
ODDT Documentation

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Installation

1.1 Requirements

- Python 2.7.x
- OpenBabel (2.3.2+) or/and RDKit (2014.03)
- Numpy (1.8+)
- Scipy (0.13+)
- Sklearn (0.13+)
- ffnet (0.7.1+) only for neural network functionality.
- joblib (0.8+)

Note: All installation methods assume that one of toolkits is installed. For detailed installation procedure visit toolkit's website (OpenBabel, RDKit)

Most convenient way of installing ODDT is using PIP. All required python modules will be installed automatically, although toolkits, either OpenBabel (`pip install openbabel`) or RDKit need to be installed manually

```
pip install oddt
```

If you want to install cutting edge version (master branch from GitHub) of ODDT also using PIP

```
pip install git+https://github.com/oddt/oddt.git@master
```

Finally you can install ODDT straight from the source

```
wget https://github.com/oddt/oddt/archive/0.1.1.tar.gz
tar zxvf 0.1.1.tar.gz
cd oddt-0.1.1/
python setup.py install
```

1.2 Common installation problems

ffnet requires numpy.distutils during installation, and you are trying to install ffnet without numpy. You have to install numpy first.

```
pip install numpy
```

Then you can install ODDT

```
pip install oddt
```

Usage Instructions

You can use any supported toolkit united under common API (for reference see [Pybel](#) or [Cinfony](#)). All methods and software which based on Pybel/Cinfony should be drop in compatible with ODDT toolkits. In contrast to it's predecessors, which were aimed to have minimalistic API, ODDT introduces extended methods and additional handles. This extensions allow to use toolkits at all it's grace and some features may be backported from others to introduce missing functionalities. To name a few:

- coordinates are returned as Numpy Arrays
- atoms and residues methods of Molecule class are lazy, ie. not returning a list of pointers, rather an object which allows indexing and iterating through atoms/residues
- Bond object (similar to Atom)
- *atom_dict*, *ring_dict*, *res_dict* - comprehensive Numpy Arrays containing common information about given entity, particularly useful for high performance computing, ie. interactions, scoring etc.
- lazy Molecule (asynchronous), which is not converted to an object in reading phase, rather passed as a string and read in when underlying object is called
- pickling introduced for Pybel Molecule (internally saved to mol2 string)

2.1 Atom, residues, bonds iteration

One of the most common operation would be iterating through molecules atoms

```
mol = oddt.toolkit.readstring('smi', 'ClCCCCl')
for atom in mol:
    print atom.idx
```

Note: mol.atoms, returns an object (AtomStack) which can be access via indexes or iterated

Iterating over residues is also very convenient, especially for proteins

```
for res in mol.residues:
    print res.name
```

Additionally residues can fetch atoms belonging to them:

```
for res in mol.residues:
    for atom in res:
        print atom.idx
```

Bonds are also iterable, similar to residues:

```
for bond in mol.bonds:
    print bond.order
    for atom in bond:
        print atom.idx
```

2.2 Reading molecules

Reading molecules is mostly identical to [Pybel](#).

Reading from file

```
for mol in oddt.toolkit.readfile('smi', 'test.smi'):
    print mol.title
```

Reading from string

```
mol = oddt.toolkit.readstring('smi', 'c1ccccc1 benzene'):
    print mol.title
```

Note: You can force molecules to be read in asynchronously, aka “lazy molecules”. Current default is not to produce lazy molecules due to OpenBabel’s Memory Leaks in OBConverter. Main advantage of lazy molecules is using them in multiprocessing, then conversion is spreaded on all jobs.

Reading molecules from file in asynchronous manner

```
for mol in oddt.toolkit.readfile('smi', 'test.smi', lazy=True):
    pass
```

This example will execute instantaneously, since no molecules were evaluated.

2.3 Numpy Dictionaries - store your molecule as an uniform structure

Most important and handy property of Molecule in ODDT are Numpy dictionaries containing most properties of supplied molecule. Some of them are straightforward, other require some calculation, ie. atom features. Dictionaries are provided for major entities of molecule: atoms, bonds, residues and rings. It was primarily used for interactions calculations, although it is applicable for any other calculation. The main benefit is marvelous Numpy broadcasting and subsetting.

Each dictionary is defined as a format in Numpy.

2.3.1 atom_dict

Atom basic information

- ‘coords’, type: float32, shape: (3) - atom coordinates
- ‘charge’, type: float32 - atom’s charge
- ‘atomicnum’, type: int8 - atomic number
- ‘*atomtype’, type: a4 - Sybyl atom’s type

- `'hybridization'`, type: `int8` - atoms hybridization
- `'neighbors'`, type: `float32`, shape: (4,3) - coordinates of non-H neighbors coordinates for angles (max of 4 neighbors should be enough)

Residue information for current atom

- `'resid'`, type: `int16` - residue ID
- `'resname'`, type: `a3` - Residue name (3 letters)
- `'isbackbone'`, type: `bool` - is atom part of backbone

Atom properties

- `'isacceptor'`, type: `bool` - is atom H-bond acceptor
- `'isdonor'`, type: `bool` - is atom H-bond donor
- `'isdonorh'`, type: `bool` - is atom H-bond donor Hydrogen
- `'ismetal'`, type: `bool` - is atom a metal
- `'ishydrophobe'`, type: `bool` - is atom hydrophobic
- `'isaromatic'`, type: `bool` - is atom aromatic
- `'isminus'`, type: `bool` - is atom negatively charged/chargable
- `'isplus'`, type: `bool` - is atom positively charged/chargable
- `'ishalogen'`, type: `bool` - is atom a halogen

Secondary structure

- `'isalpha'`, type: `bool` - is atom a part of alpha helix
- `'isbeta'`, type: `bool` - is atom a part of beta strand

2.3.2 ring_dict

- `'centroid'`, type: `float32`, shape: 3 - coordinates of ring's centroid
- `'vector'`, type: `float32`, shape: 3 - normal vector for ring
- `'isalpha'`, type: `bool` - is ring a part of alpha helix
- `'isbeta'`, type: `bool` - is ring a part of beta strand

2.3.3 res_dict

- `'id'`, type: `int16` - residue ID
- `'resname'`, type: `a3` - Residue name (3 letters)
- `'N'`, type: `float32`, shape: 3 - coordinates of backbone N atom
- `'CA'`, type: `float32`, shape: 3 - coordinates of backbone CA atom
- `'C'`, type: `float32`, shape: 3 - coordinates of backbone C atom
- `'isalpha'`, type: `bool` - is residue a part of alpha helix
- `'isbeta'`, type: `bool` - is residue a part of beta strand

Note: All aforementioned dictionaries are generated “on demand”, and are cached for molecule, thus can be shared between calculations. Caching of dictionaries brings incredible performance gain, since in some applications their generation is the major time consuming task.

Get all acceptor atoms:

```
mol.atom_dict['is_acceptor']
```

ODDT API documentation

3.1 oddt package

3.1.1 Subpackages

oddt.docking package

Submodules

oddt.docking.AutodockVina module

class `oddt.docking.AutodockVina.autodock_vina` (*protein=None, auto_ligand=None, size=(10, 10, 10), center=(0, 0, 0), exhaustiveness=8, num_modes=9, energy_range=3, seed=None, prefix_dir='/tmp', n_cpu=1, executable=None, autocleanup=True*)

Bases: `object`

Autodock Vina docking engine, which extends it's capabilities: automatic box (autocentering on ligand).

Parameters **protein:** `oddt.toolkit.Molecule` object (default=None)

Protein object to be used while generating descriptors.

auto_ligand: `oddt.toolkit.Molecule` object or `string` (default=None) Ligand use to center the docking box. Either ODDT molecule or a file (opened based on extension and read to ODDT molecule). Box is centered on geometric center of molecule.

size: `tuple, shape=[3]` (default=(10,10,10)) Dimensions of docking box (in Angstroms)

center: `tuple, shape=[3]` (default=(0,0,0)) The center of docking box in cartesian space.

exhaustiveness: `int` (default=8) Exhaustiveness parameter of Autodock Vina

num_modes: `int` (default=9) Number of conformations generated by Autodock Vina

energy_range: `int` (default=3) Energy range cutoff for Autodock Vina

seed: `int` or `None` (default=None) Random seed for Autodock Vina

prefix_dir: `string` (default=/tmp) Temporary directory for Autodock Vina files

executable: string or None (default=None) Autodock Vina executable location in the system. It's really necessary if autodetection fails.

autocleanup: bool (default=True) Should the docking engine clean up after execution?

Attributes

tmp_dir

Methods

<i>clean()</i>	
<i>dock</i> (ligands[, protein, single])	Automated docking procedure.
<i>predict_ligand</i> (ligand)	Local method to score one ligand and update it's scores.
<i>predict_ligands</i> (ligands)	Method to score ligands lazily
<i>score</i> (ligands[, protein, single])	Automated scoring procedure.
<i>set_protein</i> (protein)	Change protein to dock to.

clean()

dock (ligands, protein=None, single=False)

Automated docking procedure.

Parameters **ligands:** iterable of `oddt.toolkit.Molecule` objects

Ligands to dock

protein: `oddt.toolkit.Molecule` object or None Protein object to be used. If None, then the default one is used, else the protein is new default.

single: bool (default=False) A flag to indicate single ligand docking (performance reasons (eg. there is no need for subdirectory for one ligand))

Returns **ligands** : array of `oddt.toolkit.Molecule` objects

Array of ligands (scores are stored in `mol.data` method)

predict_ligand (ligand)

Local method to score one ligand and update it's scores.

Parameters **ligand:** `oddt.toolkit.Molecule` object

Ligand to be scored

Returns **ligand:** `oddt.toolkit.Molecule` object

Scored ligand with updated scores

predict_ligands (ligands)

Method to score ligands lazily

Parameters **ligands:** iterable of `oddt.toolkit.Molecule` objects

Ligands to be scored

Returns **ligand:** iterator of `oddt.toolkit.Molecule` objects

Scored ligands with updated scores

score (*ligands*, *protein=None*, *single=False*)

Automated scoring procedure.

Parameters **ligands**: iterable of `oddt.toolkit.Molecule` objects

Ligands to score

protein: `oddt.toolkit.Molecule` object or `None` Protein object to be used. If `None`, then the default one is used, else the protein is new default.

single: **bool (default=False)** A flag to indicate single ligand scoring (performance reasons (eg. there is no need for subdirectory for one ligand))

Returns **ligands** : array of `oddt.toolkit.Molecule` objects

Array of ligands (scores are stored in `mol.data` method)

set_protein (*protein*)

Change protein to dock to.

Parameters **protein**: `oddt.toolkit.Molecule` object

Protein object to be used.

tmp_dir

`oddt.docking.AutodockVina.parse_vina_docking_output` (*output*)

Function parsing Autodock Vina docking output to a dictionary

Parameters **output** : string

Autodock Vina standard output (STDOUT).

Returns **out** : dict

dictionary containing scores computed by Autodock Vina

`oddt.docking.AutodockVina.parse_vina_scoring_output` (*output*)

Function parsing Autodock Vina scoring output to a dictionary

Parameters **output** : string

Autodock Vina standard output (STDOUT).

Returns **out** : dict

dictionary containing scores computed by Autodock Vina

`oddt.docking.AutodockVina.random` () → x in the interval [0, 1).

Module contents

```
class oddt.docking.autodock_vina (protein=None, auto_ligand=None, size=(10, 10, 10), center=(0, 0, 0), exhaustiveness=8, num_modes=9, energy_range=3, seed=None, prefix_dir='/tmp', n_cpu=1, executable=None, autocleanup=True)
```

Bases: object

Autodock Vina docking engine, which extends its capabilities: automatic box (autocentering on ligand).

Parameters **protein**: `oddt.toolkit.Molecule` object (default=None)

Protein object to be used while generating descriptors.

auto_ligand: `oddt.toolkit.Molecule` object or string (default=None) Ligand use to center the docking box. Either ODDT molecule or a file (opened based on extension and read to ODDT molecule). Box is centered on geometric center of molecule.

size: tuple, shape=[3] (default=(10,10,10)) Dimensions of docking box (in Angstroms)

center: tuple, shape=[3] (default=(0,0,0)) The center of docking box in cartesian space.

exhaustiveness: int (default=8) Exhaustiveness parameter of Autodock Vina

num_modes: int (default=9) Number of conformations generated by Autodock Vina

energy_range: int (default=3) Energy range cutoff for Autodock Vina

seed: int or None (default=None) Random seed for Autodock Vina

prefix_dir: string (default=/tmp) Temporary directory for Autodock Vina files

executable: string or None (default=None) Autodock Vina executable location in the system. It's really necessary if autodetection fails.

autocleanup: bool (default=True) Should the docking engine clean up after execution?

Attributes

tmp_dir

Methods

<i>clean()</i>	
<i>dock</i> (ligands[, protein, single])	Automated docking procedure.
<i>predict_ligand</i> (ligand)	Local method to score one ligand and update its scores.
<i>predict_ligands</i> (ligands)	Method to score ligands lazily
<i>score</i> (ligands[, protein, single])	Automated scoring procedure.
<i>set_protein</i> (protein)	Change protein to dock to.

`clean()`

dock (ligands, protein=None, single=False)
Automated docking procedure.

Parameters **ligands:** iterable of `oddt.toolkit.Molecule` objects

Ligands to dock

protein: `oddt.toolkit.Molecule` object or None Protein object to be used. If None, then the default one is used, else the protein is new default.

single: bool (default=False) A flag to indicate single ligand docking (performance reasons (eg. there is no need for subdirectory for one ligand))

Returns **ligands** : array of `oddt.toolkit.Molecule` objects

Array of ligands (scores are stored in `mol.data` method)

predict_ligand (*ligand*)

Local method to score one ligand and update it's scores.

Parameters **ligand:** oddt.toolkit.Molecule object

Ligand to be scored

Returns ligand: oddt.toolkit.Molecule object

Scored ligand with updated scores

predict_ligands (*ligands*)

Method to score ligands lazily

Parameters **ligands:** iterable of oddt.toolkit.Molecule objects

Ligands to be scored

Returns ligand: iterator of oddt.toolkit.Molecule objects

Scored ligands with updated scores

score (*ligands, protein=None, single=False*)

Automated scoring procedure.

Parameters **ligands:** iterable of oddt.toolkit.Molecule objects

Ligands to score

protein: oddt.toolkit.Molecule object or None Protein object to be used. If None, then the default one is used, else the protein is new default.

single: bool (default=False) A flag to indicate single ligand scoring (performance reasons (eg. there is no need for subdirectory for one ligand))

Returns **ligands** : array of oddt.toolkit.Molecule objects

Array of ligands (scores are stored in mol.data method)

set_protein (*protein*)

Change protein to dock to.

Parameters **protein:** oddt.toolkit.Molecule object

Protein object to be used.

tmp_dir

oddt.scoring package

Subpackages

oddt.scoring.descriptors package

Submodules

oddt.scoring.descriptors.binana module Internal implementation of binana software (<http://nbcrc.ucsd.edu/data/sw/hosted/binana/>)

class `oddt.scoring.descriptors.binana.binana_descriptor` (*protein=None*)

Bases: `object`

Descriptor build from binana script (as used in NNScore 2.0)

Parameters **protein:** `oddt.toolkit.Molecule` object (default=None)

Protein object to be used while generating descriptors.

Methods

<code>build</code> (ligands[, protein])	Descriptor building method
<code>set_protein</code> (protein)	One function to change all relevant proteins

build (*ligands*, *protein=None*)

Descriptor building method

Parameters **ligands:** array-like

An array of generator of `oddt.toolkit.Molecule` objects for which the descriptor is computed

protein: `oddt.toolkit.Molecule` object (default=None) Protein object to be used while generating descriptors. If none, then the default protein (from constructor) is used. Otherwise, protein becomes new global and default protein.

Returns `descs`: numpy array, shape=[*n_samples*, 351]

An array of binana descriptors, aligned with input ligands

set_protein (*protein*)

One function to change all relevant proteins

Parameters **protein:** `oddt.toolkit.Molecule` object

Protein object to be used while generating descriptors. Protein becomes new global and default protein.

Module contents

`oddt.scoring.descriptors.atoms_by_type` (*atom_dict*, *types*, *mode='atomic_nums'*)

Returns atom dictionaries based on given criteria. Currently we have 3 types of atom selection criteria:

- atomic numbers [`'atomic_nums'`]
- Sybyl Atom Types [`'atom_types_sybyl'`]
- AutoDock4 atom types [`'atom_types_ad4'`] (<http://autodock.scripps.edu/faqs-help/faq/where-do-i-set-the-autodock-4-force-field-parameters>)

Parameters **atom_dict:** `oddt.toolkit.Molecule.atom_dict`

Atom dictionary as implemented in `oddt.toolkit.Molecule` class

types: array-like List of atom types/numbers wanted.

Returns out: dictionary of shape=[len(types)]

A dictionary of queried atom types (types are keys of the dictionary). Values are of `oddt.toolkit.Molecule.atom_dict` type.

```
class oddt.scoring.descriptors.autodock_vina_descriptor (protein=None,
                                                         vina_scores=['vina_affinity',
                                                         'vina_gauss1', 'vina_gauss2',
                                                         'vina_repulsion',
                                                         'vina_hydrophobic',
                                                         'vina_hydrogen'])
```

Bases: object

Methods

```
build(ligands[, protein, single])
set_protein(protein)
```

build (*ligands*, *protein*=None, *single*=False)

set_protein (*protein*)

```
class oddt.scoring.descriptors.close_contacts (protein=None,                                cutoff=4,
                                                         mode='atomic_nums', ligand_types=None,
                                                         protein_types=None, aligned_pairs=False)
```

Bases: object

Close contacts descriptor which tallies atoms of type X in certain cutoff from atoms of type Y.

Parameters **protein:** `oddt.toolkit.Molecule` or None (default=None)

Default protein to use as reference

cutoff: int or list, shape=[n,] or shape=[n,2] (default=4) Cutoff for atoms in Angstroms given as an integer or a list of ranges, eg. [0, 4, 8, 12] or [[0,4],[4,8],[8,12]]. Upper bound is always inclusive, lower exclusive.

mode: string (default='atomic_nums') Method of atoms selection, as used in *atoms_by_type*

ligand_types: array List of ligand atom types to use

protein_types: array List of protein atom types to use

aligned_pairs: bool (default=False) Flag indicating should permutation of types should be done, otherwise the atoms are treated as aligned pairs.

Methods

```
build(ligands[, protein, single]) Builds descriptors for series of ligands
```

build (*ligands*, *protein*=None, *single*=False)

Builds descriptors for series of ligands

Parameters **ligands:** iterable of `oddt.toolkit.Molecules` or `oddt.toolkit.Molecule`

A list or iterable of ligands to build the descriptor or a single molecule.

protein: `oddt.toolkit.Molecule` or `None` (default=`None`) Default protein to use as reference

single: `bool` (default=`False`) Flag indicating if the ligand is single.

class `oddt.scoring.descriptors.fingerprints` (*fp='fp2', toolkit='ob'*)
Bases: `object`

Methods

`build`(*mols*[, *single*])

build (*mols*, *single=False*)

oddt.scoring.functions package

Submodules

oddt.scoring.functions.NNScore module

`oddt.scoring.functions.NNScore.generate_descriptor` (*packed*)

class `oddt.scoring.functions.NNScore.nnscore` (*protein=None, n_jobs=-1, **kwargs*)
Bases: `oddt.scoring.scorer`

Methods

<i><code>fit</code></i> (<i>ligands</i> , <i>target</i> , * <i>args</i> , ** <i>kwargs</i>)	Trains model on supplied ligands and target values
<i><code>gen_training_data</code></i> (<i>pdbbind_dir</i> [, ...])	
<i><code>load</code></i> (<i>filename</i>)	
<i><code>predict</code></i> (<i>ligands</i> , * <i>args</i> , ** <i>kwargs</i>)	Predicts values (eg.
<i><code>predict_ligand</code></i> (<i>ligand</i>)	Local method to score one ligand and update it's scores.
<i><code>predict_ligands</code></i> (<i>ligands</i>)	Method to score ligands lazily
<i><code>save</code></i> (<i>filename</i>)	Saves scoring function to a pickle file.
<i><code>score</code></i> (<i>ligands</i> , <i>target</i> , * <i>args</i> , ** <i>kwargs</i>)	Methods estimates the quality of prediction as squared correlation coefficient (R^2)
<i><code>set_protein</code></i> (<i>protein</i>)	Proxy method to update protein in all relevant places.
<i><code>train</code></i> (<i>[sf_pickle]</i>)	

fit (*ligands*, *target*, **args*, ***kwargs*)
Trains model on supplied ligands and target values

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [*n_samples*] or [*n_samples*, *n_outputs*] Estimated target values.

gen_training_data (*pdbbind_dir*, *pdbbind_version='2007'*, *sf_pickle=''*)

classmethod `load (filename='')`

predict (*ligands*, *args, **kwargs)

Predicts values (eg. affinity) for supplied ligands

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

Returns predicted: np.array or array of np.arrays of shape = [n_ligands]

Predicted scores for ligands

predict_ligand (*ligand*)

Local method to score one ligand and update it's scores.

Parameters **ligand:** oddt.toolkit.Molecule object

Ligand to be scored

Returns ligand: oddt.toolkit.Molecule object

Scored ligand with updated scores

predict_ligands (*ligands*)

Method to score ligands lazily

Parameters **ligands:** iterable of oddt.toolkit.Molecule objects

Ligands to be scored

Returns ligand: iterator of oddt.toolkit.Molecule objects

Scored ligands with updated scores

save (*filename*)

Saves scoring function to a pickle file.

Parameters **filename:** string

Pickle filename

score (*ligands*, *target*, *args, **kwargs)

Methods estimates the quality of prediction as squared correlation coefficient (R^2)

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

Returns r2: float

Squared correlation coefficient (R^2) for prediction

set_protein (*protein*)

Proxy method to update protein in all relevant places.

Parameters **protein:** oddt.toolkit.Molecule object

New default protein

```
train(sf_pickle='')
```

oddt.scoring.functions.RFScore module

```
class oddt.scoring.functions.RFScore.rfscore (protein=None, n_jobs=-1, version=1, spr=0,  
                                              **kwargs)
```

Bases: `oddt.scoring.scorer`

Methods

<code>fit(ligands, target, *args, **kwargs)</code>	Trains model on supplied ligands and target values
<code>gen_training_data(pdbbind_dir[, ...])</code>	
<code>load([filename, version])</code>	
<code>predict(ligands, *args, **kwargs)</code>	Predicts values (eg.
<code>predict_ligand(ligand)</code>	Local method to score one ligand and update it's scores.
<code>predict_ligands(ligands)</code>	Method to score ligands lazily
<code>save(filename)</code>	Saves scoring function to a pickle file.
<code>score(ligands, target, *args, **kwargs)</code>	Methods estimates the quality of prediction as squared correlation coefficient (R^2)
<code>set_protein(protein)</code>	Proxy method to update protein in all relevant places.
<code>train([home_dir, sf_pickle])</code>	

```
fit (ligands, target, *args, **kwargs)
```

Trains model on supplied ligands and target values

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

```
gen_training_data (pdbbind_dir, pdbbind_version='2007', home_dir=None, sf_pickle='')
```

```
classmethod load (filename='', version=1)
```

```
predict (ligands, *args, **kwargs)
```

Predicts values (eg. affinity) for supplied ligands

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

Returns predicted: np.array or array of np.arrays of shape = [n_ligands]

Predicted scores for ligands

```
predict_ligand (ligand)
```

Local method to score one ligand and update it's scores.

Parameters **ligand:** oddt.toolkit.Molecule object

Ligand to be scored

Returns ligand: oddt.toolkit.Molecule object

Scored ligand with updated scores

predict_ligands (*ligands*)

Method to score ligands lazily

Parameters **ligands:** iterable of `oddt.toolkit.Molecule` objects

Ligands to be scored

Returns ligand: iterator of `oddt.toolkit.Molecule` objects

Scored ligands with updated scores

save (*filename*)

Saves scoring function to a pickle file.

Parameters **filename:** string

Pickle filename

score (*ligands, target, *args, **kwargs*)

Methods estimates the quality of prediction as squared correlation coefficient (R^2)

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = `[n_samples]` or `[n_samples, n_outputs]` Estimated target values.

Returns `r2`: float

Squared correlation coefficient (R^2) for prediction

set_protein (*protein*)

Proxy method to update protein in all relevant places.

Parameters **protein:** `oddt.toolkit.Molecule` object

New default protein

train (*home_dir=None, sf_pickle=''*)

Module contents

class `oddt.scoring.functions.rfscore` (*protein=None, n_jobs=-1, version=1, spr=0, **kwargs*)

Bases: `oddt.scoring.scorer`

Methods

<code>fit(ligands, target, *args, **kwargs)</code>	Trains model on supplied ligands and target values
<code>gen_training_data(pdbbind_dir[, ...])</code>	
<code>load([filename, version])</code>	
<code>predict(ligands, *args, **kwargs)</code>	Predicts values (eg.
<code>predict_ligand(ligand)</code>	Local method to score one ligand and update it's scores.
<code>predict_ligands(ligands)</code>	Method to score ligands lazily
<code>save(filename)</code>	Saves scoring function to a pickle file.
<code>score(ligands, target, *args, **kwargs)</code>	Methods estimates the quality of prediction as squared correlation coefficient (R^2)
<code>set_protein(protein)</code>	Proxy method to update protein in all relevant places.
<code>train([home_dir, sf_pickle])</code>	

fit (*ligands*, *target*, **args*, ***kwargs*)

Trains model on supplied ligands and target values

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

gen_training_data (*pdbind_dir*, *pdbind_version*=‘2007’, *home_dir*=None, *sf_pickle*=‘’)

classmethod load (*filename*=‘’, *version*=1)

predict (*ligands*, **args*, ***kwargs*)

Predicts values (eg. affinity) for supplied ligands

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

Returns predicted: np.array or array of np.arrays of shape = [n_ligands]

Predicted scores for ligands

predict_ligand (*ligand*)

Local method to score one ligand and update it’s scores.

Parameters **ligand:** oddt.toolkit.Molecule object

Ligand to be scored

Returns ligand: oddt.toolkit.Molecule object

Scored ligand with updated scores

predict_ligands (*ligands*)

Method to score ligands lazily

Parameters **ligands:** iterable of oddt.toolkit.Molecule objects

Ligands to be scored

Returns ligand: iterator of oddt.toolkit.Molecule objects

Scored ligands with updated scores

save (*filename*)

Saves scoring function to a pickle file.

Parameters **filename:** string

Pickle filename

score (*ligands*, *target*, **args*, ***kwargs*)

Methods estimates the quality of prediction as squared correlation coefficient (R^2)

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

Returns r2: float

Squared correlation coefficient (R^2) for prediction

set_protein (*protein*)

Proxy method to update protein in all relevant places.

Parameters **protein:** oddt.toolkit.Molecule object

New default protein

train (*home_dir=None, sf_pickle=''*)

class oddt.scoring.functions.nnscore (*protein=None, n_jobs=-1, **kwargs*)

Bases: *oddt.scoring.scorer*

Methods

<i>fit</i> (ligands, target, *args, **kwargs)	Trains model on supplied ligands and target values
<i>gen_training_data</i> (pdbbind_dir[, ...])	
<i>load</i> ([filename])	
<i>predict</i> (ligands, *args, **kwargs)	Predicts values (eg.
<i>predict_ligand</i> (ligand)	Local method to score one ligand and update it's scores.
<i>predict_ligands</i> (ligands)	Method to score ligands lazily
<i>save</i> (filename)	Saves scoring function to a pickle file.
<i>score</i> (ligands, target, *args, **kwargs)	Methods estimates the quality of prediction as squared correlation coefficient (R^2)
<i>set_protein</i> (protein)	Proxy method to update protein in all relevant places.
<i>train</i> ([sf_pickle])	

fit (*ligands, target, *args, **kwargs*)

Trains model on supplied ligands and target values

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

gen_training_data (*pdbbind_dir, pdbbind_version='2007', sf_pickle=''*)

classmethod **load** (*filename=''*)

predict (*ligands, *args, **kwargs*)

Predicts values (eg. affinity) for supplied ligands

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

Returns predicted: np.array or array of np.arrays of shape = [n_ligands]

Predicted scores for ligands

predict_ligand (*ligand*)

Local method to score one ligand and update it's scores.

Parameters **ligand:** `oddt.toolkit.Molecule` object

Ligand to be scored

Returns ligand: `oddt.toolkit.Molecule` object

Scored ligand with updated scores

predict_ligands (*ligands*)

Method to score ligands lazily

Parameters **ligands:** iterable of `oddt.toolkit.Molecule` objects

Ligands to be scored

Returns ligand: iterator of `oddt.toolkit.Molecule` objects

Scored ligands with updated scores

save (*filename*)

Saves scoring function to a pickle file.

Parameters **filename:** `string`

Pickle filename

score (*ligands*, *target*, **args*, ***kwargs*)

Methods estimates the quality of prediction as squared correlation coefficient (R^2)

Parameters **ligands:** array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = `[n_samples]` or `[n_samples, n_outputs]` Estimated target values.

Returns `r2`: float

Squared correlation coefficient (R^2) for prediction

set_protein (*protein*)

Proxy method to update protein in all relevant places.

Parameters **protein:** `oddt.toolkit.Molecule` object

New default protein

train (*sf_pickle*='')

oddt.scoring.models package

Submodules

oddt.scoring.models.classifiers module

`oddt.scoring.models.classifiers.randomforest`

alias of `RandomForestClassifier`

`oddt.scoring.models.classifiers.svm`

alias of `SVC`

oddt.scoring.models.neuralnetwork module

class `oddt.scoring.models.neuralnetwork.neuralnetwork` (*shape=None, full_conn=True, biases=True, random_weights=True, normalize=True, reduce_empty_dims=True*)

Bases: `object`

shape: shape of a NN given as a tuple

Methods

`fit(input_descriptors, target_values[, ...])`
`get_params([deep])`
`predict(input_descriptors)`
`score(X, y)`
`set_params(args)`

fit (*input_descriptors, target_values, train_alg='tnc', **kwargs*)

get_params (*deep=True*)

predict (*input_descriptors*)

score (*X, y*)

set_params (*args*)

oddt.scoring.models.regressors module Collection of regressors models

`oddt.scoring.models.regressors.randomforest`

alias of `RandomForestRegressor`

`oddt.scoring.models.regressors.svm`

alias of `SVR`

`oddt.scoring.models.regressors.pls`

alias of `PLSRegression`

class `oddt.scoring.models.regressors.neuralnetwork` (*shape=None, full_conn=True, biases=True, random_weights=True, normalize=True, reduce_empty_dims=True*)

Bases: `object`

shape: shape of a NN given as a tuple

Methods

`fit(input_descriptors, target_values[, ...])`
`get_params([deep])`
`predict(input_descriptors)`
`score(X, y)`
`set_params(args)`

```

fit (input_descriptors, target_values, train_alg='inc', **kwargs)
get_params (deep=True)
predict (input_descriptors)
score (X, y)
set_params (args)
oddt.scoring.models.regressors.mlr
alias of LinearRegression

```

Module contents

Module contents

```

oddt.scoring.cross_validate (model, cv_set, cv_target, n=10, shuffle=True, n_jobs=1)
Perform cross validation of model using provided data

```

Parameters **model**: object

Model to be tested

cv_set: array-like of shape = [**n_samples**, **n_features**] Estimated target values.

cv_target: array-like of shape = [**n_samples**] or [**n_samples**, **n_outputs**] Estimated target values.

n: integer (default = 10) How many folds to be created from dataset

shuffle: bool (default = True) Should data be shuffled before folding.

n_jobs: integer (default = 1) How many CPUs to use during cross validation

Returns r2: array of shape = [n]

R² score for each of generated folds

```

class oddt.scoring.ensemble_descriptor (descriptor_generators)
Bases: object

```

Proxy class to build an ensemble of descriptors with an API as one

Parameters **models**: array

An array of models

Methods

```

    build(mols, *args, **kwargs)
    set_protein(protein)

```

```

build (mols, *args, **kwargs)

```

```

set_protein (protein)

```

```

class oddt.scoring.ensemble_model (models)
Bases: object

```

Proxy class to build an ensemble of models with an API as one

Parameters models: array

An array of models

Methods

<i>fit</i> (X, y, *args, **kwargs)
<i>predict</i> (X, *args, **kwargs)
<i>score</i> (X, y, *args, **kwargs)

fit (X, y, *args, **kwargs)

predict (X, *args, **kwargs)

score (X, y, *args, **kwargs)

class `oddt.scoring.scorer` (*model_instance*, *descriptor_generator_instance*, *score_title*='score')

Bases: object

Scorer class is parent class for scoring functions.

Parameters model_instance: model

Model compatible with sklearn API (fit, predict and score methods)

descriptor_generator_instance: array of descriptors Descriptor generator object

score_title: string Title of score to be used.

Methods

<i>fit</i> (ligands, target, *args, **kwargs)	Trains model on supplied ligands and target values
<i>load</i> (filename)	Loads scoring function from a pickle file.
<i>predict</i> (ligands, *args, **kwargs)	Predicts values (eg.
<i>predict_ligand</i> (ligand)	Local method to score one ligand and update it's scores.
<i>predict_ligands</i> (ligands)	Method to score ligands lazily
<i>save</i> (filename)	Saves scoring function to a pickle file.
<i>score</i> (ligands, target, *args, **kwargs)	Methods estimates the quality of prediction as squared correlation coefficient (R^2)
<i>set_protein</i> (protein)	Proxy method to update protein in all relevant places.

fit (*ligands*, *target*, *args, **kwargs)

Trains model on supplied ligands and target values

Parameters ligands: array-like of ligands

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

classmethod load (*filename*)

Loads scoring function from a pickle file.

Parameters `filename: string`

Pickle filename

Returns `sf: scorer-like object`

Scoring function object loaded from a pickle

predict (*ligands*, *args, **kwargs)

Predicts values (eg. affinity) for supplied ligands

Parameters `ligands: array-like of ligands`

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

Returns `predicted: np.array or array of np.arrays of shape = [n_ligands]`

Predicted scores for ligands

predict_ligand (*ligand*)

Local method to score one ligand and update it's scores.

Parameters `ligand: oddt.toolkit.Molecule object`

Ligand to be scored

Returns `ligand: oddt.toolkit.Molecule object`

Scored ligand with updated scores

predict_ligands (*ligands*)

Method to score ligands lazily

Parameters `ligands: iterable of oddt.toolkit.Molecule objects`

Ligands to be scored

Returns `ligand: iterator of oddt.toolkit.Molecule objects`

Scored ligands with updated scores

save (*filename*)

Saves scoring function to a pickle file.

Parameters `filename: string`

Pickle filename

score (*ligands*, *target*, *args, **kwargs)

Methods estimates the quality of prediction as squared correlation coefficient (R^2)

Parameters `ligands: array-like of ligands`

Ground truth (correct) target values.

target: array-like of shape = [n_samples] or [n_samples, n_outputs] Estimated target values.

Returns `r2: float`

Squared correlation coefficient (R^2) for prediction

set_protein (*protein*)

Proxy method to update protein in all relevant places.

Parameters **protein**: `oddt.toolkit.Molecule` object

New default protein

oddt.toolkits package

Submodules

oddt.toolkits.ob module

class `oddt.toolkits.ob.Atom` (*OAtom*)

Bases: `pybel.Atom`

Attributes

<i>atomicmass</i>
<i>atomicnum</i>
<i>cidx</i>
<i>coordidx</i>
<i>coords</i>
<i>exactmass</i>
<i>formalcharge</i>
<i>heavyvalence</i>
<i>heterovalence</i>
<i>hyb</i>
<i>idx</i>
<i>implicitvalence</i>
<i>isotope</i>
<i>neighbors</i>
<i>partialcharge</i>
<i>residue</i>
<i>spin</i>
<i>type</i>
<i>valence</i>
<i>vector</i>

atomicmass

atomicnum

cidx

coordidx

coords

exactmass

formalcharge

heavyvalence

heterovalence
hyb
idx
implicitvalence
isotope
neighbors
partialcharge
residue
spin
type
valence
vector

class oddt.toolkits.ob.**AtomStack** (*OBMol*)
 Bases: object

class oddt.toolkits.ob.**Bond** (*OBBond*)
 Bases: object

Attributes

atoms

isrotor

order

atoms
isrotor
order

class oddt.toolkits.ob.**BondStack** (*OBMol*)
 Bases: object

class oddt.toolkits.ob.**Fingerprint** (*fingerprint*)
 Bases: pybel.Fingerprint

Attributes

bits

raw

bits
raw

class oddt.toolkits.ob.**Molecule** (*OBMol=None, source=None, protein=False*)
 Bases: pybel.Molecule

Attributes

<i>OBMol</i>	
<i>atom_dict</i>	
<i>atoms</i>	
<i>bonds</i>	
<i>canonic_order</i>	Returns np.array with canonic order of heavy atoms in the molecule
<i>charge</i>	
<i>charges</i>	
<i>clone</i>	
<i>conformers</i>	
<i>coords</i>	
<i>data</i>	
<i>dim</i>	
<i>energy</i>	
<i>exactmass</i>	
<i>formula</i>	
<i>molwt</i>	
<i>num_rotors</i>	
<i>res_dict</i>	
<i>residues</i>	
<i>ring_dict</i>	
<i>spin</i>	
<i>sssr</i>	
<i>title</i>	
<i>unitcell</i>	

Methods

<i>addh()</i>	Add hydrogens.
<i>calccharges</i> ([model])	Estimates atomic partial charges in the molecule.
<i>calcdesc</i> ([descnames])	Calculate descriptor values.
<i>calcfp</i> ([fptype])	Calculate a molecular fingerprint.
<i>clone_coords</i> (source)	
<i>convertdbonds</i> ()	Convert Dative Bonds.
<i>draw</i> ([show, filename, update, usecoords])	Create a 2D depiction of the molecule.
<i>localopt</i> ([forcefield, steps])	Locally optimize the coordinates.
<i>make3D</i> ([forcefield, steps])	Generate 3D coordinates.
<i>removeh</i> ()	Remove hydrogens.
<i>write</i> ([format, filename, overwrite, opt])	

OBMol

addh()

Add hydrogens.

atom_dict

atoms

bonds

calccharges (*model='mmff94'*)

Estimates atomic partial charges in the molecule.

Optional parameters:

model – default is “mmff94”. See the **charges** variable for a list of available charge models (in shell, *obabel -L charges*)

This method populates the *partialcharge* attribute of each atom in the molecule in place.

calcdesc (*descnames=[]*)

Calculate descriptor values.

Optional parameter: **descnames** – a list of names of descriptors

If **descnames** is not specified, all available descriptors are calculated. See the **descs** variable for a list of available descriptors.

calcfp (*fptype='FP2'*)

Calculate a molecular fingerprint.

Optional parameters:

fptype – the fingerprint type (default is “FP2”). See the **fps** variable for a list of available fingerprint types.

canonic_order

Returns np.array with canonic order of heavy atoms in the molecule

charge

charges

clone

clone_coords (*source*)

conformers

convertdbonds ()

Convert Dative Bonds.

coords

data

dim

draw (*show=True, filename=None, update=False, usecoords=False*)

Create a 2D depiction of the molecule.

Optional parameters: **show** – display on screen (default is True) **filename** – write to file (default is None)

update – update the coordinates of the atoms to those

determined by the structure diagram generator (default is False)

usecoords – don't calculate 2D coordinates, just use the current coordinates (default is False)

Tkinter and Python Imaging Library are required for image display.

energy

exactmass

formula

localopt (*forcefield='mmff94', steps=500*)

Locally optimize the coordinates.

Optional parameters:

forcefield – default is “mmff94”. See the **forcefields** variable for a list of available forcefields.

steps – default is 500

If the molecule does not have any coordinates, `make3D()` is called before the optimization. Note that the molecule needs to have explicit hydrogens. If not, call `addh()`.

make3D (*forcefield='mmff94', steps=50*)

Generate 3D coordinates.

Optional parameters:

forcefield – default is “mmff94”. See the **forcefields** variable for a list of available forcefields.

steps – default is 50

Once coordinates are generated, hydrogens are added and a quick local optimization is carried out with 50 steps and the MMFF94 forcefield. Call `localopt()` if you want to improve the coordinates further.

molwt

num_rotors

removeh ()

Remove hydrogens.

res_dict

residues

ring_dict

spin

sssr

title

unitcell

write (*format='smi', filename=None, overwrite=False, opt=None*)

class `oddt.toolkits.ob.Residue` (*OBResidue*)

Bases: `object`

Represent a Pybel residue.

Required parameter: `OBResidue` – an Open Babel `OBResidue`

Attributes: `atoms`, `idx`, `name`.

(refer to the Open Babel library documentation for more info).

The original Open Babel atom can be accessed using the attribute: `OBResidue`

Attributes

atoms

idx

Continued on next page

Table 3.23 – continued from previous page

name

atoms**idx****name**`oddt.toolkits.ob.pickle_mol (self)``oddt.toolkits.ob.readfile (format, filename, opt=None, lazy=False)``oddt.toolkits.ob.unpickle_mol (source)`**oddt.toolkits.rdk module**

rdkit - A Cinfony module for accessing the RDKit from CPython

Global variables: Chem and AllChem - the underlying RDKit Python bindings
informats - a dictionary of supported input formats
outformats - a dictionary of supported output formats
descs - a list of supported descriptors
fps - a list of supported fingerprint types
forcefields - a list of supported forcefields

class `oddt.toolkits.rdk.Atom (Atom)`

Bases: object

Represent an rdkit Atom.

Required parameters: Atom – an RDKit Atom

Attributes: atomicnum, coords, formalcharge

The original RDKit Atom can be accessed using the attribute: Atom

Attributes

atomicnum

coords

formalcharge

idx

Note that this index is 1-based and RDKit's internal index in 0-based.

neighbors

partialcharge

atomicnum**coords****formalcharge****idx**

Note that this index is 1-based and RDKit's internal index in 0-based. Changed to be compatible with OpenBabel

neighbors**partialcharge**

class `oddt.toolkits.rdk.AtomStack (Mol)`

Bases: object

```
class oddt.toolkits.rdk.Fingerprint (fingerprint)
```

Bases: object

A Molecular Fingerprint.

Required parameters: fingerprint – a vector calculated by one of the fingerprint methods

Attributes: fp – the underlying fingerprint object bits – a list of bits set in the Fingerprint

Methods: The “|” operator can be used to calculate the Tanimoto coeff. For example, given two Fingerprints ‘a’, and ‘b’, the Tanimoto coefficient is given by:

$$\text{tanimoto} = a \mid b$$

Attributes

raw

raw

```
class oddt.toolkits.rdk.Molecule (Mol=None, source=None, protein=False)
```

Bases: object

Represent an rdkit Molecule.

Required parameter: Mol – an RDKit Mol or any type of cinfony Molecule

Attributes: atoms, data, formula, molwt, title

Methods: addh(), calcfp(), calcdesc(), draw(), localopt(), make3D(), removeh(), write()

The underlying RDKit Mol can be accessed using the attribute: Mol

Attributes

<i>Mol</i>	
<i>atom_dict</i>	
<i>atoms</i>	
<i>canonic_order</i>	Returns np.array with canonic order of heavy atoms in the molecule
<i>charges</i>	
<i>clone</i>	
<i>coords</i>	
<i>data</i>	
<i>formula</i>	
<i>molwt</i>	
<i>num_rotors</i>	
<i>res_dict</i>	
<i>ring_dict</i>	
<i>sssr</i>	
<i>title</i>	

Methods

<code>addh()</code>	Add hydrogens.
<code>calcdesc([descnames])</code>	Calculate descriptor values.
<code>calcfp([fptype, opt])</code>	Calculate a molecular fingerprint.
<code>clone_coords(source)</code>	
<code>draw([show, filename, update, usecoords])</code>	Create a 2D depiction of the molecule.
<code>localopt([forcefield, steps])</code>	Locally optimize the coordinates.
<code>make3D([forcefield, steps])</code>	Generate 3D coordinates.
<code>removeh()</code>	Remove hydrogens.
<code>write([format, filename, overwrite])</code>	Write the molecule to a file or return a string.

Mol

addh()

Add hydrogens.

atom_dict

atoms

calcdesc (*descnames*=[])

Calculate descriptor values.

Optional parameter: *descnames* – a list of names of descriptors

If *descnames* is not specified, all available descriptors are calculated. See the *descs* variable for a list of available descriptors.

calcfp (*fptype*='rdkit', *opt*=None)

Calculate a molecular fingerprint.

Optional parameters:

fptype – the fingerprint type (default is “rdkit”). See the *fps* variable for a list of available fingerprint types.

opt – a dictionary of options for fingerprints. Currently only used for radius and bitInfo in Morgan fingerprints.

canonic_order

Returns np.array with canonic order of heavy atoms in the molecule

charges

clone

clone_coords (*source*)

coords

data

draw (*show*=True, *filename*=None, *update*=False, *usecoords*=False)

Create a 2D depiction of the molecule.

Optional parameters: *show* – display on screen (default is True) *filename* – write to file (default is None)
update – update the coordinates of the atoms to those

determined by the structure diagram generator (default is False)

usecoords – don’t calculate 2D coordinates, just use the current coordinates (default is False)

Aggdraw or Cairo is used for 2D depiction. Tkinter and Python Imaging Library are required for image display.

formula

localopt (*forcefield='uff', steps=500*)

Locally optimize the coordinates.

Optional parameters:

forcefield – default is “uff”. See the **forcefields variable** for a list of available forcefields.

steps – default is 500

If the molecule does not have any coordinates, make3D() is called before the optimization.

make3D (*forcefield='uff', steps=50*)

Generate 3D coordinates.

Optional parameters:

forcefield – default is “uff”. See the **forcefields variable** for a list of available forcefields.

steps – default is 50

Once coordinates are generated, a quick local optimization is carried out with 50 steps and the UFF force-field. Call localopt() if you want to improve the coordinates further.

molwt

num_rotors

removeh ()

Remove hydrogens.

res_dict

ring_dict

sssr

title

write (*format='smi', filename=None, overwrite=False, **kwargs*)

Write the molecule to a file or return a string.

Optional parameters:

format – see the **informats variable for a list of available** output formats (default is “smi”)

filename – default is None **overwrite** – if the output file already exists, should it be overwritten? (default is False)

If a filename is specified, the result is written to a file. Otherwise, a string is returned containing the result.

To write multiple molecules to the same file you should use the Outputfile class.

class `oddt.toolkits.rdk.MoleculeData` (*Mol*)

Bases: object

Store molecule data in a dictionary-type object

Required parameters: Mol – an RDKit Mol

Methods and accessor methods are like those of a dictionary except that the data is retrieved on-the-fly from the underlying Mol.

```
Example: >>> mol = readfile("sdf", 'head.sdf').next() >>> data = mol.data >>> print data {'Comment': 'CO-
RINA 2.61 0041 25.10.2001', 'NSC': '1'} >>> print len(data), data.keys(), data.has_key("NSC") 2 ['Com-
ment', 'NSC'] True >>> print data['Comment'] CORINA 2.61 0041 25.10.2001 >>> data['Comment'] = 'This
is a new comment' >>> for k,v in data.iteritems(): ... print k, "->", v Comment -> This is a new comment NSC
-> 1 >>> del data['NSC'] >>> print len(data), data.keys(), data.has_key("NSC") 1 ['Comment'] False
```

Methods

<code>clear()</code>
<code>has_key(key)</code>
<code>items()</code>
<code>iteritems()</code>
<code>keys()</code>
<code>update(dictionary)</code>
<code>values()</code>

clear()

has_key (*key*)

items ()

iteritems ()

keys ()

update (*dictionary*)

values ()

class `oddt.toolkits.rdk.Outputfile` (*format, filename, overwrite=False*)

Bases: `object`

Represent a file to which *output* is to be sent.

Required parameters:

format - see the `outformats` variable for a list of available output formats

filename

Optional parameters:

overwrite – if the output file already exists, should it be overwritten? (default is False)

Methods: `write(molecule)` `close()`

Methods

<code>close()</code>	Close the Outputfile to further writing.
<code>write(molecule)</code>	Write a molecule to the output file.

close ()

Close the Outputfile to further writing.

write (*molecule*)

Write a molecule to the output file.

Required parameters: molecule

class `oddt.toolkits.rdk.Smarts` (*smartspattern*)

Bases: object

Initialise with a SMARTS pattern.

Methods

findall(molecule) Find all matches of the SMARTS pattern to a particular molecule.

findall (*molecule*)

Find all matches of the SMARTS pattern to a particular molecule.

Required parameters: molecule

`oddt.toolkits.rdk.base_feature_factory = <rdkit.Chem.rdMolChemicalFeatures.MolChemicalFeatureFactory object>`

Global feature factory based on BaseFeatures.fdef

`oddt.toolkits.rdk.descs = ['fr_C_O_noCOO', 'PEOE_VSA3', 'Chi4v', 'fr_Ar_COO', 'fr_SH', 'Chi4n', 'SMR_VSA10']`

A list of supported descriptors

`oddt.toolkits.rdk.forcefields = ['uff']`

A list of supported forcefields

`oddt.toolkits.rdk.fps = ['rdkit', 'layered', 'maccs', 'atompairs', 'torsions', 'morgan']`

A list of supported fingerprint types

`oddt.toolkits.rdk.informats = {'inchi': 'InChI', 'mol2': 'Tripos MOL2 file', 'sdf': 'MDL SDF file', 'smi': 'SMILES'}`

A dictionary of supported input formats

`oddt.toolkits.rdk.outformats = {'inchikey': 'InChIKey', 'sdf': 'MDL SDF file', 'can': 'Canonical SMILES', 'smi': 'SMILES'}`

A dictionary of supported output formats

`oddt.toolkits.rdk.readfile` (*format, filename, *args, **kwargs*)

Iterate over the molecules in a file.

Required parameters:

format - see the **informats** variable for a list of available input formats

filename

You can access the first molecule in a file using the `next()` method of the iterator:

```
mol = readfile("smi", "myfile.smi").next()
```

You can make a list of the molecules in a file using: `mols = list(readfile("smi", "myfile.smi"))`

You can iterate over the molecules in a file as shown in the following code snippet: `>>> atomtotal = 0 >>> for mol in readfile("sdf", "head.sdf"): ... atomtotal += len(mol.atoms) ... >>> print atomtotal 43`

`oddt.toolkits.rdk.readstring` (*format, string, **kwargs*)

Read in a molecule from a string.

Required parameters:

format - see the **informats** variable for a list of available input formats

string

Example: `>>> input = "C1=CC=CS1" >>> mymol = readstring("smi", input) >>> len(mymol.atoms) 5`

Module contents

3.1.2 Submodules

3.1.3 oddt.datasets module

Datasets wrapped in convinient models

```
class oddt.datasets.pdbbind(home, version=None, default_set=None, data_file=None, opt={})  
    Bases: object
```

Attributes

<i>activities</i>
<i>ids</i>

activities

ids

3.1.4 oddt.interactions module

Module calculates interactions between two molecules (proein-protein, protein-ligand, small-small). Currently following interactions are implemented:

- hydrogen bonds
- halogen bonds
- pi stacking (parallel and perpendicular)
- salt bridges
- hydrophobic contacts
- pi-cation
- metal coordination
- pi-metal

```
oddt.interactions.close_contacts(x, y, cutoff, x_column='coords', y_column='coords')  
    Returns pairs of atoms which are within close contac distance cutoff.
```

Parameters **x, y** : atom_dict-type numpy array

Atom dictionaries generated by oddt.toolkit.Molecule objects.

cutoff [float] Cutoff distance for close contacts

x_column, ycolumn [string, (default='coords')] Column containing coordinates of atoms (or pseudo-atoms, i.e. ring centroids)

Returns **x_, y_** : atom_dict-type numpy array

Aligned pairs of atoms in close contact for further processing.

`oddt.interactions.hbond_acceptor_donor(mol1, mol2, cutoff=3.5, base_angle=120, tolerance=30)`

Returns pairs of acceptor-donor atoms, which meet H-bond criteria

Parameters **mol1, mol2** : `oddt.toolkit.Molecule` object

Molecules to compute H-bond acceptor and H-bond donor pairs

cutoff [float, (default=3.5)] Distance cutoff for A-D pairs

base_angle [int, (default=120)] Base angle determining allowed direction of hydrogen bond formation, which is divided by the number of neighbors of acceptor atom to establish final directional angle

tolerance [int, (default=30)] Range (+/- tolerance) from perfect direction ($\text{base_angle}/\text{n_neighbors}$) in which H-bonds are considered as strict.

Returns **a, d** : `atom_dict`-type numpy array

Aligned arrays of atoms forming H-bond, firstly acceptors, secondly donors.

strict [numpy array, dtype=bool] Boolean array align with atom pairs, informing whether atoms form 'strict' H-bond (pass all angular cutoffs). If false, only distance cutoff is met, therefore the bond is 'crude'.

`oddt.interactions.hbond(mol1, mol2, *args, **kwargs)`

Calculates H-bonds between molecules

Parameters **mol1, mol2** : `oddt.toolkit.Molecule` object

Molecules to compute H-bond acceptor and H-bond donor pairs

cutoff [float, (default=3.5)] Distance cutoff for A-D pairs

base_angle [int, (default=120)] Base angle determining allowed direction of hydrogen bond formation, which is divided by the number of neighbors of acceptor atom to establish final directional angle

tolerance [int, (default=30)] Range (+/- tolerance) from perfect direction ($\text{base_angle}/\text{n_neighbors}$) in which H-bonds are considered as strict.

Returns **mol1_atoms, mol2_atoms** : `atom_dict`-type numpy array

Aligned arrays of atoms forming H-bond

strict [numpy array, dtype=bool] Boolean array align with atom pairs, informing whether atoms form 'strict' H-bond (pass all angular cutoffs). If false, only distance cutoff is met, therefore the bond is 'crude'.

`oddt.interactions.halogenbond_acceptor_halogen(mol1, mol2, base_angle_acceptor=120, base_angle_halogen=180, tolerance=30, cutoff=4)`

Returns pairs of acceptor-halogen atoms, which meet halogen bond criteria

Parameters **mol1, mol2** : `oddt.toolkit.Molecule` object

Molecules to compute halogen bond acceptor and halogen pairs

cutoff [float, (default=4)] Distance cutoff for A-H pairs

base_angle_acceptor [int, (default=120)] Base angle determining allowed direction of halogen bond formation, which is divided by the number of neighbors of acceptor atom to establish final directional angle

base_angle_halogen [int (default=180)] Ideal base angle between halogen bond and halogen-neighbor bond

tolerance [int, (default=30)] Range (+/- tolerance) from perfect direction (base_angle/n_neighbors) in which halogen bonds are considered as strict.

Returns **a, h** : atom_dict-type numpy array

Aligned arrays of atoms forming halogen bond, firstly acceptors, secondly halogens

strict [numpy array, dtype=bool] Boolean array align with atom pairs, informing whether atoms form 'strict' halogen bond (pass all angular cutoffs). If false, only distance cutoff is met, therefore the bond is 'crude'.

`oddt.interactions.halogenbond(mol1, mol2, **kwargs)`

Calculates halogen bonds between molecules

Parameters **mol1, mol2** : oddt.toolkit.Molecule object

Molecules to compute halogen bond acceptor and halogen pairs

cutoff [float, (default=4)] Distance cutoff for A-H pairs

base_angle_acceptor [int, (default=120)] Base angle determining allowed direction of halogen bond formation, which is divided by the number of neighbors of acceptor atom to establish final directional angle

base_angle_halogen [int (default=180)] Ideal base angle between halogen bond and halogen-neighbor bond

tolerance [int, (default=30)] Range (+/- tolerance) from perfect direction (base_angle/n_neighbors) in which halogen bonds are considered as strict.

Returns **mol1_atoms, mol2_atoms** : atom_dict-type numpy array

Aligned arrays of atoms forming halogen bond

strict [numpy array, dtype=bool] Boolean array align with atom pairs, informing whether atoms form 'strict' halogen bond (pass all angular cutoffs). If false, only distance cutoff is met, therefore the bond is 'crude'.

`oddt.interactions.pi_stacking(mol1, mol2, cutoff=5, tolerance=30)`

Returns pairs of rings, which meet pi stacking criteria

Parameters **mol1, mol2** : oddt.toolkit.Molecule object

Molecules to compute ring pairs

cutoff [float, (default=5)] Distance cutoff for Pi-stacking pairs

tolerance [int, (default=30)] Range (+/- tolerance) from perfect direction (parallel or perpendicular) in which pi-stackings are considered as strict.

Returns **r1, r2** : ring_dict-type numpy array

Aligned arrays of rings forming pi-stacking

strict_parallel [numpy array, dtype=bool] Boolean array align with ring pairs, informing whether rings form 'strict' parallel pi-stacking. If false, only distance cutoff is met, therefore the stacking is 'crude'.

strict_perpendicular [numpy array, dtype=bool] Boolean array align with ring pairs, informing whether rings form 'strict' perpendicular pi-stacking (T-shaped, T-face, etc.). If false, only distance cutoff is met, therefore the stacking is 'crude'.

`oddt.interactions.salt_bridge_plus_minus(mol1, mol2, cutoff=4)`

Returns pairs of plus-minus atoms, which meet salt bridge criteria

Parameters **mol1, mol2** : `oddt.toolkit.Molecule` object

Molecules to compute plus and minus pairs

cutoff [float, (default=4)] Distance cutoff for A-H pairs

Returns **plus, minus** : atom_dict-type numpy array

Aligned arrays of atoms forming salt bridge, firstly plus, secondly minus

`oddt.interactions.salt_bridges(mol1, mol2, *args, **kwargs)`

Calculates salt bridges between molecules

Parameters **mol1, mol2** : `oddt.toolkit.Molecule` object

Molecules to compute plus and minus pairs

cutoff [float, (default=4)] Distance cutoff for plus-minus pairs

Returns **mol1_atoms, mol2_atoms** : atom_dict-type numpy array

Aligned arrays of atoms forming salt bridges

`oddt.interactions.hydrophobic_contacts(mol1, mol2, cutoff=4)`

Calculates hydrophobic contacts between molecules

Parameters **mol1, mol2** : `oddt.toolkit.Molecule` object

Molecules to compute hydrophobe pairs

cutoff [float, (default=4)] Distance cutoff for hydrophobe pairs

Returns **mol1_atoms, mol2_atoms** : atom_dict-type numpy array

Aligned arrays of atoms forming hydrophobic contacts

`oddt.interactions.pi_cation(mol1, mol2, cutoff=5, tolerance=30)`

Returns pairs of ring-cation atoms, which meet pi-cation criteria

Parameters **mol1, mol2** : `oddt.toolkit.Molecule` object

Molecules to compute ring-cation pairs

cutoff [float, (default=5)] Distance cutoff for Pi-cation pairs

tolerance [int, (default=30)] Range (+/- tolerance) from perfect direction (perpendicular) in which pi-cation are considered as strict.

Returns **r1** : ring_dict-type numpy array

Aligned rings forming pi-stacking

plus2 [atom_dict-type numpy array] Aligned cations forming pi-cation

strict_parallel [numpy array, dtype=bool] Boolean array align with ring-cation pairs, informing whether they form 'strict' pi-cation. If false, only distance cutoff is met, therefore the interaction is 'crude'.

`oddt.interactions.acceptor_metal(mol1, mol2, base_angle=120, tolerance=30, cutoff=4)`

Returns pairs of acceptor-metal atoms, which meet metal coordination criteria Note: This function is directional (mol1 holds acceptors, mol2 holds metals)

Parameters **mol1, mol2** : `oddt.toolkit.Molecule` object

Molecules to compute acceptor and metal pairs

cutoff [float, (default=4)] Distance cutoff for A-M pairs

base_angle [int, (default=120)] Base angle determining allowed direction of metal coordination, which is divided by the number of neighbors of acceptor atom to establish final directional angle

tolerance [int, (default=30)] Range (+/- tolerance) from perfect direction (base_angle/n_neighbors) in metal coordination are considered as strict.

Returns **a, d** : atom_dict-type numpy array

Aligned arrays of atoms forming metal coordination, firstly acceptors, secondly metals.

strict [numpy array, dtype=bool] Boolean array align with atom pairs, informing whether atoms form 'strict' metal coordination (pass all angular cutoffs). If false, only distance cutoff is met, therefore the interaction is 'crude'.

`oddt.interactions.pi_metal(mol1, mol2, cutoff=5, tolerance=30)`

Returns pairs of ring-metal atoms, which meet pi-metal criteria

Parameters **mol1, mol2** : `oddt.toolkit.Molecule` object

Molecules to compute ring-metal pairs

cutoff [float, (default=5)] Distance cutoff for Pi-metal pairs

tolerance [int, (default=30)] Range (+/- tolerance) from perfect direction (perpendicular) in which pi-metal are considered as strict.

Returns **r1** : ring_dict-type numpy array

Aligned rings forming pi-metal

m [atom_dict-type numpy array] Aligned metals forming pi-metal

strict_parallel [numpy array, dtype=bool] Boolean array align with ring-metal pairs, informing whether they form 'strict' pi-metal. If false, only distance cutoff is met, therefore the interaction is 'crude'.

3.1.5 oddt.metrics module

Metrics for estimating performance of drug discovery methods implemented in ODDT

`oddt.metrics.roc(y_true, y_score, pos_label=None, sample_weight=None, drop_intermediate=True)`
 Compute Receiver operating characteristic (ROC)

Note: this implementation is restricted to the binary classification task.

Read more in the [User Guide](#).

Parameters **y_true** : array, shape = [n_samples]

True binary labels in range {0, 1} or {-1, 1}. If labels are not binary, pos_label should be explicitly given.

y_score : array, shape = [n_samples]

Target scores, can either be probability estimates of the positive class or confidence values.

pos_label : int

Label considered as positive and others are considered negative.

sample_weight : array-like of shape = [n_samples], optional

Sample weights.

drop_intermediate : boolean, optional (default=True)

Whether to drop some suboptimal thresholds which would not appear on a plotted ROC curve. This is useful in order to create lighter ROC curves.

New in version 0.17: parameter *drop_intermediate*.

Returns **fpr** : array, shape = [>2]

Increasing false positive rates such that element i is the false positive rate of predictions with score \geq thresholds[i].

tpr : array, shape = [>2]

Increasing true positive rates such that element i is the true positive rate of predictions with score \geq thresholds[i].

thresholds : array, shape = [n_thresholds]

Decreasing thresholds on the decision function used to compute fpr and tpr. *thresholds[0]* represents no instances being predicted and is arbitrarily set to $\max(y_score) + 1$.

See also:

roc_auc_score Compute Area Under the Curve (AUC) from prediction scores

Notes

Since the thresholds are sorted from low to high values, they are reversed upon returning them to ensure they correspond to both `fpr` and `tpr`, which are sorted in reversed order during their calculation.

References

[R1]

Examples

```
>>> import numpy as np
>>> from sklearn import metrics
>>> y = np.array([1, 1, 2, 2])
>>> scores = np.array([0.1, 0.4, 0.35, 0.8])
>>> fpr, tpr, thresholds = metrics.roc_curve(y, scores, pos_label=2)
>>> fpr
array([ 0. ,  0.5,  0.5,  1. ])
>>> tpr
array([ 0.5,  0.5,  1. ,  1. ])
>>> thresholds
array([ 0.8 ,  0.4 ,  0.35,  0.1 ])
```

`oddt.metrics.auc(x, y, reorder=False)`

Compute Area Under the Curve (AUC) using the trapezoidal rule

This is a general function, given points on a curve. For computing the area under the ROC-curve, see `roc_auc_score()`.

Parameters `x` : array, shape = [n]

x coordinates.

`y` : array, shape = [n]

y coordinates.

reorder : boolean, optional (default=False)

If True, assume that the curve is ascending in the case of ties, as for an ROC curve. If the curve is non-ascending, the result will be wrong.

Returns `auc` : float

See also:

roc_auc_score Computes the area under the ROC curve

precision_recall_curve Compute precision-recall pairs for different probability thresholds

Examples

```
>>> import numpy as np
>>> from sklearn import metrics
>>> y = np.array([1, 1, 2, 2])
>>> pred = np.array([0.1, 0.4, 0.35, 0.8])
>>> fpr, tpr, thresholds = metrics.roc_curve(y, pred, pos_label=2)
>>> metrics.auc(fpr, tpr)
0.75
```

`oddt.metrics.roc_auc(y_true, y_score, pos_label=None, ascending_score=True)`

Computes ROC AUC score

Parameters `y_true` : array, shape=[n_samples]

True binary labels, in range {0,1} or {-1,1}. If positive label is different than 1, it must be explicitly defined.

y_score [array, shape=[n_samples]] Scores for tested series of samples

pos_label: int Positive label of samples (if other than 1)

ascending_score: bool (default=True) Indicates if your score is ascending. Ascending score increases with decreasing activity. In other words it ascends on ranking list (where actives are on top).

Returns ef : float

Enrichment Factor for given percentage in range 0:1

`oddt.metrics.roc_log_auc(y_true, y_score, pos_label=None, ascending_score=True, log_min=0.001, log_max=1.0)`

Computes area under semi-log ROC for random distribution.

Parameters y_true : array, shape=[n_samples]

True binary labels, in range {0,1} or {-1,1}. If positive label is different than 1, it must be explicitly defined.

y_score [array, shape=[n_samples]] Scores for tested series of samples

pos_label: int Positive label of samples (if other than 1)

ascending_score: bool (default=True) Indicates if your score is ascending. Ascending score increases with decreasing activity. In other words it ascends on ranking list (where actives are on top).

log_min [float (default=0.001)] Minimum logarithm value for estimating AUC

log_max [float (default=1.)] Maximum logarithm value for estimating AUC.

Returns auc : float

semi-log ROC AUC

`oddt.metrics.enrichment_factor(y_true, y_score, percentage=1, pos_label=None)`

Computes enrichment factor for given percentage, i.e. EF_1% is enrichment factor for first percent of given samples.

Parameters y_true : array, shape=[n_samples]

True binary labels, in range {0,1} or {-1,1}. If positive label is different than 1, it must be explicitly defined.

y_score [array, shape=[n_samples]] Scores for tested series of samples

percentage [int or float] The percentage for which EF is being calculated

pos_label: int Positive label of samples (if other than 1)

Returns ef : float

Enrichment Factor for given percentage in range 0:1

`oddt.metrics.random_roc_log_auc(log_min=0.001, log_max=1.0)`

Computes area under semi-log ROC for random distribution.

Parameters log_min : float (default=0.001)

Minimum logarithm value for estimating AUC

log_max [float (default=1.)] Maximum logarithm value for estimating AUC.

Returns auc : float

semi-log ROC AUC for random distribution

`oddt.metrics.rmse(y_true, y_pred)`

Compute Root Mean Squared Error (RMSE)

Parameters y_true : array-like of shape = [n_samples] or [n_samples, n_outputs]

Ground truth (correct) target values.

y_pred [array-like of shape = [n_samples] or [n_samples, n_outputs]] Estimated target values.

Returns rmse : float

A positive floating point value (the best value is 0.0).

3.1.6 oddt.spatial module

Spatial functions included in ODDT Mainly used by other modules, but can be accessed directly.

`oddt.spatial.angle(p1, p2, p3)`

Returns an angle from a series of 3 points (point #2 is centroid). Angle is returned in degrees.

Parameters p1,p2,p3 : numpy arrays, shape = [n_points, n_dimensions]

Triplets of points in n-dimensional space, aligned in rows.

Returns angles : numpy array, shape = [n_points]

Series of angles in degrees

`oddt.spatial.angle_2v(v1, v2)`

Returns an angle between two vecors. Angle is returned in degrees.

Parameters v1,v2 : numpy arrays, shape = [n_vectors, n_dimensions]

Pairs of vectors in n-dimensional space, aligned in rows.

Returns angles : numpy array, shape = [n_vectors]

Series of angles in degrees

`oddt.spatial.dihedral(p1, p2, p3, p4)`

Returns an dihedral angle from a series of 4 points. Dihedral is returned in degrees. Function distinguishes clockwise and antyclockwise dihedrals.

Parameters p1,p2,p3,p4 : numpy arrays, shape = [n_points, n_dimensions]

Quadruplets of points in n-dimensional space, aligned in rows.

Returns angles : numpy array, shape = [n_points]

Series of angles in degrees

`oddt.spatial.distance(XA, XB, metric='euclidean', p=2, V=None, VI=None, w=None)`

Computes distance between each pair of the two collections of inputs.

The following are common calling conventions:

1. `Y = cdist(XA, XB, 'euclidean')`

Computes the distance between m points using Euclidean distance (2-norm) as the distance metric between the points. The points are arranged as m n -dimensional row vectors in the matrix X .

2. `Y = cdist(XA, XB, 'minkowski', p)`

Computes the distances using the Minkowski distance $\|u - v\|_p$ (p -norm) where $p \geq 1$.

3. `Y = cdist(XA, XB, 'cityblock')`

Computes the city block or Manhattan distance between the points.

4. `Y = cdist(XA, XB, 'seuclidean', V=None)`

Computes the standardized Euclidean distance. The standardized Euclidean distance between two n -vectors u and v is

$$\sqrt{\sum (u_i - v_i)^2 / V[x_i]}.$$

V is the variance vector; $V[i]$ is the variance computed over all the i 'th components of the points. If not passed, it is automatically computed.

5. `Y = cdist(XA, XB, 'sqeuclidean')`

Computes the squared Euclidean distance $\|u - v\|_2^2$ between the vectors.

6. `Y = cdist(XA, XB, 'cosine')`

Computes the cosine distance between vectors u and v ,

$$1 - \frac{u \cdot v}{\|u\|_2 \|v\|_2}$$

where $\|*\|_2$ is the 2-norm of its argument $*$, and $u \cdot v$ is the dot product of u and v .

7. `Y = cdist(XA, XB, 'correlation')`

Computes the correlation distance between vectors u and v . This is

$$1 - \frac{(u - \bar{u}) \cdot (v - \bar{v})}{\|(u - \bar{u})\|_2 \|(v - \bar{v})\|_2}$$

where \bar{v} is the mean of the elements of vector v , and $x \cdot y$ is the dot product of x and y .

8. `Y = cdist(XA, XB, 'hamming')`

Computes the normalized Hamming distance, or the proportion of those vector elements between two n -vectors u and v which disagree. To save memory, the matrix X can be of type boolean.

9. `Y = cdist(XA, XB, 'jaccard')`

Computes the Jaccard distance between the points. Given two vectors, u and v , the Jaccard distance is the proportion of those elements $u[i]$ and $v[i]$ that disagree where at least one of them is non-zero.

10. `Y = cdist(XA, XB, 'chebyshev')`

Computes the Chebyshev distance between the points. The Chebyshev distance between two n -vectors u and v is the maximum norm-1 distance between their respective elements. More precisely, the distance is given by

$$d(u, v) = \max_i |u_i - v_i|.$$

11. `Y = cdist(XA, XB, 'canberra')`

Computes the Canberra distance between the points. The Canberra distance between two points u and v is

$$d(u, v) = \sum_i \frac{|u_i - v_i|}{|u_i| + |v_i|}.$$

12.Y = cdist(XA, XB, 'braycurtis')

Computes the Bray-Curtis distance between the points. The Bray-Curtis distance between two points u and v is

$$d(u, v) = \frac{\sum_i (u_i - v_i)}{\sum_i (u_i + v_i)}$$

13.Y = cdist(XA, XB, 'mahalanobis', VI=None)

Computes the Mahalanobis distance between the points. The Mahalanobis distance between two points u and v is $(u - v)(1/V)(u - v)^T$ where $(1/V)$ (the `VI` variable) is the inverse covariance. If `VI` is not `None`, `VI` will be used as the inverse covariance matrix.

14.Y = cdist(XA, XB, 'yule')

Computes the Yule distance between the boolean vectors. (see *yule* function documentation)

15.Y = cdist(XA, XB, 'matching')

Computes the matching distance between the boolean vectors. (see *matching* function documentation)

16.Y = cdist(XA, XB, 'dice')

Computes the Dice distance between the boolean vectors. (see *dice* function documentation)

17.Y = cdist(XA, XB, 'kulsinski')

Computes the Kulsinski distance between the boolean vectors. (see *kulsinski* function documentation)

18.Y = cdist(XA, XB, 'rogerstanimoto')

Computes the Rogers-Tanimoto distance between the boolean vectors. (see *rogerstanimoto* function documentation)

19.Y = cdist(XA, XB, 'russellrao')

Computes the Russell-Rao distance between the boolean vectors. (see *russellrao* function documentation)

20.Y = cdist(XA, XB, 'sokalmichener')

Computes the Sokal-Michener distance between the boolean vectors. (see *sokalmichener* function documentation)

21.Y = cdist(XA, XB, 'sokalsneath')

Computes the Sokal-Sneath distance between the vectors. (see *sokalsneath* function documentation)

```
22.Y = cdist(XA, XB, 'wminkowski')
```

Computes the weighted Minkowski distance between the vectors. (see *wminkowski* function documentation)

```
23.Y = cdist(XA, XB, f)
```

Computes the distance between all pairs of vectors in X using the user supplied 2-arity function f. For example, Euclidean distance between the vectors could be computed as follows:

```
dm = cdist(XA, XB, lambda u, v: np.sqrt(((u-v)**2).sum()))
```

Note that you should avoid passing a reference to one of the distance functions defined in this library. For example,:

```
dm = cdist(XA, XB, sokalsneath)
```

would calculate the pair-wise distances between the vectors in X using the Python function *sokalsneath*. This would result in *sokalsneath* being called $\binom{n}{2}$ times, which is inefficient. Instead, the optimized C version is more efficient, and we call it using the following syntax:

```
dm = cdist(XA, XB, 'sokalsneath')
```

Parameters **XA** : ndarray

An m_A by n array of m_A original observations in an n -dimensional space. Inputs are converted to float type.

XB : ndarray

An m_B by n array of m_B original observations in an n -dimensional space. Inputs are converted to float type.

metric : str or callable, optional

The distance metric to use. If a string, the distance function can be 'braycurtis', 'canberra', 'chebyshev', 'cityblock', 'correlation', 'cosine', 'dice', 'euclidean', 'hamming', 'jaccard', 'kulsinski', 'mahalanobis', 'matching', 'minkowski', 'rogerstanimoto', 'russellrao', 'seuclidean', 'sokalmichener', 'sokalsneath', 'sqeuclidean', 'wminkowski', 'yule'.

w : ndarray, optional

The weight vector (for weighted Minkowski).

p : scalar, optional

The p-norm to apply (for Minkowski, weighted and unweighted)

V : ndarray, optional

The variance vector (for standardized Euclidean).

VI : ndarray, optional

The inverse of the covariance matrix (for Mahalanobis).

Returns **Y** : ndarray

A m_A by m_B distance matrix is returned. For each i and j , the metric $\text{dist}(u=XA[i], v=XB[j])$ is computed and stored in the ij th entry.

Raises ValueError

An exception is thrown if XA and XB do not have the same number of columns.

Examples

Find the Euclidean distances between four 2-D coordinates:

```
>>> from scipy.spatial import distance
>>> coords = [(35.0456, -85.2672),
...           (35.1174, -89.9711),
...           (35.9728, -83.9422),
...           (36.1667, -86.7833)]
>>> distance.cdist(coords, coords, 'euclidean')
array([[ 0.        ,  4.7044,  1.6172,  1.8856],
       [ 4.7044,  0.        ,  6.0893,  3.3561],
       [ 1.6172,  6.0893,  0.        ,  2.8477],
       [ 1.8856,  3.3561,  2.8477,  0.        ]])
```

Find the Manhattan distance from a 3-D point to the corners of the unit cube:

```
>>> a = np.array([[0, 0, 0],
...               [0, 0, 1],
...               [0, 1, 0],
...               [0, 1, 1],
...               [1, 0, 0],
...               [1, 0, 1],
...               [1, 1, 0],
...               [1, 1, 1]])
>>> b = np.array([[0.1, 0.2, 0.4]])
>>> distance.cdist(a, b, 'cityblock')
array([[ 0.7],
       [ 0.9],
       [ 1.3],
       [ 1.5],
       [ 1.5],
       [ 1.7],
       [ 2.1],
       [ 2.3]])
```

3.1.7 oddt.virtualscreening module

ODDT pipeline framework for virtual screening

class oddt.virtualscreening.**virtualscreening** (*n_cpu=-1, verbose=False*)

Virtual Screening pipeline stack

Parameters **n_cpu**: int (default=-1)

The number of parallel procesors to use

verbose: bool (default=False) Verbosity flag for some methods

Methods

<code>apply_filter(expression[, filter_type, ...])</code>	Filtering method, can use raw expressions (strings to be evaled in if statement)
<code>dock(engine, protein, *args, **kwargs)</code>	Docking procedure.
<code>fetch()</code>	
<code>load_ligands(fmt, ligands_file, *args, **kwargs)</code>	Loads file with ligands.
<code>score(function[, protein])</code>	Scoring procedure.
<code>write(fmt, filename[, csv_filename])</code>	Outputs molecules to a file
<code>write_csv(csv_filename[, keep_pipe])</code>	Outputs molecules to a csv file

apply_filter (*expression*, *filter_type*='expression', *soft_fail*=0)

Filtering method, can use raw expressions (strings to be evaled in if statement, can use `oddt.toolkit.Molecule` methods, eg. 'mol.molwt < 500') Currently supported presets:

- Lipinski Rule of 5 ('r5' or 'l5')
- Fragment Rule of 3 ('r3')

Parameters expression: string or list of strings

Expresion(s) to be used while filtering.

filter_type: 'expression' or 'preset' (default='expression') Specify filter type: 'expression' or 'preset'. Default strings are treated as expressions.

soft_fail: int (default=0) The number of faulures molecule can have to pass filter, aka. soft-fails.

dock (*engine*, *protein*, **args*, ***kwargs*)

Docking procedure.

Parameters engine: string

Which docking engine to use.

fetch ()

load_ligands (*fmt*, *ligands_file*, **args*, ***kwargs*)

Loads file with ligands.

Parameters file_type: string

Type of molecular file

ligands_file: string Path to a file, which is loaded to pipeline

score (*function*, *protein*=None, **args*, ***kwargs*)

Scoring procedure.

Parameters function: string

Which scoring function to use.

protein: oddt.toolkit.Molecule Default protein to use as reference

write (*fmt*, *filename*, *csv_filename*=None, ***kwargs*)

Outputs molecules to a file

Parameters file_type: string

Type of molecular file

ligands_file: string Path to a output file

csv_filename: string Optional path to a CSV file

write_csv (*csv_filename*, *keep_pipe=False*, ***kwargs*)

Outputs molecules to a csv file

Parameters **csv_filename: string**

Optional path to a CSV file

keep_pipe: bool (default=False) If set to True, the ligand pipe is sustained.

3.1.8 Module contents

Open Drug Discovery Toolkit

Universal and easy to use resource for various drug discovery tasks, ie docking, virtual screening, rescoring.

toolkit [module,] Toolkits backend module, currently OpenBabel [ob] and RDKit [rdk]. This setting is toolkit-wide, and sets given toolkit as default

References

To be announced.

Documentation Indices and tables

- [genindex](#)
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Bibliography

[R1] [Wikipedia entry for the Receiver operating characteristic](#)

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