Developing a Python package

An overview of functionality and tools

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Topics

Why make a Python package?

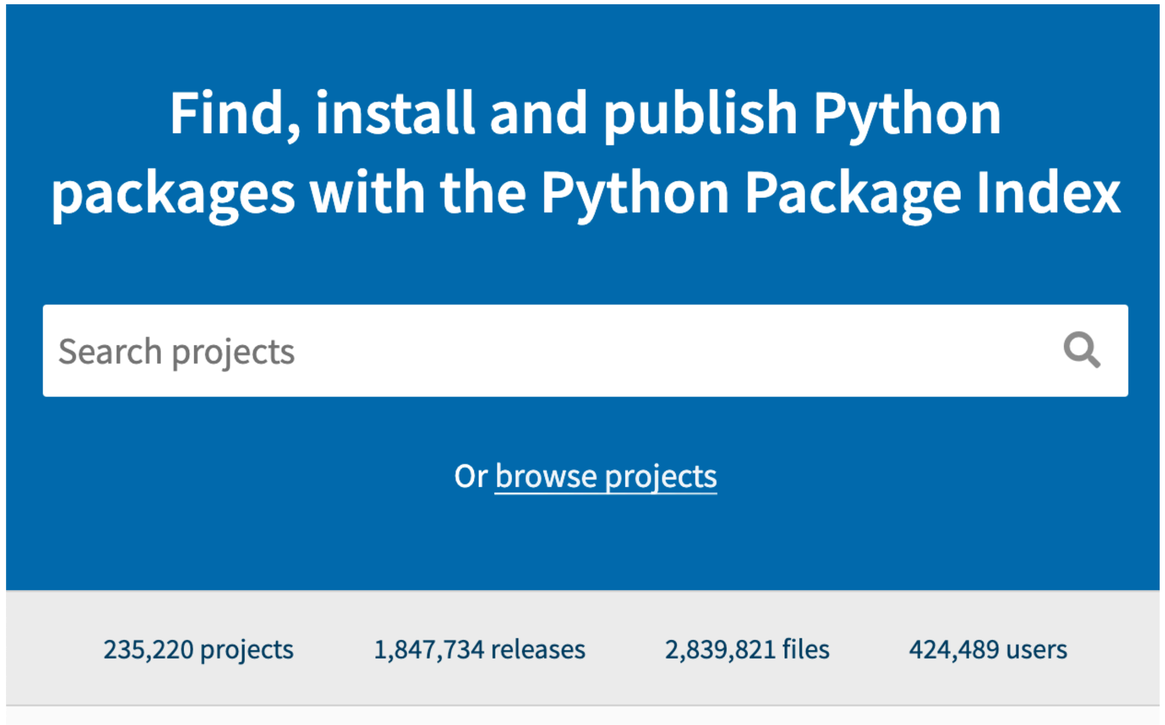
Command line vs. import

Testing

Documentation

Why Python package?

- Multiple options to distribute (GitHub, PyPI, etc.)
- Users can automatically install package and its dependencies
- Standardized structure for important parts of complex software
- Turning existing code into a package: not as much extra work as it may seem!



Your package can be imported...

in demask/homologs.py:

```python
def find_homologs(
    seqfile: str,
    blastp: str,
    db: str,
    threads: int = 1,
    evalue_cutoff: float = 0.01,
    bitscore_cutoff: float = None,
    nseqs: int = 300,
    outfile: str = None,
    outdir: str = None,
):
    """Find protein homologs using blastp.

    For each query sequence, an output file in a2m (FASTA) format will
    be produced containing the query sequence and the most similar
    homologs up to a specified number (default 300).

    Args:
```

user script:

```python
from demask.homologs import find_homologs

find_homologs("seq.fa", "blastp", "/path/to/db", outfile="homologs.a2m")
```

...or it can be run from the command line

in demask/homologs.py:

```
if __name__ == "__main__":
    args = parse_args()
    del args.config
    find_homologs(**vars(args))
```

```
dan@laptop ~> python3 -m demask.homologs -s seq.fa -o homologs.a2m
```

Tailor for scripts vs. command line.

e.g. function inputs and output are Python objects, but it can read/write files instead if run from command line:

```
if __name__ == "__main__":
    args = parse_args()
    outfile = args.outfile
    if outfile is None:
        inbase, inext = os.path.splitext(args.infile)
        outext = ".txt" if inext != ".txt" else "_demask.txt"
        outfile = inbase + outext
    del args.config, args.outfile
    predictions = run_demask(**vars(args))
    with open(outfile, "w") as out:
        out.write("\t".join(["pos", "WT", "var", "score"]) + "\n")
        for pred in predictions:
            out.write("{}\t{}\t{}\t{:.4f}\n".format(*pred))
```

Unit testing with unittest

```python
class TestProfiles(unittest.TestCase):
    def test_get_weights(self):
        seqs = read_fasta("test/P46937.a2m", as_dict=False)
        aln = seq_matrix(seqs)[:, 1:]
        wts = get_weights(aln)
        self.assertTrue(np.all(wts > 0) and np.all(wts < 1))

    def test_get_aligned_profile(self):
        # Ensure sum of each row of output array is > 0 and <= 1.
        seqs = read_fasta("test/P46937.a2m", as_dict=False)
        aln = seq_matrix(seqs)[:, 1:]
        wts = get_weights(aln)
        profile = get_aligned_profile(aln, wts)
        sums = np.sum(profile, axis=1)
        self.assertTrue(np.all(sums > 0) and np.all(sums <= 1.00))

    def test_gaps_in_query(self):
        # demask should accept gaps in query, e.g. for true MSA input.
        seqs1 = read_fasta("test/test_aln_ungapped.a2m", as_dict=False)
        aln1 = seq_matrix(seqs1)
        seqs2 = read_fasta("test/test_aln_gapped.a2m", as_dict=False)
        aln2 = seq_matrix(seqs2)
        self.assertTrue(aln1.shape == aln2.shape and np.all(aln1 == aln2))

    def test_no_homologs(self):
        seqs = read_fasta("test/random.a2m", as_dict=False)
        aln = seq_matrix(seqs)[:, 1:]
        wts = get_weights(aln)
        profile = get_aligned_profile(aln, wts)
        self.assertTrue(np.all(profile == 1/20))


class TestPredict(unittest.TestCase):
    def setUp(self):
        self.seqs = read_fasta("test/P46937.a2m", as_dict=False)
```

```
dan@laptop ~/d/DeMaSk (master)> python3 test.py
...........F.F..
======================================================================
FAIL: test_compute_scores_string (__main__.TestPredict)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "test.py", line 129, in test_compute_scores_string
    self.assertEqual(len(predictions), len(self.seqs[0]) * 18)
AssertionError: 9576 != 9072

======================================================================
FAIL: test_get_aligned_profile (__main__.TestProfiles)
----------------------------------------------------------------------
Traceback (most recent call last):
  File "test.py", line 98, in test_get_aligned_profile
    self.assertTrue(np.all(sums > 0) and np.all(sums <= 1.00))
AssertionError: False is not true

----------------------------------------------------------------------
Ran 16 tests in 0.872s

FAILED (failures=2)
dan@laptop ~/d/DeMaSk (master) [1]>
```

```
dan@laptop ~/d/DeMaSk (master)> python3 test.py
................
----------------------------------------------------------------------
Ran 16 tests in 1.022s

OK
dan@laptop ~/d/DeMaSk (master)>
```

Command line help with argparse or configargparse

```python
def parse_args():
    p = configargparse.ArgParser(
        description=(
            "Predict fitness impact of all possible substitutions in "
            "a query protein."
        )
    )
    p.add(
        "-i",
        "--infile",
        required=True,
        help=(
            "Name of the file containing a sequence alignment in A2M (FASTA)
            "format, with the query protein as the first sequence."
        ),
    )
    p.add("-o", "--outfile", default=None, help="Name of new file to write sc
    dirname = os.path.dirname(__file__)
    config = os.path.join(dirname, "..", "config.ini")
    p.add(
        "-c",
        "--config",
        is_config_file=True,
        metavar="FILE",
        default=config,
        help=("Configuration file.  Defaults to 'config.ini' in the demask di
    )
    matrix = os.path.join(dirname, "..", "data", "matrix.txt")
    p.add(
        "-m",
        "--matrix",
        metavar="FILE",
        default=matrix,
        help=(
            "File containing the directional substitution matrix.  "
            "Defaults to the file at 'demask/data/matrix.txt'."
        ),
```

```
[dan@laptop ~> python3 -m demask.predict -h
usage: predict.py [-h] -i INFILE [-o OUTFILE] [-c FILE] [-m FILE]
                  [--coefs FILE] [-n NSEQS] [-w WEIGHT_THRESHOLD]

Predict fitness impact of all possible substitutions in a query protein. Args
that start with '--' (eg. -i) can also be set in a config file (specified via
-c). Config file syntax allows: key=value, flag=true, stuff=[a,b,c] (for
details, see syntax at https://goo.gl/R74nmi). If an arg is specified in more
than one place, then commandline values override config file values which
override defaults.

optional arguments:
  -h, --help            show this help message and exit
  -i INFILE, --infile INFILE
                        Name of the file containing a sequence alignment in
                        A2M (FASTA) format, with the query protein as the
                        first sequence.
  -o OUTFILE, --outfile OUTFILE
                        Name of new file to write scores to.
  -c FILE, --config FILE
                        Configuration file. Defaults to 'config.ini' in the
                        demask directory.
  -m FILE, --matrix FILE
                        File containing the directional substitution matrix.
                        Defaults to the file at 'demask/data/matrix.txt'.
  --coefs FILE          File containing the intercept, entropy, and identity
                        coefficients. Defaults to the file at
                        'demask/data/coefficients.txt'.
  -n NSEQS, --nseqs NSEQS
                        Maximum number of supporting sequences per query
                        sequence. Defaults to 300.
  -w WEIGHT_THRESHOLD, --weight_threshold WEIGHT_THRESHOLD
                        Sequence identity threshold used for sequence
                        weighting
```

Documentation with Sphinx

```python
def run_demask(
    infile: str,
    matrix: str,
    coefs: str,
    nseqs: int = 300,
    weight_threshold: float = 0.8,
) -> list:
    """Predict fitness for all substitutions in a query sequence.

    Args:
        infile: Name of the file containing a sequence alignment in
          A2M (FASTA) format, with the query protein as the first
          sequence.
        matrix: Name of the file containing the directional
          substitution matrix.
        coefs: Name of the file containing the intercept, entropy, and
          identity coefficients, with one name and value, separated by
          a tab, per line.
        nseqs: Maximum number of sequences in the alignment to use.
          Sequence weights can take a long time to compute for huge
          sequence counts.
        weight_threshold: Sequence identity threshold used for
          sequence weighting.  Sequences are weighted by the inverse
          of the number of sequences within this percent identity.

    Returns:
        A list of tuples, each containing the position, WT AA, variant
        AA, and score for each prediction.

    """
    seqs = read_fasta(infile, as_dict=False)
    seqs = seqs[: min(len(seqs), nseqs + 1)]  # +1 for query.
    aligned = seq_matrix(seqs)
    query = aligned[:, 0].T  # Query seq minus any gaps
```

demask.predict.run_demask(*infile, matrix, coefs, nseqs=300, weight_threshold=0.8*)

Predict fitness for all substitutions in a query sequence.

Parameters

- **infile** (`str`) – Name of the file containing a sequence alignment in A2M (FASTA) format, with the query protein as the first sequence.
- **matrix** (`str`) – Name of the file containing the directional substitution matrix.
- **coefs** (`str`) – Name of the file containing the intercept, entropy, and identity coefficients, with one name and value, separated by a tab, per line.
- **nseqs** (`int`) – Maximum number of sequences in the alignment to use. Sequence weights can take a long time to compute for huge sequence counts.
- **weight_threshold** (`float`) – Sequence identity threshold used for sequence weighting. Sequences are weighted by the inverse of the number of sequences within this percent identity.

Return type

`list`

Returns

A list of tuples, each containing the position, WT AA, variant AA, and score for each prediction.

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Branch: master ▾ algographics / docs /

Dan and Dan Moved some functions into extras subp

..	
_build	Moved some function
_static/png	Moved some function
API.rst	Moved some function
Makefile	Moved some function
conf.py	Moved some function
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Colors

Colors are represented as objects of the
HSL (hue, saturation, lightness) color sp

```
outline = ag.Circle(c=(200, 200), r=
color = ag.Color(
    hue=ag.Uniform(min=0.6, max=0.8)
)
x = ex.fill_spots(outline)
ag.set_styles(x, "fill", color)
```

Resources

- Testing Python code: https://docs.python-guide.org/writing/tests/
- Sphinx: https://www.sphinx-doc.org/
- Read the Docs: https://readthedocs.org/
- Documentation guide: https://docs.python-guide.org/writing/documentation/
- Python Package Index: https://pypi.org/