

# databases

## **Database or databank?**

## Initially

- Databank (in UK)
- Database (in the USA)

**Solution** 

The abbreviation *db*

What is a Database?

A **structured collection** of data held in computer storage; *esp.* one that incorporates software to make it accessible in a variety of ways; *transf.*, any **large collection** of information.

OR

A *database* is a computerized archive used to store and organize data in such a way that information can be retrieved easily via a variety of search criteria.

Although data retrieval is the main purpose of all databases, biological databases often have a higher level of requirement, known as *knowledge discovery*, which refers to the identification of connections between pieces of information that were not known when the information was first entered.

37 Oxford Dictionary

## What is a database?

- A collection of data
  - structured
  - searchable (index)
  - updated periodically (release)
  - cross-referenced (<u>hyperlinks</u>)
- -> table of contents
- -> new edition
- -> links with other db

- Includes also associated tools (software) necessary for access, updating, information insertion, information deletion....
- Data storage management: flat files, relational databases...

## Database: a flat file

Originally, databases all used a flat file format, which is a long text file that contains many entries separated by a *delimiter* 

Within each entry are a number of fields separated by tabs or commas. Except for the raw values in each field, the entire text file does not contain any hidden instructions for computers to search for specific information or to create reports based on certain fields from each record. The text file can be considered a single table.

Thus, to search a flat file for a particular piece of information, a computer has to read through the entire file, an obviously inefficient process. This is manageable for a small database, but as database size increases or data types become more complex, this database style can become very difficult for information retrieval.  Relational databases use a set of tables to organize data. Each table, also called a *relation*, is made up of columns and rows.

 The columns in a table are indexed according to a common feature called an *attribute*, so they can be cross-referenced in other tables.

 To execute a query in a relational database, the system selects linked data items from different tables and combines the information into one report. Flat FileName, States, Course number, Course name|John Smith, Texas, Biol 689,<br/>Bioinformatics|Jane Doe, Kansas, Bich 441, Biochemistry|William Brown,<br/>Illinois, Chem 289, Organic Chemistry|Jennifer Taylor, New York, Hort 201,<br/>Horticulture|Howard Douglas, Texas, Math 172, Calculus

#### Table A

Table	B
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Table C

Student #	Name	State
1	John Smith	Texas
2	Jane Doe	Kansas
3	William Brown	Illinois
4	Jennifer Taylor	New York
5	Howard Douglas	Texas

Student #	Course #	
1	Biol 689	
2	Bich 441	
3	Chem 289	
4	Hort 201	
5	Math 172	

Course #	Course name
Biol 689	Bioinformatics
Bich 441	Biochemistry
Chem 289	Organic chemistry
Hort 201	Horticulture
Math 172	Calculus

**Figure 2.1:** Example of constructing a relational database for five students' course information originally expressed in a flat file. By creating three different tables linked by common fields, data can be easily accessed and reassembled.

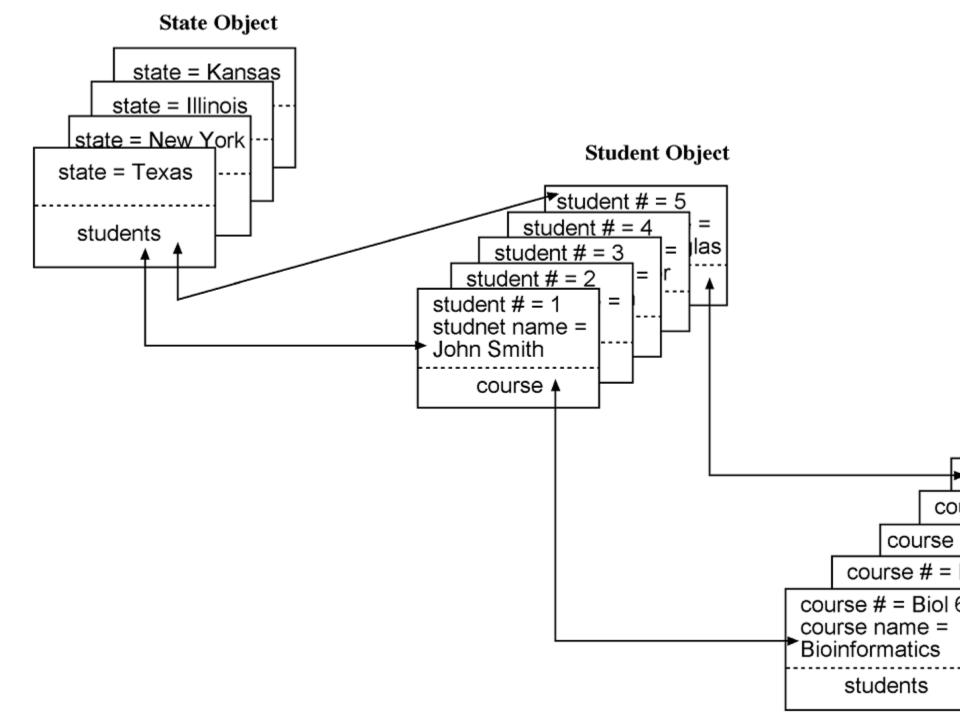
#### Some databases in the field of molecular biology...

AATDB, ACEDb, ACUTS, ADB, AFDB, AGIS, AMSdb, ARR, AsDb, BBDB, BCGD, Beanref, Biolmage, BioMagResBank, BIOMDB, BLOCKS, BovGBASE, BOVMAP, BSORF, BTKbase, CANSITE, CarbBank, CARBHYD, CATH, CAZY, CCDC, CD40Lbase, CGAP, ChickGBASE, Colibri, COPE, CottonDB, CSNDB, CUTG, CyanoBase, dbCFC, dbEST, dbSTS, DDBJ, DGP, DictyDb, Picty\_cDB, DIP, DOGS, DOMO, DPD, DPInteract, ECDC, ECGC, ECO2DBASE, EcoCyc, EcoGene, EMBL, EMD db, ENZYME, EPD, EpoDB, ESTHER, FlyBase, FlyView, GCRDB, GDB, GENATLAS, Genbank, GeneCards, Genline, GenLink, GENOTK, GenProtEC, GIFTS GPCRDB, GRAP, GRBase, gRNAsdb, GRR, GSDB, HAEMB, HAMSTERS, HEART-2DPAGE, HEXAdb, HGMD, HIDB, HIDC, HIVdb, HotMolecBase, HOVERGEN, HPDB, HSC-2DPAGE, ICN, ICTVDB, IL2RGbase, IMGT, Kabat, KDNA, KEGG, Klotho, LGIC, MAD, MaizeDb, MDB, Medline, Mendel, MEROPS, MGDB, MGI, MHCPEP5 Micado, MitoDat, MITOMAP, MJDB, MmtDB, Mol-R-Us, MPDB, MRR, MutBase, MycDB, NDB, NRSub, O-lycBase, OMIA, OMIM, OPD, ORDB, OWL, PAHdb, PatBase, PDB, PDD, Pfam, PhosphoBase, PigBASE, PIR, PKR, PMD, PPDB, PRESAGE, PRINTS, ProDom, Prolysis, PROSITE, PROTOMAP, RatMAP, RDP, REBASE, RGP, SBASE, SCOP, SegAnaiRef, SGD, SGP, SheepMap, Soybase, SPAD, SRNA db, SRPDB, STACK, StyGene, Sub2D, SubtiList, SWISS-2DPAGE, SWISS-3DIMAGE, SWISS-MODEL Repository, SWISS-PROT, TelDB, TGN, tmRDB, TOPS, TRANSFAC, TRR, UniGene, URNADB, V BASE, VDRR, VectorDB, WDCM, WIT, WormPep, YEPD, YPD, YPM, etc ..... !!!!

42

## **Object-Oriented Databases**

- Store data as objects.
- An object can be considered as a unit that combines data and mathematical routines that act on the data.
- Structured such that the objects are linked by a set of pointers defining predetermined relationships b/w the objects.
- Programming languages like C++ are used to create object-oriented databases.
- OOD is more flexible; data can be structured based on hierarchical relationships.
- OOD lacks the rigorous mathematical foundation of the relational databases
- There is also a risk that some of the relationships between objects may be misrepresented



## **Biological Databases:**

- Based on their contents, biological databases can be roughly divided into three categories:
- Primary databases contain original biological data. They are archives of raw sequence or structural data submitted by the scientific community. GenBank and Protein Data Bank (PDB) are examples of primary databases.
- Secondary databases contain computationally processed or manually curated information, based on original information from primary databases. Translated protein sequence databases containing functional annotation belong to this category. Examples are SWISS-Prot and Protein Information Resources (PIR).
- Specialized databases are those that cater to a particular research interest. For example, Flybase, HIV sequence database, and Ribosomal Database Project are databases that specialize in a particular organism or a particular type of data.

	Jor Diological Databases / Walla	
Databases and Retrieval Systems	Brief Summary of Content	URL
AceDB	Genome database for Caenorhabditis elegans	www.acedb.org
DDBJ	Primary nucleotide sequence database in Japan	www.ddbj.nig.ac.jp
EMBL	Primary nucleotide sequence database in Europe	www.ebi.ac.uk/embl/index.html
Entrez	NCBI portal for a variety of biological databases	www.ncbi.nlm.nih.gov/gquery/gque
ExPASY	Proteomics database	http://us.expasy.org/
FlyBase	A database of the <i>Drosophila</i> genome	http://flybase.bio.indiana.edu/
FSSP	Protein secondary structures	www.bioinfo.biocenter.helsinki.fi:808
GenBank	Primary nucleotide sequence database in NCBI	www.ncbi.nlm.nih.gov/Genbank
HIV databases	HIV sequence data and related immunologic information	www.hiv.lanl.gov/content/index
Microarray gene	DNA microarray data and analysis tools	www.ebi.ac.uk/microarray

#### **TABLE 2.1.** Major Biological Databases Available Via the World Wide Web

## Interconnection between Biological Databases

- There is a demand for linking different databases
- The main barrier is format incompatibility
- One solution to networking the databases is COBRA
- Works in a way similar to HTML labeling database entries using a set of common tags
- XML also helps in bridging databases. In this format, each biological record is broken down into small, basic components that are labeled with a hierarchical nesting of tags

## PITFALLS OF BIOLOGICAL DATABASES

- Overreliance on sequence information and related annotations
- High levels of redundancy in the primary sequence databases
- The solution is RefSeq, SWISS-PROT, *Gene Ontology* etc.

## INFORMATION RETRIEVAL FROM BIOLOGICAL DATABASES

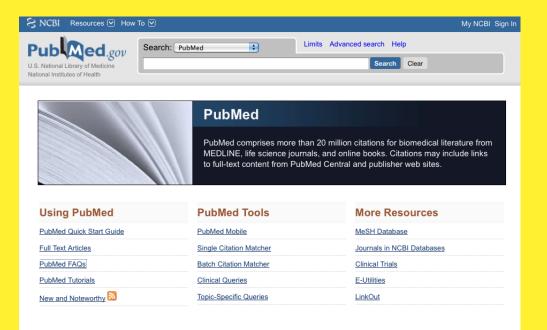
 Major goal in developing databases is to provide efficient and user friendly access to the data stored. There are a number of retrieval systems for biological data. The most popular retrieval systems for biological databases are Entrez and Sequence Retrieval Systems (SRS) that provide access to multiple databases for retrieval of search integrated results.

## Entrez

- It is a gateway that allows text-based searches for a wide variety of data, including annotated genetic sequence information, structural information, as well as citations and abstracts, full papers, and taxonomic data.
- The key feature of Entrez is its ability to integrate information, which comes from cross-referencing between NCBI databases based on preexisting and logical relationships between individual entries

### PubMed (Medline)

- MEDLINE covers the fields of medicine, nursing, dentistry, veterinary medicine, public health, and preclinical sciences
- Contains citations from approximately 5,200 worldwide journals in 37 languages; 60 languages for older journals.
- Contains over 20 million citations since 1948
- Contains links to biological db and to some journals
- New records are added to PreMEDLINE daily!



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#### A search by authors:

#### "Esser" [au] AND "martin" [au]

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#### A search by title word:

#### "Wolbachia pipientis" [ti]

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Clinical Alerts ClinicalTrials.gov PubMed Central	PMID: 16030207 [PubMed - indexed for MEDLINE]	A V

## **Database Search Strategies**

- General search principles not limited to sequence (or to biology).
- Start with broad keywords and narrow the search using more specific terms.
- Try variants of spelling, numbers, etc.
- Search many databases.
- Be persistent!!

## Searching PubMed

- Structureless searches
  - Automatic term mapping
- Structured searches
  - Tags, e.g. [au], [ta], [dp], [ti]
  - Boolean operators, e.g. AND, OR, NOT, ()
- Additional features
  - Subsets, limits
  - Clipboard, history

**Start working:** 

**Search PubMed** 

- 1. cuban cigars
- **2. cuban OR cigars**
- 3. "cuban cigars"
- 4. cuba\* cigar\*
- 5. (cuba\* cigar\*) NOT smok\*
- 6. Fidel Castro
- 7. "fidel castro"
- 8. #6 NOT #7

## "Details" and "History" in PubMed

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# The **OMIM** (Online Mendelian Inheritance in Man)

- Genes and genetic disorders
- Edited by team at Johns Hopkins
- Updated daily

### MIM Number Prefixes

\* gene with known sequence gene with known sequence and phenotype # phenotype description, molecular basis known % mendelian phenotype or locus, molecular basis unknown other, mainly phenotypes with no prefix suspected mendelian basis

## **Searching OMIM**

- Search Fields
  - Name of trait, e.g., hypertension
  - Cytogenetic location, e.g., 1p31.6
  - Inheritance, e.g., autosomal dominant
  - Gene, e.g., coagulation factor VIII

## **OMIM search tags**

All Fields Allelic Variant Chromosome Clinical Synopsis Gene Map Gene Name Reference [ALL] [AV] or [VAR] [CH] or [CHR] [CS] or [CLIN] [GM] or [MAP] [GN] or [GENE] [RE] or [REF]

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**Start working:** 

**Search OMIM** 

How many types of hemophilia are there? For how many is the affected gene known? What are the genes involved in hemophilia A? What are the mutations in hemophilia A?