COMP5310: Principles of Data Science

W4: Data Transformation and Storage with Python and SQL

Presented by

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Based on slides by previous lecturers of this unit of study

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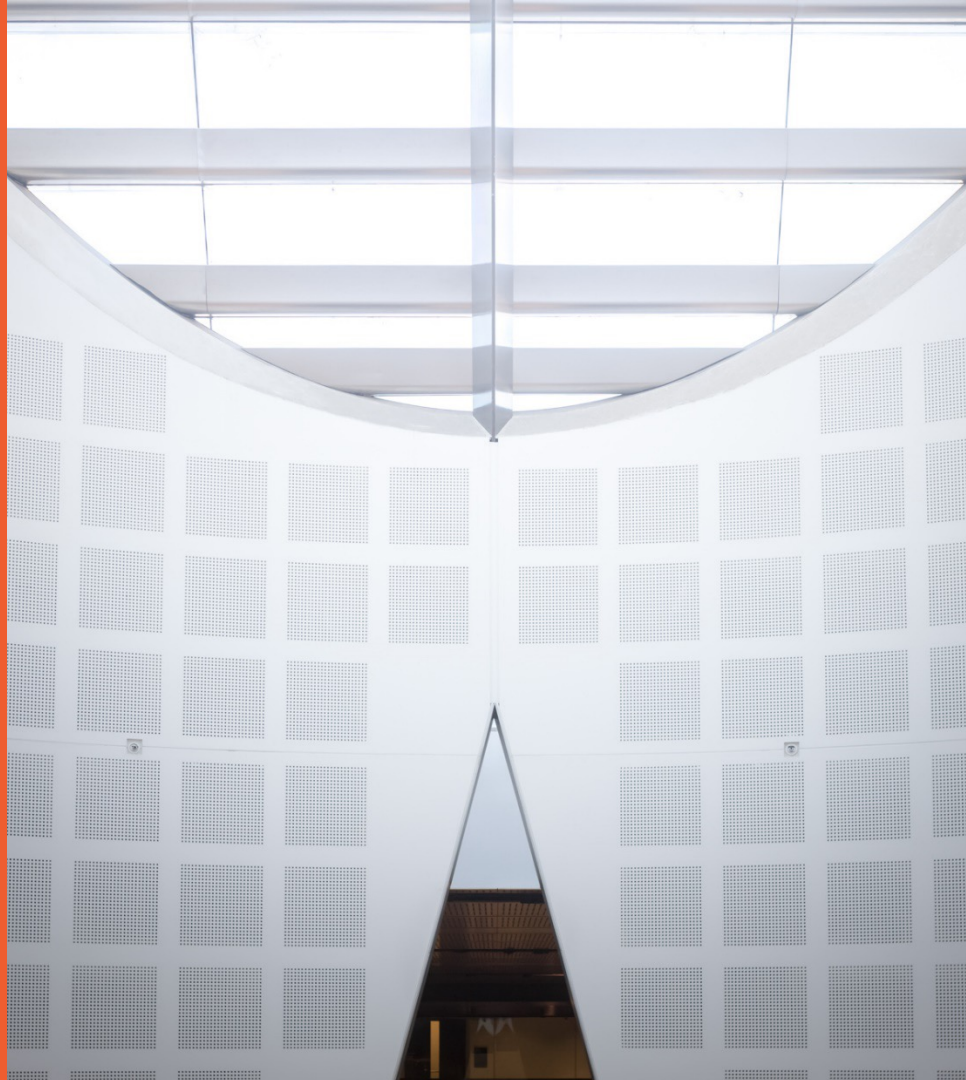


Last week: Data Exploration with Python

Objective

- Learn Python tools for exploring a new data set programmatically.

Lecture

- Pandas
- Descriptive statistics, e.g., median, quartiles, IQR, outliers.
- Descriptive visualisation, e.g., boxplots.

Readings

- Data Science from Scratch: Ch 5

Exercises

- matplotlib: Visualisation.
- pandas: Descriptive stats.

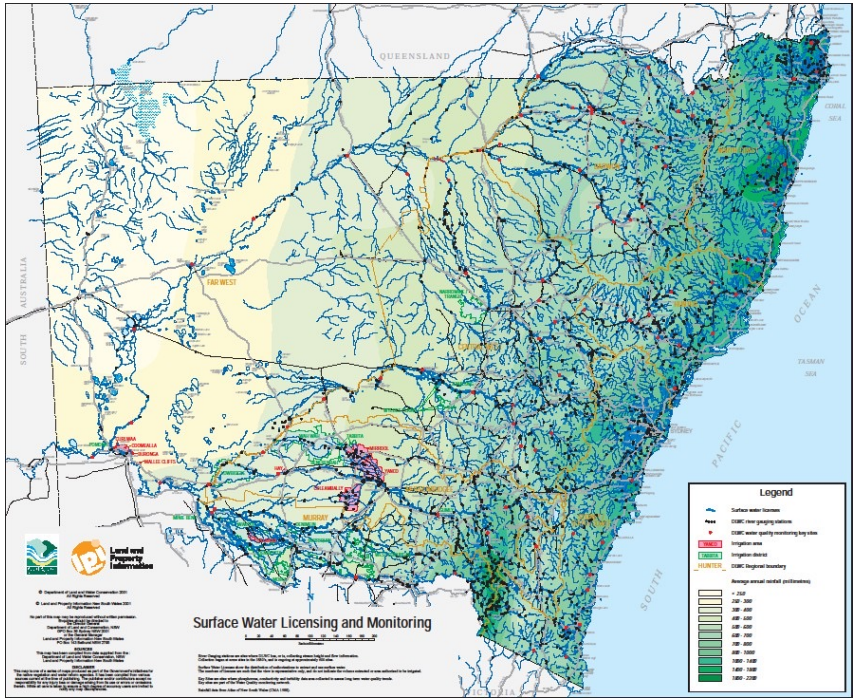
TO-DO in W3

- Ed Lessons Python modules 7-9.
- Ed Lessons SQL modules 18-19.
- Load project data with Python. Clean and prepare data

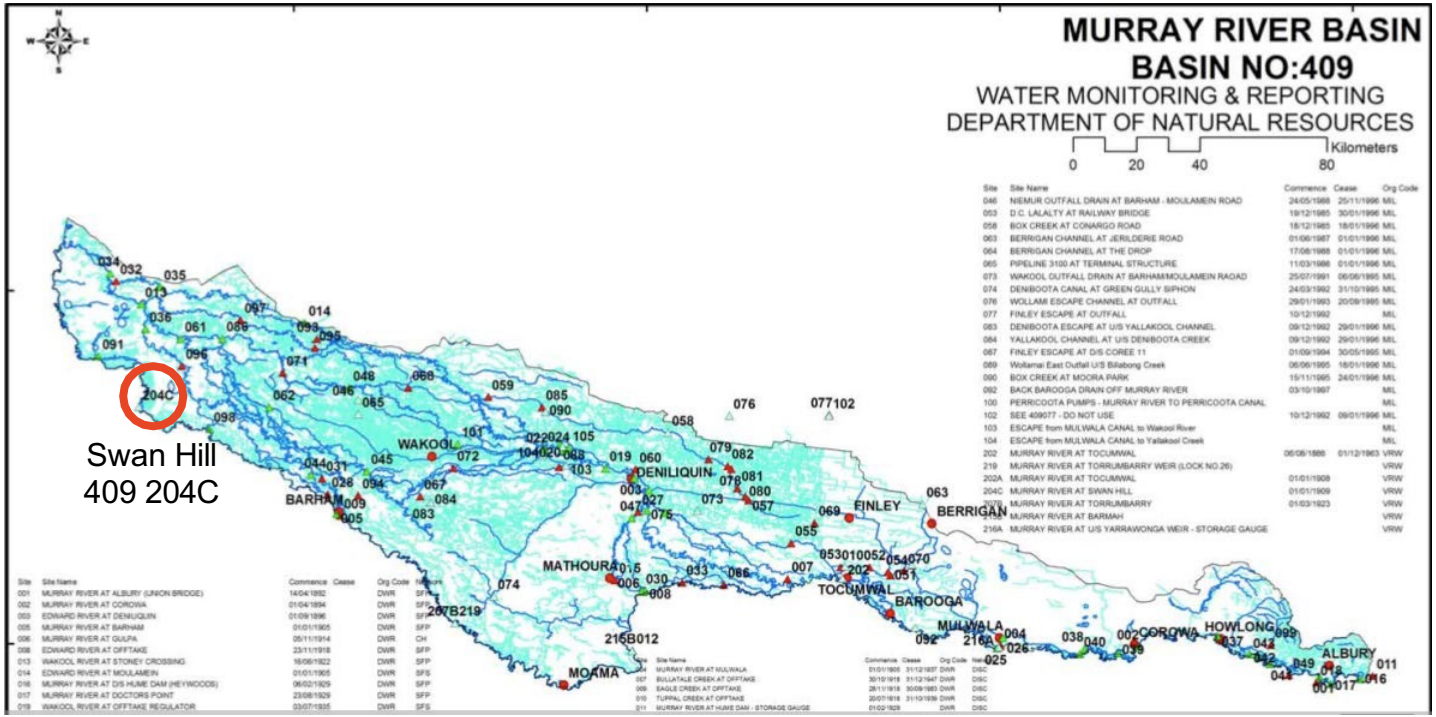
NEW SCENARIO

New data set

- Water measurements:
  - Automatic monitoring stations that are distributed over a large area.
  - Periodically send their measured values to a central authority.
  - Time-series data of:
    - Water level.
    - Water flow.
    - Water temperature.
    - Salinity (via measuring electric conductivity) or other hydraulic properties.



Example: Murray river basin in NSW



[Source: www.waterinfo.nsw.gov.au]

Where do we get data from?

- You or your organization might have it already, or a colleagues provides you access to data.
  - Typical exchange formats: CSV, Excel, XML/JSON.
- Download from an online data server
  - Still typically in CSV or Excel, etc., but now problems with meta-data.
- Scrap the web yourself or use APIs of resources.
- Cf. Data Science from Scratch, chapter 9.

- Our data set comes from a colleague in Excel format.

Water dataset

- Contains four CSV data files:
  - Measurements.csv
  - Organisations.csv
  - Sensors.csv
  - Stations.csv

- Let's have a look.

RELATIONAL DATABASES

Relational databases

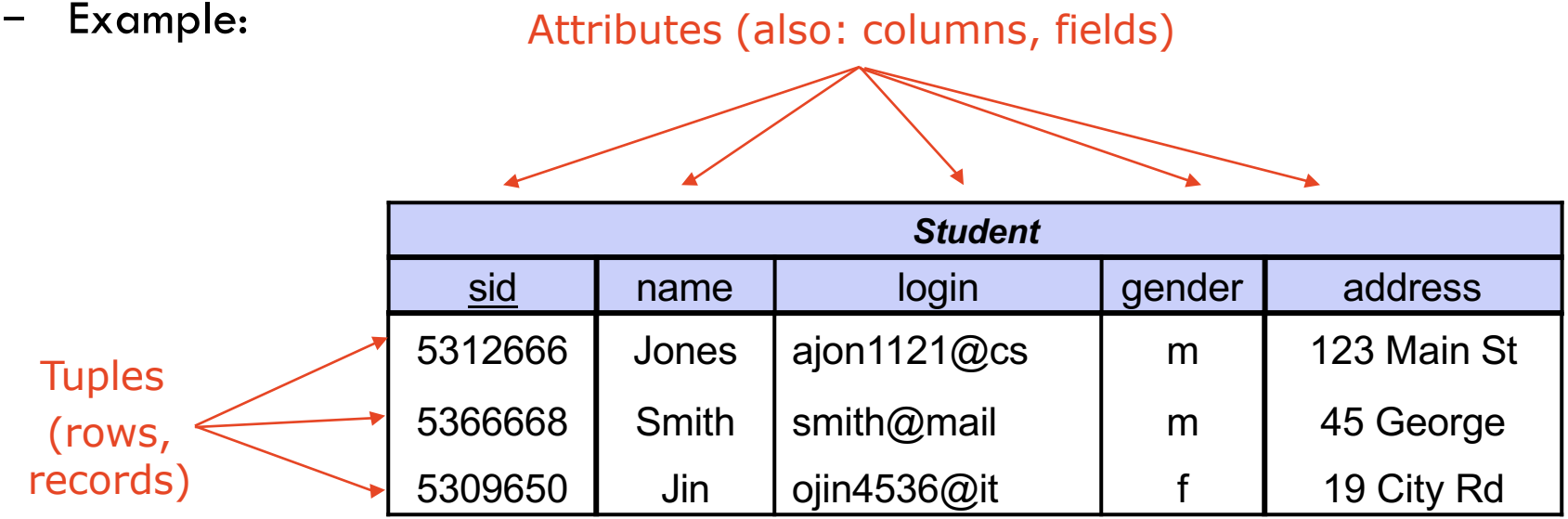
- Today's goal is to store the data in a relational database.

- The relational data model is the most widely used model today.
  - In the **relational model,** a database is a collection of one or more **relations.**
  - Each relation is a table with rows and columns.
  - Each relation has a schema, which describes the columns, or fields.

- This sounds like a spreadsheet, but as we will see, it has some differences.

Definition of relation

- Informal definition:
  - A relation is a named, two-dimensional table of data
- Table consists of rows (record) and columns (attribute or field)
- Example:



Student

sid	name	login	gender	address
5312666	Jones	ajon1121@cs	m	123 Main St
5366668	Smith	smith@mail	m	45 George
5309650	Jin	ojin4536@it	f	19 City Rd

Relation Schema vs Relation Instance

- Formally, a relation R consists of a relation schema and a relation instance
- A **relation schema** specifies name of relation, and name and data type (domain) of each attribute.
  - $R = (A_1, A_2, \ldots, A_n)$ is a ***relation schema***
    - $A_1, A_2, \ldots, A_n$ are ***attributes***, *each having a* ***data type***
  - e.g. `Student(sid: string, name: string, login: string, addr: string, gender: char)`
- A **relation instance** is a **set** of tuples (*a table*) for a schema
  - Each tuple has the same number of fields as attributes defined in schema
  - Values of a field in a tuple must conform to the data type defined in schema
  - Relation instance often abbreviated as just relation

Some remarks

- Not all tables qualify as a relation:
  - Every relation must have a unique name.
  - Attributes (columns) in tables must have unique names.
    - The order of the columns is irrelevant.
  - All tuples in a relation have the same structure
    - Constructed from the same set of attributes.
  - Every attribute value is atomic (not multivalued, not composite).
  - Every row is unique.
    - Can't have two rows with exactly the same values for all their fields.
  - The order of the rows is immaterial.
- RDBMS **table** extends mathematical **relation**
  - RDBMS allows duplicate rows, supports an order of tuples or attributes, and allows null 'values' for unknown information

DB CREATION

SQL – The Structured Query Language

- SQL is the standard declarative language for interacting with RDBMS.
- Supported commands from roughly two categories:
  - **DDL** (Data Definition Language).
    - Create, drop, or alter the relation schema.
    - Example: `CREATE TABLE name (list_of_columns)`
  - **DML** (Data Manipulation Language).
    - For retrieval of information also called query language.
    - `INSERT`, `DELETE`, `UPDATE`
    - `SELECT` … `FROM` … `WHERE`

Creating Tables in SQL

- Creation of tables/relations:

```
CREATE TABLE name ( list-of-columns );
```

  - Example: Create the Student table.

```
CREATE TABLE Student (sid INTEGER,
                      name VARCHAR(20),
                     login VARCHAR(20),
                    gender CHAR,
                   address VARCHAR(50) );
```

  - This actually specifies the schema information
  - Note that the type of each field is specified, and enforced by the DBMS whenever tuples are added or modified.

SQL DML Statements

- Insertion of new data into a table/relation.
  - Syntax:
```
INSERT INTO table (list-of-columns)
VALUES (list-of-expression)
```
  - Example:
```
INSERT INTO Students (sid, name)
VALUES (53688, "Smith")
```
- Updating of tuples in a table/relation.
  - Syntax:
```
UPDATE table
SET column = expression
WHERE search_condition
```
  - Example:
```
UPDATE students
SET gpa = gpa - 0.1
WHERE gpa >= 3.3
```
- Deleting of tuples from a table/relation
  - Syntax: `DELETE FROM table WHERE search_condition`
  - Example: `DELETE FROM students WHERE name = "Smith"`

Integrity constraints

- When creating a table, we can specify *integrity constraints* for columns.
  - A variety of rules to maintain the integrity of data when it is manipulated
  - The rule must be satisfied for *any* instance of the database; e.g., *domain constraints.*
- Integrity constraints are declared in the schema
  - They are specified when the schema is defined.
  - Declared integrity constraints are checked when relations are modified.
- A *legal* instance of a relation is one that satisfies all specified integrity constraints.
  - If integrity constraints are declared, DBMS will not allow illegal instances.
  - Stored data is more faithful to real-world meaning.
  - Avoids data entry errors, too!

Domain constraints

- *Domain constraints* restrict attributes to valid domains.
  - **NULL/NOT NULL:** whether an attribute is allowed to become NULL (unknown).
  - **DEFAULT:** to specify a default value.
  - **CHECK(condition):** a Boolean condition that must hold for every tuple in the DB instance.
- Example:

```
CREATE TABLE Student
 (
   sid            INTEGER          PRIMARY KEY,
   name           VARCHAR(20)      NOT NULL,
   gender         CHAR             CHECK (gender IN ('M','F','T')),
   birthday       DATE             NULL,
   country        VARCHAR(20),
   level          INTEGER          DEFAULT 1 CHECK (level BETWEEN 1 and 5)
 );
```

level ≥ 1 and level ≤ 5

1 ≤ level ≤ 5

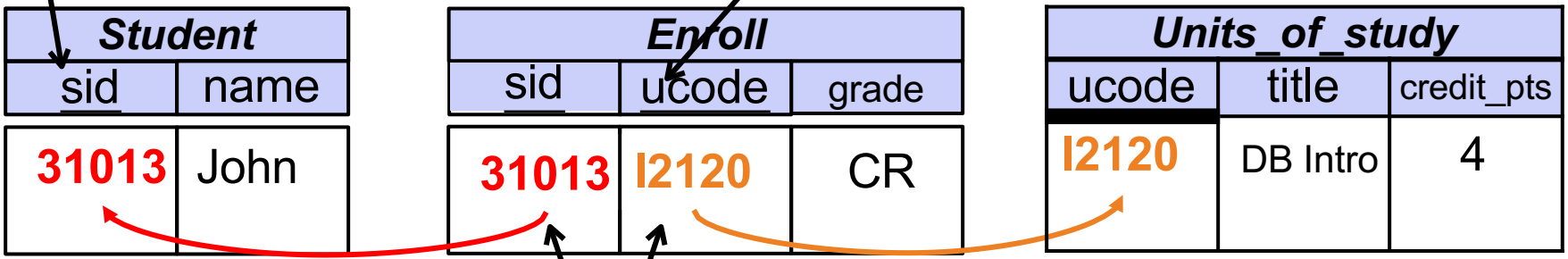
Relational keys

- **Key:** **unique, minimal** identifier of a relation.
  - Examples include employee numbers, social security numbers, etc. This is how we can guarantee that all rows are unique.
  - Keys can be **simple** (single attribute) or **composite** (multiple attributes).
- If there's at least one key for a relation, we call each of them a ***candidate key***, and one of the keys is chosen (by DBA) to be the ***primary key (PK)***
  - If we just say **key**, we typically mean ***candidate key***
- **Foreign keys:** identifiers that enable a **dependent relation** to refer to its **parent relation**
  - Must refer to a candidate key of the parent relation.
  - Like a "logical pointer".

Example: Relational keys

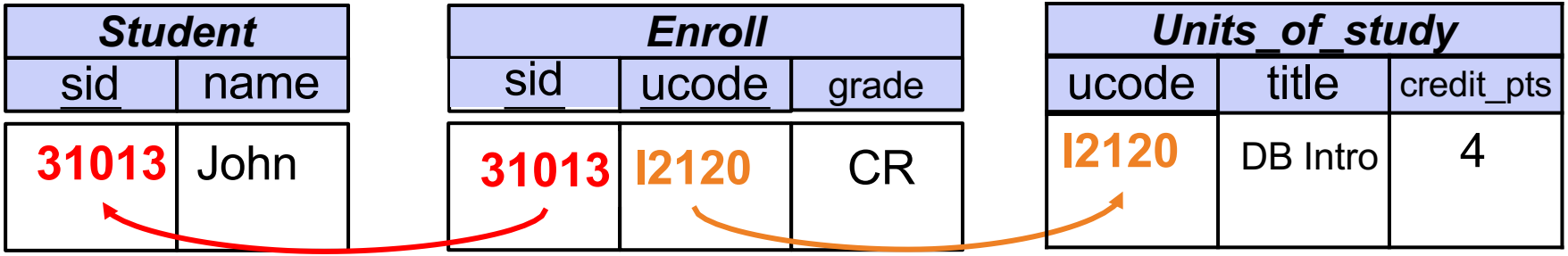
Primary key identifies each tuple of a relation.

Composite Primary Key consisting of more than one attribute.



Foreign key is a (set of) attribute(s) in one relation that "refers" to a tuple in another relation (like a "logical pointer").

Quiz: candidate key



For the student table:

Can sid be a candidate key? Y

Can sid, name be a candidate key? N

For the Enroll table:

Can sid be a candidate key? N

Can sid, ucode be a candidate key? Y

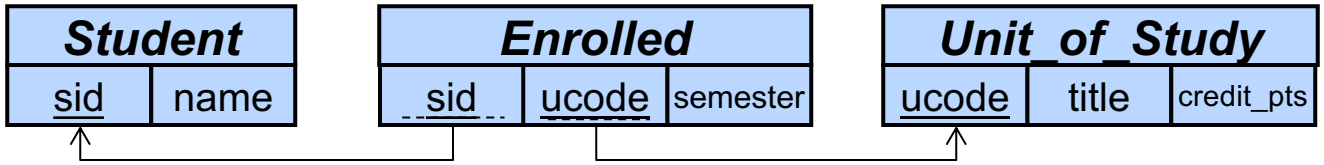
Can sid, ucode, semester be a candidate key? N

~~semester~~ grade

Key & Foreign Key in SQL

- Primary keys and foreign keys can be specified as part of the SQL **CREATE TABLE** statement:
  - The **PRIMARY KEY** clause lists attributes that comprise the primary key.
  - The **UNIQUE** clause lists attributes that comprise a candidate key.
  - The **FOREIGN KEY** clause lists the attributes that comprise the foreign key and the name of the relation referenced by the foreign key.
- Note that, SQL does not require every table to have a key
- By default, foreign key references the primary key of the referenced table
  - **FOREIGN KEY** (sid) **REFERENCES** Student
- Reference columns in the referenced table can be explicitly specified
  - but must be declared as primary or candidate keys
  - **FOREIGN KEY** (lecturer) **REFERENCES** Lecturer(empid)
- Tip: Name them using **CONSTRAINT** clauses
  - **CONSTRAINT** Student_PK **PRIMARY KEY** (sid)

Example: Primary & Foreign Keys




```
CREATE TABLE Student ( sid INTEGER, … ,
    CONSTRAINT Student_PK PRIMARY KEY (sid)
);
CREATE TABLE UoS  ( ucode CHAR(8), … ,
    CONSTRAINT UoS_PK PRIMARY KEY (ucode)
);
CREATE TABLE Enrolled ( sid INTEGER, ucode CHAR(8), semester VARCHAR,
    CONSTRAINT Enrolled_FK1 FOREIGN KEY (sid) REFERENCES Student,
    CONSTRAINT Enrolled_FK2 FOREIGN KEY (ucode) REFERENCES UoS,
    CONSTRAINT Enrolled_PK  PRIMARY KEY (sid,ucode)
);
```

Key constraint

- **Key Constraint:**
  No two distinct tuples can have the same values in all key attributes
- Careful: If used carelessly, this can prevent the storage of database instances that arise in practice!
- Example:

```
CREATE TABLE Enrolled  (
  sid    INTEGER,
  cid    CHAR(8),
  grade CHAR(2),
  PRIMARY KEY (sid,cid) );
```

"For a given student and course, there is a single grade."

```
CREATE TABLE Enrolled  (
  sid    INTEGER,
  cid    CHAR(8),
  grade CHAR(2),
  PRIMARY KEY (sid)
  UNIQUE (cid, grade) );
```

"Students can take only one course and receive a single grade for that course; further, no two students in a course receive the same grade."

Foreign key constraint

- **Foreign Key Constraint (Referential Integrity):**
  For each tuple in the referring relation whose foreign key value is α, there must be a tuple in the referred relation with a candidate key that also has value α
  - e.g. Enrolled(*sid*: integer, ucode: string, semester: string)
    sid is a foreign key referring to Student:

sid	ucode	semester
1234	COMP5138	2012S1
3456	COMP5138	2012S1
5678	COMP5138	2012S2
5678	COMP5338	2013S1

Q: What can we say about the Student relation?

Keys and NULLs

- PRIMARY KEY
  - Up to one per table, and must be unique
  - Automatically disallow NULL values

- UNIQUE (candidate key)
  - Possibly many *candidate keys* (specified using UNIQUE)

- FOREIGN KEY
  - By default, allows NULL values
  - If there must be a parent tuple, then must combine with NOT NULL constraint

DATABASE LOADING WITH PYTHON

Accessing PostgreSQL from Python: psycopg2

- First, we need to import the psycopg2 module, then connect to Postgresql.
- ***Note:*** You obviously need to provide your own login name.

```
import psycopg2

def pgconnect():
    # please replace with your own details
    YOUR_DBNAME = ' '
    YOUR_USERNAME = ' '
    YOUR_PW     = ' '
    try:
        conn = psycopg2.connect(host='localhost',
                                database=YOUR_DBNAME,
                                user=YOUR_USERNAME,
                                password=YOUR_PW)
        print('connected')
    except Exception as e:
        print("unable to connect to the database")
        print(e)
    return conn
```

Accessing PostgreSQL from Python: psycopg2

- How to execute an SQL statement on an open connection “conn”.
  - We prepared a helper function which encapsulates all the error handling:

```
def pgexec( conn, sqlcmd, args, msg ):
    """ utility function to execute some SQL statement
        can take optional arguments to fill in (dictionary)
        error and transaction handling built-in """
    retval = False
    with conn:
        with conn.cursor() as cur:
            try:
                if args is None:
                    cur.execute(sqlcmd)
                else:
                    cur.execute(sqlcmd, args)
                print("success: " + msg)
                retval = True
            except Exception as e:
                print("db error: ")
                print(e)
    return retval
```

Exercise: Data loading with Python

- In Jupyter notebook.
  - Load CSV data into Python.
  - Helper functions for connecting and querying postgresql.
    - Important: Edit your login details in the pgconnect() function.
  - Check content of Organisation table.
- **Your task:** Doing the same for the “Measurements” and “Stations” data.
  - Table creation & data loading in Python.
- Any other observations?

Technical data cleaning issues

- Interpretation of data format and meta-data.
- Differences in naming conventions.
  - Excel headers with spaces and quotes, which both are not allowed in DBMS.
- Inconsistent or missing data entries.
- “Shape” of data.

Accessing PostgreSQL from Python: psycopg2

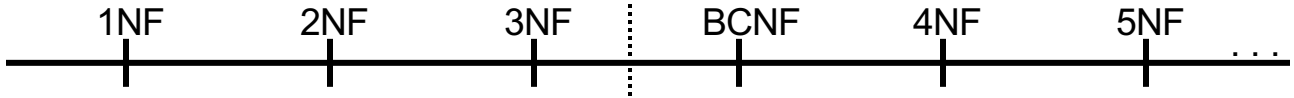
- Example: Creating a table and loading some data.

```
data_organisations = list(csv.DictReader(open('water_data/Organisations.csv')))
# 1st: login to database
conn = pgconnect()

# 2nd: ensure that the schema is in place
organisation_schema = """CREATE TABLE IF NOT EXISTS Organisation (
                         code VARCHAR(20) PRIMARY KEY,
                         orgName    VARCHAR(150)
                       )"""
pgexec (conn, organisation_schema, None, "Create Table Organisation")

# 3nd: load data
# IMPORTANT: make sure the header line of CSV is without spaces!
insert_stmt = """INSERT INTO Organisation(code,orgName)
                       VALUES (%(Code)s, %(Organisation)s)"""
for row in data_organisations:
    pgexec (conn, insert_stmt, row, "row inserted")
```

DATA MODELING

Relational database theory

- ***Redundant*** data may cause anomalies when manipulating data
- Relational database theory identifies several normal forms
  - Each normal form is characterized by a set of restrictions
  - A relation needs to be decomposed if it does not satisfy the restrictions



Student

sid	name
31013	John

Enroll

sid	ucode	grade
31013	I2120	CR

Units_of_study

ucode	title	credit_pts
I2120	DB Intro	4

Relational database theory issues

- The modelling process in relational database known as OLTP (Online Transactional Processing) focuses on normalization process which yields a flexible model.
  - Making it easy to maintain dynamic relationships between business entities.
- It is effective and efficient for operational databases – a lot of updates.
- However, a fully normalized data model can perform very inefficiently for queries.
- Historical data are usually large with static relationships:
  - Unnecessary joins may take unacceptably long time
- How to proceed with a database approach?
  - **OLAP: Online Analytical Processing (Data Warehousing Approach).**

What is a data warehouse?

- Subject-oriented.
  - Organized by subject, not by application.
  - Used for analysis, data mining, etc.
- Integrated.
  - Constructed by integrating multiple, heterogeneous data sources.
    - Relational databases, flat files, on-line transaction record.
- Time variant.
  - Large volume of historical data (Gb, Tb).
  - Time attributes are important.
- Non-volatile.
  - Updates infrequent or does not occur.
  - May be append-only.

Conceptual modeling of data warehouses

- Modeling data warehouses: dimensions & measures instead of relational model.
- Data warehouse contains a **large** central table (**fact table**).
  - Contains the data without redundancy.
- A set of **dimension tables**.

Data warehouses: Fact Tables

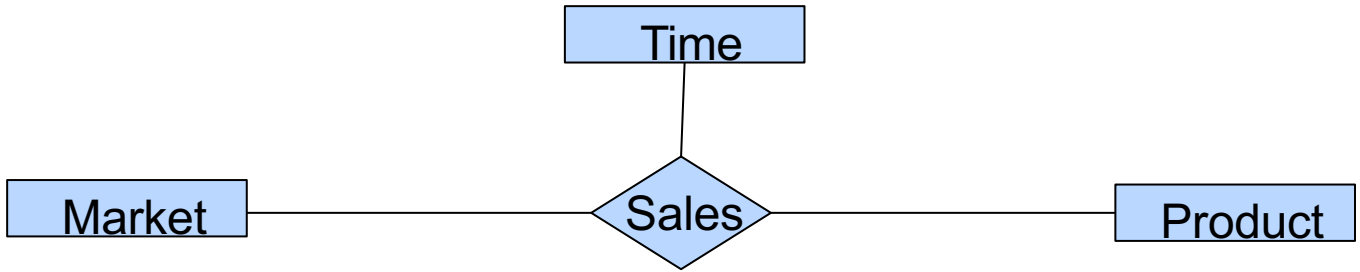
- Relational "data warehouse" applications are centered around a fact table.
  - For example, a supermarket application might be based on a table Sales (market_id, product_id, time_id, sales_amt).

market_id	product_id	time_id	sales_amt
M1	P1	T1	3000
M1	P2	T1	1000
M1	P3	T1	500
M2	P1	T1	100
M2	P2	T1	1100
M2	P3	…	…
…	…		

- The table can be viewed as multidimensional.
  - Collection of numeric measures, which depend on a set of dimensions.
  - E.g., market_id, product_id, time_id are the dimensions that represent specific supermarkets, products, and time intervals.
  - Sales_amt is a function of the other three.

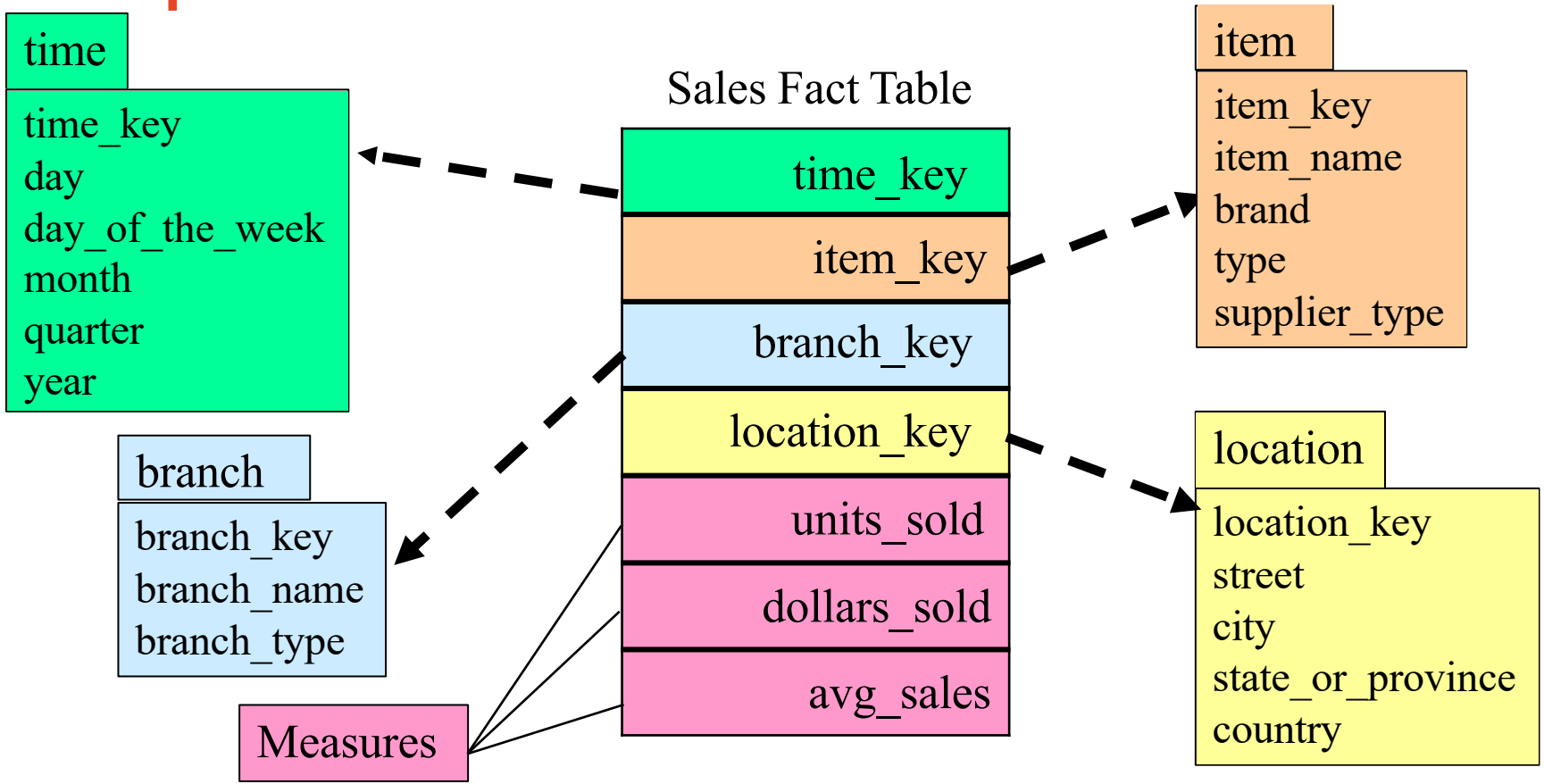
Data warehousing: Star schema

- The fact table and dimension tables linked to it look like a star.
  - This is called a **star schema**.
- Most common modelling paradigm.



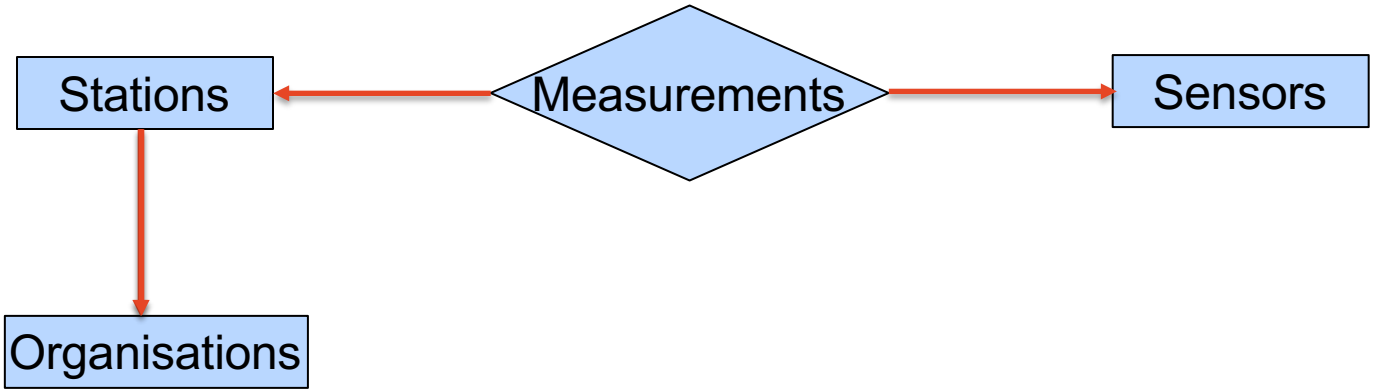
- If we map this to relations:
  - 1 central fact table.
  - n dimension tables with foreign key relationships from the fact table.
- The fact table holds the FKs referencing the dimension tables.

Example of star schema

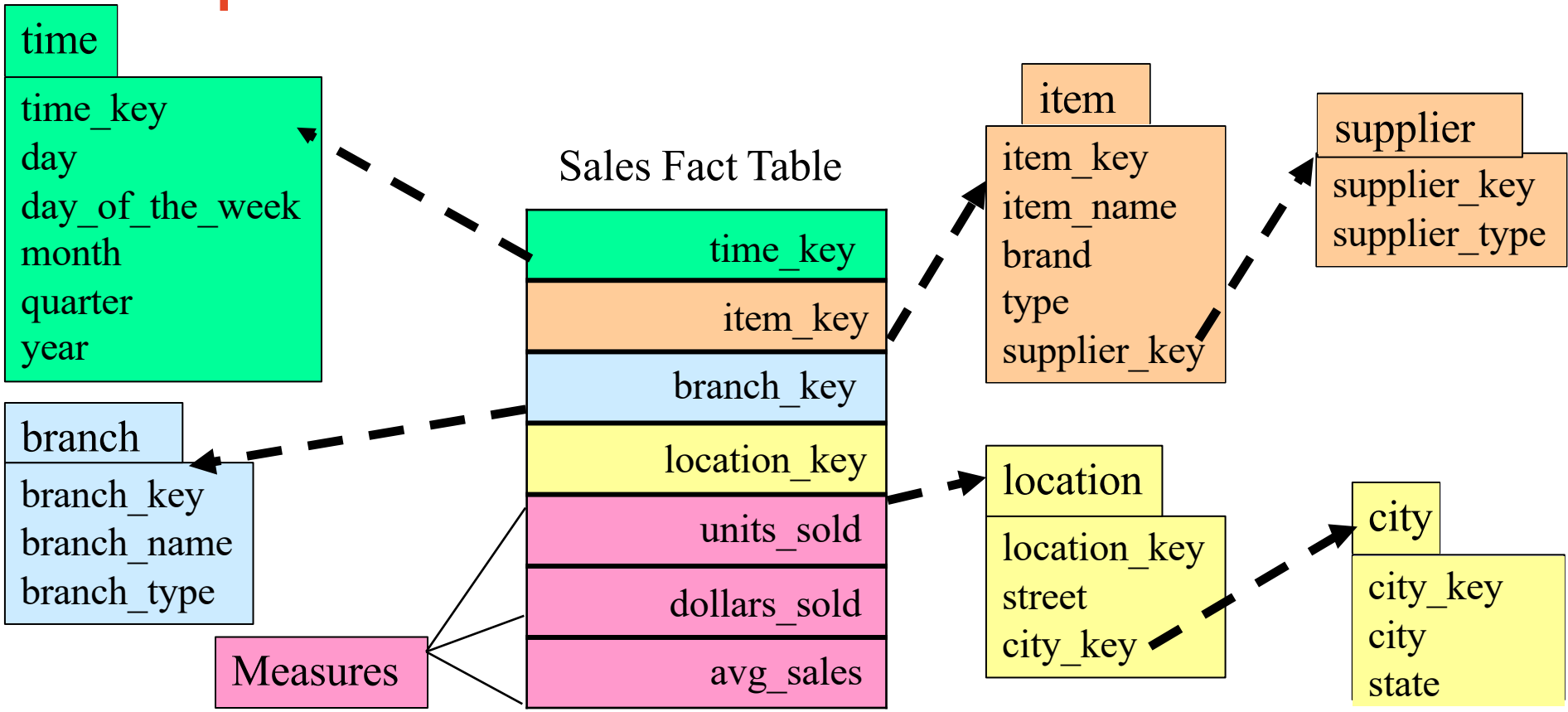


Data warehousing: Snowflake schema

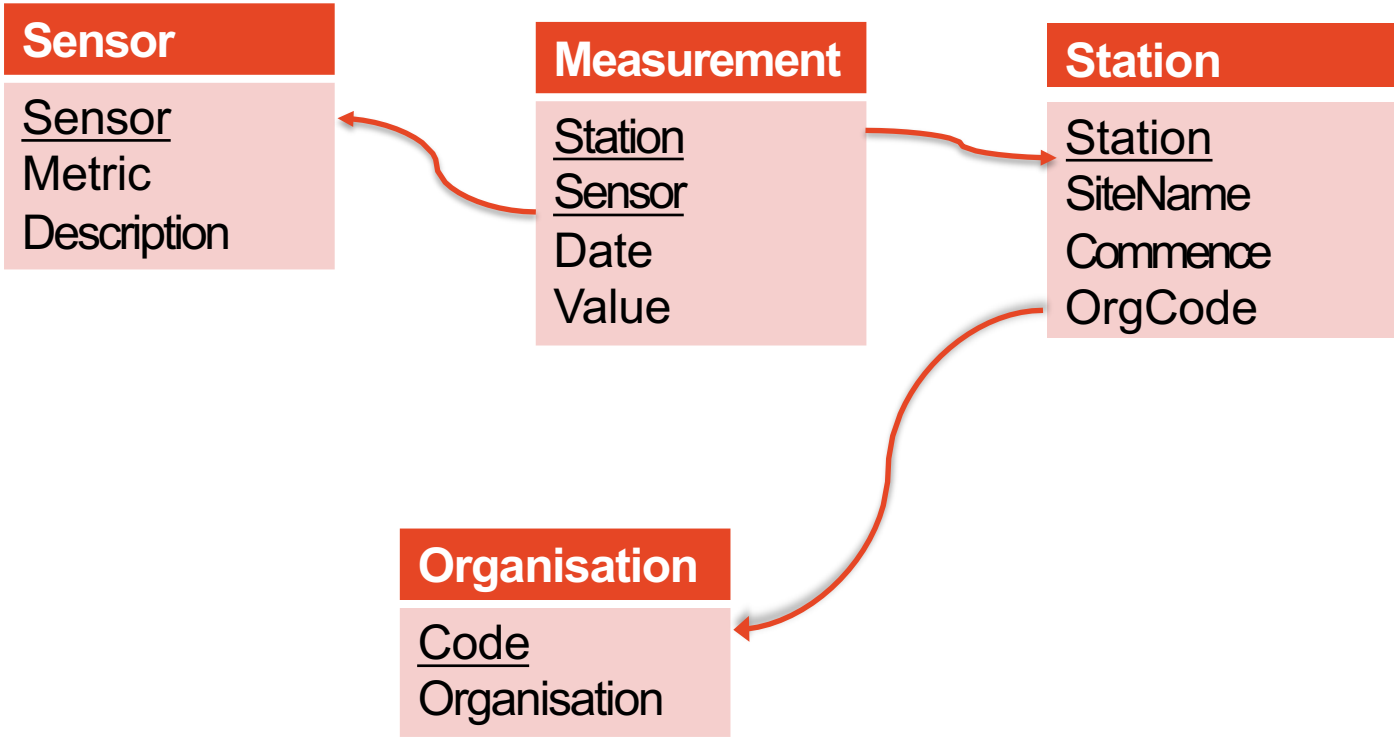
- A refinement of a star schema where some dimensional hierarchy is **normalized** into a set of smaller dimension tables, forming a shape similar to a snowflake.
- Measurements are the facts; the rest describes the dimensions.



Example of snowflake schema



Modeling our water data set



Questions to ask

- Useful to have a theoretical framework.
- **BUT**:
  - Do you need a relational database?
  - How much data do you have and what are you trying to do with it?
- Talk to your data engineers, database administrators.
- No-SQL options: document databases, key-value databases, wide-column stores, graph databases.

Review

W4 review: Data transformation and storage with Python and SQL

Objective

- Use Python and PostgreSQL to extract, clean, transform and store data.

Lecture

- DB Access from Python.
- Data cleaning and preprocessing.
- Data Modeling and DB Creation.
- Data Loading/Storage.

Readings

- Data Science from Scratch: Ch 24

Exercises

- Python/Jupyter to load data.
- Psycopg2.
- PostgreSQL to store data.

TO-DO in W4

- Ed Lessons Python modules 10-12.
- Ed Lessons SQL modules 20-21.