
bio*bitsDocumentation*

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Various bioinformatics scripts

All documentation is hosted at <http://bio-bits.readthedocs.org/en/latest>

TODO

- Include existing scripts

Contents:

1.1 Installation

It is recommended to install into a virtualenv. If you know what you are doing and don't want to install into virtualenv, then you can skip right to step 3

1. Setup Virtualenv

It is assumed you have virtualenv already installed. If not see <https://virtualenv.pypa.io/en/latest/installation.html>

```
virtualenv env
```

2. Activate virtualenv

```
. env/bin/activate
```

3. Install dependencies

```
pip install -r requirements.txt
```

For python 2.6 you will need to also install some additional packages

```
pip install -r requirements-py26.txt
```

4. Install bio_bits

```
python setup.py install
```

1.2 Scripts

1.2.1 rename_fasta

Many times you find you have a fasta file where the identifiers are all wrong and you want to rename them all via some mapping file.

Take the example where you have the following fasta file(example.fasta):

```
>id1
ATGC
>id2
ATGC
>id3
ATGC
```

You want to rename each identifier(id1, id2, id3) based on a mapping you have. In a file called renamelist.csv you would have the following:

```
#From, To
id1, samplename1
id2, samplename2
id3, samplename3
```

Then to rename your fasta without replacing the original file you have two options:

1. Rename without replacing original file

```
rename_fasta renamelist.csv example.fasta > renamedfasta.fasta
```

2. Rename replacing original file's contents

```
reanme_fasta renamelist.csv example.fasta --inplace
```

Rename Mapping File Syntax

The file you specify as the rename map file is a simple comma separated text file.

The following rules apply to the format:

- The first entry is the identifier to find in the supplied fasta file.
- The second entry is what to replace the found identifier with
- Any line beginning with a pound sign(#) will be ignored by the renamer

Missing identifiers that are in fasta but not rename file

In the case where your fasta file contains an identifier that is not in the rename map file you supply, an error will be displayed in the console telling you as such:

```
idwhatever is not in provided mapping
```

1.2.2 beast_checkpoint

beast_checkpoint is a fork of <https://gist.github.com/trvrbr/5277297> that has been rewritten in python and slightly improved as the ruby script seemed to have a few errors.

It accepts any previously run or terminated beast run and will generate an xml file that essentially starts from the last generated tree/log state.

Since beast is random in nature, there does not appear to be a way to restart the run exactly from the same state that it left off.

Example

We will use the benchmark2.xml file that comes with Beast 1.8 This file is located in:

```
BEASTv1.8.0/examples/Benchmarks/benchmark2.xml
```

First you need to fix the benchmark2.xml because each taxa has a trailing space and that is annoying

```
$> sed 's/ "/"/' benchmark2.xml > beast.xml
```

Now run beast for about half of the iterations and hit CTRL-C to kill it This benchmark is set to run 1,000,000 iterations so around 500,000 you can kill it. Notice we are using a predefined seed

```
$> seed=1234567890
$> mkdir run1
$> cp beast.xml run1/beast.xml
$> beast -seed $seed -beagle_SSE beast.xml
```

Now we will want to re-run beast from that last state. We can use beast_checkpoint to do so by supplying the original xml and the produced trees and log files. We will put the new xml into a new directory since the .trees and .log files would create an error or possibly be overwritten.

NOTE If your fileLog and treeFileLog do not have the same logEvery then when beast exits you may end up with more/less tree states than log states. For now you will have to manually edit the files and ensure that the last tree state matches the last log state.

Todo

Could be possible to get beast_checkpoint to check for that scenario and use the last tree state that matches the last log state

```
$> mkdir run2
$> beast_checkpoint beast.xml *.trees *.log > run2/beast.xml
```

Now you can simply just re-run beast on the new xml using the same seed

```
$> cd run2
$> beast -seed $seed -beagle_SSE beast.xml
```

Tracer

If you name your runs sequentially as we did in the example(aka, run1, run2,...) then you can easily load all log files into tracer via the command line as follows

```
tracer run*/*.log
```

LogCombiner

After you have run all your beast checkpointed xml files you will probably want to combine them with logcombiner which comes with beast

1.2.3 beast_wrapper

Beast wrapper is intended as a helper script to run beast. At this point it just runs beast with the same arguments you would normally give to beast from the command line and just adds a estimated time left column to the console output

Example

```
$> beast_wrapper -beagle_SSE my_beast.xml
...
state      Posterior      Prior      Likelihood      rootHeight      my_beast.ucl.d.mean      location
0      -86527.5880      -6850.8316      -79676.7564      57.6772      1.16103E-3      4.86012
20000      -29044.3753      -1123.5287      -27920.8466      288.102      3.02471E-4      0.11891
40000      -25517.9525      -979.5343      -24538.4182      211.705      1.35118E-4      0.25060
60000      -24212.1250      -1040.4103      -23171.7147      188.454      1.05572E-4      0.18908
80000      -24097.9354      -1019.8099      -23078.1256      182.242      1.53593E-4      0.12857
100000      -24121.5382      -1105.6545      -23015.8837      178.060      1.26907E-4      0.10367
120000      -23930.6897      -1105.7390      -22824.9507      187.411      1.01885E-4      0.34214
140000      -23869.4856      -1087.1915      -22782.2942      178.535      8.76375E-5      0.26128
```

1.2.4 group_references

group_references splits an alignment file by reference into separate FASTQ files. group_references takes a SAM or BAM file as input, and can optionally be given an output directory where the FASTQ files will be saved. If not output directory name is provided, the files will be saved in the new folder group_references_out.

```
$> group_references contigs.bam
$> group_references contigs.bam --outdir split_fastqs
```

1.2.5 degen

Find genes where a sequence has degenerate bases.

How-to

Usage: degen.py <fasta> <options>

Options:

```
--gb-id=<accession_id>  Accession id for reference
--gb-file=<gbfile>      Local Genbank file for reference
--tab-file=<tabfile>    TSV/CSV file for reference with fields name,start,end
```

Example:

```
degen sequence.fasta --gb-id 12398.91
degen sequence.fasta --gb-file tests/testinput/sequence.gb
degen sequence.fasta --tab-file tests/testinput/degen.tab
degen sequence.fasta --tab-file tests/testinput/degen.csv
```

Output:

Gene name, degenerate position, degenerate base:

anchored capsid protein	85	R
anchored capsid protein	88	Y
membrane glycoprotein precursor	509	R
nonstructural protein NS5	8513	Y
nonstructural protein NS5	8514	Y
nonstructural protein NS5	8515	Y
anchored capsid protein	85	R
anchored capsid protein	88	Y
membrane glycoprotein precursor	509	R
nonstructural protein NS5	8513	Y
nonstructural protein NS5	8514	Y
nonstructural protein NS5	8515	Y

Gene/Tab File

degen.tab could look like:

genename	start	stop
foo	1	2
bar	9	33

The headers do not matter, but the start field must always come before the stop field, so the below example would also be valid:

start	GENEName	stop
1	foo	2
9	bar	33

or optionally without headers:

1	foo	2
9	bar	33

alternatively, with commas in place of tabs:

name, start, stop
foo, 1, 2
bar, 9, 33

You can also specify a coding region(CDS) in your file as well:

name, start, stop
CDS, 3, 33
foo, 1, 2
bar, 9, 33

Genbank File

As downloaded from NCBI's entrez database. Use this option if you don't have internet access.

An example

LOCUS	KJ189367	10452 bp ss-RNA	linear	VRL 10-FEB-2014
DEFINITION	Dengue virus 1 isolate DENV-1/PR/BID-V8188/2010, complete genome.			
ACCESSION	KJ189367			
VERSION	KJ189367.1 GI:582052497			
DBLINK	BioProject: PRJNA31235			

```

KEYWORDS      .
SOURCE        Dengue virus 1
ORGANISM      Dengue virus 1
               Viruses; ssRNA viruses; ssRNA positive-strand viruses, no DNA
               stage; Flaviviridae; Flavivirus; Dengue virus group.
REFERENCE     1 (bases 1 to 10452)
AUTHORS       Zody,M.C., Newman,R.M., Henn,M., Munoz-Jordan,J., McElroy,K.L.,
               Santiago,G., Poon,T.W., Charlebois,P., Weiner,B., Yang,X.,
               Piper,M.E., Fitzgerald,M., McCowan,C., Young,S., Gargeya,S.,
               Levin,J., Malboeuf,C., Qu,J., Ireland,A., Chapman,S.B., Murphy,C.,
               Wortman,J., Nusbaum,C. and Birren,B.
CONSRTM       Genome Resources in Dengue Consortium; The Broad Institute Genomics
               Platform; The Broad Institute Genome Sequencing Center for
               Infectious Disease; Centers for Disease Control and Prevention
               Division of Vector Borne Infectious Diseases; CDC Dengue Branch
               Puerto Rico
TITLE         Direct Submission
JOURNAL       Submitted (22-JAN-2014) Broad Institute of MIT & Harvard, 7
               Cambridge Center, Cambridge, MA 02142, USA
COMMENT       ##Assembly-Data-START##
               Assembly Method      :: Vicuna v. 1
               Sequencing Technology :: Illumina
               ##Assembly-Data-END##
FEATURES
  source      Location/Qualifiers
               1..10452
               /organism="Dengue virus 1"
               /mol_type="genomic RNA"
               /isolate="DENV-1/PR/BID-V8188/2010"
               /isolation_source="cell supernatant"
               /host="Homo sapiens"
               /db_xref="taxon:11053"
               /country="Puerto Rico"
               /collection_date="2010"
               /note="cell passage history: C6/36 1; cohort population:
               Dengue Surveillance;
               type: 1"
  5'UTR       1..83
               /note="indels in UTR have not been validated"
  CDS         84..10262
               /codon_start=1
               /product="polyprotein"
               /protein_id="AH143750.1"
               /db_xref="GI:582052498"
               /translation="MNNQRKKTGRPSFNMLKRARNRVSTGSQIAKRFSKGLLSQGQPM
               KLVMAFIAFLRFLAIPPTAGILARWSSFKNKGAIKVLRGFKKEISSMLNIMNRRKRSV
               TMLLMLLPTALAFHLTTTRGGEPHMIVSKQERGKSLLFKTSAGVNMCTLIAMDIGELCE
               DTMTYKCPRITEAEPDDVDCWCNATDTWVTYGTCSQTGEHRREKRSVALAPHVGLGLE
               TRTETWMSSEGAWKQIQRVETWALRHGFTVIAFFLAHAIGTSITQKGIIFILLMLVT
               PSMAMRCVGVIGNRDFVEGLSGATWVDVVLEHGSCVTTMAKNKPTLDIELLKTEVTNPA
               VLRKLCIEAKISNTTDSRCPTQGEATLVEEQDANFVCRRTFVDRGWGNGCGLFGKGS
               LLTCAKFKCVTKLEGKIVQYENLKYSVIVTVHTGDQHQVGNETTEHGTIATITPQAPT
               SEIQLTDYGALTDCSPRTGLDFNEMVLLTMKEKSWLVHKQWFLDLPLPWTSGASTSQ
               ETWNRQDLLVTFKTAHAKKQEVVVLGSQEGAMHTALTGATEIQTSGTTTIFAGHLKCR
               LKMDKLTLLKGMSYVMCTGSFKLEKEVAETQHGTVLVQVKYEGTDAPCKIPFSTQDEKG
               VTQNGRLITANPIVTDKEKPVNIETEPFFGESYIVVGAGEKALKLSWFKRGSSIGKMF
               EATARGARRMAILGDTAWDFSGIGGVFTSVGKLVHQIFGTAYGVLFSGVSWTMKIGIG
               ILLTWLGLNSRSTLSMTCIVGMVTLYLGVMVQADSGCVINWKGRELKCGSGIFVTN
               EVHTWTEQYKFQADSPKRLSAAIGKAWEEGVCGIRSATRLNIMWKQISNELNHILLE

```

```

NDMKFTVVVGDANGILAQGGKMIRPQPMHKEYSWKSWGKAKIIGADIQNTTFIIDGPD
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MGYWIESEKNETWKLARASFIEVKTCTWPKSHTLWSNGVLESEMIIPKIYGGPISQHN
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GSPIVNREGKIVGLYNGNVTTSGTYVSAIAQAKASQEGPLPEIEDEVFKRNLTIMD
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AAAFMTATPPGSVEAFPQSNV IQDEERDIPERSWNSGYDWITDFPGKT VWFVPSIK
SGNDIANCLRNKGRV IQLSRKTFDTEYQKTKNNDWDYVVTDI SEMGANFRADRVID
PRRCLKPVI LKDGPERVILAGPMPVTAASAAQRRGRIGRNQNKEGDQYVYMGQPLNND
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DLPVWLSYKVASEGFQYSDRRWCFDGERNNQVLEENMDVEIWTKEGERKKLRPRWLDA
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LLETTKKDLGIGYVAAENHQHATMLD VDLHPASAWTLYAVATTVITPMMRHTIENTTA
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TKGGPGHEEPIPMATYGNLVKLHSGKDVFFMPPEKCDTLLCDIGESSPNPTIEEGRT
LRVLKMVEPWLRGNQFCIKILNPYMP SVVETLERMQRKHGGMLVRNPLSRNSTHEMYW
VSCGTGNIVSAVNMTSRMLLNRF TMAHRKPTYERD VDLGAGTRHVAVEPEVANLDIIG
QRIENIKNEHKSTWHYDEDNPYKTWAYHGSYEVKPSGSASSMVNGVVRLLTKP WDVIP
MVTQIAMTDTTPFGQQRVFEKVDTRTPRAKR GTTQIMEVTAKWLWGFLSRNKKPRIC
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GKVRKDIPQWEP SKGWNWQVQVFC SHHFHQLIMKDGREIVVPCRNQDELVGRARVSQ
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HQWMTTEDMLS VWNRVWIDENPW MENKTHVSSWEEVPYLGKREDQWCGSLIGLTARAT
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mat_peptide 426..923
               /product="membrane glycoprotein precursor"
mat_peptide 924..2408
               /product="envelope protein"
mat_peptide 2409..3464
               /product="nonstructural protein NS1"
mat_peptide 3465..4118
               /product="nonstructural protein NS2A"
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               /product="nonstructural protein NS2B"
mat_peptide 4509..6365
               /product="nonstructural protein NS3"

```

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mat_peptide	6747..6815	/product="2K peptide"				
mat_peptide	6816..7562	/product="nonstructural protein NS4B"				
mat_peptide	7563..10259	/product="nonstructural protein NS5"				
3'UTR	10263..10452	/note="indels in UTR have not been validated"				
ORIGIN						
1	catctggacc	gacaagaaca	gtttcgaatc	ggaagcttgc	ttaacgtagt	tctaacagtt
61	ttttattaga	gagcagatct	ctgatgaaca	accaacggaa	aaagacgggt	cgaccgtctt
121	tcaatatgct	gaaacgcgcg	agaaaccgcg	tgtcaactgg	ttcacagttg	gcgaagagat
181	tctcaaaagg	attgctttca	ggccaaggac	ccatgaaatt	ggtgatggct	ttcatagcat
241	ttctaagatt	tctagccata	cccccaacag	caggaatttt	ggctagatgg	agctcattca
301	agaagaatgg	agcaattaaa	gtgttacggg	gtttcaaaaa	agagatctca	agcatgttga
361	acataatgaa	caggaggaaa	agatccgtga	ccatgctcct	catgctgctg	cccacagccc
421	tggcgtttca	tttgaccaca	cgagggggag	agccacacat	gatagttagt	aagcaggaaa
481	gaggaaagtc	actcttgttt	aagacctctg	cgggcgtcaa	tatgtgcacc	ctcattgcga
541	tggacttggg	agagttatgt	gaggacacaa	tgacctacaa	atgcccccg	atcactgagg
601	cggaaccaga	tgacgttgac	tgctggtgca	atgccacaga	cacatgggtg	acctatggga
661	cgtgtttctca	aaccggcgaa	caccgacgag	agaaacgttc	cgtggcactg	gccccacacg
721	tgggacttgg	tctagaaaca	agaaccgaaa	catggatgtc	ctctgaaggc	gcctggaaac
781	aaatacaaa	agtggaaact	tgggctttga	gacaccagg	attcacgggt	atagcctttt
841	ttttagcaca	tgctatagga	acatccatca	ctcagaaagg	gatcattttc	atcttgctga
901	tgctggtgac	accatcaatg	gccatgcatg	gcgtgggaat	aggcaacaga	gacttcgttg
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1081	ctgccgtctt	gcgcaaactg	tgcaattgaag	ctaaaatatc	aaacaccacc	accgattcaa
1141	gatgtccaac	acaaggagag	gccacactgg	tggagaagaca	agacgcgaac	tttgtgtgtc
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1681	tgggatcaca	ggaaggagca	atgcatactg	cgttgactgg	ggcgacagaa	atccagacgt
1741	caggaaacgac	aacaatcttc	gcaggacacc	tgaaatgcag	actaaaaatg	gataaactga
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1861	ctgagaccca	gcatggaact	gttctagtgc	agggtcaaata	tgaaggaaaca	gacgcgccat
1921	gcaagatccc	cttttcgacc	caagatgaga	aaggagtgc	ccagaatggg	agattgataa
1981	cagccaatcc	catagttact	gacaaagaaa	aaccagtcaa	cattgagaca	gaaccacctt
2041	ttggtgagag	ctacatcgtg	gtaggggcag	gcgaaaaagc	tttgaaacta	agctggttca
2101	agagagggaag	cagcataggg	aaaatgttcg	aagcaaccgc	ccgaggagca	cgaaggatgg
2161	ctatcctggg	agacaccgca	tgggacttcg	gttctatagg	aggagtgttt	acatctgtgg
2221	gaaaattgg	acaccagatt	tttggaaaccg	catatgggg	tctgttttagc	ggtgtttctt
2281	ggaccatgaa	aataggaata	gggattctgc	tgacatggtt	gggattaaat	tcaaggagca
2341	cgtcactttc	gatgacgtgc	attgtagtgt	gcatggtcac	actgtacct	ggagtcatgg
2401	ttcaagcgga	ttcgggatgt	gtgatcaact	ggaagggcag	agaacttaaa	tgcggaagtg
2461	gcatttttgt	cactaatgaa	gtccacactt	ggacagagca	atacaaattc	caggctgact
2521	ccccaaaaag	actgtcagca	gccattggaa	aggcgtggga	ggagggcggt	tgtggaattc
2581	gatcagccac	gcgtcttgag	aacatcatgt	ggaagcagat	atcaaataaa	ttgaaccaca
2641	ttttacttga	gaatgacatg	aaattcacag	tggtttagg	agatgccaac	ggaattttgg
2701	ccaagggaaa	aaaaatgatt	aggccacaac	ccatggaaca	caaataactca	tggaaaagct
2761	ggggaaaagc	taaaatcata	ggagcagaca	tacaaaatac	caccttcatt	atcgacggcc

```

2821 cagacacccc agaatgtcct gatggccaaa gagcatggaa catttgggaa gttgaggact
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3061 tagaagtcaa aacatgcacc tggccgaaat ctcacactct atggagcaat ggagttttgg
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3241 acttgtgtga aggaccaca gttgttgtgg atgaacattg tggaaatcga ggtccatctc
3301 tcagaaccac aacagtcaca ggaaagataa tccatgaatg gtgttgca ga tccctgcacgc
3361 tacccccctt acgtttcaga ggagaagacg ggtgttggtg tggcatggaa atcagaccag
3421 tgaaggagaa ggaggagaat ctagttaggt caatggctct tgcagggcca ggagaagtgg
3481 acagtttttc attaggaata ctatgcgtat caataatgat tgaagaagtg atgagatcca
3541 gatggagtag aaagatgctg atgactggaa cactggctgt cttcctcctt cttataatgg
3601 cacaactgac atggaatgat ctgattaggt tatgcatcat ggtcggagct aacgcttcag
3661 acaggatggg gatgggaaca acgtacctag ccttgatggc tactttcaaa atgagaccaa
3721 tgttcgtgtg agggctatta ttccgcagac taacatccag agaagttctt ctcctaacga
3781 ttggattaag cctggtggca tccgtggagc taccaaattc cttggaggag ctaggggatg
3841 gacttgcaat gggatcatg atgttaaaat tgttgactga atttcagcca caccagttat
3901 ggaccacctt attgtctctg acatttgtca aaacaactct ctcattggat tatgcatgga
3961 aaacaacggc tatggcactg tctatcgtat ctctctttcc tttatgcctg tctacgacct
4021 cccaaaaaac aacatggctt ccggtgctgt taggatcttt tggatgcaaa ccattaacca
4081 tgtttcttat aacagaaaaat aaaatctggg gaaggaaaag ttggccctc aatgaaggaa
4141 ttatggctat tggaaatagtc agcattctac taagctcact cctcaaaaat gatgtgccgt
4201 tggccggggc attaatagct ggaggcatgc taatagcatg ttatgtcata tccggtagct
4261 caccgattt atcattggag aaagcggctg aagtatcctg ggaacaagaa gcagaacact
4321 ccggtgcctc acacagcata ttagtagagg tccaagatga tggaaactatg aaaataaaag
4381 atgaagagag ggatgacaca ctaccatac tccttaaagc aactttgctg gcagttctcag
4441 gagtgtaccc aatgtcaata ccagcaactc tttttgtgtg gtatttttgg cagaaaaaga
4501 aacagagatc aggagtgtta tgggacacac ccagccctcc ggaagtggaa agagcagttc
4561 ttgataatgg catctataga atcttgcaaa gaggattgtt gggcaggtcc caagtaggag
4621 tgggagtttt ccaagacggc gtgtccaca caatgtggca cgttaccagg ggagctgtcc
4681 ttatgtacca aggaagaga ctggaaccaa gctgggccag tgtgaaaaag gacttgatct
4741 catatggagg aggttggagg ttccaaggat catggaacac gggagaagaa gtgcaggtaa
4801 tagctgttga accaggaaaa aacccccaaa atgtacagac aacgccgggc acctttaaga
4861 ctctgaagg cgaagttgga gccatagctc tagattttcaa acccggcaca tctggatctc
4921 ccactgtgaa cagagagggg aaaatagttg gtctgtatgg aaatggagtg gtgacaacaa
4981 ttggaacctc cgtcagtgcc attgccaaag ctaaagcatc acaggaaggg ccttaccag
5041 agattgagga cgaggtatth aagaaaagaa acttaacaat aatggacctg caccaggat
5101 caggaaaaac aagaagatat cttccagcca tagtccgtga ggccataaaa aggaaactgc
5161 gtacgttaat cctggtctcc acaagagttg tcgctctga aatggcagag gcaactcaagg
5221 gaatgccaat aagatatcag acaacagcag tgaagagtga acacacagga agggagatag
5281 ttgacctcat gtgccacgct acttttacca tgcgtctctt atccccagtg agagttccca
5341 attacaacat gatcattatg gatgaagcac attttaccga tccagctagc atagcggcca
5401 gaggttacat ctcaaccgga gtgggtatgg gtgaagcagc tgcgatcttt atgacagcca
5461 ctccccagg atcgggtggag gcctttccac agagcaatgc agttatccaa gatgaggaaa
5521 gagacattcc tgagagatca tggaaactcag gctacgactg gatcactgac tttccaggta
5581 aaacagtctg gtttgttcca agcattaaat caggaaatga cattgccaac tgtttaagaa
5641 agaacggaaa acgggtaatc caattgagca gaaaaacctt tgacactgag taccagaaaa
5701 caaaaaacaa tgactgggac tatgttgtca caacagacat ttctgaaatg ggggcaaat
5761 tccgggccga cagggttaata gaccaaggc ggtgcttgaa accggtaata ctaaaagatg
5821 gtccagagcg tgcattcta gccggaccga tgccagtgac tgcggccagt gctgccaga
5881 ggagaggaag aattggaagg aaccaaaca aggaaggtga tcagtatgtt tatatgggac
5941 agcctttaaa taatgatgag gatcacgctc attggacaga agcaaaaatg ctcttgaca
6001 atataaacac accagaaggg atcatcccag ccctttttga gccagagaga gaaaagagtg
6061 cagcaataga cggggagtac agactgcggg gagaagcaag gaaaacgttc gtggagctca
6121 tgagaagagg agatctacca gtttggctat cctacaaagt agcctcagaa ggtttccagt
6181 actccgacag aaggtggtgc tttgatggg aaaggaacaa ccagggtgtg gaggagaaca
6241 tggacgtgga gatctggaca aaggaaggag aaagaaagaa attgcgacct cgctggttgg

```

```

6301 acgccagaac atactctgat ccattggccc tgcgcgagtt taaagagttc gcagcaggaa
6361 gaagaagtgt ctcaggtgac ctgatatagg aaatagggaa acttccacaa cattedgagt
6421 taagagccca gaatgctctg gacaacttgg tcatgttgca caattccgaa caaggaggaa
6481 aagcctacag acatgccatg gaggaactac cagacaccat agaaacattg atgctactag
6541 ctttgatagc tgtgttgact ggtggagtga cgctgttctt cctatcagga aaaggcctag
6601 ggaaaacatc cattggcttg ctctgtgtga cggcctcaag cgcactgtta tggatggcca
6661 gtgtggagcc ccattggata gcggcctcca tcatactaga gttctttttg atggtgctgc
6721 tcattccaga gccagacaga cagcgcactc cacaggacaa ccagctagca tatgtgtgga
6781 taggtttgtt attcatgata ctgacagtgg cagccaatga gatgggatta ttggaaacca
6841 caaagaaaga cctggggatt ggctatgtag ccgccgaaaa ccaccaacat gccacaatgc
6901 tggacgtaga cctacacca gcttcagcct ggaccctcta tgcagttagc acaacagtca
6961 tcaactccat gatgagacac acaattgaaa atacaacggc aaacatttcc ctgaccgcca
7021 ttgcaaatca ggcagctata ttgatgggag ttgacaaggg atggccaata tcgaagatgg
7081 acataggagt tcactttctc gccttagggg gctattccca ggtgaacca ttgacactga
7141 cagcggcggg gttgatgtta gtggctcatt atgccataat tggaccagga ctgcaagcaa
7201 agggcactag agaagcccaa aaaaggacag cagccggaat aatgaaaaat ccaaccgtag
7261 acgggattgt tgcaatagac ttggatcctg tggtttatga tgcaaaattt gaaaaacaac
7321 taggccaat aatgttactg atactttgta catcacagat cctcttgatg cggaccacat
7381 gggccttggt tgaatccatc aactgggcta ctggaccctc gaccactctc tgggagggat
7441 ctcaaggaaa attctggaat accacaatag cagtgtccat ggcaaatatt ttcaggggaa
7501 gttatctagc aggagcaggt ctggctttct cattgatgaa atcttttagga ggaggtagga
7561 gaggcacggg agctcaaggg gaaacactgg gagagaaatg gaaaagacag ttgaaccaac
7621 tgagcaagtc agaattcaac acctacaaaa ggagtgggat tatggaggtg gacagatccg
7681 aagccaaaga gggactgaaa agaggagaaa caaccaaaca tgcagtgtca agaggaaacg
7741 ccaaaactgag gtggtttgtg gagaggaaac tcgtgaaacc agaaggaaaa gtcatagacc
7801 tcggttggtg aagaggtggc tggatcatatt attgtgctgg gctgaagaaa gttactgaag
7861 tgaagggata caaaaagga ggacctggac atgaggaacc tatccaatg ggcacctatg
7921 gatggaacct agtaaaacta cactctggaa aggatgtatt ttttatgcca cctgagaaat
7981 gtgacactct tctgtgtgat attggtgagt cctctccgaa tccaactata gaagaaggaa
8041 gaacgttacg tgttctaaaa atggtggaac catggctcag aggaaaccaa ttctgcataa
8101 aaatcctaaa tccttacatg ccaagtgtgg tagaaactct ggagcgaatg caaagaaaac
8161 atggagggat gctagtgcga aaccactct caagaaattc taccatgaa atgtattggg
8221 tttcatgtgg aacaggaaac attgtgtcgg cagtgaacat gacatccaga atgttactga
8281 accgattcac aatggctcac aggaagccaa catatgaaag agacgtggac ttaggcgctg
8341 gaacaagaca tgtggcagtg gaaccagagg tagccaacct agatatcatt ggccagagga
8401 tagaaaaatg aaaaaatgaa cacaagtcaa catggcatta tgatgaggac aatccatata
8461 aaacatgggc ctatcatgga tcatatgagg tcaagccatc aggatcagcc tcatctatgg
8521 tgaatggagt ggtgagattg ctacgaaac catgggatgt catcccatg gtcacacaaa
8581 tagctatgac tgataccaca cccttggac aacagagagt gtttaaagag aaagttgaca
8641 cgcgcacacc aagagcaaaa cgaggcacia cacagattat ggaggtgaca gccaagtggg
8701 tatggggttt ctttccaga acaaaaaaac ccagaatctg cacaagagag gagttcacia
8761 gaaaggttag gtcaaacgcg gcaataggag cagtgttcgt tgatgaaaac caatggaact
8821 cagcaaaaaga agcagtggaa gacgaaaggt tttgggatct tgtgcacaga gagagggagc
8881 ttcataaaca gggaaaatgt gccacgtgtg tctacaacat gatggggaag agagagaaaa
8941 aattaggaga gtttgaaaag gcaaaaggaa gtcgtgcaat atggtacatg tggctgggag
9001 cacgctttct ggagttcgaa gcccttgggt ttatgaatga agatcactgg tttagttagg
9061 agaattcact cagtggagtg gaaggagaag gactgcacia acttgatac atactcagag
9121 acatatcaaa gattccgggg ggaaatatgt atgcagatga tacagccgga tgggacacia
9181 gagttaacaga ggatgacctc cagaatgagg ctaaaatcac tgacatcatg gagcctgaac
9241 atgctctatt ggctacgtca atttttaagc tgacttatca aaacaagggt gtgaggggtg
9301 aaagaccagc aaaaaatgga accgtgatgg atgttatatc cagacgtgat cagagaggga
9361 gtggacaggt cggaacttat ggcttaata ctttcaccaa tatggaggtc caactaataa
9421 gacaaatgga gtctgaggga atctttttac ccagcgaatt ggaaaccccc aacctagctg
9481 agagggctct tgactgggta gaaaaacatg gcgcgaaaag gctgaaacga atggcaatca
9541 gcgagatga ttgcgtggtg aaaccaattg acgacaggtt cgcaacagcc ttaacagctc
9601 tgaatgacat gggaaaagta aggaaagaca taccgcagtg ggaaccttca aaaggatgga
9661 atgattggca gcaagtgcct ttttgttcac accatttcca ccaactgatc atgaaggatg
9721 ggagggaaat agtggtgcca tgccgcaacc aagatgaact tgtgggcagg gctagagtat

```

```

9781 cacaaggcgc cggatggagc ctgagagaaa ctgcttgccct aggcaagtca tatgcacaaa
9841 tgtggcagct gatgtacttc cacaggagag acctgagact agcggctaac gctatctgtt
9901 cagccgtccc agttgattgg gtcccaacca gccgcacaac ctggtcaatc catgcccacc
9961 accaatggat gacaacagaa gacatgttat cagtgtggaa tagggtttgg atagacgaaa
10021 acccatggat ggagaacaaa actcatgtat ccagttggga agaagttcca tacctaggaa
10081 aaagggaaga tcaatggtgt ggatccctga taggcttgac agcgagggcc acctgggcca
10141 ccaacataca agtagccata aaccaagtga gaaggctcat cggaatgag aattatttag
10201 attacatgac atcaatgaag agattcaaga atgagagtga ttccgaagga gcactctggt
10261 aagtcaacac actcatgaaa taaaggaaaa tagaagatca aacaaagtaa gaagtcaggc
10321 cagattaagc catagcacgg aaagagctat gctgcctgtg agccccgtcc aaggacgtaa
10381 aatgaagtca ggccgaaagc cacggattga gcaagccgtg ctgcctgtgg ctccatcgtg
10441 ggatgtagc tc
//

```

1.2.6 parallel_blast

Parallel blast is a wrapper script around the blast commands as well as diamond. It utilizes GNU Parallel to run the commands in parallel by splitting up the input fasta files and distributes them across multiple subprocesses. If it detects that it is running inside of a PBS or SGE job it will run the job on multiple hosts that may be allocated to the job.

parallel_blast requires that you have gnu parallel installed and in your environments PATH as well as diamond and/or blastn/blastx/blastp.

- [diamond](#)
- [blast](#)
- [GNU parallel](#)

Usage

You can get all the arguments that can be supplied via the following

```
$> parallel_blast --help
```

Examples

For the examles below assume you have an input fasta in the current directory called input.fasta

Running blastn

```

$> parallel_blast input.fasta output.blast --ninst 4 --db /path/to/nt \
--blast_exe blastn --task megablast --blast_options "--value 0.01"
[cmd] /path/to/parallel -u --pipe --block 10 --restart > --sshlogin 4/: /path/to/blastn -task megab

```

Notice how we had to quote the additional --blast_options

Running diamond Diamond v0.7.9 is the version that was tested with parallel_blast. As diamond is still in development the options may change in future versions and parallel_blast may not run them correctly. Please submit a new issue if you find any issues.

```

$> parallel_blast input.fasta out.blast --ninst 4 --db /path/to/diamondnr \
--blast_exe diamond --task blastx --blast_options "--tmpdir dtmp"
[cmd] /path/to/parallel -u --pipe --block 10 --restart > --cat --sshlogin 1/: /path/to/diamond blast

```

Notice how even though we specified `--ninst 4` that `--sshlogin 1/:` was used and `--threads 4` was set instead.

Note In recent versions of diamond, diamond outputs a daa binary file instead of a tab separated file. `parallel_blast` automatically converts the diamond output from daa to tab format for you but leaves the daa file behind(Same name as the output file you specify, but with the extension .daa)

Command that is run You will notice in the examples above that when you run `parallel_blast` that it outputs the command that it is running in case you want to copy/paste it and run it yourself sometime.

You might notice that the command does not include all the quoted arguments such as the `--restart` argument which should be `--restart ">"` as well as the `--outfmt` which should be quoted as `--outfmt "6 ..."`. If you intend on rerunning the command you will have to add the quotes manually.

Running inside of a PBS or SGE Job

`parallel_blast` is able to detect if it is running inside of a PBS or SGE job by looking to see if `PBS_NODEFILE` or `PE_HOSTFILE` is set in the environment's variables.

If it finds either of them it will run the job by supplying `--sshlogin` for each host it finds in the file.

`PBS_NODEFILE` and `PE_HOSTFILE` have different syntax so `parallel_blast` first builds a CPU,NODENAME list from them.

PBS_NODEFILE

This file is parsed and counts how many of each unique host is listed such that the following `PBS_NODEFILE`:

```
node1.localhost
node2.localhost
node2.localhost
node3.localhost
node3.localhost
node3.localhost
```

would run 1 instance on `node1.localhost`, 2 instances on `node2.localhost` and 3 instances on `node3.localhost`

PE_HOSTFILE

This file is almost in the exact syntax that `parallel_blast` uses so it is almost a 1-to-1 mapping.

Diamond and multiple hosts

Since diamond utilizes threads much more efficiently than blast, for each unique host in a job only 1 instance is launched but the `-p` option is set to the number of CPUS for each host listed in the `PE_HOSTFILE` or `PBS_NODEFILE`

1.2.7 degen_regions

Finds all degenerate bases in a given fasta input file that may contain multiple sequeces and reports their position as well as the annotated gene name that contains them.

The fasta file must be previously aligned to the query sequence. That is, if you are using a genbank annotation file or having the script download it for you, you should have aligned all your input sequences to that sequence.

The annotation is retrieved via supplied genbank accession, genbank file path or gene tab/csv file.

Usage

You can view the usage of `degen_regions` via:

```
degen_regions --help
```

Using Genbank Files

If you already have downloaded the genbank annotation file (typically the extension is `.gb`) you can use the `-gb-file` argument

The following will use the test input fasta file as well as the test input genbank file to find all degenerate bases and will put the output in a tab separated file called `output.tsv`

```
degen_regions -i tests/Den4_MAAPS_TestData16.fasta -o output.tsv --gb-file tests/testinginput/sequence.g
```

Fetching Genbank Files Automatically

If you want the script to automatically fetch the Genbank annotation file from the internet you can use the `-gb-id` option and specify an accession number.

```
degen_regions -i tests/Den4_MAAPS_TestData16.fasta -o output.tsv --gb-id KJ189367
```

Using tab/csv file of gene annotation info

If you have a tab/csv file of gene annotations you can supply that using the `-tab-file` argument

You can read more about the format of the tab/csv annotation file in the [degen docs](#)

```
degen_regions -i tests/Den4_MAAPS_TestData16.fasta -o output.tsv --gb-file tests/testinginput/sequence.g
```

Manually specify CDS

You can use the `--cds` argument to set the coding region. This argument should be comma separated such as `start, stop`. Specifying this argument will override any other cds found in the tab file, genbank file or fetched genbank file.

The following would mark all locations as NON-CODING as you are specifying that only position 1 is coding

```
degen_regions -i tests/Den4_MAAPS_TestData16.fasta -o output.tsv --gb-file tests/testinginput/sequence.g
```

Without Gene Information

The gene information is optional. If it is not provided the output file will not be annotated with the gene information; otherwise, the output will look the same (you will also lose the “non-coding region” flag.)

```
degen_regions -i tests/Den4_MAAPS_TestData16.fasta -o output.tsv
```

Output

The output is a simple tab separated file

seq id	nt Position	aa position	nt composition	aa compos.
721	991	331	WCA	S/T
721	1307	436	AYA	I/T
721	1826	609	AYA	I/T
721	1865	622	GRA	E/G
721	7766	2589	ARA	K/R
2055_Den4/AY618992_1/Thailand/2001/Den4_1	1927	643	RAC	D/N
2055_Den4/AY618992_1/Thailand/2001/Den4_1	2833	945	YCG	P/S
2055_Den4/AY618992_1/Thailand/2001/Den4_1	3565	1189	YAT	H/Y
2055_Den4/AY618992_1/Thailand/2001/Den4_1	6271	2091	RAA	E/K
2055_Den4/AY618992_1/Thailand/2001/Den4_1	8656	2886	YAT	H/Y
2055_Den4/AY618992_1/Thailand/2001/Den4_1	8998	3000	YAG	*/Q
2055_Den4/AY618992_1/Thailand/2001/Den4_1	9811	3271	YCC	P/S
2055_Den4/AY618992_1/Thailand/2001/Den4_1	10542	3515	AGN	NON-CODING
2055_Den4/AY618992_1/Thailand/2001/Den4_1	10543	3515	NNN	NON-CODING
2055_Den4/AY618992_1/Thailand/2001/Den4_1	10541	3514	NNN	NON-CODING
2055_Den4/AY618992_1/Thailand/2001/Den4_1	10539	3514	NNN	NON-CODING
2055_Den4/AY618992_1/Thailand/2001/Den4_1	10546	3516	NNN	NON-CODING
2055_Den4/AY618992_1/Thailand/2001/Den4_1	10544	3515	NNN	NON-CODING
2055_Den4/AY618992_1/Thailand/2001/Den4_1	10542	3515	NNN	NON-CODING
1942_Den4/AY618992_1/Thailand/2001/Den4_1	4540	1514	RTA	I/V
1942_Den4/AY618992_1/Thailand/2001/Den4_1	10177	3393	MCA	P/T
1942_Den4/AY618992_1/Thailand/2001/Den4_1	10546	3516	NNN	NON-CODING
1942_Den4/AY618992_1/Thailand/2001/Den4_1	10544	3515	NNN	NON-CODING
1942_Den4/AY618992_1/Thailand/2001/Den4_1	10542	3515	NNN	NON-CODING
1875_Den4/AY618992_1/Thailand/2001/Den4_1	1514	505	AYG	M/T
1875_Den4/AY618992_1/Thailand/2001/Den4_1	3056	1019	ARA	K/R
1875_Den4/AY618992_1/Thailand/2001/Den4_1	3058	1020	KCA	A/S
1875_Den4/AY618992_1/Thailand/2001/Den4_1	3073	1025	WTT	F/I
1875_Den4/AY618992_1/Thailand/2001/Den4_1	3491	1164	AYC	I/T
1875_Den4/AY618992_1/Thailand/2001/Den4_1	3895	1299	RTG	M/V
1875_Den4/AY618992_1/Thailand/2001/Den4_1	7445	2482	GYA	A/V
948_Den4/AY618992_1/Thailand/2001/Den4_1	2819	940	ARC	N/S
871_Den4/AY618992_1/Thailand/2001/Den4_1	2947	983	RCC	A/T
871_Den4/AY618992_1/Thailand/2001/Den4_1	3058	1020	KCA	A/S
871_Den4/AY618992_1/Thailand/2001/Den4_1	3073	1025	WTT	F/I
871_Den4/AY618992_1/Thailand/2001/Den4_1	3116	1039	GYG	A/V
871_Den4/AY618992_1/Thailand/2001/Den4_1	3181	1061	RTW	I/V
871_Den4/AY618992_1/Thailand/2001/Den4_1	3179	1060	RTW	I/V
871_Den4/AY618992_1/Thailand/2001/Den4_1	3338	1113	ART	N/S
871_Den4/AY618992_1/Thailand/2001/Den4_1	3362	1121	ARA	K/R
871_Den4/AY618992_1/Thailand/2001/Den4_1	3373	1125	WCR	S/T
871_Den4/AY618992_1/Thailand/2001/Den4_1	3371	1124	WCR	S/T
871_Den4/AY618992_1/Thailand/2001/Den4_1	4314	1439	ATV	I/M
871_Den4/AY618992_1/Thailand/2001/Den4_1	7045	2349	WCC	S/T
871_Den4/AY618992_1/Thailand/2001/Den4_1	10536	3513	GAW	NON-CODING
871_Den4/AY618992_1/Thailand/2001/Den4_1	10537	3513	YCA	NON-CODING
947_Den4/AY618992_1/Thailand/2001/Den4_1	2971	991	YTY	F/L
947_Den4/AY618992_1/Thailand/2001/Den4_1	2969	990	YTY	F/L
947_Den4/AY618992_1/Thailand/2001/Den4_1	6763	2255	YTT	F/L

1793_Den4/AY618992_1/Thailand/2001/Den4_1	223	75	MAG	K/Q
1793_Den4/AY618992_1/Thailand/2001/Den4_1	556	186	RCC	A/T
1793_Den4/AY618992_1/Thailand/2001/Den4_1	586	196	RGT	G/S
1793_Den4/AY618992_1/Thailand/2001/Den4_1	613	205	YCA	P/S
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2875	959	YCG	P/S
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2943	982	AAN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2944	982	NNG	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2942	981	NNG	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2976	993	ATN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2977	993	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2975	992	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2973	992	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2980	994	NTG	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2987	996	ANN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2986	996	ANN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2989	997	NGT	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2996	999	TNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2995	999	TNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3001	1001	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2999	1000	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	2997	1000	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3004	1002	NCC	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3073	1025	NTT	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3086	1029	ARC	N/S
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3095	1032	CNG	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3116	1039	GNG	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3144	1049	GAN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3159	1054	GAN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3160	1054	NNC	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3158	1053	NNC	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3206	1069	GNC	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3235	1079	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3233	1078	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3231	1078	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3238	1080	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3236	1079	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3234	1079	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3241	1081	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3239	1080	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3237	1080	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3244	1082	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3242	1081	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3240	1081	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3247	1083	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3245	1082	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3243	1082	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3250	1084	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3248	1083	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3246	1083	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3253	1085	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3251	1084	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3249	1084	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3256	1086	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3254	1085	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3252	1085	NNN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3316	1106	NGG	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3337	1113	NAT	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3341	1114	GNA	GAPFOUND

1793_Den4/AY618992_1/Thailand/2001/Den4_1	3408	1137	ATN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3412	1138	NTG	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3493	1165	MCC	P/T
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3509	1170	ANT	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	3837	1280	TTN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	6185	2062	ARG	K/R
1793_Den4/AY618992_1/Thailand/2001/Den4_1	6187	2063	RAR	E/K
1793_Den4/AY618992_1/Thailand/2001/Den4_1	6185	2062	RAR	E/K
1793_Den4/AY618992_1/Thailand/2001/Den4_1	6614	2205	TYT	F/S
1793_Den4/AY618992_1/Thailand/2001/Den4_1	6650	2217	ARA	K/R
1793_Den4/AY618992_1/Thailand/2001/Den4_1	8630	2877	ART	N/S
1793_Den4/AY618992_1/Thailand/2001/Den4_1	8844	2949	AAN	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	9938	3313	AYT	I/T
1793_Den4/AY618992_1/Thailand/2001/Den4_1	9941	3314	GRC	D/G
1793_Den4/AY618992_1/Thailand/2001/Den4_1	10015	3339	RTT	I/V
1793_Den4/AY618992_1/Thailand/2001/Den4_1	10087	3363	NGR	GAPFOUND
1793_Den4/AY618992_1/Thailand/2001/Den4_1	10085	3362	NGR	GAPFOUND
1901_Den4/AY618992_1/Thailand/2001/Den4_1	15	6	AAN	NON-CODING
1901_Den4/AY618992_1/Thailand/2001/Den4_1	111	38	TTN	GAPFOUND
1901_Den4/AY618992_1/Thailand/2001/Den4_1	2279	760	GYT	A/V
1901_Den4/AY618992_1/Thailand/2001/Den4_1	8798	2933	ARA	K/R
1901_Den4/AY618992_1/Thailand/2001/Den4_1	10195	3399	RAG	E/K
1901_Den4/AY618992_1/Thailand/2001/Den4_1	10366	3456	RGG	NON-CODING
1934_Den4/AY618992_1/Thailand/2001/Den4_1	15	6	AAN	NON-CODING
1934_Den4/AY618992_1/Thailand/2001/Den4_1	111	38	TTN	GAPFOUND
1934_Den4/AY618992_1/Thailand/2001/Den4_1	998	333	GMT	A/D
1934_Den4/AY618992_1/Thailand/2001/Den4_1	4515	1506	TTM	F/L
1934_Den4/AY618992_1/Thailand/2001/Den4_1	8798	2933	ARA	K/R

1.2.8 plot_muts

Plot mutations either by comparing two sequences or by comparing a bunch of sequences to another sequence.

This command is still under a bit of development so bare with the nuances

Usage

You can view the usage of degen_regions via:

```
plot_muts --help
```

Example comparing multiple sequences against a query sequence

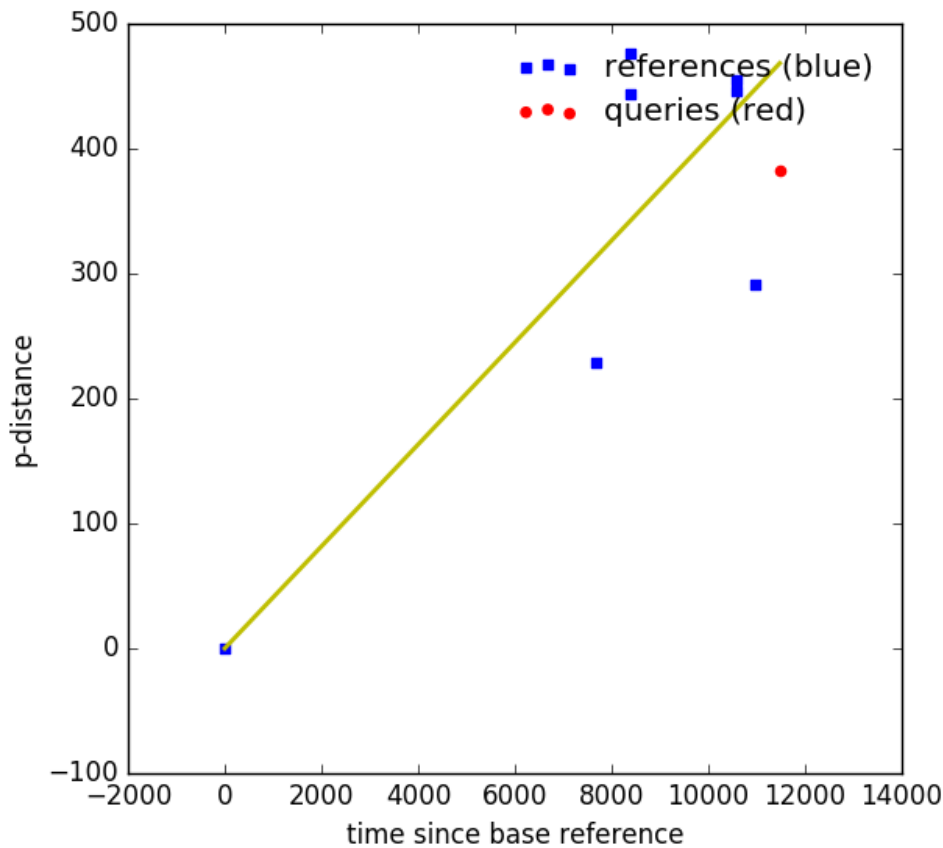
--refs is a fasta file containing multiple sequences where the sequence that has the earliest date will be used as the base reference.

--query is a fasta file containing a single sequence to be plotted in a different color to see how it compares.

```
plot_muts --refs tests/testinput/refs.fas --query tests/testinput/query.fas --out plot.png
```

The --out option is optional. If it is not provided, the plot will pop up on the user's screen automatically. If this does not work, try saving the image using --out instead.

Example Output



Plot muts also outputs a csv file named after the `--out` with `.csv` appended

```
name,dates,p-dist
Ref_gi|499073378|gb|KC807176.1|_Houston_virus_strain_V3982_complete_genome____2004,8401,476
Ref_gi|499073386|gb|KC807178.1|_Houston_virus_strain_16757_complete_genome____2010,10592,455
Ref_gi|499073382|gb|KC807177.1|_Houston_virus_strain_16740_complete_genome____2010,10592,446
Ref_gi|499073374|gb|KC807175.1|_Houston_virus_strain_V3872_complete_genome____2004,8401,444
Query_A12x2520____08_16_2012,11478,383
Ref_gi|557884407|gb|KF522691.1|_Nam_Dinh_virus_isolate_SZ11706Z_complete_genome____2011,10957,291
Ref_gi|341819796|gb|DQ458789.2|_Nam_Dinh_virus_isolate_02VN178_complete_genome____2002,7670,229
BaseRef_gi|499073354|gb|KC807170.1|_Ngewotan_virus_strain_JKT9982_complete_genome____1981,0,0
```

Input File Requirements

The input must be fasta format. Both the query and ref files can have any number of sequences.

The year should be the last part of the ID, preceded by a quadruple underscore. e.g.:

```
>some|info|blah_blah____2001_09_2010
>some____1995
>some____09/09/2012
```

If the ID uses '/' rather than underscore, plot_muts currently accepts the year as the *fourth* field. e.g.:

```
>some/info/blah/1995
>some/info/blah/1995/more/info
```

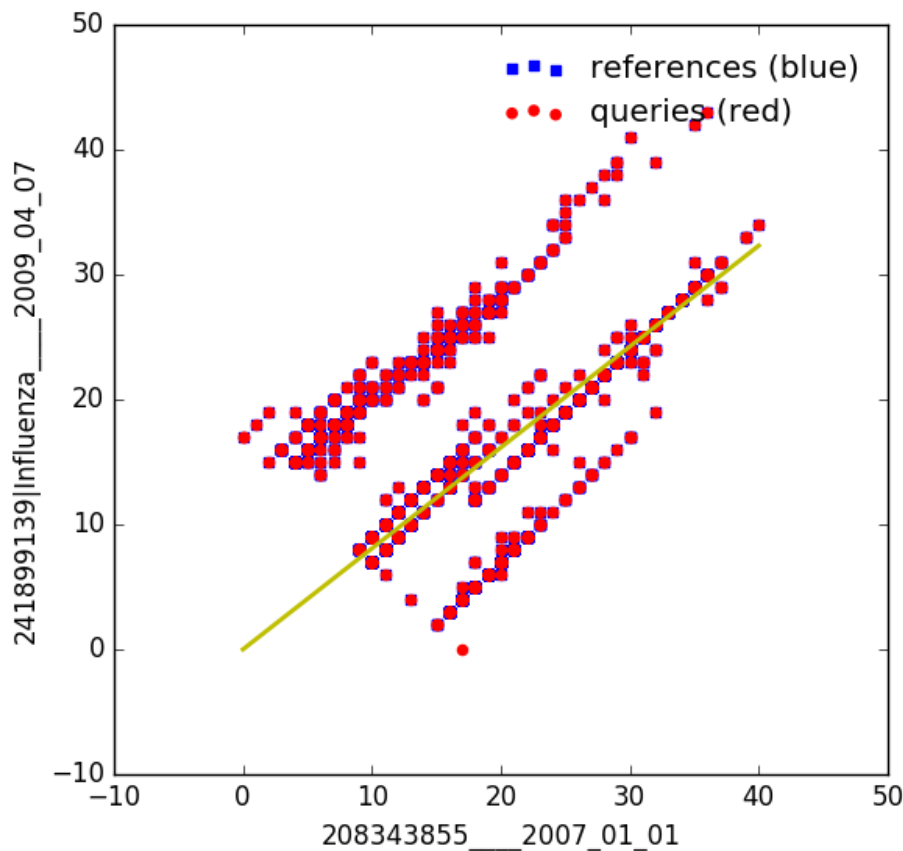
Example using cluster method to use two references as x and y axis

This is useful when you only have two references and no dates as all the sequences will be compared against these two sequences to give you a ‘clustered’ view

--refs is a fasta file that contains two references. The first being the x-axis and the second representing the y-axis
 --queries is a fasta file that contains multiple sequences that will be plotted against the --refs sequences

```
plot_muts --query tests/testinput/ha/refall.ha.fasta --refs tests/testinput/ha/refall.ha.fasta --clus
```

Example Output



Generating html graphics that are interactive

For both --cluster and non-cluster graphics you can optionally supply --html which will utilize the bokeh python project to build an interactive html output that you can open in your web browser.

1.2.9 fasta

fasta is a very simple script to help mangle fasta files.

- Supports converting multiline sequences into single line
- Supports splitting fasta file into separate files each named after the identifier
- Supports disambiguating ambiguous sequences

Usage

```
fasta --help
```

Examples

The following examples all use the test fasta file found under `tests/testinput/col.fasta`

```
>sequence1 some description !@#$$%^&*()_+=[ ]{}.,></?';:"
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT
GGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGG
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
>sequence2!@#$$%^&*()_+=[ ]{}.,></?';:"
AAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAAA
TTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTTT
GGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGGG
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
```

Convert column fasta into single lines

The following is a simple shell pipeline using fasta to ensure all sequences are on one line

```
$> cat tests/testinput/col.fasta | fasta -
```

Or if you want to you can read straight from a fasta file

```
$> fasta tests/testinput/col.fasta
```

Convert single line fasta into column fasta

The following would convert single line fasta sequences into column formatted fasta. It defaults to using 80 characters for each column

```
$> fasta tests/testinput/col.fasta
```

You can verify that it is wrapping correctly by simply piping the fasta command back into itself and then comparing to the original input file.

Here you can see we do that and then use diff to show there is no difference between the original file(`col.fasta`) and the new one(`newline.fasta`)

```
$> cat tests/testinput/col.fasta | fasta - | fasta --wrap - > newfile.fasta
$> diff tests/testinput/col.fasta newfile.fasta
```

There will be no output as there is no difference between `newfile.fasta` and `tests/testinput/col.fasta`

Simple shell pipeline using fasta

The following is a simple shell pipeline to count how many A's there are in the sequence lines. There should be 160 since col.fasta is 80 characters per line and only the first line of each sequence has A and there are 2 sequences.

```
$> fasta tests/testinput/col.fasta | grep -v '>' | grep -Eo '[Aa]' | wc -l
160
```

Split fasta file into separate files named after identifiers

The following example shows how you can split a fasta file into multiple fasta files each named after an identifier in the original

```
$> fasta tests/testinput/col.fasta --split
$> ls -l *.fasta
sequence1.fasta
sequence2_____.fasta
```

Note The reason sequence2 has such a long name is because it is replacing all punctuation characters with underscores. col.fasta is a test file that has a bunch of punctuation, hence all the underscores.

Similar to above, you can use input from standard input as the fasta input file

```
$> cat tests/testinput/col.fasta | fasta --split -
$> ls -l *.fasta
sequence1.fasta
sequence2_____.fasta
```

Disambiguate ambiguous sequences

You can turn sequences that have ambiguous bases in them into all permutations of the same sequence with the ambiguous bases turned into non-ambiguous bases.

There is an upper limit of 100 for how many sequences can be generated to avoid creating thousands of sequences or consuming all of your computer's RAM.

If a sequence would generate more than 100 sequences, it will generate a message such as:

```
Sequence too_many has 7 ambiguous bases that would produce 128 permutations and was skipped
```

and it will be skipped.

```
$> fasta --disambiguate tests/testinput/ambiguous.fasta > disambiguous.fasta
```

1.3 AMOS

AMOS is a file format that is similar to any assembly file format such as ACE or SAM. It contains information about each read that is used to assemble each contig.

The format is broken into different message blocks. For the Ray assembler, it produces an AMOS file that is broken into 3 types of message blocks

- RED

```
{RED
iid:\d+
eid:\d+
seq:
[ATGC]+
.
qlt:
[A-Z]+
}
```

iid Integer identifier

eid Same as iid?

seq Sequence data

qlt Should be quality, but is only a series of D's from Ray assembler

- TLE

```
{TLE
src:\d+
off:\d+
clr:\d+, \d+
}
```

src RED iid that was used

off One would think offset, but unsure what it actually means

clr Not sure what this is either

- CTG

```
{CTG
iid:\d+
eid:\w+
com:
.*$
.
seq:
[ATGC]+
.
qlt:
[A-Z]+
.
{TLE
...
}
}
```

iid integer id of contig

eid contig name

com Communication software that generated this contig

seq Contig sequence data

qlt Supposed to be contig quality data, but for Ray it only produces D's

TLE 0 or more TLE blocks that represent RED sequences that compose the contig

1.3.1 Parsing

bio_bits contains an interface to parse a given file handle that has been opened on an AMOS file.

To read in the AMOS file you simply do the following

```
from bio_bits import amos
a = None
with open('AMOS.afg') as fh:
    a = amos.AMOS(fh)
```

CTG

To get information about the contigs(CTG) you can access the `.ctgs` attribute. The contigs are indexed based on their iid so to get the sequence of contig iid 1 you would do the following:

```
ctg = a.ctgs[1]
seq = ctg.seq
```

To retrieve all the reads(RED) that belong to a specific contig:

```
reads = []
for tle in ctg.tlelist:
    reads.append(a.reds[tle.src])
```

RED

To get information about the reads(RED) you can access the `.reds` attribute. The reds are indexed based on their iid so to get the sequence of red iid 1 you would do the following:

```
red = a.reds[1]
seq = red.seq
```

If you want to convert a RED entry into anything you can use the `.format` method. The `.format` method allows you to utilize any of the properties of a RED object such as `.iid`, `.eid`, `.seq`, `.qlt`. You can see in the examples below how to do this.

1.3.2 Examples

Here is an example of how to convert all RED blocks into a single fastq file

```
from bio_bits import amos

# Fastq format string
fastq_fmt = '@{iid}\n{seq}\n+\n{n}{qlt}'

with open('amos.fastq', 'w') as fh_out:
    with open('AMOS.afg') as fh_in:
        for iid, red in amos.AMOS(fh_in).reds.items():
            fq = red.format(fastq_fmt)
            fh_out.write(fq + '\n')
```

1.4 CHANGELOG

1.4.1 Version 1.4.0

- Switched to conda install
- Added continuous delivery

1.4.2 Version 1.3.2

- fasta added `--disambiguate` option to turn ambiguous sequences into all permutations possible

1.4.3 Version 1.3.1

- plot_muts added `--cluster` and `--html` options
- fasta added `--split` and `--wrap` options

1.4.4 Version 1.3.0

- Added fasta script that removes newlines from fasta sequences

1.4.5 Version 1.2.1

- Fixed some python3 and python2.6 incompatibility issues
- Fixed some old bio_pieces references
- Added some simple tests for plot_muts

1.4.6 Version 1.2.0

- Renamed project to bio_bits to fix naming issue with other project
- GPL License added
- degen_regions script added
- parallel_blast added
- plot_muts script added

1.4.7 Version 1.1.0

- Renamed parse_contigs to group_references to better name functionality
- group_references now supports bam files

1.4.8 Version 1.0.0

- Version bump. Starting here we will employ semantic versioning
- Added version script to get version from project

1.4.9 Version 0.1.0

- Started project over to setup for Continuous Integration testing
- Added rename_fasta that can rename fasta sequence identifiers based on a input rename file
- Added travis, coveralls, readthedocs
- Added amos file parser that is specific to Ray assembler amos format
- Added format functionality for amos classes such that it is easy to convert to different formats
- Added amos2fastq to pull sequences out of AMOS files organized by their contigs.
- Added vcfcats.py, a commandline app for filtering and comparing vcf files.
- Completed documentation for vcfcats
- Added beast_checkpoint script and documentation
- Added beast_wrapper script that prints estimated time column in beast output
- Added beast_est_time script that allows you to easily get estimated time left from already running beast run

1.5 TODO

Todo

Could be possible to get beast_checkpoint to check for that scenario and use the last tree state that matches the last log state

(The original entry is located in /home/docs/checkouts/readthedocs.org/user_builds/bio-bits/checkouts/latest/docs/scripts/beast_checkpoint.rst, line 52.)

Indices and tables

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