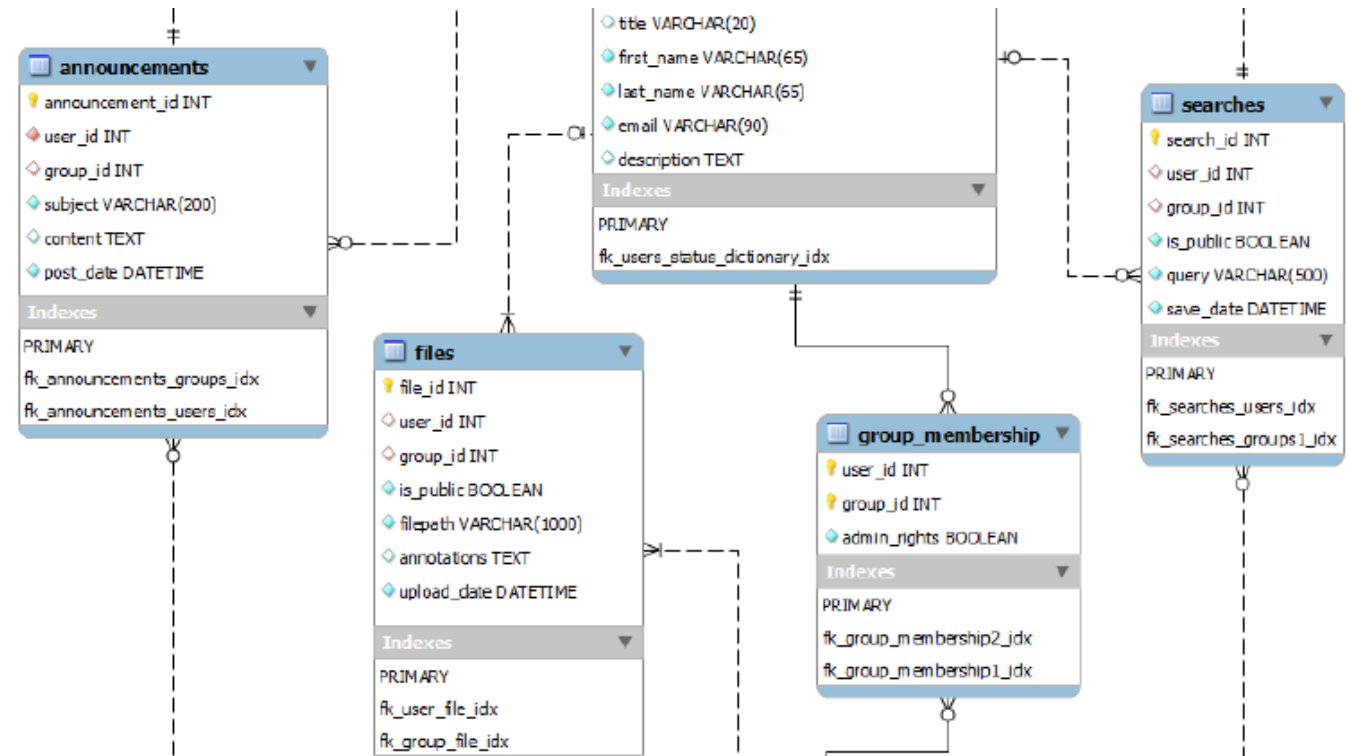




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11 February 2025

Introduction to Database Design and Normalisation



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Module engagement QR code



If you are unable to scan this code, please contact SAS Admin – seeaadmin@cranfield.ac.uk



Problems of data storage

Tabular data storage - spreadsheets, comma-separated value (CSV) files...

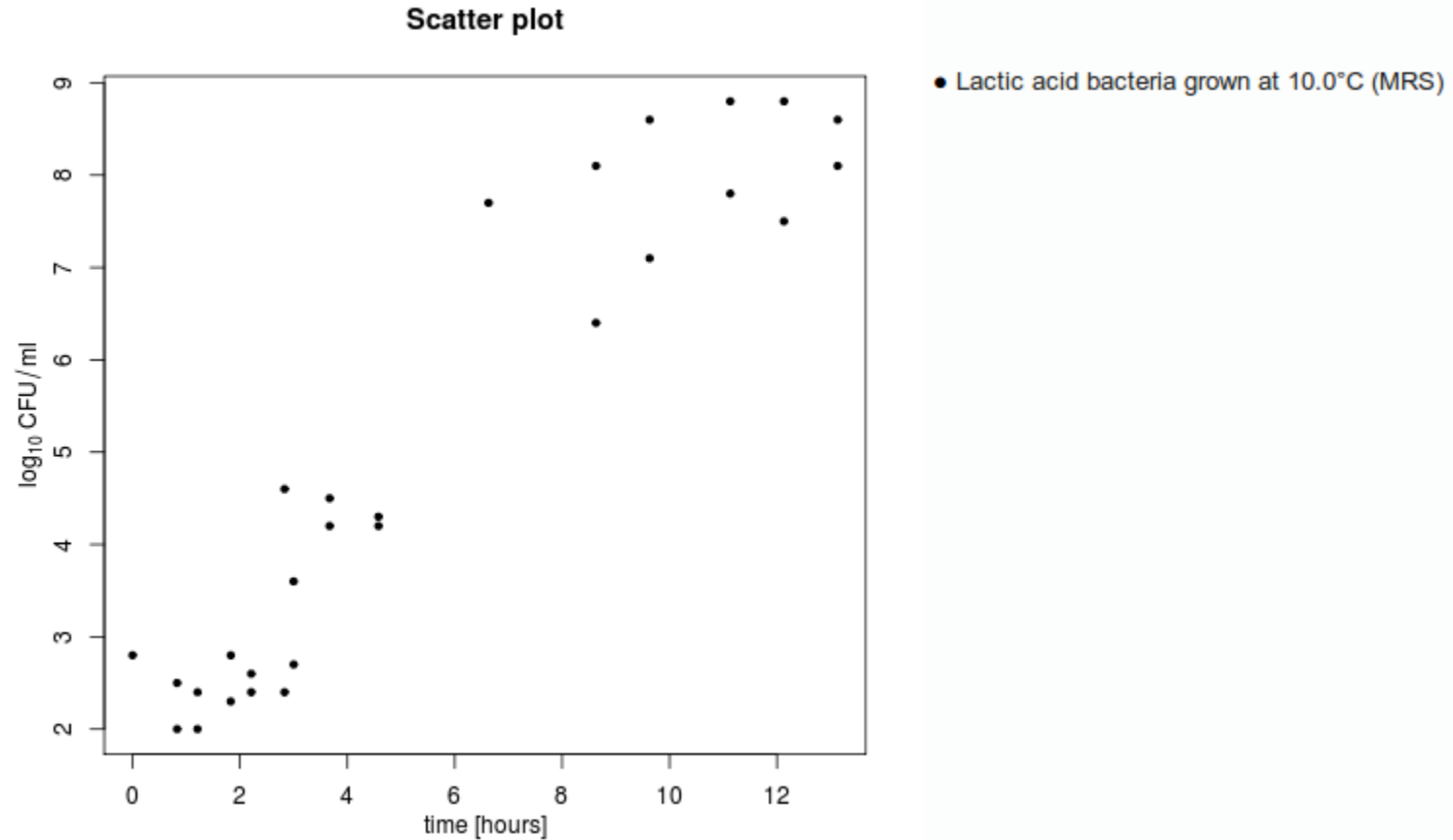
Experiment	Authors	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	7	2	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	11	1	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	16	2.3	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	21	1	0
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	0	1	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	72	1.3	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	96	1.8	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	122	2.8	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	144	2	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	168	2	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	192	5.2	7

Redundant data, no integrity protection, no associated query system

Spreadsheet available on Canvas!

Example data

Time series of bacterial growth in specific conditions:





Problems of data storage

Experiment	Authors	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	7	2	0

Experiment	-	alphanumeric experiment identifier
Authors	-	list of authors
Medium	-	name of medium used for microorganism growth
Organism	-	name of studied organism
Is Fungus	-	1 if organism is a fungus, 0 if it is not
Time	-	time point of data collection [hours]
CFU	-	\log_{10} of Colony Forming Unit concentration
Temperature	-	temperature during experiment [°C]



Problems of data storage

You could make it prettier...

Experiment	Authors	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
					2	1.3	
					7	2	
					11	1	
					16	2.3	
					21	1	
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	0	1	7
					72	1.3	
					96	1.8	
					122	2.8	
					144	2	
					168	2	
					192	5.2	

But does this make it better?



Databases

What is a database for?

- Storage of data
- Organising data
- Providing a system of accessing data and interacting with it



CRUD – **C**reating, **R**eading, **U**dating, **D**eleting

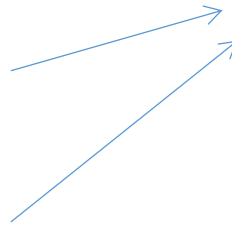


Databases

What is a database for?

- Storage of data
- Organising data
- Providing a system of accessing data and interacting with it

Minimise redundancy



CRUD – **C**reating, **R**eading, **U**psdating, **D**eleting





Databases

What is a database for?

- Storage of data
- Organising data
- Providing a system of accessing data and interacting with it

Minimise redundancy

Maintain integrity

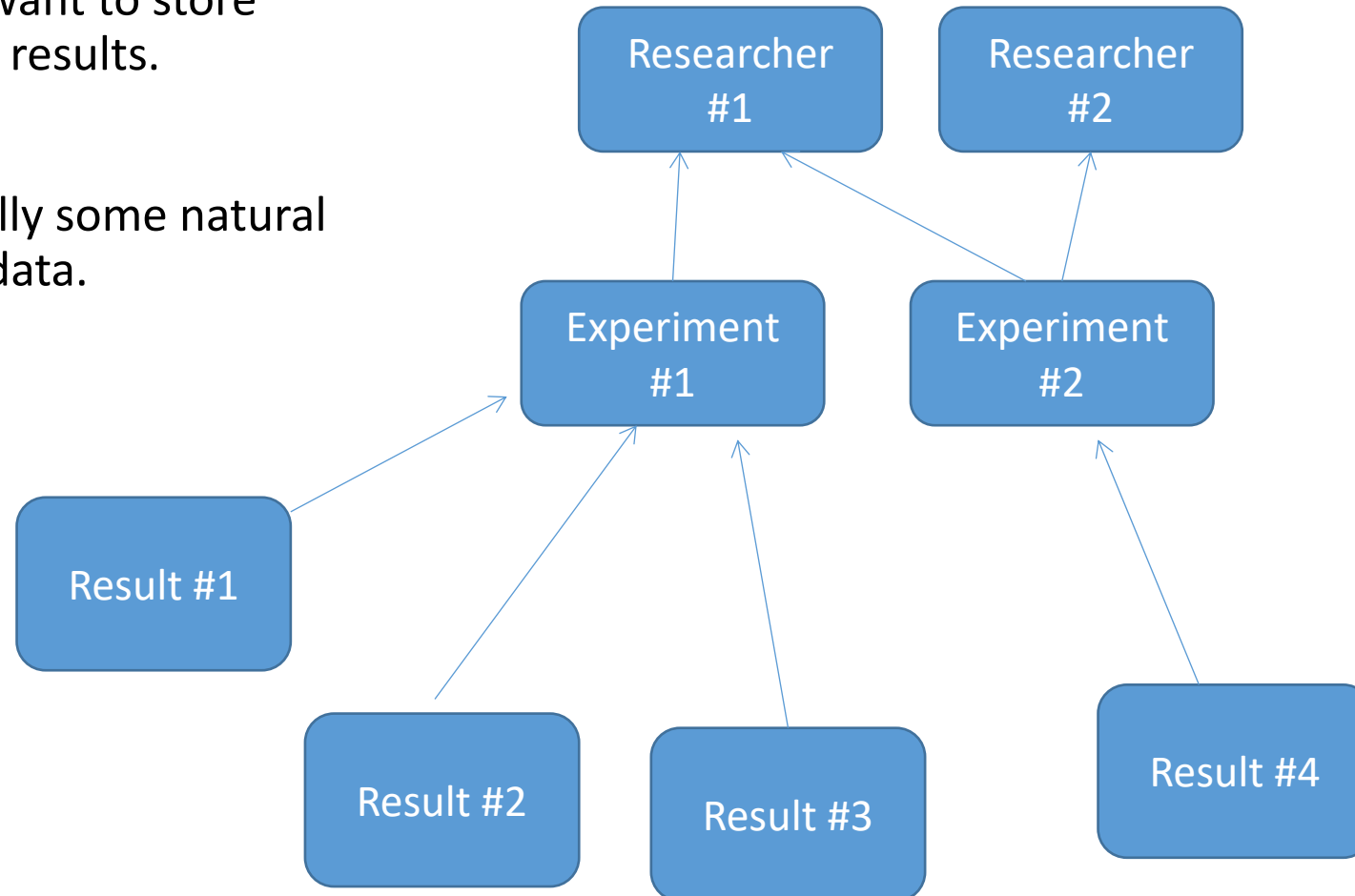
CRUD – **C**reating, **R**eading, **U**psdating, **D**eleting



Relationships between data

Let's say we want to store experimental results.

There is usually some natural hierarchy to data.



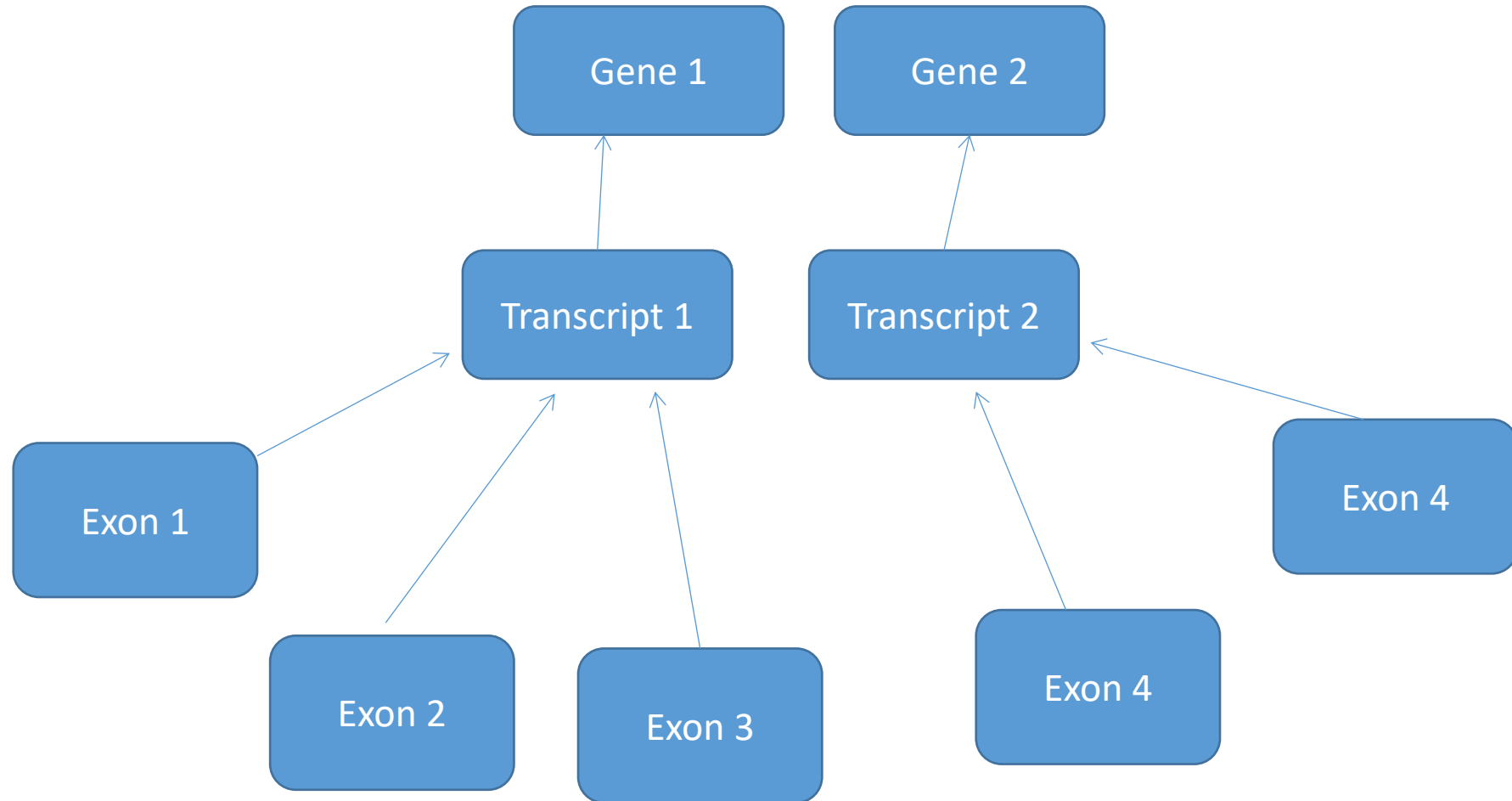


In your Java assignment

```
chr1 HAVANA gene 11869 14409 . + . gene_id "ENSG00000290825.1"; gene_type "lncRNA"; gene_name "DDX11L2"; level 2; tag "overlaps_pseudogene";
chr1 HAVANA transcript 11869 14409 . + . gene_id "ENSG00000290825.1"; transcript_id "ENST00000456328.2"; gene_type "lncRNA"; gene_name "DDX11L2"; transcript_type "lncRNA"; transcript_name "DDX11L2-202"; level 2; transcript_support_level "1"; tag "basic"; tag "Ensembl_canonical"; havana_transcript "OTTHUMT00000362751.1";
chr1 HAVANA exon 11869 12227 . + . gene_id "ENSG00000290825.1"; transcript_id "ENST00000456328.2"; gene_type "lncRNA"; gene_name "DDX11L2"; transcript_type "lncRNA"; transcript_name "DDX11L2-202"; exon_number 1; exon_id "ENSE00002234944.1"; level 2; transcript_support_level "1"; tag "basic"; tag "Ensembl_canonical"; havana_transcript "OTTHUMT00000362751.1";
chr1 HAVANA exon 12613 12721 . + . gene_id "ENSG00000290825.1"; transcript_id "ENST00000456328.2"; gene_type "lncRNA"; gene_name "DDX11L2"; transcript_type "lncRNA"; transcript_name "DDX11L2-202"; exon_number 2; exon_id "ENSE00003582793.1"; level 2; transcript_support_level "1"; tag "basic"; tag "Ensembl_canonical"; havana_transcript "OTTHUMT00000362751.1";
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chr1 HAVANA transcript 12010 13670 . + . gene_id "ENSG00000223972.6"; transcript_id "ENST00000450305.2"; gene_type "transcribed_unprocessed_pseudogene"; gene_name "DDX11L1"; transcript_type "transcribed_unprocessed_pseudogene"; transcript_name "DDX11L1-201"; level 2; transcript_support_level "NA"; hgnc_id "HGNC:37102"; ont "PGO:0000005"; ont "PGO:0000019"; tag "basic"; tag "Ensembl_canonical"; havana_gene "OTTHUMG00000000961.2"; havana_transcript "OTTHUMT000000002844.2";
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chr1 HAVANA exon 12179 12227 . + . gene_id "ENSG00000223972.6"; transcript_id "ENST00000450305.2"; gene_type "transcribed_unprocessed_pseudogene"; gene_name "DDX11L1"; transcript_type "transcribed_unprocessed_pseudogene"; transcript_name "DDX11L1-201"; exon_number 2; exon_id "ENSE00001671638.2"; level 2; transcript_support_level "NA"; hgnc_id "HGNC:37102"; ont "PGO:0000005"; ont "PGO:0000019"; tag "basic"; tag "Ensembl_canonical"; havana_gene "OTTHUMG00000000961.2"; havana_transcript "OTTHUMT000000002844.2";
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```



In your Java assignment





Relational model

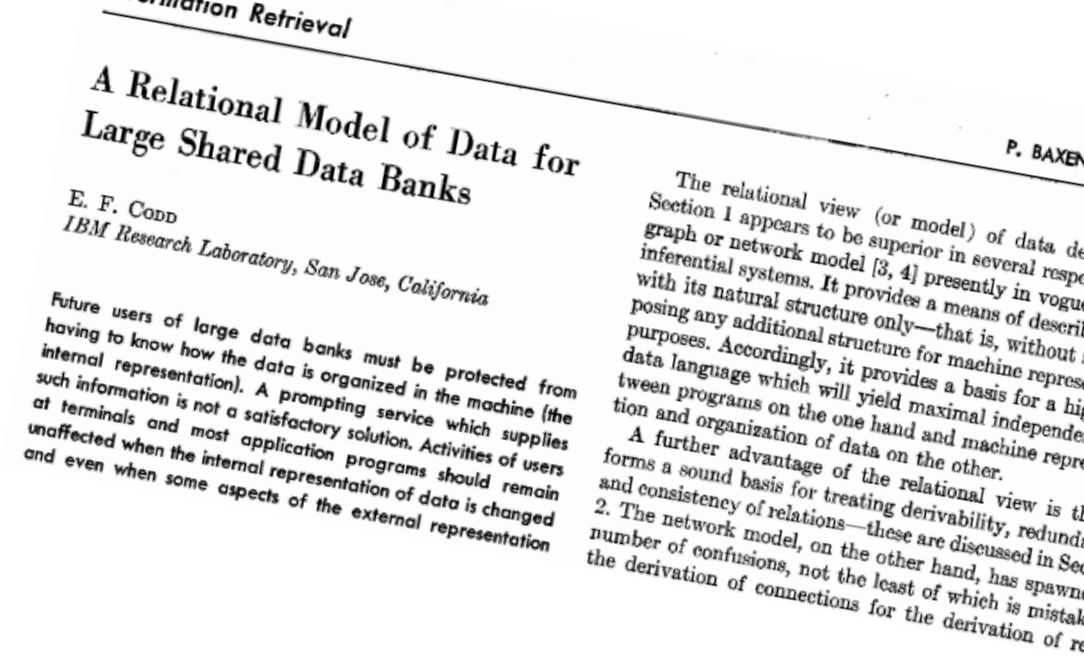
General, theoretical model for organising databases.

Introduced in the 1970s by E.F. Codd.

Currently the most popular approach, relational databases are a \$100 billion industry.

Data arranged in a collection of tables (n-ary relations subsets of the Cartesian product of n domains).

Separates the concepts of “data” and “schema” (structure of data)





Relational model

Data is stored in multiple named **tables (relations)**.

Experiments			
Experiment_ID	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
ds001b1	MRS	Lactic acid bacteria	0
ds001b2	MRS	Lactic acid bacteria	5
ds001b3	MRS	Lactic acid bacteria	10
ds001b4	MRS	Lactic acid bacteria	15
ds001d1	STAA	Brochothrix thermosphacta	0
ds001d2	STAA	Brochothrix thermosphacta	5
ds001d3	STAA	Brochothrix thermosphacta	10
ds001d4	STAA	Brochothrix thermosphacta	15



Relational model

Each table has a list of named **columns (attributes)**.

Each column has a **type (domain)**, e.g. INT for integer or CHAR for character strings.

Experiments			
Experiment_ID	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
ds001b1	MRS	Lactic acid bacteria	0
ds001b2	MRS	Lactic acid bacteria	5
ds001b3	MRS	Lactic acid bacteria	10
ds001b4	MRS	Lactic acid bacteria	15
ds001d1	STAA	Brochothrix thermosphacta	0
ds001d2	STAA	Brochothrix thermosphacta	5
ds001d3	STAA	Brochothrix thermosphacta	10
ds001d4	STAA	Brochothrix thermosphacta	15



Relational model

Each table **row (record, tuple)** represents an entry and has to be unique.

Experiments			
Experiment_ID	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
ds001b1	MRS	Lactic acid bacteria	0
ds001b2	MRS	Lactic acid bacteria	5
ds001b3	MRS	Lactic acid bacteria	10
ds001b4	MRS	Lactic acid bacteria	15
ds001d1	STAA	Brochothrix thermosphacta	0
ds001d2	STAA	Brochothrix thermosphacta	5
ds001d3	STAA	Brochothrix thermosphacta	10
ds001d4	STAA	Brochothrix thermosphacta	15



Primary Keys

In order to be unique, each table needs to have at least one unique column or combination of columns. One of them is the **Primary Key (PK)**, which serves as an identifier of that row.

There may be multiple **Candidate Keys**, but only one **Primary Key**.

Experiments			
Experiment_ID	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
ds001b1	MRS	Lactic acid bacteria	0
ds001b2	MRS	Lactic acid bacteria	5
ds001b3	MRS	Lactic acid bacteria	10
ds001b4	MRS	Lactic acid bacteria	15
ds001d1	STAA	Brochothrix thermosphacta	0
ds001d2	STAA	Brochothrix thermosphacta	5
ds001d3	STAA	Brochothrix thermosphacta	10
ds001d4	STAA	Brochothrix thermosphacta	15



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ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
ds001b1	MRS	Lactic acid bacteria	0
ds001b2	MRS	Lactic acid bacteria	5
ds001b3	MRS	Lactic acid bacteria	10
ds001b4	MRS	Lactic acid bacteria	15
ds001d1	STAA	Brochothrix thermosphacta	0
ds001d2	STAA	Brochothrix thermosphacta	5
ds001d3	STAA	Brochothrix thermosphacta	10
ds001d4	STAA	Brochothrix thermosphacta	15



But what about this?!

What are the candidate keys? What should be the Primary Key?

Employees	
First_Name	Last_Name
Tomasz	Kurowski
Fady	Mohareb
James	Smith
...	...



Compound Key

A combination of attributes which are not themselves unique can be a Candidate/Primary Key.

The key is (First_Name, Last_Name)

Employees	
First_Name	Last_Name
Tomasz	Kurowski
Fady	Mohareb
James	Smith
...	...

But is that enough?



Surrogate Key

We could simply add a unique identifier ourselves – typically an integer. This is called a **Surrogate Key**.

Non-Surrogate Keys are sometimes called **Natural Keys**.

Employees		
Employee_id	First_Name	Last_Name
1	Tomasz	Kurowski
2	Fady	Mohareb
3	James	Smith
...

Some people add surrogate keys to all tables, avoiding natural keys.

Others claim using natural keys is superior.

It depends...



Foreign Keys

Tables may also contain Foreign Keys. These refer to a Primary Key of a different table. This creates a relationship between two tables!

Child table

Measurements		
Time	CFU	Experiment_ID
1	1.8	ds001a1
2	1.3	ds001a1
7	2	ds001a1
11	1	ds001a1
16	2.3	ds001a1
1	2.3	ds001b1
7	1.6	ds001b1
11	2.4	ds001b1
16	2.5	ds001b1
21	3.5	ds001b1
28	5.1	ds001b1
32	4.3	ds001b1

Parent table

Experiments			
Experiment_ID	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
ds001b1	MRS	Lactic acid bacteria	0
ds001b2	MRS	Lactic acid bacteria	5
ds001b3	MRS	Lactic acid bacteria	10
ds001b4	MRS	Lactic acid bacteria	15
ds001d1	STAA	Brochothrix thermosphacta	0
ds001d2	STAA	Brochothrix thermosphacta	5
ds001d3	STAA	Brochothrix thermosphacta	10
ds001d4	STAA	Brochothrix thermosphacta	15



Cardinality

Experiments has a one-to-many relationship with **Measurements**

Usually symbolised by a „crow’s foot”

Child table

Measurements		
Time	CFU	Experiment_ID
1	1.8	ds001a1
2	1.3	ds001a1
7	2	ds001a1
11	1	ds001a1
16	2.3	ds001a1
1	2.3	ds001b1
7	1.6	ds001b1
11	2.4	ds001b1
16	2.5	ds001b1
21	3.5	ds001b1
28	5.1	ds001b1
32	4.3	ds001b1

Parent table

Experiments			
Experiment_ID	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
ds001b1	MRS	Lactic acid bacteria	0
ds001b2	MRS	Lactic acid bacteria	5
ds001b3	MRS	Lactic acid bacteria	10
ds001b4	MRS	Lactic acid bacteria	15
ds001d1	STAA	Brochothrix thermosphacta	0
ds001d2	STAA	Brochothrix thermosphacta	5
ds001d3	STAA	Brochothrix thermosphacta	10
ds001d4	STAA	Brochothrix thermosphacta	15



Cardinality

One-to-many relationships are the most common type in relational databases.

One-to-one relationships are also common, but usually such tables can be merged and remain separate for convenience or performance.

Many-to-many relationships are **NOT ALLOWED!**

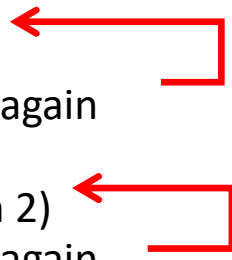


Database normalisation

How to make a „good” database?

Normal forms - list of conditions which a correct relational database should fulfil

You can treat it like a check-list:

1. Put all data in table
 2. Check if it fulfils first set of conditions (is in normal form 1)
 - a. If no, modify or split the table to make it fit and check again
 - b. If yes, move on to step 3
 3. Check if it fulfils second set of conditions (is in normal form 2)
 - a. If no, modify or split the table to make it fit and check again
 - b. If yes, move on to step 4
 4. Check if It fulfils third set of conditions (is in normal form 3)...
- 
- Two red arrows are present. The first arrow starts from the right side of step 1 and points left to step 2. The second arrow starts from the right side of step 2 and points left to step 3.

When you are more experienced you can design the whole database first, and THEN do the check-list to see if you have missed anything.



Database normalisation

1. First Normal Form (1NF)
2. Second Normal Form (2NF)
3. Third Normal Form (3NF)
4. Boyce-Codd Normalisation
5. Fourth Normal Form (4NF)
6. Domain-key Normal Form (5NF)

We will stop at 3NF!



Data normalisation

The first step is putting everything in a single table – we already have that!

Experiment	Authors	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	7	2	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	11	1	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	16	2.3	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	21	1	0
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	0	1	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	72	1.3	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	96	1.8	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	122	2.8	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	144	2	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	168	2	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	192	5.2	7

Time to normalise this!

Download the spreadsheet from Canvas



First normal form (1NF)

Criteria:

1. Each table must have a primary key (rows should not repeat)
2. Values in the table should be atomic
3. There should be no repeating groups



Criterion 1 – Primary Key

What are our **Candidate Keys**?

Experiment	Authors	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	7	2	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	11	1	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	16	2.3	0
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ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	0	1	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	72	1.3	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	96	1.8	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	122	2.8	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	144	2	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	168	2	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	192	5.2	7

Candidate Keys are unique columns or combinations of columns



Criterion 1 – Primary Key

The combination of Experiment and Time is a good candidate key

Experiment	Authors	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	7	2	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	11	1	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	16	2.3	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	21	1	0
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	0	1	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	72	1.3	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	96	1.8	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	122	2.8	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	144	2	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	168	2	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	192	5.2	7
Primary Key: (Experiment, Time)							

We could also simply add a surrogate key. How would you name it?



Criterion 2 – Atomic?

A table cell should only include a single value of a given type.

Experiment	Authors	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	7	2	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	11	1	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	16	2.3	0
ds001a1	Seintis P., Skandamis P.	CFC	Pseudomonas sp.	0	21	1	0
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	0	1	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	72	1.3	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	96	1.8	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	122	2.8	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	144	2	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	168	2	7
ds003b07	Fotinopoulou E., Skandamis P.	TSA	Staphylococcus aureus	0	192	5.2	7
Primary Key: (Experiment, Time)							

How do we split this?



Experiment	Author1	Author2	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	7	2	0
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	11	1	0
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	16	2.3	0
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	21	1	0
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	0	1	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	72	1.3	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	96	1.8	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	122	2.8	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	144	2	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	168	2	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	192	5.2	7
Primary Key: (Experiment, Time)								

Criterion 2 – Atomic?

We don't know if there are always going to be two authors.

Experiment	Author1	Author2	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	7	2	0
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	11	1	0
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	16	2.3	0
ds001a1	Seintis P.	Skandamis P.	CFC	Pseudomonas sp.	0	21	1	0
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	0	1	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	72	1.3	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	96	1.8	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	122	2.8	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	144	2	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	168	2	7
ds003b07	Fotinopoulou E.	Skandamis P.	TSA	Staphylococcus aureus	0	192	5.2	7
Primary Key: (Experiment, Time)								

...and these are the „repeating groups from criterion



Experiment	Author	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Seintis P.	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	Skandamis P.	CFC	Pseudomonas sp.	0	2	1.3	0
...
Primary Key: (Experiment, Time)							



Criterion 2 – Atomic?

This could technically work as 1NF.

Experiment	Author	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	Seintis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Skandamis P.	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	Seintis P.	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	Skandamis P.	CFC	Pseudomonas sp.	0	2	1.3	0
...
Primary Key: (Experiment, Time)							

But it introduces even more redundancy.



Criterion 2 – Atomic?

Probably best solution: split the table!
(for now, let's keep the entire primary key)

Authorships		
Name	Measurement ID	
Seintis P.	1	
Skandamis P.	1	
Seintis P.	2	
Skandamis P.		
...		
Primary Key: (Name, Experiment, Time)		
Foreign Key: (Experiment, Time)		

Measurements							
Experiment	Measurement ID	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	1	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	2	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	3	CFC	Pseudomonas sp.	0	7	2	0
ds001a1	4	CFC	Pseudomonas sp.	0	11	1	0
...	
Primary Key: (Measurement ID)							

So, are we in 1NF?



Second normal form (2NF)

Criteria:

1. Must be in 1NF
2. Non-prime attributes must depend on entire Primary Key, not only part of it

(non-prime attribute – attribute which is not part of any candidate key in the referenced table)



Authors		
Name	Experiment	Time
Seintis P.	ds001a1	1
Skandamis P.	ds001a1	1
Seintis P.	ds001a1	2
Skandamis P.	ds001a1	2
...

Primary Key: (Name, Experiment, Time)
Foreign Key: (Experiment, Time)

Experiment Data						
Experiment	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	CFC	Pseudomonas sp.	0	7	2	0
ds001a1	CFC	Pseudomonas sp.	0	11	1	0
...
Primary Key: (Experiment, Time)						



CFU depends both on the Experiment and Time, the entire Primary Key

Experiment Data						
Experiment	Medium	Organism	Is Fungus	Time	CFU	Temperature
ds001a1	CFC	Pseudomonas sp.	0	1	1.8	0
ds001a1	CFC	Pseudomonas sp.	0	2	1.3	0
ds001a1	CFC	Pseudomonas sp.	0	7	2	0
ds001a1	CFC	Pseudomonas sp.	0	11	1	0
...
Primary Key: (Experiment, Time)						



Criterion 2

We split the Experiment_Data table!

Authors		
Name	Experiment	Time
Seintis P.	ds001a1	1
Skandamis P.	ds001a1	1
Seintis P.	ds001a1	2
Skandamis P.	ds001a1	2
...
Primary Key: (Name, Experiment, Time)		
Foreign Key: (Experiment, Time)		

Experiments				
Experiment	Medium	Organism	Is Fungus	Temperature
ds001a1	CFC	Pseudomonas sp.	0	0
ds001a2	CFC	Pseudomonas sp.	0	5
ds001a3	CFC	Pseudomonas sp.	0	10
ds001a4	CFC	Pseudomonas sp.	0	15
...
Primary Key: (Experiment)				

Datapoints		
Experiment	Time	CFU
ds001a1	1	1.8
ds001a1	2	1.3
ds001a1	7	2
ds001a1	11	1
...
Primary Key: (Experiment, Time)		
Foreign Key: (Experiment)		

What about the Authors table?

The authors of a given experiment do not depend on time.



Criterion 2

That's better.

Authors	
Name	Experiment
Seintis P.	ds001a1
Skandamis P.	ds001a1
Seintis P.	ds001a2
Skandamis P.	ds001a2
...	...
Primary Key: (Name, Experiment) Foreign Key: (Experiment)	

Experiments				
Experiment	Medium	Organism	Is Fungus	Temperature
ds001a1	CFC	Pseudomonas sp.	0	0
ds001a2	CFC	Pseudomonas sp.	0	5
ds001a3	CFC	Pseudomonas sp.	0	10
ds001a4	CFC	Pseudomonas sp.	0	15
...
Primary Key: (Experiment)				

Are we in 2NF?

Datapoints		
Experiment	Time	CFU
ds001a1	1	1.8
ds001a1	2	1.3
ds001a1	7	2
ds001a1	11	1
...
Primary Key: (Experiment, Time) Foreign Key: (Experiment)		



Third normal form (3NF)

Criteria:

1. Must be in 2NF
2. Non-prime attributes must not depend on other non-prime attributes



Criterion 2

Does any non-prime attribute depends on another?

Authors	
Name	Experiment
Seintis P.	ds001a1
Skandamis P.	ds001a1
Seintis P.	ds001a2
Skandamis P.	ds001a2
...	...
Primary Key: (Name, Experiment) Foreign Key: (Experiment)	

Experiments				
Experiment	Medium	Organism	Is Fungus	Temperature
ds001a1	CFC	Pseudomonas sp.	0	0
ds001a2	CFC	Pseudomonas sp.	0	5
ds001a3	CFC	Pseudomonas sp.	0	10
ds001a4	CFC	Pseudomonas sp.	0	15
...
Primary Key: (Experiment)				

Datapoints		
Experiment	Time	CFU
ds001a1	1	1.8
ds001a1	2	1.3
ds001a1	7	2
ds001a1	11	1
...
Primary Key: (Experiment, Time) Foreign Key: (Experiment)		



Criterion 2

Is_Fungus depends on Organism!

Authors	
Name	Experiment
Seintis P.	ds001a1
Skandamis P.	ds001a1
Seintis P.	ds001a2
Skandamis P.	ds001a2
...	...
Primary Key: (Name, Experiment) Foreign Key: (Experiment)	

Experiments				
Experiment	Medium	Organism	Is Fungus	Temperature
ds001a1	CFC	Pseudomonas sp.	0	0
ds001a2	CFC	Pseudomonas sp.	0	5
ds001a3	CFC	Pseudomonas sp.	0	10
ds001a4	CFC	Pseudomonas sp.	0	15
...
Primary Key: (Experiment)				

What shall we do?

Datapoints		
Experiment	Time	CFU
ds001a1	1	1.8
ds001a1	2	1.3
ds001a1	7	2
ds001a1	11	1
...
Primary Key: (Experiment, Time) Foreign Key: (Experiment)		



Criterion 2

Looks like we are in 3NF!

Authors	
Name	Experiment
Seintis P.	ds001a1
Skandamis P.	ds001a1
Seintis P.	ds001a1
Skandamis P.	ds001a1
...	...
Primary Key: (Name, Experiment) Foreign Key: (Experiment)	

Experiments			
Experiment	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
...
Primary Key: (Experiment) Foreign Key: (Organism)			

Organisms	
Organism	Is Fungus
Pseudomonas sp.	0
Lactic acid bacteria	0
Enterobacteriaceae	0
Yeasts-moulds	1
...	...
Primary Key: (Organism)	

Datapoints		
Experiment	Time	CFU
ds001a1	1	1.8
ds001a1	2	1.3
ds001a1	7	2
ds001a1	11	1
...
Primary Key: (Experiment, Time) Foreign Key: (Experiment)		



Normalisation summed up

Data depends on:

- 1NF:** *The key,*
- 2NF:** *the whole key,*
- 3NF:** *and nothing but the key.*

So, are we done yet?



A look at our relationships

What type of relationship do Experiments and Datapoints have?

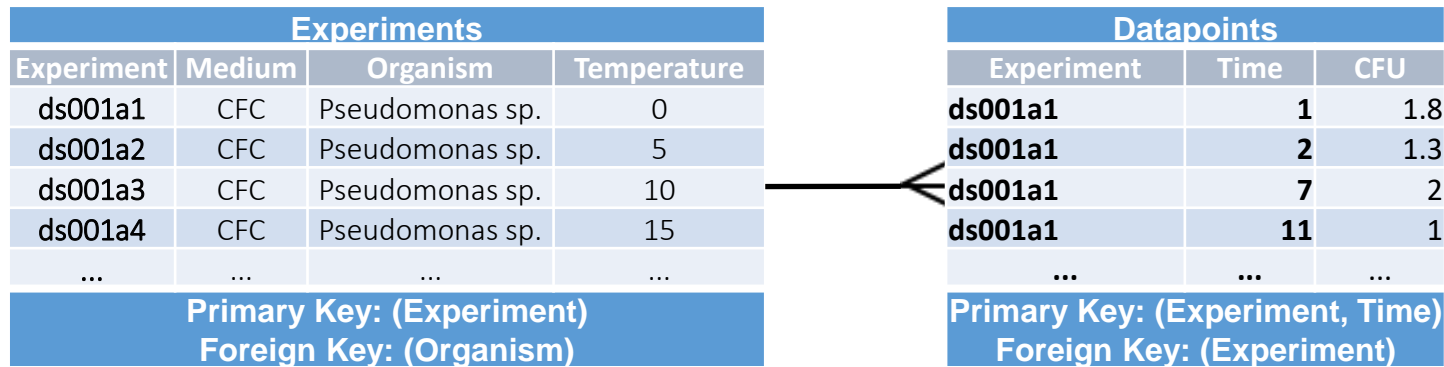
Experiments			
Experiment	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
...
Primary Key: (Experiment) Foreign Key: (Organism)			

Datapoints		
Experiment	Time	CFU
ds001a1	1	1.8
ds001a1	2	1.3
ds001a1	7	2
ds001a1	11	1
...
Primary Key: (Experiment, Time) Foreign Key: (Experiment)		



A look at our relationships

Answer: One-to-Many





A look at our relationships

What is the relationship between Organisms and Experiments?

Organisms	
Organism	Is Fungus
Pseudomonas sp.	0
Lactic acid bacteria	0
Enterobacteriaceae	0
Yeasts-moulds	1
...	...
Primary Key: (Organism)	

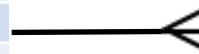
Experiments			
Experiment	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
...
Primary Key: (Experiment) Foreign Key: (Organism)			



A look at our relationships

Answer: One-to-Many

Organisms	
Organism	Is Fungus
Pseudomonas sp.	0
Lactic acid bacteria	0
Enterobacteriaceae	0
Yeasts-moulds	1
...	...
Primary Key: (Organism)	



Experiments			
Experiment	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
...
Primary Key: (Experiment) Foreign Key: (Organism)			



A look at our relationships

What about Authors and Experiments?

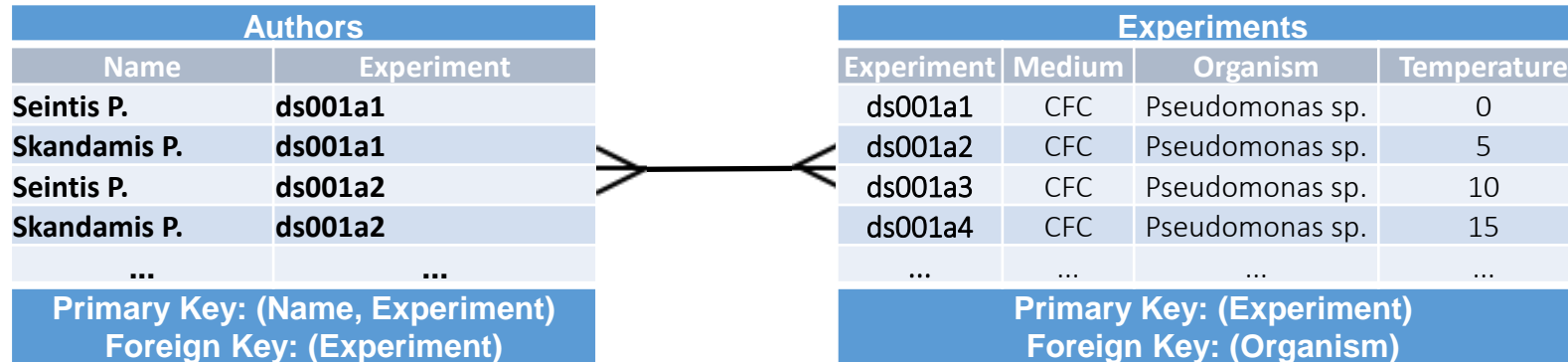
Authors	
Name	Experiment
Seintis P.	ds001a1
Skandamis P.	ds001a1
Seintis P.	ds001a2
Skandamis P.	ds001a2
...	...
Primary Key: (Name, Experiment) Foreign Key: (Experiment)	

Experiments			
Experiment	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
...
Primary Key: (Experiment) Foreign Key: (Organism)			



A look at our relationships

Many-to-Many!

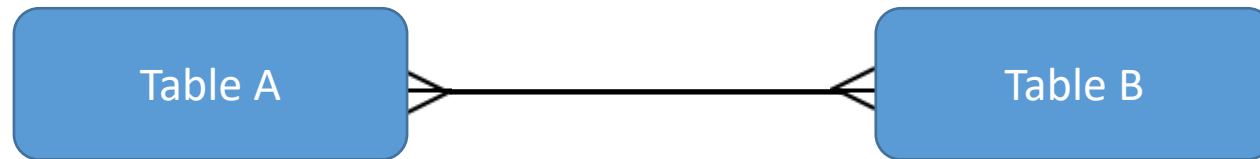


How do we fix this? This is related to higher normal forms, but...



Junction tables

Many-to-Many relationships can be represented
by introducing a **Junction Table**.



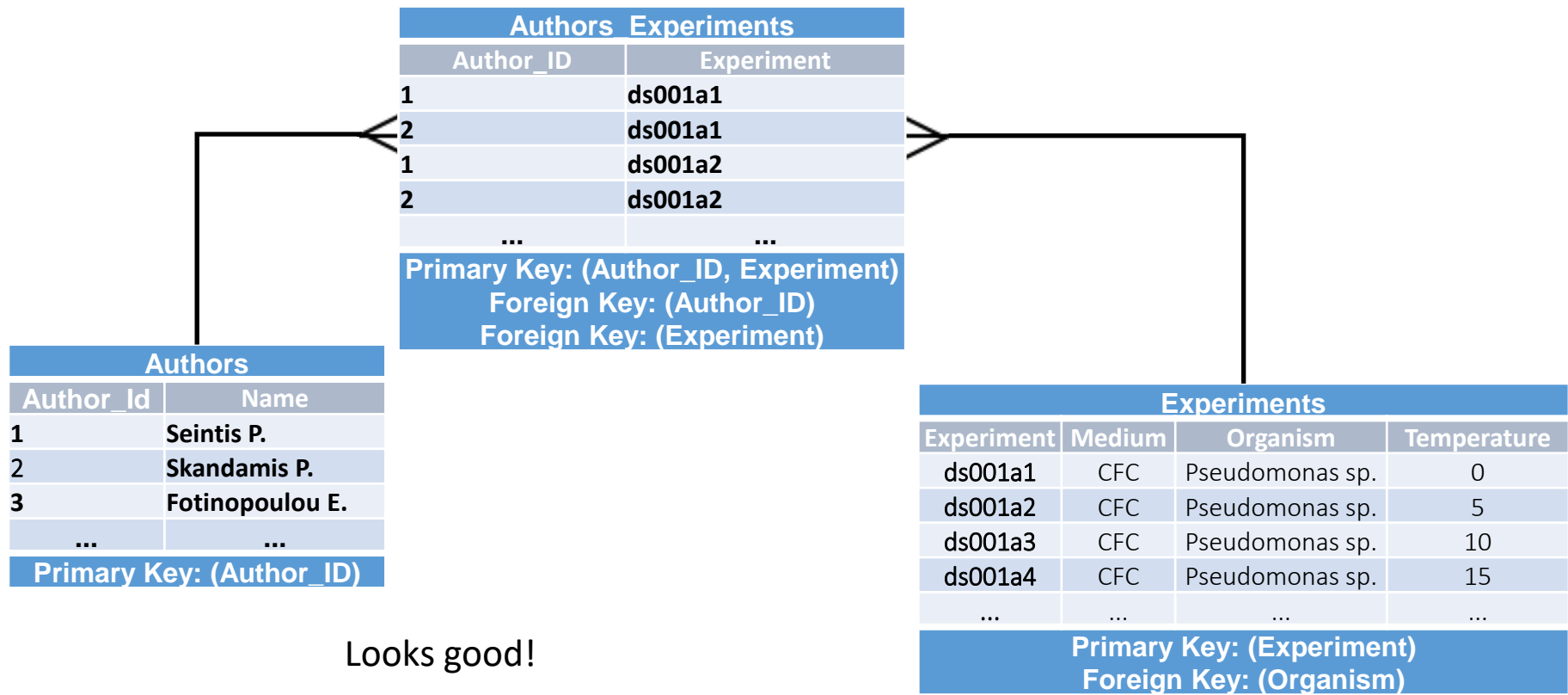
One Many-to-Many relationship is replaced by two One-to-Many relationships.

The Junction table has one Foreign Key referencing Table A, and a second Foreign Key referencing Table B.





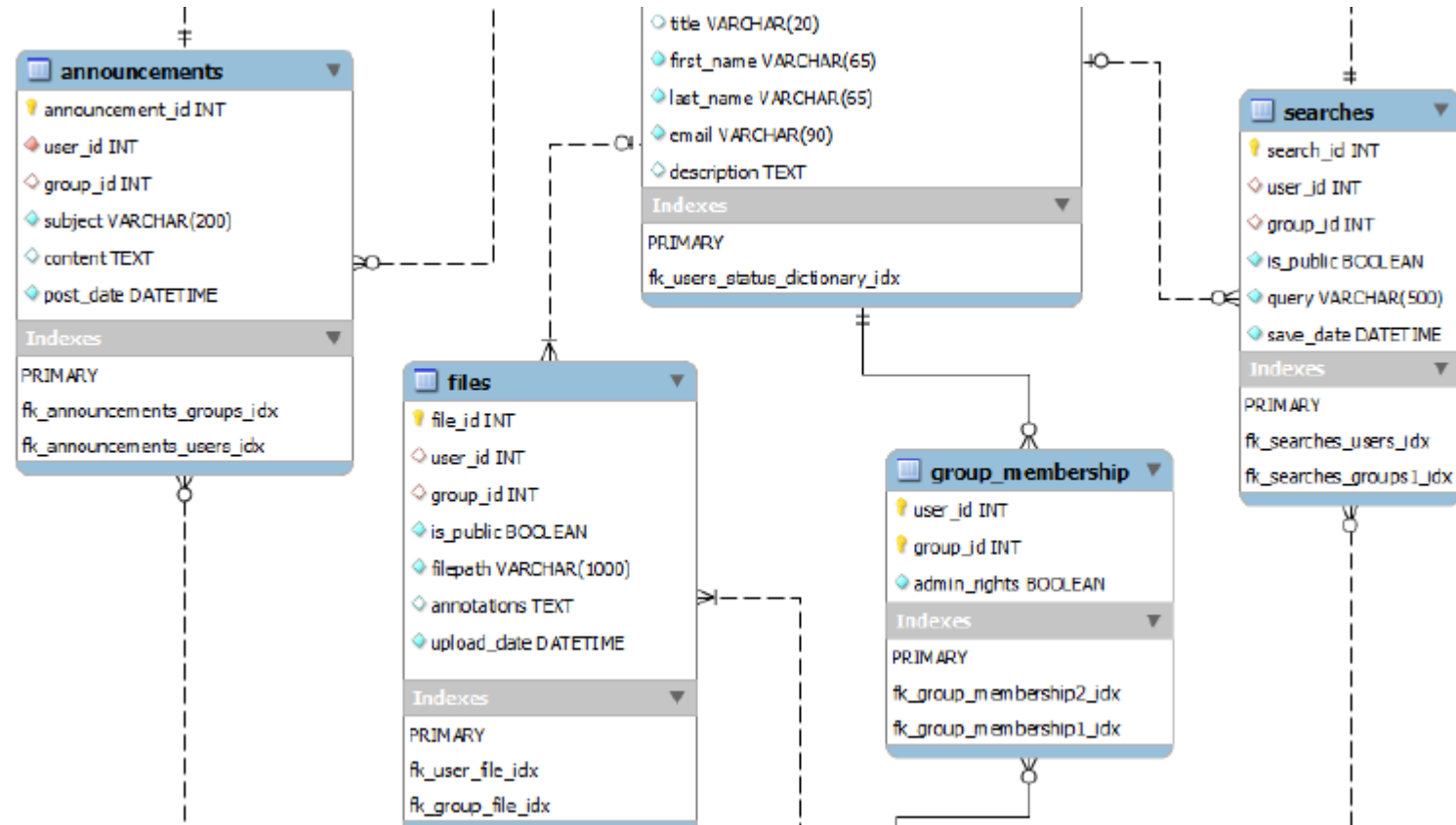
A look at our relationships



Looks good!

"Author_Experiments" is a conventional name, but it may be better to use something meaningful, like "Author_Participation"

EER diagrams





ACID – Database transactions

A transaction is a single operation on a relational database. Transactions may include **multiple** changes.

Atomicity – either succeed completely or fail completely

Consistency – any written data must respect all database constraints

Isolation – concurrent transactions are equivalent to sequential transactions

Durability – committed transactions remain committed



SQL

SQL - Structured Query Language

By far the most popular language for using relational databases.

Relatively few keywords and simple syntax.

Standardised by ISO and ANSI.

Declarative – you describe **what** you want it to do, not **how**. Relatively few keywords and simple syntax.

<https://dev.mysql.com/doc/refman/5.7/en/sql-statements.html>



SELECT

```
SELECT column1, column2  
FROM table_name  
WHERE condition;
```

```
SELECT Organism FROM Experiments  
WHERE Experiment_ID='ds001a2';
```

```
SELECT Time, CFU FROM Measurements  
WHERE Experiment_ID='ds001a2';
```

```
SELECT * FROM Experiments;
```



INSERT

```
INSERT INTO table_name (column1, column2)  
VALUES (value1, value2)  
WHERE condition;
```

```
INSERT INTO Measurements (Time, CFU)  
VALUES (15, 32.5) WHERE  
Experiment_ID='ds001b2';
```



UPDATE

```
UPDATE table_name  
SET column1=value1, column2=value2  
WHERE condition;
```

```
UPDATE Experiments  
SET Organism='E.coli', Medium='CFC'  
WHERE Experiment_ID='ds001a2';
```



DELETE

```
DELETE FROM table_name  
WHERE condition;
```

```
DELETE FROM Measurements  
WHERE Experiment_ID='ds001a2';
```



CREATE

```
CREATE TABLE table_name (  
    column1 type,  
    column2 type,  
    ...  
);
```

```
CREATE TABLE IF NOT EXISTS datapoints (  
    experiment_id VARCHAR(10),  
    time DOUBLE NOT NULL,  
    cfu DOUBLE NOT NULL,  
    PRIMARY KEY (experiment_id, time),  
    FOREIGN KEY (experiment_id)  
        REFERENCES experiments  
        (experiment_id)  
);
```



Joins

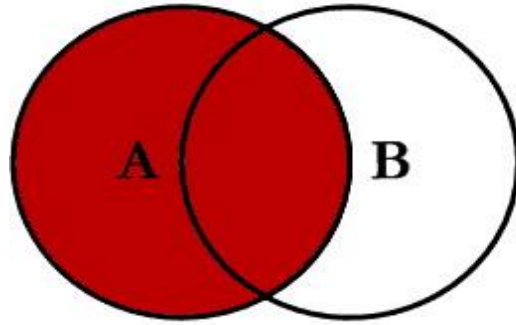
INNER JOIN: Returns all rows when there is at least one match in BOTH tables

LEFT JOIN: Return all rows from the left table, and the matched rows from the right table

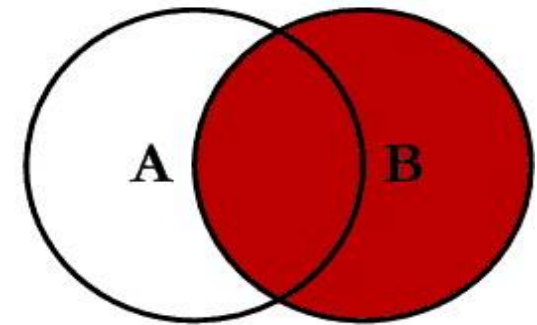
RIGHT JOIN: Return all rows from the right table, and the matched rows from the left table

FULL JOIN: Return all rows when there is a match in ONE of the tables

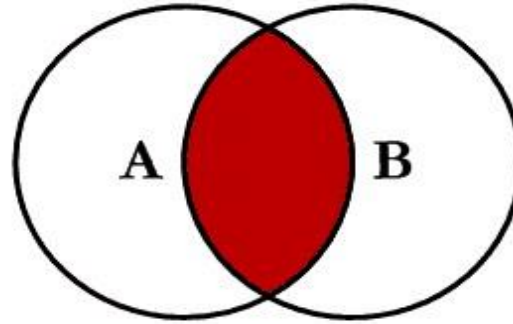
SQL JOINS



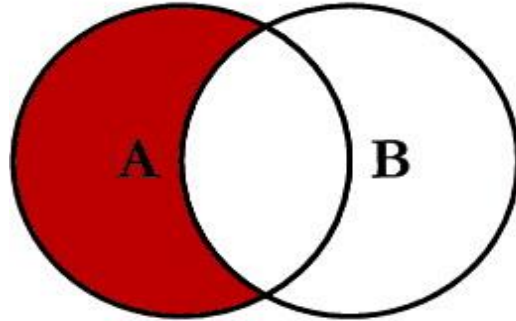
```
SELECT <select_list>
FROM TableA A
LEFT JOIN TableB B
ON A.Key = B.Key
```



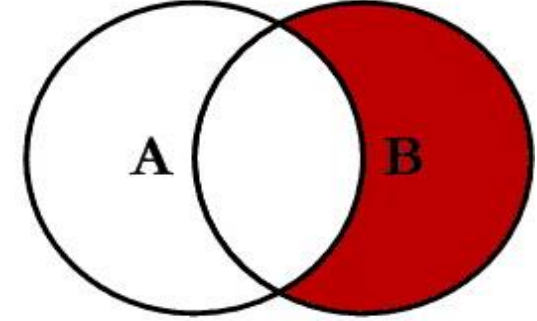
```
SELECT <select_list>
FROM TableA A
RIGHT JOIN TableB B
ON A.Key = B.Key
```



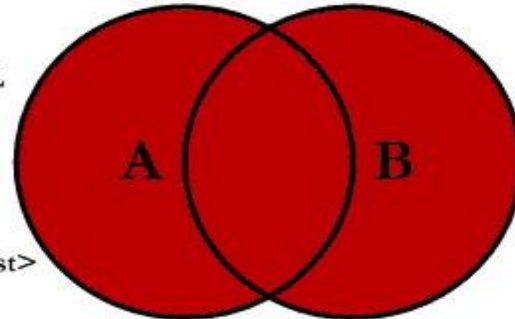
```
SELECT <select_list>
FROM TableA A
INNER JOIN TableB B
ON A.Key = B.Key
```



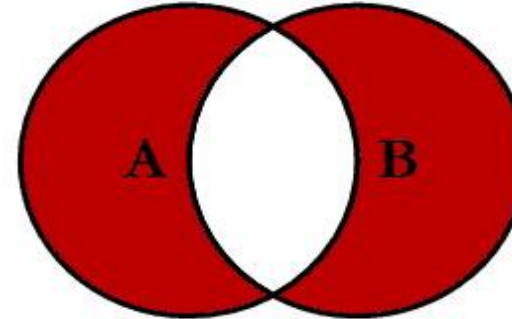
```
SELECT <select_list>
FROM TableA A
LEFT JOIN TableB B
ON A.Key = B.Key
WHERE B.Key IS NULL
```



```
SELECT <select_list>
FROM TableA A
RIGHT JOIN TableB B
ON A.Key = B.Key
WHERE A.Key IS NULL
```



```
SELECT <select_list>
FROM TableA A
FULL OUTER JOIN TableB B
ON A.Key = B.Key
```



```
SELECT <select_list>
FROM TableA A
FULL OUTER JOIN TableB B
ON A.Key = B.Key
WHERE A.Key IS NULL
OR B.Key IS NULL
```




Measurements and Experiments

Child table

Measurements		
Time	CFU	Experiment_ID
1	1.8	ds001a1
2	1.3	ds001a1
7	2	ds001a1
11	1	ds001a1
16	2.3	ds001a1
1	2.3	ds001b1
7	1.6	ds001b1
11	2.4	ds001b1
16	2.5	ds001b1
21	3.5	ds001b1
28	5.1	ds001b1
32	4.3	ds001b1

Parent table

Experiments			
Experiment_ID	Medium	Organism	Temperature
ds001a1	CFC	Pseudomonas sp.	0
ds001a2	CFC	Pseudomonas sp.	5
ds001a3	CFC	Pseudomonas sp.	10
ds001a4	CFC	Pseudomonas sp.	15
ds001b1	MRS	Lactic acid bacteria	0
ds001b2	MRS	Lactic acid bacteria	5
ds001b3	MRS	Lactic acid bacteria	10
ds001b4	MRS	Lactic acid bacteria	15
ds001d1	STAA	Brochothrix thermosphacta	0
ds001d2	STAA	Brochothrix thermosphacta	5
ds001d3	STAA	Brochothrix thermosphacta	10
ds001d4	STAA	Brochothrix thermosphacta	15



Measurements and Experiments

```
SELECT Organism, Medium, Time, CFU
```

```
FROM Experiments JOIN Measurements ON
```

```
Experiments.Experiment_ID=Measurements.Experiment_ID WHERE Temperature=0;
```

Result			
Organism	Medium	Time	CFU
Pseudomonas sp.	CFC	1	1.8
Pseudomonas sp.	CFC	2	1.3
Pseudomonas sp.	CFC	7	2
Pseudomonas sp.	CFC	11	1
Pseudomonas sp.	CFC	16	2.3
Lactic acid bacteria	MRS	1	2.3
Lactic acid bacteria	MRS	7	1.6
Lactic acid bacteria	MRS	11	2.4
Lactic acid bacteria	MRS	16	2.5
Lactic acid bacteria	MRS	21	3.5
Lactic acid bacteria	MRS	28	5.1
Lactic acid bacteria	MRS	32	4.3



RDBMS



Relational database management systems

- SQLite
- MySQL
- Oracle
- Microsoft SQL Server
- MariaDB
- PostgreSQL





NoSQL

Non-SQL...

...or Not Only SQL

Cassandra vs **MongoDB** vs **CouchDB** vs **Redis** vs **Riak** vs
HBase vs **Couchbase** vs **OrientDB** vs **Aerospike** vs **Neo4j** vs
Hypertable vs **ElasticSearch** vs **Accumulo** vs **VoltDB** vs
Scalaris vs **RethinkDB** comparison

<https://kkovacs.eu/cassandra-vs-mongodb-vs-couchdb-vs-redis>



SQLite

Free, open source.

No client-server setup - "embedded" approach.

Databases stored in local files.

Good for small projects and learning SQL.

One of the most popular pieces of software in the world – you already have it!





That's all!

MSc Applied Bioinformatics 2024-2025
Data Integration and Interaction Networks

Dr Tomasz Kurowski
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Database Design and Implementation

Following the database design discussion this morning, you are now going to implement the proposed microbial growth database using a relational database management system called **SQLite**. Unlike most traditional RDBMSes, SQLite does not depend on a separate server application (which stores and manages the data) and client application (which remotely connects to the server), but it stores databases in local files, which can be accessed using a simple local executable – one could call it an “embedded” system. This makes it less suitable for databases meant to be shared by many users, but it will make your work easier as you learn the basics of what is otherwise a full-fledged relational database system.

SQLite setup

For most uses SQLite does not require installation or significant setup. Simply download and extract the appropriate precompiled binaries for your system (Linux, Windows, or macOS), either from Canvas or the official website: <https://sqlite.org/download.html>

