COMP5310: Principles of Data Science

W4: Data Extract, Data Transformation and Storage

Presented by

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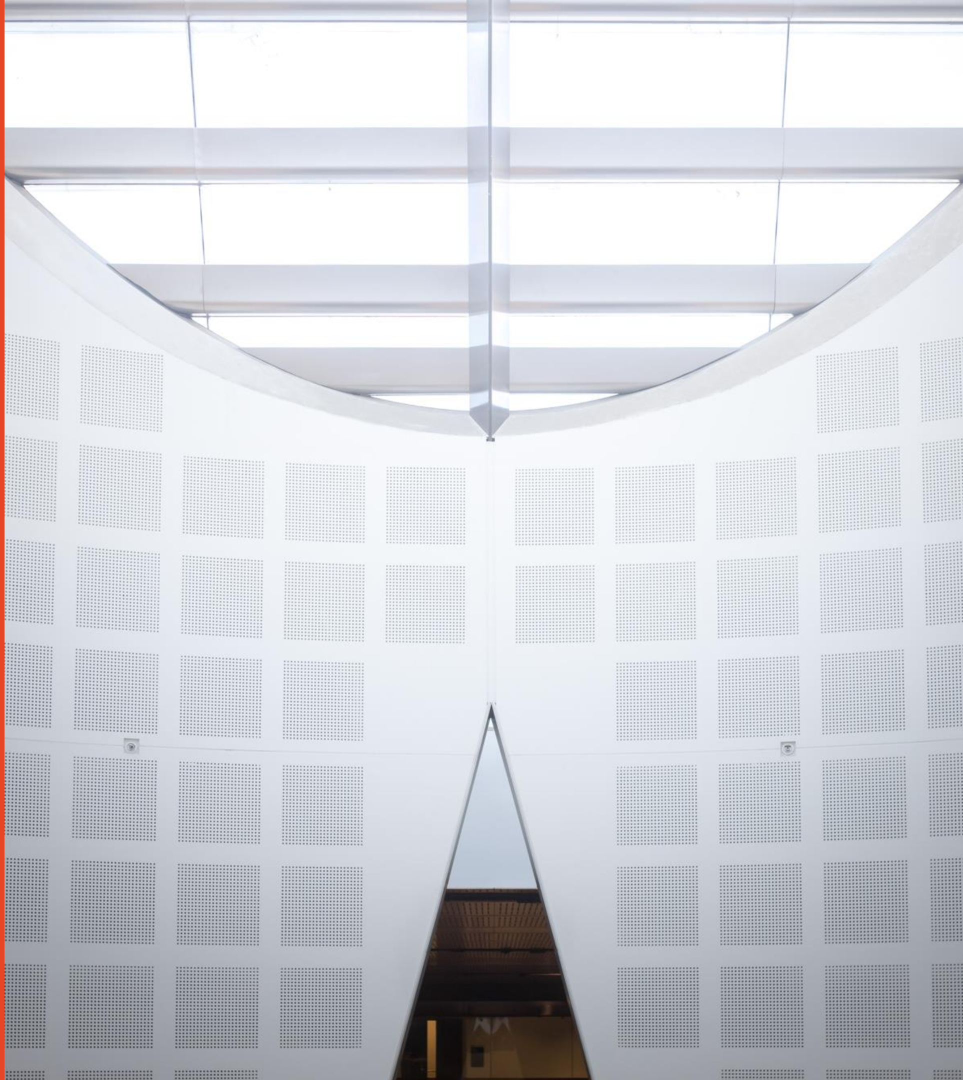


Overview of Week 4

Today: 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 9 + 10

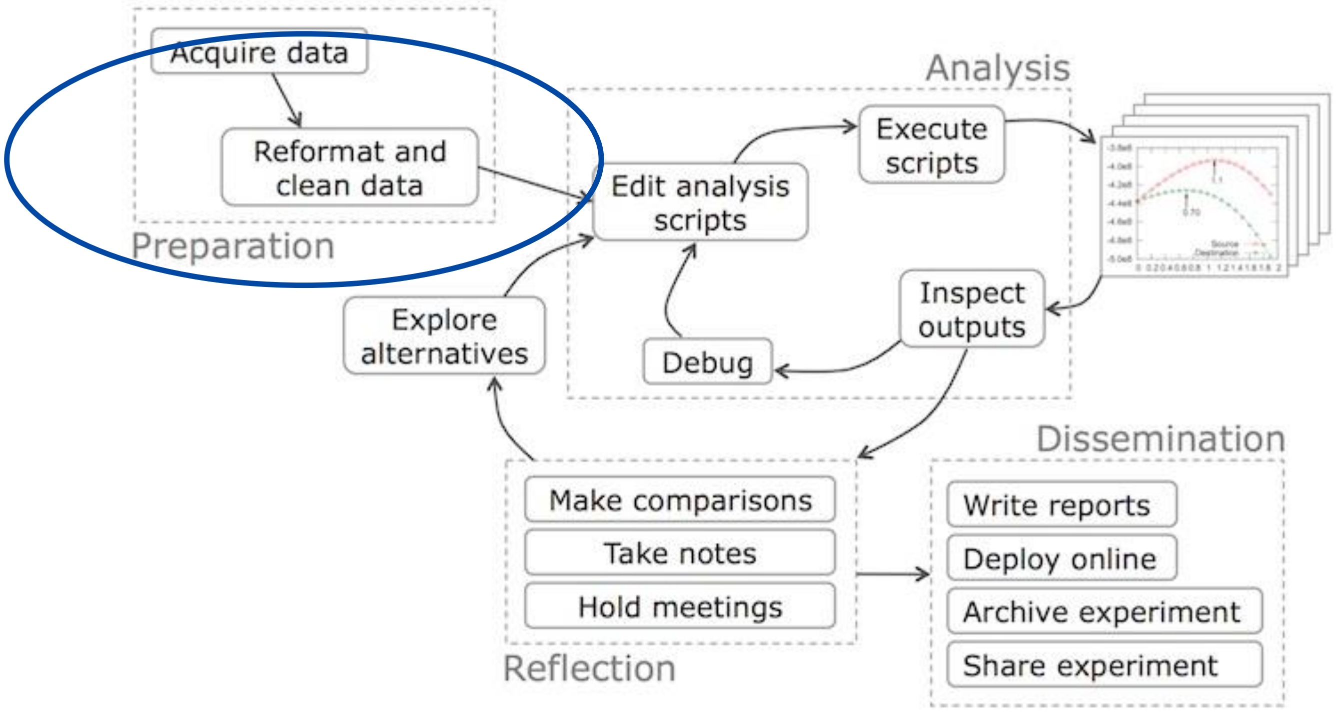
Exercises

- Python / Jupyter to load data
- psycopg2
- PostgreSQL to store data

TODO in W4

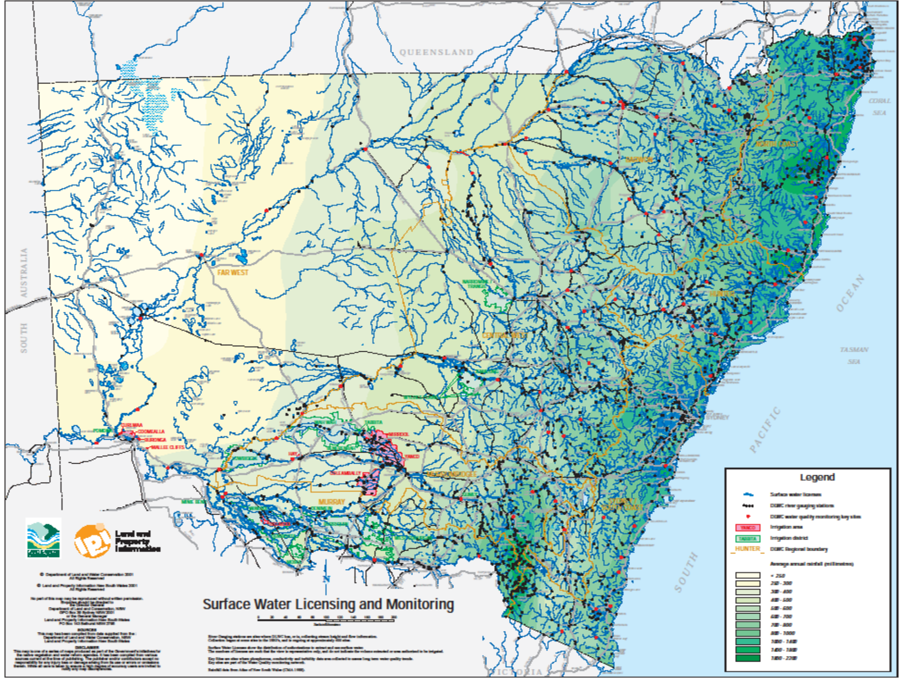
- Grok Python modules 10-12
- Grok SQL modules 20-22 (24 if you can)
- Summarise and prepare data

Exploratory Analysis Workflow



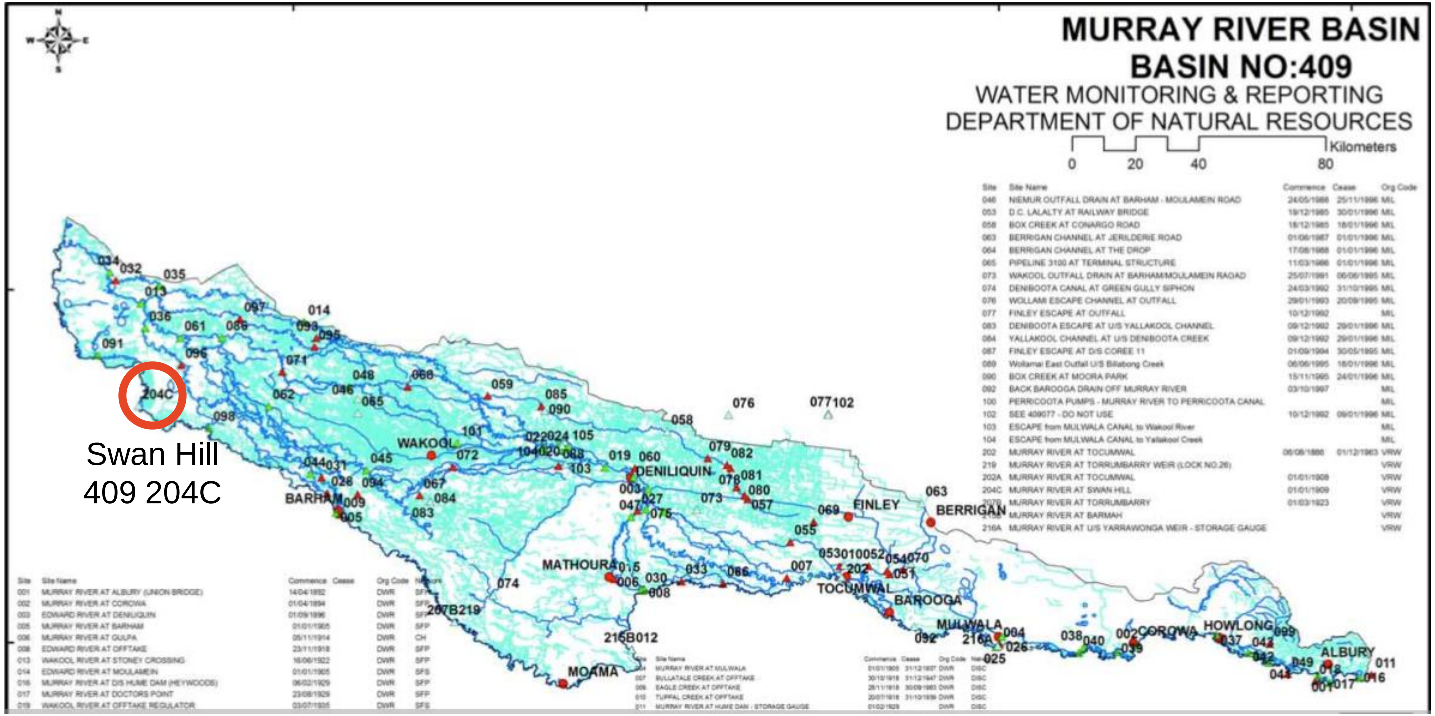
New Scenario

New Data Set



- Water measurements:
  - automatic monitoring stations
  - that are distributed over a larger area
    - (say the Murray River catchment basin)
  - that 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
- Or: Download from an online data server
  - Still typically in CSV or Excel etc, but now problems with meta-data
- Or: Scrap the web yourself or use APIs of resources
  - Cf. textbook, chapter 9

- Our data set comes from a colleague in Excel format

Relational Databases

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

- **Relational data model** is the most widely used model today
  - Main concept: **relation**, basically a table with rows and columns
  - Every 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:

Attributes (also: columns, fields)

Student				
<u>sid</u>	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

Tuples (rows, records)

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

Exercise 1: Some initial issued to be solved

- Our first attempt is for just a 1:1 mapping
  - Still: separate tables need to go to separate database relations
  - Note: CSV headers are not allowed to contain spaces or '
- Connection to Postgresql with **psql** shell tool
- Create 1:1 mapping tables in SQL
- Load CSV directly to SQL tables
  - We first try COPY command from psql
    http://www.postgresql.org/docs/current/interactive/sql-copy.html

Exercise 1: Data Loading with DB Loader

- Download data and notebook from **Canvas**
  - five CSV data files:
    - Measurements.csv
    - Organisations.csv
    - Sensors.csv
    - Stations.csv
    - Jupyter Notebook
- Upload all those files to Jupyter server
- Run notebook and do Exercise 1 for db creation and data loading with **psql**

Important:
Make sure to use the correct names including the '.csv' file extension

Reminder: Jupyter server locations

1. Login to one of these Jupyter Servers
   - https://ucpu1.ug.it.usyd.edu.au/
   - https://soit-ucpu-pro-**X**.ucc.usyd.edu.au (***X*** *= 1 or 3*)
   - Log in with unikey as username and password
   - Both servers are linked to your ICT shared folder here at Usyd
     - you need to have logged-in to one of the lab machines in the SIT building first to have this shared folder created

2. Login to our central postgresql: soit-db-pro-2.ucc.usyd.edu.au
   Your unikey with your SID as pw

Database Loading with Python

Issues with DB Loaders

- DB Loading tools such as **psql**
  - good for administration of server
  - good for bulk-loading of exported data in clean csv format (db export)
  - needs terminal access (both an advantage and a disadvantage)
  - has its limitations if format and structure of data files do not match the actual database schema
    => cleaning and transformation of data needed

- Could we do so in a programming language such as Python?

Accessing PostgreSQL from Python: psycopg2

- First, we need to import the **psycopg2** module, then connect to Postgresql
- Note: You need obviously to provide you own login name
  - Username and password are prepared by us as your unikey and your SID

```
import psycopg2

def pgconnect():
    # please replace <your_unikey> and <your_SID> with your own details
    YOUR_UNIKEY = '<your_unikey>'
    YOUR_PW     = '<your_SID>'
    try:
        conn = psycopg2.connect(host='soit-db-pro-2.ucc.usyd.edu.au',
                                database='y18s1c5310_'+YOUR_UNIKEY,
                                user='y18s1c5310_'+YOUR_UNIKEY,
                                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 (cont'd)

- 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
```

Accessing PostgreSQL from Python: psycopg2 (cont'd)

– Example: Creating a table and loading some data

```
# 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")
```

Exercise 2: Data Loading with Python

- Next part 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?
- What problems do you encounter when trying to load the table?

Transforming and Cleaning Data

Issues encountered at previous exercises

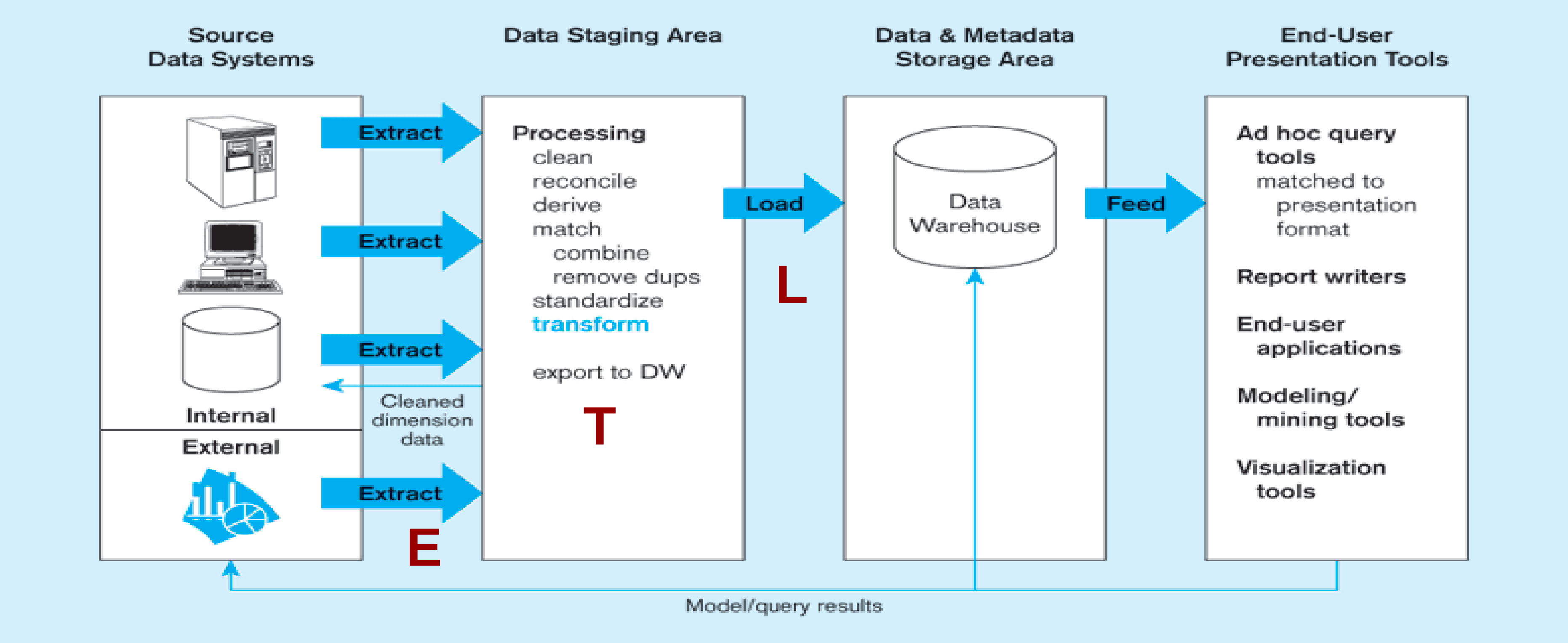
- Interpretation of data format and meta-data
- Differences in naming conventions
  - Excel headers with spaces and quotes, which both are not allowed to DBMS
- Inconsistent or missing data entries
- 'shape' of data

Cleaning and Transforming Data

- Real data is often '*dirty*'
- Important to do some data cleaning and transforming first
  - remember last week, when we had to convert strings to float
- Typical steps involved:
  - type and name conversion
  - filtering of missing or inconsistent data
  - unifying semantic data representations
  - matching of entries from different sources
- Later also:
  - **<u>Rescaling</u>** and optional dimensionality reduction

ETL Process

- This problem is well known from data warehousing
- **ETL Process:** Capture/Extract - Data Cleansing - Transform - Load



Data Cleaning in Python

- Yes, there are powerful ETL tools out there, but we do it for free in Python:
  - (1) type and name conversion
  - (2) filtering of missing or inconsistent data
  - (3) unifying semantic data representations
  - (4) matching of entries from different sources
- Last week's clean() function deals with Tasks (1) and (2)
  - int() creates integer objects, e.g., -1, 101
  - float() creates floating point object, e.g., 3.14, 2.71
  - datetime.strptime() creates datetime objects from strings
  - Filters missing / wrongly formatted data and replaces with default value
- For more complex cases (3) and (4), you would need special code though

TODO

Repeat from Week 3: A function to convert values

Use "not a number" as default value
numpy knows to ignore for some stats

```
import numpy as np
DEFAULT_VALUE = np.nan

def clean(data, column_key, convert_function, default_value):
    special_values= {} # no special values yet
    for row in data:
        old_value = row[column_key]
        new_value = default_value
        try:
            if old_value in special_values.keys():
                new_value = special_values[old_value]
            else:
                new_value = convert_function(old_value)
        except (ValueError, TypeError):
            print('Replacing {} with {} in column {}'.format(row[column_key], new_value, column_key))
        row[column_key] = new_value

# the following converts the two measurement columns to float values - or NaN
clean(data_measurements, 'Discharge', float, DEFAULT_VALUE)
clean(data_measurements, 'MeanDischarge', float, DEFAULT_VALUE)
```

Exercise 3: Data Cleaning

- Next part in Jupyter notebook
  - Apply cleaning steps to data from Stations.csv
  - Repeat for **Sensors.csv**
    - and if time also for the remaining CSVs from Canvas

- Which types of data conversions do you encounter?
- How would you resolve those?
- Any other observations regarding the source data format?

Data Modeling

Lessons Learned from Previous Exercise

- If we look closer at the 'Stations.csv' content, we see that is only partially fits a relational database model
  - **station identifier** is split over two attributes
    - BasinNo
    - Site
- Human interpretable ≠ machine readable

- So how to proceed with a database approach?

  => **OLAP: Online Analytical Processing**

Data Warehouses: Fact Tables

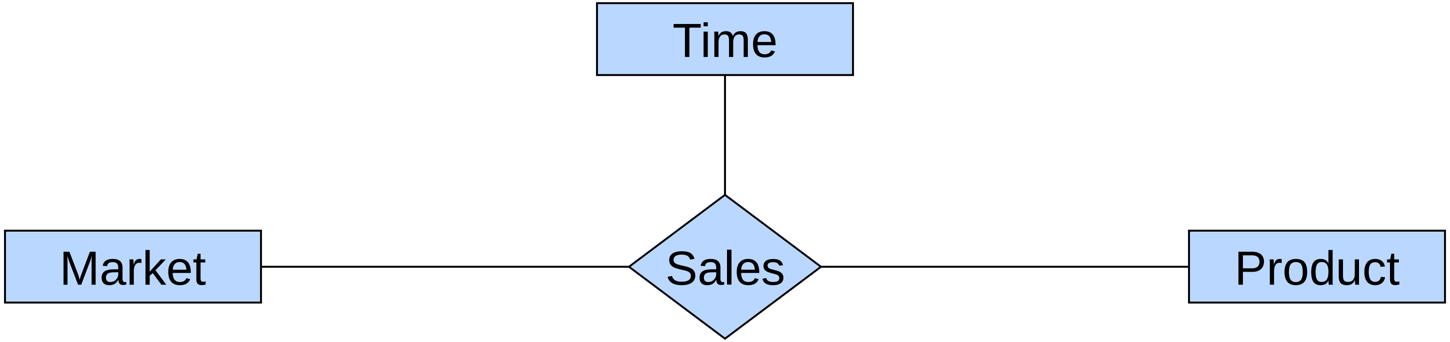
– Relational 'data warehouse' applications are centered around a ***fact table***
  – For example, a supermarket application might be based on a table
    Sales (*Market_Id*, *Product_Id*, *Time_Id*, *Sales_Amt*)

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 and dimension relations linked to it looks like a star;
- this is called a ***star schema***

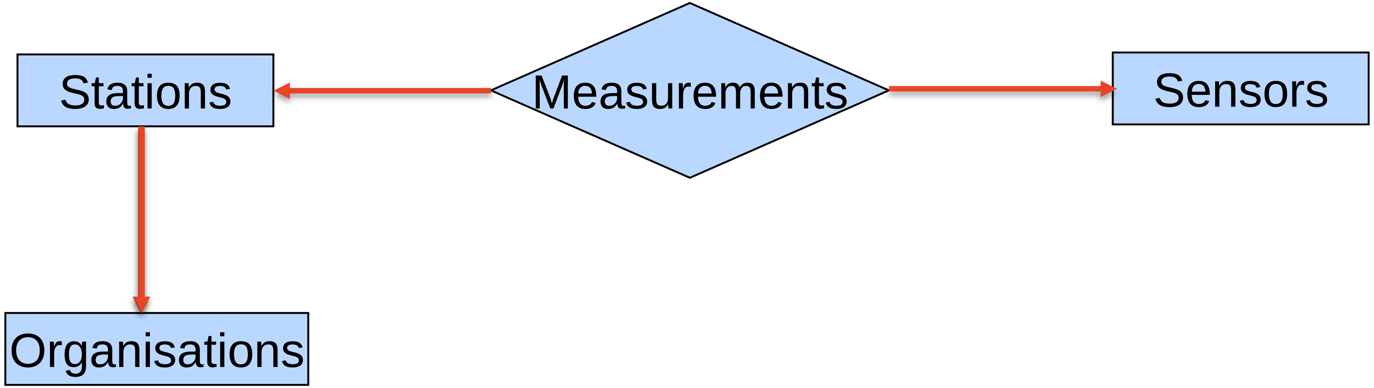


- If we map this to relations
  - 1 central fact table
  - *n* dimension tables with foreign key relationships from the fact table

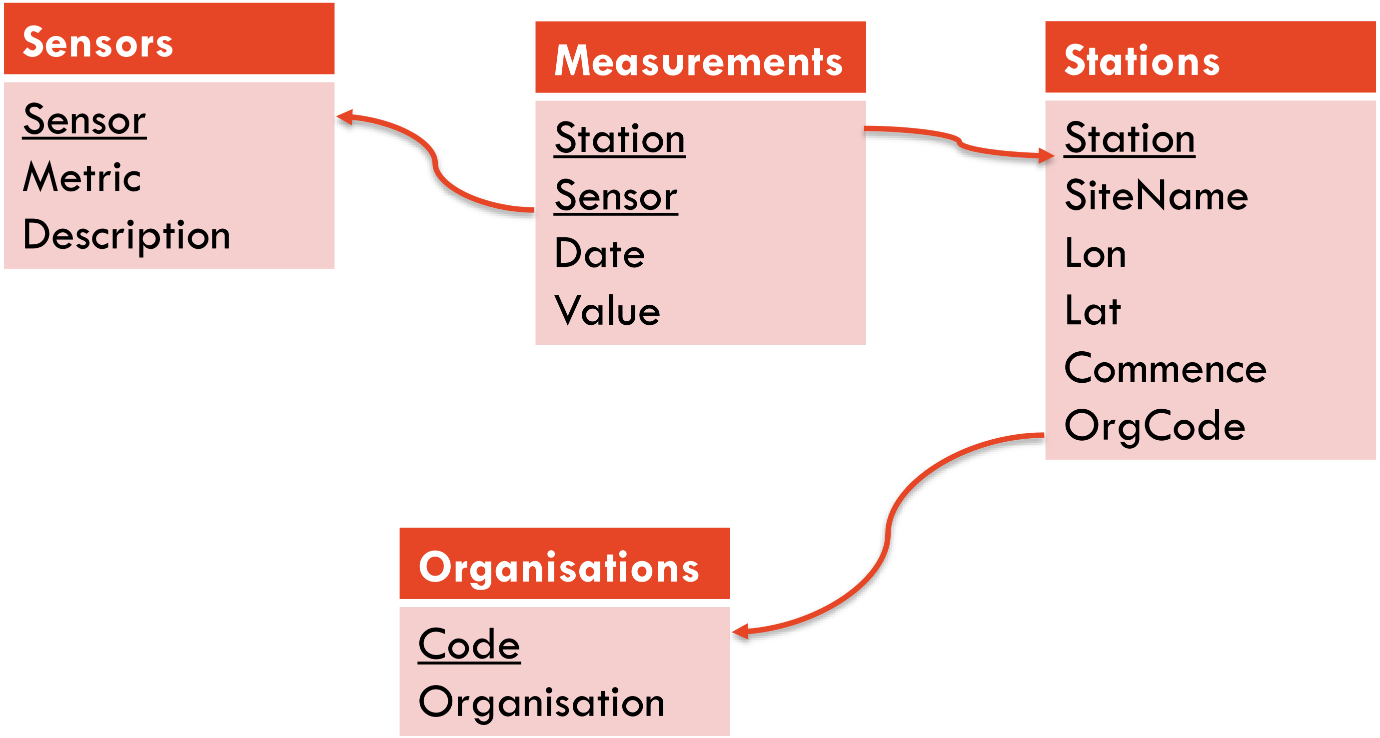
    (the fact table holds the FKs referencing the dimension tables)

Data Warehousing: Snowflake Schema

– measurements are the facts, rest describes the dimensions



Modeling our Water Data Set



DB Creation

SQL – The Structured Query Language

- SQL is the standard declarative query language for RDBMS
  - Describing what data we are interested in, but not how to retrieve it.
- 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`

Table Constraints and Relational Keys

- When creating a table, we can also specify ***Integrity Constraints*** for columns
  - eg. domain types per attribute, or **NULL** / **NOT NULL** constraints

- **Primary 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.

- **Foreign keys** are identifiers that enable a dependent relation (on the many side of a relationship) to refer to its parent relation (on the one side of the relationship)
  - Must refer to a candidate key of the parent relation
  - Like a \`logical pointer’

- Keys can be **simple** (single attribute) or **composite** (multiple attributes)

Example: Relational Keys

Primary key identifies each tuple of a relation.

Composite Primary Key consisting of more than one attribute.

Student	
sid	name
31013	John

Enroll		
sid	ucode	grade
31013	I2120	CR

Units_of_study		
ucode	title	credit_pts
I2120	DB Intro	4

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

SQL Domain Constraints

- SQL supports various domain constraints to restrict attribute 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)
 );
```

Exercise 4: Schema Creation

- Next part in Jupyter notebook
  - We provided an example schema already
    - follows the mapping rules from the previous slides

- **Your Task:** Using Python + SQL, create the full SQL schema for the given data model
    - This should give you seven separate tables as compared to the five spreadsheets which we originally had

Data Loading / Storage

Data Storing

- Where are we now?
  - We have analysed our given data set
  - Cleaned it
  - Transformed it and created a corresponding relational database
- Next, we want to store the given data in our database.
- Main approaches:
  1. Command line tools
  2. Python loader
  3. (Combination of Python loader and stored procedures)

Approach 1: PSQL Data Loader

- Postgresql offers a command to load data directly from a CSV file into a database table

  \COPY *tablename* FROM *filename* CSV [HEADER] [NULL '…']

  - Many further options
  - Try \help COPY
- Pros:
  - Relatively fast and straight-forward
  - No programming needed
- Cons:
  - Only 1:1 mapping of CSV to tables; no data cleaning or transformation
  - Stops at the first error…

Approach 2: Python Loading Code

– Example: Creating a table and loading some data

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# 1st: login to database
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for row in data_organisations:
    pgexec (conn, insert_stmt, row, "row inserted")
```

– Pros: Full flexibility; data cleaning and transformation possible

– Cons: Has to be hand-coded for each case

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* {"**,**"*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'

(Final) Exercise 5: Data Storage

- Next part in Jupyter notebook
  - Make sure you have the full SQL schema for the given data model
  - Load all CSV files into these tables

Review

Reprise Participation Marking

Requirements

- Complete Grok by end of week 6
- Submit code at end of each week
- **Jupyter Notebooks:**
  - The various exercises have placeholder cells marked as TODO:

```
# TODO: replace the content of this cell
raise NotImplementedError
```

  - The content of these cells needs to be replaced with your own solution => basis for participation marking

Output

- Code/spreadsheets from exercises
- Completion of final Python and final SQL module in Grok

Marking

- 10% of overall mark
- each week's participation assessed as: all done, partially done, no participation

Submit your Jupyter notebooks in Canvas by next Monday

Tips and Tricks

- Real data is 'dirty' – **data cleaning** and transformation essential
- Database systems are great for *shared*, *persistent* storage of *structured* data, and also for consistent updating ('life' data)
- But some caveats:
  - Schema-first
  - Relational model quite restrictive (1NF, no lists, collections etc)
  - Not too intuitive; 1:1 mapping from spreadsheets doomed to fail
  - Type-mismatches between programming languages and SQL
  - Needs to be installed and maintained
    (though much better nowadays for SQLite and PostgreSQL)
- What's the benefit?
  - Sharing! Large data sets! Querying will give us some leverage too.

Next Time

Lecture Plan

- W1: Introductions and housekeeping
- W2: Data exploration (spreadsheets)
- W3: Data exploration (Python)
- W4: Cleaning and storing data
- W5: Querying and summarising data
- W6: Hypothesis testing
  Project stage 1 due 8/Sep
- W7: Data Mining
- W8: Machine learning
- W9: From data to decisions
- W10: Unstructured data
- W11: Analysing big data
- W12: Product Thinking and Ethics*
  Project stage 2 due 27/Oct
- W13: Review
- ***Exam***

Next Lecture (10th April): Querying and Summarising Data

Objective

To be able to extract a data set from a database, as well as to leverage on the SQL capabilities for in-database data summarisation and analysis.

Lecture

– Data Gathering reprise
– SQL querying
– Summarising data with SQL
– Statistic functions support in SQL

Readings

– Data Science from Scratch, Ch 23

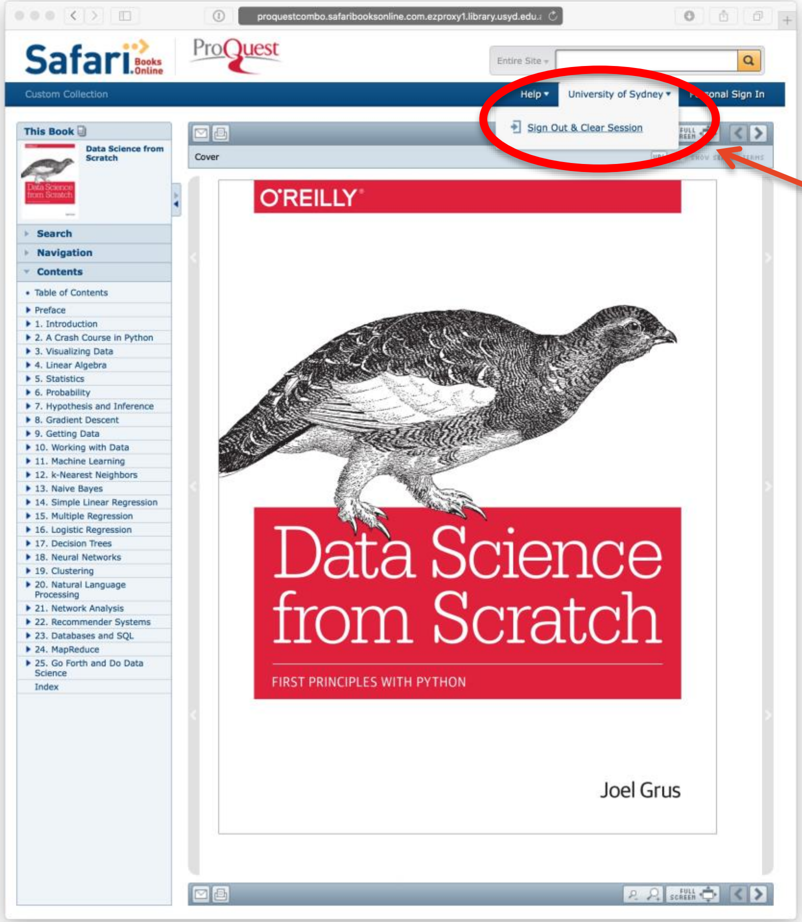
Exercises

– **[TODO]**

TODO in W5

– Finish Grok Python modules
– Finish Grok SQL modules
– project data

Online Book



don't forget to end session when finished reading

Many Good Python Resources

- Hard to make recommendations given different backgrounds
- Look online, there are many free resources and example code
- A few lists:
  - https://www.fullstackpython.com/best-python-resources.html
  - https://www.quora.com/Learning-Python/How-should-I-start-learning-Python-1

Project Stage 1

Project Stage 1: Explore, Clean, Pitch

Objective

Explore a data set and define a research question based on research/business requirement.

Activities

- Choose a data set
- Explore and summarise data set
- Clean and prepare data
- Define problem

Output

- **2-page report** summarising data, problem and explorative analysis
  - with titlepage & references: max 4p
- **1-page technical summary**
  - how did you acquire the data?
  - which tools did you use to clean and explore the data set?

Marking

- 20% of overall mark

SUGGESTED Timeline for Project Stage 1

- W1: Identify possible data sets
- W2: Identify and Explore possible data sets
- W3: Select project data set, define problem, complete exploration
- ***W4: Draft summary (problem & exploratory analysis)***
- W5: Clean and prepare data
- W6: Descriptive Stats, justification of suitability
  Submit Technical-Summary + report (3-5 pages altogether)

Project and discussion time

Time for you to talk
to tutors, instructors and each other
about data sets, data exploration
and possible research questions.