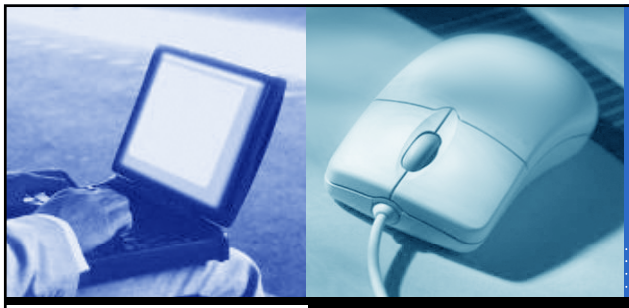
Fundamentals of Scientific Data

IST400/600

Jian Qin



Data Basics

at the low level of computing

Do you know…

- Bit?
- Byte?
- How do they form “word”?

Numbers

- Integer
  - Signed: -(2(n-1)), -(2(n-1)-1), …
  - Unsigned: …, 2^n-2, 2^n-1, 0, 1, …
- Real
  - Fixed-point
  - Scaled
  - Floating-point

Text (1)

- Character
  - ISO 8859-1
    - 8 bits/character
      - 256 possible characters
    - encodes Latin alphabet
      - e.g. works for French, but not for Russian
    - most widely supported encoding in US
  - Unicode
    - 8..32 bits/character
      - up to ~4 billion possible characters
    - encodes (potentially) all human language characters
      - (and even some nonhuman ones...)
- String: sequence of characters
  - portable, if you also know:
    - order
    - length, from one of:
      - count ("here come N characters")
      - delimiter (end-of-string character)

Text (2)

- **"Printable" Text**

  Subset of possible 1-byte characters
  - no "control" codes: newline, bell, tab, etc.
    - glyph always matches stored value
  - no "unAmerican" characters: Å, ñ, £, etc.
    - glyph read/writable on any I/O device

  Most portable type

Text (3)

- **"Binary Text"**
  - Bitwise conversion: bytes ↔ text
  - E.g.: 4 bits ↔ hexadecimal character
    - 0000..1001 ↔ 0..9
    - 1010..1111 ↔ A..F
- Most portable "byte stream"
  - inflation: byte becomes >1 character
    - less if larger radix
      - hex → 2x
      - base-64 (e.g. uuencode) → 1.25x
  - need printable chars for delimiters

Same bits, different types

binary
- 11000000010010010000111111011011

hexadecimal
- C0490FDB

ISO Latin-1
- À I control-O Û

unsigned integer
- 3,226,013,659

signed integer
- -1,068,953,637

IEEE floating-point
- -3.1415927

More information about computer numbering formats:
http://en.wikipedia.org/wiki/Computer_numbering_formats

Do you recognize these file formats?

```
("root" "x" "0" "0" "root" "/root" "/bin/sh")
("uucp" "x" "10" "14" "uucp" "/var/spool/uucp" "/sbin/nologin")
("fido" "x" "501" "501" "fidonet national mail hour" "/home/fido" "/home/bin/fido")
```

```
"REVIEW_DATE","AUTHOR","ISBN","DISCOUNTED_PRICE"
 "1985/01/21","Douglas Adams",0345391802,5.95
 "1990/01/12","Douglas Hofstadter",0465026567,9.95
 "1998/07/15","Timothy ""The Parser"" Campbell",0968411304,18.99
 "1999/12/03","Richard Friedman",0060630353,5.95
 "2001/09/19","Karen Armstrong",0345384563,9.95
 "2002/06/23","David Jones",0198504691,9.95
 "2002/06/23","Julian Jaynes",0618057072,12.50
 "2003/09/30","Scott Adams",0740721909,4.95
 "2004/10/04","Benjamin Radcliff",0804818088,4.95
 "2004/10/04","Randel Helms",0879755725,4.50
```


Metaformats (1)

- DSV – delimiter-separated values
  - CSV – comma-separated values
    - 1 record per line
    - First line: fields = variable names
    - Remaining lines: fields = variable values

DSV format: separated by colon, one record per line (mainly used in Unix)

```
Name:Password: UserID:PrincipleGroup:Gecos: HomeDirectory:Shell
smith:!:100:100:8A-74(office):/home/smith:/usr/bin/sh
guest:!:200:0::/home/guest:/usr/bin/sh
```

CSV format: mainly used in Windows system

```
"REVIEW_DATE","AUTHOR","ISBN","DISCOUNTED_PRICE"
 "1985/01/21","Douglas Adams",0345391802,5.95
 "1990/01/12","Douglas Hofstadter",0465026567,9.95
```

Metaformats (2)

- XML
  - Simple syntax
  - Plain text
  - Nested
  - Semantics
  - Suitable for complex nested or recursive structure

```
<booklist>
   <book ISBN="1-558-28592-x" availability="instock">
      <title>XML: A Primer</title>
      <price>24.99</price>
      <author>
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         </contactinfo>
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   </book>
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      <price>44.95</price>
      <author>
         <name>Charles F. Goldfarb</name>
         <name>Paul Prescod</name>
      </author>
   </book>
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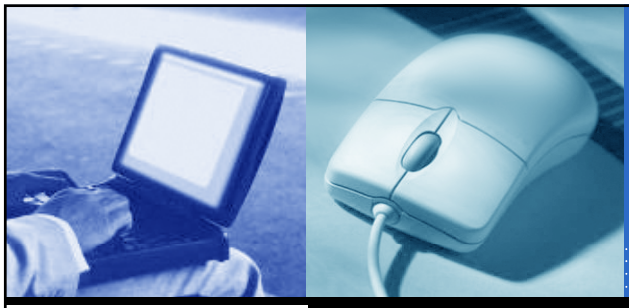
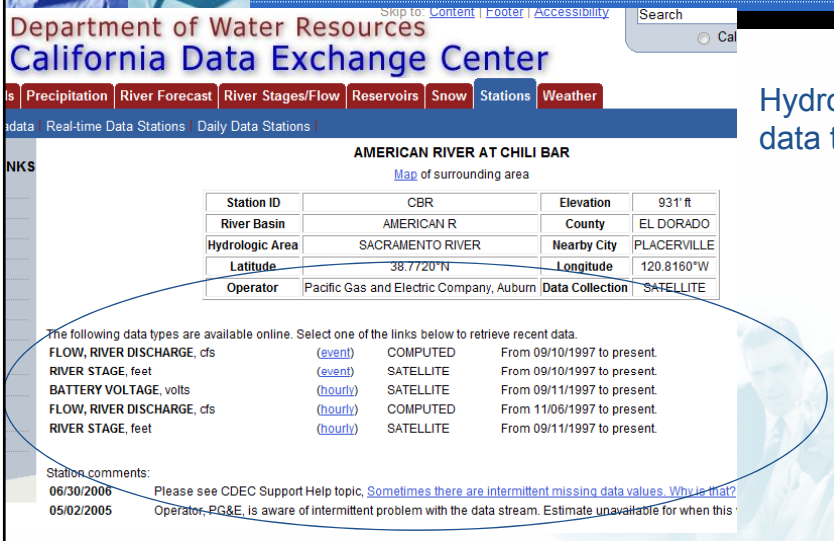


Scientific data types

A few examples

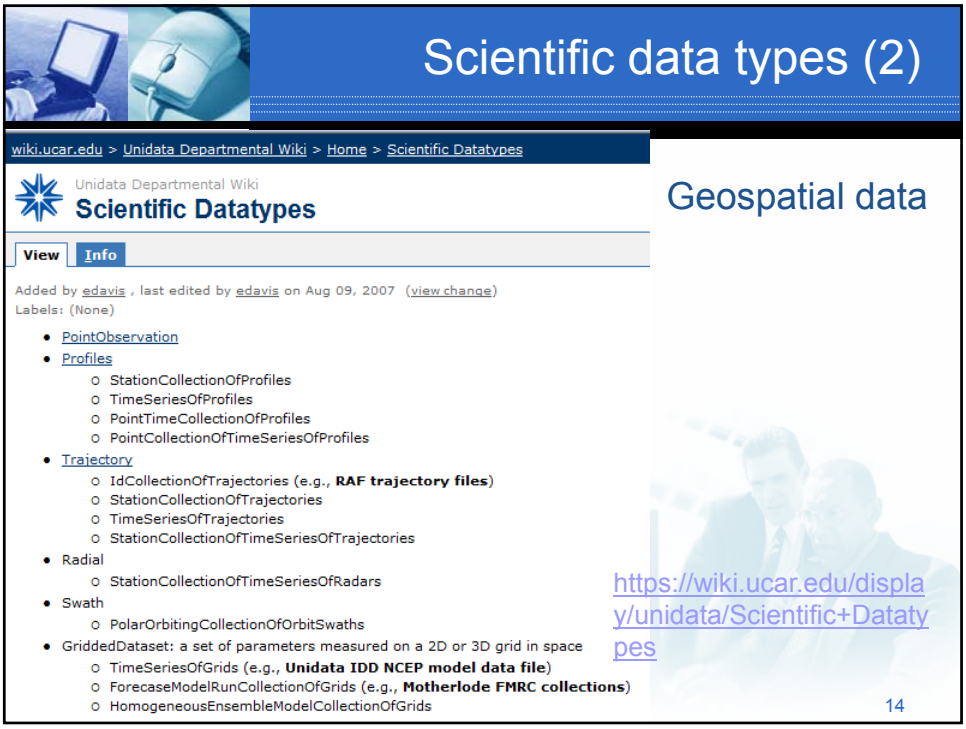
Scientific data types (1)



Hydrology data types

http://cdec.water.ca.gov/cgi-progs/staMeta?station_id=CBR

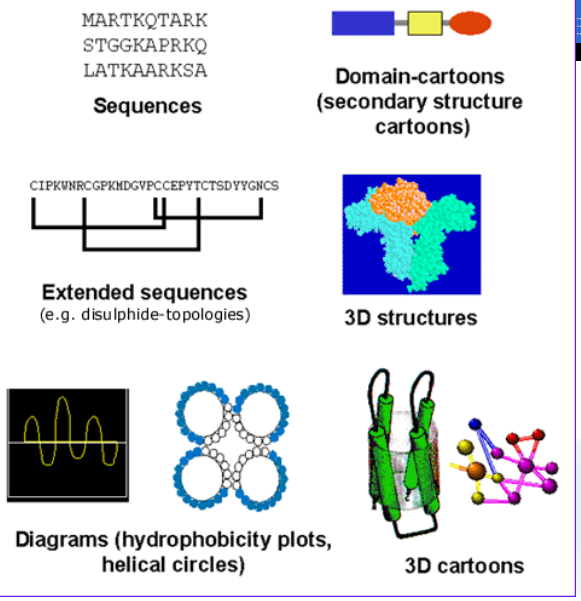
Scientific data types (2)



Geospatial data

https://wiki.ucar.edu/display/unidata/Scientific+Datatypes

Scientific data types (3)



Bioinformatics data types

http://www.ncbi.nlm.nih.gov/Education/Bioinformatics/datatypes.html

Scientific data types (4)

- Chemical data types
  - Registry number
  - Chemical name
    - One chemical has many different names
    - Chemical names are sometimes misleading
    - Slight difference in spelling of a chemical name can lead to a complete misrepresentation of the chemical substance
  - Modular formula
  - Structural formula
  - Connectivity tables

Summary of scientific data types

- Disciplinary specific
- Associated with data collection methods
  - Computed
  - Captured by instruments or satellites
- Associated with the natural phenomenon, organism, or object being described by the data
- Grouping of a set of attributes

Data formats

Scientific data formats

- Disciplinary specific formats
- Image formats (2-D)
- Image formats (3-D, MESH)
- Matrix formats
- Microarray file formats
- Communication protocols

See handout for examples

What formats are for?

- Archiving
  - Preservation for posterity
- Storage
  - Availability for “arbitrary” access
- Transmission
  - delivery across
    - hardware
    - software
    - administrative
  - system boundaries
- Analysis
  - availability for processing

Format requirements for archiving

- Critical
  - portable
  - *self-describing*
    - Assume neither software nor hardware that wrote data will be available when data are read.
- Important
  - space-efficient
    - Huge archives must fit in finite space
  - *write* speed
    - Huge archives must be writable in finite time.

Format Requirements for Storage

- Critical
  - subset retrieval
    - the piece you need is different from the piece everybody else needs
- Important
  - space-efficient
    - probably less fast storage than archival storage
  - portable
    - fast storage may be accessed by multiple hardware/software architectures

Format Requirements for Transmission

- Critical
  - convertible
    - easy to get data and metadata into and out of
  - portable
    - *readable* anywhere
  - extensible
    - can add types and structures you didn't think of yet
- Important
  - single stream for data and metadata
    - wadding everything up together reduces risk of missing critical piece and not knowing it

Format Requirements for Analysis

- Critical
  - works with *your* software
    - e.g.: data/metadata serialized for processing pipeline
    - e.g.: relevant data "chunk" fits entirely in memory (FFT, etc.)
- Important
  - works with *all* your software
    - minimize time spent converting format