ECOL 553L

Section 5
Command line tools for Genomic Data Analysis

Turning in your homework

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- within this folder, make a folder called `homework1`

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- make a file within this folder called *`<last_name>_<first_initial>`*`.txt` and put the homework answers in it

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- within this folder, make a folder called `homework1`
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- when finished move back to `~/ecol553_homework` and run `turnin homework1`

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If you run this more than once, it will overwite your old submittion

Web BLAST

nucleotide blast	Search **nucleotide** database using a **nucleotide** query *Algorithms:* blastn, megablast, discontiguous megablast
protein blast	Search **protein** database using a **protein** query *Algorithms:* blastp, psi-blast, phi-blast, delta-blast
blastx	Search **protein** database using a **translated nucleotide** query
tblastn	Search **translated nucleotide** database using a **protein** query
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Web BLAST

- First you have to pick the blast protocol

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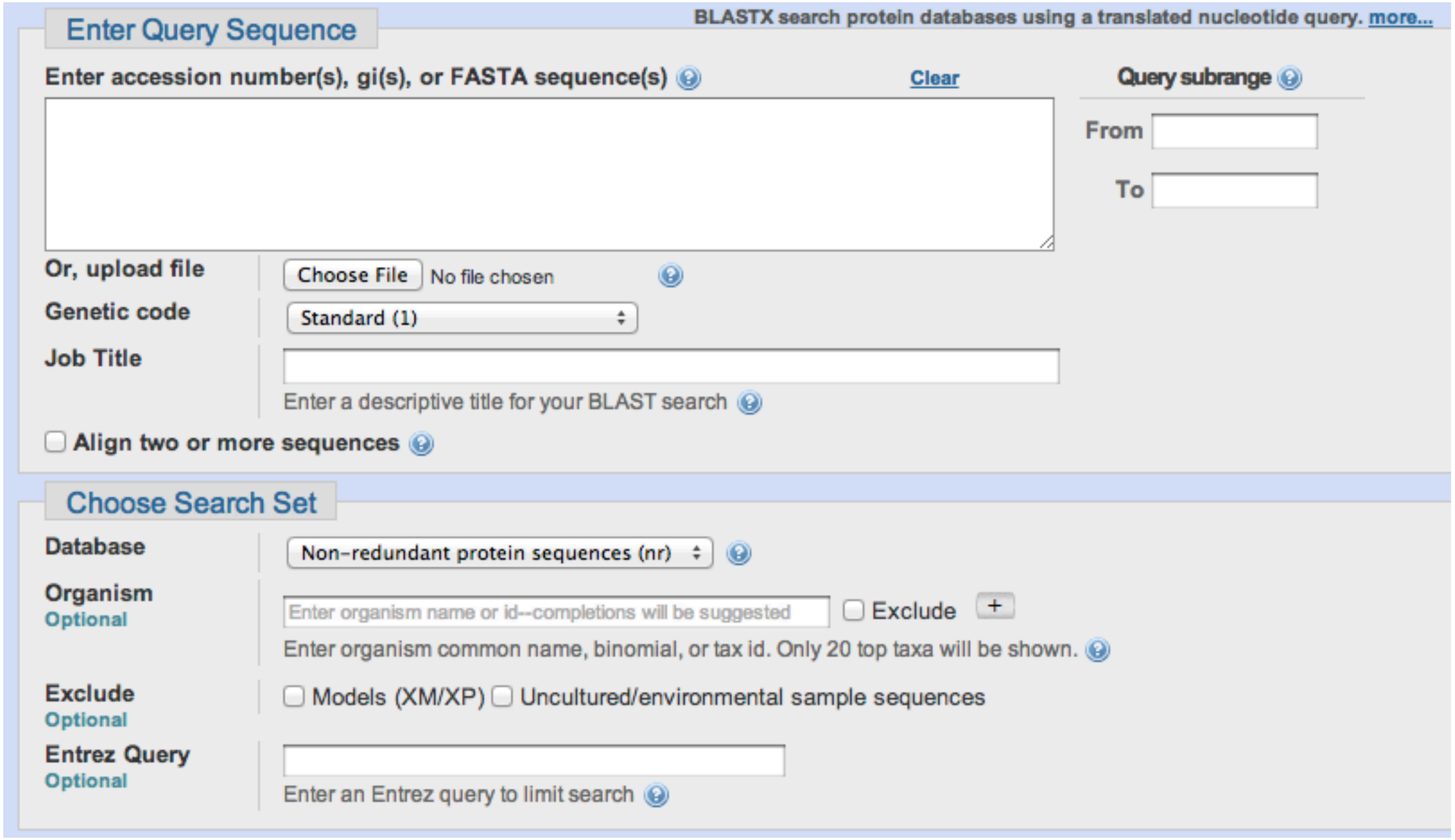
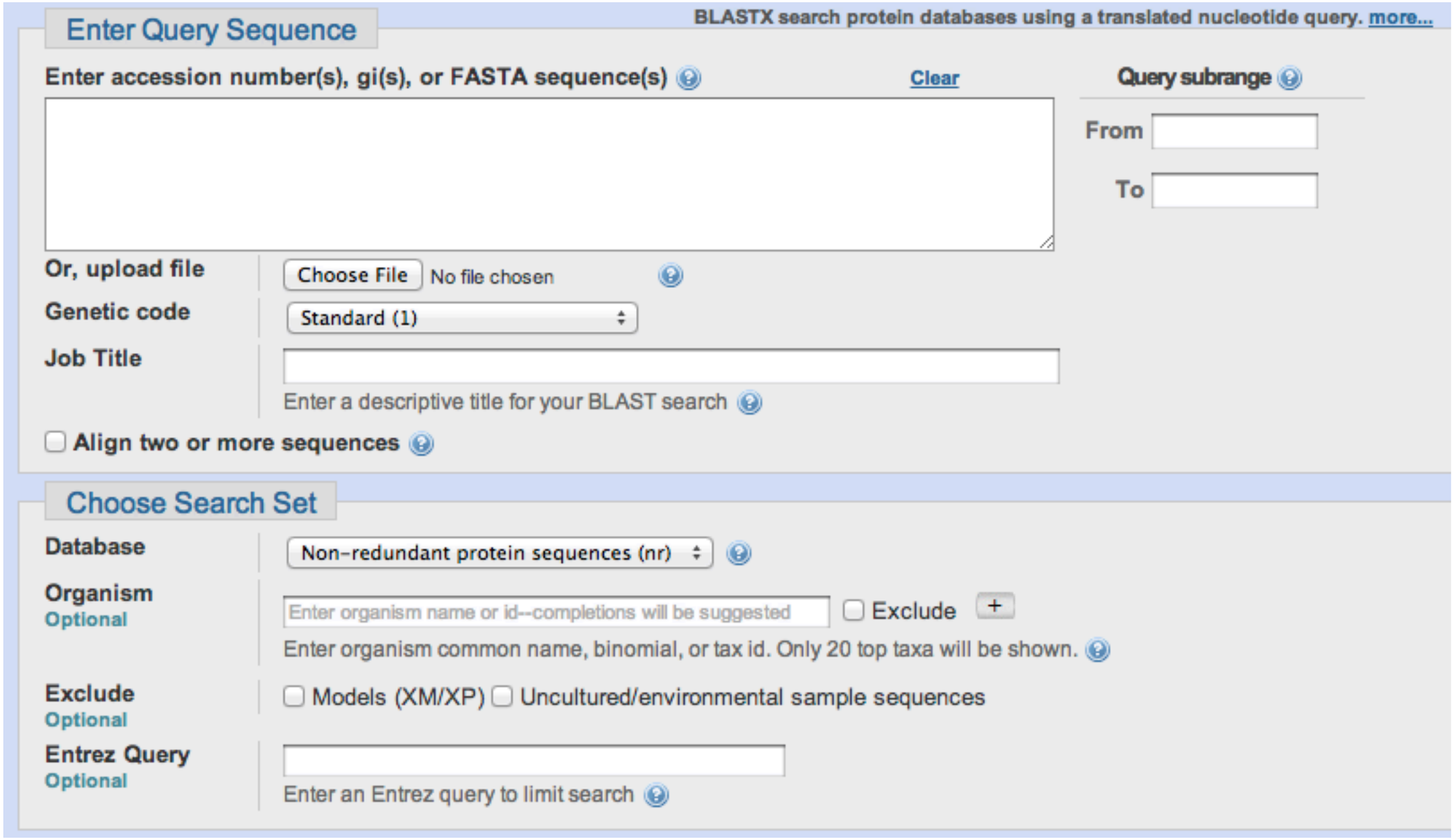
Web BLAST

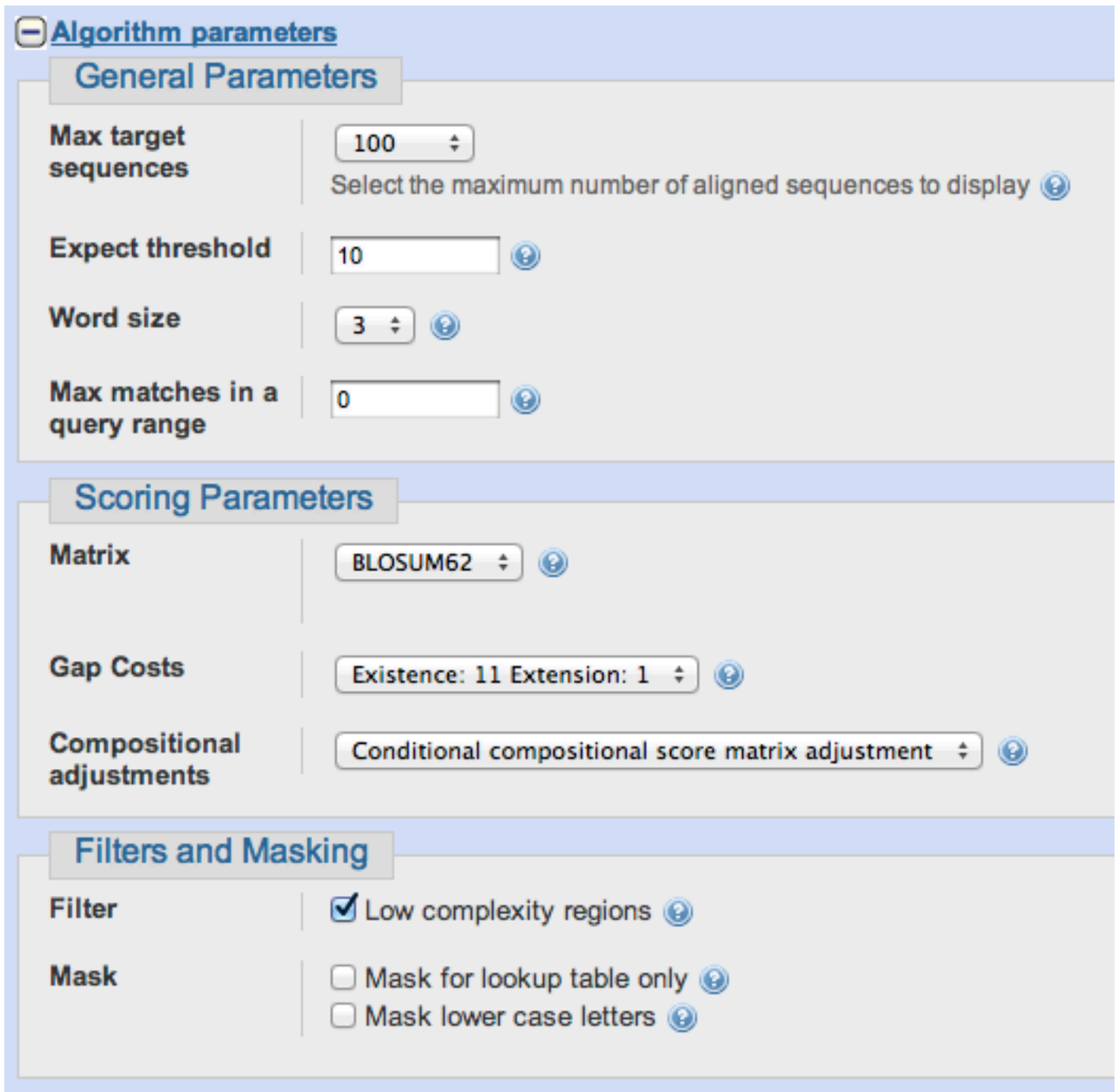

Enter Query Sequence
BLASTX search protein databases using a translated nucleotide query. more...
Enter accession number(s), gi(s), or FASTA sequence(s)
Clear
Query subrange
From
To
Or, upload file
Choose File
No file chosen
Genetic code
Standard (1)
Job Title
Enter a descriptive title for your BLAST search
Align two or more sequences
Choose Search Set
Database
Non-redundant protein sequences (nr)
Organism
Optional
Enter organism name or id--completions will be suggested
Exclude
+
Enter organism common name, binomial, or tax id. Only 20 top taxa will be shown.
Exclude
Optional
Models (XM/XP)
Uncultured/environmental sample sequences
Entrez Query
Optional
Enter an Entrez query to limit search

Web BLAST

- Input our data

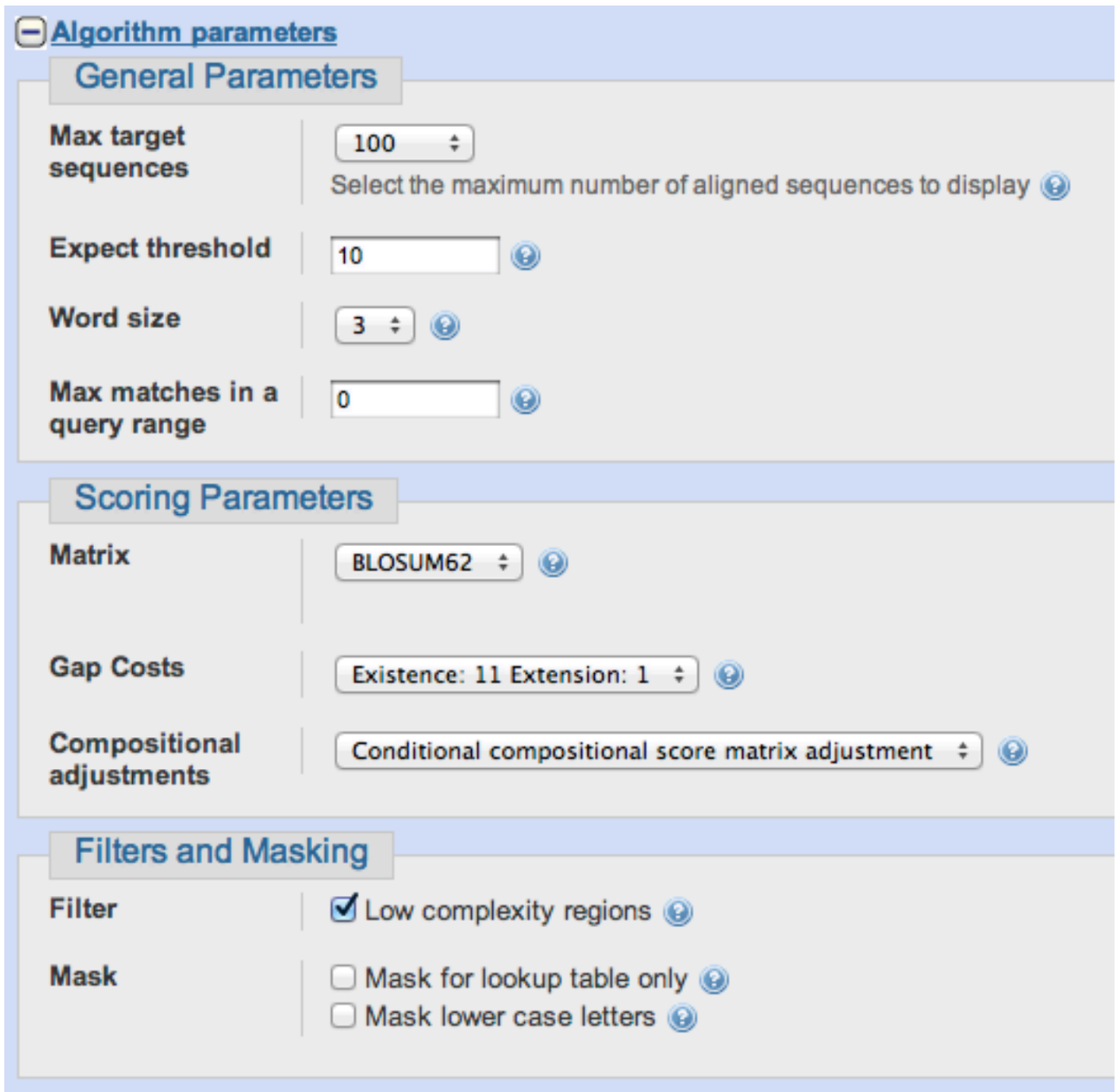


Web BLAST


Algorithm parameters
General Parameters
Max target sequences
100
Select the maximum number of aligned sequences to display
Expect threshold
10
Word size
3
Max matches in a query range
0
Scoring Parameters
Matrix
BLOSUM62
Gap Costs
Existence: 11 Extension: 1
Compositional adjustments
Conditional compositional score matrix adjustment
Filters and Masking
Filter
Low complexity regions
Mask
Mask for lookup table only
Mask lower case letters

Web BLAST

- Then you have to change the settings



DO THIS NO MORE

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  - Save Settings

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  - Not Know How Long Till It Starts/Finishes Running

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  - Not Know How Long Till It Starts/Finishes Running
  - Use A Web Browser (or your mouse)

Modules on the HPC

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  - `module avail` shows the available packages

Modules on UPG

```
deblasio@service2(login):~/ParamAdvising/core_column_svm> module avail

------------------------------------------------------ /usr/share/Modules/modulefiles ------------------------------
chkfeature  dot         module-cvs  module-info modules     mpt/2.04    null        perfboost   perfcatcher use.own

------------------------------------------------------------ /uaopt/modulefiles ------------------------------------
R/2.14.1                        exonerate/2.2                   lapack/3.4.0                    quake/0.3.0
abaqus/6.11                     fastqc/0.10.0                   lastz/1.02.00                   raxml/7.2.8
abaqus/6.9                      fftw/2.1.5                      mafft/6.923                     roche454/2.6
abyss/1.3.2                     fftw/3.3                        mathematica/8.0                 ruby/1.9.3-p0
abyss/1.3.4-kmer64              gaussian/g03-E.01               matlab/r2012a                   samtools/0.1.18
abyss/1.3.4-kmer96              gaussian/g09                    mcnp5                           seqtools/4.13.2-2-g0a83
ansys/14.0                      gnuplot/4.6.0                   mcnpx/2.6.0                     soapdenovo/1.05
apbs/1.3                        gotoblas2                       meep/1.1.1                      sparsehash/1.12
augustus/2.6.1                  grace/5.1.22                    mercurial/2.2                   tandemrepeatsfinder/4.04
autodock/4.3.2                  graphviz/2.28.0                 mothur/1.23.1                   tex/2011
bamtools/1.0.2                  gromacs/4.5.5                   mothur/1.26.0                   tophat/2.0.4
blas                            gsl/1.15                        mpich2/1.4.1p1                  trans-abyss/1.3.2
blast/ncbi-2.2.26               hdf5/1.8.8                      mrbayes/3.2.1                   trinity/r2012-03-17
blat/34                         hmmer/3.0                       muscle/3.8.31                   trinity/r2012-05-18
boost/1.48.0                    intel/2012.0.032                ncl/6.0.0                       vasp/4.6
bowtie2/2.0.0-b5                intel-mpi/2012.0.032(default)   netcdf/4.1.3                    vasp/5.2
bwa/0.6.1                       intel-mpi/2012.0.032-ia32       netcdf/4.1.3-intel              velvet/1.2.02
cd-hit/4.5.4                    irods/3.0                       nwchem/6.0                      velvet/1.2.07
clustalw/2.1                    java/1.6.0                      oases/0.2.08                    xtandem/10-12-01-1
cmake/2.8.9                     java/1.7.0                      openmpi/1.4.4
emboss/6.4.0                    lammps/20apr12                  perl/5.14.2
espresso/4.3.2                  lammps/30aug12                  python/2.7.3
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- The programs associated with that package are now available

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Using Command Line BLAST

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  - Generate Database

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Generating a BLAST Database

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- `tblastx`: compares the six-frame translations of a nucleotide query sequence against the six-frame translations of a nucleotide sequence database. Note that `tblastx` program cannot be used with the nr database on the BLAST Web page.

Searching Your New Database

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[t]blast[xnp] -db <dbTitle> -query <input_file>
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- If command lines are very long, such as `blastall` with many options, you can continue across several lines by placing a backslash (`\`) at the end of each line

Sample PBS Batch Submit File to run BLAST

```
#!/bin/sh
#PBS -N test_blast
#PBS -m bea
#PBS -M myEmail@email.arizona.edu
#PBS -W group_list=myGroup
#PBS -q standard
#PBS -l select=1:ncpus=12:mem=24Gb
#PBS -l cput=96:0:0
#PBS -l walltime=24:0:0

module load blast

cd ~deblasio/blast_dir
time blastn –db  /genome/nt -query seqs.fasta -out seqs.bln \
-evalue 1e-30 -num_descriptions 20 -num_alignments 20 \
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Where my group is your PIs netid

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Notice that the number of processors requested (8) in one more than the num_threads option. Also, the `nt` database requires a lot of memory!

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Submitting and Monitoring PBS Jobs

```
qsub <run_blast.sh>
```

```
qstat -a
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- To view the queue of PBS Jobs, run the command

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```

Submitting and Monitoring PBS Jobs

- To submit a PBS job, use the qsub command with your PBS script as the argument
  - PBS will return a job number

```
qsub <run_blast.sh>
```

- To view the queue of PBS Jobs, run the command

```
qstat -a
```

- To see details about a running job, use:

```
qstat -f <JobNumber> | more
```

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- Look at the .o file to see how much CPU time your PI's group was charged for the run and how much time remains in your group's monthly allocation.