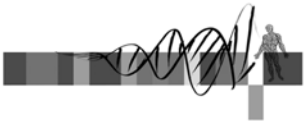

Relational Databases for Biologists: Efficiently Managing and Manipulating Your Data

Session 1:
Data Conceptualization and Database Design

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WIBR Bioinformatics and Research Computing

What is a Database?

- A collection of data
- A set of rules to manipulate data
- A method to mold information into knowledge
- Is a phonebook a database?
  - Is a phonebook with a human user a database?

Babbitt, S.	38 William St., Cambridge	555-1212
Baggins, F.	109 Auburn Ct., Boston	555-1234
Bayford, A.	1154 William St., Newton	555-8934

Why are Databases Important?

- Data -> information -> knowledge
- Efficient manipulation of large data sets
- Integration of multiple data sources
- Adding crosslinks/references to other resources

Why is a Database Useful?

- If database systems simply manipulate data, why not use existing file system and spreadsheet mechanisms?
- "Baggins" Telephone No. Lookup:
  - Human: Look for B, then A, then G …
  - Unix: grep Baggins boston_directory.txt
  - DB: SELECT * FROM directory WHERE lastName="Baggins"

Babbitt, S.	38 William St., Cambridge	555-1212
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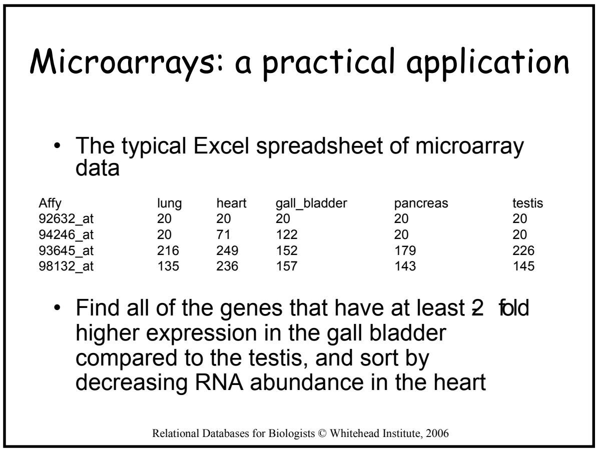
What is the Advantage of a Database?

- Find all last names that contain "th" but do not have street address that begin with "th".
  - Human: a lot of careful reading....
  - Unix: Write a directory parser and a filter.
  - DB: SELECT lastName FROM directory WHERE lastName LIKE "%th%" AND street NOT LIKE "Th%"

Why Biological Databases?

- To access and manipulate lots of data
- To manage experimental results
- To improve search sensitivity
- To improve search efficiency
- To merge multiple data sets

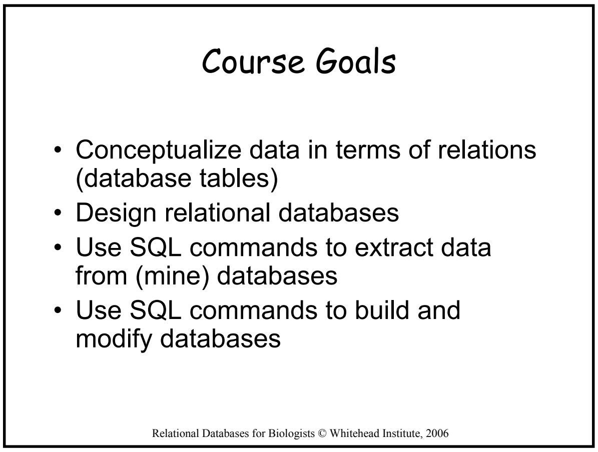


Microarrays: a practical application

- The typical Excel spreadsheet of microarray data

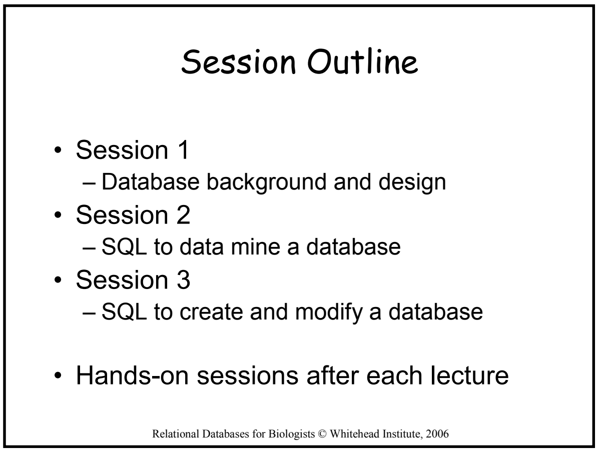
Affy	lung	heart	gall_bladder	pancreas	testis
92632_at	20	20	20	20	20
94246_at	20	71	122	20	20
93645_at	216	249	152	179	226
98132_at	135	236	157	143	145

- Find all of the genes that have at least 2 fold higher expression in the gall bladder compared to the testis, and sort by decreasing RNA abundance in the heart



Course Goals

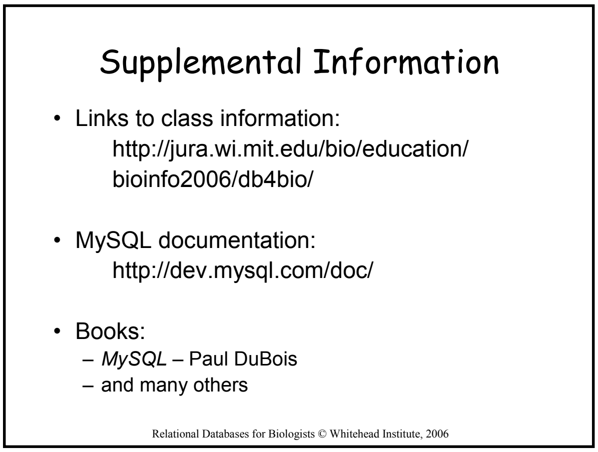
- Conceptualize data in terms of relations (database tables)
- Design relational databases
- Use SQL commands to extract data from (mine) databases
- Use SQL commands to build and modify databases



Session Outline

- Session 1
  - Database background and design
- Session 2
  - SQL to data mine a database
- Session 3
  - SQL to create and modify a database

- Hands-on sessions after each lecture

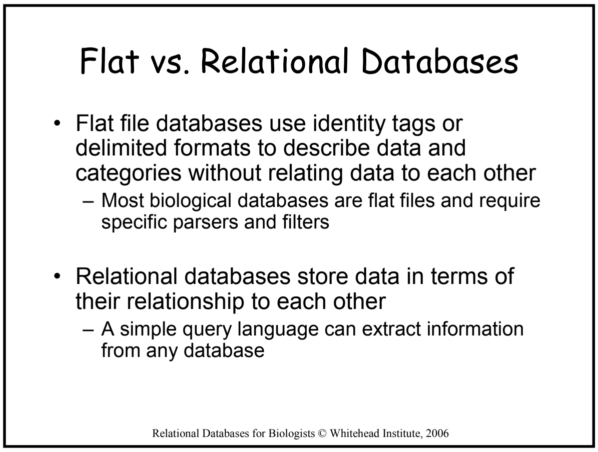


Supplemental Information

- Links to class information:
  http://jura.wi.mit.edu/bio/education/
  bioinfo2006/db4bio/

- MySQL documentation:
  http://dev.mysql.com/doc/

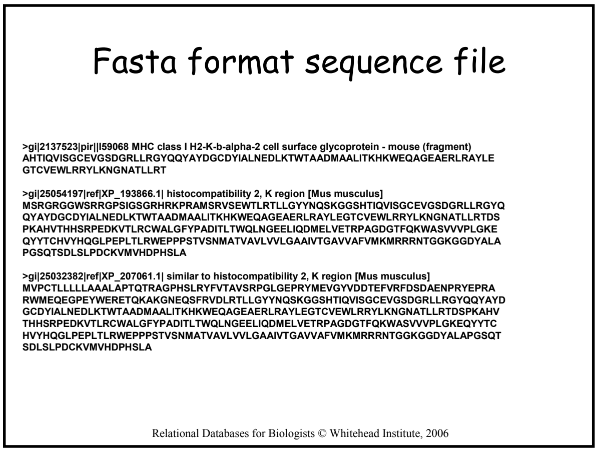
- Books:
  - *MySQL* – Paul DuBois
  - and many others



Flat vs. Relational Databases

- Flat file databases use identity tags or delimited formats to describe data and categories without relating data to each other
  - Most biological databases are flat files and require specific parsers and filters

- Relational databases store data in terms of their relationship to each other
  - A simple query language can extract information from any database



Fasta format sequence file

```
>gi|2137523|pir||I59068 MHC class I H2-K-b-alpha-2 cell surface glycoprotein - mouse (fragment)
AHTIQVISGCEVGSDGRLLRGYQQYAYDGCDYIALNEDLKTWTAADMAALITKHKWEQAGEAERLRAYLE
GTCVEWLRRYLKNGNATLLRT

>gi|25054197|ref|XP_193866.1| histocompatibility 2, K region [Mus musculus]
MSRGRGGWSRRGPSIGSGRHRKPRAMSRVSEWTLRTLLGYYNQSKGGSHTIQVISGCEVGSDGRLLRGYQ
QYAYDGCDYIALNEDLKTWTAADMAALITKHKWEQAGEAERLRAYLEGTCVEWLRRYLKNGNATLLRTDS
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>gi|25032382|ref|XP_207061.1| similar to histocompatibility 2, K region [Mus musculus]
MVPCTLLLLLAAALAPTQTRAGPHSLRYFVTAVSRPGLGEPRYMEVGYVDDTEFVRFDSDAENPRYEPRA
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GCDYIALNEDLKTWTAADMAALITKHKWEQAGEAERLRAYLEGTCVEWLRRYLKNGNATLLRTDSPKAHV
THHSRPEDKVTLRCWALGFYPADITLTWQLNGEELIQDMELVETRPAGDGTFQKWASVVVPLGKEQYYTC
HVYHQGLPEPLTLRWEPPPSTVSNMATVAVLVVLGAAIVTGAVVAFVMKMRRRNTGGKGGDYALAPGSQT
SDLSLPDCKVMVHDPHSLA
```

GenBank format sequence file

```
LOCUS       NM_205137               1111 bp    mRNA    linear   VRT 16-APR-2005
DEFINITION  Gallus gallus homeobox protein Nkx-2.8 (NKX2.8), mRNA.
ACCESSION   NM_205137 XM_444649
VERSION     NM_205137.1  GI:49170097
SOURCE      Gallus gallus (chicken)
  ORGANISM  Gallus gallus
            Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
            Archosauria; Aves; Neognathae; Galliformes; Phasianidae;
            Phasianinae; Gallus.
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                     /db_xref="GeneID:396037"
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                     /codon_start=1
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                     APYGITVSPYSYSTYYSAYGVSYGVGYTGVLTP"
ORIGIN
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       61 tatcctcagc ctggagcaga gcagcgctcc cggagccccc ggggtccgcc gcagcccttc
```

The Relational Database

- Data is composed of sets of tables and links
- Structured Query Language (SQL) to query the database
- Database management system (DBMS) to manage the data

DBMS ACID properties

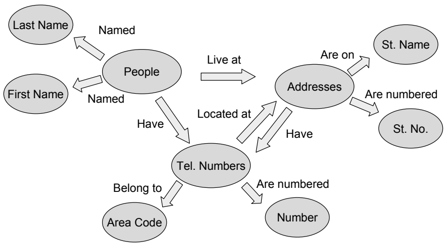
- ACID properties/model
  - Atomicity: “All or nothing” transactions
  - Consistency: Only valid data can be input
  - Isolation: Multiple user independence
  - Durability: Recovery mechanisms for system failures

Selected DBMSs

- MySQL
  - “The world's most popular open source database”, probably for biology too
  - Free; open source; small application; quick to learn
  - DBMS for this class
- PostgreSQL
  - “The world's most advanced open source database ”
  - Free; open source; somewhat larger application
- Oracle
  - “The worlds #1 database”
  - A lot more features but takes longer to learn
  - Expensive (but of course, many feel it’s worth it)
- All three are great choices and have the same core SQL functionality.

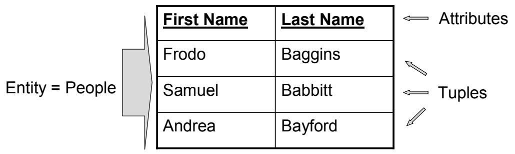
Data Conceptualization

- Data and Links (For a Phonebook)



Data Structure

- Data stored in tables with multiple columns (“attributes”).
- Each record is represented by a row (a “tuple”)



First Name	Last Name
Frodo	Baggins
Samuel	Babbitt
Andrea	Bayford

Relational Database Specifics

- Tables are relations
  - You perform operations on the tables
- No two tuples (rows) should be identical
- Each attribute for a tuple has only one value
- Tuples within a table are unordered
- Each tuple is uniquely Identified by a primary key

Primary Keys

- Primary Identifiers (IDs)
- Set of attributes that uniquely define a single, specific tuple (row)
- Must be absolutely unique
  - SSN ?
  - Phone Number ?
  - ISBN ?

First Name	Last Name	SSN
Frodo	Baggins	332-97-0123
Frodo	Binks	398-76-5327
Maro	Baggins	215-01-3965

Find the Keys

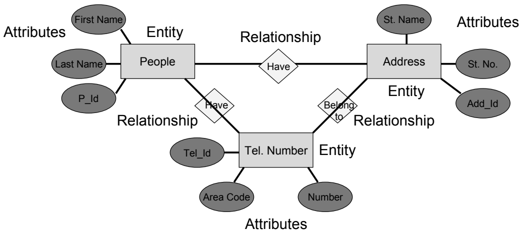
First Name	Last Name	SSN	Phone Number	Address
Frodo	Baggins	321-45-7891	123-4567	29 Hobbitville
Aragon	Elf-Wantabe	215-87-7458	258-6109	105 Imladris
Boromir	Ringer	105-91-0124	424-9706	31 Hobbitville
Bilbo	Baggins	198-02-2144	424-9706	29 Hobbitville
Legolas	Elf	330-78-4230	555-1234	135 Imladris

Design Principles

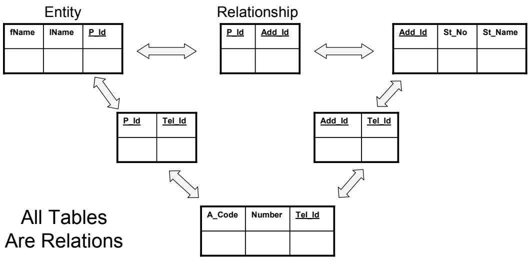
- Conceptualize the data elements (entities)
- Identify how the data is related
- Make it simple
- Avoid redundancy
- Make sure the design accurately describes the data!

Entity-Relationship Diagrams

- Expression of a database table design



E-R to Table Conversion



All Tables
Are Relations

Steps to Build an E-R Diagram

- Identify data attributes
- Conceptualize entities by grouping related attributes
- Identify relationships/links
- Draw preliminary E-R diagram
- Add cardinalities and references

Developing an E-R Diagram

- Convert a GenBank File into an E R Diagram

```
LOCUS       NM_205137               1111 bp    mRNA    linear   VRT 16-APR-2005
DEFINITION  Gallus gallus homeobox protein Nkx-2.8 (NKX2.8), mRNA.
ACCESSION   NM_205137 XM_444649
VERSION     NM_205137.1  GI:49170097
SOURCE      Gallus gallus (chicken)
ORGANISM    Gallus gallus
            Eukaryota; Metazoa; Chordata; Craniata; Vertebrata; Euteleostomi;
            Archosauria; Aves; Neognathae; Galliformes; Phasianidae;
            Phasianinae; Gallus.
FEATURES             Location/Qualifiers
     source          1..1111
                     /organism="Gallus gallus"
                     /mol_type="mRNA"
                     /db_xref="taxon:9031"
     gene            1..1111
                     /gene="NKX2.8"
                     /db_xref="GeneID:396037"
     CDS             32..613
                     /gene="NKX2.8"
                     /codon_start=1
                     /product="homeobox protein Nkx-2.8"
                     /protein_id="NP_990468.1"
                     /db_xref="GI:49170098"
                     /db_xref="GeneID:396037"
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                     LTSTQVKIWFQNRRYKCKRQRQDRSLEMATYPLPPRKVAVPVLVRNGKPCFEGSQPHL
                     APYGITVSPYSYSTYYSAYGVSYGVGYTGVLTP"
ORIGIN
        1 gagggagctc acagcgatcc cggcccggag gatgctgcgc agcccttttct cggtcgagga
       61 tatcctcagc ctggagcaga gcagcgctcc cggagccccc ggggtccgcc gcagcccttc
```

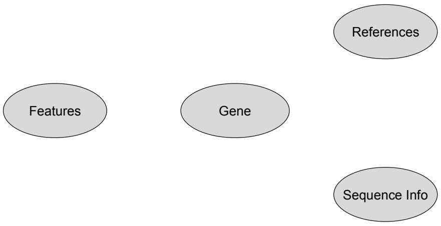
Identify Attributes

- Locus, Definition, Accession, Version, Source Organism
- Authors, Title, Journal, Medline Id, PubMed Id
- Protein Name, Protein Description, Protein Id, Protein Translation, Locus Id, GI
- A count, C count, G count, T count, Sequence

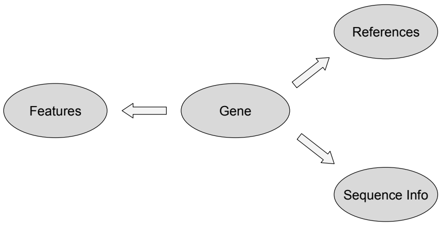
Identify Entities by Grouping

- Gene
  - Locus, Definition, Accession, Version, Source Organism
- References
  - Authors, Title, Journal, Medline Id, PubMed Id
- Features
  - Protein Name, Protein Description, Protein Id, Protein Translation, Locus Id, GI
- Sequence Information
  - A count, C count, G count, T count, Sequence

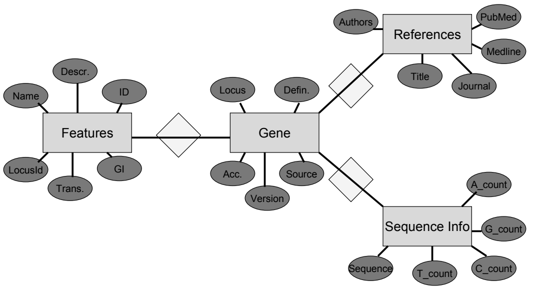
Conceptualize Entities



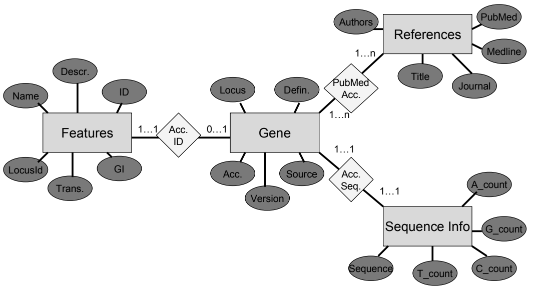
Identify Relationships



Preliminary E-R Diagram

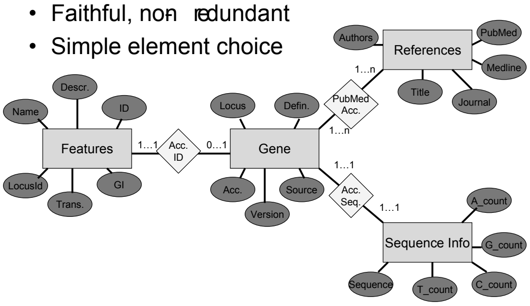


Cardinalities and References



Apply Design Principles

- Faithful, non-redundant
- Simple element choice



Summary

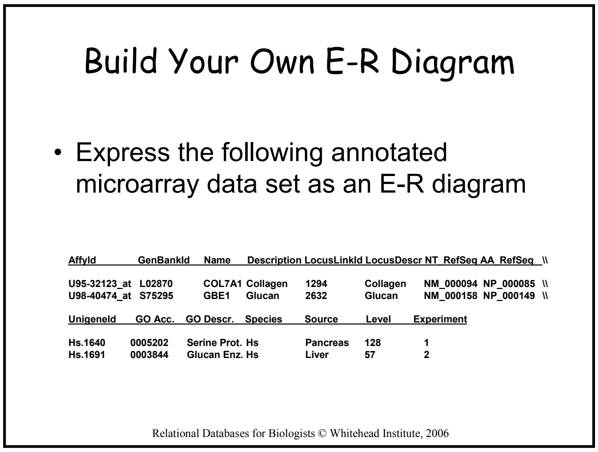
- Databases provide ACID
- Databases are composed of tables (relations)
- Relations are entities that have attributes and tuples
- Databases can be designed from E-R diagrams that are easily converted to tables
- Primary keys uniquely identify individual tuples and represent links between tables

Next class

- Using structured query language (SQL) to data mine databases
- SELECT a FROM b WHERE c = d

Database design example:

Design the db4bio database

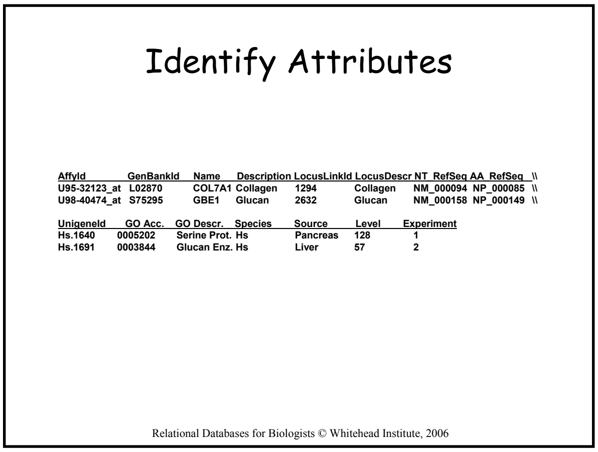


Build Your Own E-R Diagram

- Express the following annotated microarray data set as an E-R diagram

AffyId	GenBankId	Name	Description	LocusLinkId	LocusDescr	NT_RefSeq	AA_RefSeq	\\
U95-32123_at	L02870	COL7A1	Collagen	1294	Collagen	NM_000094	NP_000085	\\
U98-40474_at	S75295	GBE1	Glucan	2632	Glucan	NM_000158	NP_000149	\\

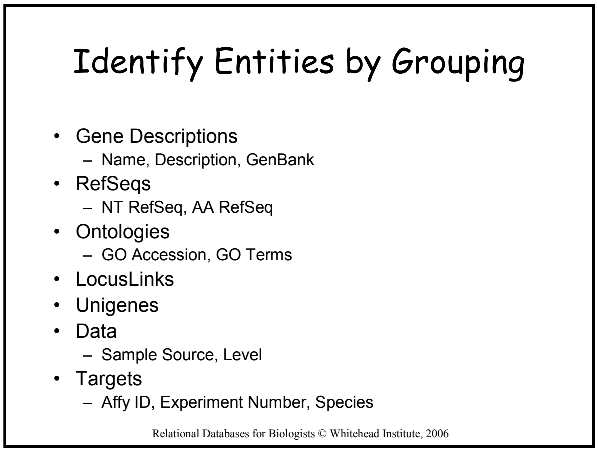
UnigeneId	GO Acc.	GO Descr.	Species	Source	Level	Experiment
Hs.1640	0005202	Serine Prot.	Hs	Pancreas	128	1
Hs.1691	0003844	Glucan Enz.	Hs	Liver	57	2



Identify Attributes

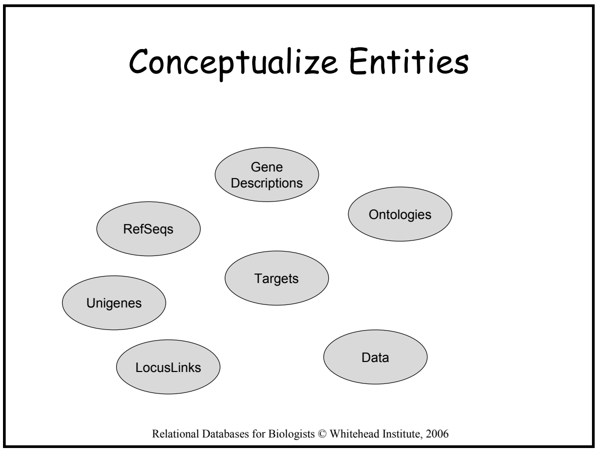
AffyId	GenBankId	Name	Description	LocusLinkId	LocusDescr	NT_RefSeq	AA_RefSeq	\\
U95-32123_at	L02870	COL7A1	Collagen	1294	Collagen	NM_000094	NP_000085	\\
U98-40474_at	S75295	GBE1	Glucan	2632	Glucan	NM_000158	NP_000149	\\

UnigeneId	GO Acc.	GO Descr.	Species	Source	Level	Experiment
Hs.1640	0005202	Serine Prot.	Hs	Pancreas	128	1
Hs.1691	0003844	Glucan Enz.	Hs	Liver	57	2

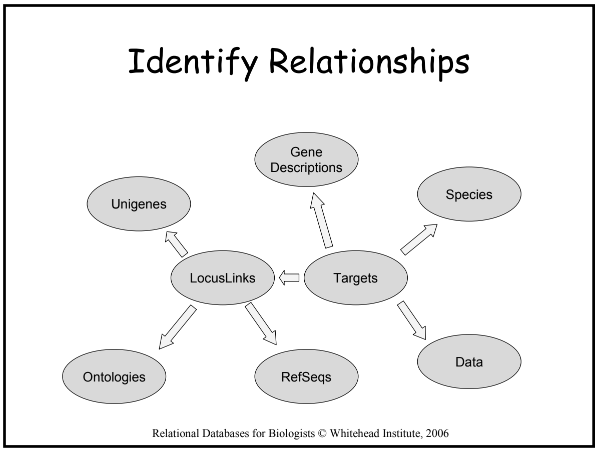


Identify Entities by Grouping

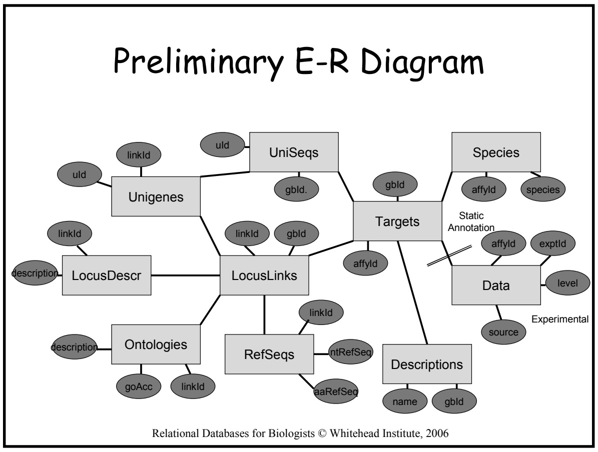
- Gene Descriptions
  - Name, Description, GenBank
- RefSeqs
  - NT RefSeq, AA RefSeq
- Ontologies
  - GO Accession, GO Terms
- LocusLinks
- Unigenes
- Data
  - Sample Source, Level
- Targets
  - Affy ID, Experiment Number, Species



Conceptualize Entities

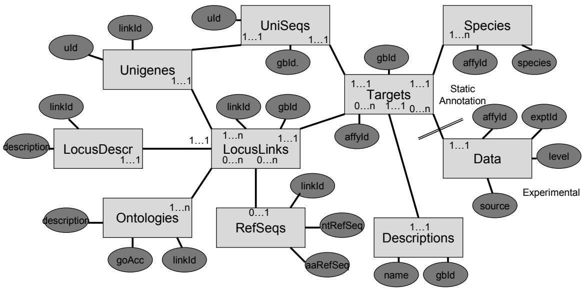


Identify Relationships

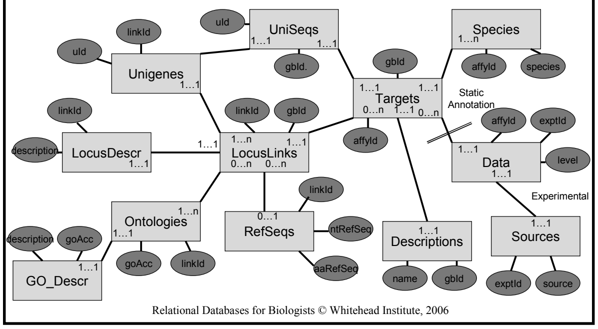


Preliminary E-R Diagram

Cardinalities and References



Apply Design Principles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