Data curation with SQL

Manage your data the “enterprise” way

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Quantitative Methods – Masterclass 2016

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Research Data Curation

In the following, we assume data curation scenarios within the following boundary conditions

- Structured data of the type that is often kept in (multiple) Excel sheets
- Possibly related multimedia objects (images, audio, video)
- Small to medium size, i.e. $< 1,000,000$ rows in tables, $< 100GB$ of data on disc
- Mainly curated by hand by a small team

Research Data Examples

Examples for this kind of research data:

- The data served by the D-PLACE app
- WALS - the World Atlas of Language Structures
- Tsammalex - a multilingual lexical database on plants and animals
- But also smaller collections, e.g. wordlists with related cognacy judgements

So, hopefully, data of the kind most of you have to deal with regularly.

What is SQL?

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Structured **Q**uery **L**anguage

is a special-purpose programming language designed for managing data held in a relational database management system (RDBMS)

(Wikipedia)

What is a RDBMS?

A relational database is a way to store and manipulate information.
Databases are arranged as ***tables****. Each table has* ***columns*** *(also known as* ***fields****) that describe the data, and* ***rows*** *(also known as* ***records****) which contain the data.*

(software carpentry)

Database Managers

- Interacting with an RDBMS means sending SQL to a Database Manager much like interacting with the R runtime system means sending R instructions.
- The Database Manager is responsible for reading and writing the data to our disc.
- Common Database Managers include
  - Oracle (”but we are not a bank!”)
  - MySQL
  - SQLite
  - PostgreSQL

SQLite

- serverless! Just a library embedded in (**many**) programs
- The database is just a file ⇒
  - easy to backup
  - easy to share - e.g. using dropbox
- Firefox embeds SQLite, and a Firefox plugin is available as GUI for SQLite databases.
- Python supports interfacing with SQLite databases out-of-the-box, via stdlib's `sqlite3` module.
- Recommended for single user (or one user at a time).

PostgreSQL

- A client-server database ⇒
  - requires some administion
  - supports concurrent (remote) users
- Very SQL-standard compliant (probably more so than any other RDBMS) ⇒ easier to learn/lookup things/debug
- Scales to GB (TB even) of data ⇒
  - so storing multimedia in the database as well is an option
  - millions of rows in a table are no problem
- Good support for many specialized datatypes, in particular GIS data

Why not Excel?

Why not Excel?

Spreadsheets - and Excel in particular

- do not scale well (once above – say – 50,000 rows, people become afraid of changing the sort order)
- do not really support typed data ...
- ...sometimes trying too hard to support it, like converting gene names such as `SEPT2` to dates `2006/09/02`
- are not really cross-platform (or cross-version) compatible
- do not really support complex (inter-related) data

Why SQL?

Typed data

Unlike e.g. CSV, SQL requires explicitly typed columns. Unfortunately the data type specification (or name) is not standardized across RDBMS.

- The usual suspects are typically supported: integer, float, boolean, text
- But there's a lot more:
  - **B**inary **L**arge **Ob**jects (**BLOB**s) can be used for multimedia content.
  - **JSON** columns (supported in SQLite and PostgreSQL) can be used to add schemaless attribute-value-pairs to any record.
  - GIS objects like polygons (supported in SQLite and PostgreSQL)

Constraints

Constraints in SQL are rules enforced for records in a table:

NOT NULL indicates that a column cannot store NULL value

UNIQUE ensures that each row for a column (or combination of columns) must have a unique value

CHECK Ensures that the value in a column meets a specific condition (e.g. to implement enumerated types, or to make sure latitudes are numbers between -90 and 90).

DEFAULT Specifies a default value for a column

Referential Integrity and Normalization

Two constraints are used to relate records between tables in a way that ensure referential integrity:

PRIMARY KEY Ensures that a column (or combination columns) have a unique identity (implies NOT NULL and UNIQUE)

FOREIGN KEY Declare a column (or combination of columns) as ”pointer” to a primary key of another record.

The typical/simplest use case for this are reference tables, e.g.

- a LANGUAGE table with ISO 639-3 codes or Glottocodes as primary key
- a SOURCE table referenced by BibTeX citation key

ACID Transactions

While not strictly a part of SQL, both – SQLite and PostgreSQL provide transactions with guaranteeing the ACID properties:

Atomicity Transactions are **all or nothing**.

Consistency Successful transactions cannot result in an invalid database state.

Isolation Transactions are isolated from one another, i.e. to the outside world they appear as happening in a series.

Durability If a transaction is **committed**, the new state is durable, i.e. written to disc.

Other advantages of SQL

- Every software developer should know SQL, so when your data is in an RDBMS, they will know how to access it.
- SQL allows you to bundle data and schema (i.e. the data description) in a single text file.

Best practices for data modeling

- Always use auto-incrementing integer primary keys – model natural (or surrogate, or composite) candidates for primary keys via unique constraints instead. ⇒
  - Changing the unique properties later is easier.
  - The schema is more predictable/intuitive (foreign keys must be integers, too).
- Choose and adhere to naming conventions for
  - tables (**either** plural **or** singular nouns)
  - primary keys
  - foreign keys (e.g. prefix with name of referenced table)
- Use and link to standard reference catalogs
  - Glottolog (maybe ISO 639-3) for languages
  - Concepticon for concepts in wordlists
  - D-PLACE for societies
  - Any other in your field?

SQL and text data

SQL databases are not particularly good at handling non-ASCII text - but better than many other environments

- They don't pretend text can contain markup (like Filemaker or Excel).
- They don't support unicode in a meaningful way out of the box, but can be taught to do a little better.

Best practices for text data

- Declare the text encoding for your databases explicitly

  SQLite:
  ```
  PRAGMA encoding = "UTF-8"
  ```

  PostgreSQL:
  ```
  createdb -E UTF-8 ...
  ```

  Note: The default encoding is your locale!

- Normalize your unicode data before insertion into the database, e.g. using Python's `unicodedata` module:

```
>>> unicodedata.normalize('NFC', u'\u0061\u0301')
u'\xe1'
```

- Or enable Unicode collation support via DUCET

```
# SELECT E'\u0061\u0301' = E'\u00e1';
 f

# SELECT collkey(E'\u0061\u0301', 'root', true, 4, false) =
      collkey(E'\u00e1', 'root', true, 4, false);
 t
```

SQL and version control

Given the power of SQL, it's not surprising that various schemes of keeping a history of changes in a database exist, e.g. using *triggers*.

Here's a simpler recipe, exploiting the fact that

- SQL commands are lines of text suitable for version control with tools like git
- SQL includes a DDL, i.e. a data description language describing the schema

SQL and version control

1. Dump your database to plain SQL (including the schema)

   SQLite:
   ```
   sqlite3 db.sqlite .dump > db.sql
   ```

   PostgreSQL:
   ```
   pg_dump -x db -f db.sql
   ```

2. Version control the dumped SQL file.
3. Start editing after restoring the database from the dump

   SQLite:
   ```
   sqlite3 db_restored.sqlite < db.sql
   ```

   PostgreSQL:
   ```
   createdb db_restored
   psql -d db_restored -f db.sql
   ```

Applicable if

- data isn't too big ($< 100,000$ rows, no blobs)
- no concurrent editing happens (although merging may work, resolving conclicts by hand may be no fun)

Weaknesses of SQL databases

- Manual data entry is not supported too well out of the box
  - generic frontend tools are often clunky
  - custom frontends, e.g. Django apps, require programming/maintenance/administration.
- SQL dumps are not really portable across SQL implementations, thus, while a good format for versioning, these are not good for data sharing.

Conclusion I

You may go straight from collecting data in Excel to analysis in R, but ...

- if you are going to collect (aggregate)
  - a lot of data
  - or over a long time
  - or with multiple collaborators
- or if analysis must be efficient/performant
- or if you want to make your data easy to repurpose/accessible from various tools/languages

...introducing SQL as data curation layer may be worth the effort!

Conclusion II

- If you find yourself experiencing the pain points of Excel already
- or if you write code to check the consistency of your data

...consider writing code instead to import your data into a SQL database with a properly constrained data model.