ME314 Introduction to Data Science and Machine Learning

Working with databases

Day 3 Lecture, 23 July 2021 - Kenneth Benoit

Plan for today

- Database systems
- JSON
- Relational data
- Normalisation
- SQL and SQLite

Database systems

RELATIONAL DATABASES

- Mainly implementations and extensions of the SQL Standard (<u>ISO/IEC</u>)
- Transactions are always ACID (atomic, consistent, isolated, durable)
- Data needs to be defined

Non-relational databases

- Key-value storage types (e.g. Amazon DynamoDB) or document storage types (e.g. CouchDB, MongoDB)
- Sometime labelled as providing ACID transactions but often only eventually consistent

JSON

- a lightweight data-interchange format that is (supposedly!) easy for humans to read and write, and easy for machines to generate or parse
- follows conventions from Javascript, but is language-independent
- Example: **Twitter data**
- built on two structures:
 - A collection of name/value pairs
 - An ordered list of values

object

- unordered set of name/value pairs. An object begins with { and ends with }
- each name is followed by : and the name/value pairs are separated by ,

array

- an ordered collection of values
- begins with [and ends with]
- array values are separated by ,

value

- can be a "string", a number, or true, false, or null, or an object or array
- can be nested

strings in JSON

- a sequence of zero or more Unicode characters, wrapped in double quotes
- uses backslash escapes, e.g.
 - "\u2708\ufe0f" represents a →
 - "this is \"quoted\"" represents "quoted"

```
In [10]:
print("It's a bird, it's a \u2708\ufe0f!!")
```

```
It's a bird, it's a \frac{1}{2}!!
```

Relational data structures

- invented by E. F. Codd at IBM in 1970
- A relational database is a collection of data organized as a set of formally defined tables
- These tables can be accessed or reassembled in many different ways without having to reorganize the underlying tables that organize the data
- RDBMS: a relational database management system. Examples include: MySQL, SQLite, PostgreSQL, Oracle. MS Access is a lite version of this too.
- The standard user and application programmer interface to a relational database is structured query language (SQL)

Example: from Database of Parties, Elections, and Governments (DPEG) relational database

```
SELECT c.countryName, c.countryAbbrev, p.* FROM party AS p
LEFT JOIN country AS c
ON p.countryID = c.countryID
```

Basic database concepts

(following on from last week)

- The basic unit is the database
- It might be stored on disk in a single file or a range of files managed by a server
- The database constists of tables which store actual data
- A table consist of at least one column whose name and data type need to be declared
- Data is stored in the rows of a table

Basic relational structures

- tables
 - also known as "relations"
 - tables define the forms of the data that are linked to other data through key relations
- keys: how tables are cross-referenced
 - primary key: an column in a table that uniquely identifies the remaining data in the table
 - **foreign key**: a field in a relational table that matches the primary key column of another table
 - join operations link tables in a structured query

Normalization

- Refers to the process of organizing a database into tables and columns, so that each table records a specific type of data, and only those columns that pertain to its topic are included
- Prevents duplication, and allows easier guarantee of data integrity
- Is more efficient
- Allows joined data to consist of merged tables, constructed through queries (more on this later)

Normal forms 1

"Normalizing" a database means creating a proper set of relations First normal form: No Repeating Elements or Groups of Elements

	countryname	partyname dat	e per108	per110
175	Austria	FPÖ Freedom Party 19901	3	0
176	Austria	GA Green Alternative 19901	0	3
177	Austria S	PÖ Social Democratic Party 19901	5	0
178	Austria	ÖVP People's Party 19901	8	0
179	Austria	FPÖ Freedom Party 19941) 1	11
180	Austria	LF Liberal Forum 19941	0	0

Here, this is violated because of the wide format of per108 and per110. To solve this, we have to move this to "long" format.

Normal forms 2

Second normal form: No Partial Dependencies on a Concatenated Key

```
countryname party date category catcount
1 Austria 42420 199010 per101 0
2 Austria 42110 199010 per101 0
3 Austria 42320 199010 per101 0
4 Austria 42520 199010 per101 5
5 Austria 42420 199410 per101 0
6 Austria 42421 199410 per101 0
```

Here, the format is still violated, because party 42420 is repeated. To solve this we need to create a party table and link to it using a foreign key.

Normal forms 3

Third normal form: No Dependencies on Non-Key Attributes. Every non-prime attribute of data in a table must be dependent on a primary key.

	countryname	party	date	category	catcount
1	Austria	42420	199010	per101	0
2	Austria	42110	199010	per101	0
3	Austria	42320	199010	per101	0
4	Austria	42520	199010	per101	5
5	Austria	42420	199410	per101	0
6	Austria	42421	199410	per101	0

Here, this is violated because election data repeats across multiple values of the category count table, when it should have its own table.

(Good explanation <u>here</u>)

Normalization: Example

SalesStaff							
<u>EmployeeID</u>	SalesPerson	SalesOffice	OfficeNumber	Customer1	Customer2	Customer3	
1003	Mary Smith	Chicago	312-555-1212	Ford	GM		
1004	John Hunt	New York	212-555-1212	Dell	HP	Apple	
1005	Martin Hap	Chicago	312-555-1212	Boeing			

This table serves multiple functions:

- identifies the organization's salespeople
- listing the sales offices and phone numbers
- associates a salesperson with a sales office
- lists each salesperson's customers

Problems

SalesStaff						
<u>EmployeeID</u>	SalesPerson	SalesOffice	OfficeNumber	Customer1	Customer2	Customer3
1003	Mary Smith	Chicago	312-555-1212	Ford	GM	
1004	John Hunt	New York	212-555-1212	Dell	HP	Apple
1005	Martin Hap	Chicago	312-555-1212	Boeing		

- What if we move the Chicago office to San Francisco?
 We would then need to update SalesOffice for every row of this table
- What if John Hunt leaves the firm?
 Removing that employee means we lose the information about New York
- What if Dell moves to having Mary Smith as a salesperson?
 Do we shift Customer2 and Customer3 left for John Hunt?

Problem: "insert anomaly"

<u>EmployeeID</u>	SalesPerson	SalesOffice	OfficeNumber	Customer1	Customer2	Customer3
1003	Mary Smith	Chicago	312-555-1212	Ford	GM	
1004	John Hunt	New York	212-555-1212	Dell	HP	Apple
1005	Martin Hap	Chicago	312-555-1212	Boeing		
???	???	Atlanta	312-555-1212			

- We cannot create a new sales office, until we also know the name of a sales person, because EmployeeID is the primary key
- The primary key uniquely identifies the data item, so we must have one

Problem: "update anomaly"

<u>EmployeeID</u>	SalesPerson	SalesOffice	OfficeNumber	Customer1	Customer2	Customer3
1003	Mary Smith	Chicago	312-555-1212	Ford	GM	
1004	John Hunt	New York	212-555-1212	Dell	HP	Apple
1005	Martin Hap	Chicago	312-555-1212	Boeing		

- If we have to update an attribute not uniquely associated with the primary key,
 then we have to change the entry multiple times
- Failure to make this update uniformly means we have inconsistent data (in this case, about the phone number of the sales office)

Problem: "deletion anomaly"

EmployeeID	SalesPerson	SalesOffice	OfficeNumber	Customer1	Customer2	Customer3
1003	Mary Smith	Chicago	312-555-1212	Ford	GM	
1004	John Hunt	New York	212-555-1212	Dell	쁖	A pple
1005	Martin Hap	Chicago	312-555-1212	Boeing		

- Deletion of one row removes more information than the item indexed by the primary key
- Here, removing John Hunt also removes information about the New York sales office, and his clients

Problem: Searching or sorting

SalesStaff						
<u>EmployeeID</u>	SalesPerson	SalesOffice	OfficeNumber	Customer1	Customer2	Customer3
1003	Mary Smith	Chicago	312-555-1212	Ford	GM	
1004	John Hunt	New York	212-555-1212	Dell	HP	Apple
1005	Martin Hap	Chicago	312-555-1212	Boeing		

- If we want to search for a specific customer, such as Ford, we have to search three fields (Customer1 - Customer3)
- How could we sort the list of customers?
- Where would we record client data, or link to the clients?

Example: Normalization

Non-Normalised Table					
ID	Name	Age	Movie	Language	
001	Tom Cruise	53	Mission Impossible, Top gun	English	
002	Brad Pitt	50	Seven, Troy	English	
003	George Clooney	54	ER, Gravity	English	

Example: solution (2NF)

Second Degree Normalised Table

ACTOR

ID	Name	Age
001	Tom Cruise	53
002	Brad Pitt	50
003	George Clooney	54

MOVIES

ID	Movie	Language
001	Mission Impossible	English
001	Top gun	English
002	Seven	English
002	Troy	English
003	ER	English
003	Gravity	English

Basic SQL syntax

- Defining data: CREATE TABLE
- Adding, changing, and deleting data: INSERT, UPDATE, DELETE
- Accessing data: SELECT
- Most functionality is part of the SELECT statement:
 - Filter: SELECT ... WHERE
 - Sort: SELECT ... ORDER BY
 - Aggregate: SELECT ... GROUP BY
 - Combining data: SELECT ... JOIN
- Adding constraints: CREATE CONSTRAINT
- Adding indexes: CREATE INDEX

SQL Syntax caveats

- SQL syntax is case-insensitive
- ; has to be added at the end of a line to terminate it (as in C-family languages, Javascript, ...)
- There is no implicit ordering of rows in SQL

Setting up the SQLite command line

INSTALLATION VIA ANACONDA

conda install sqlite

CONNECTING TO A DATABASE

```
SQLite example.db

SQLite version 3.20.1 2017-08-24 16:21:36
Enter ".help" for usage hints.
sqlite>
```

Creating a table

```
CREATE TABLE table_name (column_name column_type [, column_name column_type]);
```

Creating a table involves two things:

- 1. Giving the table a name constiting of alphanumeric characters and ____
- 2. Giving each column a name and a data type

The SQL Standard defines several common data types and most SQL implementations provide additional ones:

Туре	Description
INT, BIGINT	Integer (4- and 8-byte).
FLOAT, DOUBLE	Single or double precision floating point number (4 or 8 bytes).
TEXT	String, stored using the database encoding (UTF-8,).
BLOB	Raw binary data.
BOOLEAN	True or false.
DATE, TIMESTAMP	Date and date-time.

Compare data types available in **SQLite**, **MySQL**, and **PostgreSQL**.

EXAMPLE

```
CREATE TABLE my_table (my_integer INT, my_float FLOAT, my_text TEXT) ;
```

Adding data to a table

You probably will not do this by hand but rather via a script. This is the topic of the class.

```
INSERT INTO table_name [(column_name [, column_name])] VALUES (value1 [, value2]);
EXAMPLE

INSERT INTO my_table VALUES (1, 1.3, 'abc');
INSERT INTO my_table (my_integer, my_float, my_text) VALUES (4, 4.3, 'def');
INSERT INTO my table (my_integer, my_float) VALUES (8, 8.3);
```

INSERT documentation

Changing or deleting data in a table

As above, you probably do not want to do this by hand.

```
UPDATE table_name SET column_name = value [, column_name = value] WHERE ...;
DELETE FROM table_name WHERE ...;
```

EXAMPLE

```
UPDATE my_table SET my_float = 1.5 WHERE my_integer = 1 ;
UPDATE my_table SET my_integer = my_integer * 2 WHERE my_text = 'def' ;
DELETE FROM my_table WHERE my_integer = 8 ;
```

Retrieving data

Whenever data should be retrieved, the statement starts with SELECT.

```
select * | column_name [AS new_name] {, column_name} FROM table_name [AS other_name] ;

* selects all columns of the table
```

Example 1: Dummy table created above

```
SELECT * FROM my_table ;

1|1.3|abc
4|4.3|def
```

Example 2: Actual data

```
SELECT * FROM lecture_TBD ;
TBD
```

 This will return all the rows in the table which is not practical for tables with many rows • To just have a glance at the first X rows of the data:

```
SELECT * FROM lecture TBD LIMIT 20 ;
```

- This works the same as the head(dat, n = 20) function in R from last week
- NB: There is no implicit ordering of rows in SQL
- If the data is not explicitly ordered (will be explained shortly) there is no order whatsoever
- This is one of the main differences between SQL tables and tabular data in, e.g., an Excel sheet

Filtering data

```
SELECT ... WHERE condition ;
```

The WHERE clause is part and parcel of the power of SQL (WHERE, JOIN, and indexing)

You can test for many condition s:

- Equality: WHERE column_name = value (as used in the example above)
- Interval: WHERE column_name BETWEEN lower_value AND higher_value
- Set membership: WHERE column_name IN (value1, value2, ...)
- The set can be generated on the fly: WHERE column_name IN (SELECT myvar FROM mytable)
- Simple pattern match in strings: WHERE string_column LIKE '_ab%' (_ denotes *one* character, % denotes zero or more characters, see also GLOB and REGEX)
- Missing values: WHERE column_name IS NULL

Individual conditions can be composed with the logic operators $\,$ AND $\,$, $\,$ OR $\,$, and $\,$ NOT

Sorting data

As mentioned previously:

```
SQL does not implicitly order data.1
```

This means data can and will be returned in an arbitrary fashion (last accessed, query optimization, ...)

Work around this by explicitly ordering on variables.

```
SELECT ... ORDER BY column_name [DESC] [, column_name, ...] ;
```

EXAMPLE

```
SELECT * FROM lecture TBD WHERE TBD ;
```

Only works in SQLite because the variable rowid is created by default.

```
SELECT * FROM lecture_TBD ORDER BY rowid LIMIT 20 ;
```

¹ SQLite tables have a primary key by default called rowid (<u>see here</u>). However, the data is **not** implicitly sorted according to the rowid.

Aggregating data

```
SELECT ... GROUP BY column_name ;
```

- Data can be aggregated directly within SQL
- This works by defining a grouping variable
- The number of distinct values of the grouping variable defines the number groups
- All rows which share a value on the grouping variable are grouped together
- If there are several grouping variables, the unique combinations across all grouping variables defines the groups
- This statement puts some limits on the variables that you can select in the part
- Bare variables must be included in the GROUP BY part
- Other variables need to be aggregated with the help of a function
- The functions gets the all the rows in the group and returns a single, aggregated value
- Aggregation functions available in <u>SQLite</u>, <u>MySQL</u>, and <u>PostgreSQL</u>

Aggregating data (cont'd)

```
SELECT ... GROUP BY column_name ;
```

EXAMPLE

Count the number of rows per group:

```
SELECT country, COUNT(country) AS n FROM lecture TBD GROUP BY country;
```

Return minimum/maximum value per group:

```
SELECT country, min(XXX) AS XXX_min, max(XXX) AS XXX_max FROM lecture_TBD GROUP BY column_name ;
```

Joining tables

- The second pillar of SQL's (or more generally RDBM's) success
- Allows to combine two tables on the fly
- A single table thus does not need to contain all the relevant information
- If you know where

Types of JOINs:

- INNER JOIN retains only matching rows from tables 1 and 2
- LEFT OUTER JOIN retains all rows from table 1 and matching rows from table 2
- RIGHT OUTER JOIN retains matching rows from table 1 and all rows from table 2

Joining tables: INNER JOIN

2017530293

2017539281

Mette

Adam

Student name	Programme	
Anne	MSc in Research	
Tobias	MSc in DB Management	
Mette	MSc in DB Management	
Adam	MSc in Statistics	
	Department	
nagemen	Department of Databases	
cs	Department of Statistics	
Research	Methods Department of Methodology	
mes AS b		
Tobias	MSc in DB Management Department o	f Databases
	Anne Tobias Mette Adam nagement cs Research a.programme mes AS b programme name	Anne MSc in Research Tobias MSc in DB Management Mette MSc in DB Management Adam MSc in Statistics Department Department of Databases CS Department of Statistics Research Methods Department of Methodology a.programme, b.department mes AS b .programme; name programme department

MSc in DB Management

MSc in Statistics

Department of Databases

Department of Statistics

Joining tables: LEFT OUTER JOIN

Student ID	Student name	Programme
2017829384	Anne	MSc in Research
2017891623	Tobias	MSc in DB Management
2017530293	Mette	MSc in DB Management
2017539281	Adam	MSc in Statistics

Programme	Department	
MSc in DB Management	Department of Databases	
MSc in Statistics	Department of Statistics	

MSc in Social Research Methods Department of Methodology

The OUTER keyword is optional and often left out.

```
a.id, a.name, a.programme, b.department

FROM students AS a

LEFT JOIN programmes AS b

ON a.programme = b.programme;
id name programme

2017829384 Anne MSc in Research

2017891623 Tobias MSc in DB Management Department of Databases
```

id	d name programme		department
2017530293	Mette	MSc in DB Management	Department of Databases
2017539281	Adam	MSc in Statistics	Department of Statistics

Joining tables: RIGHT OUTER JOIN

Student name	Programme
Anne	MSc in Research
Tobias	MSc in DB Management
Mette	MSc in DB Management
Adam	MSc in Statistics
	Anne Tobias Mette

Programme	Department
MSc in DB Management	Department of Databases
MSc in Statistics	Department of Statistics

MSc in Social Research Methods Department of Methodology

SQLite does not support RIGHT OUTER JOIN so the actual syntax used for the output uses LEFT JOIN with rearranged tables

department

```
a.id, a.name, b.programme, b.department

FROM students AS a

RIGHT JOIN programmes AS b

ON a.programme = b.programme;

id name programme
```

id	name	programme	department
2017530293	Mette	MSc in DB Management	Department of Databases
2017891623	Tobias	MSc in DB Management	Department of Databases
2017539281	Adam	MSc in Statistics	Department of Statistics
		MSc in Social Research Methods	Department of Methodology

Keys, constraints and indexes

- A primary or foreign key (as mentioned at the beginning of the lecture) is a unique identifier
- In SQL, keys are mainly made of constraints
- A constraint defines a check on data entered in to a table
- If a row fails the check, SQL will signal an error and no data will be inserted in the table
- The main constraints used to build indexes are:
 - UNIQUE forces the values of a given column to be distinct
 - NOT NULL disallows NULL, i.e. missing, values
 - PRIMARY KEY is a shortcut for UNIQUE NOT NULL in most SQL implementations but not in SQLite (for historical reasons)
 - FOREIGN KEY ... foreign constraints in most SQL implementations and recent SQLite with foreign keys turned on

- CHECK (EXISTS(SELECT 1 FROM foreign_table WHERE foreign_key=local_key)) foreign key constraint implemented by hand
- Declaring a primary key also automatically creates an index in most SQL implementations (though not in SQLite)
- An **index** is, generally speaking, a lookup table for a given column which allows sorting and filtering data to be quicker
- It comes with a maintenance cost because it needs to be updated whenever new data is inserted

Setting up tables

```
CREATE TABLE students (id INT PRIMARY KEY NOT NULL, name TEXT);
CREATE TABLE programmes (id INT PRIMARY KEY NOT NULL, name TEXT, department TEXT);
CREATE TABLE allocation (
    student_id INT NOT NULL,
    programme_id INT NOT NULL,
    FOREIGN KEY(student_id) REFERENCES students(id),
    FOREIGN KEY(programme_id) REFERENCES programme(id)
    );
```

Adding data

The programmes table contains the missing row for an "MSc in Research"

Joining

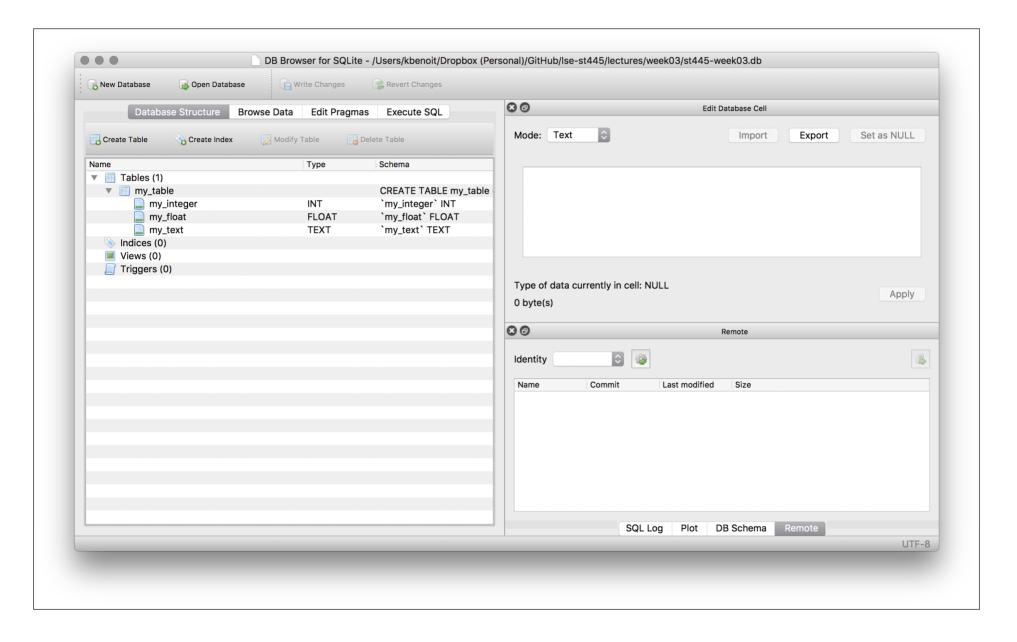
```
SELECT
    s.id AS student id,
   s.name AS student name,
   p.name AS programme name,
   p.department
FROM
    allocation AS a,
    students AS s,
   programmes AS p
WHERE
    a.student id = s.id
   AND
   a.programme id = p.id
student_id
                 student_name
                          programme_name
                                                      department
 2017829384
                          MSc in Research
                                                      Department of Research
                 Anne
 2017891623
                 Tobias
                          MSc in DB Management
                                                      Department of Databases
 2017530293
                                                      Department of Databases
                 Mette
                          MSc in DB Management
 2017539281
                 Adam
                                                      Department of Statistics
                          MSc in Statistics
(Implicit CROSS JOIN with manual implementation of the ON ...)
```

Aggregating

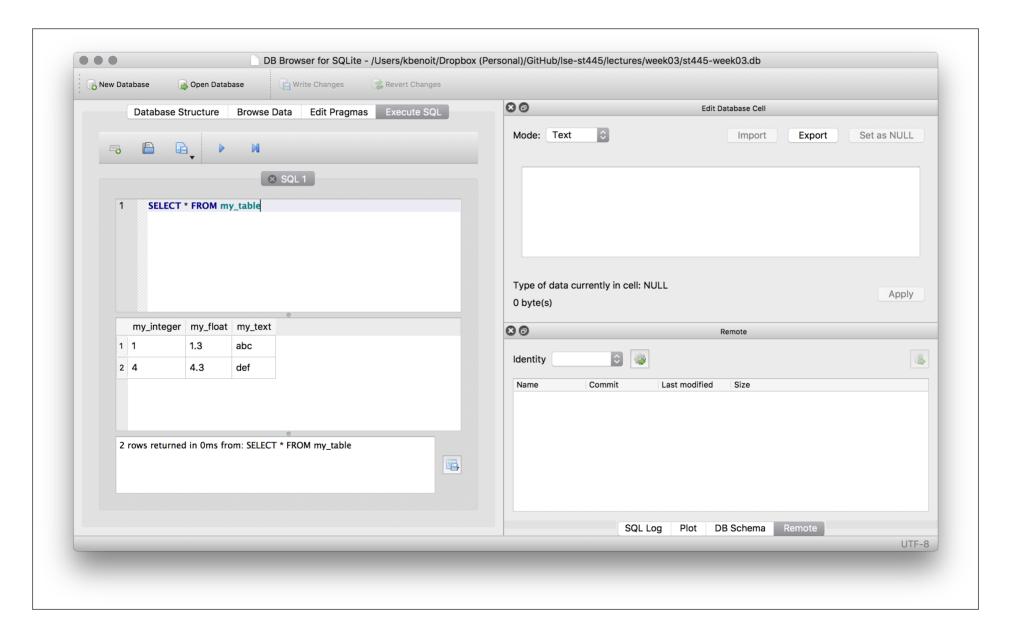
NB:

- Departments without students are omitted here
- Just to reiterate: The order of the rows is completely arbitrary

DB Browser to the rescue



DB Browser: Executing queries



More on normal forms

1NF

- each table cell should contain a single value
- each record needs to be unique, identified by a primary key
 - a primary key muust be unique and non-NULL
 - assigned when a new record is created
 - often just an (alpha)numeric identifier

2NF

- has to be in 1NF
- need a single column primary key
 - this links to other tables as their foreign keys
 - usually foreign keys are not unique in the table where they are foriegn
 - can be NULL

3NF

- has to be in 2NF
- has no transitive functional dependencies
 - a tfd occurs when changing a non-key column would chaneg any of the other non-key column values

For examples, see https://www.guru99.com/database-normalization.html