Working with Large Datasets for Scientific Modeling

AM215 - LECTURE 8

The AM215 Team

The Data Bottleneck

▒▒▒▒ Complex models are useless if data cannot be processed effectively!

- **Data too large for RAM:** Common with modern scientific instruments and simulations.
- **Slow preprocessing:** Wastes valuable research time.
- **Reproducibility nightmares:** Inconsistent data inputs lead to irreproducible results.

Today's Mission: Efficient, Scalable, Reproducible Workflows

Our goal: Build **efficient, scalable, reproducible data workflows** that empower robust scientific modeling.

We will cover:

1. **Storage Layer:** From CSV chaos to columnar efficiency (Parquet, Feather, Arrow).
2. **Compute Layer:** Choosing the right Python engine (Pandas, Polars, Dask).
3. **SQL Layer:** Reducing data *before* Python.
4. **SQL Engines:** SQLite for structured data, DuckDB for fast analytics.
5. **Integration:** Connecting SQL and Python DataFrames.
6. **Reproducibility & Testing:** Ensuring trust in your data pipelines.
7. **Code Examples:** Putting it all together.

Storage Layer: How Data Lives on Disk

CSV: The Ubiquitous Data Storage Format

A simple CSV file looks like this:

```
date,region,cases
2022-01-01,North,150
2022-01-01,South,
2022-01-02,North,155
```

Why it's popular:

- **Simple:** It's just plain text.
- **Human-readable:** You can open it in any text editor.
- **Universal:** Supported by nearly every tool, including Excel.

Why Your Go-To Format is Holding You Back

```
date,region,cases
2022-01-01,North,150
2022-01-01,South,
2022-01-02,North,155
```

The Problems:

- **Ambiguous Types:** Is 150 an integer or a string? Is the empty value NULL or an empty string?
- **Slow to Parse:** The entire file must be read line-by-line to find a specific record.
- **No Schema:** The file itself doesn't tell you the data types. This must be inferred or specified manually on every load.
- **Large on Disk:** Text is verbose. 150 takes 3 bytes; as a 16-bit integer it would take 2.

Columnar Storage to the Rescue

Parquet: The On-Disk Format

- An efficient, compressed, columnar, and typed binary format.
- **Columnar:** Stores data column by column, not row by row.
- **Compressed:** Achieves high compression ratios (e.g., using Snappy or Zstandard).
- **Typed:** Includes schema metadata in the file footer, eliminating type inference on load.

Columnar In-Memory: Apache Arrow

The Lingua Franca for Data Analytics

- **Apache Arrow** is a standardized, language-agnostic **in-memory columnar data format**.
- It provides a common data structure that different tools (Polars, DuckDB, Pandas 2.0+) can all understand.
- This enables **zero-copy** data transfer: tools can operate on the same block of memory without expensive serialization or copying.

Feather: Fast, Lightweight Arrow Storage

▒ The On-Disk Format for Speed

- A simple, fast, columnar file format for storing Arrow tables.
- It is essentially the Arrow in-memory format written directly to disk.
- **Use Case:** Ideal for short-term storage or passing data between Python processes (Inter-Process Communication) with maximum speed.
- **Trade-off:** Lacks the advanced compression and metadata features of Parquet, making it less suitable for long-term archival storage.

> **Parquet** for archival, **Feather** for speed.

Why Columnar Wins (1/3): I/O Efficiency

▒▒▒▒ Read Only What You Need

- Analytical queries often only need a few columns from a wide table.
- **Columnar storage** allows you to read just the temperature and pressure columns, skipping humidity, wind_speed, etc. on disk.
- This dramatically reduces the amount of data read from disk (I/O), which is often the slowest part of a data pipeline.

> If a query only needs 2 out of 20 columns, you can achieve a ~10x reduction in I/O.

Why Columnar Wins (2/3): Faster Computation

▒ Leveraging Modern CPUs

- Data for a single column is stored contiguously in memory.
- This layout is ideal for modern CPUs, which can perform a single instruction on multiple pieces of data at once (**SIMD** or **vectorization**).
- Operations like `sum()`, `mean()`, or applying a filter are significantly faster because the CPU can process chunks of a column in parallel.

> Columnar data "fits the shape" of the CPU, leading to massive speedups in aggregation and filtering.

Why Columnar Wins (3/3): Better Compression

▒▒▒ Reducing Storage Footprint

- Columns contain data of the same type (e.g., all integers, all strings).
- This homogeneity allows for much more effective compression algorithms.
    - **Dictionary encoding**, for example, replaces long, repeated strings (like "North America") with small integers (`0`) and stores a lookup table ("dictionary"). This is extremely efficient for columns with low cardinality.
- Better compression means smaller files on disk, which in turn means faster data transfer over networks and less storage cost.

> Smaller data on disk → faster to read → faster analysis.

Columnar vs. Row Layout

▒▒▒▒ A Fundamental Difference in Data Organization

- **Row-oriented (e.g., CSV, traditional databases):** Stores all data for a single record together.
    - Good for transactional workloads (**OLTP** - Online Transaction Processing) where you need to retrieve or update entire rows quickly (e.g., processing an order).
- **Column-oriented (e.g., Parquet, Arrow):** Stores all data for a single column together.
    - Excellent for analytical workloads (**OLAP** - Online Analytical Processing) where you often aggregate or filter on specific columns across many records (e.g., calculating average sales).

Compute Layer: How Data Is Processed in Python

Pandas: The Familiar Workhorse

- ✅ **Mature and flexible:** The standard for years, with a massive ecosystem.
- ✅ **Intuitive API** for many common data manipulation tasks.
- ❌ **Eager execution:** Operations run immediately, which can be inefficient.
- ❌ **Single-threaded and memory-bound:** Struggles with datasets larger than RAM and doesn't use modern multi-core CPUs effectively.

> **Verdict:** Great for small to medium data, but a liability for large-scale, reproducible pipelines.

Polars: The Modern Challenger

- ✅ **Extremely fast:** Built in Rust on top of Apache Arrow.
- ✅ **Lazy query optimizer:** Plans the most efficient way to execute your query, reducing memory usage and computation time.
- ✅ **Multi-threaded:** Automatically uses all available CPU cores.
- ❌ **Smaller ecosystem:** Fewer third-party integrations compared to Pandas.

> **Verdict:** The modern default for high-performance, single-machine data work.

Dask: Scaling Beyond a Single Machine

- ✅ **Out-of-core and distributed:** Can handle datasets larger than RAM by breaking them into chunks (like NumPy arrays or Pandas DataFrames) and processing them in parallel across multiple cores or machines.
- ✅ **Pandas-like API:** Provides a familiar interface for users coming from Pandas.
- ❌ **Complexity and overhead:** Requires managing a scheduler and workers, which adds complexity. Not ideal for problems that can fit on a single machine.

> **Verdict:** Use Dask when your data is truly too large for one machine, not just because it's "big."

What if Data Still Doesn't Fit?

▒ Streaming and Chunking

- Even without Dask, you can process large files by reading them in **chunks**.
- This is a form of **streaming**, where you process the data piece by piece without ever holding the entire file in memory.

```python
# Pandas can read a CSV in chunks
chunk_iter = pd.read_csv("very_large_file.csv", chunksize=1_000_000)

results = []
for chunk_df in chunk_iter:
    # Process each million-row chunk
    results.append(process_chunk(chunk_df))

final_result = pd.concat(results)
```

> This is a manual, "out-of-core" approach. Polars' lazy engine and Dask automate this process more effectively.

Choosing Your Compute Engine

▒▒▒▒ Pick the Engine Based on Scale, Not Habit

Engine	Strength	Limitation	Best Use Case
Pandas	Familiar, mature ecosystem	Single-threaded, memory-bound	Small to medium data
Polars	Fast, lazy, multi-threaded	Newer, smaller ecosystem	Fast local processing
Dask	Distributed, out-of-core	Overhead, cluster complexity	Larger-than-RAM data

> This is a scale gradient: **Pandas** (familiar) → **Polars** (optimized) → **Dask** (distributed).

Before We Scale Out, Let's Scale Smart

▒▒▒▒ The Most Efficient Memory Optimization

- **Dask** helps when your data is *already* in Python and too big for one machine.
- But what if we could avoid loading all that data in the first place?
- The most efficient memory optimization is to **not load data you don't need.**

> This is the job of the **SQL Layer**: to reduce data *before* it ever touches a Python DataFrame.

SQL Layer: Reducing Data Before Loading

Structured Query Language

Why Use SQL in a Python Workflow?

▒▒▒ Push Computation to the Data

- **Reduce data before loading:** The most effective way to manage memory is to not load data you don't need.
    - SQL is the language of data reduction.
- **Push compute to where data lives:** Databases are highly optimized for filtering, joining, and aggregating. Let them do the heavy lifting.
- **Declarative and deterministic:** A SQL query is a precise, repeatable definition of a dataset.
    - Excellent for reproducibility.

> **Core Principle:** SQL filters, aggregates, and joins **before** Python loads the data, dramatically reducing memory cost and processing time.

Relational DB Foundations

▒▒▒▒ The Language of Structured Data

A relational database organizes data into **tables** with predefined **schemas**.

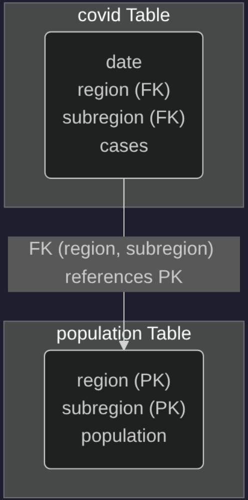
- **Schema:** A formal contract for a table's structure. It defines:
  - Column names (e.g., `date`, `region`, `cases`).
  - Data types (e.g., `TEXT`, `INTEGER`, `REAL`).
  - Constraints (e.g., `NOT NULL`, `UNIQUE`).
- **ACID Guarantees:** Transactions are Atomic, Consistent, Isolated, and Durable.
  - Ensures data integrity, which is critical for scientific reproducibility.

Primary and Foreign Keys

▒▒▒ The Language of Table Relationships

- A **Primary Key (PK)** is a column (or set of columns) that uniquely identifies each row in a table. No two rows can have the same primary key, and it cannot be NULL.
- A **Foreign Key (FK)** is a column in one table that refers to the Primary Key of another table. This creates a link between the two tables.

In our dataset, (region, subregion) together form a composite Primary Key for the population table. In the covid table, these same columns act as a Foreign Key, linking each daily report back to a specific population entry.



Core SQL Syntax

▒▒▒▒ The Verbs of Data Manipulation

SQL provides a clear, declarative syntax for retrieving and manipulating data. Let's look at the core commands.

- `SELECT ... FROM ...`: Choose columns from a table.
- `WHERE ...`: Filter rows based on a condition.
- `GROUP BY ...`: Aggregate data into summary rows.
- `JOIN ... ON ...`: Combine rows from multiple tables.
- `ORDER BY ...`: Sort the results.

We will now look at each of these in turn.

SQL: SELECT

▒▒▒▒ Choosing Columns

The SELECT statement specifies which columns you want to retrieve.

- SELECT * is a wildcard that selects **all** columns.
- SELECT column1, column2 retrieves only specific columns.
- You can use AS to create an **alias** (a new name) for a column in the output.

```sql
-- Select all columns from the covid table
SELECT * FROM covid;

-- Select only specific columns
SELECT date, region, cases FROM covid;

-- Select a column and rename it
SELECT date, cases AS daily_cases FROM covid;
```

SQL: WHERE

▒▒▒ Filtering Rows

The WHERE clause filters rows based on one or more conditions.

- Use standard comparison operators: =, !=, >, <, >=, <=.
- Combine conditions with AND and OR.
- Use BETWEEN for date or number ranges.

```sql
-- Filter for a specific region
SELECT date, region, cases
FROM covid
WHERE region = 'North';

-- Filter for a date range
SELECT date, region, cases
FROM covid
WHERE date BETWEEN '2022-01-01' AND '2022-01-31';
```

SQL: GROUP BY

▒▒▒▒ Aggregating Data

The GROUP BY clause groups rows that have the same values in specified columns into summary rows. It is almost always used with **aggregate functions** like SUM(), AVG(), COUNT(), MAX(), MIN().

```sql
-- Calculate the total cases for each region
SELECT
    region,
    SUM(cases) AS total_cases
FROM covid
GROUP BY region;
```

> This query collapses all rows for a given region into a single output row, summing up the `cases` for that entire group.

SQL: ORDER BY

▒▒▒ Sorting Results

The ORDER BY clause sorts the final result set based on one or more columns.

- ASC for ascending order (the default).
- DESC for descending order.

```sql
-- Calculate total cases per region and sort from highest to lowest
SELECT
    region,
    SUM(cases) AS total_cases
FROM covid
GROUP BY region
ORDER BY total_cases DESC;
```

A Note on Modifying Data

CREATE, INSERT, UPDATE, DELETE

While our focus is on *querying* data for analysis, SQL also includes commands for modifying the database structure and its contents.

- `CREATE TABLE`: Defines a new table and its schema.
- `INSERT INTO`: Adds new rows of data to a table.
- `UPDATE`: Modifies existing rows.
- `DELETE`: Removes rows.

These commands are part of **Data Definition Language (DDL)** and **Data Manipulation Language (DML)**. While essential for database administration, they are less central to the data *analysis* workflow we are focusing on today.

Understanding JOINs

▒▒▒▒ Combining Data from Multiple Tables

JOIN is arguably the most powerful feature of SQL. It allows you to combine rows from two or more tables based on a related column between them.

This is how we connect our covid data with our population data to calculate per-capita rates.

We will focus on the two most common types: INNER JOIN and LEFT JOIN.

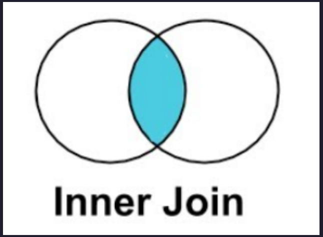
INNER JOIN

▒ Finding the Intersection

An INNER JOIN returns only the rows where the join key exists in **both** tables. It finds the intersection of the two datasets.

```
SELECT
    c.date,
    c.cases,
    p.population
FROM covid AS c
INNER JOIN population AS p
  ON c.region = p.region;
```

> If a region exists in the `covid` table but not in the `population` table (or vice-versa), it will be excluded from the result.

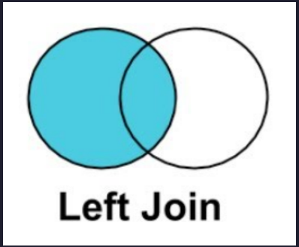


LEFT JOIN

▒▒▒▒ Keeping All Data from the "Left" Table

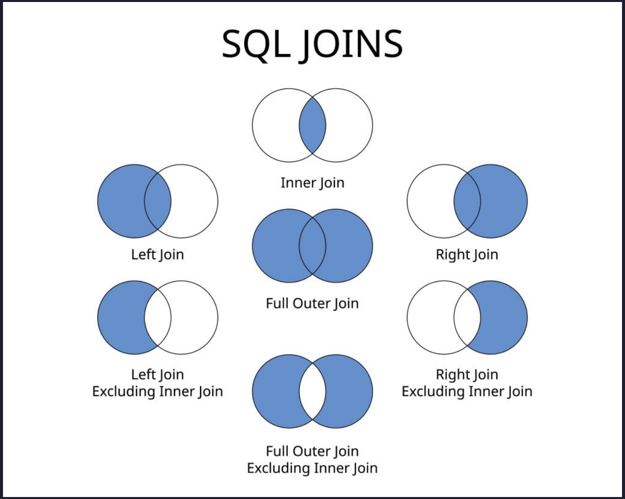
A LEFT JOIN returns **all** rows from the left table, and the matched rows from the right table. If there is no match for a row from the left table, the columns from the right table are filled with NULL.

```
SELECT
    c.date,
    c.cases,
    p.population
FROM covid AS c
LEFT JOIN population AS p
  ON c.region = p.region;
```



> Use this when you want to keep all records from one dataset (the "left" one), even if they don't have a corresponding entry in the other.

Many Types of Joins!


SQL JOINS
Inner Join
Left Join
Right Join
Full Outer Join
Left Join Excluding Inner Join
Right Join Excluding Inner Join
Full Outer Join Excluding Inner Join

SQL Engines for Scientific Computing

SQLite: The Portable, Versionable Database

- **File-based:** A complete database stored in a single, cross-platform binary file with a stable, well-documented format.
  - No server, no installation, zero configuration.
- **Portable and versionable:** You can commit your SQLite database file to Git (if small) or DVC.
- **Perfect for reproducible pipelines:** Bundling a SQLite DB with your code ensures your analysis runs on a known, consistent dataset.

> **Use Case:** Your go-to for creating a small, structured, and reproducible relational dataset that you control.

DuckDB: The Analytical Powerhouse

- **Analytical Database (OLAP):** Designed for fast, complex queries, not transactional updates.
- **Query Parquet/CSV directly:** Can run SQL on files without importing them into a database.
- **Vectorized and fast:** Extremely high performance for analytical queries.
- **In-process:** Runs inside your Python application, like SQLite.

> **Use Case:** Running fast SQL on large local Parquet or CSV files without the overhead of a traditional database.

SQLite vs. DuckDB: A Quick Comparison

Engine	Best For	Key Feature
SQLite	Structured, versioned relational data	A portable, self-contained database file
DuckDB	Fast SQL on Parquet / large files	Querying files directly without import

> They are complementary. Use **SQLite** to manage a curated, relational dataset. Use **DuckDB** for ad-hoc, high-performance analysis of raw data files.

A Note on NoSQL Databases

▒ When Would You Use Something Else?

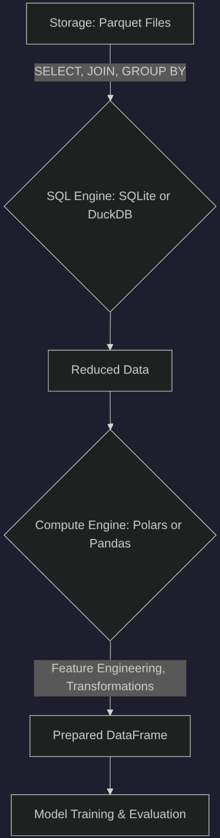
Relational databases are not the only model. Other types exist for different use cases.

Type	Example	Best For
Document	MongoDB	Semi-structured JSON-like data (e.g., web app user profiles).
Key-Value	Redis	Fast caching, session storage, real-time counters.
Graph	Neo4j	Network analysis, social graphs, recommendation engines.

> For most scientific modeling, data is **structured and relational**, making SQL databases the natural choice.

Integration: SQL + Python DataFrames

The Modern Data Pipeline


Storage: Parquet Files
SELECT, JOIN, GROUP BY
SQL Engine: SQLite or DuckDB
Reduced Data
Compute Engine: Polars or Pandas
Feature Engineering, Transformations
Prepared DataFrame
Model Training & Evaluation

Connecting to SQLite in Python

▒▒▒ The sqlite3 Module

Python's built-in `sqlite3` module provides a simple, direct interface for working with SQLite databases.

- `sqlite3.connect(path)`: Opens a connection to a database file. It will create the file if it doesn't exist.
- **Connection Object**: Represents the database session. You use it to execute commands.
- **Cursor Object**: A lower-level object for executing queries and fetching results one by one. For our purposes, `pandas` and other libraries handle the cursor for us.

For managing connections, using a `with` statement (as shown in the demo's `db.py`) is the modern best practice, as it ensures the connection is automatically closed even if errors occur.

SQL to Pandas

▒▒▒▒ The Classic Integration

`pd.read_sql` executes a SQL query and loads the results directly into a Pandas DataFrame.

```python
import pandas as pd
import sqlite3

# Assumes a SQLite connection `conn`
conn = sqlite3.connect("data/covid.sqlite")

query = """
SELECT
    r.date,
    r.region,
    r.subregion,
    r.cases,
    p.population
FROM covid AS r
JOIN population AS p
  ON r.region = p.region AND r.subregion = p.subregion
WHERE r.date >= :start_date;
"""

df = pd.read_sql(query, conn, params={"start_date": "2021-01-01"})
```

> Using parameters (`params=...`) is a critical best practice to prevent **SQL injection**, a major security vulnerability.

A Note on Security: SQL Injection

▒▒▒ Why You Should NEVER Use F-Strings for Queries

The Wrong Way (Vulnerable):

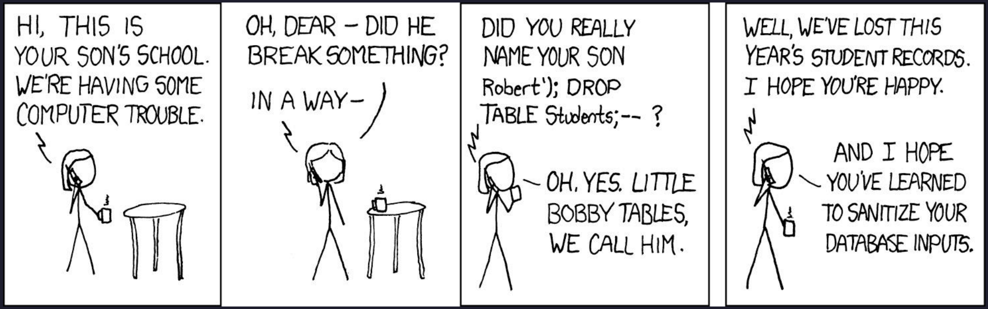
```
# User input could be malicious
user_input = "2021-01-01'; DROP TABLE population; --"

# Using an f-string injects the malicious code directly into the query
query = f"SELECT * FROM covid WHERE date >= '{user_input}';"
conn.executescript(query) # This would delete your table!
```

The Right Way (Safe):

```
# The database driver safely handles the parameter
query = "SELECT * FROM covid WHERE date >= :start_date;"
df = pd.read_sql(query, conn, params={"start_date": user_input})
```

> Parameterization separates the query's logic from the data. The database driver sanitizes the input, preventing it from being executed as code.

xkcd tried to warn you!


HI, THIS IS YOUR SON'S SCHOOL. WE'RE HAVING SOME COMPUTER TROUBLE.
OH, DEAR – DID HE BREAK SOMETHING?
IN A WAY–
DID YOU REALLY NAME YOUR SON Robert'); DROP TABLE Students;-- ?
OH. YES. LITTLE BOBBY TABLES, WE CALL HIM.
WELL, WE'VE LOST THIS YEAR'S STUDENT RECORDS. I HOPE YOU'RE HAPPY.
AND I HOPE YOU'VE LEARNED TO SANITIZE YOUR DATABASE INPUTS.

SQL to Polars

▒ High-Performance Integration

A robust way to integrate Polars is by converting from a Pandas DataFrame. This is the approach used in our demo to ensure a fair compute comparison with minimal dependencies.

```python
import pandas as pd
import polars as pl
import sqlite3

# Assumes a SQLite connection `conn` and a `query` string
df_pd = pd.read_sql(query, conn)

# Efficiently convert from Pandas to Polars
df_pl = pl.from_pandas(df_pd)
```

For the highest performance, DuckDB can query Parquet files and return a Polars DataFrame with zero-copy data transfer.

```python
import duckdb
import polars as pl

# DuckDB returns a Polars DataFrame directly
df_pl = duckdb.query("SELECT * FROM 'data/*.parquet'").pl()
```

Reproducibility: Beyond Code and Environments

▒▒▒ Pinning Data and Queries for Trustworthy Science

- **From Lecture 3:** We learned to pin **environments** (Python versions, packages) for reproducible code execution.
  - venv, uv, conda, Docker ensure consistent code behavior.
- **But reproducibility extends to data:**
  - Same inputs must always yield same outputs.
  - This requires pinning **data + queries**.
- **The Immutable Data Principle:** Never overwrite raw data.
  - Treat raw data as an unchangeable artifact.

Data Versioning Strategies

▒▒ Tracking Changes in Your Most Valuable Asset

- **Why version data?**
    - Ensures **same input → same output**, even months later.
    - Provides an audit trail for data transformations.
- **Strategies for different scales:**
    - **Git for small data:** Simple, but quickly becomes unwieldy for large files.
    - **DVC / lakeFS for large data:** Specialized tools for versioning large datasets and models.
    - **Parquet + hash digest:** Storing data in Parquet with a cryptographic hash of its contents provides a strong guarantee of immutability.

Reproducibility & Testing (1/4): Version Your Queries

▒ Treat SQL as Code

- Your SQL queries are a critical part of your analysis logic. They should be treated like any other source code.
- Store your queries in dedicated `.sql` files and commit them to version control (`git`).
- Load them into your Python code rather than embedding them as multi-line strings.

```python
# db_utils.py
from pathlib import Path

def load_query(name: str) -> str:
    query_path = Path("queries") / f"{name}.sql"
    return query_path.read_text()

# analysis.py
from db_utils import load_query
query = load_query("get_covid_data")
```

> **Anti-Pattern:** Hiding complex SQL inside scattered notebook cells or Python scripts.

Reproducibility & Testing (2/4): Separate Concerns

▒▒▒▒ Create a Data Access Layer

- Isolate all your database interaction logic into a dedicated module (e.g., `db.py` or `data_access.py`).
- This module should be responsible for:
    - Managing database connections.
    - Loading queries from `.sql` files.
    - Executing queries and returning data (e.g., as a DataFrame).
- Your main analysis code should call functions from this layer, without knowing the details of the database connection or SQL.

> This separation makes your code cleaner, easier to maintain, and vastly easier to test.

Reproducibility & Testing (3/4): Unit Testing with Mocks

▒ Isolate Your Logic from the Database

- Your unit tests for analysis functions should **never** touch a real database. (Revisiting Lec 6)
- Use **mocking** to replace the data access layer with a fake object that returns a pre-defined DataFrame.
- This makes your tests fast, reliable, and independent of any external database file.

```python
# test_analysis.py
def test_feature_engineering(mocker):
    # Create fake data that the mock will return
    fake_df = pd.DataFrame(...)
    # Patch the function in the data access layer
    mocker.patch("db_utils.load_data", return_value=fake_df)

    # Run the analysis function, which now receives the fake data
    result = create_features()
    assert "new_feature" in result.columns
```

Reproducibility & Testing (4/4): Integration Testing

▒▒▒ Verifying the Full Pipeline

- While unit tests isolate components, **integration tests** verify that they work together.
- For a data pipeline, an integration test can verify the full SQL-to-DataFrame workflow.
- Use a temporary, **in-memory SQLite database** for these tests.
  - Create a fresh database for each test run.
  - Populate it with a small, known set of test data.
  - Run your real query against it and check the result.

```python
# test_integration.py
def test_sql_to_dataframe_pipeline():
    # Create an in-memory SQLite DB
    conn = sqlite3.connect(":memory:")
    # ... create tables and insert test data ...

    # Run the real query against the temporary DB
    df = pd.read_sql(load_query("get_covid_data"), conn)
    assert len(df) == 5 # Check against known test data
```

> For cleaner and more reusable test setup, this database creation logic is perfectly suited for a `pytest` fixture.

Code Examples: Putting It All Together

Scenario: Analyzing COVID Data

▒ Comparing Pandas and Polars for a Realistic Task

- **The Data:** We have two tables in a SQLite database:
  - `covid`: Daily case counts by `(region, subregion)`.
  - `population`: Population data for each `(region, subregion)`.
- **The Goal:** Compute a 7-row rolling average of per-capita case rates.
- **The Task:**

1. Use SQL to `JOIN` the two tables.
2. Load the result into Pandas and Polars.
3. Perform the rolling average calculation in each library.
4. Compare the performance (time and memory).

> This example code mirrors a common scientific data preparation workflow: joining disparate datasets and engineering a time-series feature.

From SQL to Features with Pandas and Polars

1. **Query SQLite:** Run a parameterized SQL JOIN on `(region, subregion)` to combine COVID cases and population data.
2. **Load into Pandas:** Use `pd.read_sql` to load the query result.
3. **Load into Polars:** Convert the Pandas DataFrame to a Polars DataFrame to ensure an identical starting point for a fair comparison.
4. **Compute Rolling Feature:** In both libraries, compute a 7-row rolling per-capita case rate.
5. **Compare Performance:** Measure and compare the wall time and memory usage for the feature engineering step.

> **Goal:** Demonstrate the full, reproducible pipeline and highlight the performance characteristics of modern tools.

Key Takeaways

▒▒▒ Designing for Scale and Reproducibility

- **Parquet > CSV:** Use columnar formats for efficient, typed, and reproducible data storage.
- **SQL first, DataFrame second:** Reduce your data with SQL *before* loading it into Python for computation.
- **Pandas vs. Polars vs. Dask = Scale Choices:**
  - Start with **Pandas** for familiarity.
  - Move to **Polars** for performance on a single machine.
  - Use **Dask** for problems that exceed a single machine's memory.
- **Reproducibility is a design decision:** Version your data, your queries, and your code.

Thank you!