File Parsing

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Programming for Scientists

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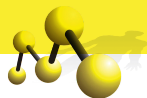
File Representations
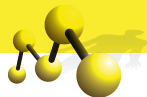
What's a File?

A sequence of bytes.

(and meta-data).

File Format Examples: FASTA format
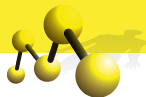
> qqq
ACTTTGTTATATATACTATCTGTATTTTC
CTGGGTGAGAGAGTGGTTGAGAGGGGGAA
CCCCCAACCACATTTCCCCACACCCCCTG
ACTTTCCTATATGTCCATTTTTATAATC
> ppp
TTTTTGGTATCTATTTTCCACTCATTCTTTAT
TACCCCAGTCATCACAAAACACACACACAACC
ATTATCTCTAATATATAATTTTACCTTT
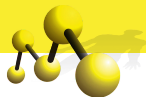
Parsing FASTA

```python
sequences = []
curseq = ''
for line in file('input.fsa'):
    if line[0] == '>':
        sequences.append(curseq)
    else:
        curseq += line.strip()
sequences.append(curseq)
```

File Format Examples (II): GenBank

```
LOCUS       SCU49845    5028 bp    DNA          PLN      21-JUN-1999
DEFINITION  Saccharomyces cerevisiae TCP1-beta gene, partial cds, and A
            (AXL2) and Rev7p (REV7) genes, complete cds.
ACCESSION   U49845
VERSION     U49845.1  GI:1293613
KEYWORDS    .
SOURCE      Saccharomyces cerevisiae (baker's yeast)
  ORGANISM  Saccharomyces cerevisiae
            Eukaryota; Fungi; Ascomycota; Saccharomycotina; Saccharomycetes;
            Saccharomycetales; Saccharomycetaceae; Saccharomyces.
...
ORIGIN
        1 gatcctccat atacaacggt atctccacct caggtttaga tctcaacaac ggaaccattg
       61 ccgacatgag acagttaggt atcgtcgaga gttacaagct aaaacgagca gtagtcagct
      121 ctgcatctga gccgctgaa gttctactaa gggtggataa catcatccgt gcaagaccaa
      181 gaaccgccaa tagacaacat atgtaacata tttaggatat acctcgaaaa taataaaccg
      241 ccacactgtc attattataa ttagaaacag aacgcaaaaa ttatccacta tataattcaa
```
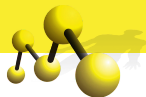
Representing Text

ASCII

- 65: A
- 66: B
- ...
- 48: 0
- 49: 1
- ...
- ...

127 code points taken.

Two File Format Classes

- Text files
- Non-text files (binary files)

| Size	Hex Value	Value	Meaning
2	42 4D	"BM"	Magic Number (66, 77)
4	46 00 00 00	70 Bytes	Size of Bitmap
2	00 00	Unused	Application Specific
2	00 00	Unused	Application Specific
4	36 00 00 00	54 bytes	The offset of data.
4	28 00 00 00	40 bytes	Size of header.
4	02 00 00 00	2 pixels	The width in pixels
4	02 00 00 00	2 pixels	The height in pixels
2	01 00	1 plane	Number of color planes.
2	18 00	24 bits	The bits/pixel.
4	00 00 00 00	0	No compression used
4	10 00 00 00	16 bytes	The size of the raw BMP data
4	13 0B 00 00	2,835 pixels/m	The horizontal resolution
4	13 0B 00 00	2,835 pixels/m	The vertical resolution
4	00 00 00 00	0	Number of colors in the palette
4	00 00 00 00	0	Means all colors are important

Size	Hex Value	Value	Meaning
3	00 00 FF	0 0 255	Red, Pixel (0,1)
3	FF FF FF	255 255 255	White, Pixel (1,1)
2	00 00	0	Padding for 4 bytes/row
3	FF 00 00	255 0 0	Blue, Pixel (0,0)
3	00 FF 00	0 255 0	Green, Pixel (1,0)
2	00 00	0	Padding for 4 bytes/row

(Wikipedia)

Text vs. Binary
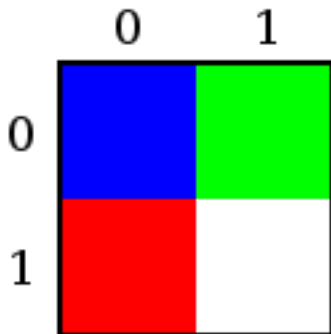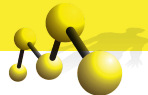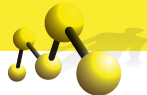
When possible, prefer text formats.
They are simpler.

Line Endings
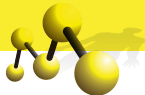
- Unix: LF (line feed)
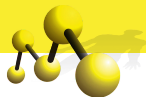- Windows: CRLF (carriage return, line feed)
- (Old Mac OS: CR)

The extra carriage returns will often show up as ^M in Unix.
Some unix text files will show up as a single ultra-long line on Windows.
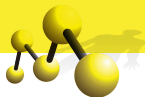
What About International Characters?

- Such as á or ç?
- Or μ?
- Or Asian characters?
- Or —?

It's a mess!

International Character Sets

- Traditional (latin-1,latin-9,latin-15,...)
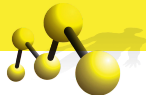- Unicode (16-bits, or 32-bits)
- UTF-8

Unicode

Unicode

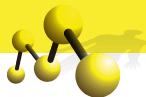Use 16 bits for (almost) all possible possible characters.

Use 32 bits for all possible characters.

Byte Order

If you have a 2 byte number, which byte do you write first?

UTF-8

Emerging standard (at some levels).

# UTF-8

Emerging standard (at some levels).
You still see errors
I saw this in an ATM receipt the other day
confirmação (which is confirma cão in UTF-8, but printed out in
Latin-15)

Text Based Formats

- Text format is not only for text
- Your Python files are text files
- Anything can be represented as a text-file

Text Formats

- Easier to parse
- Easier to debug
- Easier to transfer from one machine to the next
- Larger files (but you can compress them)

Tabular Text Formats
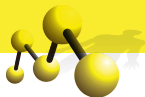
- Comma- or TAB- separated files are flexible
- Can be used to transfer from and to spreadsheet software
- Unfortunately, these are often not 100% well specified

Example: SAM Format
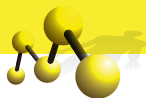
```
@HD    VN:1.0 SO:unsorted
@SQ    SN:    LN:9732
@PG    ID:bowtie2    PN:bowtie2    VN:2.0.0-beta7
FC5:1101:1441:2131    4    *    0    0    *    *    0    0    TNTCTATT
FC5:1101:1371:2227    4    *    0    0    *    *    0    0    TTGTCTCT
FC5:1101:1650:2171    4    *    0    0    *    *    0    0    GTGTAATT
FC5:1101:1599:2183    4    *    0    0    *    *    0    0    GTATATAC
FC5:1101:1539:2201    4    *    0    0    *    *    0    0    CCTTCTCA
```
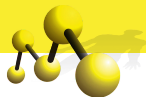
FC5:1101:1441:2131\t4\t*\t0\t0...
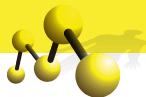
Parsing This File
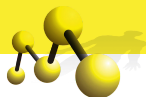
```python
ifile = open('input.sam')
matched = []
nreads = 0
for line in ifile:
    if line[0] == '@':
        continue
    nreads += 1
    tokens = line.strip().split('\t')
    if tokens[1] != '4': # Four is *unmatched*
        matched.append( (tokens[0], tokens[2], int(tokens[3

print 'Matched {0} reads out of {1} ({2:.2%})'.format(len(m
```

Conclusions

- Use UTF-8
- Prefer text-based formats (use generic compression on top)

Homework I

- Download FastQ file from course webpage
- Plot (for each base pair position) average quality & std. dev.
- Write a sequence trimmer

Homework I