File Parsing

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Programming for Scientists

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File Representions



What's a File?

A sequence of bytes.

(and meta-data).

Representing Text



ASCII

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

127 code points taken.

File Format Examples: FASTA format



> qqq ACTTTGTTATATATACTATCTGTATTTTC CTGGGTGAGAGAGTGGTTGAGAGGGGGAA CCCCCAACCACATTTCCCCACACCCCCTG ACTTTCCTATATGTCCATTTTTATAATC

> ppp TTTTTGGTATCTATTTTCCACTCATTCTTTAT TACCCCAGTCATCACAAAACACACACACACACA ATTATCTCTAATATATAATTTTACCTTT

Parsing FASTA



```
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.

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ORIGIN

 $1~{\rm gatcctccat}$ ataca
acggt atctccacct caggtttaga tctcaacaac ggaaccattg

61 ccgacatgag acagttaggt atcgtcgaga gttacaagct aaaacgagca gtagtcagct

121 ctgcatctga agccgctgaa gttctactaa gggtggataa catcatccgt gcaagaccaa

181 gaaccgccaa tagacaacat atgtaacata tttaggatat acctcgaaaa taataaaccg

241 ccacactotc attattataa ttagaaacag aacgcaaaaa ttatccacta tataattcaa. Luis Pedro Coelho (Programming for Scientists) * File Parsing * October 15, 2012 (6 / 24

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).



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

_ 12	110	DIVI	magic manibol (00, 11)					
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	8 00 00 00	40 bytes	Size of header.					
4 02	2 00 00 00	2 pixels	The width in pixels					
4 02	2 00 00 00	2 pixels	The height in pixels					
2 01	1 00	1 plane	Number of color planes.					
2 18	8 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	3 0B 00 00	2,835 pixels/m The horizontal resolution						
4 13	3 0B 00 00	2,835 pixels/m The vertical resolution						
4 00	00 00 00 00	Number of colors in the palette						
4 00	00 00 00	0 Means all colors are importan						
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Meaning

Magic Number (66, 77)

Size

2

Hex Value

42~4D

Value

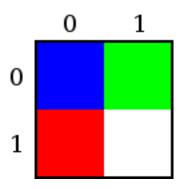
 $\rm "BM"$

Size	Hex Value	Value	Meaning
3	00 00 FF	0 0 255	Red, Pixel (0,1)
$\frac{3}{2}$	FF FF FF 00 00	255 255 255 0	White, Pixel (1,1) Padding for 4 bytes/row
3	FF 00 00	$255\ 0\ 0$	Blue, Pixel (0,0)
$\frac{3}{2}$	00 FF 00 00 00	$\begin{array}{ccc} 0 & 255 & 0 \\ 0 & & \end{array}$	Green, Pixel (1,0) Padding for 4 bytes/row

 $({\bf Wikipedia})$

Bitmap





Text vs. Binary



When possible, prefer text formats. They are simpler.

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

U										
@PG	ID:bowtie2	PN:bowtie2				VN:2.0.0-beta7				
FC5:11	01:1441:2131	4	*	0	0	*	*	0	0	TNTCTATI
FC5:11	01:1371:2227	4	*	0	0	*	*	0	0	TTGTCTCT
FC5:11	01:1650:2171	4	*	0	0	*	*	0	0	GTGTAATT
FC5:11	01:1599:2183	4	*	0	0	*	*	0	0	GTATATAC
FC5:11	01:1539:2201	4	*	0	0	*	*	0	0	CCTTCTCA

SAM Close Up



 $FC5:1101:1441:2131 \\ \\ t4 \\ t^* \\ t0 \\ t0...$

Parsing This File



```
ifile = open('input.sam')
matched = 0
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 += 1
print 'Matched \{0\} reads out of \{1\} (\{2:.2\%\})' \
             . format (matched, nreads, matched/float (nreads))
```

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



