Bioinformatics Data Management

Lecture 3

Structured Databases

MARC: Developing Bioinformatics Programs
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Bioinformatics Data Management

- The following material is the result of a curriculum development effort to provide a set of courses to support bioinformatics efforts involving students from the biological sciences, computer science, and mathematics departments. They have been developed as a part of the NIH funded project “Assisting Bioinformatics Efforts at Minority Schools” (2T36 GM008789). The people involved with the curriculum development effort include:

- Dr. Hugh B. Nicholas, Dr. Troy Wymore, Mr. Alexander Ropelewski and Dr. David Deerfield II, National Resource for Biomedical Supercomputing, Pittsburgh Supercomputing Center, Carnegie Mellon University.
- Dr. Ricardo González Méndez, University of Puerto Rico Medical Sciences Campus.
- Dr. Alade Tokuta, North Carolina Central University.
- Dr. Jaime Seguel and Dr. Bienvenido Vélez, University of Puerto Rico at Mayagüez.
- Dr. Satish Bhalla, Johnson C. Smith University.

Structured Databases: Outline

- Structured Databases at a Glance - Characteristics
- Advantages of Structured Databases
- Data Independence
- Disadvantages of Structured Databases
- Examples of Structured Databases
  - Hierarchical Databases
  - Networked Databases
  - Relational Databases
  - XML Databases

Structured Databases at a Glance

- All information organized in same way (Data Model)
- Language available to
  - describe (create) the database
  - insert data
  - manipulate data
  - update
- Language establishes an abstract data model: Data Independence
- Programs using language can work across systems
- Facilitates communication and sharing data

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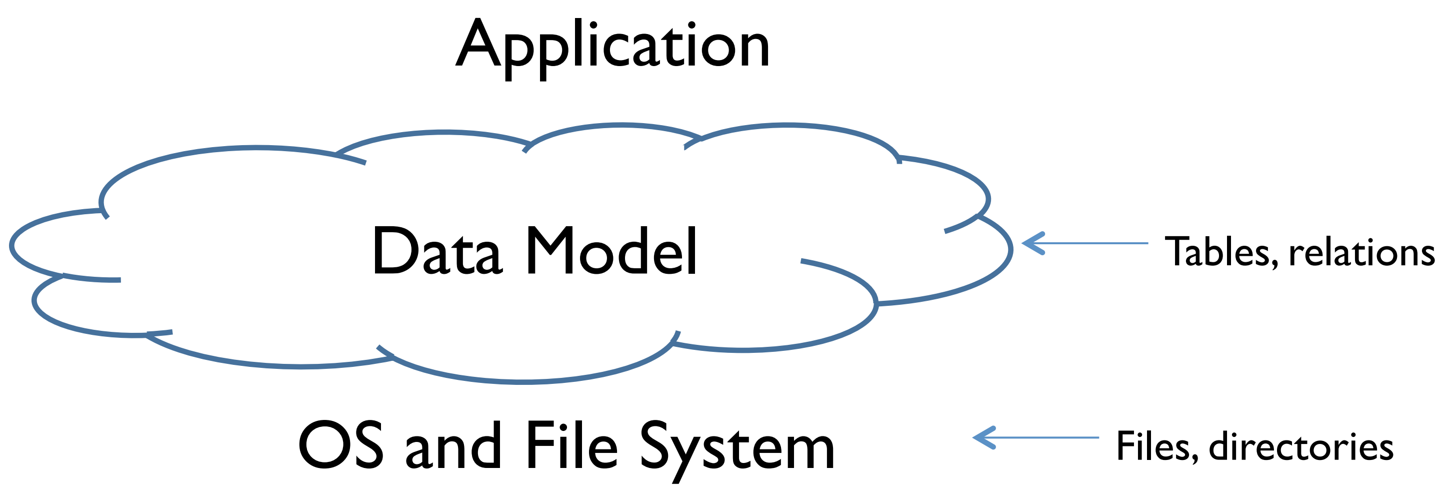
Data Independence



Objective:

Shield apps from changes in “physical” platform specific layers

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Disadvantages of Structured Databases

Model may not fit data needs

Example: How to represent proteins in table format

Approach #1 – Store one residue per column

AccNum	Name	AA1	AA2	AA3	…	AA517
AAA16331	G-gamma globin	M	G	H		
AAA51693	Aldehyde Dehydrogenase	M	L	R	…	S

Wasted space

Must make number of columns = max length of any possible sequence

What is this number?

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Disadvantages of Structured Databases

Model may not fit data needs

Approach #2 – Store one residue per rows

AccNum	AAPos	AA	Name
AAA16331	1	M	G-gamma globin
AAA16331	2	M	G-gamma globin
…	…	…	…
AAA51693	1	M	Aldehyde Dehydrogenase
…	…	…	…

Difficult to recover sequence in string form using DML

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Disadvantages of Structured Databases

Model may not fit data needs

Approach #3 – Put aminoacid sequence in one attribute

AccNum	Name	Sequence
AAA16331	G-gamma globin	"MGHFTEEDKA…."
AAA51693	Aldehyde Dehydrogenase	"MLRAAARFPGP…."
…	…	

Must analyze sequence using program outside SQL
Loose some benefits of Data Model

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A Simple Relational Example

- Intuitively model consists of tables
  - Rows are objects or "entities"
  - Columns are "attributes" of entities
  - Attributes cross reference other tables

Proteins

AccessionNum	Name	DiscBy	SeqBy
P201		2	3
Q303		2	1
R32		3	NULL

Primary key

Scientists

Num	Name	Last	Country
1	John	Doe	England
2	Jane	Doe	England
3	Hugh	Nicholas	USA

Primary key

Intuitively:
- ➢Protein P201 discovered by Jane Doe
- ➢Hugh discovered R2 and sequenced P201

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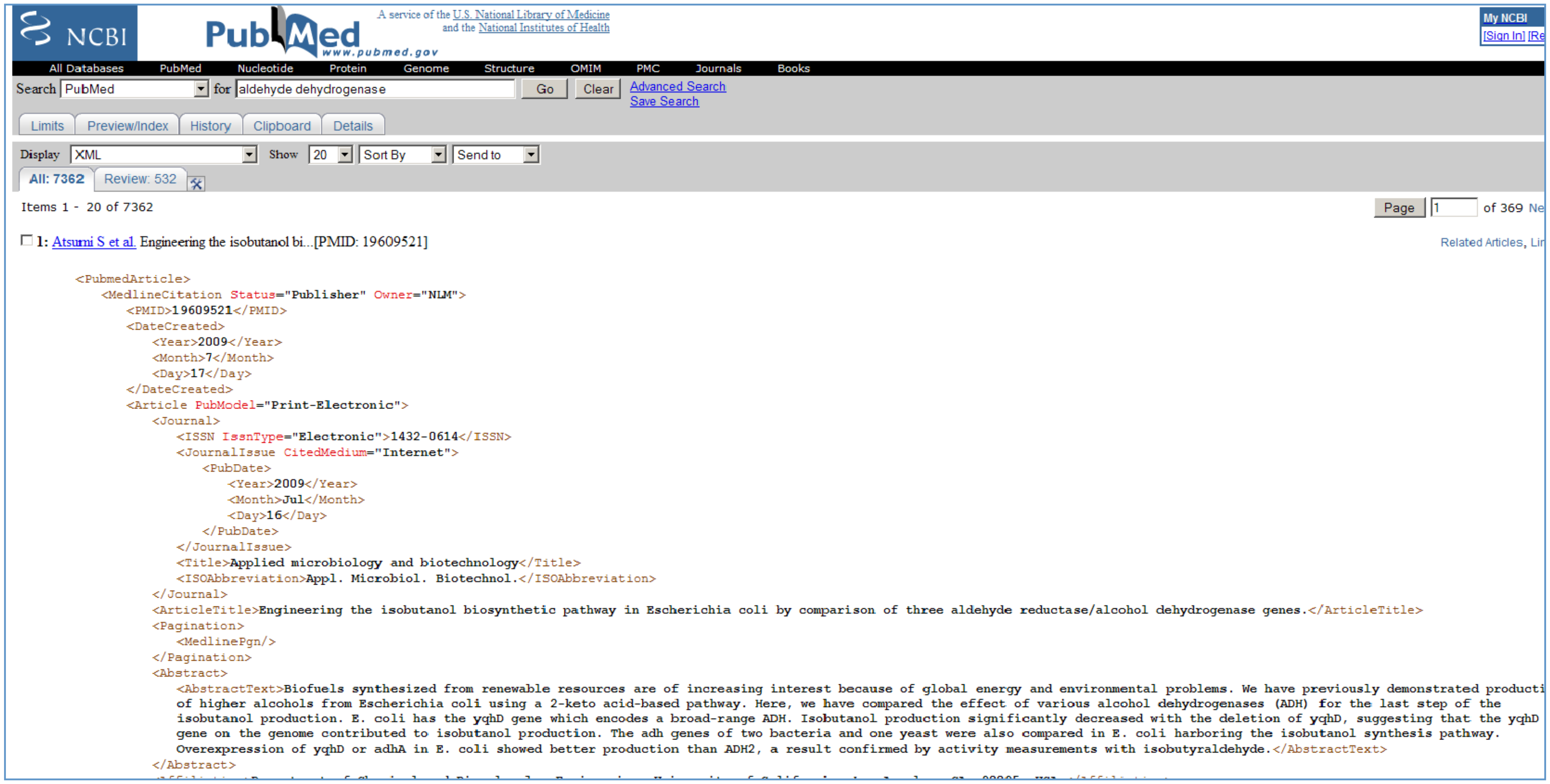
Structured Databases: Other examples

- XML Databases



1: Atsumi S et al. Engineering the isobutanol bi...[PMID: 19609521]

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                of higher alcohols from Escherichia coli using a 2-keto acid-based pathway. Here, we have compared the effect of various alcohol dehydrogenases (ADH) for the last step of the
                isobutanol production. E. coli has the yqhD gene which encodes a broad-range ADH. Isobutanol production significantly decreased with the deletion of yqhD, suggesting that the yqhD
                gene on the genome contributed to isobutanol production. The adh genes of two bacteria and one yeast were also compared in E. coli harboring the isobutanol synthesis pathway.
                Overexpression of yqhD or adhA in E. coli showed better production than ADH2, a result confirmed by activity measurements with isobutyraldehyde.</AbstractText>
            </Abstract>
```

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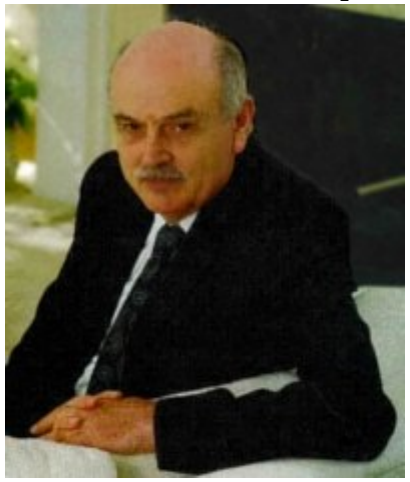
- Query language = XPATH/XQUERY

Relational Databases: Outline

- Introduction and Examples
- Relational Database Design by Example
    - entities and relational diagrams
    - normal forms
- SQL (Sequel) Language
- SQL Data Manipulation
    – Select
    – Joins
    – Updates and deletes
    – Inserts

Relational Databases: Timeline

- Originally proposed by E.F. Codd in 1970
- First research prototypes in early 80's:
  - Ingres @ UC Berkeley
  - System R @ IBM
- Today the market exceeds $20B annually


Edgar F. Codd

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Relational Databases Products

- Commercial
  - Oracle
  - MS SQL Server
  - IBM DB2
- Open Source
  - MySQL
  - Postgres
  - SQLite

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Example Relational Database Design

Goal: Store results from multiple sequence search attempts

Leverage SQL to analyze large result set

Entities to be stored: Matching sequences with scores for each search matrix

Acc#	Definition	Source	Matrix	eValue	SearchDate
P14555	Group IIA Phospholipase A2	Human	Pam70	4.18 E-32	7/21/07
P81479	Phospholipase A2 isozyme IV	Indian Green Tree Viper	Pam70	2.68 -E52	7/21/07
P14555	Group IIA Phospholipase A2	Human	Blosom80	3.47 E-33	7/20/07
P81479	Phospholipase A2 isozyme IV	Indian Green Tree Viper	Blosom80	1.20 E-54	7/20/07

Problems: Lots of redundant information

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Dealing with Redundancy

Normalization

Sequences

AccNum	Definition	Source
P14555	Group IIA Phospholipase A2	Human
P81479	Phospholipase A2 isozyme IV	Indian Green Tree Viper

Matches

Acc#	Date	Matrix	eValue
P14555	7/21/07	Pam70	4.18 E-32
P81479	7/21/07	Pam70	2.68 -E52
P14555	7/20/07	Blosom80	3.47 E-33
P81479	7/20/07	Blosom80	1.20 E-54

Foreign key

Still redundant

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Dealing with Redundancy

Normalization

Sequences

Acc#	Definition	Source
P14555	Group IIA Phospholipase A2	Human
P81479	Phospholipase A2 isozyme IV	Indian Green Tree Viper

Matches

Acc#	Run#	eValue
P14555	1	4.18 E-32
P81479	1	2.68 -E52
P14555	2	3.47 E-33
P81479	2	1.20 E-54

Runs

Run#	Matrix	Date
1	7/21/07	Pam70
2	7/20/07	Blosom80

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Basic Normal Forms

- First Normal Form
  - Table must be flat; no multi-valued attributes
- Second Normal Form
  - All non-key attributes determined by whole primary key
- Third Normal Form
  - All non-key attributes can ONLY depend on whole primary key directly
- Others…

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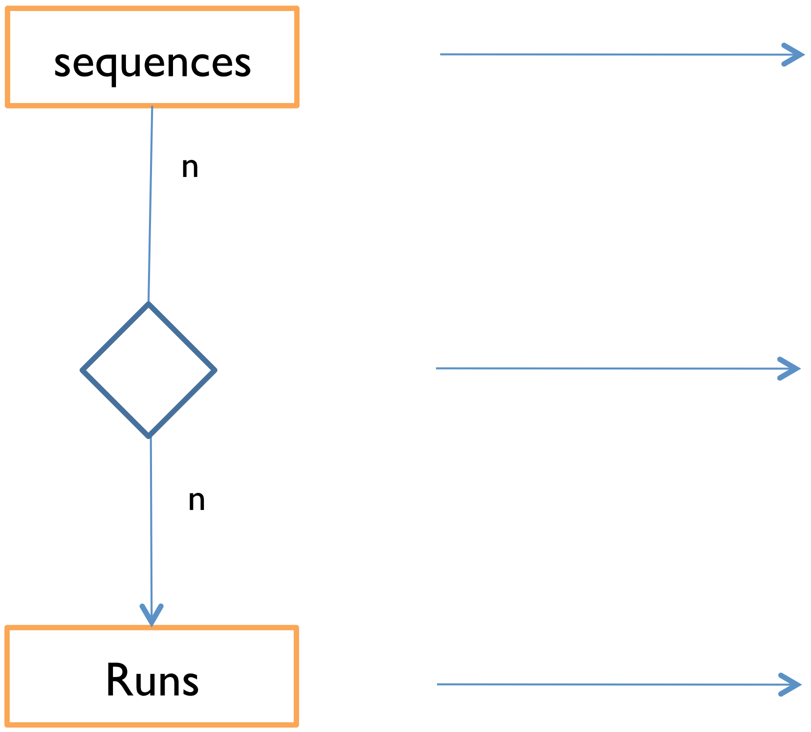
Entity Relationship Diagrams



Sequences

Acc#	Definition	Source

Matches

Acc#	Run#	eValue

Runs

Run#	Matrix	Date

N-to-N relations model as table

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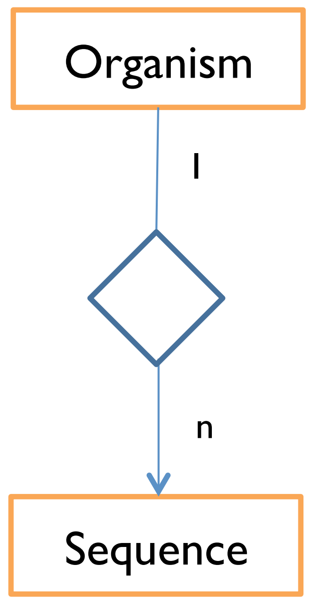
Entity Relationship Diagrams



Organism

ID	Name	Description
1	Cod worm	Pseudoterranova decipiens
2	Human	Homo sapiens

No table necessary for one-to-many rel's

Sequence

Acc#	SrcID	Name
CAA77743	1	Hemoglobin
AB647031	2	Hemoglobin

one-to-many relationships

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Simple Query Language (SQL)

- Organization
  - Data definition/schema creation
  - Data manipulation
    - Insertion
    - Manipulation
    - Updates
    - Removals
  - A standard (ISO) since 1987

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SQL Data Definition Language (DDL)

- The CREATE statement

Sequences

Acc#	Definition	Source

Runs

Run#	Matrix	Date

Matches

Acc#	Run#	eValue

```
CREATE TABLE Sequences(
            AccNum int,
            Definition varchar (255),
            Source varchar(255) )
CREATE TABLE Runs(
            RunNum int,
            Matrix varchar(255),
            Date date)
CREATE TABLE Matches(
            AccNum int,
            RunNum int,
            eValue int)
```

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SQL Data Manipulation Language (DML)

- Foundation is relational algebra
- An algebra on relations with three basic operations:

Operation	Description
Projection	Select subset of attributes of a table
Selection	Select subset of entities in a table
Join	Merge two tables into one

All three operations yield a new table as the result

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Relational Algebra - Projection

- Selects a subset of attributes or columns

Sequences

Acc#	Definition	Source
CAM22514	Hemoglobin alpha	Mus Musculus
CAO91797	Hemoglobin X	Mus Musculus
ABG47031	Hemoglobin	Homo Sapiens

$\pi_{\text{Acc\#, Source}}(\text{Sequences})$

Acc#	Source
CAM22514	Mus Musculus
CAO91797	Mus Musculus
ABG47031	Homo Sapiens

Intuitively:
Find organism that each sequence belongs to

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Relational Algebra - Selection

- Selects a subset of entities or rows

Sequences

Acc#	Definition	Source
CAM22514	Hemoglobin alpha	Mus Musculus
CAO91797	Hemoglobin X	Mus Musculus
ABG47031	Hemoglobin	Homo Sapiens

$$\downarrow$$

$\sigma_{\text{Source=Mus Musculus}}$ (Sequences)

$$\downarrow$$

Intuitively:
Find all sequences from Mus Musculus

Sequences

Acc#	Definition	Source
CAM22514	Hemoglobin alpha	Mus Musculus
CAO91797	Hemoglobin X	Mus Musculus

No reason to keep organism is result

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Relational Algebra: Projection and Selection

$\pi_{\text{Acc\#, Definition}}(\sigma_{\text{Source= Mus Musculus}}(\text{Sequences}))$

Sequences

Acc#	Definition	Source
CAM22514	Hemoglobin alpha	Mus Musculus
CAO91797	Hemoglobin X	Mus Musculus
ABG47031	Hemoglobin	Homo Sapiens

$\sigma_{\text{Source= Mus Musculus}}$ (Sequences)

Acc#	Definition	Source
CAM22514	Hemoglobin alpha	Mus Musculus
CAO91797	Hemoglobin X	Mus Musculus

$\pi_{\text{Acc\#, Definition}}$ (Sequences)

Acc#	Definition
CAM22514	Hemoglobin alpha
CAO91797	Hemoglobin X

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Relational Algebra - Natural Join

Sequences

AccNum	Definition	SourceID
CAM22514	Hemoglobin alpha	1
CAO91797	Hemoglobin X	1
ABG47031	Hemoglobin	2

Organisms

SourceID	Name
1	Mus Musculus
1	Mus Musculus
2	Homo Sapiens

Sequences $\bowtie$ Organisms

AccNum	Definition	SourceID	Name
CAM22514	Hemoglobin alpha	1	Mus Musculus
CAO91797	Hemoglobin X	1	Mus Musculus
ABG47031	Hemoglobin	2	Homo Sapiens

Requires attributes for join to have same name

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Relational Algebra - Inner Join

Sequences

AccNum	Definition	SrcID
CAM22514	Hemoglobin alpha	1
ABG47031	Hemoglobin	2
NPO34535	Hemoglobin zeta	3

Organisms

SrcID	Name
1	Mus Musculus
2	Homo Sapiens

$$\text{Sequences} \bowtie_{\text{sequences.SrcID = organisms.SrcID}} \text{Organisms}$$

AccNum	Name	SrcID	Name
CAM22514	Hemoglobin alpha	1	Mus Musculus
ABG47031	Hemoglobin	2	Homo Sapiens

Rows without matching attributes excluded

Can name attribute explicitly

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Relational Algebra - Left Join

Sequences

AccNum	Definition	SrcID
CAM22514	Hemoglobin alpha	1
ABG47031	Hemoglobin	2
NPO34535	Hemoglobin zeta	3

Organisms

SrcID	Name
1	Mus Musculus
2	Homo Sapiens

$\text{Sequences} \bowtie_{\text{sequences.SrcID = organisms.SrcID}} \text{Organisms}$

AccNum	Name	SrcID	Name
CAM22514	Hemoglobin alpha	1	Mus Musculus
ABG47031	Hemoglobin	2	Homo Sapiens
NPO34535	Hemoglobin zeta	3	NULL

Tuples (rows) on left table without matches have NULL values on attributes of right table

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SQL Select - Projection

- Selects a subset of attributes or columns

Sequences

Acc#	Definition	Source
CAM22514	Hemoglobin alpha	Mus Musculus
CAO91797	Hemoglobin X	Mus Musculus
ABG47031	Hemoglobin	Homo Sapiens

$\pi_{\text{Acc\#, Source}}(\text{Sequences})$

Acc#	Source
CAM22514	Mus Musculus
CAO91797	Mus Musculus
ABG47031	Homo Sapiens

SELECT Acc#, Source
FROM Sequences

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SQL Select - Selection

- Selects a subset of entities or rows

Sequences

Acc#	Definition	Source
CAM22514	Hemoglobin alpha	Mus Musculus
CAO91797	Hemoglobin X	Mus Musculus
ABG47031	Hemoglobin	Homo Sapiens

$\sigma_{\text{Source=Mus Musculus}}$ (Sequences)

```
SELECT *
  FROM Sequences
   WHERE Source= Mus Musculus
```

Sequences

Acc#	Definition	Source
CAM22514	Hemoglobin alpha	Mus Musculus
CAO91797	Hemoglobin X	Mus Musculus

"*" means "all" attributes

No reason to keep organism is result

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SQL Select: Projection and Selection

$\pi_{\text{Acc\#, Definition}}(\sigma_{\text{Source= Mus Musculus}}(\text{Sequences}))$

Sequences

Acc#	Definition	Source
CAM22514	Hemoglobin alpha	Mus Musculus
CAO91797	Hemoglobin X	Mus Musculus
ABG47031	Hemoglobin	Homo Sapiens

```
SELECT SeqNum,  Org
   FROM Sequences
    WHERE Source= Mus Musculus)
```

$\sigma_{\text{Source= Mus Musculus}}$ (Sequences)

Acc#	Definition	Source
CAM22514	Hemoglobin alpha	Mus Musculus
CAO91797	Hemoglobin X	Mus Musculus

$\pi_{\text{Acc\#, Definition}}$ (Sequences)

Acc#	Definition
CAM22514	Hemoglobin alpha
CAO91797	Hemoglobin X

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SQL Select - Natural Join

Sequences

AccNum	Definition	SourceID
CAM22514	Hemoglobin alpha	1
CAO91797	Hemoglobin X	1
ABG47031	Hemoglobin	2

Organisms

SourceID	Name
1	Mus Musculus
1	Mus Musculus
2	Homo Sapiens

Sequences $\bowtie$ Organisms

```
SELECT *
   FROM Sequences
   NATURAL JOIN Organisms
```

AccNum	Definition	SourceID	Name
CAM22514	Hemoglobin alpha	1	Mus Musculus
CAO91797	Hemoglobin X	1	Mus Musculus
ABG47031	Hemoglobin	2	Homo Sapiens

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SQL Select - Inner Join

Sequences

AccNum	Definition	SrcID
CAM22514	Hemoglobin alpha	1
ABG47031	Hemoglobin	2
NPO34535	Hemoglobin zeta	3

Organisms

SrcID	Name
1	Mus Musculus
2	Homo Sapiens

$\text{Sequences} \bowtie_{\text{sequences.SrcID = organisms.SrcID}} \text{Organisms}$

```
SELECT *
    FROM Sequences
    INNER JOIN Organisms
    on sequences.SrcID = organisms.SrcID
```

AccNum	Name	SrcID	Name
CAM22514	Hemoglobin alpha	1	Mus Musculus
ABG47031	Hemoglobin	2	Homo Sapiens

Rows without matching attributes excluded

Can name attribute explicitly

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SQL Select - Left Join

Sequences

AccNum	Definition	SrcID
CAM22514	Hemoglobin alpha	1
ABG47031	Hemoglobin	2
NPO34535	Hemoglobin zeta	3

Organisms

SrcID	Name
1	Mus Musculus
2	Homo Sapiens

Sequences $\bowtie_{\text{sequences.SrcID = organisms.SrcID}}$ Organisms

```
SELECT *
   FROM Sequences LEFT OUTER JOIN Organisms
      ON Sequences.SrcID = Organisms.SrcID;
```

AccNum	Name	SrcID	Name
CAM22514	Hemoglobin alpha	1	Mus Musculus
ABG47031	Hemoglobin	2	Homo Sapiens
NPO34535	Hemoglobin zeta	3	NULL

Tuples (rows) on left table without matches have NULL values on attributes of right table

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SQL UPDATE Statement

Matches

Acc#	Date	Matrix	eValue
P14555	7/21/07	Pam70	4.18 E-32
P81479	7/21/07	Pam70	2.68 -E52
P14555	7/20/07	Blosom80	3.47 E-33
P81479	7/20/07	Blosom80	1.20 E-54

```
UPDATE Matches
        SET Date = '7/22/07'
       WHERE Date = '7/21/07'
```

Matches

Acc#	Date	Matrix	eValue
P14555	7/22/07	Pam70	4.18 E-32
P81479	7/22/07	Pam70	2.68 -E52
P14555	7/20/07	Blosom80	3.47 E-33
P81479	7/20/07	Blosom80	1.20 E-54

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SQL DELETE Statement

Matches

Acc#	Date	Matrix	eValue
P14555	7/21/07	Pam70	4.18 E-32
P81479	7/21/07	Pam70	2.68 -E52
P14555	7/20/07	Blosom80	3.47 E-33
P81479	7/20/07	Blosom80	1.20 E-54

```
DELETE FROM Matches
       WHERE Date = '7/21/07'
```

Matches

Acc#	Date	Matrix	eValue
P14555	7/20/07	Blosom80	3.47 E-33
P81479	7/20/07	Blosom80	1.20 E-54

ADVICE: BE CAREFUL WITH DELETE. THERE IS NO EASY UNDO

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SQL Select with SORT BY

Matches

Acc#	Date	Matrix	eValue
P14555	7/21/07	Pam70	4.18 E-32
P81479	7/21/07	Pam70	2.68 -E52
P14555	7/20/07	Blosom80	3.47 E-33
P81479	7/20/07	Blosom80	1.20 E-54

```
SELECT * FROM Matches
         SORT BY eValue ASC
```

Matches

Acc#	Date	Matrix	eValue
P81479	7/20/07	Blosom80	1.20 E-54
P81479	7/22/07	Pam70	2.68 -E52
P14555	7/20/07	Blosom80	3.47 E-33
P14555	7/22/07	Pam70	4.18 E-32

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SQL Data Manipulation

- Grouping Results and Aggregates

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Filling-Up the database - Insert

Organisms

SrcID	Name
1	Mus Musculus
2	Homo Sapiens

```
INSERT INTO Organisms
        Values (3,'C. Elegans')
```

Organisms

SrcID	Name
1	Mus Musculus
2	Homo Sapiens
3	C. Elegans

Good when you know the attributes of all entities c-priori

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Filling-Up the database

- Approach #2: Input from file (CSV)

- Under construction

- Tricky to set data types handled correctly

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Case Study: Analyzing Results of Multiple BLAST Runs with alternative search matrices

- Steps at a Glance
  - Install and configure tools
    - Python environment including BioPython
    - Database system (SQLite)
  - Design the relational database schema
  - Write Python functions to insert results into database
  - Analyze data using SQL queries

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Case Study (Step 1): Install Tools

Windows version

- Install Python interpreter
  - Download installer from www.python.org
  - Run installer and verify installation
- Install BioPython
  - Download installer from www.biopython.org
  - Run installer and verify installation
- Install SQLiteMan
  - Download SQLiteMan query browser from www.sqliteman.com
  - Run installer and verify installation

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Case Study (Step 1): Install Tools

Mac OS version

- UNDER CONSTRUCTION

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Case Study (Step 2):Design Database Schema

Source	Accession Num	Definition	Matrix	eValue	SearchDate
Human	P14555	Group IIA Phospholipase A2	Pam70	4.18 E-32	7/21/07
Indian Green Tree Viper	P81479	Phospholipase A2 isozyme IV	Pam70	2.68 -E52	7/21/07
Human	P14555	Group IIA Phospholipase A2	Blosom80	3.47 E-33	7/20/07
Indian Green Tree Viper	P81479	Phospholipase A2 isozyme IV	Blosom80	1.20 E-54	7/20/07

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Case Study Step 3: Python Programming

- Write Python functions to:
  - Run a BLAST search for the query sequence and a specific matrix
  - Insert results into Database
    - Run SQL insert queries to populate the database
    - Create a CSV file with all results from BLAST searches and import to DB
  - Run all functions together running one Blast for each one of a set of matrices

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Case Study Step 3: Python Programming

- Run a BLAST search for the query sequence and a specific matrix

```
From Bio.Blast import NCBIWWW
from Bio.Blast import NCBIXML
from Bio import Fasta
from sys import *
import sqlite3

def searchAndStoreBlastSearch(query, matrix_id, filename):
    # Creates handle to store the results sent by NCBI website
    results_handle = NCBIWWW.qblast("blastp", "swissprot", query, expect=10,
                descriptions=2000, alignments=2000, hitlist_size=2000,
                matrix_name=matrix_id)
    # Reads results into memory
    blast_results = results_handle.read()

    # Creates and opens a file in filesystem for writing
    save_file = open(filename, 'w')

    # Store results from memory into the filesystem
    save_file.write(blast_results)

    #Close the file handler
    save_file.close()
```

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Case Study Step 3: Python Programming

- Insert results into Database: Run multiple SQL insert queries

```
def xmlToDatabase(filename, matrix_id, dbCursor, dbConn):
    blast_fileptr=open(filename)
    record=NCBIXML.parse(blast_fileptr).next()

    for alignment in record.alignments:
        hsp=alignment.hsps[0]
        storeIntoDatabase(hsp, alignment, matrix_id,dbCursor,dbConn)
    blast_fileptr.close()
```

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Case Study Step 3: Python Programming

- Insert results into Database: Run multiple SQL *insert* queries

```
def storeIntoDatabase(hsp, alignment, matrix_id, dbCursor, dbConn):
    # Insert a row of data into the table (securely)
    t = (hsp.expect, hsp.score, matrix_id, alignment.accession, alignment.title,)
    dbCursor.execute("insert into sequences values (?,?,?,?,?)",t)

    # Save (commit) the changes
    dbConn.commit()
```

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Case Study Step 3: Python Programming

- Insert results into Database: Create a CSV file with all results from BLAST searches

```
def xmlToCSV(xmlFilename, csvFilename, matrix_id):
    # Create file handler
    blast_fileptr=open(xmlFilename)
    # Parse xml file into biopython object
    record=NCBIXML.parse(blast_fileptr).next()
    # Create csv file writer
    csvFileWriter = csv.writer(open(csvFilename,'wb'))
    # Iterate over record alignments
    for alignment in record.alignments:
        # Extract high score pairwise alignment object
        hsp=alignment.hsps[0]
        # Create record vector
        record = [hsp.expect, hsp.score, matrix_id, alignment.accession, alignment.title,]
        # Store record vector into csv file
        csvFileWriter.writerow( record )
    # Close file handler
    blast_fileptr.close()
```

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Case Study Step 3: Python Programming

- Use all functions to run one Blast for each of a sequence of search matrices

```
Matrixname=['PAM70','BLOSUM80']
FileName=['TestPAM70.xml','TestBLOSUM80.xml']
dbFileName='data.db3'
```

```
def doIt():
    print "Import fasta file"
    query_file = open('P00624.fasta')
    fasta = Fasta.Iterator(query_file)
    query = fasta.next()
    query_file.close()
    print "Creating database interface"
    dbConnection = sqlite3.connect(dbFileName)
    dbCursor = dbConnection.cursor()

    # Create tables
    dbCursor.execute("DROP TABLE IF EXISTS sequences")

    dbCursor.execute("CREATE TABLE IF NOT EXISTS sequences (expect real, score int, matrix text, \
                                                            accession text, description text)")
    print "Iterate over matrixes"
    for i in range(0,len(MatrixName)):
        print "Sending blast search"
        searchAndStoreBlastSearch(query, MatrixName[i], FileName[i])
        print "Processing blase search"
        xmlToDatabase(FileName[i], MatrixName[i], dbCursor, dbConnection)
    print "Program done"
```

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Case Study Step 3: Python Programming

- Run all functions together running one Blast for each one of a set of matrices
- Import CSV version

```
MatrixName=['PAM70','BLOSUM80']
TableName=['PAM70','BLOSUM80']
FileName=['TestPAM70.xml','TestBLOSUM80.xml']
CsvFileName=['TestPAM70.csv','TestBLOSUM80.csv']

def doIt():
    query_file = open('P00624.fasta')
    fasta = Fasta.Iterator(query_file)
    query = fasta.next()
    query_file.close()
    for i in range(0,len(MatrixName)):
        searchAndStoreBlastSearch(query, MatrixName[i], FileName[i])
        xmlToCSV(FileName[i], CsvFileName[i], MatrixName[i])
```

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Case Study (Step 3): Import CSV File

- UNDER CONSTRUCTION

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Case Study (Step 4): Analyze Data

- Analyze data using SQL
- Example 1: Finding top matches
  - Display sequences sorted by average score/run and number of runs where they appeared

```
select *, COUNT(matrix) as total
    from sequences
    group by accession
    order by total desc
```

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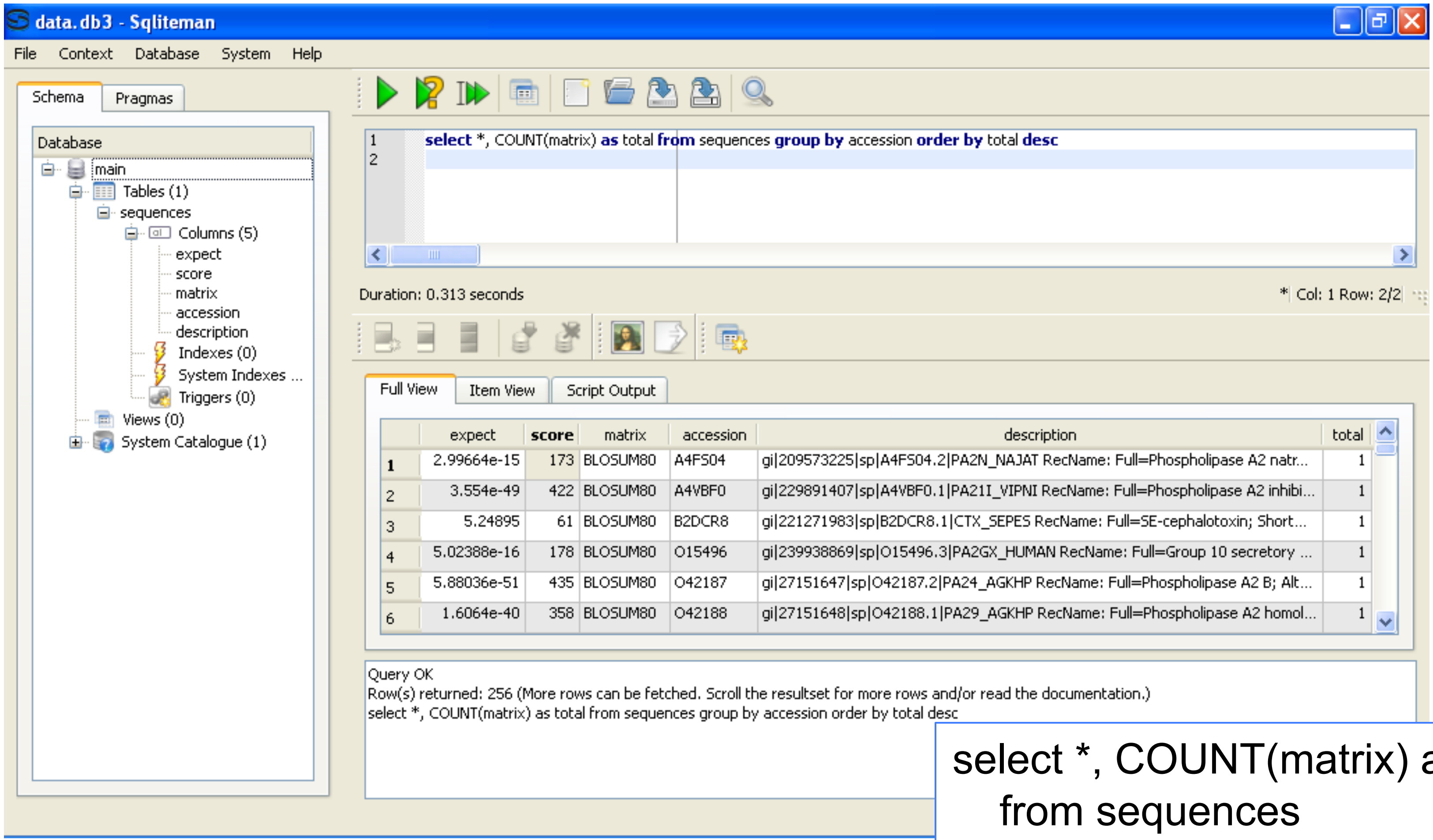
Case Study (Step 4): Analyze Data



```
select *, COUNT(matrix) as total from sequences group by accession order by total desc
```

Duration: 0.313 seconds

* Col: 1 Row: 2/2

	expect	score	matrix	accession	description	total
1	2.99664e-15	173	BLOSUM80	A4FS04	gi|209573225|sp|A4FS04.2|PA2N_NAJAT RecName: Full=Phospholipase A2 natr...	1
2	3.554e-49	422	BLOSUM80	A4VBF0	gi|229891407|sp|A4VBF0.1|PA21I_VIPNI RecName: Full=Phospholipase A2 inhibi...	1
3	5.24895	61	BLOSUM80	B2DCR8	gi|221271983|sp|B2DCR8.1|CTX_SEPES RecName: Full=SE-cephalotoxin; Short...	1
4	5.02388e-16	178	BLOSUM80	O15496	gi|239938869|sp|O15496.3|PA2GX_HUMAN RecName: Full=Group 10 secretory ...	1
5	5.88036e-51	435	BLOSUM80	O42187	gi|27151647|sp|O42187.2|PA24_AGKHP RecName: Full=Phospholipase A2 B; Alt...	1
6	1.6064e-40	358	BLOSUM80	O42188	gi|27151648|sp|O42188.1|PA29_AGKHP RecName: Full=Phospholipase A2 homol...	1

```
Query OK
Row(s) returned: 256 (More rows can be fetched. Scroll the resultset for more rows and/or read the documentation.)
select *, COUNT(matrix) as total from sequences group by accession order by total desc
```

```
select *, COUNT(matrix) as total
    from sequences
    group by accession
    order by total desc
```

Display sequences sorted by average score/run and number of runs where they appeared

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Case Study (Step 4): Analyze Data

- Analyze data using SQL
- Example 2: Finding discriminating matrices
  - Display sequences that only showed up in one matrix run

```
select *, COUNT(matrix) as total
    from sequences
    group by accession
    having total = 1
```

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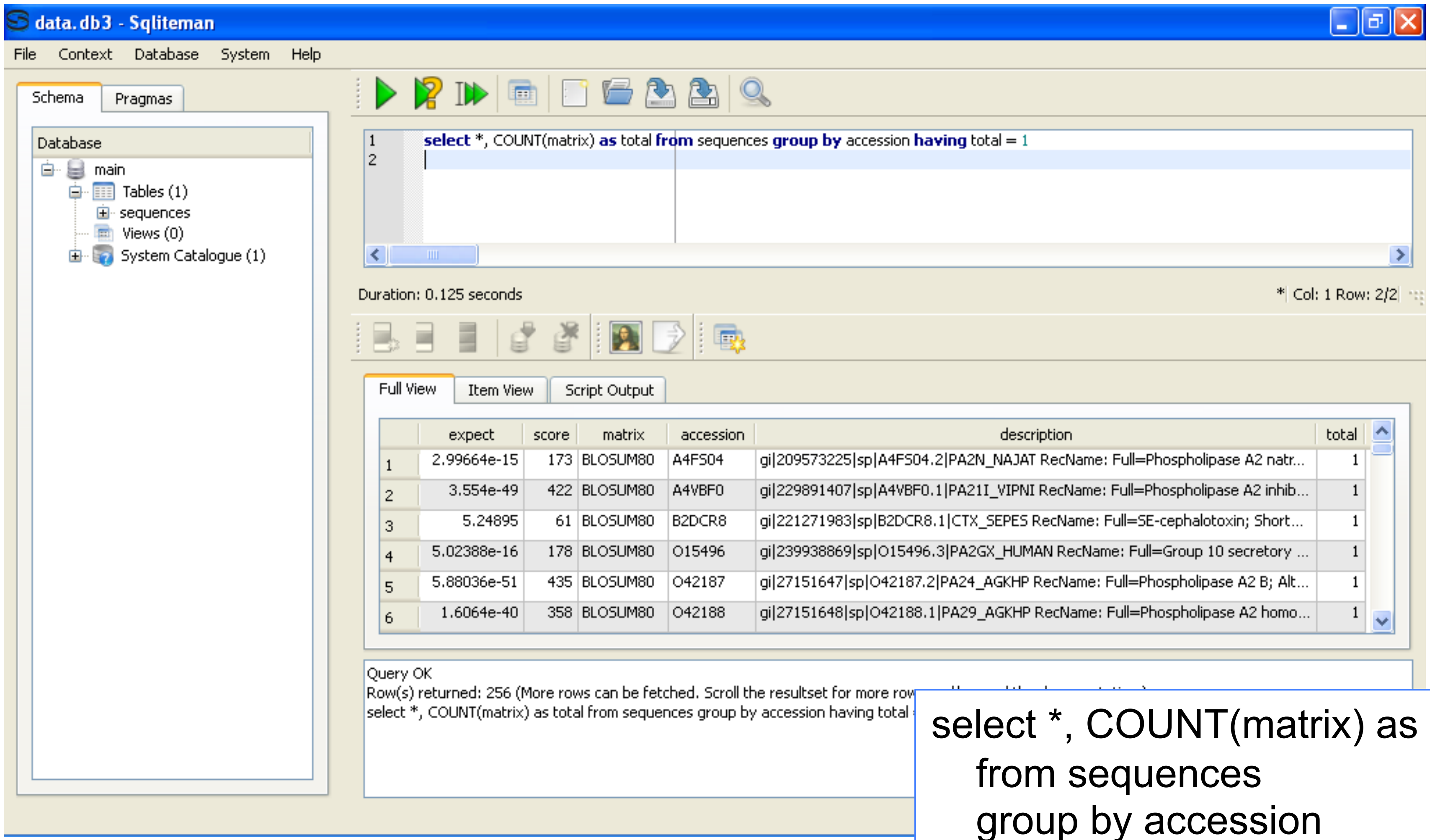
Case Study (Step 4): Analyze Data



```
select *, COUNT(matrix) as total from sequences group by accession having total = 1
```

Duration: 0.125 seconds   * Col: 1 Row: 2/2

	expect	score	matrix	accession	description	total
1	2.99664e-15	173	BLOSUM80	A4FS04	gi|209573225|sp|A4FS04.2|PA2N_NAJAT RecName: Full=Phospholipase A2 natr...	1
2	3.554e-49	422	BLOSUM80	A4VBF0	gi|229891407|sp|A4VBF0.1|PA21I_VIPNI RecName: Full=Phospholipase A2 inhib...	1
3	5.24895	61	BLOSUM80	B2DCR8	gi|221271983|sp|B2DCR8.1|CTX_SEPES RecName: Full=SE-cephalotoxin; Short...	1
4	5.02388e-16	178	BLOSUM80	O15496	gi|239938869|sp|O15496.3|PA2GX_HUMAN RecName: Full=Group 10 secretory ...	1
5	5.88036e-51	435	BLOSUM80	O42187	gi|27151647|sp|O42187.2|PA24_AGKHP RecName: Full=Phospholipase A2 B; Alt...	1
6	1.6064e-40	358	BLOSUM80	O42188	gi|27151648|sp|O42188.1|PA29_AGKHP RecName: Full=Phospholipase A2 homo...	1

```
Query OK
Row(s) returned: 256 (More rows can be fetched. Scroll the resultset for more row
select *, COUNT(matrix) as total from sequences group by accession having total
```

Display sequences that only showed up in one matrix run

```
select *, COUNT(matrix) as total
    from sequences
    group by accession
    having total = 1
```

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Case Study: Step 4

- Generate Graphic Reports using Excel

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