S1 PlasClass documentation

PlasClass is fully documented at https://github.com/Shamir-Lab/PlasClass. We outline the installation and usage instructions here.

Installing PlasClass

PlasClass is written in Python3 and requires NumPy and scikit-learn. To install PlasClass do:

```
git clone https://github.com/Shamir-Lab/PlasClass.git
cd PlasClass
python setup.py install
```

We recommend using a virtual environment.

After installation, run the tests to see that PlasClass is installed and working correctly on your system:

```
python test/test.py
```

Classifying sequences in a fasta file

The classify_fasta.py script can be used to classify the sequences in a fasta file. It is invoked as follows:

```
python classify_fasta.py -f <input file> [-o <output file>] [-p <# processes>]
```

The required option is:

- `-f/--fasta`: String - the fasta file to be classified.

The two optional options are:

- `-o/--outfile`: String - the name of the output file.
  Default: `<in>.probs.out` (<in> is the path to the fasta file).
- `-p/--num_processes`: Integer - the number of processes to use. Default: 8.
The output file is a tab separated file with each line containing a sequence header and the corresponding score. The sequences are in the same order as in the input fasta file.

**Calling the PlasClass module**

The classifier can also be imported and called directly in a Python program. For example, once the `plasclass` module has been installed the following lines of code can be used:

```python
from plasclass import plasclass
my_classifier = plasclass()
my_classifier.classify(seqs)
```

The `plasclass()` constructor takes 3 optional parameters:

- `n_procs`: Integer - Number of processes to use (default: 1)
- `scales`: Integer array - Scales of the sequence length bins (default: `[1000,10000,100000,500000]`)
- `ks`: Integer array - Values of the k-mer lengths to use (default: `[3,4,5,6,7]`)

The sequence(s) to classify, `seqs`, can be either a single string or a list of strings. The strings must be uppercase. The function `plasclass.classify(seqs)` returns a list of plasmid scores, one per input sequence, in the same order as the input.

**Training PlasClass models**

The user can train models by providing two fasta files with plasmid and bacterial reference sequences to the `train.py` script. Required options are:

- `-p/--plasmid`: String - the fasta file of the plasmid references.
- `-c/--chromosome`: String - the fasta file of the chromosome references.
- `-o/--outdir`: String - the path of the output directory.

Default: directory of script.

The optional options are:
- **-n/--num_processes**: Integer - the number of processes to use.
  
  Default: 16.

- **-k/--kmer**: String - comma separated list of the k-mer sizes to use.
  
  Default: 3,4,5,6,7.

- **-l/--lengths**: String - comma separated list of the sequence lengths to use.
  
  Default: 1000,10000,100000,500000.

The models will be created in the output directory and should be put into the `data` directory of the PlasClass module to be used. Note that if k-mer and sequence lengths other than the default are used, then these must be specified when calling the `plasclass()` constructor.