Data Loading, Manipulation, and Visualization

Introdução Engenharia Informática

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Data Formats and Structures

The Spectrum of Data Structure i

Understanding the underlying organization of data is the first step in the pipeline.

1. **Structured Data**

    - **Definition:** Data that adheres to a pre-defined data model and is therefore straightforward to analyze.
    - **Format:** Rows and columns (Tabular).
    - **Schema:** Rigid (Schema-on-write).
    - **Examples:** Relational Databases (SQL), Excel files.

The Spectrum of Data Structure ii

2. **Unstructured Data**
   - **Definition:** Information that either does not have a pre-defined data model or is not organized in a pre-defined manner.
   - **Format:** Text, Binary, Media.
   - **Schema:** None (Schema-on-read).
   - **Examples:** PDF documents, Video, Audio, Plain Text emails, Social Media posts.

The Spectrum of Data Structure iii

3. **Semi-Structured Data**
    - **Definition:** Data that does not reside in a relational database but has organizational properties that make it easier to analyze. It uses “tags” or “markers” to separate semantic elements and enforce hierarchies.
    - **Format:** Hierarchical trees or Key-Value pairs.
    - **Examples:** JSON, XML, YAML, NoSQL databases.

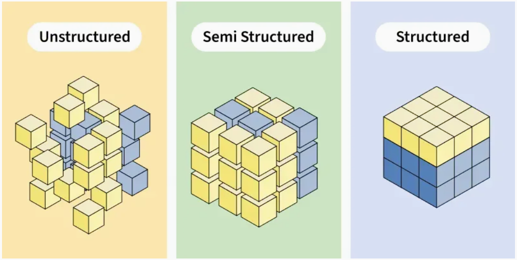


Figure 1: Ilustration of [Un|Semi]Structured organization

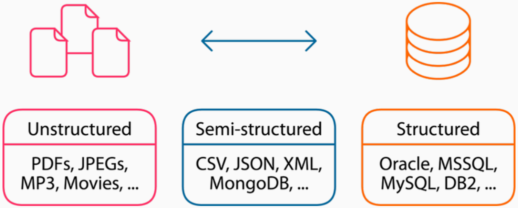

Unstructured
PDFs, JPEGs, MP3, Movies, ...
Semi-structured
CSV, JSON, XML, MongoDB, ...
Structured
Oracle, MSSQL, MySQL, DB2, ...

Figure 2: Examples of [Un|Semi]Structured Files

Semi-Structured Formats i

CSV (Comma Separated Values)

- **Structure:** Flat text file where lines are rows and commas separate columns.
- **Pros:** Universally supported, extremely lightweight.
- **Cons:** No support for types (everything is a string/number), no nesting/hierarchy.

Semi-Structured Formats ii

XML (eXtensible Markup Language)

- **Structure:** Tree-based structure using custom opening/closing tags.
- **Pros:** Standard for legacy web services (SOAP), supports complex hierarchy and schemas (XSD).
- **Cons:** Verbose (heavy storage footprint due to repeated tags), harder to parse than JSON.

Semi-Structured Formats iii

JSON (JavaScript Object Notation)

- **Structure:** Key-Value pairs using brackets `{}` for objects and `[]` for arrays.
- **Pros:** The standard for modern Web APIs (REST), native mapping to Python Dictionaries, human-readable.
- **Cons:** Keys are repeated for every record (verbose).

Semi-Structured Formats iv

YAML (YAML Ain’t Markup Language)

- **Structure:** Relies on whitespace indentation to define hierarchy.
- **Pros:** The most human-readable format; perfect for configuration files (Docker, Kubernetes).
- **Cons:** Indentation errors can break the file easily; parsing can be slower than JSON.

Semi-Structured Formats v

BSON (Binary JSON)

- **Structure:** A binary-encoded serialization of JSON-like documents.
- **Pros:** Optimized for speed (traversal) and space; supports types JSON does not (e.g., `Date`, `BinData`).
- **Cons:** Not human-readable without a decoder. Used primarily in MongoDB.

Example: “Employee Record” i

Here is a dataset containing two records represented in all formats. Note how “lists” of employees are handled.

1. CSV

No native nesting. “Skills” list requires a custom separator (e.g., pipe |).

```
id,name,skills,active
1,"Jane Doe","Python|SQL",true
2,"Bob Smith","Java|C++",false
```

Example: “Employee Record” ii

2. XML

Requires a root tag to wrap multiple children.

```xml
<employees>
    <employee id="1">
        <name>Jane Doe</name>
        <skills><skill>Python</skill><skill>SQL</skill>
        </skills>
        <active>true</active>
    </employee>
    <employee id="2">
        <name>Bob Smith</name>
        <skills><skill>Java</skill><skill>C++</skill>
        </skills>
        <active>false</active>
    </employee>
</employees>
```

Example: “Employee Record” iii

3. JSON

JSON uses square brackets [ ] to denote a list.

```
{"employees": [{
      "id": 1, "name": "Jane Doe",
      "skills": ["Python", "SQL"], "active": true
    },
    {
      "id": 2, "name": "Bob Smith",
      "skills": ["Java", "C++"], "active": false
    }]
}
```

Example: “Employee Record” iv

4. YAML

YAML uses dashes – to denote list items.

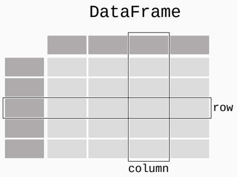
```
employees:
  - id: 1
    name: Jane Doe
    skills: [Python, SQL]
    active: true
  - id: 2
    name: Bob Smith
    skills:
      - Java
      - C++
    active: false
```

Data Loading & Manipulation

The DataFrame Concept

A **DataFrame** is the central data structure in data science (used by R, Pandas, Polars, Spark).

- **Conceptual Model:** An in-memory spreadsheet.
- **Structure:**
  - **Index:** Labels for rows (axis 0).
  - **Columns:** Labels for variables (axis 1).
  - **Cells:** The intersection holding the data.
- **Homogeneity:** A single column usually holds a single data type (e.g., all Integers), but different columns can hold different types.



Pandas

- **Core Philosophy:** Eager execution. Code runs line-by-line immediately, making debugging and exploration intuitive.
- **Key Architecture:**
  - **Single-Threaded:** Primarily runs on a single CPU core.
  - **Index-Based:** Relies heavily on explicit row labels (Indices) for data alignment, which is crucial for time-series analysis.
- **Why use it?**
  - **Unrivaled Ecosystem:** It is the default input for Scikit-Learn, Matplotlib, and thousands of other libraries.
  - **Maturity:** If a data problem exists, there is a StackOverflow answer for how to solve it in Pandas.

Polars

- **Core Philosophy:** Lazy Evaluation. It builds an optimized query plan before execution to minimize work and memory usage.
- **Key Architecture:**
  - **Multi-Threaded (Rust):** Written in Rust to bypass Python limitations, utilizing **all available CPU cores** for parallel processing.
  - **Apache Arrow:** Uses a columnar memory format that allows for zero-copy data transfer and efficient caching.
- **Why use it?**
  - **Performance:** Significantly faster than Pandas on large datasets (10x-100x speedups are common).
  - **Streaming:** Can process datasets larger than your computer's RAM.

Library Comparison: Pandas vs. Polars

Feature	**Pandas**	**Polars**
History	Created in 2008. The industry standard.	Newer (2020s). Built for performance.
Backend	Python/C / Cython.	**Rust** (Safety & Speed).
Execution	**Eager**: Runs line-by-line immediately.	**Lazy & Eager**: Can optimize the whole query plan before running.
Parallelism	Single-threaded (mostly).	**Multi-threaded** (Native parallelization).
Memory	Copies data often (High RAM usage).	**Arrow Memory Format** (Zero-copy, efficient).

Data Cleaning: Missing Values (Imputation) i

Data often has gaps (`NaN` or `Null`). You must decide to **drop** them or **fill** them. Missing data can be filled in with the mean (continous values) or mode (discrete values).

- **Pandas Approach:**

```python
# Drop rows with any missing values
df.dropna()


# Fill with Mean (Imputation)
mean_val = df['salary'].mean()
df['salary'].fillna(mean_val, inplace=True)
```

Data Cleaning: Missing Values (Imputation) ii

- **Polars Approach:**

```python
# Drop rows with any missing values
df.drop_nans()

# Fill with Mean
df.with_columns(
    pl.col("salary")
    .fill_null(pl.col("salary")
    .mean())
)
```

Data Cleaning: Outliers with IQR i

Outliers are extreme values that deviate from other observations. We use the **Interquartile Range (IQR)** to detect them.

The Math:

1. **Q1 (25th Percentile):** The middle number between the smallest number and the median.
2. **Q3 (75th Percentile):** The middle number between the median and the highest number.
3. **IQR Formula:**

$$IQR = Q_3 - Q_1$$

Data Cleaning: Outliers with IQR ii

The Filter: Data D is an outlier if:

$$D < (Q_1 - 1.5 \times IQR) \quad \text{or} \quad D > (Q_3 + 1.5 \times IQR)$$

Implementation (Pandas):

```
Q1 = df['age'].quantile(0.25)
Q3 = df['age'].quantile(0.75)
IQR = Q3 - Q1
# Filtering
df_clean = df[~((df['age'] < (Q1 - 1.5 * IQR)) |
(df['age'] > (Q3 + 1.5 * IQR)))]
```

Data Cleaning: Outliers with IQR iii

Implementation (Polars):

```
Q1 = df["age"].quantile(0.25, interpolation="linear")
Q3 = df["age"].quantile(0.75, interpolation="linear")
IQR = Q3 - Q1
# Filtering
df_clean = df.filter(
    pl.col("age").is_between(q1 - 1.5 * iqr, q3 + 1.5 * iqr)
)
```

Data Scaling i

Scaling the data can help to balance the impact of all variables on the distance calculation and can help to improve the performance of the algorithm.

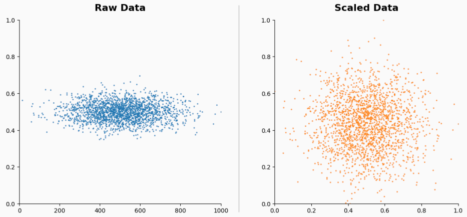


Figure 4: Scaling Data

Data Scaling ii

A. Min-Max Scaling (Normalization)

- **Goal:** Squeeze data into a range $[0, 1]$.
- **Formula:**

$$X_{norm} = \frac{X - X_{min}}{X_{max} - X_{min}}$$

- **Usage:** Image processing (pixels 0-255), Neural Networks.

B. Standard Scaling (Z-Score Standardization)

- **Goal:** Center data around Mean=0 with Std Dev=1.

Data Scaling iii

- **Formula:**
$$Z = \frac{X - \mu}{\sigma}$$
- **Usage:** PCA, Logistic Regression, Clustering.

Statistics: Correlation & Summaries i

Summaries (Central Tendency & Dispersion):

- **Mean:** Average.
- **Median:** Middle value (Robust to outliers).
- **Mode:** Most frequent value.
- **Quartiles:** Distribution checkpoints (25%, 50%, 75%).

Correlation (Pearson):

- Measures linear relationship between -1 (perfect negative) and $+1$ (perfect positive).
- 0 means no linear correlation.

Code Example:

Statistics: Correlation & Summaries ii

```python
# Pandas/Polars Summary
# Returns count, mean, std,
# min, 25%, 50%, 75%, max
print(df.describe())

# Pandas Correlation Matrix
print(df.corr())
```

Data Visualization

Matplotlib vs. Seaborn i

Matplotlib:

- **Role:** The engine.
- **Philosophy:** “Make easy things easy and hard things possible.”
- **Control:** Granular control over every axis, tick, line style, and canvas element.
- **Syntax:** Imperative (Step-by-step construction).

Seaborn:

- **Role:** The interface.
- **Philosophy:** “Draw attractive and informative statistical graphics.”

Matplotlib vs. Seaborn ii

- **Control:** Automates color mapping, legends, and statistical aggregation.
- **Syntax:** Declarative (Describe *what* you want, not how to draw it).

Best Plots for Analysis Types i

1. **Analysis: Distribution (Univariate)**

- **Goal:** See the spread and shape of data.
- **Plot: Histogram** or **KDE** (Kernel Density Estimate).
- **Example:** `sns.histplot(data=df, x="price", kde=True)`

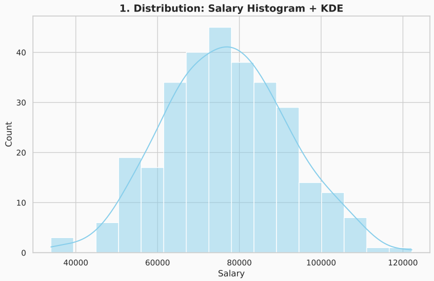


Figure 5: Distribution

Best Plots for Analysis Types ii

2. Analysis: Correlation (Bivariate)

- **Goal:** See how two variables relate.
- **Plot: Scatter Plot** or **Heatmap**.
- **Example:** `sns.scatterplot(data=df, x="age", y="salary")`

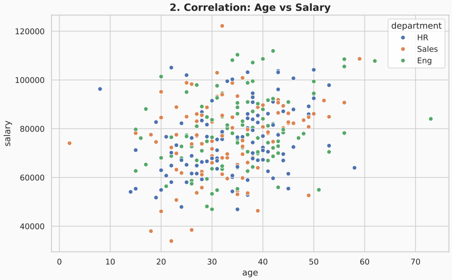


Figure 6: Correlation

Best Plots for Analysis Types iii

3. Analysis: Comparison (Categorical)

- **Goal:** Compare values across groups.
- **Plot: Bar Chart** (aggregates) or **Box Plot** (distributions).
- **Example:** `sns.boxplot(data=df, x="department", y="salary")`

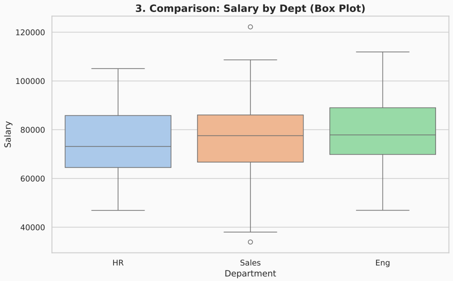


Figure 7: Comparison

Best Plots for Analysis Types iv

4. Analysis: Comparison (Distribution Density)

- **Goal:** Compare the distribution and probability.
- **Plot: Violin Plot**.
- **Example:** `sns.violinplot(data=df, x="department", y="salary")`

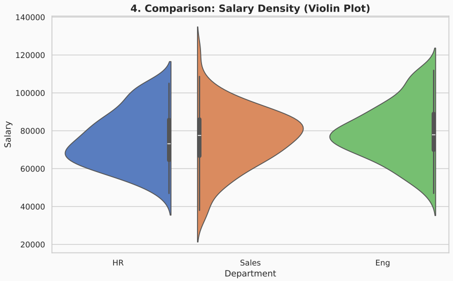


Figure 8: Comparison

Exporting: Raster vs. Vector i

When saving your figures (`plt.savefig`), the extension determines the technology.

Feature	**Raster (Bitmap)**	**Vector**
Formats	`.png`, `.jpg`, `.bmp`	`.pdf`, `.svg`, `.eps`
Composition	Grid of colored pixels.	Mathematical formulas (paths, curves).
Scalability	Loses quality when zoomed (pixelates).	Infinite scalability (sharp at any zoom).
File Size	Large for high resolution.	Small (unless containing thousands of scatter points).
Usage	Web, PowerPoints, Quick previews.	**Academic Papers, Printing, Posters.**

Jupyter Notebooks

The Interactive Framework i

Jupyter (JUlia, PYThon, R) is a web-based interactive computing platform. It is a JSON document containing an ordered list of input/output cells.

The Interactive Framework ii

Key Features

1. **Literate Programming:** Mixes executable code with narrative text (Markdown), equations (“LaTeX”), and images.
2. **The Kernel:** The computational engine (e.g., IPython) runs in the background. It maintains the “state” (variables remain in memory between cells).
3. **Visualization:** Plots render inline directly below the code that generated them.

Effective Usage Workflow i

1. The "Markdown" Cell Use for documentation. Supports headers (`#`), bolding (`**`), and lists to explain methodology *before* the code.

2. The "Code" Cell Runs Python. The last line of a cell is automatically printed (no `print()` needed).

3. Magic Commands

- `%matplotlib inline`: Embeds plots in the notebook.
- `%timeit`: Runs a line multiple times to benchmark performance.
- `!pip install X`: Runs shell commands to install libraries inside the notebook.

Further Reading

Further Reading

- **Pandas Documentation:** pandas.pydata.org - The definitive guide.
- **Polars User Guide:** pola.rs - Essential for high-performance data manipulation.
- **Seaborn Gallery:** seaborn.pydata.org - Visual inspiration for plots.
- **Matplotlib Anatomy of a Plot:** matplotlib.org - Understanding the object hierarchy.
- **Project Jupyter:** jupyter.org