1}{m}\cdot m\cdot\frac{m}{n} = \frac{m\cdot m}{m\cdot n} = \frac{m}{n}$$

Adjusted AP

$$\text{Adjusted AP} = \frac{\text{AP} - \frac{m}{n}}{1-\frac{m}{n}}$$

This tells us how far above random our AP is, scaled relative to the best possible AP (which is 1).

- $= 1$ model ranks all outliers perfectly (AP = 1)
- $= 0$ model performs no better than random (AP = $\frac{m}{n}$)
- < 0 model ranks outliers worse than random (AP < $\frac{m}{n}$)

Isolation Forests (Overall Idea)

Assume dataset $X = \{x_1, \cdots, x_n\}$, with $x_i \in \mathbb{R}^d$. We consider a point an outlier if it can be easily separated from the rest of the data.

The high level work flow:

1. Randomly select a subsample $\bar{X} \subseteq X$
2. Recursively split $\bar{X}$ by:
   (a) Choosing a random feature $j \in \{1, \cdots, d\}$
   (b) Choosing a random threshold τ along that feature
3. Continue splitting until:
   (a) The data point is isolated (in a node by itself), or
   (b) A maximum depth is reached
4. Repeat the process multiple times to build a forest of such trees
5. A data point is scored as an outlier if it consistently gets isolated with fewer splits (i.e., ends up closer to the root)

Isolation Trees

Isolation Trees

The core data structure for isolation forests. Each inner node is defined as (S, h, j, τ, l, r) where:

- S: the set of points currently at this node
- h: the height (depth) of this node in the tree
- $j \in \{1, \cdots, d\}$: randomly chosen split feature
- τ: randomly chosen threshold for that feature
- l: left child node = points with $x_j < \tau$
- r: right child node = points with $x_j \geq \tau$

The root is just the top node with $S = X$ and $h = 0$

A node becomes a leaf node if any of the following holds:

1. It contains only one point (point is isolated)
2. All points in it are identical
3. The current depth h reaches a pre-defined limit h_{lim}

Isolation Tree Construction Algorithm

Given a dataset X and a maximum height parameter h_{lim}, construct an isolation tree as follows:

1. Initialize:
   - Tree $T \leftarrow \emptyset$
   - Queue of open nodes $O \leftarrow \{o\}$, where $o = (S = X, h = 0, \cdot, \cdot, \cdot, \cdot)$
2. While $O \neq \emptyset$:
   (a) Remove a node v from O
   (b) If v satisfies any leaf condition:
   - (1) $|S| = 1$, or
   - (2) all points in S are identical, or
   - (3) $h \geq h_{\text{lim}}$

   then add v to T
   (c) Else:
   - Choose a random split feature $j \in \{1, \ldots, d\}$
   - Choose a random threshold $\tau \in [\min(x_j), \max(x_j)]$
   - Split S into:
     - $S_l = \{x \in S \mid x_j < \tau\}$
     - $S_r = S \setminus S_l$
   - Create left and right children:
     - $l = (S_l, h + 1, \cdot, \cdot, \cdot, \cdot)$
     - $r = (S_r, h + 1, \cdot, \cdot, \cdot, \cdot)$
   - Add v to T, and add l, r to O
3. Return tree T

Example: Building an Isolation Tree (2D Data)

Dataset: 3 points in $\mathbb{R}^2$

Point	x	y
A	1	3
B	2	2
C	4	6

1. **Root node:** $S = \{A, B, C\}$, $h = 0$
   - Randomly choose feature $j = 1$ (i.e., x)
   - Randomly pick threshold $\tau = 2.5$
   - Split:
     - Left: $x < 2.5 \Rightarrow \{A, B\}$
     - Right: $x \geq 2.5 \Rightarrow \{C\}$ (leaf node)
2. **Left child:** $S = \{A, B\}$, $h = 1$
   - Randomly choose feature $j = 2$ (i.e., y)
   - Randomly pick threshold $\tau = 2.5$
   - Split:

- Left: $y < 2.5 \Rightarrow \{B\}$ (leaf)
- Right: $y \geq 2.5 \Rightarrow \{A\}$ (leaf)

Final Tree Structure:

```
        Root: x < 2.5
        /          \
   y < 2.5        Leaf: {C}
    /    \
{B}      {A}
```

From Tree to Forest

An Isolation Forest is $\mathcal{F} = \{(T, \bar{X}) \mid \bar{X} \subseteq X\}$ with each isolation tree T built on a different $\bar{X}$

Subsets $\bar{X}$ are sampled without replacement from the full dataset. Each subset has size ψ, where $\psi \leq n$ (hyperparameter), the default is $\psi = \min(n, 256)$

Another hyperparameter is $|\mathcal{F}|$ (number of trees), by default $= 100$

> Note
>
> We use subsampling to (a) sparsify the data, i.e. remove dense regions that can mask outliers hence make outliers more visible. (b) cover different views because each sparse subsample may expose different outlier patterns hence increase robustness and generalizability

Outlier Score

Given an isolation forest $\mathcal{F}$ and a data point $x \in X$, we want to define an outlier score $s(x) \in (0, 1)$.

First we should identify trees containing x:

$$\mathcal{F}(x) = \{T \in \mathcal{F} \mid x \text{ was included in the training subset } \bar{X} \text{ for tree } T\}$$

Then we should compute path lengths, for each tree $T \in \mathcal{F}(x)$, compute:

$$\ell_T(x) = \text{path length from root to leaf that isolates } x$$

Then we average all path lenghts:

$$\ell(x) = \frac{1}{|\mathcal{F}(x)|} \sum_{T \in \mathcal{F}(x)} \ell_T(x)$$

This is the average number of splits needed to isolate x.

Next we should normalize with expected value. Let $c(\psi)$ be the expected path length in a random tree of size ψ. This is not dependent on x, just on tree size. We define the score as:

$$s(x) = 2^{-\ell(x)/c(\psi)}$$

- For outliers, they will be isolated quickly, i.e. $\ell(x) \ll c(\psi)$, so $\frac{\ell(x)}{c(\psi)} \ll 1$, thus: $s(x) = 2^{\text{small}} \rightarrow$ close to 1
- For normal points, they will be harder to isolate, i.e. $\ell(x) \approx c(\psi)$, so $s(x) \approx 0.5$
- For very dense regions, they will be the hardest to isolate, i.e. $\ell(x) > c(\psi)$, so $s(x) \ll 0.5 \rightarrow$ close to 0

Note: $s(x)$ is a global, model-based outlier score.

How the expected path length $c(\psi)$ and the maximum depth h_{lim} are computed?

We use properties of **Binary Search Trees (BSTs)**

- Isolation Trees and BSTs are both binary trees
- Both recursively split data into two parts
- The path to isolate a point in an iTree is like an unsuccessful search in a BST (you reach a leaf but do not find the key)

We want to know the expected number of splits needed to isolate a point among ψ data points, assuming completely random partitioning. This is mathematically equivalent to: The expected length of an unsuccessful search in a Binary Search Tree (BST) built from ψ randomly inserted elements.

The expected path length $\mathbb{E}[\ell(x)]$ for a point in a random BST with ψ nodes (unsuccessful search) is:

$$c(\psi) = 2H(\psi - 1) - \frac{2(\psi - 1)}{\psi}$$

Where $H(n) = \sum_{i=1}^{n} \frac{1}{i}$ is the **harmonic** number. It has an approximation (for large n) as follows:

$$H(n) \approx \ln(n) + \gamma \qquad \gamma \approx 0.577$$

Moreover, a perfectly balanced binary tree with ψ elements has depth $log_2(\psi)$

These formulae come from classical analysis of average-case behavior in binary search trees.

We borrow that to calculate our $c(\psi)$ and h_{lim}

Problem: Incomplete Isolation

In an isolation tree T, each node v stores a subset $v.S \subseteq X$ of the data. A point $x \in X$ is considered isolated when it reaches a leaf node v with $v.S = \{x\}$.

However, not all trees fully isolate every point because:

- Tree growth may stop early due to the depth limit h_{lim}
- This results in leaf nodes v where $|v.S| > 1$

In such cases, we don't know the full number of splits needed to isolate x.

Solution: Approximating Path Length $\ell_T(x)$

Let v be the leaf node reached by x, and let d be its depth in the tree. Then define:

- If $|v.S| = 1$: $\ell_T(x) = d$
- If $|v.S| > 1$: $\ell_T(x) = d + c(|v.S|)$

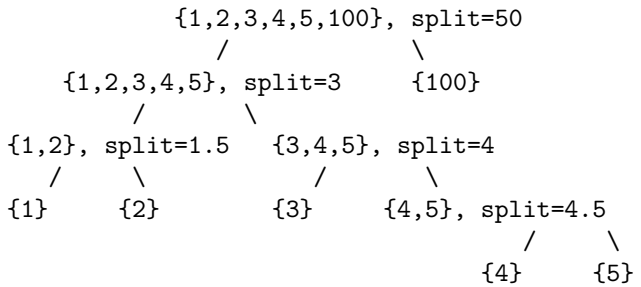
Here, $c(|v.S|)$ is the expected path length in a random isolation tree of size $|v.S|$.

This accounts for the average number of additional splits that would be required to isolate x if the tree had continued to grow.

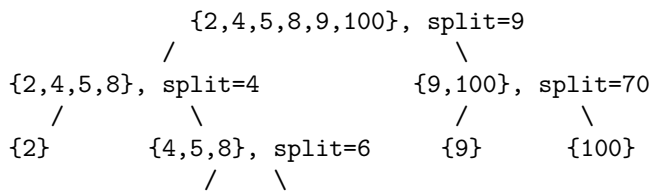
Very Simple Example (1D)

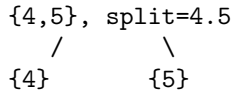
Consider $X = \{1, 2, 3, 4, 5, 6, 7, 8, 9, 100\}$, $\psi = 6$ hence $c(\psi) = 2.9$, and $|\mathcal{F}| = 3$

$T_1 : \{1, 2, 3, 4, 5, 100\}$

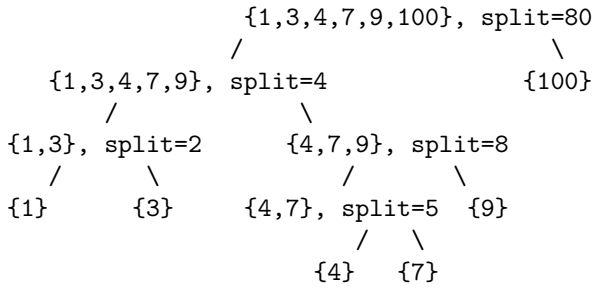


$T_2 : \{2, 4, 5, 8, 9, 100\}$





$T_3 : \{1, 3, 4, 7, 9, 100\}$



Path lengths of data points in the three isolation trees:

Tree	Point	Depth (Path Length)
Tree 1	1	3
	2	3
	3	3
	4	4
	5	4
	100	1
Tree 2	2	2
	4	4
	5	4
	8	3
	9	2
	100	2
Tree 3	1	3
	3	3
	4	4
	7	4
	9	3
	100	1

Average path lengths for data points appearing in multiple trees:

Data Point	Average Path Length
1	3.0
2	2.5
3	3.0
4	4.0
5	4.0
9	2.5
100	1.33

$$c(\psi) = 2 \cdot H(\psi - 1) - \frac{2(\psi - 1)}{\psi} \text{where } H(n) = \sum_{i=1}^{n} \frac{1}{i}$$

$$
\begin{aligned}
c(6) &= 2 \cdot H(5) - \frac{2 \cdot 5}{6} \\
&= 2\left(1 + \frac{1}{2} + \frac{1}{3} + \frac{1}{4} + \frac{1}{5}\right) - \frac{10}{6} \\
&= 2\,(1 + 0.5 + 0.333 + 0.25 + 0.2) - 1.\overline{6} \\
&= 2 \cdot 2.283 - 1.\overline{6} \\
&= 4.566 - 1.666... \\
&\approx 2.9
\end{aligned}
$$

Isolation Forest scores:

Data Point	**Average Path Length**	**Score** $s(x) = 2^{-\ell(x)/2.9}$
1	3.0	0.50
2	2.5	0.56
3	3.0	0.50
4	4.0	0.41
5	4.0	0.41
9	2.5	0.56
100	1.33	0.73

Local Outlier Factor (LOF)

Given a dataset $X = \{x_1, \cdots, x_n\}$ and a distance function $d : X \times X \to \mathbb{R}_{\geq 0}$, we want to detect outliers based on how *sparse* a point's local neighborhood is.

A point $x \in X$ is considered as **local outlier** iff its neighborhood is less dense than the neighborhoods of its neighbors.

k-Distance: Let $x \in X$. Sort all other points by distance to x: $y_1, y_2, \cdots, y_{n-1}$ such that $d(x, y_1) \leq d(x, y_2) \leq \cdots$. Then define $d_k(x) = d(x, y_k)$ as the distance from x to its k^{th} nearest neighbor.

K-Neighborhood: Define $N_k(x) = \{y \in X \mid d(x, y) \leq d_k(x)\}$ as the set of points that lie within distance $d_k(x)$

Example: $X = \{1, 2, 3, 5, 8, 9\}$, $d(x, y) = |x - y|$, point of interest is $x = 3$.

k-Distnaces: $d(3, 1) = 2, d(3, 2) = 1, d(3, 5) = 2, d(3, 8) = 5, d(3, 9) = 6$

Sort data points by distance to $x = 3$: $\{2(1), 1(2), 5(2), 8(5), 9(6)\}$

For $k = 2$, we can compute $d_k(x) = d_2(3) = 2$

K-Neighborhood: $N_2(3) = \{y \in X \mid d(x, y) \leq d_2(3)\} = \{1, 2, 5\}$

Note: although $k = 2$, we got 3 neighbors, i.e. we may have $|N_k(x)| > k$ if multiple data points have same distance.

The Non-Symmetric Behavior

Consider $X = \{1, 2, 3, 10\}$, at $k = 2$ we want to compute $N_2(2)$ and $N_2(10)$

Here are the distances from 2:

Point	Distance
1	1
3	1
10	8

Sorting: $\{1(1), 3(1), 10(8)\}$.

$d_2(2) = 1 \qquad N_2(2) = \{1, 3\}$

Here are the distances from 10:

Point	Distance
1	9
2	8
3	7

Sorting: $\{3(7), 2(8), 1(9)\}$.

$d_2(10) = 8 \qquad N_2(10) = \{2, 3\}$

Notice that $10 \notin N_2(2)$ but $2 \in N_2(10)$

Naive Local Density

- Find the k-nearest neighbors of point x. This gives us $N_k(x)$
- For each neighbor $y \in N_k(x)$, compute the distance $d(x, y)$
- Take the average of those distances
- Take the inverse of that average

$$\text{density}_k(x) = \left(\frac{1}{|N_k(x)|} \sum_{y \in N_k(x)} d(x, y) \right)^{-1}$$

- If x is close to its neighbors, the average distance is small, inverse is large, high density
- If x is far from its neighbors, the average distance is large, inverse is small, low density

Problems:

- Highly sensitive to small changes in distances
- If neighbors are very close, denominator becomes very small, density explodes
- Small difference in distance leads to huge variance in density

Local Reachability Density (LRD)

We want to measure local density in a way that's robust to small distance differences, solving problems from the previous "inverse mean distance" approach.

Instead of using raw distance $d(x, y)$, we use the **k-reachability distance**:

$$\text{reach-dist}_k(x, y) = \max(d_k(y), d(x, y))$$

- $d(x, y)$: the actual distance between x and y
- $d_k(y)$: the k-distance of y, i.e. the distance from y to its k-th nearest neighbor

This avoids overestimating density when points are very close just by chance.

$$\text{density}_k(x) = \text{LRD}_k(x) = \left(\frac{1}{|N_k(x)|} \sum_{y \in N_k(x)} \text{reach-dist}_k(x, y) \right)^{-1}$$

Given that, we can define the Local Outlier Factor (local outlier score):

$$\text{LOF}_k(x) = \frac{1}{|N_k(x)|} \sum_{y \in N_k(x)} \frac{\text{LRD}_k(y)}{\text{LRD}_k(x)}$$

- The formula computes the average ratio between the densities of x's neighbors and x's own density.
- Measures how isolated x is w.r.t. its neighborhood.
- Relative measure of density.
- Range: $[0, \infty]$
- $\approx 1 \rightarrow x$'s neighborhood has similar density to its neighbors
- $< 1 \rightarrow x$ is in a denser area than its neighborhoods
- $> 1 \rightarrow x$ is in a sparser area than its neighbors $\rightarrow$ potential outlier

Max and Min Reachability Distance in a Cluster

Assume cluster $C = \{A, B, C, D\}$ and $d_k(x, y) = \text{reach-dist}_k(x, y)$. We can define a max/min reachability distance in C if we look at all pairs of distinct points in C, compute $d_k(x, y)$ for each, and pick the largest/smallest one.

$$M_k(C) = \max_{x \neq y \in C} d_k(x, y) \qquad m_k(C) = \min_{x \neq y \in C} d_k(x, y)$$

Example, $d_k(A, B) = 5, d_k(A, C) = 7, d_k(A, D) = 6, d_k(B, C) = 4, d_k(B, D) = 8, d_k(C, D) = 3$

$$M_k(C) = 8 \qquad m_k(C) = 3$$

Relative k-reachability distance spread

We can furthur define a measure that tells us how uniform the reachability distances are inside our cluster C (measuring the spread of the cluster):

$$\epsilon(C) = \frac{M_k(C)}{m_k(C)} - 1 \qquad \text{in our case } \frac{8}{3} - 1 \approx 1.67$$

- If max and min are close, $\frac{M_k(C)}{m_k(C)} \approx 1$, $\epsilon(C) \approx 0$, meaning, tight and homogenous cluster

Two-hop neighborhood

Remember, the k-neighborhood of a point x is given by $N_k(x)$, given that, we can define $N_k^2(x)$ as the set of all points that are neighbors of any of x's neighbors (it includes points two hops away in the k-nearest-neighborhood)

$$N_k^2(x) = \{z \in X \mid \exists y \in N_k(x) : z \in N_k(y)\}$$

Example, assume query point x, and $N_2(x) = \{A, B\}$, assume that $N_2(A) = \{x, C\}, N_2(B) = \{x, D\}$ then $N_2^2(x) = \{C, D\}$

Bounding LRD

Remember, we defined local density as the inverse of the average of all distances:

$$\text{LRD}_k(x) = \left(\frac{1}{|N_k(x)|} \sum_{y \in N_k(x)} d_k(x, y) \right)^{-1}$$

But if all those neighbors are in the same cluster, then $d_k(x, y)$ is always going to be between $[m_k(C), M_k(C)]$

Two Edge Cases:

1. If all the neighbors are within the minimum distance then the average distance is $\frac{|N_k(x)|m_k(C)}{|N_k(x)|} = m_k(C)$ then $\text{LRD}_k(x) = \frac{1}{m_k(C)}$ (the highest possible density)
2. If all the neighbors are within the maximum distance then the average distance is $\frac{|N_k(x)|M_k(C)}{|N_k(x)|} = M_k(C)$ then $\text{LRD}_k(x) = \frac{1}{M_k(C)}$ (the lowest possible density)

Which means:

$$\frac{1}{M_k(C)} \leq \text{LRD}_k(x) \leq \frac{1}{m_k(C)}$$

Bounding $\text{LOF}_k(x)$

Remember, we defined the outlier factor for a point x as the average of how dense each neighbor is compared to x

$$\text{LOF}_k(x) = \frac{1}{|N_k(x)|} \sum_{y \in N_k(x)} \frac{\text{LRD}_k(y)}{\text{LRD}_k(x)}$$

We assume the following:

- $x \in C$ (query point is in the cluster)
- $N_k^2(x) \subseteq C$ (all neighbors and their neighbors are also in C)

Which means that:

$$\frac{1}{M_k(C)} \leq \text{LRD}_k(x), \text{LRD}_k(y) \leq \frac{1}{m_k(C)}$$

If we look at the ratio $\frac{\text{LRD}_k(y)}{\text{LRD}_k(x)}$, we have two edge cases:

First one:

- $\text{LRD}_k(y) = \frac{1}{m_k(C)}$ (neighbor is extremely dense)

- $\text{LRD}_k(x) = \frac{1}{M_k(C)}$ (x is extremely sparse)

$$\text{Then } \frac{\text{LRD}_k(y)}{\text{LRD}_k(x)} = \frac{1/m_k(C)}{1/M_k(C)} = \frac{M_k(C)}{m_k(C)} = \epsilon(C) + 1$$

Second one:

- $\text{LRD}_k(y) = \frac{1}{M_k(C)}$ (neighbor is extremely sparse)
- $\text{LRD}_k(x) = \frac{1}{m_k(C)}$ (x is extremely dense)

$$\text{Then } \frac{\text{LRD}_k(y)}{\text{LRD}_k(x)} = \frac{1/M_k(C)}{1/m_k(C)} = \frac{m_k(C)}{M_k(C)} = \frac{1}{\epsilon(C) + 1}$$

Since $LOF_k(x)$ is an average of those ratios, it must lie between those extremes. So we conclude:

$$\frac{1}{\epsilon(C) + 1} \leq \text{LOF}_k(x) \leq \epsilon(C) + 1$$

If the cluster is tight, $\epsilon(C) \approx 0$, $\text{LOF}_k(x) \approx 1$, then x is similar to its neighbors (not an outlier)

Exercise - LOF (2D)

Consider Euclidean distance and $k = 2$, calculate LOF for point D:

Point	X	Y
A	0	1
B	1	1
C	1	0
D	3	-1

First, we calculate the 2-neighborhood:

$$N_2(x) = \{y \in X \mid d(x, y) \leq d_2(x)\} \qquad \forall x \in X$$

for $x = A$:

$$d(A, B) = \sqrt{(0-1)^2 + (1-1)^2} = \sqrt{1+0} = 1$$
$$d(A, C) = \sqrt{(0-1)^2 + (1-0)^2} = \sqrt{1+1} = \sqrt{2}$$
$$d(A, D) = \sqrt{(0-3)^2 + (1-(-1))^2} = \sqrt{9+4} = \sqrt{13}$$

- Points sorted by distance: $\{B(1), C(\sqrt{2}), D(\sqrt{13})\}$
- $d_2(A) = \sqrt{2}$
- $N_2(A) = \{y \in X \mid d(A, y) \leq \sqrt{2}\} = \{B, C\}$

for $x = B$:

$$d(B, A) = \sqrt{(1-0)^2 + (1-1)^2} = \sqrt{1+0} = 1$$
$$d(B, C) = \sqrt{(1-1)^2 + (1-0)^2} = \sqrt{0+1} = 1$$
$$d(B, D) = \sqrt{(1-3)^2 + (1-(-1))^2} = \sqrt{4+4} = \sqrt{8}$$

- Points sorted by distance: $\{A(1), C(1), D(\sqrt{8})\}$
- $d_2(B) = 1$
- $N_2(B) = \{y \in X \mid d(B, y) \leq 1\} = \{A, C\}$

for $x = C$:

$$d(C, A) = \sqrt{(1-0)^2 + (0-1)^2} = \sqrt{1+1} = \sqrt{2}$$
$$d(C, B) = \sqrt{(1-1)^2 + (0-1)^2} = \sqrt{0+1} = 1$$
$$d(C, D) = \sqrt{(1-3)^2 + (0-(-1))^2} = \sqrt{4+1} = \sqrt{5}$$

- Points sorted by distance: $\{B(1), A(\sqrt{2}), D(\sqrt{5})\}$
- $d_2(C) = \sqrt{2}$
- $N_2(C) = \{y \in X \mid d(C, y) \leq \sqrt{2}\} = \{B, A\}$

For $x = D$:

$$d(D, A) = \sqrt{(3-0)^2 + (-1-1)^2} = \sqrt{9+4} = \sqrt{13}$$
$$d(D, B) = \sqrt{(3-1)^2 + (-1-1)^2} = \sqrt{4+4} = \sqrt{8}$$
$$d(D, C) = \sqrt{(3-1)^2 + (-1-0)^2} = \sqrt{4+1} = \sqrt{5}$$

- Points sorted by distance: $\{C(\sqrt{5}), B(\sqrt{8}), A(\sqrt{13})\}$
- $d_2(D) = \sqrt{8}$
- $N_2(D) = \{y \in X \mid d(D, y) \leq \sqrt{8}\} = \{C, B\}$

Then we calculate k-reachability distances:

For $x = A$ $\quad N_2(A) = \{B, C\}$, we calculate:

$$\text{reach-dist}_k(x, y) = \max(d_k(y), d(x, y))$$
$$\text{reach-dist}_2(A, B) = \max(d_2(B), d(A, B)) = \max(1, 1) = 1$$
$$\text{reach-dist}_2(A, C) = \max(d_2(C), d(A, C)) = \max(\sqrt{2}, \sqrt{2}) = \sqrt{2}$$

For $x = B$ $\quad N_2(B) = \{A, C\}$, we calculate:

$$\text{reach-dist}_k(x, y) = \max(d_k(y), d(x, y))$$
$$\text{reach-dist}_2(B, A) = \max(d_2(A), d(B, A)) = \max(\sqrt{2}, 1) = \sqrt{2}$$
$$\text{reach-dist}_2(B, C) = \max(d_2(C), d(B, C)) = \max(\sqrt{2}, 1) = \sqrt{2}$$

For $x = C$ $\quad N_2(C) = \{A, B\}$, we calculate:

$$\text{reach-dist}_k(x, y) = \max(d_k(y), d(x, y))$$
$$\text{reach-dist}_2(C, A) = \max(d_2(A), d(C, A)) = \max(\sqrt{2}, \sqrt{2}) = \sqrt{2}$$
$$\text{reach-dist}_2(C, B) = \max(d_2(B), d(C, B)) = \max(1, 1) = 1$$

For $x = D$ $\quad N_2(D) = \{C, B\}$, we calculate:

$$\text{reach-dist}_k(x, y) = \max(d_k(y), d(x, y))$$
$$\text{reach-dist}_2(D, C) = \max(d_2(C), d(D, C)) = \max(\sqrt{2}, \sqrt{5}) = \sqrt{5}$$
$$\text{reach-dist}_2(D, B) = \max(d_2(B), d(D, B)) = \max(1, \sqrt{8}) = \sqrt{8}$$

Then we compute $\text{LRD}_k(x) \quad \forall x \in X$

for $x = A$:

$$\text{LRD}_2(x) = \left(\frac{1}{|N_2(x)|} \sum_{y \in N_2(x)} \text{reach-dist}_2(x, y) \right)^{-1}$$
$$\text{LRD}_2(A) = \left(\frac{1}{|N_2(A)|} \sum_{y \in N_2(A)} \text{reach-dist}_2(A, y) \right)^{-1}$$
$$\text{LRD}_2(A) = \left(\frac{1}{2} (\text{reach-dist}_2(A, B) + \text{reach-dist}_2(A, C)) \right)^{-1}$$
$$\text{LRD}_2(A) = \left(\frac{1+\sqrt{2}}{2} \right)^{-1} \approx 0.83$$

for $x = B$:

$$\text{LRD}_2(x) = \left(\frac{1}{|N_2(x)|} \sum_{y \in N_2(x)} \text{reach-dist}_2(x, y) \right)^{-1}$$

$$\text{LRD}_2(B) = \left(\frac{1}{|N_2(B)|} \sum_{y \in N_2(B)} \text{reach-dist}_2(B, y) \right)^{-1}$$

$$\text{LRD}_2(B) = \left(\frac{1}{2} (\text{reach-dist}_2(B, A) + \text{reach-dist}_2(B, C)) \right)^{-1}$$

$$\text{LRD}_2(B) = \left(\frac{2\sqrt{2}}{2} \right)^{-1} = \sqrt{2}^{-1} \approx 0.71$$

for $x = C$:

$$\text{LRD}_2(x) = \left(\frac{1}{|N_2(x)|} \sum_{y \in N_2(x)} \text{reach-dist}_2(x, y) \right)^{-1}$$

$$\text{LRD}_2(C) = \left(\frac{1}{|N_2(C)|} \sum_{y \in N_2(C)} \text{reach-dist}_2(C, y) \right)^{-1}$$

$$\text{LRD}_2(C) = \left(\frac{1}{2} (\text{reach-dist}_2(C, A) + \text{reach-dist}_2(C, B)) \right)^{-1}$$

$$\text{LRD}_2(C) = \left(\frac{\sqrt{2} + 1}{2} \right)^{-1} \approx 0.83$$

for $x = D$:

$$\text{LRD}_2(x) = \left(\frac{1}{|N_2(x)|} \sum_{y \in N_2(x)} \text{reach-dist}_2(x, y) \right)^{-1}$$

$$\text{LRD}_2(D) = \left(\frac{1}{|N_2(D)|} \sum_{y \in N_2(D)} \text{reach-dist}_2(D, y) \right)^{-1}$$

$$\text{LRD}_2(D) = \left(\frac{1}{2} \left(\text{reach-dist}_2(D, C) + \text{reach-dist}_2(D, B) \right) \right)^{-1}$$

$$\text{LRD}_2(D) = \left(\frac{\sqrt{5} + \sqrt{8}}{2} \right)^{-1} \approx 0.40$$

Now we can compute $\text{LOF}_k(x)$ for $x = D, k = 2$:

$$\text{LOF}_k(x) = \frac{1}{|N_k(x)|} \sum_{y \in N_k(x)} \frac{\text{LRD}_k(y)}{\text{LRD}_k(x)}$$

$$\text{LOF}_2(D) = \frac{1}{|N_2(D)|} \sum_{y \in N_2(D)} \frac{\text{LRD}_2(y)}{\text{LRD}_2(D)}$$

$$\text{LOF}_2(D) = \frac{1}{2} \left(\frac{\text{LRD}_2(B)}{\text{LRD}_2(D)} + \frac{\text{LRD}_2(C)}{\text{LRD}_2(D)} \right)$$

$$\text{LOF}_2(D) = \frac{1}{2} \left(\frac{0.71}{0.40} + \frac{0.83}{0.40} \right) \approx 1.93$$

Potential Exercise Discussion

Question 1

You are given the following:

- Total data points: $n = 6$
- Ground truth outliers: $O = \{x_2, x_5\}$, so $m = 2$
- Model ranking: $[x_3,\ x_2,\ x_1,\ x_6,\ x_5,\ x_4]$

Tasks:

1. Compute actual $P@k$ for $k = 1$ to 6
2. Compute max possible $P@k$ for each k
3. Compute expected $P@k$ under random ranking
4. Compute adjusted $P@2$
5. Compute average precision (AP)
6. Compute expected AP and adjusted AP

Question 2

Create Isolation Forest and give the model ranking. Assume data points $X = \{(1,1),(2,2),(3,1),(4,2),(5,1),(50,50)\}$, $|\mathcal{F}| = 3$, and $\psi = 4,\ c(4) \approx 2.1$