CMSC423: Bioinformatic Algorithms, Databases and Tools
Lecture 4

Writing bioinformatics software

Biological databases

Writing bioinformatics software

Libraries/utilities

- Bio::Perl (Perl)
- BioJava (Java)
- BioPython (Python)
- BioRuby (Ruby)
- seqAn (C++)
- Bioconductor (R)
- Chado (SQL)

Bio::Perl

- http://www.bioperl.org

```
use Bio::Perl;

my $seq = read_sequence(“mytest.fa”, “fasta”);
my $gbseq = read_sequence(“mytest.gb”, “genbank”);

write_sequence(“>test.fasta”, 'fasta', $gbseq);
```

' vs “ ?

Bio::Perl

- Homework question #5

```
use Bio:Perl;

while ($seq = read_sequence(“test.fa”, 'fasta')) {
    if ($seq ->length() > 500) {
        print $seq->primary_id(), “\n”;
    }
}
```

Note: you still need to write your own version...

Bio::Perl

- Other useful stuff

```
$seqio = new Bio::SeqIO(-format => 'largefasta',
                        -file   => 't/data/genomic-seq.fasta');
$pseq = $seqio->next_seq();

$gb = new Bio::DB::GenBank;
$seq1 = $gb->get_Seq_by_id('MUSIGHBA1');

etc...
```

BioJava

- http://www.biojava.org

```
import org.biojava.bio.*;
String filename = args[0];
     BufferedInputStream is =
        new BufferedInputStream(new FileInputStream(filename));
     //get the appropriate Alphabet
     Alphabet alpha =
   AlphabetManager.alphabetForName(args[1]);

     //get a SequenceDB of all sequences in the file
     SequenceDB db = SeqIOTools.readFasta(is, alpha);
```

BioJava

- Question 5

```
BufferedReader br =
          new BufferedReader(new FileReader(args[0]));

 String format = args[1];
 String alphabet = args[2];

 SequenceIterator iter =
 (SequenceIterator)SeqIOTools.fileToBiojava(format,alphabet, br);
while (iter.hasNext()){
    Sequence seq = iter.nextSequence();
    if (seq.length() > 500) {System.out.println(seq.getName());}
}
```

BioJava...more

- Same as Bio::Perl:
  - can directly connect to databases
  - various sequence manipulations (reverse complement, translate, etc.)
  - basic bioinformatics algorithms
  - etc.

BioPython

- http://www.biopython.org

```
from Bio import SeqIO
handle = open(“file.fasta”)
seq_record = SeqIO.parse(handle, “fasta”)

SeqIO.write(my_records, handle2, "fasta")
```

BioPython

- Question 5

```
from Bio import SeqIO
handle = open("test.fasta")
for seq_record in SeqIO.parse(handle, "fasta") :
    if len(seq_record) > 500 :
        print seq_record.id
handle.close()
```

BioPython...more

- Same as Bio::Perl:
  - can directly connect to databases
  - various sequence manipulations (reverse complement, translate, etc.)
  - basic bioinformatics algorithms
  - etc.

BioRuby

- http://www.bioruby.org

```
require 'bio'

input_seq = ARGF.read      # reads all files inarguments

my_naseq = Bio::Sequence::NA.new(input_seq)
```

BioRuby

- Question 5

```
#!/usr/bin/env ruby

require 'bio'

ff = Bio::FlatFile.new(Bio::FastaFormat, ARGF)
ff.each_entry do |f|
  if f.length > 500
    puts f.entry_id
  end
end
```

BioRuby...more

- Same as Bio::Perl:
  - can directly connect to databases
  - various sequence manipulations (reverse complement, translate, etc.)
  - basic bioinformatics algorithms
  - etc.

SeqAn

- http://www.seqan.de

```
#include <seqan/sequence.h>
#include <seqan/file.h>

using namespace seqan;
using namespace std;

String <Dna> seq;
String<char> name;
fstream f;
f.open(“test.fasta”);
readMeta(f, name, Fasta());
readMeta(f, seq, Fasta());
```

SeqAn

- Question 5

```
String <Dna> seq;
String<char> name;
fstream f;
f.open(“test.fasta”);
while (! f.eof()){
    readMeta(f, name, Fasta());
    readMeta(f, seq, Fasta());
    if (length(seq)){
        cout << name << endl;
    }
}
```

SeqAn...more

- Not quite as much as Perl/Java/Python, but still lots of utilities (including graph algorithms)

R/BioConductor

- http://www.bioconductor.org
- Mainly for statistical applications, e.g. microarray analysis

```
library("affy")
library("geneplotter")
library("gplots")


data <- ReadAffy()
eset <- rma(data)
e <- exprs(eset)
heatmap.2(e, margin=c(15,15), trace="none",
  col=redgreen(25), cexRow=0.5)
```

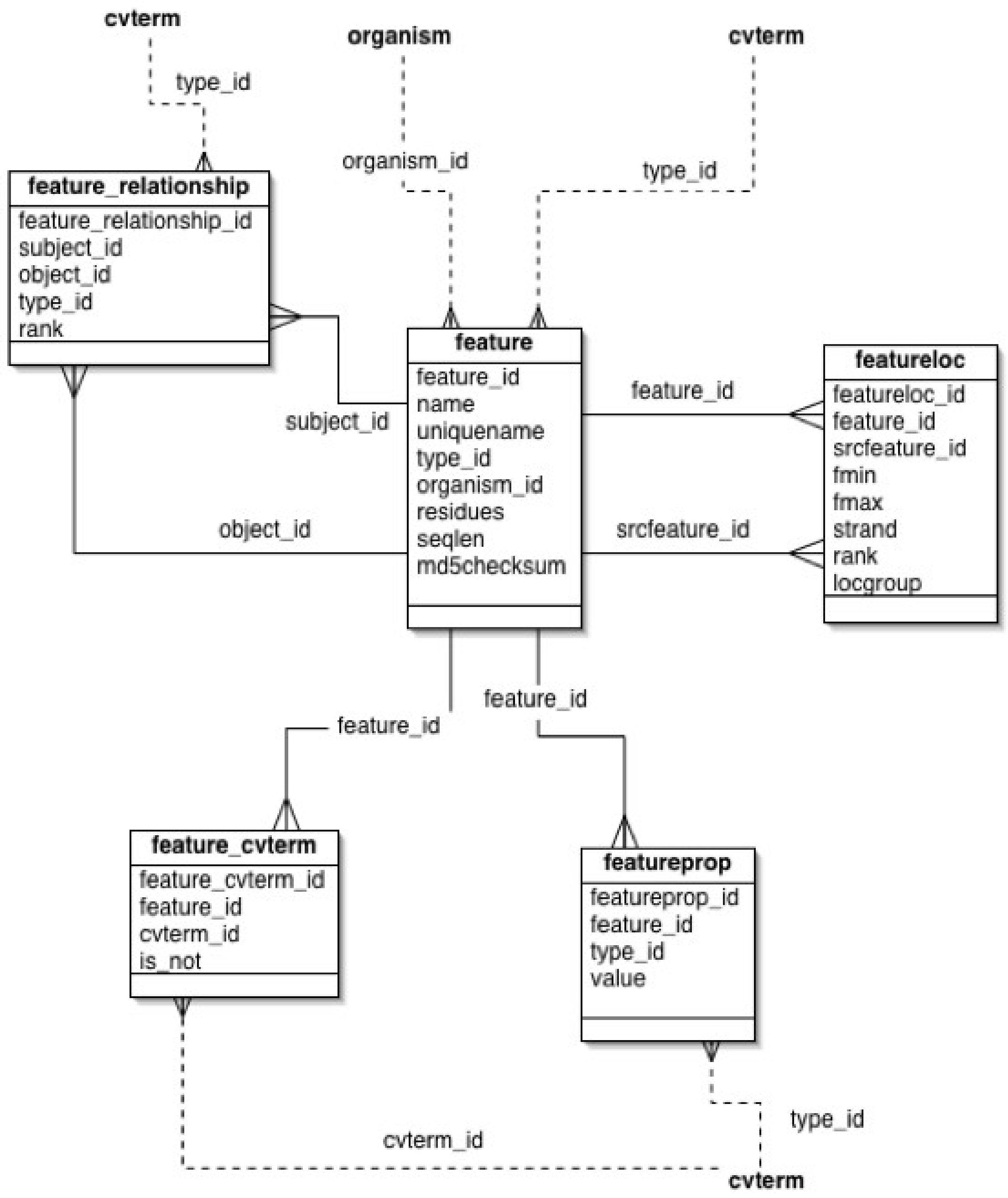
R/BioConductor

- Book has lots of examples
- Worth learning more about it – easy to do various cool things
- example... if time

Chado

- http://www.gmod.org
- Relational schema for storing biological data types in a relational database (e.g. MySQL, Oracle, Sybase, ...)

```
SELECT o.organism_id,o.abbreviation,o.genus,o.species,
           o.common_name,  count(f.feature_id) as n_features,
           o.comment
  FROM organism o LEFT JOIN feature f USING (organism_id)
  GROUP by o.organism_id,o.abbreviation,o.genus,o.species,
                o.common_name,o.comment
  ORDER BY o.genus,o.species
```


cvterm
type_id
organism
organism_id
cvterm
type_id
feature_relationship
feature_relationship_id
subject_id
object_id
type_id
rank
feature
feature_id
name
uniquename
type_id
organism_id
residues
seqlen
md5checksum
featureloc
featureloc_id
feature_id
srcfeature_id
fmin
fmax
strand
rank
locgroup
subject_id
object_id
feature_id
srcfeature_id
feature_id
feature_id
feature_cvterm
feature_cvterm_id
feature_id
cvterm_id
is_not
featureprop
featureprop_id
feature_id
type_id
value
type_id
cvterm_id
cvterm

Chado...more

- Bio... generally provide ability to interface with relational database.
- Understanding SQL and Chado is useful irrespective of language used.
- Relational DB particularly useful for web services
- Gbrowse example....if time

Programming for bioinformatics

- Details of specialized libraries beyond scope of course
- Good software engineering practices are essential
- Often, “correct” is undefined – output of program defines correctness
- Pitfalls – e.g. papers retracted from Science due to software bugs

- Key – be proactive and learn by yourselves from online resources!