Introduction: Elements of Biological Data Models

Prof. Daniel P. Miranker

Objectives:

- What is the course about?
  - Why is "data model" deserving of an entire course?
- How is the course organized?
  - What will I learn, and what is expected of me?

AFQ:

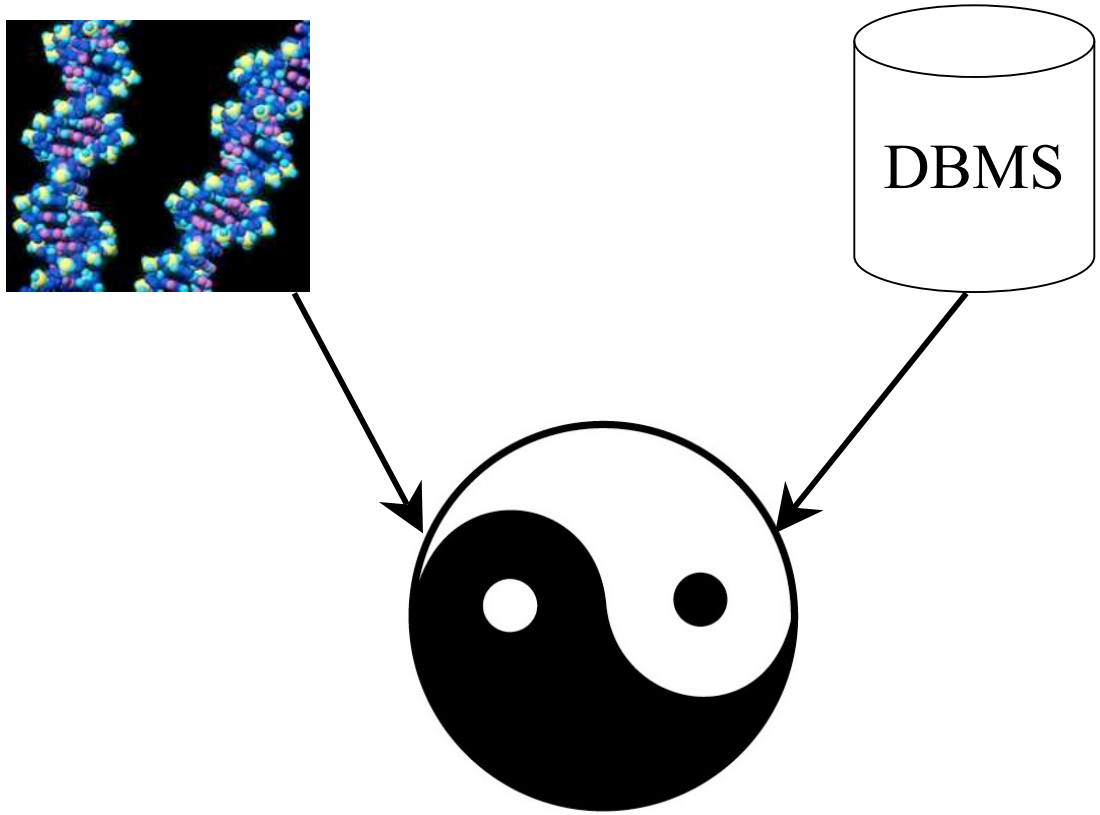
AFQ: Answers to Your First Questions

- Is this class only useful for biologists?
  - No, approaching computers from the data model is a (the) broadly accepted way of thinking about organizing computer systems. The biology applications are a means to understanding these ideas.
- How much biology do I need to know?
  - Almost none. It will be covered in class. The contemporary developments in biology that are creating the data are so new, even biology majors don't know the story.
- Is there a lot of programming in this class?
  - Yes and no. You will be in a computer lab almost every week. You will not be writing out lines of code. You will get some visibility into this today.
  - Also, model solutions/programs are available for every homework. You are welcome to use the model code. Some team programming will be encouraged

Context of the Course

1. Genomic Revolution

2. A Discipline of Engineering
   Software is [finally] emerging



Goal: Learn about engineering large software systems through a biological application

Practical Goals:

(intended)

1. Be the non-software developer who can speak to the engineers.

(unintended)

2. If your goal is a job as a software developer, you'll walk out of this class very employable.

What is a data model?

http://www.utexas.edu/its/windows/database/datamodeling/dm/overview.html

Data Model: A data model is a conceptual representation of the data structures that are required by a database application.

Key phrase: *conceptual representation*

- *Think about it.*
- *Principles, Methods and Tools*

The Revolution In Biology

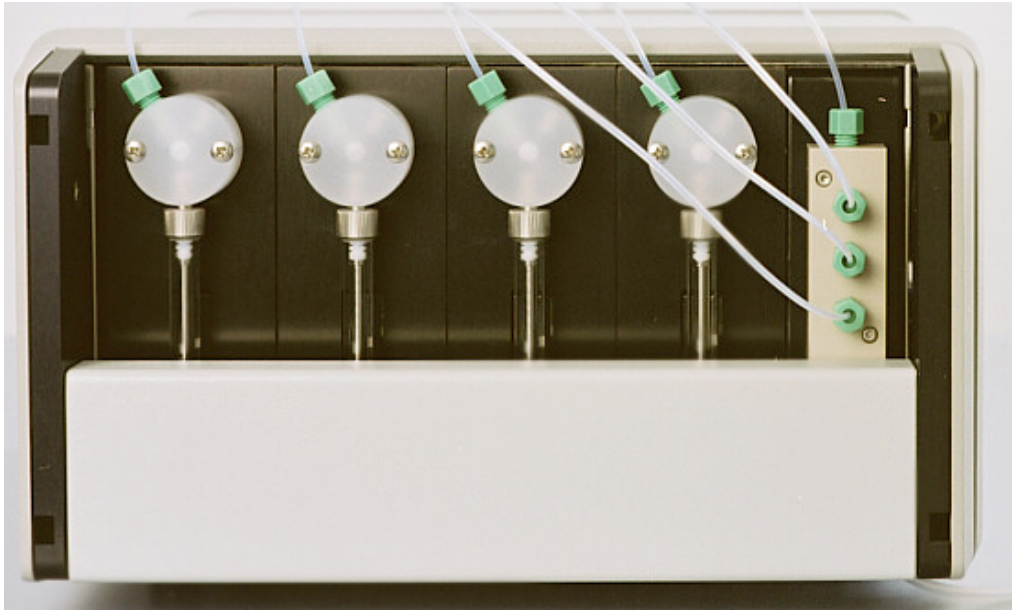
- "Post-genomic era" = After the human genome was first completely sequenced, 2000.
  - Grand challenge initiated ~1990
  - (3.3 billion nucleotides, A,C,G &T)

- How was the human genome sequenced?
  - Man or machine?

→Biologists discovered robots could do lab work (better).

- Not C3PO, but more like welding arms

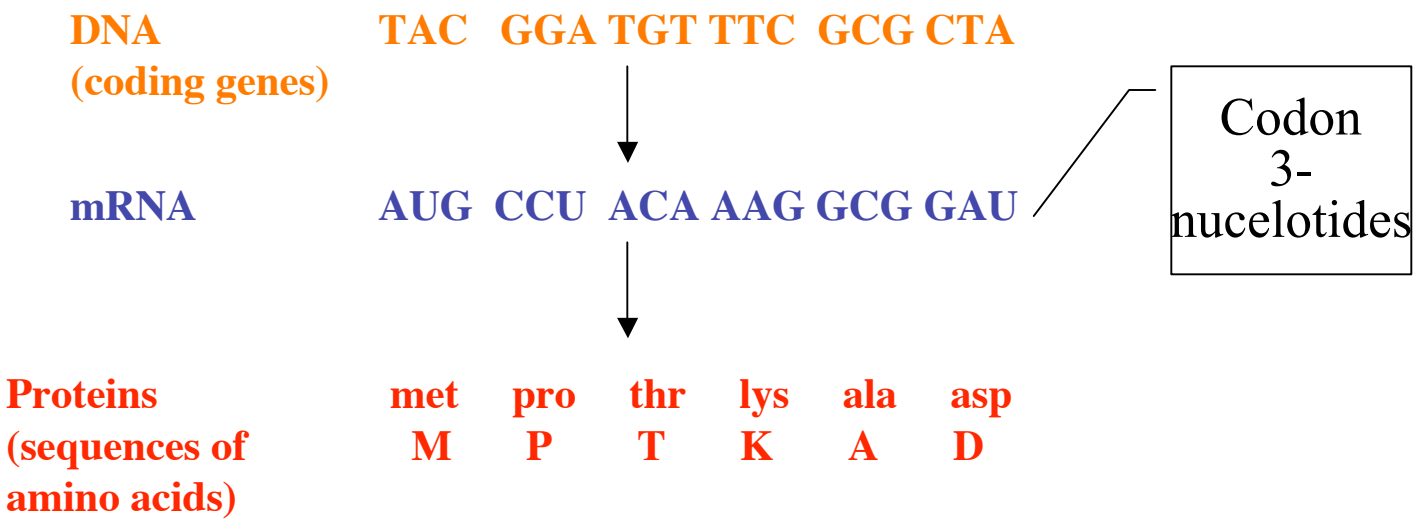
Industrial Automation Makes it into Biology Labs.



- Mostly by the use of microfluidic pumps

  Keyword: **“High-throughput”**

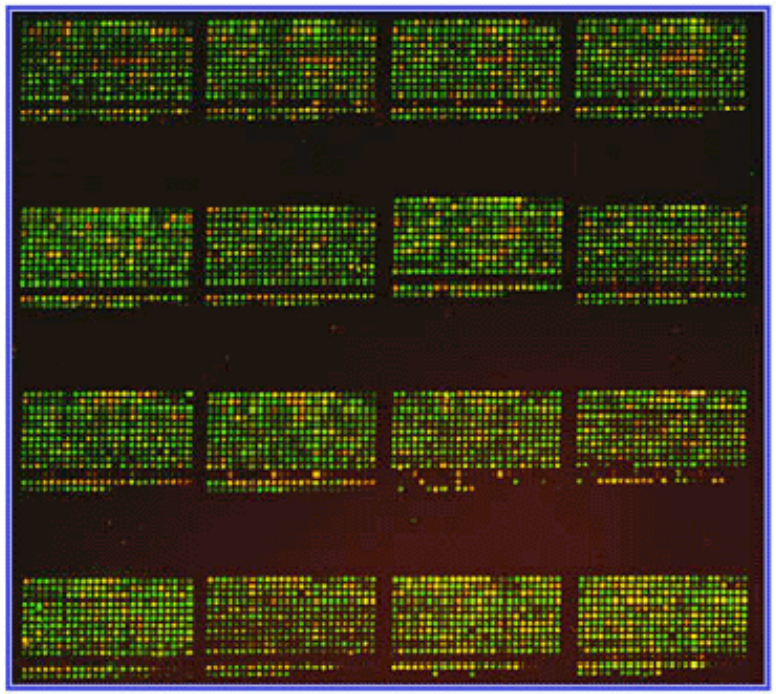
Biological dogma



Three Major Sources of Biological Data

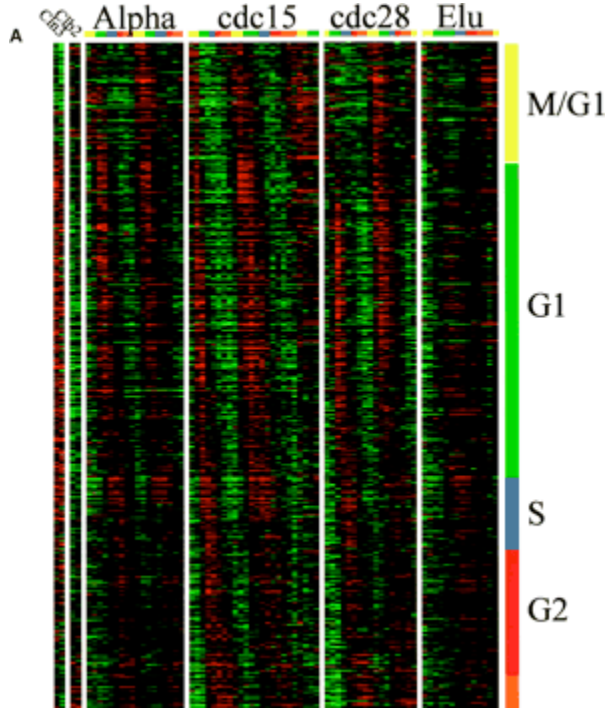
1. Sequencing machines
   - Determine DNA sequences
2. DNA chips (misnomer)
   - Measures mRNA
3. Mass-spectroscopy
   – Measures proteins

Gene Expression Chips



RNA vs. DNA

Raw data



Processed Yeast Cell Cycle [Alter]
Each row one gene

- Each spot fluoresces if mRNA is present
- 64,000 – 4,000,000 spot per chip, record red, green

Mass-Spectrometers with Liquid Chromatography:

- Can process whole cell lysate ie. All the proteins in a cell

→ 17,000 spectra in 12 hours., each spectra 30,000 real numbers

More coming every day (two, right here at UT)

Biology is feeling swamped by data.

- evangelists speak to exponential growth of data.

Role of a Database? *Biology*

- Databases are assuming the role of laboratory notebooks
  - Previously, data was
    - Hard earned
    - Manually transcribed
  - Now,
    - High throughput machines
    - 1,000 - 100,000 data elements at once.
- Archival Recording of Information
    - Data
    - What is the data
    - How was it captured (provenance)

Role of a Database?
Computer Engineering

- Stores the input for functions and algorithms.
    - (starting point for doing other things.)
- How is the data used?

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Data Model: A data model is a conceptual representation of the data structures that are required by a database application.

Key phrase: *conceptual representation*

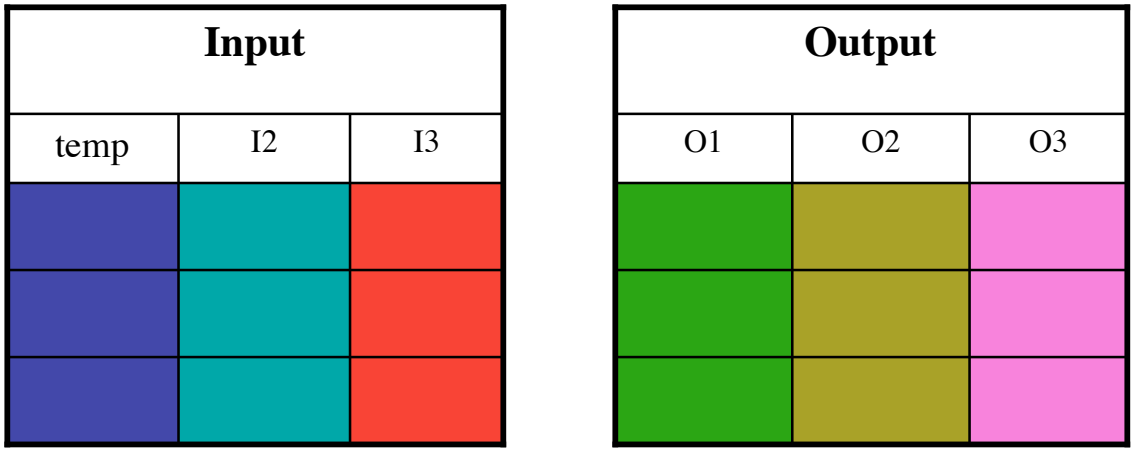
- *Think about it.*
- *Principles, Methods and Tools*

What goes wrong?

Example:

Hypothesis1, temp. dependent?

Experiment 1, build a database for it:



What goes wrong? (2)

- Scientific Method: New Hypothesis

  Hypothesis 2,pressure dependent?

  Experiment 2, build a database for it:

Input		
pres	I2	I3

Output		
O1	O2	O3

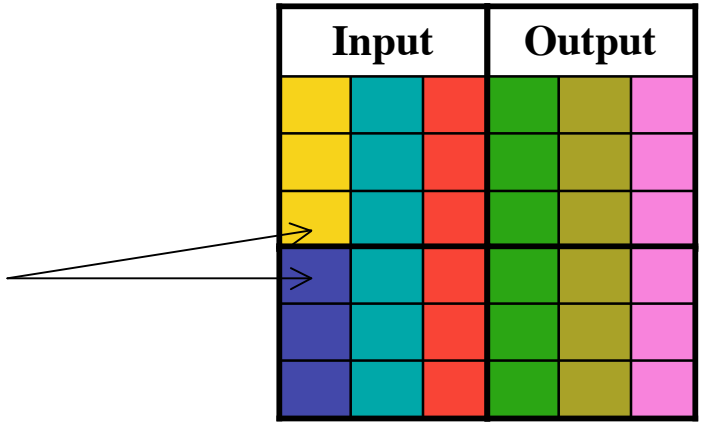
This goes wrong:

- Some time later

Hypothesis, both temp & pressure dependent?

Experiment 3 - NOT, just analyze the previous experiments together

The schema don't match



Goals/Content of Course

1. Mini-course in Data/Software Engineering
   - Process & methods for organizing data/programs

2. Tools to support this
   - A picture says a thousand words…

3. Walk through developing an application

Data Modeling In the Context of Database Design

- 1. planning and analysis
- 2. conceptual design // logic without the details
- 3. logical design
- 4. physical design
- 5. implementation

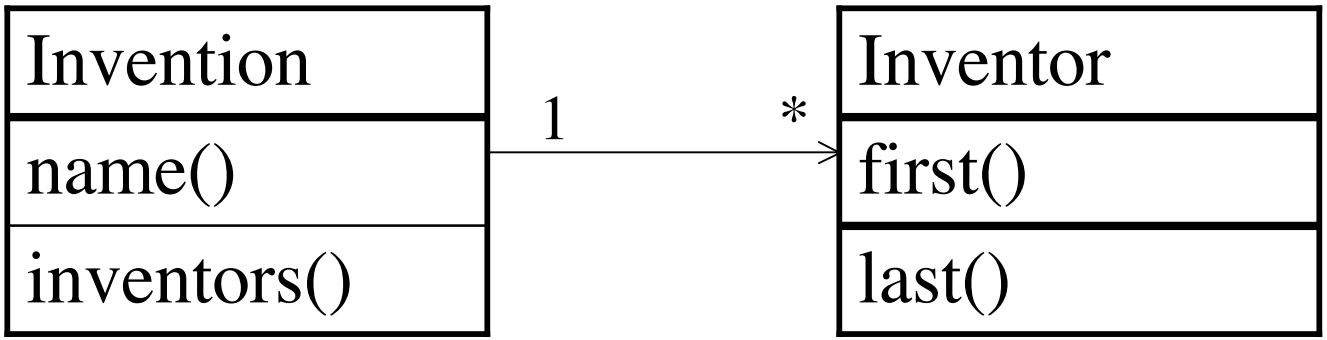
Inventor - Invention as DB Tables

Invention	
iid	name
1	structure
2	sequencing_machine
3	expression_chips

Inventor		
iid	first	last
1	Francis	Crick
1	James	Watson
1	Rosalyn	Franklin
1	Maurice	Wilkens
2	Lee	Hood
3	David	Botstein

Inventor-Invention, Object Model

A list of inventions, each with their list of inventors



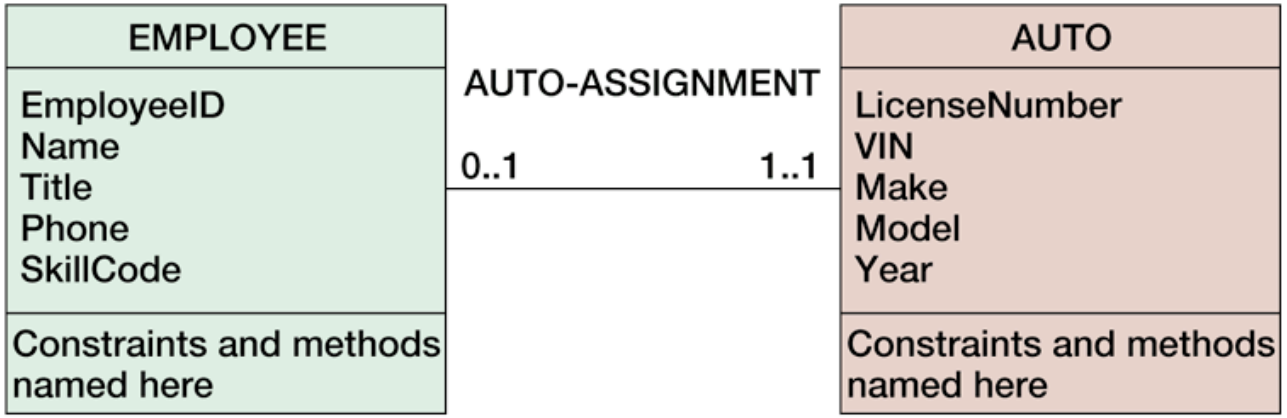
Computer Aided Software Engineering (CASE)

- Computer's help Civil Engineer's and Architects (CAD)
- Why not, have computer's help write software?

- The can & do:
  - We will learn to use Rational Rose

Just to show you a pretty picture (1)

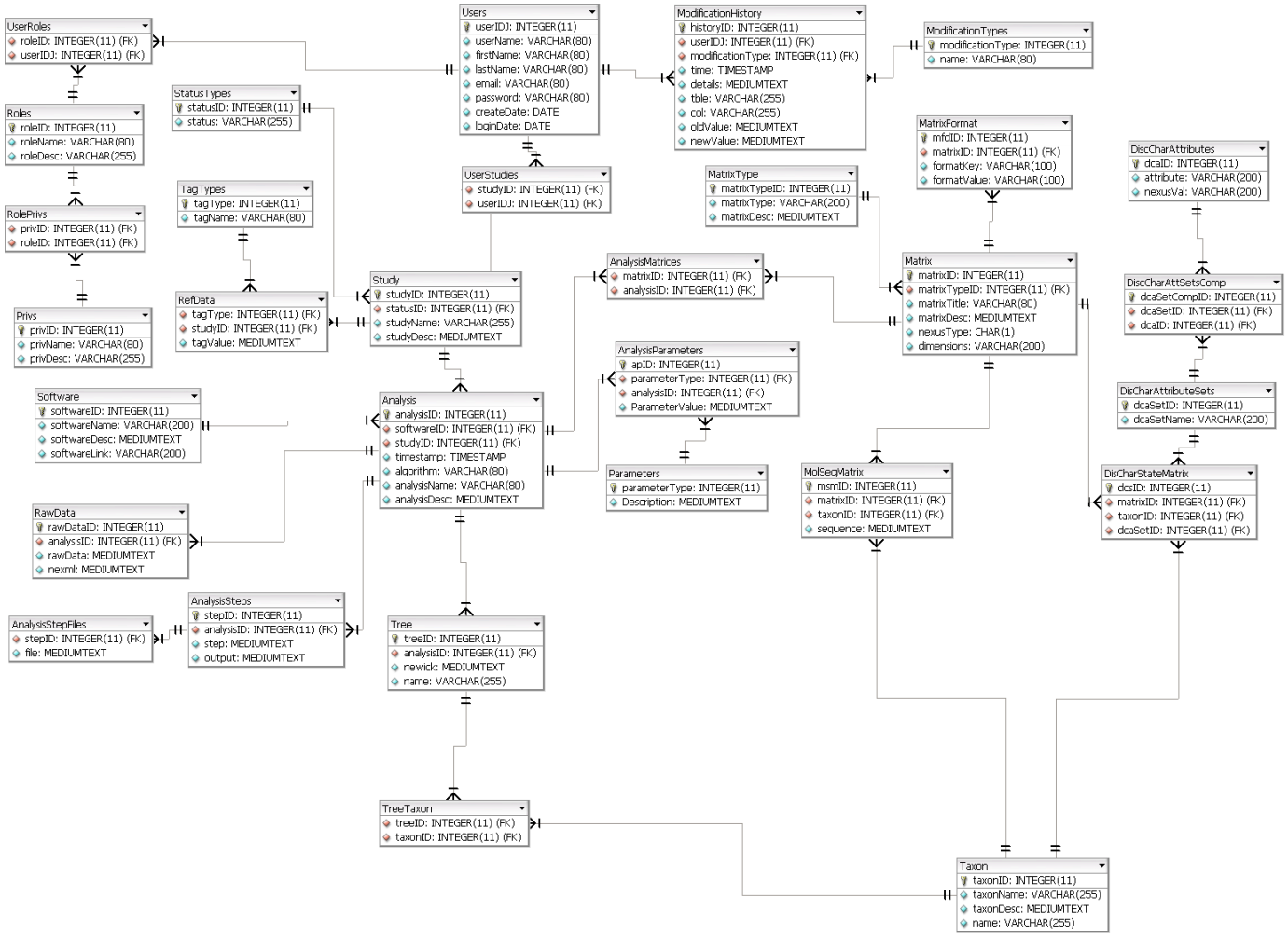
Figure 2.27a UML Representation of a 1:1 Relationship



(a)

Code Generated by Rational Rose for Inventors/Inventions

```
CREATE TABLE T_Invention (
    iname VARCHAR ( 255 ) NOT NULL,
    T_Invention_ID INTEGER NOT NULL,
    CONSTRAINT PK_T_Invention0 PRIMARY KEY (T_Invention_ID)
    );
CREATE TABLE T_Inventor (
    Firnname VARCHAR ( 255 ) NOT NULL,
    LastName VARCHAR ( 255 ) NOT NULL,
    name SMALLINT NOT NULL,
    T_Inventor_ID INTEGER NOT NULL,
    T_Invention_ID INTEGER NOT NULL,
    CONSTRAINT PK_T_Inventor1 PRIMARY KEY (T_Inventor_ID)
    );
CREATE INDEX TC_T_Inventor1 ON T_Inventor (T_Invention_ID );
ALTER TABLE T_Inventor ADD CONSTRAINT FK_T_Inventor0
    FOREIGN KEY (T_Invention_ID) REFERENCES T_Invention
    (T_Invention_ID)
    ON DELETE NO ACTION ON UPDATE NO ACTION;
```

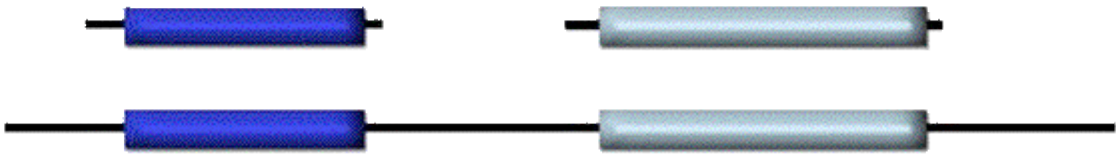


A commercial database has an average of _____ attributes per table

Application Example:

- Rosetta Sequence Analysis to
  - determine gene/protein function

Rosetta Stone Method Identifies Protein Fusions



Monomeric proteins that are found fused in another organism are likely to be functionally related and physically interacting.

Marcotte EM, Pellegrini M, Ng HL, Rice DW, Yeates TO, Eisenberg D, Detecting protein function and protein-protein interactions from genome sequences. *Science* 285(5428):751-3, 1999

Introduce self & Administrivia

Student's turn

- Name, dept., year
- Why did you register for this course
  - (especially if you are not a biology major)
- What are you hoping to get out of this course?