Data & Databases

DBW

Outline

- Data modeling and Databases
- Concept and types of Databases
  - SQL vs NoSQL
- Data modelling
- Database design
- ETLs
- Interaction with Web apps
- MySQL
- SQL Language

What is data modeling?

- All applications manage data
- Simple data can be managed with primitive data types and simple arrays (dictionaries, …)
- Complex data require to design a data model
- Data models provide Classes in object-oriented programming and are the basis for designing database structures.

What is a database?

- Collection of data organized and stored according to some purpose.
  - Pile of papers, Flat text file, indexed store,…
- Ideally, data is organized following a specific data model
- Provide permanent storage for data structures
- DBMS (Database management software) takes care of storing and retrieving data
  - MySQL, PostgreSQL, SQLite, Oracle, Access, MongoDB, …
- Types
  - Relational DB, Column DB, Document DB, XML DB, …

Databases & Web Applications

- Databases are used for
  - Storing Data
  - Storing Meta-Data
  - Managing user/session credentials

- Databases always need an access application
  - Databases can be accessed but this not practical for end users (permanent conections, not enough expertise)
  - Most usual way is a **REST API** (a web service)

REST-ful APIs

Web services to serve “resources” (data) using only HTTP (GET, POST, PUT)

/api/{store}/{id}/option.format?options

/api/pdb/2ki5/entry

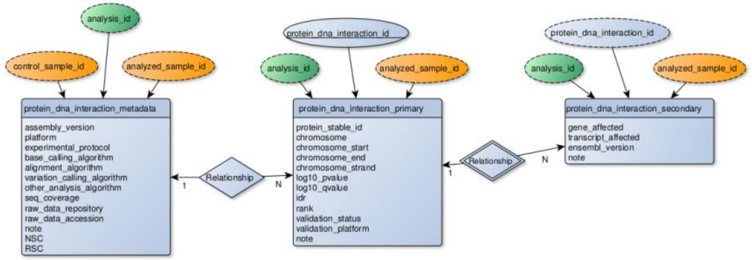
{JSON} <xml />

OPEN API INITIATIVE

SQL *vs* noSQL

Oracle, MySQL, PostgreSQL,…

- Poorer scaling abilities
- A.C.I.D. (**A**tomicity, **C**onsistency, **I**solation, **D**urability)
- Do not map transparently on object-oriented data
- More difficult design
- Static design
- Libraries everywhere



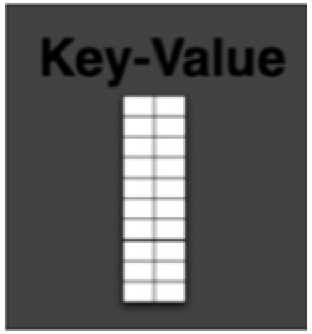
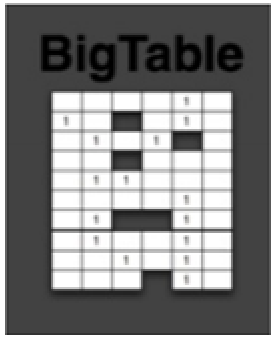
Google BigTable, MongoDB, Hbase, …

- Great scalability, but require larger resources
- B.A.S.E. (**B**asically **A**vailable, **S**oft state, **E**ventually consistent)
- Map complex data structures directly. No additional design
- Libraries everywhere
- Align better with “modern” data representations (JSON or XML)

Relational databases (SQL)

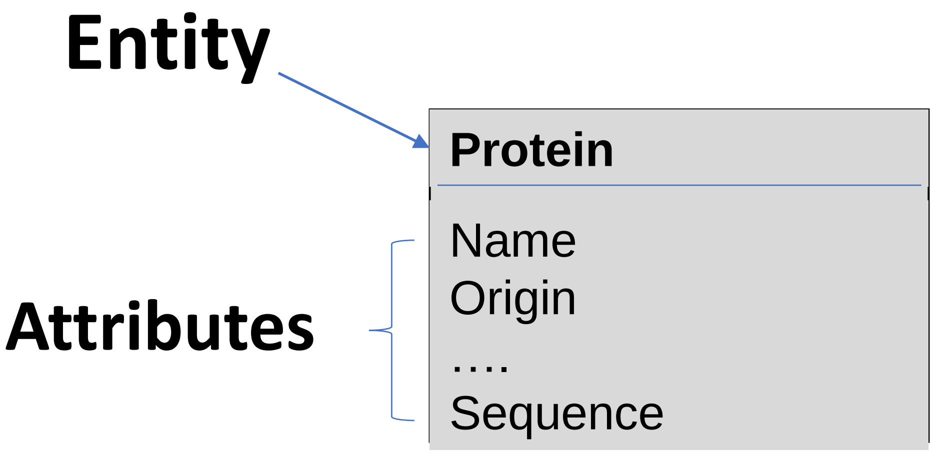
- Most used in general, and especially in bioinformatics
  - This is changing, however…
- Data organized in “tables”
  - Tables contain a number of “records” (rows)
  - Each record has a number of “fields” (columns)
- “Relational” means that logical relationships could be established between fields on different tables.
- Efficiency on data management depends on a “correct” DB design.

NoSQL Databases

Key - Value	Document Based	Column Based	Graph Based
			
amazon DynamoDB	mongoDB	cassandra	AllegroGraph Franz Inc.
	CouchDB relax	HBASE	Neo4j

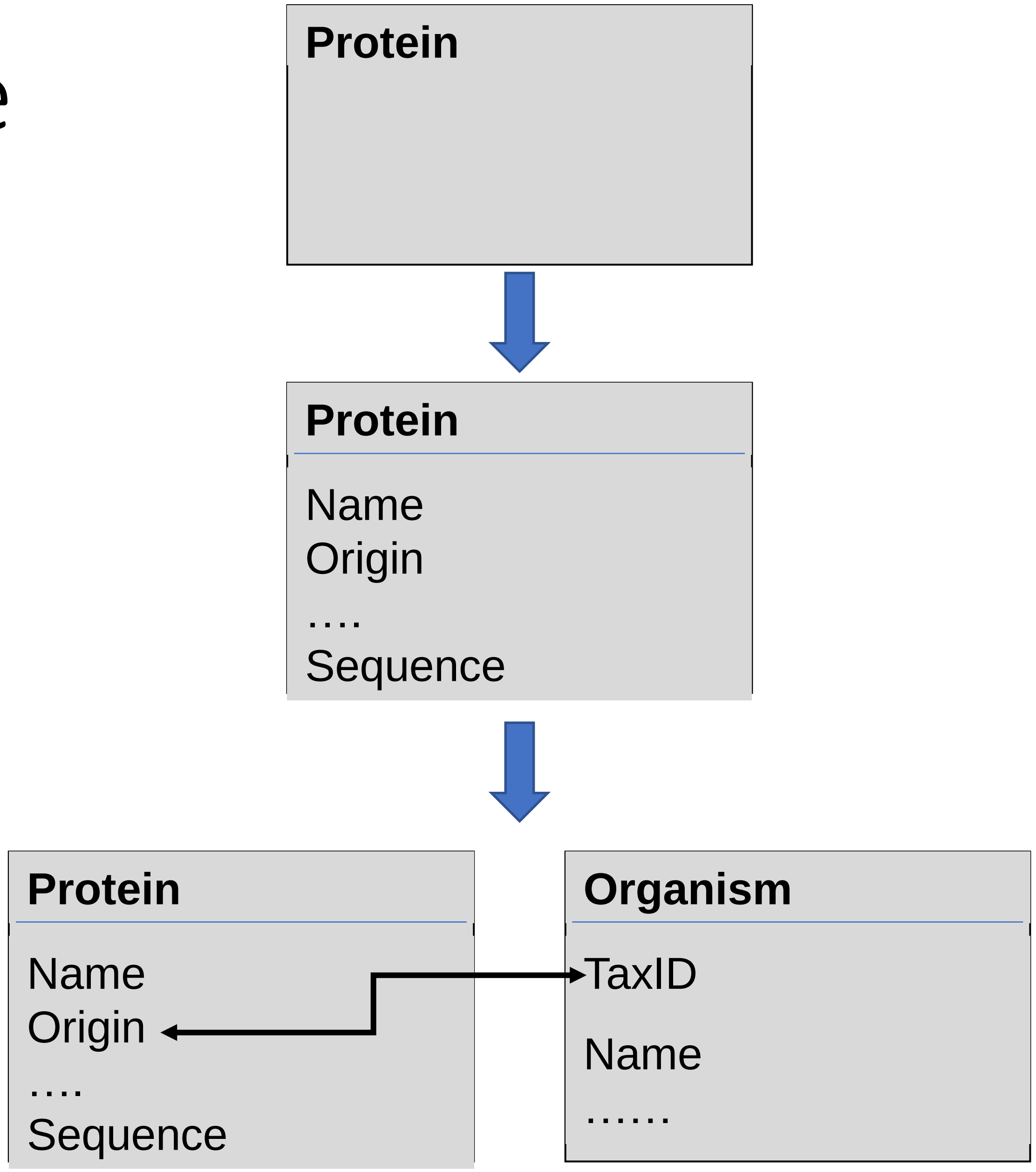
Data modeling

- **Aim:** Define the structure of data types and components to be managed by the application
- First step in designing any application
- Data entities: everything that should be stored/managed
- Entity attributes: information about the entity



Data modeling procedure

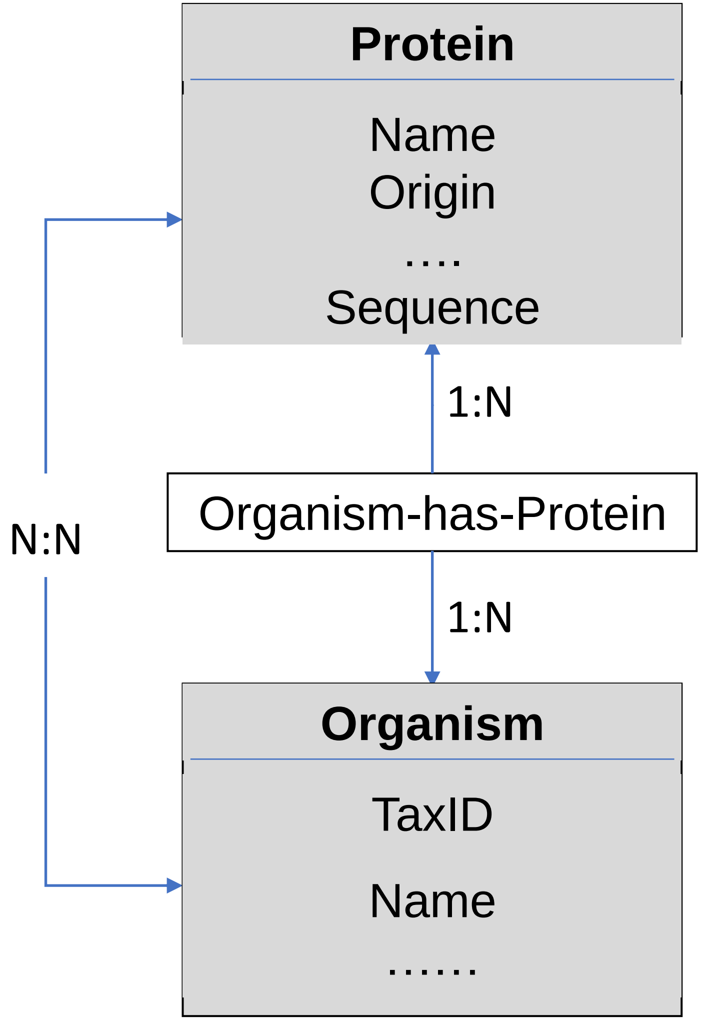
- Identify data entities
  - Data items that "exist" by themselves
- Decide on data attributes
  - Details of every data entity
- Identify data relationships
  - Which attributes relate data entities
- If a Database is involved
  - Define unique identifiers (always useful)
  - Normalize



Relationships

- Associations between entities
  - Relational DBs include explicit keys
  - O-Oriented DBs and languages often “denormalize” date including nested objects

- **1:1** Rare, entities should be merged (common primary key)
  - May be necessary to improve efficiency
- **1:N** most common
  - The “N” classe includes “1” primary key as attribute
- **N:N** A new “hidden” entity exists.
  - The new entity is 1:N to the original entities. Add attributes as necessary.



NoSQL databases do not handle (in general) relationship, but the concept should be considered in the design

Database (SQL) design phylosophy

- Structure of data should be
  - Compact with minimum redundancies
    - Data stored only once (consistency)
    - Space saving
  - Structure oriented to retrieval
    - Most Bioinformatics DBs are store once, retrieve many
    - Obtaining data quick is required
  - Able to grow
    - Data evolves, structure should be flexible
- Relational DBs requires known and fixed data structures
- For unforeseen data structures, use noSQL approach!!

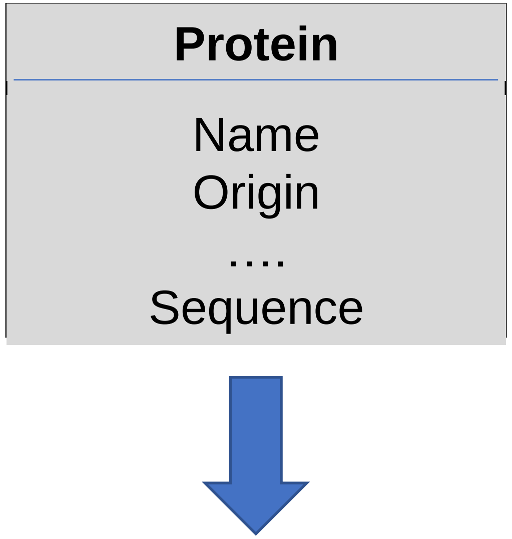
Physical DB design

- Depends on the language/Database type

- Traditional Relational Databases
  - Saving space and avoiding redundancies is the main issue

- NoSQL databases / O-O Programming
  - Space is not an issue, data can be redundant (but consistent), efficiency in insertion/retrieval is the main issue

Physical DB design



- Entities become classes, tables, collections, …
- Attributes become fields (Columns in tables)
- Unique identifiers become primary keys
  - not NULL, never changes
  - Unique identification of a record
  - Can be a combination of several fields
- In SQL DBs Relationships become “foreign keys”

ID	Name	Origin	Sequence
P9WKE1	Thymidylate kinase	8332	MLIAIEGVDGAG KRTLVE…
P04183	Thymidine kinase, cytosolic	9606	MSCINLPTVLPGS PSK…
…	…	…	…

- Keys are usually integers (often with auto-increment), although can be any field.

Normalization of Relational DBs

- Rules to Reduce (eliminate) data redundancies
  - Avoids inconsistencies
  - Allows non-complete insertions or deletions
  - Make easier queries

- 1st Normal Form (1NF)
  - Unique identifiers. Records are independent to each other. All attributes have single values. *Lists of values show hidden entities*

- 2nd Normal Form (2NF)
  - All attributes depend entirely on the entity. *Attribute is misplaced or a new entity*

- 3rd Normal Form (3NF)
  - Data attributes are independent to each other. *Show hidden entitites.*

ETLs

- Extract, Transform, & Load
  - Software designed to populate DBs from the original data sources
  - Normally offline command-line scripts
  - Typically scripting languages (Perl, Python)
  - Data is usually obtained from text files or from Web Services

- Extract:
  - Parsing data input

- Transform:
  - Do the necessary modifications on the data
  - Add new “calculated” fields if necessary

- Load
  - Insert into the DB

From Web apps

- Server side
  - Server-side languages include specific drivers and helpers
  - The usual ones issues database commands (SQL, JSON, …)
    - $result = $db -> mysql_query(“SELECT ^ FROM foo”);
    - $result = $foo_collection->find(array(‘_id’ => ‘any_id’));

  - More elaborated drivers map DB tables/objects into program objects
    - Interaction with DB is made in the background
    - Common in pure o-o languages and programming frameworks

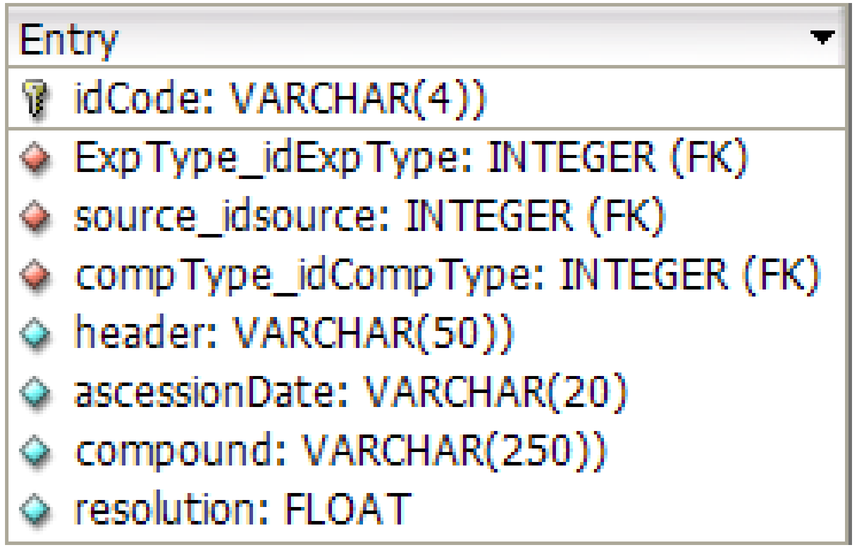
  - DB connections are persistent . Connection is usually made once at the initialization phase for each script.

- Client side
  - Jquery / AJAX may include direct DB connections (not recommended)

MySQL

- Created in 1979 by Michael Widenius
- MySQL 1.0 in 1995
- Uses SQL as query language
- Used in most bioinformatics applications
  - Free, easy to install
  - Now (v $\geq$ 5.x) has most features of a commercial DBMS

- MariaDB is an open source replacement (no differences)
- Drivers
  - PHP: mysqli
  - Python: mysql.connector, pymysql, mysqldb, …




```
CREATE TABLE Entry (
  idCode VARCHAR(4)) NOT NULL,
  ExpType_idExpType INTEGER UNSIGNED NOT
   NULL,
  source_idsource INTEGER UNSIGNED NOT
   NULL,
  compType_idCompType INTEGER UNSIGNED
   NOT NULL,
  header VARCHAR(50)) NULL,
  ascessionDate VARCHAR(20) NULL,
  compound VARCHAR(250)) NULL,
  resolution FLOAT NULL,
  PRIMARY KEY(idCode),
  INDEX
   Entry_FKIndex1(compType_idCompType),
  INDEX Entry_FKIndex3(source_idsource),
  INDEX Entry_FKIndex4(ExpType_idExpType)
);
```

MySQL numeric data types

- Integer (Tinyint, smallint, mediumint, **int**, bigint)
- Bit = Bool = tinyint(1)
- Float (M,D)
- Double (M,D)
- Decimal (M,D) (=dec, fixed)

MySQL text data types

- Char(n), **varchar(n)** (char is fixed length!)
- Binary(n), varbinary(n)
- Tinyblob, **blob(n)**, mediumblob, longblob
- Tinytext, **text(n)**, mediumtext, longtext
- Enum (‘val1’, ‘val2’,…)
- Set (‘val1’, ‘val2’,…)

- Check character sets!!

MySQL Date/time types

- Date yyyy-mm-dd
- Datetime yyyy-mm-dd hh:mm:ss
- Timestamp
- Time hh:mm:ss
- Year (2|4)

- Be careful with order, can depend on O.S.!!
  - Safe alternative use string: YYYY-MM-DD:HH-MM

Data initialization

- DEFAULT constant
- Auto-increment
- NOT NULL
- ZEROFILL (left padding)
- SIGNED/UNSIGNED

Table types

- MyISAM.
  - Each table, index, etc. is a file
- **InnoDB**.
  - Default, transaction safe, allows advanced operations
- Memory
  - Hash indexes
- Merge
  - Several MyISAM identical tables accessed together
- Archive
  - Good for long term storage (no Update or delete)
- Federated
  - Distributed among diferent servers
- NDB
  - Fast
- CSV
  - Text oriented
- Blackhole

Basic SQL

- Table manipulation
  - CREATE TABLE, ALTER TABLE, DROP TABLE, RENAME TABLE, CREATE INDEX, DROP INDEX
  - Usually done with helper software (Mysql Workbench, PhpMyAdmin)

- Storing data
  - INSERT INTO table (col1, col2,…) VALUES (val1,val2,…)
  - LOAD DATA INFILE ‘file_name’
  - REPLACE
    - Like INSERT but replaces rows with the same primary key
  - UPDATE table SET col1=val1, coln=valn WHERE ‘some_condition’

- Retrieving data
  - SELECT col1, …. FROM table1, table2,… WHERE ‘some condition’ ORDER BY col