
PyBrain Documentation

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The documentation is build up in the following parts: first, there is the quickstart tutorial which aims at getting you started with PyBrain as quickly as possible. This is the right place for you if you just want get a feel for the library or if you never used PyBrain before.

Although the quickstart uses supervised learning with neural networks as an example, this does not mean that that's it. PyBrain is not only about supervised learning and neural networks.

While the quickstart should be read sequentially, the tutorial chapters can mostly be read independently of each other.

In case this does not suffice, we also have an API reference, the *Module Index*. Most of the packages and modules of PyBrain are auto-documented there.

If at any point the documentation does not suffice, you can always get help at the pybrain Google Group at <http://groups.google.com/group/pybrain>.

INSTALLATION

Quick answer:

```
$ git clone git://github.com/pybrain/pybrain.git  
$ python setup.py install
```

Long answer: We keep more detailed installation instructions (including dependencies) up-to-date in a wiki at <http://wiki.github.com/pybrain/pybrain/installation>.

QUICKSTART

2.1 Building a Network

To go through the quickstart interactively, just fire up Python and we will make everything in the interpreter:

```
$ python
Python 2.5.2 (r252:60911, Sep 17 2008, 11:21:23)
[GCC 4.0.1 (Apple Inc. build 5465)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

In PyBrain, networks are composed of Modules which are connected with Connections. You can think of a network as a directed acyclic graph, where the nodes are Modules and the edges are Connections. This makes PyBrain very flexible but it is also not necessary in all cases.

2.1.1 The buildNetwork Shortcut

Thus, there is a simple way to create networks, which is the `buildNetwork` shortcut:

```
>>> from pybrain.tools.shortcuts import buildNetwork
>>> net = buildNetwork(2, 3, 1)
```

This call returns a network that has two inputs, three hidden and a single output neuron. In PyBrain, these layers are Module objects and they are already connected with `FullConnection` objects.

2.1.2 Activating a Network

The net is already initialized with random values - we can already calculate its output:

```
>>> net.activate([2, 1])
array([-0.98646726])
```

For this we use the `.activate()` method, which expects a list, tuple or an array as input.

2.1.3 Examining the structure

How can we examine the structure of our network somewhat closer? In PyBrain, every part of a network has a name by which you can access it. When building networks with the `buildNetwork` shortcut, the parts are named automatically:

```
>>> net['in']
<LinearLayer 'in'>
>>> net['hidden0']
<SigmoidLayer 'hidden0'>
>>> net['out']
<LinearLayer 'out'>
```

The hidden layers have numbers at the end in order to distinguish between those.

2.1.4 More sophisticated Networks

Of course, we want more flexibility when building up networks. For instance, the hidden layer is constructed with the sigmoid squashing function per default: but in a lot of cases, this is not what we want. We can also supply different types of layers:

```
>>> from pybrain.structure import TanhLayer
>>> net = buildNetwork(2, 3, 1, hiddenclass=TanhLayer)
>>> net['hidden0']
<TanhLayer 'hidden0'>
```

There is more we can do. For example, we can also set a different class for the output layer:

```
>>> from pybrain.structure import SoftmaxLayer
>>> net = buildNetwork(2, 3, 2, hiddenclass=TanhLayer, outclass=SoftmaxLayer)
>>> net.activate((2, 3))
array([ 0.6656323,  0.3343677])
```

We can also tell the network to use a bias:

```
>>> net = buildNetwork(2, 3, 1, bias=True)
>>> net['bias']
<BiasUnit 'bias'>
```

This approach has of course some restrictions: for example, we can only construct a feedforward topology. But it is possible to create very sophisticated architectures with PyBrain, and it is also one of the library's strength to do so.

2.2 Building a DataSet

In order for our networks to learn anything, we need a dataset that contains inputs and targets. PyBrain has the `pybrain.dataset` package for this, and we will use the `SupervisedDataSet` class for our needs.

2.2.1 A customized DataSet

The `SupervisedDataSet` class is used for standard supervised learning. It supports input and target values, whose size we have to specify on object creation:

```
>>> from pybrain.datasets import SupervisedDataSet
>>> ds = SupervisedDataSet(2, 1)
```

Here we have generated a dataset that supports two dimensional inputs and one dimensional targets.

2.2.2 Adding samples

A classic example for neural network training is the XOR function, so let's just build a dataset for this. We can do this by just adding samples to the dataset:

```
>>> ds.addSample((0, 0), (0,))
>>> ds.addSample((0, 1), (1,))
>>> ds.addSample((1, 0), (1,))
>>> ds.addSample((1, 1), (0,))
```

2.2.3 Examining the dataset

We now have a dataset that has 4 samples in it. We can check that with python's idiomatic way of checking the size of something:

```
>>> len(ds)
4
```

We can also iterate over it in the standard way:

```
>>> for inpt, target in ds:
...     print inpt, target
...
[ 0.  0.] [ 0.]
[ 0.  1.] [ 1.]
[ 1.  0.] [ 1.]
[ 1.  1.] [ 0.]
```

We can access the input and target field directly as arrays:

```
>>> ds['input']
array([[ 0.,  0.],
       [ 0.,  1.],
       [ 1.,  0.],
       [ 1.,  1.]])
>>> ds['target']
array([[ 0.],
       [ 1.],
       [ 1.],
       [ 0.]])
```

It is also possible to clear a dataset again, and delete all the values from it:

```
>>> ds.clear()
>>> ds['input']
array([], shape=(0, 2), dtype=float64)
>>> ds['target']
array([], shape=(0, 1), dtype=float64)
```

2.3 Training your Network on your Dataset

For adjusting parameters of modules in supervised learning, PyBrain has the concept of trainers. Trainers take a module and a dataset in order to train the module to fit the data in the dataset.

A classic example for training is backpropagation. PyBrain comes with backpropagation, of course, and we will use the `BackpropTrainer` here:

```
>>> from pybrain.supervised.trainers import BackpropTrainer
```

We have already build a dataset for XOR and we have also learned to build networks that can handle such problems. Let's just connect the two with a trainer:

```
>>> net = buildNetwork(2, 3, 1, bias=True, hiddenclass=TanhLayer)
>>> trainer = BackpropTrainer(net, ds)
```

The trainer now knows about the network and the dataset and we can train the net on the data:

```
>>> trainer.train()
0.31516384514375834
```

This call trains the net for one full epoch and returns a double proportional to the error. If we want to train the network until convergence, there is another method:

```
>>> trainer.trainUntilConvergence()
...
```

This returns a whole bunch of data, which is nothing but a tuple containing the errors for every training epoch.

TUTORIALS

3.1 Introduction

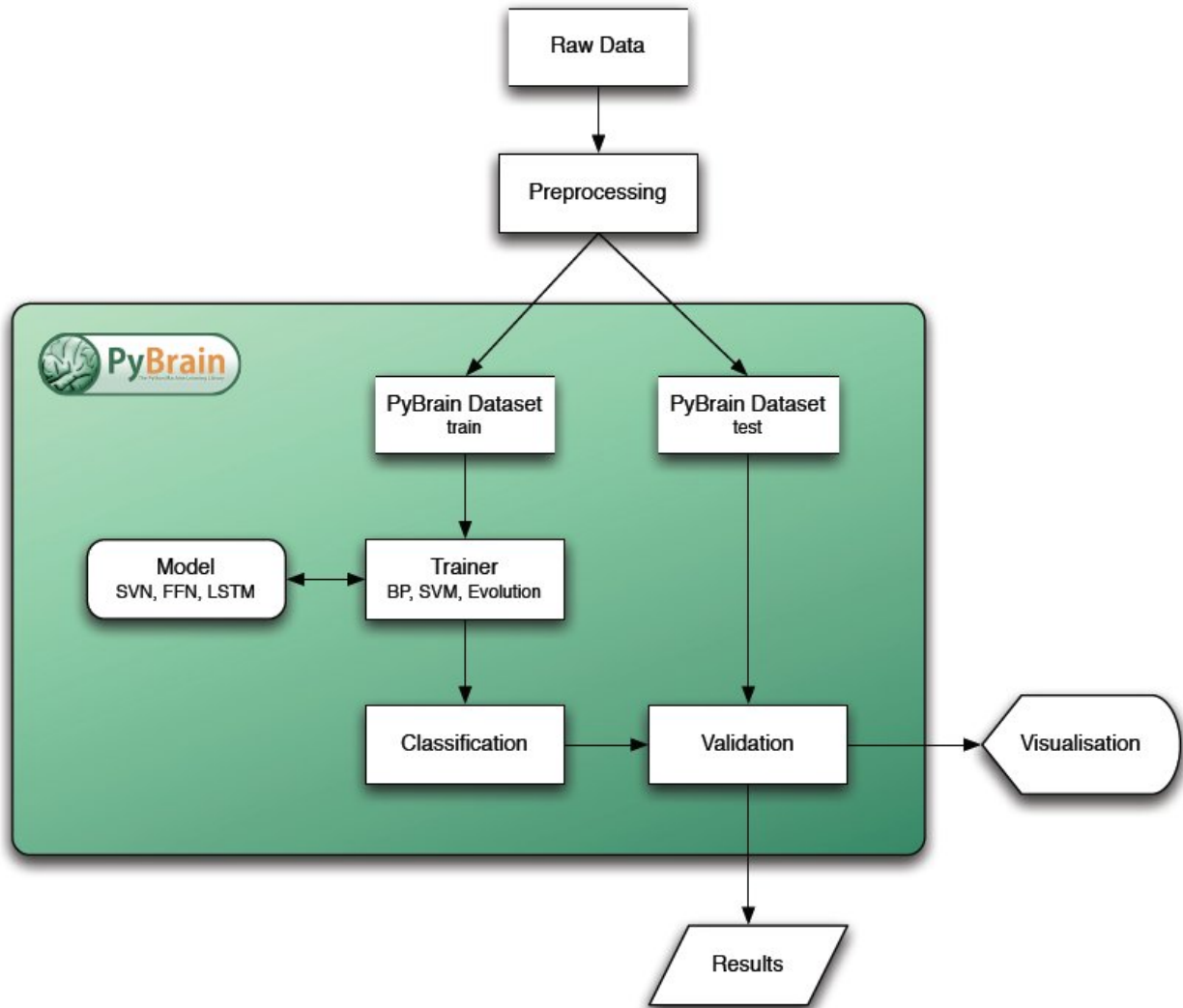
PyBrain's concept is to encapsulate different data processing algorithms in what we call a `Module`. A minimal `Module` contains a forward implementation depending on a collection of free parameters that can be adjusted, usually through some machine learning algorithm.

Modules have an input and an output buffer, plus corresponding error buffers which are used in error backpropagation algorithms.

They are assembled into objects of the class `Network` and are connected via `Connection` objects. These may contain a number of adjustable parameters themselves, such as weights.

Note that a `Network` itself is again a `Module`, such that it is easy to build hierarchical networks as well. Shortcuts exist for building the most common network architectures, but in principle this system allows almost arbitrary connectionist systems to be assembled, as long as they form a directed acyclic graph.

The free parameters of the `Network` are adjusted by means of a `Trainer`, which uses a `Dataset` to learn the optimum parameters from examples. For reinforcement learning experiments, a simulation environment with an associated optimization task is used instead of a `Dataset`.



3.2 Building Networks with Modules and Connections

This chapter will guide you to use PyBrain's most basic structural elements: the `FeedForwardNetwork` and `RecurrentNetwork` classes and with them the `Module` class and the `Connection` class. We have already seen how to create networks with the `buildNetwork` shortcut - but since this technique is limited in some ways, we will now explore how to create networks from the ground up.

3.2.1 Feed Forward Networks

We will start with a simple example, building a multi layer perceptron.

First we make a new `FeedForwardNetwork` object:

```
>>> from pybrain.structure import FeedForwardNetwork
>>> n = FeedForwardNetwork()
```

Next, we're constructing the input, hidden and output layers:

```
>>> from pybrain.structure import LinearLayer, SigmoidLayer
>>> inLayer = LinearLayer(2)
>>> hiddenLayer = SigmoidLayer(3)
>>> outLayer = LinearLayer(1)
```

There are a couple of different classes of layers. For a complete list check out the `modules` package.

In order to use them, we have to add them to the network:

```
>>> n.addInputModule(inLayer)
>>> n.addModule(hiddenLayer)
>>> n.addOutputModule(outLayer)
```

We can actually add multiple input and output modules. The net has to know which of its modules are input and output modules, in order to forward propagate input and to back propagate errors.

It still needs to be explicitly determined how they should be connected. For this we use the most common connection type, which produces a full connectivity between layers, by connecting each neuron of one layer with each neuron of the other. This is implemented by the `FullConnection` class:

```
>>> from pybrain.structure import FullConnection
>>> in_to_hidden = FullConnection(inLayer, hiddenLayer)
>>> hidden_to_out = FullConnection(hiddenLayer, outLayer)
```

As with modules, we have to explicitly add them to the network:

```
>>> n.addConnection(in_to_hidden)
>>> n.addConnection(hidden_to_out)
```

All the elements are in place now, so we can do the final step that makes our MLP usable, which is to call the `.sortModules()` method:

```
>>> n.sortModules()
```

This call does some internal initialization which is necessary before the net can finally be used: for example, the modules are sorted topologically.

3.2.2 Examining a Network

We can actually print networks and examine their structure:

```
>>> print n
FeedForwardNetwork-6
Modules:
[<LinearLayer 'LinearLayer-3'>, <SigmoidLayer 'SigmoidLayer-7'>, <LinearLayer 'LinearLayer-8'>]
Connections:
[<FullConnection 'FullConnection-4': 'LinearLayer-3' -> 'SigmoidLayer-7'>, <FullConnection 'FullConn
```

Note that the output on your machine will not necessarily be the same.

One way of using the network is to call its `'activate()'` method with an input to be transformed:

```
>>> n.activate([1, 2])
array([-0.11302355])
```

Again, this might look different on your machine - the weights of the connections have already been initialized randomly. To have a look at those parameters, just check the `.params` field of the connections:

We can access the trainable parameters (weights) of a connection directly, or read all weights of the network at once:

```
>>> in_to_hidden.params
array([ 1.37751406,  1.39320901, -0.24052686, -0.67970042, -0.5999425 , -1.27774679])
>>> hidden_to_out.params
array([-0.32156782,  1.09338421,  0.48784924])
```

The network encapsulating the modules actually holds the parameters too. You can check them out here:

```
>>> n.params
array([ 1.37751406,  1.39320901, -0.24052686, -0.67970042, -0.5999425 ,
        -1.27774679, -0.32156782,  1.09338421,  0.48784924])
```

As you can see, the last three parameters of the network equal the parameters of the second connection.

3.2.3 Naming your Networks structure

In some settings it makes sense to give the parts of a network explicit identifiers. The structural components are derived from the `Named` class, which means that they have an attribute `.name` by which you can identify it by. If no name is given, a new name will be generated automatically.

Subclasses can also be named by passing the `name` argument on initialization:

```
>>> LinearLayer(2)
<LinearLayer 'LinearLayer-11'>
>>> LinearLayer(2, name="foo")
<LinearLayer 'foo'>
```

By using names for your networks, printouts look more concise and readable. They also ensure that your network components are named in the same way every time you run your program.

3.2.4 Using Recurrent Networks

In order to allow recurrency, networks have to be able to “look back in time”. Due to this, the `RecurrentNetwork` class is different from the `FeedForwardNetwork` class in the substantial way, that the complete history is saved. This is actually memory consuming, but necessary for some learning algorithms.

To create a recurrent network, just do as with feedforward networks but use the appropriate class:

```
>>> from pybrain.structure import RecurrentNetwork
>>> n = RecurrentNetwork()
```

We will quickly build up a network that is the same as in the example above:

```
>>> n.addInputModule(LinearLayer(2, name='in'))
>>> n.addModule(SigmoidLayer(3, name='hidden'))
>>> n.addOutputModule(LinearLayer(1, name='out'))
>>> n.addConnection(FullConnection(n['in'], n['hidden'], name='c1'))
>>> n.addConnection(FullConnection(n['hidden'], n['out'], name='c2'))
```

The `RecurrentNetwork` class has one additional method, `.addRecurrentConnection()`, which looks back in time one timestep. We can add one from the hidden to the hidden layer:


```
>>> n.addRecurrentConnection(FullConnection(n['hidden'], n['hidden'], name='c3'))
```

If we now activate the network, we will get different outputs each time:

```
>>> n.sortModules()
>>> n.activate((2, 2))
array([-0.1959887])
>>> n.activate((2, 2))
array([-0.19623716])
>>> n.activate((2, 2))
array([-0.19675801])
```

Of course, we can clear the history of the network. This can be done by calling the *reset* method:

```
>>> n.reset()
>>> n.activate((2, 2))
array([-0.1959887])
>>> n.activate((2, 2))
array([-0.19623716])
>>> n.activate((2, 2))
array([-0.19675801])
```

After the call to `.reset()`, we are getting the same outputs as just after the objects creation.

3.3 Classification with Feed-Forward Neural Networks

This tutorial walks you through the process of setting up a dataset for classification, and train a network on it while visualizing the results online.

First we need to import the necessary components from PyBrain.

```
from pybrain.datasets          import ClassificationDataSet
from pybrain.utilities         import percentError
from pybrain.tools.shortcuts   import buildNetwork
from pybrain.supervised.trainers import BackpropTrainer
from pybrain.structure.modules import SoftmaxLayer
```

Furthermore, pylab is needed for the graphical output.

```
from pylab import ion, ioff, figure, draw, contourf, clf, show, hold, plot
from scipy import diag, arange, meshgrid, where
from numpy.random import multivariate_normal
```

To have a nice dataset for visualization, we produce a set of points in 2D belonging to three different classes. You could also read in your data from a file, e.g. using `pylab.load()`.

```
means = [(-1,0), (2,4), (3,1)]
cov = [diag([1,1]), diag([0.5,1.2]), diag([1.5,0.7])]
alldata = ClassificationDataSet(2, 1, nb_classes=3)
for n in xrange(400):
    for klass in range(3):
        input = multivariate_normal(means[klass], cov[klass])
        alldata.addSample(input, [klass])
```

Randomly split the dataset into 75% training and 25% test data sets. Of course, we could also have created two different datasets to begin with.

```
tstdata, trndata = alldata.splitWithProportion( 0.25 )
```

For neural network classification, it is highly advisable to encode classes with one output neuron per class. Note that this operation duplicates the original targets and stores them in an (integer) field named 'class'.

```
trndata._convertToOneOfMany( )
tstdata._convertToOneOfMany( )
```

Test our dataset by printing a little information about it.

```
print "Number of training patterns: ", len(trndata)
print "Input and output dimensions: ", trndata.indim, trndata.outdim
print "First sample (input, target, class):"
print trndata['input'][0], trndata['target'][0], trndata['class'][0]
```

Now build a feed-forward network with 5 hidden units. We use the shortcut `buildNetwork()` for this. The input and output layer size must match the dataset's input and target dimension. You could add additional hidden layers by inserting more numbers giving the desired layer sizes.

The output layer uses a softmax function because we are doing classification. There are more options to explore here, e.g. try changing the hidden layer transfer function to linear instead of (the default) sigmoid.

See Also:

Description `buildNetwork()` for more info on options, and the Network tutorial [Building Networks with Modules and Connections](#) for info on how to build your own non-standard networks.

```
fnn = buildNetwork( trndata.indim, 5, trndata.outdim, outclass=SoftmaxLayer )
```

Set up a trainer that basically takes the network and training dataset as input. For a list of trainers, see `trainers`. We are using a `BackpropTrainer` for this.

```
trainer = BackpropTrainer( fnn, dataset=trndata, momentum=0.1, verbose=True, weightdecay=0.01)
```

Now generate a square grid of data points and put it into a dataset, which we can then classify to obtain a nice contour field for visualization. Therefore the target values for this data set can be ignored.

```
ticks = arange(-3., 6., 0.2)
X, Y = meshgrid(ticks, ticks)
# need column vectors in dataset, not arrays
griddata = ClassificationDataSet(2, 1, nb_classes=3)
for i in xrange(X.size):
    griddata.addSample([X.ravel()[i], Y.ravel()[i]], [0])
griddata._convertToOneOfMany() # this is still needed to make the fnn feel comfy
```

Start the training iterations.

```
for i in range(20):
```

Train the network for some epochs. Usually you would set something like 5 here, but for visualization purposes we do this one epoch at a time.

```
...
    trainer.trainEpochs( 1 )
```

Evaluate the network on the training and test data. There are several ways to do this - check out the `pybrain.tools.validation` module, for instance. Here we let the trainer do the test.

```
...
trnresult = percentError( trainer.testOnClassData(),
                          trndata['class'] )
tstresult = percentError( trainer.testOnClassData(
    dataset=tstdata ), tstdata['class'] )

print "epoch: %4d" % trainer.totalepochs, \
      "  train error: %5.2f%%" % trnresult, \
      "  test error: %5.2f%%" % tstresult
```

Run our grid data through the FNN, get the most likely class and shape it into a square array again.

```
...
out = fnn.activateOnDataset(griddata)
out = out.argmax(axis=1) # the highest output activation gives the class
out = out.reshape(X.shape)
```

Now plot the test data and the underlying grid as a filled contour.

```
...
figure(1)
ioff() # interactive graphics off
clf() # clear the plot
hold(True) # overplot on
for c in [0,1,2]:
    here, _ = where(tstdata['class']==c)
    plot(tstdata['input'][here,0],tstdata['input'][here,1],'o')
if out.max()!=out.min(): # safety check against flat field
    contourf(X, Y, out) # plot the contour
ion() # interactive graphics on
draw() # update the plot
```

Finally, keep showing the plot until user kills it.

```
ioff()
show()
```

3.4 Using Datasets

Datasets are useful for allowing comfortable access to training, test and validation data. Instead of having to mangle with arrays, PyBrain gives you a more sophisticated datastructure that allows easier work with your data.

For the different tasks that arise in machine learning, there is a special dataset type, possibly with a few sub-types. The different types share some common functionality, which we'll discuss first.

A dataset can be seen as a collection of named 2d-arrays, called *fields* in this context. For instance, if DS implements `DataSet`:

```
inp = DS['input']
```

returns the input field. The last dimension of this field corresponds to the input dimension, such that

```
inp[0,:]
```

would yield the first input vector. In most cases there is also a field named ‘target’, which follows the same rules. However, didn’t we say we will spare you the array mangling? Well, in most cases you will want iterate over a dataset like so:

```
for inp, targ in DS:
    ...
```

Note that whether you get one, two, or more sample rows as a return depends on the number of *linked fields* in the DataSet: These are fields containing the same number of samples and assumed to be used together, like the above ‘input’ and ‘target’ fields. You can always check the DS.link property to see which fields are linked.

Similarly, DataSets can be created by adding samples one-by-one – the cleaner but slower method – or by assembling them from arrays.

```
for inp, targ in samples:
    DS.appendLinked(inp, targ)
# or alternatively, with ia and ta being arrays:
assert(ia.shape[0] == ta.shape[0])
DS.setField('input', ia)
DS.setField('target', ta)
```

In the latter case DS cannot check the linked array dimensions for you, otherwise it would not be possible to build a dataset from scratch.

You may add your own linked or unlinked data to the dataset. However, note that many training algorithms iterate over the linked fields and may fail if their number has changed:

```
DS.addField('myfield')
DS.setField('myfield', myarray)
DS.linkFields('input','target','myfield') # must provide complete list here
```

A useful utility method for quick generation of randomly picked training and testing data is also provided:

```
>>> len(DS)
100
>>> TrainDS, TestDS = DS.splitWithProportion(0.8)
>>> len(TrainDS), len(TestDS)
(80, 20)
```

3.4.1 supervised – Dataset for Supervised Regression Training

As the name says, this simplest form of a dataset is meant to be used with supervised learning tasks. It is comprised of the fields ‘input’ and ‘target’, the pattern size of which must be set upon creation:

```
>>> from pybrain.datasets import SupervisedDataSet
>>> DS = SupervisedDataSet( 3, 2 )
>>> DS.appendLinked( [1,2,3], [4,5] )
>>> len(DS)
1
>>> DS['input']
array([[ 1.,  2.,  3.]])
```

3.4.2 *sequential – Dataset for Supervised Sequences Regression Training*

This dataset introduces the concept of *sequences*. With this we are moving further away from the array mangling towards something more practical for sequence learning tasks. Essentially, its patterns are subdivided into sequences of variable length, that can be accessed via the methods

```
getNumSequences()
getSequence(index)
getSequenceLength(index)
```

Creating a `Sequentialdataset` is no different from its parent, since it still contains only ‘input’ and ‘target’ fields. `Sequentialdataset` inherits from `SupervisedDataSet`, which can be seen as a special case with a sequence length of 1 for all sequences.

To fill the dataset with content, it is advisable to call `newSequence()` at the start of each sequence to be stored, and then add patterns by using `appendLinked()` as above. This way, the class handles indexing and such transparently. One can theoretically construct a `Sequentialdataset` directly from arrays, but messing with the `index` field is not recommended.

A typical way of iterating over a sequence dataset `DS` would be something like:

```
for i in range(DS.getNumSequences):
    for input, target in DS.getSequenceIterator(i):
        # do stuff
```

3.4.3 *classification – Datasets for Supervised Classification Training*

The purpose of this dataset is to facilitate dealing with classification problems, whereas the above are more geared towards regression. Its ‘target’ field is defined as integer, and it contains an extra field called ‘class’ which is basically an automated backup of the targets, for reasons that we be apparent shortly. For the most part, you don’t have to bother with it. Initialization requires something like:

```
DS = ClassificationDataSet(inputdim, nb_classes=2, class_labels=['Fish', 'Chips'])
```

The labels are optional, and mainly used for documentation. Target dimension is supposed to be 1. The targets are class labels starting from zero. If for some reason you don’t know beforehand how many you have, or you fiddled around with the `setField()` method, it is possible to regenerate the class information using `assignClasses()`, or `calculateStatistics()`:

```
>>> DS = ClassificationDataSet(2, class_labels=['Urd', 'Verdandi', 'Skuld'])
>>> DS.appendLinked([ 0.1, 0.5 ], [0])
>>> DS.appendLinked([ 1.2, 1.2 ], [1])
>>> DS.appendLinked([ 1.4, 1.6 ], [1])
>>> DS.appendLinked([ 1.6, 1.8 ], [1])
>>> DS.appendLinked([ 0.10, 0.80 ], [2])
>>> DS.appendLinked([ 0.20, 0.90 ], [2])

>>> DS.calculateStatistics()
{0: 1, 1: 3, 2: 2}
>>> print DS.classHist
{0: 1, 1: 3, 2: 2}
>>> print DS.nClasses
3
>>> print DS.getClass(1)
Verdandi
```

```
>>> print DS.getField('target').transpose()
[[0 1 1 1 2 2]]
```

When doing classification, many algorithms work better if classes are encoded into one output unit per class, that takes on a certain value if the class is present. As an advanced feature, `ClassificationDataSet` does this conversion automatically:

```
>>> DS._convertToOneOfMany(bounds=[0, 1])
>>> print DS.getField('target')
[[1 0 0]
 [0 1 0]
 [0 1 0]
 [0 1 0]
 [0 0 1]
 [0 0 1]]
>>> print DS.getField('class').transpose()
[[0 1 1 1 2 2]]
>>> DS._convertToClassNb()
>>> print DS.getField('target').transpose()
[[0 1 1 1 2 2]]
```

In case you want to do sequence classification, there is also a `SequenceClassificationDataSet`, which combines the features of this class and the `Sequentialdataset`.

3.4.4 importance – Datasets for Weighted Supervised Training

This is another extension of `Sequentialdataset` that allows assigning different weights to patterns. Essentially, it works like its parent, except comprising another linked field named 'importance', which should contain a value between 0.0 and 1.0 for each pattern. A `Sequentialdataset` is a special case with all weights equal to 1.0.

We have packed this functionality into a different class because it is rarely used and drains some computational resources. So far, there is no corresponding non-sequential dataset class.

3.5 Black-box Optimization

This tutorial will illustrate how to use the optimization algorithms in PyBrain.

Very many practical problems can be framed as optimization problems: finding the best settings for a controller, minimizing the risk of an investment portfolio, finding a good strategy in a game, etc. It always involves determining a certain number of *variables* (the *problem dimension*), each of them chosen from a set, that maximizing (or minimize) a given *objective function*.

The main categories of optimization problems are based on the kinds of sets the variables are chosen from:

- all real numbers: continuous optimization
- real numbers with bounds: constrained optimization
- integers: integer programming
- combinations of the above
- others, e.g. graphs

These can be further classified according to properties of the objective function (e.g. continuity, explicit access to partial derivatives, quadratic form, etc.). In black-box optimization the objective function is a black box, i.e. there are

no conditions about it. The optimization tools that PyBrain provides are all for the most general, black-box case. They fall into 2 groups:

- `BlackBoxOptimizer` are applicable to all kinds of variable sets
- `ContinuousOptimizer` can only be used for continuous optimization

We will introduce the optimization framework for the more restrictive kind first, because that case is simpler.

3.5.1 Continuous optimization

Let's start by defining a simple objective function for (numpy arrays of) continuous variables, e.g. the sum of squares:

```
>>> def objF(x): return sum(x**2)
```

and an initial guess for where to start looking:

```
>>> x0 = array([2.1, -1])
```

Now we can initialize one of the optimization algorithms, e.g. CMAES:

```
>>> from pybrain.optimization import CMAES
>>> l = CMAES(objF, x0)
```

By default, all optimization algorithms *maximize* the objective function, but you can change this by setting the `minimize` attribute:

```
>>> l.minimize = True
```

Note: We could also have done that upon construction: `CMAES(objF, x0, minimize = True)`

Stopping criteria can be algorithm-specific, but in addition, it is always possible to define the following ones:

- maximal number of evaluations
- maximal number of learning steps
- reaching a desired value

```
>>> l.maxEvaluations = 200
```

Now that the optimizer is set up, all we need to use is the `learn()` method, which will attempt to optimize the variables until a stopping criterion is reached. It returns a tuple with the best evaluable (= array of variables) found, and the corresponding fitness:

```
>>> l.learn()
(array([-1.59778097e-05, -1.14434779e-03]), 1.3097871509722648e-06)
```

3.5.2 General optimization: using `Evolvable`

Our approach to doing optimization in the most general setting (no assumptions about the variables) is to let the user define a subclass of `Evolvable` that implements:

- a `copy()` operator,
- a method for generating random other points: `randomize()`,
- `mutate()`, an operator that does a small step in search space, according to *some* distance metric,

- (optionally) a `crossover()` operator that produces *some* combination with other evolvables of the same class.

The optimization algorithm is then initialized with an instance of this class and an objective function that can evaluate such instances.

Here's a minimalistic example of such a subclass with a single constrained variable (and a bias to do mutation steps toward larger values):

```
>>> from random import random
>>> from pybrain.structure.evolvables.evolvable import Evolvable
>>> class SimpleEvo(Evolvable):
...     def __init__(self, x): self.x = max(0, min(x, 10))
...     def mutate(self):      self.x = max(0, min(self.x + random() - 0.3, 10))
...     def copy(self):        return SimpleEvo(self.x)
...     def randomize(self):    self.x = 10*random()
...     def __repr__(self):     return '<-%.2f->' + str(self.x)
```

which can be optimized using, for example, `HillClimber`:

```
>>> from pybrain.optimization import HillClimber
>>> x0 = SimpleEvo(1.2)
>>> l = HillClimber(lambda x: x.x, x0, maxEvaluations = 50)
>>> l.learn()
(<-10.00->, 10)
```

3.5.3 Optimization in Reinforcement Learning

This section illustrates how to use optimization algorithms in the reinforcement learning framework.

As our objective function we use any episodic task, e.g:

```
>>> from pybrain.rl.environments.cartpole.balancetask import BalanceTask
>>> task = BalanceTask()
```

Then we construct a module that can interact with the task, for example a neural network controller,

```
>>> from pybrain.tools.shortcuts import buildNetwork
>>> net = buildNetwork(task.outdim, 3, task.indim)
```

and we choose any optimization algorithm, e.g. a simple `HillClimber`.

Now, we have 2 (equivalent) ways for connecting those:

1. using the same syntax as before, where the task plays the role of the objective function directly:

```
>>> HillClimber(task, net, maxEvaluations = 100).learn()
```

2. or, using the agent-based framework:

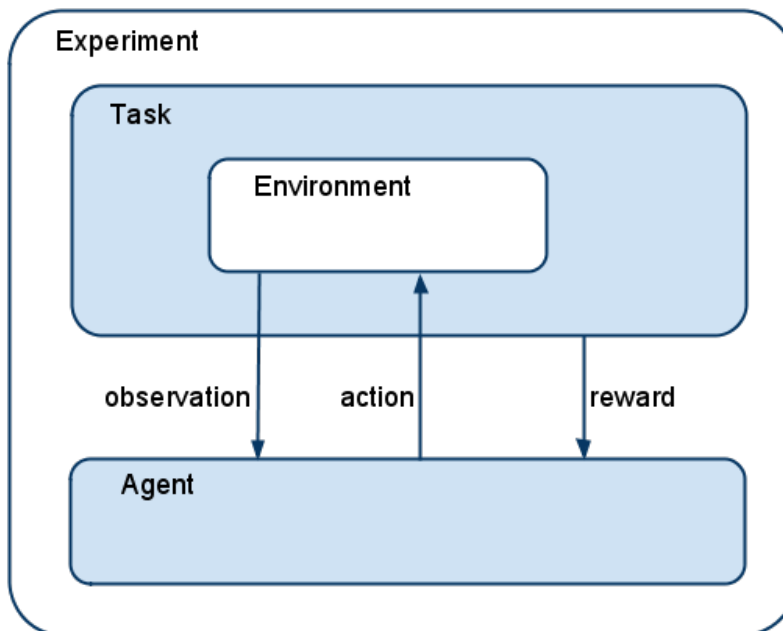
```
>>> from pybrain.rl.agents import OptimizationAgent
>>> from pybrain.rl.experiments import EpisodicExperiment
>>> agent = OptimizationAgent(net, HillClimber())
>>> exp = EpisodicExperiment(task, agent)
>>> exp.doEpisodes(100)
```

Note: This is very similar to the typical (non-optimization) reinforcement learning setup, the key difference being the use of a `LearningAgent` instead of an `OptimizationAgent`.


```
>>> from pybrain.rl.learners import ENAC
>>> from pybrain.rl.agents import LearningAgent
>>> agent = LearningAgent(net, ENAC())
>>> exp = EpisodicExperiment(task, agent)
>>> exp.doEpisodes(100)
```

3.6 Reinforcement Learning

A reinforcement learning (RL) task in PyBrain always consists of a few components that interact with each other: Environment, Agent, Task, and Experiment. In this tutorial we will go through each of them, create the instances and explain what they do.



But first of all, we need to import some general packages and the RL components from PyBrain:

```
from scipy import *
import sys, time

from pybrain.rl.environments.mazes import Maze, MDP MazeTask
from pybrain.rl.learners.valuebased import ActionValueTable
from pybrain.rl.agents import LearningAgent
from pybrain.rl.learners import Q, SARSA
```

```
from pybrain.rl.experiments import Experiment
from pybrain.rl.environments import Task
```

Note: You can directly run the code in this tutorial by running the script `docs/tutorials/rl.py`.

For later visualization purposes, we also need to initialize the plotting engine (interactive mode).

```
import pylab
pylab.gray()
pylab.ion()
```

The Environment is the world, in which the agent acts. It receives input with the `performAction()` method and returns an output with `getSensors()`. All environments in PyBrain are located under `pybrain/rl/environments`.

One of these environments is the maze environment, which we will use for this tutorial. It creates a labyrinth with free fields, walls, and an goal point. An agent can move over the free fields and needs to find the goal point. Let's define the maze structure, a simple 2D numpy array, where 1 is a wall and 0 is a free field:

```
structure = array([[1, 1, 1, 1, 1, 1, 1, 1, 1],
                  [1, 0, 0, 1, 0, 0, 0, 0, 1],
                  [1, 0, 0, 1, 0, 0, 1, 0, 1],
                  [1, 0, 0, 1, 0, 0, 1, 0, 1],
                  [1, 0, 0, 1, 0, 1, 1, 0, 1],
                  [1, 0, 0, 0, 0, 0, 1, 0, 1],
                  [1, 1, 1, 1, 1, 1, 1, 0, 1],
                  [1, 0, 0, 0, 0, 0, 0, 0, 1],
                  [1, 1, 1, 1, 1, 1, 1, 1, 1]])
```

Then we create the environment with the structure as first parameter and the goal field tuple as second parameter:

```
environment = Maze(structure, (7, 7))
```

Next, we need an agent. The agent is where the learning happens. It can interact with the environment with its `getAction()` and `integrateObservation()` methods.

The agent itself consists of a controller, which maps states to actions, a learner, which updates the controller parameters according to the interaction it had with the world, and an explorer, which adds some explorative behavior to the actions. All standard agents already have a default explorer, so we don't need to take care of that in this tutorial.

The controller in PyBrain is a module, that takes states as inputs and transforms them into actions. For value-based methods, like the Q-Learning algorithm we will use here, we need a module that implements the `ActionValueInterface`. There are currently two modules in PyBrain that do this: The `ActionValueTable` for discrete actions and the `ActionValueNetwork` for continuous actions. Our maze uses discrete actions, so we need a table:

```
controller = ActionValueTable(81, 4)
controller.initialize(1.)
```

The table needs the number of states and actions as parameters. The standard maze environment comes with the following 4 actions: north, south, east, west.

Then, we initialize the table with 1 everywhere. This is not always necessary but will help converge faster, because unvisited state-action pairs have a promising positive value and will be preferred over visited ones that didn't lead to the goal.

Each agent also has a learner component. Several classes of RL learners are currently implemented in PyBrain: black box optimizers, direct search methods, and value-based learners. The classical Reinforcement Learning mostly

consists of value-based learning, in which of the most well-known algorithms is the Q-Learning algorithm. Let's now create the agent and give it the controller and learner as parameters.

```
learner = Q()
agent = LearningAgent(controller, learner)
```

So far, there is no connection between the agent and the environment. In fact, in PyBrain, there is a special component that connects environment and agent: the task. A task also specifies what the goal is in an environment and how the agent is rewarded for its actions. For episodic experiments, the Task also decides when an episode is over. Environments usually bring along their own tasks. The Maze environment for example has a MDP Maze Task, that we will use. MDP stands for “markov decision process” and means here, that the agent knows its exact location in the maze. The task receives the environment as parameter.

```
task = MDP Maze Task(environment)
```

Finally, in order to learn something, we create an experiment, tell it both task and agent (it knows the environment through the task) and let it run for some number of steps or infinitely, like here:

```
experiment = Experiment(task, agent)

while True:
    experiment.doInteractions(100)
    agent.learn()
    agent.reset()

    pylab.pcolor(controller.params.reshape(81,4).max(1).reshape(9,9))
    pylab.draw()
```

Above, the experiment executes 100 interactions between agent and environment, or, to be exact, between the agent and the task. The task will process the agent's actions, possibly scale it and hand it over to the environment. The environment responds, returns the new state back to the task which decides what information should be given to the agent. The task also gives a reward value for each step to the agent.

After 100 steps, we call the agent's `learn()` method and then reset it. This will make the agent forget the previously executed steps but of course it won't undo the changes it learned.

Then the loop is repeated, until a desired behavior is learned.

In order to observe the learning progress, we visualize the controller with the last two code lines in the loop. The ActionValueTable consists of a scalar value for each state/action pair, in this case 81x4 values. A nice way to visualize learning is to only consider the maximum value over all actions for each state. This value is called the state-value V and is defined as $V(s) = \max_a Q(s, a)$.

We plot the new table after learning and resetting the agent, *inside* the while loop. Running this code, you should see the shape of the maze and a change of colors for the free fields. During learning, colors may jump and change back and forth, but eventually the learning should converge to the true state values, having higher scores (brighter fields) the closer they are to the goal.

ADVANCED

4.1 Fast networks for PyBrain

Writing a neural networking framework in Python imposes certain speed restrictions upon it. Python is just not as fast as languages such as C++ or Fortran.

Due to this, PyBrain has its own spin-off called *arac*, which is a re-implementation of its neural networking facilities that integrates transparently with it.

Depending on the configuration of your system, speedups of **5-10x faster** can be expected. This speedup might be even higher (ranging into the hundreds) if you use sophisticated topologies such as MDRNNs. If you want some numbers on your system, there is a comparison script shipped with PyBrain at `examples/arac/benchmark.py`.

4.1.1 Installation

However, the installation process is less easy than for pure Python PyBrain. On the other hand, it's mostly about installing an additional library and telling PyBrain to use fast networks.

You will find detailed installation instructions for *arac* on the [arac wiki](#).

This instructions are work in progress. If you run into difficulties, ask on the PyBrain mailing list.

4.1.2 Usage

Once you have installed it, there are three ways to use fast networks.

First, the shortcut `buildNetwork` has a keyword `fast` which builds an *arac* network instead:

```
>>> from pybrain.tools.shortcuts import buildNetwork
>>> n = buildNetwork(2, 3, 1, fast=True)
>>> n.activate((2, 3))
array([-0.20781205])
```

As you can see by examining the network, it is a special class:

```
>>> n
<_FeedForwardNetwork '_FeedForwardNetwork-8'>
```

which is prefixed with an underscore, the Python convention for naming C implementations of already existing classes. We can import these classes directly from *arac* and use them in the same way as PyBrain classes:

```
>>> from arac.pybrainbridge import _FeedForwardNetwork, _RecurrentNetwork
```

The third method is to construct a network as a PyBrain network and call the method `convertToFastNetwork` afterwards:

```
>>> n = buildNetwork(2, 3, 1, fast=False)
>>> n.convertToFastNetwork()
<_FeedForwardNetwork '_FeedForwardNetwork-18'>
```

However, be cautious with the last method since changes to the PyBrain network are not reflected in the arac network.

4.1.3 Limitations

Since arac is implemented in C++ and currently maintained by only a single person, arac development is likely to be slower than PyBrain's. This might lead to certain features (e.g. layer types) to be implemented later than the pure python versions. This also applies to custom layer types. As soon as you have your layer type, you will not be able to use fast networks anymore – except if you chose to also implement them for arac yourself.

4.2 Using ODE Environments

4.2.1 Using an existing ODE environment

This tutorial walks you through the process of setting up an existing ODE Environment for use as a testbed for RL or optimization algorithms.

First we need the following additional packages that are not required for PyBrain (in addition to SciPy):

- matplotlib
- python-tk
- python-pyode
- python-opengl (if you also want to view what is happening, very recommended)

You also need to exchange the following two `.py` files with custom versions:

```
cd pybrain/pybrain/rl/environments/ode/xode_changes/
sudo cp * /usr/lib/python2.6/dist-packages/xode/ (or there ever your dist-packages are)
```

You can test if all your settings are ok by starting following example:

```
cd ~/pybrain/examples/rl/
python johnnie_pgpe.py
```

... and then view whats happening by using the viewer:

```
cd ~/pybrain/pybrain/rl/environments/ode
python viewer.py
```

Existing ODE Environments that are tested are:

- Johnnie (a biped humanoid robot modeled after the real robot Johnnie (<http://www.amm.mw.tum.de>))

- CCRL (a robot with two 7 DoF Arms and simple grippers, modeled after the real robot at the CCRL of TU Munich. (<http://www.lsr.ei.tum.de/>)
- PencilBalancer (a robot that balances pencils in a 2D way, modeled after the real robot from Jörg Conradt. (<http://www.ini.uzh.ch/~conradt/Projects/PencilBalancer/>)

4.2.2 Creating your own learning task in an existing ODE environment

This tutorial walks you through the process of setting up a new task within an existing ODE Environment. It assumes that you have taken the steps described in the section *Using an existing ODE environment*.

For all ODE environments there can be found a standard task in `pybrain/rl/environments/ode/tasks`

We take as an example again the Johnnie environment. You will find that the first class in the `johnnie.py` file in the above described location is named `JohnnieTask` and inherits from `EpisodicTask`.

The necessary methods that you need to define your own task are described already in that basic class:

- `__init__(self, env)` - the constructor
- `performAction(self, action)` - processes and filters the output from the controller and communicates it to the environment.
- `isFinished(self)` - checks if the maximum number of timesteps has been reached or if other break condition has been met.
- `res(self)` - resets counters rewards and similar.

If we take a look at the `StandingTask` (the next class in the file) we see that only little has to be done to create an own task. First of all the class must inherit from `JohnnieTask`. Then, the constructor has to be overwritten to declare some variables and constants for the specific task. In this case there were some additional position sensors added and normalized for reward calculation. As normally last step the `getReward` Method has to be overwritten, because the reward definition is normally what defines the task. In this case just the vertical head position is returned (with some clipping to prevent the robot from jumping to get more reward). That is already enough to create a task that is sufficiently defined to make a proper learning method (like PGPE in the above mentioned and testable example `johnnie_pgpe.py`) learn a controller that let the robot stand complete upright without falling.

For some special cases you maybe are forced to rewrite the `performAction` method and the `isFinished` method, but that special cases are out of scope of this HowTo. If you need to make such changes and encounter problems please feel free to contact the PyBrain mailing list.

4.2.3 Creating your own ODE environment

This tutorial walks you through the process of setting up a new ODE Environment. It assumes that you are already familiar with the sections *Using an existing ODE environment* and *Creating your own learning task in an existing ODE environment* and have taken the necessary steps explained there.

If you want to your own environment you need the following:

- Environment that inherits from `ODEEnvironment`
- Agent that inherits from `OptimizationAgent`
- Tasks that inherit from `EpisodicTask`

For all ODE environments, an instance can be found in `pybrain/rl/environments/ode/instances/`

We take as an example again the Johnnie environment. You will find that the first class in the `johnnie.py` file in the location described above is named `JohnnieEnvironment` and inherits from `ODEEnvironment`.

You will see that there is not much to do on the PyBrain side to generate the environment class. First loading the corresponding XODE file is necessary to provide PyBrain with the specification of the simulation. How to generate the corresponding XODE file will be shown later in this HowTo. Then the standard sensors are added like the JointSensors, the corresponding JointVelocitySensors and also the actuators for every joint. Because this kind of sensors and actuators are needed in every simulation they are already added in the environment and assumed to exist by later stages of PyBrain.

The next part is a bit more involved. First, member variables that state the number of action dimensions and number of sensors have to be set.

```
self.actLen = self.getActionLength()
self.obsLen = len(self.getSensors())
```

Next, 3 lists are generated for every action dimension. The first list is called `torqueList` and states the fraction of the global maximal force that can be applied to the joints. The second list states the maximum angle, the third list states the minimum angle for every joint. (`cHighList` and `cLowList`) For example:

```
self.torqueList = array([0.2, 0.2, 0.2, 0.5, 0.5, 2.0, 2.0, 2.0, 2.0, 0.5, 0.5],)
self.cHighList = array([1.0, 1.0, 0.5, 0.5, 0.5, 1.5, 1.5, 1.5, 1.5, 0.25, 0.25],)
self.cLowList = array([-0.5, -0.5, -0.5, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, -0.25, -0.25],)
```

The last thing to do is how much simulation steps ODE should make before getting an update from the controller and sending new sensor values back, called `stepsPerAction`.

4.2.4 Creating your own XODE instance

Now we want to specify a instantiation in a XODE file. If you do not know ODE very well, you can use a script that is shipped with PyBrain and can be found in `pybrain/rl/environments/ode/tools/xodetools.py`

The first part of the file is responsible for parsing the simplified XODE code to a regular XODE file, that can be ignored. For an example, look at the Johnnie definition by searching for `class XODEJohnnie(XODEfile)`

The instantiation of what you want to simulate in ODE is defined in this tool as a class that inherits from `XODEfile`. The class consists only of a constructor. Here all parts of the simulated object are defined. The parts are defined in an global coordinate system. For examples the row

```
self.insertBody('arm_left', 'cappedCylinder', [0.25, 7.5], 5, pos=[2.06, -2.89, 0],
               euler=[90, 0, 0], passSet=['total'], mass=2.473)
```

creates the left arm (identifier 'arm_left') of Johnnie as an cylinder with round endings ('cappedCylinder') with a diameter of 0.25 and a length of 7.5 ([0.25, 7.5]) with a density of 5 (that will be overwritten if the optional value mass is given at the end of the command), an initial position of `pos = [2.06, -2.89, 0]`, turned by 90 degrees around the x-Axis (`euler = [90, 0, 0]`, all capped cylinders are by default aligned with the y-Axis) the passSet named 'total' (will be explained soon) and the optional mass of the part.

"passSet" is used to define parts that can penetrate each other. That is especially necessary for parts that have a joint together, but can also be usable in other cases. All parts that are part of the same passSet can penetrate each other. Multiple passSet names can be given delimited by a ",". Types that are understood by this tool are:

- cylinder
- cappedCylinder
- box

Next we have to define the joints that connect the parts. Types of joints that are understood by this tool are:

- fixed, for a stiff fixed joint.

- hinge, one dimensional joint.
- universal joint, experimental 2D joint.

A joint between two parts is inserted in the model by `insertJoint`, giving the identifier of the first part, then the identifier of the second part. Next the type of joint is stated (e.g. 'hinge'). The axis around the joint will rotate is stated like `axis={'x':1, 'y':0, 'z':0}` and the anchor point in global coordinates is defined by something like `anchor=(2.06,0.86,0)`. Add all parts and joints for your model.

Finally with `centerOn(identifier)` the camera position is fixed to that part and with `insertFloor(y=??)` a floor can be added.

Now go to the end of the file and state:

```
name = YourClass('../models/name')
name.writeXODE()
```

and execute the file with

```
python xodetools.py
```

And you have created an instantiation of your model that can be read in in the above environment.

What is missing is a default task for the new environment. In the previous “HowTo create your own learning task in an existing ODE environment” we saw how such a standard task looks for the Johnnie environment. To create our own task we have to create a file with the name of our environment in `pybrain/rl/environments/ode/tasks/`

The new task has to import the following packages:

```
from pybrain.rl.environments import EpisodicTask from pybrain.rl.environments.ode.sensors import *
```

And whatever is needed from `scipy` and similar.

The new class should inherit from `EpisodicTask` like in the `JohnnieTask`. Next we create the constructor that takes the environment with `def __init__(self, env)`.

It is important that the constructor of `EpisodicTask` is called.

```
EpisodicTask.__init__(self, env)
```

The following member variables are mandatory:

```
self.maxPower = 100.0    #Overall maximal torque - is multiplied with relative max
                        #torque for individual joint to get individual max torque
self.reward_history = []
self.count = 0           #timestep counter
self.epiLen = 500        #time steps for one episode
```

In contrast to the `ODEEnvironment` standard settings some changes might be needed:

- `self.env.FricMu` if you need higher or lower friction for your task,
- `self.env.dt` if you need more timely resolution.

Next the sensor and actuator limits must be set, usually between -1 and 1:

```
# normalize standard sensors to (-1, 1)
self.sensor_limits = []
#Angle sensors
for i in range(self.env.actLen):
    # Joint velocity sensors
```

```
self.sensor_limits.append((self.env.cLowList[i], self.env.cHighList[i]))
for i in range(self.env.actLen):
    self.sensor_limits.append((-20, 20))
#Normalize all actor dimensions to (-1, 1)
self.actor_limits = [(-1, 1)]*env.actLen
```

The next method that is needed is the `performAction` method, the standard setting looks like that:

```
def performAction(self, action):
    """ Filtered mapping towards performAction of the underlying environment """
    EpisodicTask.performAction(self, action)
```

If you want to control the wanted angels instead of the forces you may include this simple PD mechanism:

```
#The joint angles
isJoints = self.env.getSensorByName('JointSensor')
#The joint angular velocities
isSpeeds = self.env.getSensorByName('JointVelocitySensor')
#norm output to action interval
act = (action+1.0)/2.0*(self.env.cHighList-self.env.cLowList)+self.env.cLowList
#simple PID
action = tanh((act - isJoints - isSpeeds) * 16.0) * self.maxPower * self.env.torqueList
```

Now we have to define the `isFinished()` method:

```
def isFinished(self):
    """ returns true if episode timesteps has reached episode length and resets the task """
    if self.count > self.epiLen:
        self.res()
        return True
    else:
        self.count += 1
        return False
```

You are certainly free to include other breaking conditions.

Finally we define a `reset()` method:

```
def res(self):
    """ sets counter and history back, increases incremental counter """
    self.count = 0
    self.reward_history.append(self.getTotalReward())
```

We don't need a `getReward()` function here, because the method from `EpisodicTask` that returns always 0.0 is taken over. This is the default task that is used to create specific tasks. Please take a look at [Creating your own learning task in an existing ODE environment](#) for how to create a task that gives actual reward.

If you have done all steps right you now have a new ODE environment with a corresponding task that you can test by creating an experiment. Or you can try to copy an existing example like the `johnnie_pgpe.py` and replace the environment and the task definition with your new environment and task.

API

5.1 connections – Structural Components: Connections

class FullConnection (**args, **kwargs*)

Connection which fully connects every element from the first module's output buffer to the second module's input buffer in a matrix multiplicative manner.

whichBuffers (*paramIndex*)

Return the index of the input module's output buffer and the output module's input buffer for the given weight.

class IdentityConnection (**args, **kwargs*)

Connection which connects the *i*'th element from the first module's output buffer to the *i*'th element of the second module's input buffer.

class SharedConnection (*mother, *args, **kwargs*)

A shared connection can link different couples of modules, with a single set of parameters.

class SharedFullConnection (*mother, *args, **kwargs*)

Shared version of FullConnection.

class MotherConnection (*nbparams, **args*)

The container for the shared parameters of connections (just a container with a constructor, actually).

5.2 evolvable – Container Component: Evolvable

class Evolvable ()

The interface for all Evolvables, i.e. which implement mutation, randomize and copy operators.

copy ()

By default, returns a full deep-copy - subclasses should implement something faster, if appropriate.

mutate (***args*)

Vary some properties of the underlying module, so that it's behavior changes, (but not too abruptly).

newSimilarInstance ()

Generates a new Evolvable of the same kind.

randomize ()

Sets all variable parameters to random values.

5.3 modules – Structural Components: Modules

class BiasUnit (*name=None*)

Bases: `pybrain.structure.modules.neuronlayer.NeuronLayer`

A simple bias unit with a single constant output.

class GaussianLayer (*dim, name=None*)

Bases: `pybrain.structure.modules.neuronlayer.NeuronLayer`,
`pybrain.structure.parametercontainer.ParameterContainer`

A layer implementing a gaussian interpretation of the input. The mean is the input, the sigmas are stored in the module parameters.

setSigma (*sigma*)

Wrapper method to set the sigmas (the parameters of the module) to a certain value.

class LinearLayer (*dim, name=None*)

Bases: `pybrain.structure.modules.neuronlayer.NeuronLayer`

The simplest kind of module, not doing any transformation.

__init__ (*dim, name=None*)

Create a layer with *dim* number of units.

class LSTMLayer (*dim, peepholes=False, name=None*)

Bases: `pybrain.structure.modules.neuronlayer.NeuronLayer`,
`pybrain.structure.parametercontainer.ParameterContainer`

Long short-term memory cell layer.

The input consists of 4 parts, in the following order: - input gate - forget gate - cell input - output gate

class MDLSTMLayer (*dim, dimensions=1, peepholes=False, name=None*)

Bases: `pybrain.structure.modules.neuronlayer.NeuronLayer`,
`pybrain.structure.parametercontainer.ParameterContainer`

Multi-dimensional long short-term memory cell layer.

The cell-states are explicitly passed on through a part of the input/output buffers (which should be connected correctly with IdentityConnections).

The input consists of 4 parts, in the following order: - input gate - forget gates (1 per dim) - cell input - output gate - previous states (1 per dim)

The output consists of two parts: - cell output - current state

Attention: this module has to be used with care: it's last <size> input and outputs are reserved for transmitting internal states on flattened recursive multi-dim networks, and so its connections have always to be sliced!

class SigmoidLayer (*dim, name=None*)

Bases: `pybrain.structure.modules.neuronlayer.NeuronLayer`

Layer implementing the sigmoid squashing function.

__init__ (*dim, name=None*)

Create a layer with *dim* number of units.

class SoftmaxLayer (*dim, name=None*)

Bases: `pybrain.structure.modules.neuronlayer.NeuronLayer`

A layer implementing a softmax distribution over the input.

```
__init__(dim, name=None)
    Create a layer with dim number of units.
```

```
class StateDependentLayer (dim, module, name=None, onesigma=True)
    Bases: pybrain.structure.modules.neuronlayer.NeuronLayer,
            pybrain.structure.parametercontainer.ParameterContainer
```

```
class TanhLayer (dim, name=None)
    Bases: pybrain.structure.modules.neuronlayer.NeuronLayer

    A layer implementing the tanh squashing function.
```

```
__init__(dim, name=None)
    Create a layer with dim number of units.
```

5.4 networks – Structural Components: Networks

```
class Network (name=None, **args)
    Bases: pybrain.structure.modules.module.Module, pybrain.structure.parametercontainer.ParameterContainer
```

Abstract class for linking different modules with connections.

```
activate (inpt)
    Do one transformation of an input and return the result.
```

```
activateOnDataset (dataset)
    Run the module's forward pass on the given dataset unconditionally and return the output.
```

```
addConnection (c)
    Add the given connection to the network.
```

```
addInputModule (m)
    Add the given module to the network and mark it as an input module.
```

```
addModule (m)
    Add the given module to the network.
```

```
addOutputModule (m)
    Add the given module to the network and mark it as an output module.
```

```
reset ()
    Reset all component modules and the network.
```

```
sortModules ()
    Prepare the network for activation by sorting the internal datastructure.

    Needs to be called before activation.
```

```
class FeedForwardNetwork (*args, **kwargs)
    Bases: pybrain.structure.networks.feedforward.FeedForwardNetworkComponent,
            pybrain.structure.networks.network.Network
```

FeedForwardNetworks are networks that do not work for sequential data. Every input is treated as independent of any previous or following inputs.

```
class RecurrentNetwork (*args, **kwargs)
    Bases: pybrain.structure.networks.recurrent.RecurrentNetworkComponent,
            pybrain.structure.networks.network.Network
```

Class that implements networks which can work with sequential data.

Until `.reset()` is called, the network keeps track of all previous inputs and thus allows the use of recurrent connections and layers that look back in time.

addRecurrentConnection (*c*)

Add a connection to the network and mark it as a recurrent one.

5.5 actionvalues – RL Components: ActionValues

class ActionValueInterface ()

Interface for different ActionValue modules, like the ActionValueTable or the ActionValueNetwork.

class ActionValueTable (*numStates, numActions, name=None*)

Bases: `pybrain.structure.modules.table.Table`, `pybrain.rl.learners.valuebased.interface.ActionValueInterface`

A special table that is used for Value Estimation methods in Reinforcement Learning.

getMaxAction (*state*)

Return the action with the maximal value for the given state.

initialize (*value=0.0*)

Initialize the whole table with the given value.

class ActionValueNetwork (*dimState, numActions, name=None*)

Bases: `pybrain.structure.modules.module.Module`, `pybrain.rl.learners.valuebased.interface.ActionValueInterface`

getActionValues (*state*)

Run forward activation for each of the actions and returns all values.

getMaxAction (*state*)

Return the action with the maximal value for the given state.

5.6 agents – RL Components: Agents

class Agent ()

An agent is an entity capable of producing actions, based on previous observations. Generally it will also learn from experience. It can interact directly with a Task.

getAction ()

Return a chosen action. :rtype: by default, this is assumed to be a numpy array of doubles. :note: This method is abstract and needs to be implemented.

giveReward (*r*)

Reward or punish the agent. :key r: reward, if C{r} is positive, punishment if C{r} is negative :type r: double

integrateObservation (*obs*)

Integrate the current observation of the environment. :arg obs: The last observation returned from the environment :type obs: by default, this is assumed to be a numpy array of doubles

newEpisode ()

Inform the agent that a new episode has started.

class LoggingAgent (*indim, outdim*)

Bases: `pybrain.rl.agents.agent.Agent`

This agent stores actions, states, and rewards encountered during interaction with an environment in a ReinforcementDataSet (which is a variation of SequentialDataSet). The stored history can be used for learning and

is erased by resetting the agent. It also makes sure that `integrateObservation`, `getAction` and `giveReward` are called in exactly that order.

getAction ()

Step 2: store the action in a temporary variable until reward is given.

giveReward (*r*)

Step 3: store observation, action and reward in the history dataset.

integrateObservation (*obs*)

Step 1: store the observation received in a temporary variable until action is called and reward is given.

newEpisode ()

Indicate the beginning of a new episode in the training cycle.

reset ()

Clear the history of the agent.

class LearningAgent (*module, learner=None*)

Bases: `pybrain.rl.agents.logging.LoggingAgent`

LearningAgent has a module, a learner, that modifies the module, and an explorer, which perturbs the actions. It can have learning enabled or disabled and can be used continuously or with episodes.

getAction ()

Activate the module with the last observation, add the exploration from the explorer object and store the result as last action.

learn (*episodes=1*)

Call the learner's learn method, which has access to both module and history.

learning

Return whether the agent currently learns from experience or not.

newEpisode ()

Indicate the beginning of a new episode in the training cycle.

reset ()

Clear the history of the agent and resets the module and learner.

class OptimizationAgent (*module, learner*)

Bases: `pybrain.rl.agents.agent.Agent`

A simple wrapper to allow optimizers to conform to the RL interface. Works only in conjunction with Episodic-Experiment.

5.7 experiments – RL Components: Experiments

class Experiment (*task, agent*)

An experiment matches up a task with an agent and handles their interactions.

doInteractions (*number=1*)

The default implementation directly maps the methods of the agent and the task. Returns the number of interactions done.

class EpisodicExperiment (*task, agent*)

Bases: `pybrain.rl.experiments.experiment.Experiment`

The extension of Experiment to handle episodic tasks.

doEpisodes (*number=1*)

Do one episode, and return the rewards of each step as a list.

class ContinuousExperiment (*task, agent*)

Bases: `pybrain.rl.experiments.experiment.Experiment`

The extension of Experiment to handle continuous tasks.

doInteractionsAndLearn (*number=1*)

Execute a number of steps while learning continuously. no reset is performed, such that consecutive calls to this function can be made.

5.8 explorers – RL Components: Explorers

class Explorer (*indim, outdim, name=None, **args*)

An Explorer object is used in Agents, receives the current state and action (from the controller Module) and returns an explorative action that is executed instead the given action.

activate (*state, action*)

The super class commonly ignores the state and simply passes the action through the module. implement `_forwardImplementation()` in subclasses.

newEpisode ()

Inform the explorer about the start of a new episode.

5.8.1 Continuous Explorers

class NormalExplorer (*dim, sigma=0.0*)

A continuous explorer, that perturbs the resulting action with additive, normally distributed random noise. The exploration has parameter(s) sigma, which are related to the distribution's standard deviation. In order to allow for negative values of sigma, the real std. derivation is a transformation of sigma according to the `expln()` function (see `pybrain.tools.functions`).

class StateDependentExplorer (*statedim, actiondim, sigma=-2.0*)

A continuous explorer, that perturbs the resulting action with additive, normally distributed random noise. The exploration has parameter(s) sigma, which are related to the distribution's standard deviation. In order to allow for negative values of sigma, the real std. derivation is a transformation of sigma according to the `expln()` function (see `pybrain.tools.functions`).

activate (*state, action*)

The super class commonly ignores the state and simply passes the action through the module. implement `_forwardImplementation()` in subclasses.

newEpisode ()

Randomize the matrix values for exploration during one episode.

5.8.2 Discrete Explorers

class DiscreteExplorer ()

Bases: `pybrain.rl.explorers.explorer.Explorer`

Discrete explorers choose one of the available actions from the set of actions. In order to know which actions are available and which action to choose, discrete explorers need access to the module (which has to of class `ActionValueTable`).

`_setModule (module)`

Tells the explorer the module (which has to be ActionValueTable).

class `EpsilonGreedyExplorer` (*epsilon=0.29999999999999999, decay=0.99990000000000001*)

Bases: `pybrain.rl.explorers.discrete.discrete.DiscreteExplorer`

A discrete explorer, that executes the original policy in most cases, but sometimes returns a random action (uniformly drawn) instead. The randomness is controlled by a parameter $0 \leq \text{epsilon} \leq 1$. The closer epsilon gets to 0, the more greedy (and less explorative) the agent behaves.

`_forwardImplementation (inbuf, outbuf)`

Draws a random number between 0 and 1. If the number is less than epsilon, a random action is chosen. If it is equal or larger than epsilon, the greedy action is returned.

class `BoltzmannExplorer` (*tau=2.0, decay=0.99950000000000006*)

Bases: `pybrain.rl.explorers.discrete.discrete.DiscreteExplorer`

A discrete explorer, that executes the actions with probability that depends on their action values. The boltzmann explorer has a parameter tau (the temperature). for high tau, the actions are nearly equiprobable. for tau close to 0, this action selection becomes greedy.

`activate (state, action)`

The super class ignores the state and simply passes the action through the module. implement `_forwardImplementation()` in subclasses.

`_forwardImplementation (inbuf, outbuf)`

Draws a random number between 0 and 1. If the number is less than epsilon, a random action is chosen. If it is equal or larger than epsilon, the greedy action is returned.

class `DiscreteStateDependentExplorer` (*epsilon=0.20000000000000001, decay=0.99980000000000002*)

Bases: `pybrain.rl.explorers.discrete.discrete.DiscreteExplorer`

A discrete explorer, that directly manipulates the ActionValue estimator (table or network) and keeps the changes fixed for one full episode (if episodic) or slowly changes it over time.

TODO: currently only implemented for episodes

`activate (state, action)`

Save the current state for state-dependent exploration.

`_forwardImplementation (inbuf, outbuf)`

Activate the copied module instead of the original and feed it with the current state.

5.9 learners – RL Components: Learners

5.9.1 Abstract classes

The top of the learner hierarchy is more conceptual than functional. The different classes distinguish algorithms in such a way that we can automatically determine when an algorithm is not applicable for a problem.

class `Learner` ()

Top-level class for all reinforcement learning algorithms. Any learning algorithm changes a policy (in some way) in order to increase the expected reward/fitness.

`learn ()`

The main method, that invokes a learning step.

class `EpisodicLearner` ()

Bases: `pybrain.rl.learners.learner.Learner`

Assumes the task is episodic, not life-long, and therefore does a learning step only after the end of each episode.

class DataSetLearner ()

Bases: `pybrain.rl.learners.learner.EpisodicLearner`

A class for learners that learn from a dataset, which has no target output but only a reinforcement signal for each sample. It requires a ReinforcementDataSet object (which provides state-action-reward tuples).

class ExploringLearner ()

Bases: `pybrain.rl.learners.learner.Learner`

A Learner determines how to change the adaptive parameters of a module.

class DirectSearchLearner ()

Bases: `pybrain.rl.learners.learner.Learner`

The class of learners that (in contrast to value-based learners) searches directly in policy space.

5.9.2 Value-based Learners

class ValueBasedLearner ()

Bases: `pybrain.rl.learners.learner.ExploringLearner`, `pybrain.rl.learners.learner.DataSetLearner`, `pybrain.rl.learners.learner.EpisodicLearner`

An RL algorithm based on estimating a value-function.

batchMode

Does the algorithm run in batch mode or online?

explorer

Return the internal explorer.

module

Return the internal module.

offPolicy

Does the algorithm work on-policy or off-policy?

class Q (alpha=0.5, gamma=0.9899999999999999)

Bases: `pybrain.rl.learners.valuebased.valuebased.ValueBasedLearner`

learn ()

Learn on the current dataset, either for many timesteps and even episodes (`batchMode = True`) or for a single timestep (`batchMode = False`). Batch mode is possible, because Q-Learning is an off-policy method.

In `batchMode`, the algorithm goes through all the samples in the history and performs an update on each of them. if `batchMode` is `False`, only the last data sample is considered. The user himself has to make sure to keep the dataset consistent with the agent's history.

class QLambda (alpha=0.5, gamma=0.9899999999999999, qlambda=0.9000000000000002)

Bases: `pybrain.rl.learners.valuebased.valuebased.ValueBasedLearner`

Q-lambda is a variation of Q-learning that uses an eligibility trace.

class SARSA (alpha=0.5, gamma=0.9899999999999999)

Bases: `pybrain.rl.learners.valuebased.valuebased.ValueBasedLearner`

State-Action-Reward-State-Action (SARSA) algorithm.

In `batchMode`, the algorithm goes through all the samples in the history and performs an update on each of them. if `batchMode` is `False`, only the last data sample is considered. The user himself has to make sure to keep the dataset consistent with the agent's history.

```
class NFQ()
    Bases: pybrain.rl.learners.valuebased.valuebased.ValueBasedLearner
    Neuro-fitted Q-learning
```

5.9.3 Direct-search Learners

```
class PolicyGradientLearner()
    Bases: pybrain.rl.learners.directsearch.directsearch.DirectSearchLearner,
           pybrain.rl.learners.learner.DataSetLearner, pybrain.rl.learners.learner.ExploringLearner
```

PolicyGradientLearner is a super class for all continuous direct search algorithms that use the log likelihood of the executed action to update the weights. Subclasses are ENAC, GPOMDP, or REINFORCE.

```
learn()
    calls the gradient calculation function and executes a step in direction of the gradient, scaled with a small
    learning rate alpha.
```

```
class Reinforce()
    Bases: pybrain.rl.learners.directsearch.policygradient.PolicyGradientLearner
```

Reinforce is a gradient estimator technique by Williams (see “Simple Statistical Gradient-Following Algorithms for Connectionist Reinforcement Learning”). It uses optimal baselines and calculates the gradient with the log likelihoods of the taken actions.

```
class ENAC()
    Bases: pybrain.rl.learners.directsearch.policygradient.PolicyGradientLearner
```

Episodic Natural Actor-Critic. See J. Peters “Natural Actor-Critic”, 2005. Estimates natural gradient with regression of log likelihoods to rewards.

Note: Black-box optimization algorithms can also be seen as direct-search RL algorithms, but are not included here.

5.10 tasks – RL Components: Tasks

```
class Task(environment)
    A task is associating a purpose with an environment. It decides how to evaluate the observations, potentially
    returning reinforcement rewards or fitness values. Furthermore it is a filter for what should be visible to the
    agent. Also, it can potentially act as a filter on how actions are transmitted to the environment.
```

```
denormalize(actors)
    The function scales the parameters from -1 and 1 to the given interval (min, max) for each actor.
```

```
getObservation()
    A filtered mapping to getSample of the underlying environment.
```

```
getReward()
    Compute and return the current reward (i.e. corresponding to the last action performed)
```

```
normalize(sensors)
    The function scales the parameters to be between -1 and 1. e.g. [(-pi, pi), (0, 1), (-0.001, 0.001)]
```

```
performAction(action)
    A filtered mapping towards performAction of the underlying environment.
```

```
setScaling(sensor_limits, actor_limits)
    Expects scaling lists of 2-tuples - e.g. [(-3.14, 3.14), (0, 1), (-0.001, 0.001)] - one tuple per parameter,
```

giving min and max for that parameter. The functions normalize and denormalize scale the parameters between -1 and 1 and vice versa. To disable this feature, use 'None'.

class EpisodicTask (*environment*)

Bases: `pybrain.rl.environments.task.Task`, `pybrain.rl.environments.fitness_evaluator.FitnessEvaluator`

A task that consists of independent episodes.

addReward ()

A filtered mapping towards performAction of the underlying environment.

discount

Discount factor

f (*x*)

An episodic task can be used as an evaluation function of a module that produces actions from observations, or as an evaluator of an agent.

getTotalReward ()

Return the accumulated reward since the start of the episode

isFinished ()

Is the current episode over?

performAction (*action*)

Execute one action.

reset ()

Re-initialize the environment

5.11 optimization – Black-box Optimization Algorithms

5.11.1 The two base classes

class BlackBoxOptimizer (*evaluator=None, initEvaluable=None, **kwargs*)

The super-class for learning algorithms that treat the problem as a black box. At each step they change the policy, and get a fitness value by invoking the FitnessEvaluator (provided as first argument upon initialization).

Evaluable objects can be lists or arrays of continuous values (also wrapped in ParameterContainer) or subclasses of Evolvable (that define its methods).

__init__ (*evaluator=None, initEvaluable=None, **kwargs*)

The evaluator is any callable object (e.g. a lambda function). Algorithm parameters can be set here if provided as keyword arguments.

setEvaluator (*evaluator, initEvaluable=None*)

If not provided upon construction, the objective function can be given through this method. If necessary, also provide an initial evaluable.

learn (*additionalLearningSteps=None*)

The main loop that does the learning.

minimize

Minimize cost or maximize fitness? By default, all functions are maximized.

maxEvaluations

Stopping criterion based on number of evaluations.

maxLearningSteps

Stopping criterion based on number of learning steps.

desiredEvaluation

Is there a known value of sufficient fitness?

verbose

provide console output during learning

storeAllEvaluations

Store all evaluations (in the `._allEvaluations` list)?

storeAllEvaluated

Store all evaluated instances (in the `._allEvaluated` list)?

numParameters

dimension of the search space, if applicable

class ContinuousOptimizer (*evaluator=None, initEvaluable=None, **kwargs*)

Bases: `pybrain.optimization.optimizer.BlackBoxOptimizer`

A more restricted class of black-box optimization algorithms that assume the parameters to be necessarily an array of continuous values (which can be wrapped in a `ParameterContainer`).

__init__ (*evaluator=None, initEvaluable=None, **kwargs*)

The evaluator is any callable object (e.g. a lambda function). Algorithm parameters can be set here if provided as keyword arguments.

5.11.2 General Black-box optimizers

class RandomSearch (*evaluator=None, initEvaluable=None, **kwargs*)

Every point is chosen randomly, independently of all previous ones.

class HillClimber (*evaluator=None, initEvaluable=None, **kwargs*)

The simplest kind of stochastic search: hill-climbing in the fitness landscape.

class StochasticHillClimber (*evaluator=None, initEvaluable=None, **kwargs*)

Stochastic hill-climbing always moves to a better point, but may also go to a worse point with a probability that decreases with increasing drop in fitness (and depends on a temperature parameter).

temperature

The larger the temperature, the more explorative (less greedy) it behaves.

5.11.3 Continuous optimizers

class NelderMead (*evaluator=None, initEvaluable=None, **kwargs*)

Do the optimization using a simple wrapper for scipy's `fmin`.

class CMAES (*evaluator=None, initEvaluable=None, **kwargs*)

CMA-ES: Evolution Strategy with Covariance Matrix Adaptation for nonlinear function minimization. This code is a close transcription of the provided matlab code.

class OriginalNES (*evaluator=None, initEvaluable=None, **kwargs*)

Reference implementation of the original Natural Evolution Strategies algorithm (CEC-2008).

class ExactNES (*evaluator=None, initEvaluable=None, **kwargs*)

A new version of NES, using the exact instead of the approximate Fisher Information Matrix, as well as a number of other improvements. (GECCO 2009).

baselineType

Type of baseline. The most robust one is also the default.

class FEM (*evaluator=None, initEvaluable=None, **kwargs*)
Fitness Expectation-Maximization (PPSN 2008).

Finite difference methods

class FiniteDifferences (*evaluator=None, initEvaluable=None, **kwargs*)
Basic finite difference method.

perturbation ()
produce a parameter perturbation

class PGPE (*evaluator=None, initEvaluable=None, **kwargs*)
Bases: `pybrain.optimization.finitedifference.fd.FiniteDifferences`
Policy Gradients with Parameter Exploration (ICANN 2008).

epsilon
Initial value of sigmas

exploration
exploration type

perturbation ()
Generate a difference vector with the given standard deviations

sigmaLearningRate
specific settings for sigma updates

wDecay
lasso weight decay (0 to deactivate)

class SimpleSPSA (*evaluator=None, initEvaluable=None, **kwargs*)
Bases: `pybrain.optimization.finitedifference.fd.FiniteDifferences`
Simultaneous Perturbation Stochastic Approximation.
This class uses SPSA in general, but uses the likelihood gradient and a simpler exploration decay.

Population-based

class ParticleSwarmOptimizer (*evaluator=None, initEvaluable=None, **kwargs*)
Particle Swarm Optimization

size determines the number of particles.

boundaries should be a list of (min, max) pairs with the length of the dimensionality of the vector to be optimized (default: +-10). Particles will be initialized with a position drawn uniformly in that interval.

memory indicates how much the velocity of a particle is affected by its previous best position.

sociality indicates how much the velocity of a particle is affected by its neighbours best position.

inertia is a damping factor.

best (*particlelist*)
Return the particle with the best fitness from a list of particles.

class GA (*evaluator=None, initEvaluable=None, **kwargs*)
Standard Genetic Algorithm.

crossOver (*parents, nbChildren*)
generate a number of children by doing 1-point cross-over

mutated (*indiv*)
mutate some genes of the given individual

mutationProb
mutation probability

produceOffspring ()
produce offspring by selection, mutation and crossover.

select ()
select some of the individuals of the population, taking into account their fitnesses

Returns list of selected parents

selectionSize
the number of parents selected from the current population

topProportion
selection proportion

tournament
selection scheme

5.11.4 Multi-objective Optimization

class MultiObjectiveGA (*evaluator=None, initEvaluable=None, **kwargs*)
Multi-objective Genetic Algorithm: the fitness is a vector with one entry per objective. By default we use NSGA-II selection.

5.12 classification – Datasets for Supervised Classification Training

class ClassificationDataSet (*inp, target=1, nb_classes=0, class_labels=None*)
Bases: `pybrain.datasets.supervised.SupervisedDataSet`
Specialized data set for classification data. Classes are to be numbered from 0 to `nb_classes-1`.

__init__ (*inp, target=1, nb_classes=0, class_labels=None*)
Initialize an empty dataset.

inp is used to specify the dimensionality of the input. While the number of targets is given by implicitly by the training samples, it can also be set explicitly by *nb_classes*. To give the classes names, supply an iterable of strings as *class_labels*.

calculateStatistics ()
Return a class histogram.

getClass (*idx*)
Return the label of given class.

splitByClass (*cls_select*)
Produce two new datasets, the first one comprising only the class selected (`0..nClasses-1`), the second one containing the remaining samples.

castToRegression (*values*)
Converts data set into a `SupervisedDataSet` for regression. Classes are used as indices into the value array given.

`_convertToOneOfMany` (*bounds*=(0, 1))

Converts the target classes to a 1-of-k representation, retaining the old targets as a field *class*.

To supply specific bounds, set the *bounds* parameter, which consists of target values for non-membership and membership.

`_convertToClassNb` ()

The reverse of `_convertToOneOfMany`. Target field is overwritten.

class `SequenceClassificationDataSet` (*inp*, *target*, *nb_classes*=0, *class_labels*=None)

Bases: `pybrain.datasets.sequential.SequentialDataSet`,
`pybrain.datasets.classification.ClassificationDataSet`

Defines a dataset for sequence classification. Each sample in the sequence still needs its own target value.

`__init__` (*inp*, *target*, *nb_classes*=0, *class_labels*=None)

Initialize an empty dataset.

inp is used to specify the dimensionality of the input. While the number of targets is given by implicitly by the training samples, it can also be set explicitly by *nb_classes*. To give the classes names, supply an iterable of strings as *class_labels*.

5.13 importance – Datasets for Weighted Supervised Training

class `ImportanceDataSet` (*indim*, *targetdim*)

Bases: `pybrain.datasets.sequential.SequentialDataSet`

Allows setting an importance value for each of the targets of a sample.

`addSample` (*inp*, *target*, *importance*=None)

adds a new sample consisting of input, target and importance.

Parameters

- *inp* – the input of the sample
- *target* – the target of the sample

Key importance the importance of the sample. If left None, the importance will be set to 1.0

5.14 sequential – Dataset for Supervised Sequences Regression Training

class `SequentialDataSet` (*indim*, *targetdim*)

Bases: `pybrain.datasets.supervised.SupervisedDataSet`

A `SequentialDataSet` is like a `SupervisedDataSet` except that it can keep track of sequences of samples. Indices of a new sequence are stored whenever the method `newSequence()` is called. The last (open) sequence is considered a normal sequence even though it does not have a following “new sequence” marker.

`endOfSequence` (*index*)

Return True if the marker was moved over the last element of sequence *index*, False otherwise.

Mostly used like `.endOfData()` with while loops.

`evaluateModuleMSE` (*module*, *averageOver*=1, ***args*)

Evaluate the predictions of a module on a sequential dataset and return the MSE (potentially average over a number of epochs).

getCurrentSequence ()

Return the current sequence, according to the marker position.

getNumSequences ()

Return the number of sequences. The last (open) sequence is also counted in, even though there is no additional 'newSequence' marker.

getSequence (index)

Returns the sequence given by *index*.

A list of arrays is returned for the linked arrays. It is assumed that the last sequence goes until the end of the dataset.

getSequenceIterator (index)

Return an iterator over the samples of the sequence specified by *index*.

getSequenceLength (index)

Return the length of the given sequence. If *index* is pointing to the last sequence, the sequence is considered to go until the end of the dataset.

gotoSequence (index)

Move the internal marker to the beginning of sequence *index*.

newSequence ()

Marks the beginning of a new sequence. this function does nothing if called at the very start of the data set. Otherwise, it starts a new sequence. Empty sequences are not allowed, and an EmptySequenceError exception will be raised.

removeSequence (index)

Remove the *index*'th sequence from the dataset and places the marker to the sample following the removed sequence.

splitWithProportion (proportion=0.5)

Produce two new datasets, each containing a part of the sequences.

The first dataset will have a fraction given by *proportion* of the dataset.

Note: This documentation comprises just a subjective excerpt of available methods. See the source code for additional functionality.

5.15 supervised – Dataset for Supervised Regression Training

class SupervisedDataSet (inp, target)

Bases: pybrain.datasets.dataset.DataSet

SupervisedDataSets have two fields, one for input and one for the target.

__init__ (inp, target)

Initialize an empty supervised dataset.

Pass *inp* and *target* to specify the dimensions of the input and target vectors.

__len__ ()

Return the length of the linked data fields. If no linked fields exist, return the length of the longest field.

addSample (inp, target)

Add a new sample consisting of *input* and *target*.

batches (label, n, permutation=None)

Yield batches of the size of *n* from the dataset.

A single batch is an array of with *dim* columns and *n* rows. The last batch is possibly smaller.

If permutation is given, batches are yielded in the corresponding order.

clear (*unlinked=False*)

Clear the dataset.

If linked fields exist, only the linked fields will be deleted unless *unlinked* is set to True. If no fields are linked, all data will be deleted.

copy ()

Return a deep copy.

class **loadFromFile** (*filename, format=None*)

Return an instance of the class that is saved in the file with the given filename in the specified format.

randomBatches (*label, n*)

Like *.batches()*, but the order is random.

class **reconstruct** (*filename*)

Read an incomplete data set (option *arrayonly*) into the given one.

saveToFile (*filename, format=None, **kwargs*)

Save the object to file given by filename.

splitWithProportion (*proportion=0.5*)

Produce two new datasets, the first one containing the fraction given by *proportion* of the samples.

5.16 svmunit – LIBSVM Support Vector Machine Unit

class **SVMUnit** (*indim=0, outdim=0, model=None*)

This unit represents an Support Vector Machine and is implemented through the LIBSVM Python interface. It functions somewhat like a Model or a Network, but combining it with other PyBrain Models is currently discouraged. Its main function is to compare against feed-forward network classifications. You cannot get or set model parameters, but you can load and save the entire model in LIBSVM format. Sequential data and backward passes are not supported. See the corresponding example code for usage.

__init__ (*indim=0, outdim=0, model=None*)

Initializes as empty module.

If *model* is given, initialize using this LIBSVM model instead. *indim* and *outdim* are for compatibility only, and ignored.

forwardPass (*values=False*)

Produce the output from the current input vector, or process a dataset.

If *values* is False or 'class', output is set to the number of the predicted class. If True or 'raw', produces decision values instead. These are stored in a dictionary for multi-class SVM. If *prob*, class probabilities are produced. This works only if probability option was set for SVM training.

activateOnDataset (*dataset, values=False*)

Run the module's forward pass on the given dataset unconditionally and return the output as a list.

Parameter *dataset* – A non-sequential supervised data set.

Key values Passed trough to *forwardPass()* method.

getNbClasses ()

return number of classes the current model uses

```

reset ()
    Reset input and output buffers

setModel (model)
    Set the SVM model.

loadModel (filename)
    Read the SVM model description from a file

saveModel (filename)
    Save the SVM model description from a file

```

5.17 svmtrainer – LIBSVM Support Vector Machine Trainer

class SVMTrainer (*svmunittest, dataset, modelfile=None, plot=False*)

A class performing supervised learning of a DataSet by an SVM unit. See the remarks on SVMUnit above. This whole class is a bit of a hack, and provided mostly for convenience of comparisons.

__init__ (*svmunittest, dataset, modelfile=None, plot=False*)

Initialize data and unit to be trained, and load the model, if provided.

The passed *svmunittest* has to be an object of class SVMUnit that is going to be trained on the ClassificationDataSet object dataset. Compared to FNN training we do not use a test data set, instead 5-fold cross-validation is performed if needed.

If *modelfile* is provided, this model is loaded instead of training. If *plot* is True, a grid search is performed and the resulting pattern is plotted.

train (*search=False, **kwargs*)

Train the SVM on the dataset. For RBF kernels (the default), an optional meta-parameter search can be performed.

Key search optional name of grid search class to use for RBF kernels: 'GridSearch' or 'GridSearchDOE'

Key log2g base 2 log of the RBF width parameter

Key log2c base 2 log of the slack parameter

Key searchlog filename into which to dump the search log

Key others ...are passed through to the grid search and/or libsvm

setParams (***kwargs*)

Set parameters for SVM training. Apart from the ones below, you can use all parameters defined for the LIBSVM svm_model class, see their documentation.

Key searchlog Save a list of coordinates and the achieved CV accuracy to this file.

load (*filename*)

no training at all - just load the SVM model from a file

save (*filename*)

save the trained SVM

class GridSearch (*problem, targets, cmin, cmax, cstep=None, crossval=5, plotflag=False, maxdepth=8, searchlog='gridsearch_results.txt', **params*)

Helper class used by SVMTrainer to perform an exhaustive grid search, and plot the resulting accuracy surface, if desired. Adapted from the LIBSVM python toolkit.

```
__init__(problem, targets, cmin, cmax, cstep=None, crossval=5, plotflag=False, maxdepth=8,
          searchlog='gridsearch_results.txt', **params)
```

Set up (log) grid search over the two RBF kernel parameters C and gamma.

Parameters

- *problem* – the LIBSVM svm_problem to be optimized, ie. the input and target data
- *targets* – unfortunately, the targets used in the problem definition have to be given again here
- *cmin* – lower left corner of the log2C/log2gamma window to search
- *cmax* – upper right corner of the log2C/log2gamma window to search

Key cstep step width for log2C and log2gamma (ignored for DOE search)

Key crossval split dataset into this many parts for cross-validation

Key plotflag if True, plot the error surface contour (regular) or search pattern (DOE)

Key maxdepth maximum window bisection depth (DOE only)

Key searchlog Save a list of coordinates and the achieved CV accuracy to this file

Key others ...are passed through to the cross_validation method of LIBSVM

search()

iterate successive parameter grid refinement and evaluation; adapted from LIBSVM grid search tool

setParams(kwargs)**

set parameters for SVM training

```
class GridSearchDOE(problem, targets, cmin, cmax, cstep=None, crossval=5, plotflag=False, maxdepth=8,
                    searchlog='gridsearch_results.txt', **params)
```

Same as GridSearch, but implements a design-of-experiments based search pattern, as described by C. Staelin, <http://www.hpl.hp.com/techreports/2002/HPL-2002-354R1.pdf>

search(cmin=None, cmax=None)

iterate parameter grid refinement and evaluation recursively

5.18 trainers – Supervised Training for Networks and other Modules

```
class BackpropTrainer(module, dataset=None, learningrate=0.01, lrdecay=1.0, momentum=0.0, verbose=False, batchlearning=False, weightdecay=0.0)
```

Trainer that trains the parameters of a module according to a supervised dataset (potentially sequential) by backpropagating the errors (through time).

```
__init__(module, dataset=None, learningrate=0.01, lrdecay=1.0, momentum=0.0, verbose=False, batchlearning=False, weightdecay=0.0)
```

Create a BackpropTrainer to train the specified *module* on the specified *dataset*.

The learning rate gives the ratio of which parameters are changed into the direction of the gradient. The learning rate decreases by *lrdecay*, which is used to multiply the learning rate after each training step. The parameters are also adjusted with respect to *momentum*, which is the ratio by which the gradient of the last timestep is used.

If *batchlearning* is set, the parameters are updated only at the end of each epoch. Default is False.

weightdecay corresponds to the weightdecay rate, where 0 is no weight decay at all.

setData (*dataset*)

Associate the given dataset with the trainer.

testOnClassData (*dataset=None, verbose=False, return_targets=False*)

Return winner-takes-all classification output on a given dataset.

If no dataset is given, the dataset passed during Trainer initialization is used. If *return_targets* is set, also return corresponding target classes.

train ()

Train the associated module for one epoch.

trainEpochs (*epochs=1, *args, **kwargs*)

Train on the current dataset for the given number of *epochs*.

Additional arguments are passed on to the train method.

trainOnDataset (*dataset, *args, **kwargs*)

Set the dataset and train.

Additional arguments are passed on to the train method.

trainUntilConvergence (*dataset=None, maxEpochs=None, verbose=None, continueEpochs=10, validationProportion=0.25*)

Train the module on the dataset until it converges.

Return the module with the parameters that gave the minimal validation error.

If no dataset is given, the dataset passed during Trainer initialization is used. *validationProportion* is the ratio of the dataset that is used for the validation dataset.

If *maxEpochs* is given, at most that many epochs are trained. Each time validation error hits a minimum, try for *continueEpochs* epochs to find a better one.

Note: This documentation comprises just a subjective excerpt of available methods. See the source code for additional functionality.

class RPropMinusTrainer (*module, etaminus=0.5, etaplus=1.2, deltamin=9.999999999999995e-07, deltamax=5.0, delta0=0.10000000000000001, **kwargs*)

Train the parameters of a module according to a supervised dataset (possibly sequential) by RProp without weight backtracking (aka RProp-, cf. [Igel&Huesken, Neurocomputing 50, 2003]) and without ponderation, ie. all training samples have the same weight.

__init__ (*module, etaminus=0.5, etaplus=1.2, deltamin=9.999999999999995e-07, deltamax=5.0, delta0=0.10000000000000001, **kwargs*)

Set up training algorithm parameters, and objects associated with the trainer.

Parameter *module* – the module whose parameters should be trained.

Key etaminus factor by which step width is decreased when overstepping (0.5)

Key etaplus factor by which step width is increased when following gradient (1.2)

Key delta step width for each weight

Key deltamin minimum step width (1e-6)

Key deltamax maximum step width (5.0)

Key delta0 initial step width (0.1)

Note: See the documentation of [BackpropTrainer](#) for inherited methods.

5.19 tools – Some Useful Tools and Macros

Neural network tools

buildNetwork (*layers, **options)

Build arbitrarily deep networks.

layers should be a list or tuple of integers, that indicate how many neurons the layers should have. *bias* and *outputbias* are flags to indicate whether the network should have the corresponding biases; both default to True.

To adjust the classes for the layers use the *hiddenclass* and *outclass* parameters, which expect a subclass of *NeuronLayer*.

If the *recurrent* flag is set, a *RecurrentNetwork* will be created, otherwise a *FeedForwardNetwork*.

If the *fast* flag is set, faster arac networks will be used instead of the pybrain implementations.

class NNregression (DS, **kwargs)

Learns to numerically predict the targets of a set of data, with optional online progress plots.

__init__ (DS, **kwargs)

Initialize with the training data set DS. All keywords given are set as member variables. The following are particularly important:

Key hidden number of hidden units

Key tds test data set for checking convergence

Key vds validation data set for final performance evaluation

Key epoinc number of epochs to train for, before checking convergence (default: 5)

initGraphics (ymax=10, xmax=-1)

initialize the interactive graphics output window, and return a handle to the plot

setupNN (trainer=<class 'pybrain.supervised.trainers.rprop.RPropMinusTrainer'>, hidden=None, **trnargs)

Constructs a 3-layer FNN for regression. Optional arguments are passed on to the Trainer class.

runTraining (convergence=0, **kwargs)

Trains the network on the stored dataset. If convergence is >0, check after that many epoch increments whether test error is going down again, and stop training accordingly. CAVEAT: No support for Sequential datasets!

saveTrainingCurve (learnfname)

save the training curves into a file with the given name (CSV format)

saveNetwork (fname)

save the trained network to a file

class NNclassifier (DS, **kwargs)

Learns to classify a set of data, with optional online progress plots.

__init__ (DS, **kwargs)

Initialize the classifier: the least we need is the dataset to be classified. All keywords given are set as member variables.

initGraphics (ymax=10, xmax=-1)

initialize the interactive graphics output window, and return a handle to the plot

setupNN (trainer=<class 'pybrain.supervised.trainers.rprop.RPropMinusTrainer'>, hidden=None, **trnargs)

Setup FNN and trainer for classification.

setupRNN (*trainer=<class 'pybrain.supervised.trainers.backprop.BackpropTrainer'>*, *hidden=None*, ***trnargs*)
 Setup an LSTM RNN and trainer for sequence classification.

runTraining (*convergence=0*, ***kwargs*)
 Trains the network on the stored dataset. If convergence is >0, check after that many epoch increments whether test error is going down again, and stop training accordingly.

saveTrainingCurve (*learnfname*)
 save the training curves into a file with the given name (CSV format)

saveNetwork (*fname*)
 save the trained network to a file

Dataset tools

convertSequenceToTimeWindows (*DSseq*, *NewClass*, *winsize*)

Converts a sequential classification dataset into time windows of fixed length. Assumes the correct class is given at the last timestep of each sequence. Incomplete windows at the sequence end are pruned. No overlap between windows.

Parameters

- *DSseq* – the sequential data set to cut up
- *winsize* – size of the data window
- *NewClass* – class of the windowed data set to be returned (gets initialised with in-dim*winsize, outdim)

Training performance validation tools

class Validator ()

This class provides methods for the validation of calculated output values compared to their destined target values. It does not know anything about modules or other pybrain stuff. It just works on arrays, hence contains just the core calculations.

The class has just classmethods, as it is used as kind of namespace instead of an object definition.

class ESS (*output*, *target*)

Returns the explained sum of squares (ESS).

Parameters

- *output* – array of output values
- *target* – array of target values

class MSE (*output*, *target*, *importance=None*)

Returns the mean squared error. The multidimensional arrays will get flattened in order to compare them.

Parameters

- *output* – array of output values
- *target* – array of target values

Key importance each squared error will be multiplied with its corresponding importance value. After summing up these values, the result will be divided by the sum of all importance values for normalization purposes.

class **classificationPerformance** (*output, target*)
Returns the hit rate of the outputs compared to the targets.

Parameters

- *output* – array of output values
- *target* – array of target values

class **ModuleValidator** ()

This class provides methods for the validation of calculated output values compared to their destined target values. It especially handles pybrains modules and dataset classes. For the core calculations, the Validator class is used.

The class has just classmethods, as it is used as kind of namespace instead of an object definition.

class **MSE** (*module, dataset*)
Returns the mean squared error.

Parameters

- *module* – Object of any subclass of pybrain’s Module type
- *dataset* – Dataset object at least containing the fields ‘input’ and ‘target’ (for example SupervisedDataSet)

class **calculateModuleOutput** (*module, dataset*)
Calculates the module’s output on the dataset. Can be called with any type of dataset.

Parameter *dataset* – Any Dataset object containing an ‘input’ field.

class **classificationPerformance** (*module, dataset*)
Returns the hit rate of the module’s output compared to the targets stored inside dataset.

Parameters

- *module* – Object of any subclass of pybrain’s Module type
- *dataset* – Dataset object at least containing the fields ‘input’ and ‘target’ (for example SupervisedDataSet)

class **validate** (*valfunc, module, dataset*)
Abstract validate function, that is heavily used by this class. First, it calculates the module’s output on the dataset. In advance, it compares the output to the target values of the dataset through the valfunc function and returns the result.

Parameters

- *valfunc* – A function expecting arrays for output, target and importance (optional). See Validator.MSE for an example.
- *module* – Object of any subclass of pybrain’s Module type
- *dataset* – Dataset object at least containing the fields ‘input’ and ‘target’ (for example SupervisedDataSet)

class **CrossValidator** (*trainer, dataset, n_folds=5, valfunc=<bound method type.classificationPerformance of <class 'pybrain.tools.validation.ModuleValidator'>>, **kwargs*)
Class for crossvalidating data. An object of CrossValidator must be supplied with a trainer that contains a module and a dataset. Then the dataset is shuffled and split up into n parts of equal length.

A clone of the trainer and its module is made, and trained with n-1 parts of the split dataset. After training, the module is validated with the n’t part of the dataset that was not used during training.

This is done for each possible combination of n-1 dataset pieces. The the mean of the calculated validation results will be returned.

setArgs (***kwargs*)

Set the specified member variables.

Key max_epochs maximum number of epochs the trainer should train the module for.

Key verbosity set verbosity level

validate ()

The main method of this class. It runs the crossvalidation process and returns the validation result (e.g. performance).

testOnSequenceData (*module, dataset*)

Fetch targets and calculate the modules output on dataset. Output and target are in one-of-many format. The class for each sequence is determined by first summing the probabilities for each individual sample over the sequence, and then finding its maximum.

Auxiliary functions

semilinear (*x*)

This function ensures that the values of the array are always positive. It is $x+1$ for $x \geq 0$ and $\exp(x)$ for $x < 0$.

semilinearPrime (*x*)

This function is the first derivative of the semilinear function (above). It is needed for the backward pass of the module.

sigmoid (*x*)

Logistic sigmoid function.

sigmoidPrime (*x*)

Derivative of logistic sigmoid.

tanhPrime (*x*)

Derivative of tanh.

safeExp (*x*)

Bounded range for the exponential function (won't produce inf or NaN).

ranking (*R*)

Produces a linear ranking of the values in R.

multivariateNormalPdf (*z, x, sigma*)

The pdf of a multivariate normal distribution (not in scipy). The sample *z* and the mean *x* should be 1-dim-arrays, and *sigma* a square 2-dim-array.

simpleMultivariateNormalPdf (*z, detFactorSigma*)

Assuming *z* has been transformed to a mean of zero and an identity matrix of covariances. Needs to provide the determinant of the factorized (real) covariance matrix.

multivariateCauchy (*mu, sigma, onlyDiagonal=True*)

Generates a sample according to a given multivariate Cauchy distribution.

5.20 utilities – Simple but useful Utility Functions

Tools for binary encodings

one_to_n (*val, maxval*)

Returns a 1-in-n binary encoding of a non-negative integer.

n_to_one (*arr*)

Returns the reverse of a 1-in-n binary encoding.

int2gray (*i*)

Returns the value of an integer in Gray encoding.

asBinary (*i*)

Produces a string from an integer's binary representation. (preceding zeros removed).

Tools for sets

reachable (*stepFunction, start, destinations*)

Determines the subset of destinations that can be reached from a set of starting positions, while using stepFunction (which produces a list of neighbor states) to navigate. Uses breadth-first search.

crossproduct (*ss, row=None, level=0*)

Returns the cross-product of the sets given in *ss*.

Matrix tools

triu2flat (*m*)

Flattens an upper triangular matrix, returning a vector of the non-zero elements.

flat2triu (*a, dim*)

Produces an upper triangular matrix of dimension *dim* from the elements of the given vector.

blockList2Matrix (*l*)

Converts a list of matrices into a corresponding big block-diagonal one.

blockCombine (*l*)

Produce a matrix from a list of lists of its components.

Stochastic index choices

drawIndex (*probs, tolerant=False*)

Draws an index given an array of probabilities.

Key tolerant if set to True, the array is normalized to sum to 1.

drawGibbs (*vals, temperature=1.0*)

Return the index of the sample drawn by a softmax (Gibbs).

5.21 nearoptimal – Near Optimal Locality Sensitive Hashing

class MultiDimHash (*dim, omega=4, prob=0.80000000000000004*)

Class that represents a datastructure that enables nearest neighbours search and methods to do so.

__init__ (*dim, omega=4, prob=0.80000000000000004*)

Create a hash for arrays of dimension *dim*.

The hyperspace will be split into hypercubes with a sidelength of $\omega * \sqrt{\sqrt{\text{dim}}}$, that is $\omega * \text{radius}$.

Every point in the d -dimensional euclidean space will be hashed to its correct bucket with a probability of prob .

insert (*point*, *satellite*)

Put a point and its satellite information into the hash structure.

knn (*point*, *k*)

Return the k approximate nearest neighbours of the item in the current hash.

Mind that the probabilistic nature of the data structure might not return a nearest neighbor at all and not the nearest neighbour.

See Also:

[Near-Optimal Hashing Algorithms for Approximate Nearest Neighbor in High Dimensions](#) Paper that describes the algorithm used in this module by Alexandr Andoni and Piotr Indyk.

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