BIT05 - Databanktechnologie

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Overview

The student is able to
- Solve exercises on both normalisation and database creation
- Create a database model
- Recognise several database types
- Use online databases

Course material
- Slides on LEHO

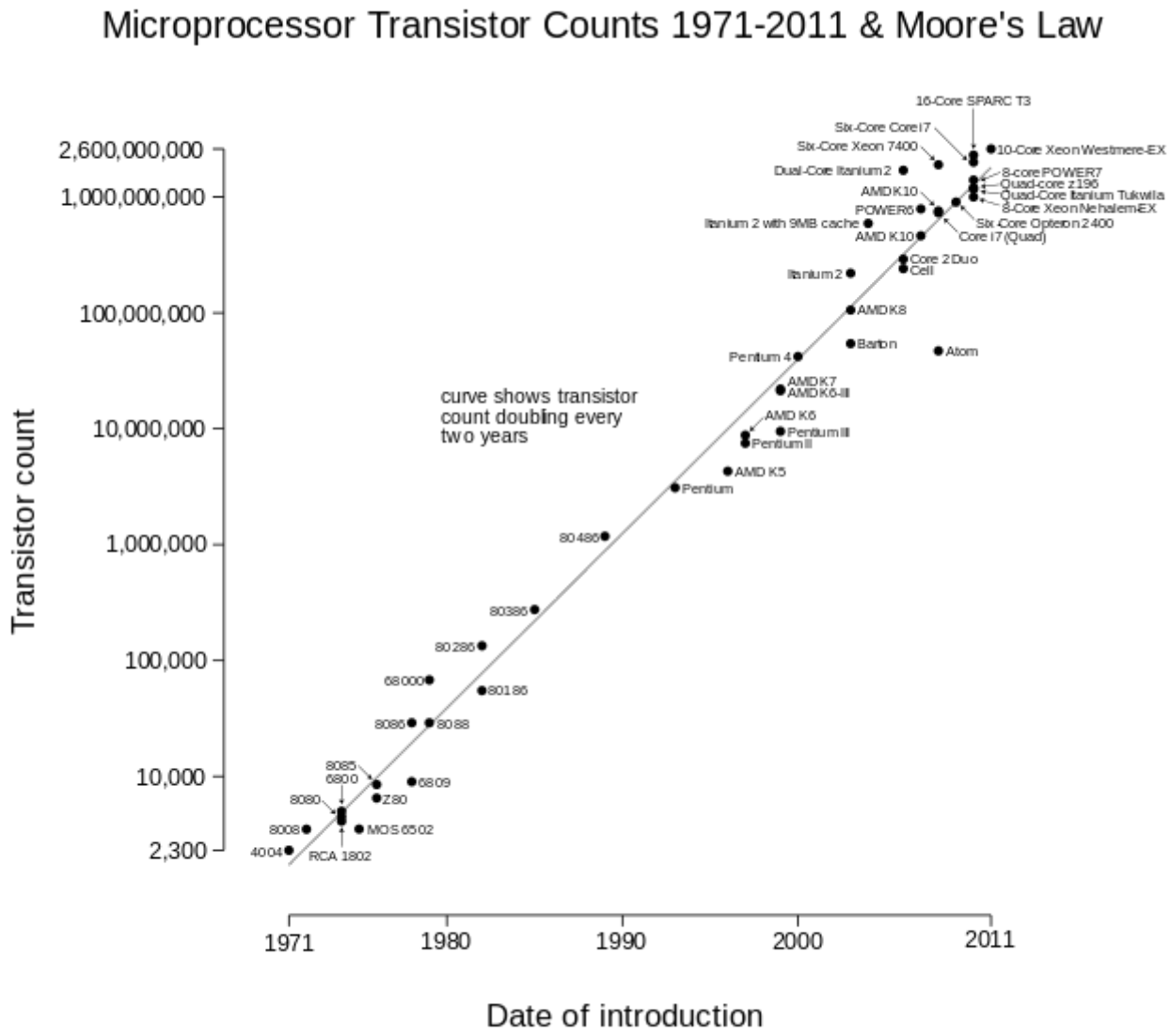
Examination
- Theoretical and practical part

Requirements

- A working internet connection

Lecture 1 – Introduction & relational databases 1

Introduction



Introduction

IBM 3380

1985

~ 1,000,000 USD

8 x 2.5 GB = 20 GB storage!

SanDisk microSD

2017

€ 84! (bol.com)

200 GB storage

Introduction

1 genome

+ 10 year

20 labs

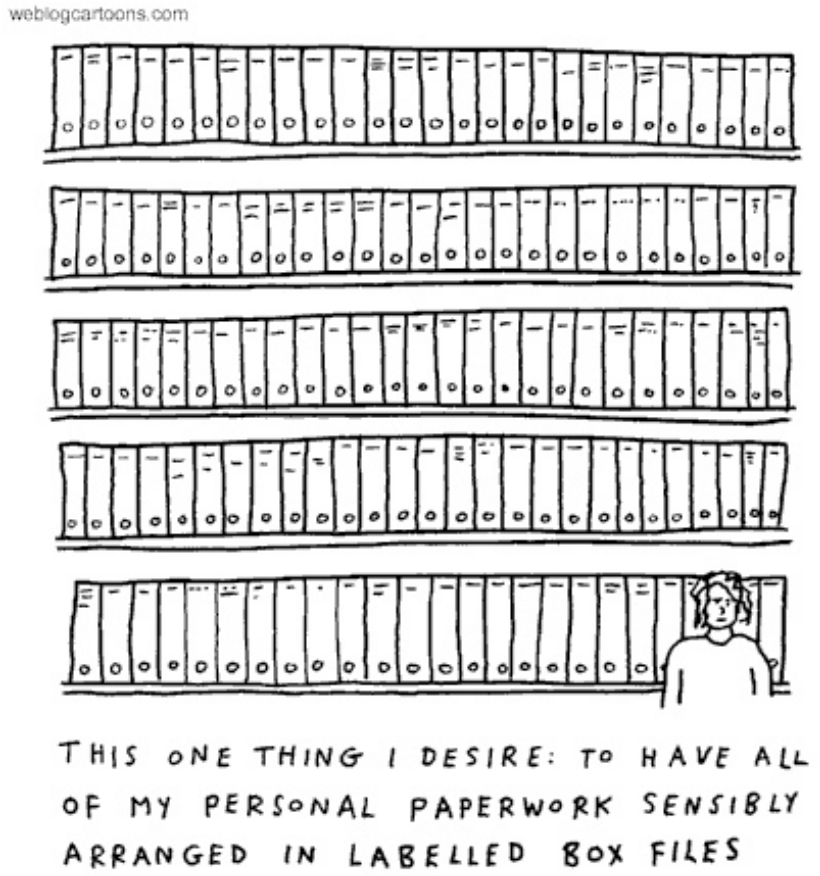
~ 3 billion USD

6 genomes

1 - 3,5 days

~ 1000 USD

Introduction



Storage

Structured storage

Introduction

Database

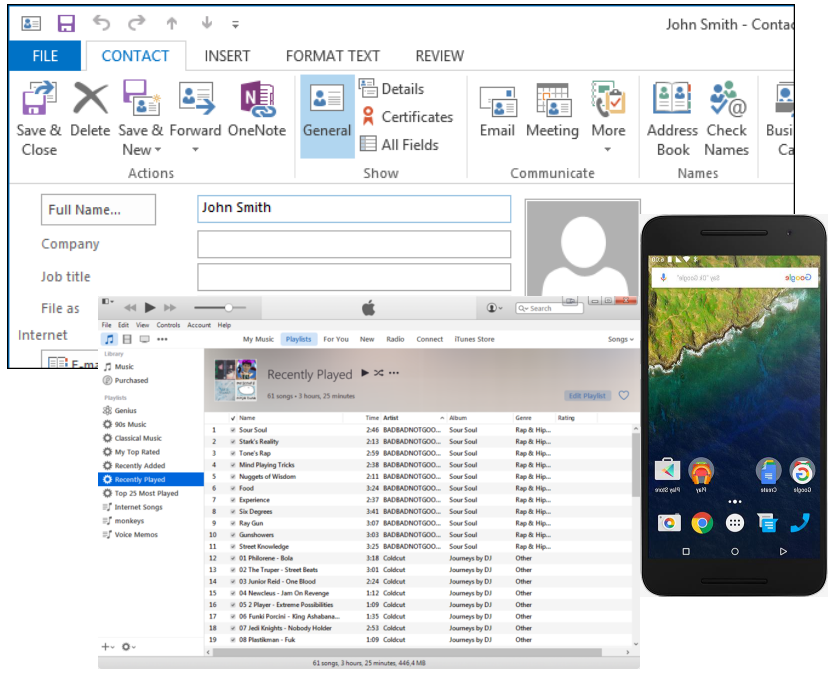
- Mechanism used to store information
- Collection of data (numbers, dates, text, …)
- Structured storage of data
- Efficient interaction with data
    - CRUD

- **Used everywhere!**

Introduction

Database driven websites

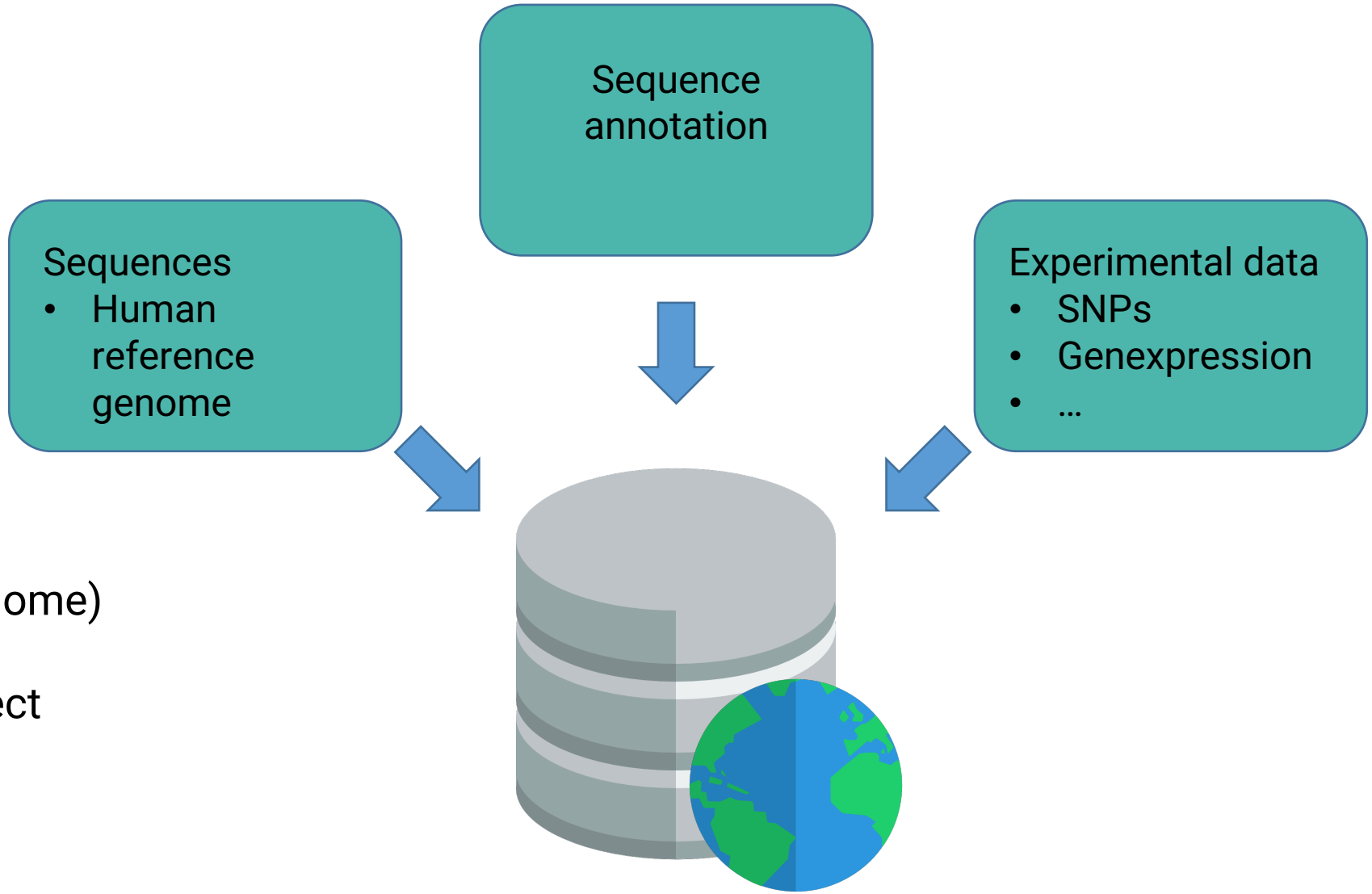
Company databases (customers, stock, data warehousing)



Local databases

Introduction

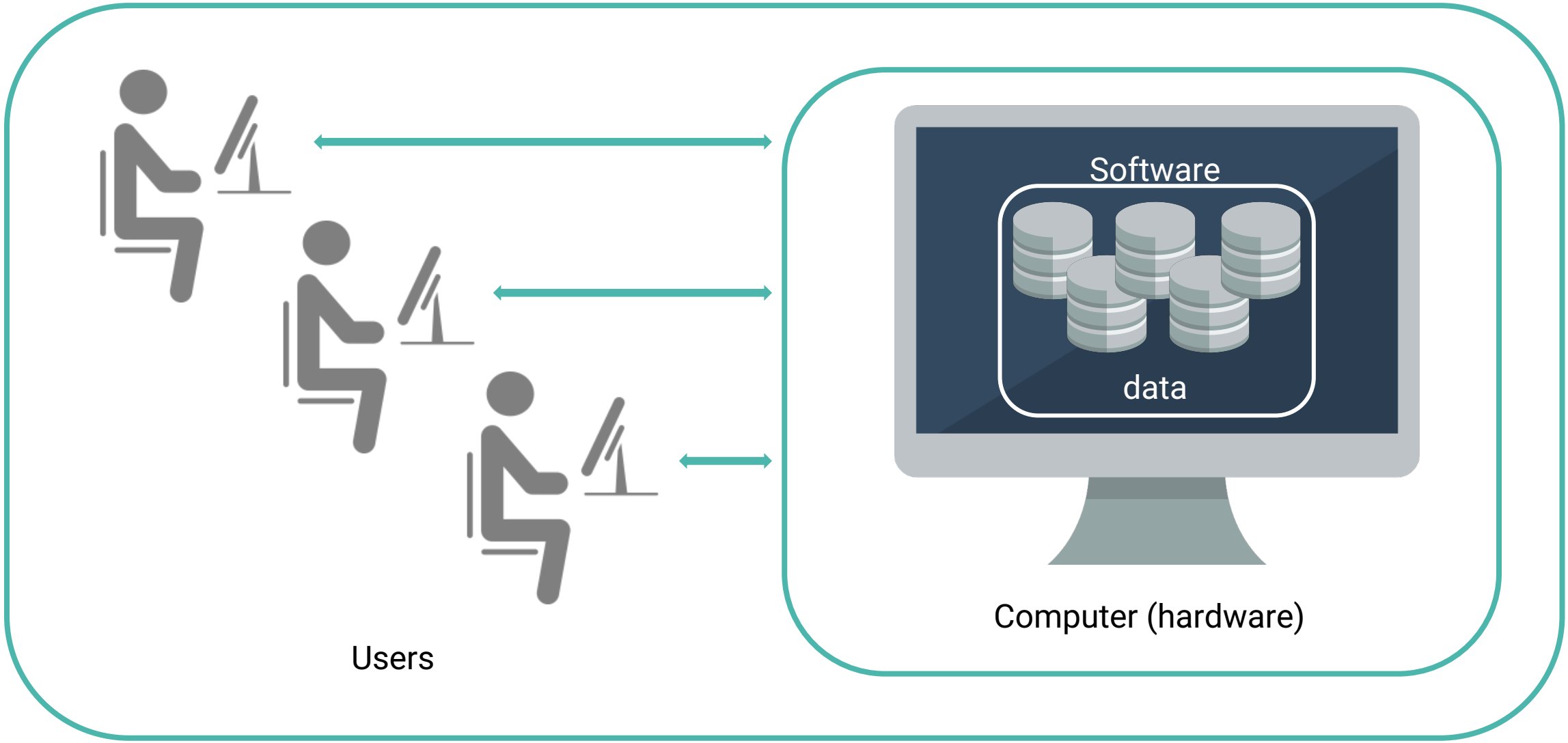
Databases in research



Examples:

- Ensembl, UCSC (genome)
- Encode project
- 1000 genomes project
- …

Introduction

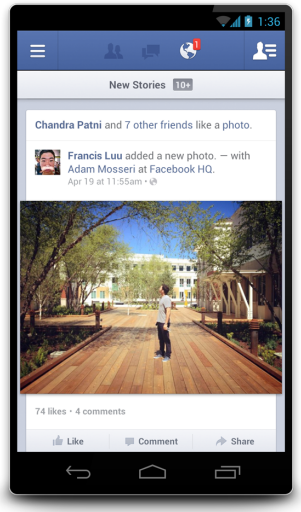


Introduction

Database system

- Hardware
  - Processor and internal memory
  - Personal laptop – server cluster
- Data
  - Structured storage
  - Little redundancy
  - Shared (single-user vs. multi-user)
- Software
  - Database Management System (DBMS)
    - Data storage
    - Data retrieval
    - Data manipulation
- Users
  - Authentication & authorization
  - Administrator > end-user

Introduction



View level

View 1

View 2

...

View N

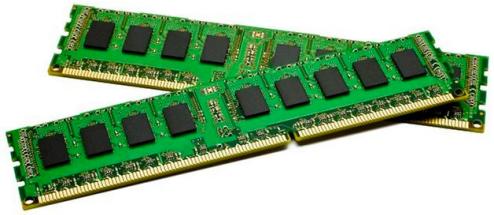
Patients
Patient_id INT PK
Patient_name
Demographic_Info INT FK
Indexes
PRIMARY id

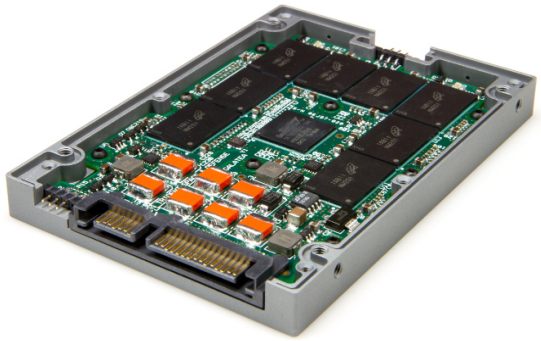
Medication
Medication_id INT PK
Patient_id INT FK
Medication_name
Indexes
PRIMARY id

Diagnoses
Diagnosis_id INT PK
Patient_id INT FK
Diagnosis
Indexes
PRIMARY id

Logical level

Logical data independence





Physical level

Physical data independence

Introduction

A good database system

- Sufficient amount of storage
  - Think ahead
- Easily accessible
  - Centralised system
- Secured against non-users
  - Per user rights
- Easily maintainable
  - Add, edit, delete data
- Controlled input
  - All data in same format
- Quick!
  - Queries need to be run within a certain time
- Little redundancy
  - Do not store the same information twice (or more)
  - Application dependable
- Clear structure

Introduction

Database Management System (DBMS)

- A **database management system** (**DBMS**) is a computer software application that interacts with the user, other applications, and the database itself to capture and analyse data
- Shields users from hardware and storage details
- Most important software component, though not the only one (development tools, …)

- Used for
  - Data storage
  - Data retrieval
  - Data manipulation
  - Authentication & authorization

Introduction

Database Management System (DBMS) examples

- MySQL

- Oracle

- Access

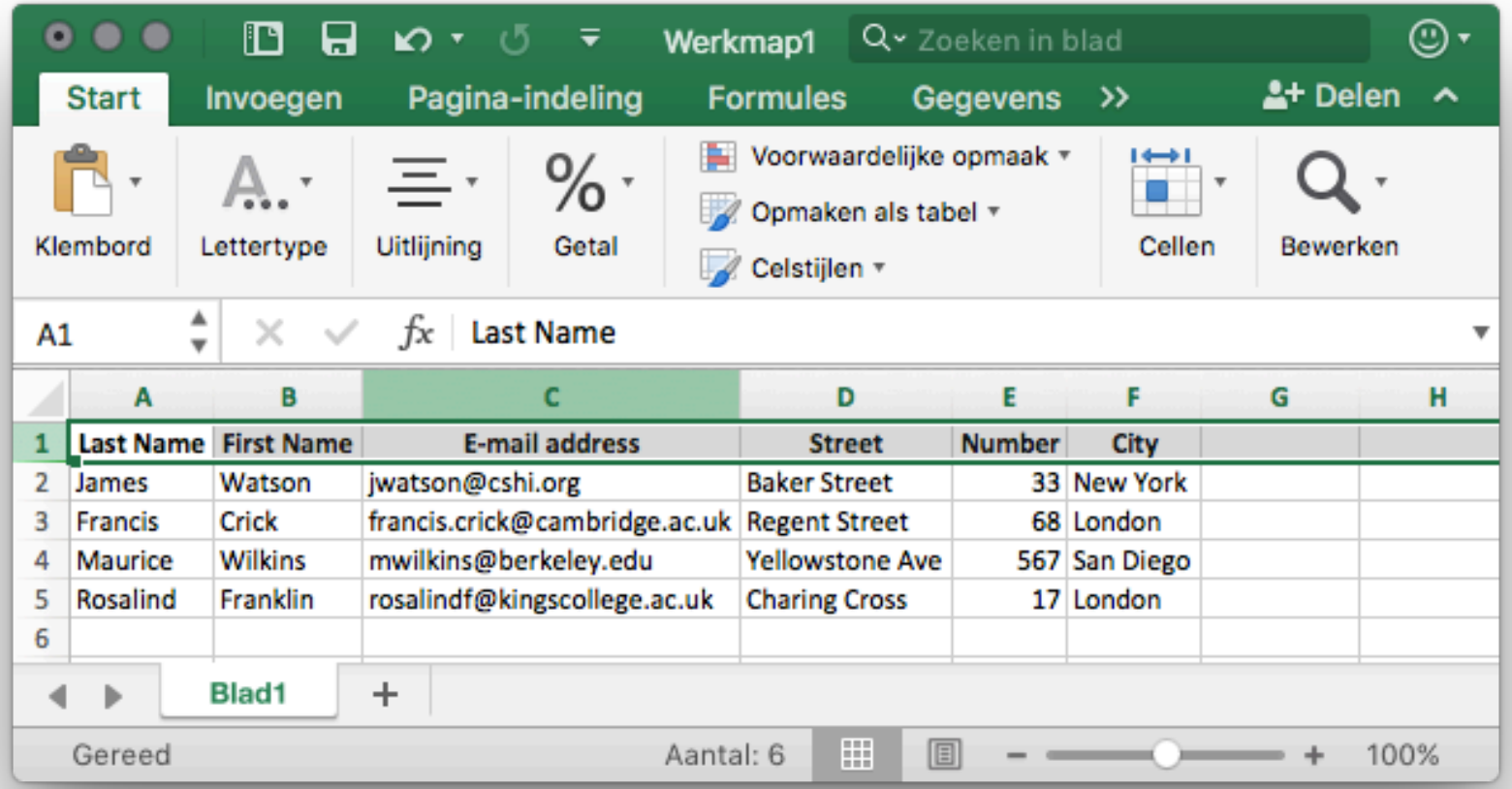
- Sybase, Informix, DB2, Ingres, SQL Server, SQLite
- NoSQL systems

- NewSQL systems

Introduction

Relational databases

- Rigid structure
- 2 dimensional *tables*
  - Columns (fields)
  - Rows (records)



	A	B	C	D	E	F	G	H
1	Last Name	First Name	E-mail address	Street	Number	City		
2	James	Watson	jwatson@cshi.org	Baker Street	33	New York		
3	Francis	Crick	francis.crick@cambridge.ac.uk	Regent Street	68	London		
4	Maurice	Wilkins	mwilkins@berkeley.edu	Yellowstone Ave	567	San Diego		
5	Rosalind	Franklin	rosalindf@kingscollege.ac.uk	Charing Cross	17	London		
6								

Introduction

Relational databases

- Model objects (entities) and their relationships
- E.g. *a store sells products to customers*
  - Entities:
    - Customers
      Attributes: name, address, telephone number, …
    - Products
      Attributes: name, price, …
  - Relationships:
    - Sale
      Attributes: quantity, timestamp, …

Introduction

Relational Database Management Systems (RDBMS)

- Enforce data integrity
  - Honours constraints on columns
- Enforce referential integrity
  - Honours constraints on relations

! 12 rules of Edgar Codd!

Introduction

Relational Database Management Systems (RDBMS)

- Commercial products
  - Oracle
  - DB2 (IBM)
  - MS SQL Server (Microsoft)
- Open-source
  - **MySQL (Oracle)**
  - PostgreSQL
  - SQLite

Introduction

Relational Database with MySQL

- Most used RDBMS
- Open source
- Free of charge (paying versions exist)
- Wordpress, Twitter, Facebook, …

- http://www.mysql.com

Introduction

Installing MySQL on your system

- Linux
  - http://dev.mysql.com/doc/refman/5.7/en/linux-installation.html
- Mac
  - http://dev.mysql.com/doc/refman/5.7/en/osx-installation.html
- Windows
  - http://dev.mysql.com/doc/refman/5.7/en/windows-installation.html

Introduction

Starting/stopping/restarting MySQL

- Linux/Mac

```
$ /etc/init.d/mysqld start    service mysqld start      service mysql start
$ /etc/init.d/mysqld stop     service mysqld stop       service mysql stop
$ /etc/init.d/mysqld restart  service mysqld restart    service mysql restart
```

- Windows

```
$ C:\> "C:\Program Files\MySQL\MySQL Server 5.7\bin\mysqld”
$ C:\> "C:\Program Files\MySQL\MySQL Server 5.7\bin\mysqladmin" -u root shutdown
```

Introduction

Check whether or not MySQL is running correctly

- Linux/Mac

```
$ service mysqld status       (service mysql status)
mysql start/running, process 3394
$ ps -ef | grep mysql
mysql 3394 1 0 12:09 ? 00:00:00 /usr/sbin/mysqld
$ netstat -ltpn | grep mysql
tcp 0 0 0.0.0.0:3306 0.0.0.0:* LISTEN 3394/mysqld
```

- Windows

```
$ C:\> "C:\Program Files\MySQL\MySQL Server 5.7\bin\mysqlshow"
$ C:\> "C:\Program Files\MySQL\MySQL Server 5.7\bin\mysqlshow" -u root mysql
$ C:\> "C:\Program Files\MySQL\MySQL Server 5.7\bin\mysqladmin" version status proc
$ C:\> "C:\Program Files\MySQL\MySQL Server 5.7\bin\mysql" test
```

  Or check running services through *Control Panel*

Introduction

Exercises

- Install MySQL
- Start the service
- Check whether or not the service has been started

Introduction

The MySQL monitor

- To connect or log on to a MySQL database service

  ```
  $ mysql
  ```

- Many options, check the manual

  ```
  $ man mysql
  ```

  or

  ```
  $ mysql --help
  ```

Introduction

The MySQL monitor

- Most important options

```
$ mysql [options] [database]
    -u uname | --user=name
            default: UNIX account
    -p [pwd] | --password[=pwd]
            default: <none>
    -h hname | --host=name
            default: localhost
    -P prt | --port=prt
            default: 3306
```

Introduction

Exercises

- Connect to the database and execute the following commands

```
mysql> select current_user;
mysql> show databases;
```

Introduction

Securing the server

```
$ mysql_secure_installation
```

- Set password for root accounts
- Remove anonymous-user accounts
- Remove remote root login
- Remove test database

Introduction

Securing the server – extra

- Prevent any external access to the database server
  - Add to global config file (*/etc/mysql/my.cnf*)

```
[mysqld]
bind-address = 127.0.0.1
```

Introduction

Exercises

- Secure your MySQL installation
  - Drop test database
  - Set root user password
- Repeat previous exercise(s) and mind the differences

Introduction

Database users

- Database users and OS users are completely independent from each other
  - No user specified --> OS user is taken
  - Database superadmin --> *root@localhost* (all rights, including dropping databases)
- Not a good idea to always connect as root!!!

Introduction

Exercises

- Create a database user
  - Choose a username and password you can remember, but that is still safe
  - Hostname: *localhost*
- Try to connect as this user and execute following SQL statements

```
mysql> select current_user;
mysql> show databases;
```

Introduction

Database user - privileges

- Created user has very limited privileges
- Grant privileges *prv* on table *tbl* in database *db*

```
mysql> GRANT prv ON db.tbl TO user@host;
```

- Some wild cards
  - All privileges, specify `all` as *prv*
  - All databases, specify * as *db*
  - All tables, specify * as *tbl*
- The given database and table names do not have to exist (yet)

Introduction

The options file

- Avoid retyping of password with every connection, create options file
  - `.my.cnf`
  - Located in home directory
  - Protect from others: mode 600
- Contains *key=value* pairs in [sections]
  - Provided as (invisible) command line parameters

Introduction

The options file - example

- Put password in options file
  - Command line parameters of mysql

    $ mysql --password=*pwd*
- Options file could look like this

```
[client]
password=pwd
user=username
```

Introduction

Exercises

- Create an options file and put your password in it
  - Make sure the options file protected on the OS level
- Try to connect as to the database without specifying a password

Introduction

SQL: Structured Query Language

- **Data Definition Language** (DDL) statements: design (create, alter, drop, …) database
  `CREATE TABLE, DROP DATABASE`
- **Data Manipulation Language** (DML) statements: manage data
  - **C**reate: add new data
  - **R**ead: collect data
  - **U**pdate: alter data
  - **D**elete: remove data

  `SELECT, INSERT, UPDATE, DELETE`
- **Data Control Language** (DCL) statements: manage database rights
  `GRANT, REVOKE`

- **Transaction Control Language** (TCL) statements: manage DML tasks (group, undo, …)

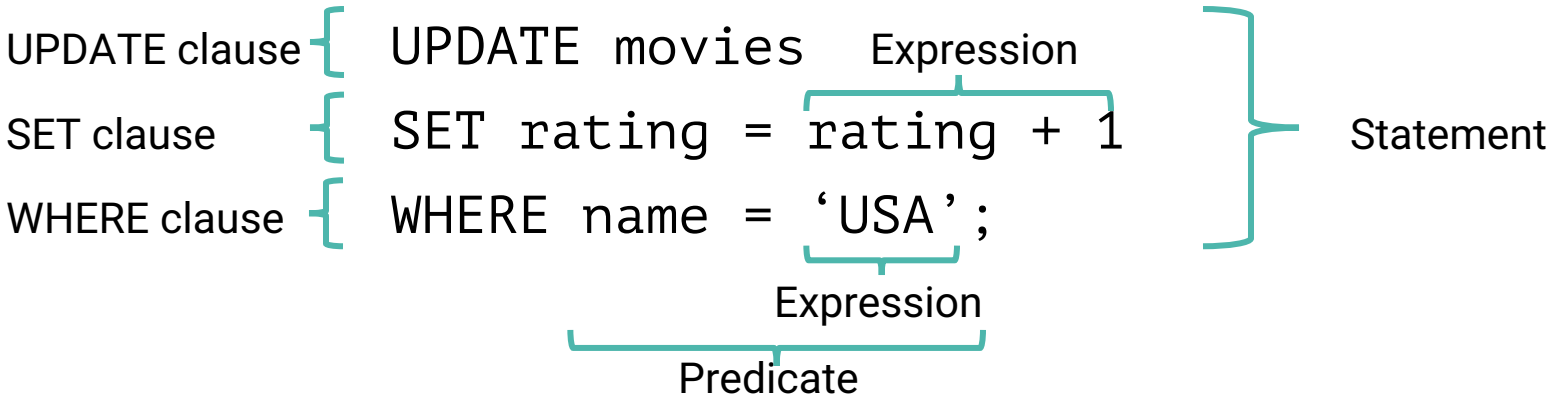
Introduction

SQL: Structured Query Language

- Clauses: components of statements and queries
- Expressions: produce scalar values, or tables consisting of columns and rows of data
- Predicates: conditions or Booleans, used to limit effects of statements and queries
- Queries: retrieve data based on specific criteria
- Statements: effect on schemata and data, control transactions, connections, …
  - End with semicolon (“;”)
- Whitespace: generally ignored, used for readability

Introduction

SQL: Structured Query Language



Introduction

The MySQL monitor (again)

- Several ways to execute SQL statements using the MySQL monitor
  - Interactively

    ```
    $ mysql [database]
    mysql> stmt
    ```

  - From the command line

    ```
    $ mysql [database] -e 'stmt'
    ```

  - From a file or a pipe (stdin)

    ```
    $ mysql [database] < stmt_file
    $ cat stmt_file | mysql [database]
    ```

Introduction

Creating a database

- Only database users with significant privileges can create databases
  - From the command line

    `$ mysqladmin [opt] create` *`dbname`*

    `mysqladmin` has the same command line options as `mysql`
  - From within the mysql monitor

    `mysql> create database` *`dbname`*

Introduction

Exercises

- As *root@localhost*, create database '*`biodb`*'
- Grant all privileges to the database user you created before
- Download the `1.sql` (first take a look at the contents)
- Execute all SQL statements in the file

Introduction

Hierarchy

- A single MySQL service can have multiple databases

  ```
  mysql > SHOW databases;
  ```

- A particular database *db* can have multiple tables

  ```
  mysql > USE db;
  mysql > SHOW tables;
  ```

- A particular table *tbl* can have multiple columns or fields

  ```
  mysql > SHOW columns FROM tbl;
  mysql > SHOW create table tbl;
  ```

Introduction

Exercises

- Connect to the database service as a normal user
- What databases do you see?
- What tables are defined in *biodb*?
- What are the column names?

Relational databases with MySQL

- MySQL database = collection of tables
  - Table = set columns with specific types
    - Number, text, date, …
    - Each row in same format
    - Only 1 value per field

Student_number	Name	Last_name	Birthdate	Sex
0293826	John	Doe	1991-10-02	M
0293749	Mel	Trotter	1991-04-11	V
0328273	Bill	Schuette	1990-12-01	M

Relational databases with MySQL

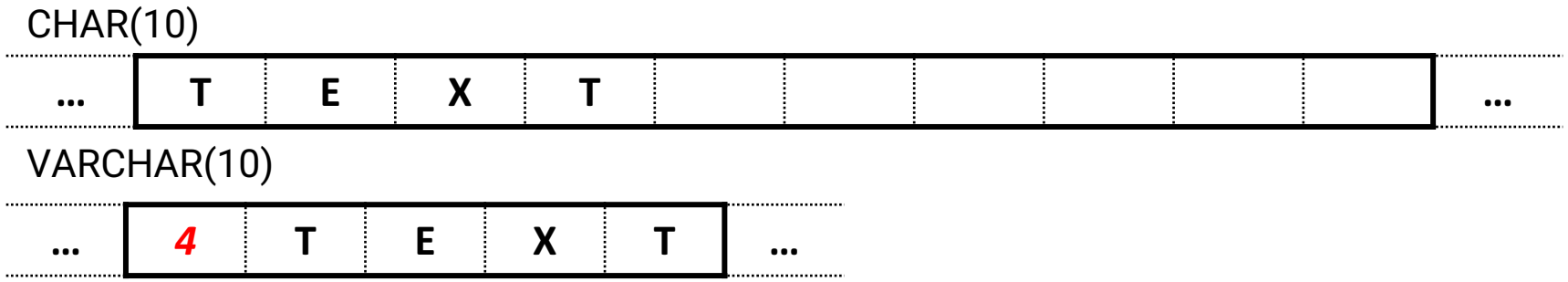
Column types

- INT
  - Integer
  - SIGNED: -2 147 483 648 tot 2 147 483 647
  - UNSIGNED: 0 tot 4 294 967 295
  - TINYINT, BIGINT, SMALLINT
- FLOAT & DOUBLE
  - Numbers with decimal point
  - FLOAT: 7 digits after decimal point, DOUBLE: 15 digits after decimal point
- DATE
  - YYYY-MM-DD
  - DATETIME
    - YYYY-MM-DD HH:MM:SS
    - ! TIMESTAMP ! No dates < 1970 and > 2038

Relational databases with MySQL

Column types

- VARCHAR & CHAR
  - String with a certain number of characters
  - Define max number of characters e.g. VARCHAR(200)
  - VARCHAR: up to 65 535 characters
  - CHAR: up to 255 characters, spaces are added to reach required length



  - VARCHAR is more efficient in storage, CHAR is faster for reading data
  - Similar for INT vs BIGINT vs ...

Relational databases with MySQL

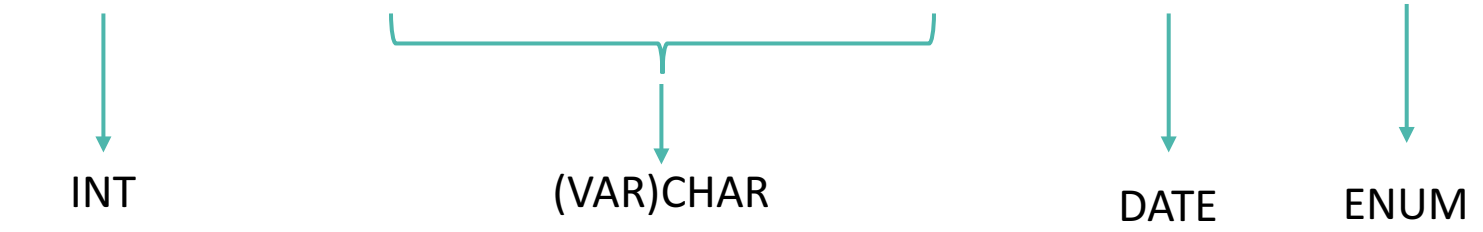
Column types

- TEXT & BLOB
  - Used for texts that are not queried often or do not have to be searchable
  - BLOB for binary data (images, …)
- ENUM
  - List of permitted values
    - E.g. Set of colours: ’red’, ‘green’, ‘blue’
  - Very efficient

Relational databases with MySQL

Column types

Student_number	Name	Last_name	Birthdate	Sex
0293826	John	Doe	1991-10-02	M
0293749	Mel	Trotter	1991-04-11	V
0328273	Bill	Schuette	1990-12-01	M



Relational databases with MySQL

Column types

- Every row has to be unique
  - DBMS is able to distinguish separate rows

Student_number	Name	Last_name	Birthdate	Sex
0293826	John	Doe	1991-10-02	M
0293749	Mel	Trotter	1991-04-11	V
0328273	Bill	Schuette	1990-12-01	M

Primary key: column that makes sure every row is unique!

- Usually first column
- INT
- auto_increment: adds 1 to each value automatically

Relational databases with MySQL

Constraints

On top of column types, there are some additional requirements per column

- Primary key
  - Only 1 PK per table, all values must be unique
- UNIQUE
  - All values (or combinations) must be unique
- NOT NULL
  - Field can not be empty when adding data (empty = null)
- Default
  - Default value for a field
- Foreign key
  - Same constraints as referenced column
  - Security when adjusting linked data possible

Relational databases with MySQL

Summary – database structure

MySQL database

→ table

→ row

→ column

column type

constraint(s)

Relational databases with MySQL

`INSERT` – add new rows

```
INSERT INTO tbl (col1, col2) VALUES (val1, val2);
INSERT INTO students (student_number, name, last_name) VALUES
(2654897, ‘Glenn’, ‘Walker’);
```

- Be aware!
  - Not all columns need to be included in query, unmentioned columns are given the default value for that column
  - Empty column gets null value
  - Columns with NOT NULL constraint required a value
  - Strings are written between quotes

Relational databases with MySQL

`SELECT`– retrieve rows

```
SELECT columns FROM tbl;
SELECT * FROM modorg;
SELECT genus, species FROM modorg;
```

- *`columns`*
  - List of columns, separated by comma
  - * for all columns
  - Use of arithmic operators (+, -, …) and other functions (min, max, …) on columns is possible
- *`tbl`*
  - Single table or multiple tables joined together
  - Subquery
  - View

Relational databases with MySQL

`ORDER BY` – sort rows

```
SELECT columns FROM tbl ORDER BY col1 [asc|desc] [, col2
[asc|desc]...];
```

When using `SELECT` statements, the data is displayed in no particular order

→ use `ORDER BY` clause

- *colX*: a column or a column alias
- *asc*: ascending order (default)
- *desc*: descending order

Relational databases with MySQL

Exercices

- Show the names (genus & species) of all model organisms in the order of the publishing date of the draft
- Show the names (genus & species) of all model organisms sorted by the number of chromosomes (most chromosomes on top) and then alphabetically by name

Relational databases with MySQL

Calculated rows

- You can add columns in a query that calculate some value using other columns of the same row
- Lot of functions and operators readily available

```
mysql> SELECT 6*7;
mysql> SELECT concat(class, “ “, genus) FROM modorg;
mysql> SELECT now();
```

Relational databases with MySQL

Calculated rows – numbers

- Operators

  `+, -, *, /, %`

- Functions

  ```
  sqrt(x), power(x, y), …
  exp(x), ln(x), …
  sin(x), cos(x)
  round(x), ceil(x), floor(x), …
  rand(), rand(x)
  ```

Relational databases with MySQL

Calculated rows – strings

- Functions

```
length(s)
concat(s1, …)
upper(s), lower(s)
trim(s), ltrim(s), rtrim(s)
substr(s, …)
reverse(s)
truncate(s)
```

Relational databases with MySQL

Calculated rows – dates

- Functions

```
currentdate(), now()
year(d), month(d), week(d)
dayofmonth(d), dayofweek(d)
hour(d), minute(d), second(d)
```

Relational databases with MySQL

Exercices

- Show
  - Model organism full name (as one column)
  - Genome size (as Gb), rounded to 4 digits
  - Average chromosome size
  - Publication year

  of all rows sorted by average chromosome size (largest on top)

Relational databases with MySQL

Column aliases

- Columns can be renamed
  `SELECT` *`col`* `[AS]` *`alias`* …
- The aliases can be used in the `ORDER BY` clause

Relational databases with MySQL

Exercices

- Show
  - Model organism full name (as one column) as name
  - Average chromosome size as avgsize
  - Publication year as pubyear

  of all rows sorted by avgsize (largest on top)

Relational databases with MySQL

`WHERE` – filter rows

```
SELECT columns FROM tbl WHERE condition(s) [ORDER BY sortcol];
```

- *conditions*
  - One or more conditions, combined with `AND`, `OR`, `NOT`, `XOR`
  - Only row for which the `condition(s)` evaluates `TRUE` are selected
  - Unable to use column aliases in `condition(s)`

Relational databases with MySQL

Filtering rows – conditions

- Numerical comparison operators
  - `=`
  - `!=` or `<>`
  - `<`, `<=`, `>`, `>=`
  - `between` *x* `and` *y* (inclusive)

- E.g. select all organisms with more than 10 chromosomes

```
SELECT genus, species FROM modorg WHERE nchr > 10;
```

Relational databases with MySQL

Filtering rows – conditions

- String comparison operators
  - =
  - `!=` or `<>`
  - `<`, `<=`, `>`, `>=` (lexical)
  - `like “pattern”`
    matches a pattern
    - `_` (A single character)
    - % (zero or more characters)
  - `rlike “regex”` [MySQL]
    matches a regular expression

- E.g. select all mammals

```
SELECT genus, species FROM modorg WHERE class = “mammals”;
```

Relational databases with MySQL

Filtering rows – conditions

- Dealing with NULL-values
  - Testing for NULL-ness

    `SELECT … WHERE col IS NULL;`

    `SELECT … WHERE col IS NOT NULL;`
  - Substitution of NULL-values

    `SELECT ifnull(col, value) …`
    this function returns
    - *col* if *col* is NOT NULL
    - *value* if *col* is NULL

    e.g. `SELECT genus, species, ifnull(nchr, 0) FROM modorg;`

Relational databases with MySQL

Filtering rows – conditions

- Boolean logic
  - *not x*
    Evaluates TRUE if *x* is FALSE
  - *x and y*
    Evaluates TRUE if both *x* and *y* are TRUE
  - *x or y*
    Evaluates TRUE if *x* or *y* is TRUE, or both
  - *x xor y (exclusive or)*
    Evaluates TRUE if *x* or *y* is TRUE, but not both

Relational databases with MySQL

Exercises

- Select all mammals with genomes published after 2005
- Select all organisms that have an average chromosome size between 10 and 100 Mbp
- Select all organisms whose genus starts with A, B, C, D, or E

Relational databases with MySQL

Filtering rows – duplicates

- Eliminate duplicate rows
  `SELECT DISTINCT(`*`cols`*`) FROM …`
  → Each combination of *`cols`* is unique

Relational databases with MySQL

Filtering rows – limiting output

- Limit the number of rows in a result set
  `SELECT … LIMIT` *n* `[OFFSET` *r*`];`

- Result set is limited to a maximum of *n* rows
- If an offset *r* is given, the first *r* rows are skipped
- Mostly used in combination with `ORDER BY`

Relational databases with MySQL

Exercises

- Give an overview of all organism classes in the dataset (sorted alphabetically)
- Show the organism names of the top 3 largest genome sizes

Relational databases with MySQL

Aggregation

- Queries are concentrated on particular rows
- Possible to calculate a single result across multiple rows
  e.g. maximum genome size?
- SQL allows you to
  - Specify criteria to group rows together
  - Calculate a single value per group
  - Filter grouped data

Relational databases with MySQL

Aggregation

- Functions
  - `count(col)`, `count(*)`, `count(distinct col)`
  - `sum(col)`
  - `min(col)`, `max(col)`
  - `avg(col)`, `stddev(col)`, `variance(col)`

Relational databases with MySQL

Exercises

- All these queries return a row count. What is the result and why?

```
SELECT count(*) FROM modorg;
SELECT count(nchr) FROM modorg;
SELECT count(class) FROM modorg;
SELECT count(DISTINCT class) FROM modorg;
```

- How many mammals are in the database?

Relational databases with MySQL

`GROUP BY` - aggregation

- Sort data into groups for aggregation purposes

  ```
  SELECT [col,] aggregatefunctions FROM src [WHERE cond] GROUP BY
  col [ORDER BY …];
  ```

- All rows with the same value in *`col`* are grouped
- For each group, the aggregate function is calculated
- No sense in select other columns than *`col`*

Relational databases with MySQL

Exercises

- How many organisms are present in the dataset for each class?
  Note the sort order.
- Show the minimum and the maximum genome sizes for each class.
  Take only those organisms into account for which genome sizes are known.
  Sort the results such that the biggest maximum genome size is on top.

Relational databases with MySQL

Aggregation – filtering

- Filter results based on the results of aggregate functions using HAVING clause

```
SELECT [col, ] aggregatefunctions FROM src [WHERE cond1] GROUP BY col HAVING cond2 [ORDER BY …];
```

- Column aliases can be used in *cond2*

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```
SELECT
    [ALL | DISTINCT | DISTINCTROW ]
      [HIGH_PRIORITY]
      [STRAIGHT_JOIN]
      [SQL_SMALL_RESULT] [SQL_BIG_RESULT] [SQL_BUFFER_RESULT]
      [SQL_CACHE | SQL_NO_CACHE] [SQL_CALC_FOUND_ROWS]
    select_expr [, select_expr ...]
    [FROM table_references
    [WHERE where_condition]
    [GROUP BY {col_name | expr | position}
      [ASC | DESC], ... [WITH ROLLUP]]
    [HAVING where_condition]
    [ORDER BY {col_name | expr | position}
      [ASC | DESC], ...]
    [LIMIT {[offset,] row_count | row_count OFFSET offset}]
    [PROCEDURE procedure_name(argument_list)]
    [INTO OUTFILE 'file_name'
        [CHARACTER SET charset_name]
        export_options
      | INTO DUMPFILE 'file_name'
      | INTO var_name [, var_name]]
    [FOR UPDATE | LOCK IN SHARE MODE]]
```

http://dev.mysql.com/doc/refman/5.5/en/select.html

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Execution order

1. Input columns are determined
2. `WHERE` – input columns are filtered
3. `GROUP BY` – sorting & grouping of filtered input
4. Aggregation functions are calculated
5. `HAVING` – aggregation functions are filtered
6. `ORDER BY` – output is sorted
7. `LIMIT/OFFSET` – output is chopped

Relational databases with MySQL

Exercises

- For each class with more than 1 organism, show the average number of chromosomes. Sort the result such that the biggest average is on top.

Relational databases with MySQL

Database upgrade

- Download `bioinf_testdb.sql`
- Create a new database `bioinf_testdb`

```
mysql> CREATE database bioinf_testdb;
```

- Grant your user all rights on this database
- Create the tables and insert the data

```
$ mysql bioinf_testdb < bioinf_testdb.sql
```

Relational databases with MySQL

Exercises

- Find the gene named *HOTAIR* in the `gene` table (bioinf_testdb)
  - In addition to the gene name and the chromosomal position, return the size of the gene
- Find the known lincRNA that is located the most distal on the p-arm of chromosome 14 (see figure below for hint)
- Find genes related to prostate cancer (use `description` field)
- Return a list of genes located on chromosome X in alphabetical order

A	T	G	G	C	T	A	T	A	C
1	2	3	4	5	6	7	8	9	10