Modular Toolkit for Data Processing (MDP)

This document is also available online: http://mdp-toolkit.sourceforge.net/tutorial.html

Tutorial

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Homepage: http://mdp-toolkit.sourceforge.net

Version: 2.6

This is a guide to basic and some more advanced features of the MDP library. Besides the present tutorial, you can learn more about MDP by using the standard Python tools. All MDP nodes have doc-strings, the public attributes and methods have telling names: All information about a node can be obtained using the `help` and `dir` functions within the Python interpreter. In addition to that, an automatically generated API is available.

Note

Code snippets throughout the script will be denoted by:

```
>>> print "Hello world!"
Hello world!
```

To run the following code examples don't forget to import mdp in your Python session with:

```
>>> import mdp
```

You'll find all the code of this tutorial within the `demo` directory in the MDP installation path.

Contents

Introduction

The use of the Python programming language in computational neuroscience has been growing steadily during the past few years. The maturation of two important open source projects, the scientific libraries NumPy and SciPy, gives access to a large collection of scientific functions that rivals in size and speed with well known commercial alternatives like The MathWorks™ Matlab©. Furthermore, the flexible and dynamic nature of Python offers the scientific programmer the opportunity to quickly develop efficient and structured software while maximizing prototyping and reusability capabilities.

The Modular toolkit for Data Processing (MDP) package contributes to this growing community a library of widely used data processing algorithms, and the possibility to combine them according to a pipeline analogy to build more complex data processing software.

MDP has been designed to be used as-is and as a framework for scientific data processing development.

From the user's perspective, MDP consists of a collection of supervised and unsupervised learning algorithms, and other data processing units (*nodes*) that can be combined into data processing sequences (*flows*) and more complex feed-forward network architectures. Given a set of input data, MDP takes care of successively training or executing all nodes in the network. This allows the user to specify complex algorithms as a series of simpler data processing steps in a natural way.

The base of available algorithms is steadily increasing and includes, to name but the most common, Principal Component Analysis (PCA and NIPALS), several Independent Component Analysis algorithms (CuBICA, FastICA, TDSEP, JADE, and XSFA), Slow Feature Analysis, Gaussian Classifiers, Restricted Boltzmann Machine, and Locally Linear Embedding (see the Node List section for a more exhaustive list and references).

Particular care has been taken to make computations efficient in terms of speed and memory. To reduce memory requirements, it is possible to perform learning using batches of data, and to define the internal parameters of the nodes to be single precision, which makes the usage of very large data sets possible. Moreover, the `parallel` subpackage offers a parallel implementation of the basic nodes and flows.

From the developer's perspective, MDP is a framework that makes the implementation of new supervised and unsupervised learning algorithms easy and straightforward. The basic class, `Node`, takes care of tedious tasks like numerical type and dimensionality checking, leaving the developer free to concentrate on the implementation of the learning and execution phases. Because of the common interface, the node then automatically integrates with the rest of the library and can be used in a network together with other nodes. A node can have multiple training phases and even an undetermined number of phases. This allows the implementation of algorithms that need to collect some statistics on the whole input before proceeding with the actual training, and others that need to iterate over a training phase until a convergence criterion is satisfied. The ability to train each phase using chunks of input data is maintained if the chunks are given as an iterable. Moreover, crash recovery is optionally available: in case of failure, the current state of the flow is saved for later inspection.

MDP is distributed under the open source LGPL license. It has been written in the context of theoretical research in neuroscience, but it has been designed to be helpful in any context where trainable data processing algorithms are used. Its simplicity on the user's side, the variety of readily available algorithms, and the reusability of the implemented nodes make it also a useful educational tool.

With over 10,000 downloads since its first public release in 2004, MDP has become a widely used Python scientific software. It has minimal dependencies, requiring only the NumPy numerical extension, is completely platform-independent, and is available as a package in the GNU/Linux Debian distribution and the Python(x,y) scientific Python distribution.

As the number of its users and contributors is increasing, MDP appears to be a good candidate for becoming a community-driven common repository of user-supplied, freely available, Python implemented data processing algorithms.

Quick Start

Using MDP is as easy as:

```
>>> import mdp
>>> # perform pca on some data x
...
>>> y = mdp.pca(x)
>>> # perform ica on some data x using single precision
...
>>> y = mdp.fastica(x, dtype='float32')
```

MDP requires the numerical Python extensions NumPy or SciPy. At import time MDP will select `scipy` if available, otherwise `numpy` will be loaded. You can force the use of a numerical extension by setting the environment variable `MDPNUMX=numpy` or `MDPNUMX=scipy`.

> **An important remark**
> Input array data is typically assumed to be two-dimensional and ordered such that observations of the same variable are stored on rows and different variables are stored on columns.

Nodes

A *node* is the basic building block of an MDP application. It represents a data processing element, like for example a learning algorithm, a data filter, or a visualization step (see the Node List section for an exhaustive list and references).

Each node can have one or more training phases, during which the internal structures are learned from training data (e.g. the weights of a neural network are adapted or the covariance matrix is estimated) and an execution phase, where new data can be processed forwards (by processing the data through the node) or backwards (by applying the inverse of the transformation computed by the node if defined).

Nodes have been designed to be applied to arbitrarily long sets of data: if the underlying algorithms supports it, the internal structures can be updated incrementally by sending multiple batches of data (this is equivalent to online learning if the chunks consists of single observations, or to batch learning if the whole data is sent in a single chunk). It is thus possible to perform computations on amounts of data that would not fit into memory or to generate data on-the-fly.

A `Node` also defines some utility methods, like for example `copy` and `save`, that return an exact copy of a node and save it in a file, respectively. Additional methods may be present, depending on the algorithm.

Node Instantiation

Nodes can be obtained by creating an instance of the `Node` class.

Each node is characterized by an input dimension (i.e., the dimensionality of the input vectors), an output dimension, and a `dtype`, which determines the numerical type of the internal structures and of the output signal. By default, these attributes are inherited from the input data if left unspecified. The constructor of each node class can require other task-specific arguments. The full documentation is always available in the doc-string of the node's class.

Some examples of node instantiation:

- Create a node that performs Principal Component Analysis (PCA) whose input dimension and `dtype` are inherited from the input data during training. Output dimensions default to input dimensions.

```
>>> pcanode1 = mdp.nodes.PCANode()
>>> pcanode1
PCANode(input_dim=None, output_dim=None, dtype=None)
```

- Setting `output_dim = 10` means that the node will keep only the first 10 principal components of the input.

  ```
  >>> pcanode2 = mdp.nodes.PCANode(output_dim = 10)
  >>> pcanode2
  PCANode(input_dim=None, output_dim=10, dtype=None)
  ```

  The output dimensionality can also be specified in terms of the explained variance. If we want to keep the number of principal components which can account for 80% of the input variance, we set:

  ```
  >>> pcanode3 = mdp.nodes.PCANode(output_dim = 0.8)
  >>> pcanode3.desired_variance
  0.80000000000000004
  ```

- If `dtype` is set to `float32` (32-bit float), the input data is cast to single precision when received and the internal structures are also stored as `float32`. `dtype` influences the memory space necessary for a node and the precision with which the computations are performed.

  ```
  >>> pcanode4 = mdp.nodes.PCANode(dtype = 'float32')
  >>> pcanode4
  PCANode(input_dim=None, output_dim=None, dtype='float32')
  ```

  You can obtain a list of the numerical types supported by a node lookng at its `supported_dtypes` property:

  ```
  >>> pcanode4.supported_dtypes
  [dtype('float32'), dtype('float64')]
  ```

  This attribute is a list of `numpy.dtype` objects.

- A `PolynomialExpansionNode` expands its input in the space of polynomials of a given degree by computing all monomials up to the specified degree. Its constructor needs as first argument the degree of the polynomials space (3 in this case).

  ```
  >>> expnode = mdp.nodes.PolynomialExpansionNode(3)
  ```

Node Training

Some nodes need to be trained to perform their task. For example, the Principal Component Analysis (PCA) algorithm requires the computation of the mean and covariance matrix of a set of training data from which the principal eigenvectors of the data distribution are estimated.

This can be done during a training phases by calling the `train` method. MDP supports both supervised and unsupervised training, and algorithms with multiple training phases.

Some examples of node training:

- Create some random data to train the node

  ```
  >>> x = mdp.numx_rand.random((100, 25))  # 25 variables, 100 observations
  ```

- Analyzes the batch of data `x` and update the estimation of mean and covariance matrix:

  ```
  >>> pcanode1.train(x)
  ```

  At this point the input dimension and the `dtype` have been inherited from `x`:

  ```
  >>> pcanode1
  PCANode(input_dim=25, output_dim=None, dtype='float64')
  ```

- We can train our node with more than one chunk of data. This is especially useful when the input data is too long to be stored in memory or when it has to be created on-the-fly. (See also the Iterables section):

  ```
  >>> for i in range(100):
  ...     x = mdp.numx_rand.random((100, 25))
  ...     pcanode1.train(x)
  >>>
  ```

- Some nodes don't need to or cannot be trained:

```
>>> expnode.is_trainable()
False
```

Trying to train them anyway would raise an `IsNotTrainableException`.

- The training phase ends when the `stop_training`, `execute`, `inverse`, and possibly some other node-specific methods are called. For example we can finalyze the PCA algorithm by computing and selecting the principal eigenvectors

```
>>> pcanode1.stop_training()
```

- If the `PCANode` was declared to have a number of output components dependent on the input variance to be explained, we can check after training the number of output components and the actually explained variance:

```
>>> pcanode3.train(x)
>>> pcanode3.stop_training()
>>> pcanode3.output_dim
16
>>> pcanode3.explained_variance
0.85261144755506446
```

It is now possible to access the trained internal data. In general, a list of the interesting internal attributes can be found in the class documentation.

```
>>> avg = pcanode1.avg            # mean of the input data
>>> v = pcanode1.get_projmatrix() # projection matrix
```

- Some nodes, namely the one corresponding to supervised algorithms, e.g. Fisher Discriminant Analysis (FDA), may need some labels or other supervised signals to be passed during training. Detailed information about the signature of the `train` method can be read in its doc-string.

```
>>> fdanode = mdp.nodes.FDANode()
>>> for label in ['a', 'b', 'c']:
...     x = mdp.numx_rand.random((100, 25))
...     fdanode.train(x, label)
>>>
```

- A node could also require multiple training phases. For example, the training of `fdanode` is not complete yet, since it has two training phases: The first one computing the mean of the data conditioned on the labels, and the second one computing the overall and within-class covariance matrices and solving the FDA problem. The first phase must be stopped and the second one trained:

```
>>> fdanode.stop_training()
>>> for label in ['a', 'b', 'c']:
...     x = mdp.numx_rand.random((100, 25))
...     fdanode.train(x, label)
>>>
```

The easiest way to train multiple phase nodes is using flows, which automatically handle multiple phases (see the Flows section).

Node Execution

Once the training is finished, it is possible to execute the node:

- The input data is projected on the principal components learned in the training phase:

```
>>> x = mdp.numx_rand.random((100, 25))
>>> y_pca = pcanode1.execute(x)
```

- Calling a node instance is equivalent to executing it:

```
>>> y_pca = pcanode1(x)
```

- The input data is expanded in the space of polynomials of degree 3:

```
>>> x = mdp.numx_rand.random((100, 5))
>>> y_exp = expnode(x)
```

- The input data is projected to the directions learned by FDA:

```
>>> x = mdp.numx_rand.random((100, 25))
>>> y_fda = fdanode(x)
```

- Some nodes may allow for optional arguments in the `execute` method. As always the complete information can be found in the doc-string.

Node Inversion

If the operation computed by the node is invertible, the node can also be executed *backwards*, thus computing the inverse transformation:

- In the case of PCA, for example, this corresponds to projecting a vector in the principal components space back to the original data space:

```
>>> pcanode1.is_invertible()
True
>>> x = pcanode1.inverse(y_pca)
```

- The expansion node in not invertible:

```
>>> expnode.is_invertible()
False
```

  Trying to compute the inverse would raise an `IsNotInvertibleException`.

Writing your own nodes: subclassing Node

MDP tries to make it easy to write new nodes that interface with the existing data processing elements.

The `Node` class is designed to make the implementation of new algorithms easy and intuitive. This base class takes care of setting input and output dimension and casting the data to match the numerical type (e.g. float or double) of the internal variables, and offers utility methods that can be used by the developer.

To expand the MDP library of implemented nodes with user-made nodes, it is sufficient to subclass `Node`, overriding some of the methods according to the algorithm one wants to implement, typically the `_train`, `_stop_training`, and `_execute` methods.

In its namespace MDP offers references to the main modules `numpy` or `scipy`, and the subpackages `linalg`, `random`, and `fft` as `mdp.numx`, `mdp.numx_linalg`, `mdp.numx_rand`, and `mdp.numx_fft`. This is done to possibly support additional numerical extensions in the future. For this reason it is recommended to refer to the `numpy` or `scipy` numerical extensions through the MDP aliases `mdp.numx`, `mdp.numx_linalg`, `mdp.numx_fft`, and `mdp.numx_rand` when writing `Node` subclasses. This shall ensure that your nodes can be used without modifications should MDP support alternative numerical extensions in the future.

We'll illustrate all this with some toy examples.

- We start by defining a node that multiplies its input by 2.

  Define the class as a subclass of `Node`:

```
>>> class TimesTwoNode(mdp.Node):
```

  This node cannot be trained. To specify this, one has to overwrite the `is_trainable` method to return False:

```
...     def is_trainable(self):
...         return False
```

  Execute only needs to multiply `x` by 2:

```
...     def _execute(self, x):
...         return 2*x
```

  Note that the `execute` method, which should never be overwritten and which is inherited from the `Node` parent class, will perform some tests, for example to make sure that `x` has the right rank, dimensionality and casts it to have the right `dtype`. After that the user-supplied `_execute` method is called. Each subclass has to handle the `dtype` defined by the user or inherited by the input data, and make sure that internal structures are stored consistently. To help with this the `Node` base class has a method called `_refcast(array)` that casts the input `array` only when its `dtype` is different from the `Node` instance's `dtype`.

  The inverse of the multiplication by 2 is of course the division by 2:

```
...     def _inverse(self, y):
...         return y/2
...
>>>
```

Test the new node:

```
>>> node = TimesTwoNode(dtype = 'int32')
>>> x = mdp.numx.array([[1.0, 2.0, 3.0]])
>>> y = node(x)
>>> print x, '* 2 =  ', y
[ [ 1.  2.  3.]] * 2 =   [ [2 4 6]]
>>> print y, '/ 2 =', node.inverse(y)
[ [2 4 6]] / 2 = [ [1 2 3]]
```

- We then define a node that raises the input to the power specified in the initializer:

```
>>> class PowerNode(mdp.Node):
```

We redefine the init method to take the power as first argument. In general one should always give the possibility to set the `dtype` and the input dimensions. The default value is `None`, which means that the exact value is going to be inherited from the input data:

```
...     def __init__(self, power, input_dim=None, dtype=None):
```

Initialize the parent class:

```
...         super(PowerNode, self).__init__(input_dim=input_dim, dtype=dtype)
```

Store the power:

```
...         self.power = power
```

`PowerNode` is not trainable...

```
...     def is_trainable(self):
...         return False
```

... nor invertible:

```
...     def is_invertible(self):
...         return False
```

It is possible to overwrite the function `_get_supported_dtypes` to return a list of `dtype` supported by the node:

```
...     def _get_supported_dtypes(self):
...         return ['float32', 'float64']
```

The supported types can be specified in any format allowed by the `numpy.dtype` constructor. The interface method `get_supported_dtypes` converts them and sets the property `supported_dtypes`, which is a list of `numpy.dtype` objects.

The `_execute` method:

```
...     def _execute(self, x):
...         return self._refcast(x**self.power)
...
>>>
```

Test the new node:

```
>>> node = PowerNode(3)
>>> x = mdp.numx.array([[1.0, 2.0, 3.0]])
>>> y = node(x)
>>> print x, '**', node.power, '=', node(x)
[ [ 1.  2.  3.]] ** 3 = [ [  1.   8.  27.]]
```

- We now define a node that needs to be trained. The `MeanFreeNode` computes the mean of its training data and subtracts it from the input during execution:

```
>>> class MeanFreeNode(mdp.Node):
...     def __init__(self, input_dim=None, dtype=None):
...         super(MeanFreeNode, self).__init__(input_dim=input_dim,
...                                            dtype=dtype)
```

We store the mean of the input data in an attribute. We initialize it to `None` since we still don't know how large is an input vector:

```
...         self.avg = None
```

Same for the number of training points:

```
...         self.tlen = 0
```

The subclass only needs to overwrite the `_train` method, which will be called by the parent `train` after some testing and casting has been done:

```
...     def _train(self, x):
...         # Initialize the mean vector with the right
...         # size and dtype if necessary:
...         if self.avg is None:
...             self.avg = mdp.numx.zeros(self.input_dim,
...                                       dtype=self.dtype)
```

Update the mean with the sum of the new data:

```
...         self.avg += mdp.numx.sum(x, axis=0)
```

Count the number of points processed:

```
...         self.tlen += x.shape[0]
```

Note that the `train` method can have further arguments, which might be useful to implement algorithms that require supervised learning. For example, if you want to define a node that performs some form of classification you can define a `_train(self, data, labels)` method. The parent `train` checks `data` and takes care to pass the `labels` on (cf. for example `mdp.nodes.FDANode`).

The `_stop_training` function is called by the parent `stop_training` method when the training phase is over. We divide the sum of the training data by the number of training vectors to obtain the mean:

```
...     def _stop_training(self):
...         self.avg /= self.tlen
...         if self.output_dim is None:
...             self.output_dim = self.input_dim
```

Note that we `input_dim` are set automatically by the `train` method, and we want to ensure that the node has `output_dim` set after training. For nodes that do not need training, the setting is performed automatically upon execution. The `_execute` and `_inverse` methods:

```
...     def _execute(self, x):
...         return x - self.avg
...     def _inverse(self, y):
...         return y + self.avg
...
>>>
```

Test the new node:

```
>>> node = MeanFreeNode()
>>> x = mdp.numx_rand.random((10,4))
>>> node.train(x)
>>> y = node(x)
>>> print 'Mean of y (should be zero): ', mdp.numx.mean(y, 0)
Mean of y (should be zero):  [  0.00000000e+00   2.22044605e-17
-2.22044605e-17   1.11022302e-17]
```

- It is also possible to define nodes with multiple training phases. In such a case, calling the `train` and `stop_training` functions multiple times is going to execute successive training phases (this kind of node is much easier to train using Flows). Here we'll define a node that returns a meanfree, unit variance signal. We define two training phases: first we compute the mean of the signal and next we sum the squared, mean-free input to compute the standard deviation (of course it is possible to solve this problem in one single step - remember this is just a toy example).

```
>>> class UnitVarianceNode(mdp.Node):
...     def __init__(self, input_dim=None, dtype=None):
...         super(UnitVarianceNode, self).__init__(input_dim=input_dim,
...                                                dtype=dtype)
...         self.avg = None # average
...         self.std = None # standard deviation
...         self.tlen = 0
```

The training sequence is defined by the user-supplied method `_get_train_seq`, that returns a list of tuples, one for each training phase. The tuples contain references to the training and stop-training methods of each of them. The default output of this method is `[(_train, _stop_training)]`, which explains the standard behavior illustrated above. We overwrite the method to return the list of our training/stop_training methods:

```
...     def _get_train_seq(self):
...         return [(self._train_mean, self._stop_mean),
...                 (self._train_std, self._stop_std)]
```

Next we define the training methods. The first phase is identical to the one in the previous example:

```
...     def _train_mean(self, x):
...         if self.avg is None:
...             self.avg = mdp.numx.zeros(self.input_dim,
...                                       dtype=self.dtype)
...         self.avg += mdp.numx.sum(x, 0)
...         self.tlen += x.shape[0]
...     def _stop_mean(self):
...         self.avg /= self.tlen
```

The second one is only marginally different and does not require many explanations:

```
...     def _train_std(self, x):
...         if self.std is None:
...             self.tlen = 0
...             self.std = mdp.numx.zeros(self.input_dim,
...                                       dtype=self.dtype)
...         self.std += mdp.numx.sum((x - self.avg)**2., 0)
...         self.tlen += x.shape[0]
...     def _stop_std(self):
...         # compute the standard deviation
...         self.std = mdp.numx.sqrt(self.std/(self.tlen-1))
```

The `_execute` and `_inverse` methods are not surprising, either:

```
...     def _execute(self, x):
...         return (x - self.avg)/self.std
...     def _inverse(self, y):
...         return y*self.std + self.avg
>>>
```

Test the new node:

```
>>> node = UnitVarianceNode()
>>> x = mdp.numx_rand.random((10,4))
>>> # loop over phases
... for phase in range(2):
...     node.train(x)
...     node.stop_training()
...
...
```

```
>>> # execute
... y = node(x)
>>> print 'Standard deviation of y (should be one): ', mdp.numx.std(y, axis=0)
Standard deviation of y (should be one):  [ 1.  1.  1.  1.]
```

- In our last example we'll define a node that returns two copies of its input. The output is going to have twice as many dimensions.

```
>>> class TwiceNode(mdp.Node):
...     def is_trainable(self): return False
...     def is_invertible(self): return False
```

When `Node` inherits the input dimension, output dimension, and `dtype` from the input data, it calls the methods `set_input_dim`, `set_output_dim`, and `set_dtype`. Those are the setters for `input_dim`, `output_dim` and `dtype`, which are Python properties. If a subclass needs to change the default behavior, the internal methods `_set_input_dim`, `_set_output_dim` and `_set_dtype` can be overwritten. The property setter will call the internal method after some basic testing and internal settings. The private methods `_set_input_dim`, `_set_output_dim` and `_set_dtype` are responsible for setting the private attributes `_input_dim`, `_output_dim`, and `_dtype` that contain the actual value.

Here we overwrite `_set_input_dim` to automatically set the output dimension to be twice the input one, and `_set_output_dim` to raise an exception, since the output dimension should not be set explicitly.

```
...     def _set_input_dim(self, n):
...         self._input_dim = n
...         self._output_dim = 2*n
...     def _set_output_dim(self, n):
...         raise mdp.NodeException, "Output dim can not be set explicitly!"
```

The `_execute` method:

```
...     def _execute(self, x):
...         return mdp.numx.concatenate((x, x), 1)
...
>>>
```

Test the new node

```
>>> node = TwiceNode()
>>> x = mdp.numx.zeros((5,2))
>>> x
array([[0, 0],
       [0, 0],
       [0, 0],
       [0, 0],
       [0, 0]])
>>> node.execute(x)
array([[0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0]])
```

Flows

A *flow* is a sequence of nodes that are trained and executed together to form a more complex algorithm. Input data is sent to the first node and is successively processed by the subsequent nodes along the sequence.

Using a flow as opposed to handling manually a set of nodes has a clear advantage: The general flow implementation automatizes the training (including supervised training and multiple training phases), execution, and inverse execution (if defined) of the whole sequence.

Crash recovery is optionally available: in case of failure the current state of the flow is saved for later inspection. A subclass of the basic flow class (`CheckpointFlow`) allows user-supplied checkpoint functions to be executed at the end of each phase, for example to save the internal structures of a node for later analysis. Flow objects are Python containers. Most of the builtin `list` methods are available. A `Flow` can be saved or copied using the corresponding `save` and `copy` methods.

Flow instantiation, training and execution

For example, suppose we need to analyze a very high-dimensional input signal using Independent Component Analysis (ICA). To reduce the computational load, we would like to reduce the input dimensionality of the data using PCA. Moreover, we would like to find the data that produces local maxima in the output of the ICA components on a new test set (this information could be used for instance to characterize the ICA filters).

We start by generating some input signal at random (which makes the example useless, but it's just for illustration...). Generate 1000 observations of 20 independent source signals:

```
>>> inp = mdp.numx_rand.random((1000, 20))
```

Rescale x to have zero mean and unit variance:

```
>>> inp = (inp - mdp.numx.mean(inp, 0))/mdp.numx.std(inp, 0)
```

We reduce the variance of the last 15 components, so that they are going to be eliminated by PCA:

```
>>> inp[:,5:] /= 10.0
```

Mix the input signals linearly:

```
>>> x = mdp.utils.mult(inp,mdp.numx_rand.random((20, 20)))
```

`x` is now the training data for our simulation. In the same way we also create a test set `x_test`.

```
>>> inp_test = mdp.numx_rand.random((1000, 20))
>>> inp_test = (inp_test - mdp.numx.mean(inp_test, 0))/mdp.numx.std(inp_test, 0)
>>> inp_test[:,5:] /= 10.0
>>> x_test = mdp.utils.mult(inp_test, mdp.numx_rand.random((20, 20)))
```

- We could now perform our analysis using only nodes, that's the lengthy way...

  1. Perform PCA:

     ```
     >>> pca = mdp.nodes.PCANode(output_dim=5)
     >>> pca.train(x)
     >>> out1 = pca(x)
     ```

  2. Perform ICA using CuBICA algorithm:

     ```
     >>> ica = mdp.nodes.CuBICANode()
     >>> ica.train(out1)
     >>> out2 = ica(out1)
     ```

  3. Find the three largest local maxima in the output of the ICA node when applied to the test data, using a `HitParadeNode`:

     ```
     >>> out1_test = pca(x_test)
     >>> out2_test = ica(out1_test)
     >>> hitnode = mdp.nodes.HitParadeNode(3)
     >>> hitnode.train(out2_test)
     >>> maxima, indices = hitnode.get_maxima()
     ```

- ... or we could use flows, which is the best way:

  ```
  >>> flow = mdp.Flow([mdp.nodes.PCANode(output_dim=5), mdp.nodes.CuBICANode()])
  ```

  Note that flows can be built simply by concatenating nodes:

  ```
  >>> flow = mdp.nodes.PCANode(output_dim=5) + mdp.nodes.CuBICANode()
  ```

  Train the resulting flow:

  ```
  >>> flow.train(x)
  ```

  Now the training phase of PCA and ICA are completed. Next we append a `HitParadeNode` which we want to train on the test data:

  ```
  >>> flow.append(mdp.nodes.HitParadeNode(3))
  ```

  As before, new nodes can be appended to an existing flow by adding them ot it:

```
>>> flow += mdp.nodes.HitParadeNode(3)
```

Train the `HitParadeNode` on the test data:

```
>>> flow.train(x_test)
>>> maxima, indices = flow[2].get_maxima()
```

A single call to the `flow`'s `train` method will automatically take care of training nodes with multiple training phases, if such nodes are present.

Just to check that everything works properly, we can calculate covariance between the generated sources and the output (should be approximately 1):

```
>>> out = flow.execute(x)
>>> cov = mdp.numx.amax(abs(mdp.utils.cov2(inp[:,:5], out)), axis=1)
>>> print cov
[ 0.98992083  0.99244511  0.99227319  0.99663185  0.9871812 ]
```

The `HitParadeNode` is an analysis node and as such does not interfere with the data flow.

Note that flows can be executed by calling the `Flow` instance directly:

```
>>> out = flow(x)
```

Flow inversion

Flows can be inverted by calling their `inverse` method. In the case where the flow contains non-invertible nodes, trying to invert it would raise an exception. In this case, however, all nodes are invertible. We can reconstruct the mix by inverting the flow:

```
>>> rec = flow.inverse(out)
```

Calculate covariance between input mix and reconstructed mix: (should be approximately 1)

```
>>> cov = mdp.numx.amax(abs(mdp.utils.cov2(x/mdp.numx.std(x,axis=0),
...                                        rec/mdp.numx.std(rec,axis=0))))
>>> print cov
[ 0.99839606  0.99744461  0.99616208  0.99772863  0.99690947
  0.99864056  0.99734378  0.98722502  0.98118101  0.99407939
  0.99683096  0.99756988  0.99664384  0.99723419  0.9985529
  0.99829763  0.9982712   0.99721741  0.99682906  0.98858858]
```

Flows are container type objects

`Flow` objects are defined as Python containers, and thus are endowed with most of the methods of Python lists.

You can loop through a `Flow`:

```
>>> for node in flow:
...     print repr(node)
...
PCANode(input_dim=20, output_dim=5, dtype='float64')
CuBICANode(input_dim=5, output_dim=5, dtype='float64')
HitParadeNode(input_dim=5, output_dim=5, dtype='float64')
HitParadeNode(input_dim=5, output_dim=5, dtype='float64')
>>>
```

You can get slices, `pop`, `insert`, and `append` nodes:

```
>>> len(flow)
4
>>> print flow[::2]
[PCANode, HitParadeNode]
>>> nodetoberemoved = flow.pop(-1)
>>> nodetoberemoved
HitParadeNode(input_dim=5, output_dim=5, dtype='float64')
>>> len(flow)
3
```

Finally, you can concatenate flows:

```
>>> dummyflow = flow[1:].copy()
>>> longflow = flow + dummyflow
>>> len(longflow)
4
```

The returned flow must always be consistent, i.e. input and output dimensions of successive nodes always have to match. If you try to create an inconsistent flow you'll get an exception.

Crash recovery

If a node in a flow fails, you'll get a traceback that tells you which node has failed. You can also switch the crash recovery capability on. If something goes wrong you'll end up with a pickle dump of the flow, that can be later inspected.

To see how it works let's define a bogus node that always throws an `Exception` and put it into a flow:

```
>>> class BogusExceptNode(mdp.Node):
...     def train(self,x):
...         self.bogus_attr = 1
...         raise Exception, "Bogus Exception"
...     def execute(self,x):
...         raise Exception, "Bogus Exception"
...
>>> flow = mdp.Flow([BogusExceptNode()])
```

Switch on crash recovery:

```
>>> flow.set_crash_recovery(1)
```

Attempt to train the flow:

```
>>> flow.train(x)
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
  [...]
mdp.linear_flows.FlowExceptionCR:
----------------------------------------
! Exception in node #0 (BogusExceptNode):
Node Traceback:
Traceback (most recent call last):
  [...]
Exception: Bogus Exception
----------------------------------------
A crash dump is available on: "/tmp/MDPcrash_LmISO_.pic"
```

You can give a file name to tell the flow where to save the dump:

```
>>> flow.set_crash_recovery('/home/myself/mydumps/MDPdump.pic')
```

Iterables

Python allows user-defined classes to support iteration, as described in the Python docs. A class is a so called iterable if it defines a method `__iter__` that returns an iterator instance. An iterable is typically some kind of container or collection (e.g. `list` and `tuple` are iterables).

The iterator instance must have a `next` method that returns the next element in the iteration. In Python an iterable also has to have an `__iter__` method itself that returns `self` instead of a new iterator. It is important to understand that an iterator only manages a single iteration. After this iteration it is spend and cannot be used for a second iteration (it cannot be restarted). An iterable on the other hand can create as many iterators as needed and therefore supports multiple iterations. Even though both iterables and iterators have an `__iter__` method they are semantically very different (duck-typing can be misleading in this case).

In the context of MDP this means that an iterator can only be used for a single training phase, while iterables also support multiple training phases. So if you use a node with multiple training phases and train it in a flow make sure that you provide an iterable for this node (otherwise an exception will be raised). For nodes with a single training phase you can use either an iterable or an iterator.

A convenient implementation of the iterator protocol is provided by generators: see this article for an introduction, and the official PEP for a complete description.

Let us define two bogus node classes to be used as examples of nodes:

```
>>> class BogusNode(mdp.Node):
...     """This node does nothing."""
...     def _train(self, x):
...         pass
...
>>> class BogusNode2(mdp.Node):
...     """This node does nothing. But it's not trainable nor invertible.
...     """
...     def is_trainable(self): return False
...     def is_invertible(self): return False
...
>>>
```

This generator generates `blocks` input blocks to be used as training set. In this example one block is a 2-dimensional time series. The first variable is [2,4,6,....,1000] and the second one [0,1,3,5,...,999]. All blocks are equal, this of course would not be the case in a real-life example.

In this example we use a progress bar to get progress information.

```
>>> def gen_data(blocks):
...     for i in mdp.utils.progressinfo(xrange(blocks)):
...         block_x = mdp.numx.atleast_2d(mdp.numx.arange(2,1001,2))
...         block_y = mdp.numx.atleast_2d(mdp.numx.arange(1,1001,2))
...         # put variables on columns and observations on rows
...         block = mdp.numx.transpose(mdp.numx.concatenate([block_x,block_y]))
...         yield block
...
>>>
```

The `progressinfo` function is a fully configurable text-mode progress info box tailored to the command-line die-hards. Have a look at its doc-string and prepare to be amazed!

Let's define a bogus flow consisting of 2 `BogusNode`:

```
>>> flow = mdp.Flow([BogusNode(),BogusNode()], verbose=1)
```

Train the first node with 5000 blocks and the second node with 3000 blocks. Note that the only allowed argument to `train` is a sequence (list or tuple) of iterables or iterators. In case you don't want or need to use incremental learning and want to do a one-shot training, you can use as argument to `train` a single array of data:

block-mode training

```
>>> flow.train([gen_data(5000),gen_data(3000)])
Training node #0 (BogusNode)
[===================================100%==================================>]

Training finished
Training node #1 (BogusNode)
[===================================100%==================================>]

Training finished
Close the training phase of the last node
```

one-shot training using one single set of data for both nodes

```
>>> flow = BogusNode() + BogusNode()
>>> block_x = mdp.numx.atleast_2d(mdp.numx.arange(2,1001,2))
>>> block_y = mdp.numx.atleast_2d(mdp.numx.arange(1,1001,2))
>>> single_block = mdp.numx.transpose(mdp.numx.concatenate([block_x,block_y]))
>>> flow.train(single_block)
```

If your flow contains non-trainable nodes, you must specify a `None` for the non-trainable nodes:

```
>>> flow = mdp.Flow([BogusNode2(),BogusNode()], verbose=1)
>>> flow.train([None, gen_data(5000)])
```

```
Training node #0 (BogusNode2)
Training finished
Training node #1 (BogusNode)
[==================================100%==================================>]

Training finished
Close the training phase of the last node
```

You can use the one-shot training:

```
>>> flow = mdp.Flow([BogusNode2(),BogusNode()], verbose=1)
>>> flow.train(single_block)
Training node #0 (BogusNode2)
Training finished
Training node #1 (BogusNode)
Training finished
Close the training phase of the last node
```

Iterators can always be safely used for execution and inversion, since only a single iteration is needed:

```
>>> flow = mdp.Flow([BogusNode(),BogusNode()], verbose=1)
>>> flow.train([gen_data(1), gen_data(1)])
Training node #0 (BogusNode)
Training finished
Training node #1 (BosgusNode)
[==================================100%==================================>]

Training finished
Close the training phase of the last node
>>> output = flow.execute(gen_data(1000))
[==================================100%==================================>]
>>> output = flow.inverse(gen_data(1000))
[==================================100%==================================>]
```

Execution and inversion can be done in one-shot mode also. Note that since training is finished you are not going to get a warning

```
>>> output = flow(single_block)
>>> output = flow.inverse(single_block)
```

If a node requires multiple training phases (e.g., `GaussianClassifierNode`), `Flow` automatically takes care of using the iterable multiple times. In this case generators (and iterators) are not allowed, since they are spend after yielding the last data block.

However, it is fairly easy to wrap a generator in a simple iterable if you need to:

```
>>> class SimpleIterable(object):
...     def __init__(self, blocks):
...         self.blocks = blocks
...     def __iter__(self):
...         # this is a generator
...         for i in range(self.blocks):
...             yield generate_some_data()
>>>
```

Note that if you use random numbers within the generator, you usually would like to reset the random number generator to produce the same sequence every time:

```
>>> class RandomIterable(object):
...     def __init__(self):
...         self.state = None
...     def __iter__(self):
...         if self.state is None:
...             self.state = mdp.numx_rand.get_state()
...         else:
...             mdp.numx_rand.set_state(self.state)
...         for i in range(2):
```

```
...             yield mdp.numx_rand.random((1,4))
>>> iterable = RandomIterable()
>>> for x in iterable:
...     print x
...
[[ 0.99586495  0.53463386  0.6306412   0.09679571]]
[[ 0.51117469  0.46647448  0.95089738  0.94837122]]
>>> for x in iterable:
...     print x
...
[[ 0.99586495  0.53463386  0.6306412   0.09679571]]
[[ 0.51117469  0.46647448  0.95089738  0.94837122]]
```

Checkpoints

It can sometimes be useful to execute arbitrary functions at the end of the training or execution phase, for example to save the internal structures of a node for later analysis. This can easily be done by defining a `CheckpointFlow`. As an example imagine the following situation: you want to perform Principal Component Analysis (PCA) on your data to reduce the dimensionality. After this you want to expand the signals into a nonlinear space and then perform Slow Feature Analysis to extract slowly varying signals. As the expansion will increase the number of components, you don't want to run out of memory, but at the same time you want to keep as much information as possible after the dimensionality reduction. You could do that by specifying the percentage of the total input variance that has to be conserved in the dimensionality reduction. As the number of output components of the PCA node now can become as large as the that of the input components, you want to check, after training the PCA node, that this number is below a certain threshold. If this is not the case you want to abort the execution and maybe start again requesting less variance to be kept.

Let start defining a generator to be used through the whole example:

```
>>> def gen_data(blocks,dims):
...     mat = mdp.numx_rand.random((dims,dims))-0.5
...     for i in xrange(blocks):
...         # put variables on columns and observations on rows
...         block = mdp.utils.mult(mdp.numx_rand.random((1000,dims)), mat)
...         yield block
...
>>>
```

Define a `PCANode` which reduces dimensionality of the input, a `PolynomialExpansionNode` to expand the signals in the space of polynomials of degree 2 and a `SFANode` to perform SFA:

```
>>> pca = mdp.nodes.PCANode(output_dim=0.9)
>>> exp = mdp.nodes.PolynomialExpansionNode(2)
>>> sfa = mdp.nodes.SFANode()
```

As you see we have set the output dimension of the `PCANode` to be `0.9`. This means that we want to keep at least 90% of the variance of the original signal. We define a `PCADimensionExceededException` that has to be thrown when the number of output components exceeds a certain threshold:

```
>>> class PCADimensionExceededException(Exception):
...     """Exception base class for PCA exceeded dimensions case."""
...     pass
...
>>>
```

Then, write a `CheckpointFunction` that checks the number of output dimensions of the `PCANode` and aborts if this number is larger than `max_dim`:

```
>>> class CheckPCA(mdp.CheckpointFunction):
...     def __init__(self,max_dim):
...         self.max_dim = max_dim
...     def __call__(self,node):
...         node.stop_training()
...         act_dim = node.get_output_dim()
...         if act_dim > self.max_dim:
...             errstr = 'PCA output dimensions exceeded maximum '+\
```

```
...                       '(%d > %d)'%(act_dim,self.max_dim)
...             raise PCADimensionExceededException, errstr
...         else:
...             print 'PCA output dimensions = %d'%(act_dim)
...
>>>
```

Define the CheckpointFlow:

```
>>> flow = mdp.CheckpointFlow([pca, exp, sfa])
```

To train it we have to supply 3 generators and 3 checkpoint functions:

```
>>> flow.train([gen_data(10, 50), None, gen_data(10, 50)],
...            [CheckPCA(10), None, None])
Traceback (most recent call last):
  File "<stdin>", line 2, in ?
  [...]
__main__.PCADimensionExceededException: PCA output dimensions exceeded maximum (25 > 10)
```

The training fails with a `PCADimensionExceededException`. If we only had 12 input dimensions instead of 50 we would have passed the checkpoint:

```
>>> flow[0] = mdp.nodes.PCANode(output_dim=0.9)
>>> flow.train([gen_data(10, 12), None, gen_data(10, 12)],
...            [CheckPCA(10), None, None])
PCA output dimensions = 6
```

We could use the built-in `CheckpoinSaveFunction` to save the `SFANode` and analyze the results later :

```
>>> pca = mdp.nodes.PCANode(output_dim=0.9)
>>> exp = mdp.nodes.PolynomialExpansionNode(2)
>>> sfa = mdp.nodes.SFANode()
>>> flow = mdp.CheckpointFlow([pca, exp, sfa])
>>> flow.train([gen_data(10, 12), None, gen_data(10, 12)],
...            [CheckPCA(10),
...             None,
...             mdp.CheckpointSaveFunction('dummy.pic',
...                                        stop_training = 1,
...                                        protocol = 0)])
...
PCA output dimensions = 7
```

We can now reload and analyze the `SFANode`:

```
>>> fl = file('dummy.pic')
>>> import cPickle
>>> sfa_reloaded = cPickle.load(fl)
>>> sfa_reloaded
SFANode(input_dim=35, output_dim=35, dtype='d')
```

Don't forget to clean the rubbish:

```
>>> fl.close()
>>> import os
>>> os.remove('dummy.pic')
```

Node Extensions

First note that dealing with the node extension mechanism should be considered advanced usage, so you can skip this section.

The node extension mechanism makes it possible to dynamically add methods or class attributes for specific features to node classes (e.g. for parallelization the nodes need a `_fork` and `_join` method). Note that methods are just a special case of class attributes, the extension mechanism treats them like any other class attributes. It is also possible for users to define new extensions to introduce new functionality for MDP nodes without having to directly modify any MDP code. The node extension mechanism basically enables some form of *Aspect-oriented programming* (AOP) to deal with *cross-cutting concerns* (i.e., you want to add a new aspect to node classes which

are spread all over MDP and possibly your own code). In the AOP terminology any new methods you introduce contain *advice* and the *pointcut* is effectively defined by the calling of these methods.

Without the extension mechanism the adding of new aspects to nodes would be done through inheritance, deriving new node classes that implement the aspect for the parent node class. This is fine unless one wants to use multiple aspects, requiring multiple inheritance for every combination of aspects one wants to use. Therefore this approach does not scale well with the number of aspects.

The node extension mechanism does not directly depend on inheritance, instead it adds the methods or class attributes to the node classes dynamically at runtime (like *method injection*). This makes it possible to activate extensions just when they are needed, reducing the risk of interference between different extensions. One can also use multiple extensions at the same time, as long as there is no interference, i.e., both extensions do not use any attributes with the same name.

The node extension mechanism uses a special Metaclass, which allows it to define the node extensions as classes derived from nodes (bascially just what one would do without the extension mechanism). This keeps the code readable and avoids some problems when using automatic code checkers (like the background pylint checks in the Eclipse IDE with PyDev).

In MDP the node extension mechanism is currently used by the `parallel` package and for the the HTML representation in the `hinet` package, so the best way to learn more is to look there. We also use these packages in the following examples.

Using Extensions

First of all you can get all the available node extensions by calling the `get_extensions` function, or to get just a list of their names use `get_extensions().keys()`. Be careful not to modify the dict returned by `get_extensions`, since this will actually modify the registered extensions. The currently activated extensions are returned by `get_active_extensions`. To activate an extension use `activate_extension`, e.g. to activate the parallel extension use `mdp.activate_extension("parallel")`. Alternatively you can use the function decorator `@with_extension("parallel"` In the future we will also support the new `with` statement in Python. Activating an extension adds the available extensions attributes to the supported nodes. An extension can be deactivated with `deactivate_extension` (if you use the function decorator this is done automatically at the end).

Writing Extension Nodes

Suppose you have written your own nodes and would like to make them compatible with a particular extension (e.g. add the required methods). The first way to do this is by using multiple inheritance to derive from the base class of this extension and your custom node class. For example the parallel extension of the SFA node is defined in a class `ParallelSFANode(ParallelExtensionNode, mdp.nodes.SFANode)`. Here `ParallelExtensionNode` is the base class of the extension. Then you define the required methods or attributes just like in a normal class. If you want you could even use the new `ParallelSFANode` class like a normal class, ignoring the extension mechanism. Note that your extension node is automatically registered in the extension mechanism (through a little metaclass magic).

For methods you can alternatively use the `extension_method` function decorator. You define the extension method like a normal function, but add the function decorator on top, for example:

```
>>> @mdp.extension_method("html", mdp.hinet.Rectangular2dSwitchboard)
... def _html_representation(self):
...     pass
...
>>>
```

The first decorator argument is the name of the extension, the second is the class you want to extend. You can also specify the method name as a third argument, then the name of the function is ignored (this allows you to get rid of warnings about multiple functions with the same name).

Creating Extensions

To create a new node extension you just have to create a new extension base class. For example the HTML representation extension in `mdp.hinet` is created with

```
>>> class  HTMLExtensionNode(mdp.ExtensionNode, mdp.Node):
...     """Extension node for HTML representations of individual nodes."""
...     extension_name = "html"
...     def html_representation(self):
...         pass
...     def _html_representation(self):
```

```
...         pass
...
>>>
```

Note that you must derive from `ExtensionNode`. If you also derive from `mdp.Node` then the methods (and attributes) in this class are the default implementation for the `mdp.Node` class. So they will be used by all nodes without a more specific implementation. If you do not derive from `mdp.Node` then there is no such default implementation. You can also derive from a more specific node class if your extension only applies to these specific nodes.

When you define a new extension then you must define the `extension_name` attribute. This magic attribute is used to register the new extension and you can activate or deactivate the extension by using this name.

Note that extensions can override attributes and methods that are defined in a node class. The original attributes can still be accessed by prefixing the name with `_non_extension_` (the prefix string is also available as `mdp.ORIGINAL_ATTR_PREFIX`). On the other hand one extension is not allowed to override attributes that were defined by another currently active extension.

The extension mechanism uses some magic to make the behavior more intuitive with respect to inheritance. Basically methods or attributes defined by extensions shadow those which are not defined in the extension. Here is an example:

```
>>> class TestExtensionNode(mdp.ExtensionNode):
...     extension_name = "test"
...     def _execute(self):
...         return 0
...
>>> class TestNode(mdp.Node):
...     def _execute(self):
...         return 1
...
>>> class ExtendedTestNode(TestExtensionNode, TestNode):
...     pass
...
>>>
```

After this extension is activated any calls of `_execute` in instances of `TestNode` will return 0 instead of 1. The `_execute` from the extension base-class shadows the method from `TestNode`. This makes it easier to share behavior for different classes. Without this magic one would have to explicitly override `_execute` in `ExtendedTestNode` (or derive the extension base-class from `Node`, but that would give this behavior to all node classes). Note that there is a `verbose` argument in `activate_extension` which can help with debugging.

Hierarchical Networks

In case the desired data processing application cannot be defined as a sequence of nodes, the `hinet` subpackage makes it possible to construct arbitrary feed-forward architectures, and in particular hierarchical networks.

Building blocks

The `hinet` package contains three basic building blocks (which are all nodes themselves) to construct hierarchical node networks: `Layer`, `FlowNode`, `Switchboard`.

- The first building block is the `Layer` node, which works like a horizontal version of flow. It acts as a wrapper for a set of nodes that are trained and executed in parallel. For example, we can combine two nodes with 100 dimensional input to construct a layer with a 200-dimensional input

  ```
  >>> node1 = mdp.nodes.PCANode(input_dim=100, output_dim=10)
  >>> node2 = mdp.nodes.SFANode(input_dim=100, output_dim=20)
  >>> layer = mdp.hinet.Layer([node1, node2])
  >>> layer
  Layer(input_dim=200, output_dim=30, dtype=None)
  ```

  The first half of the 200 dimensional input data is then automatically assigned to `node1` and the second half to `node2`. We can train and execute a `Layer` just like any other node. Note that the dimensions of the nodes must be already set when the layer is constructed.

- In order to be able to build arbitrary feed-forward node structures, `hinet` provides a wrapper class for flows (i.e., vertical stacks of nodes) called `FlowNode`. For example, we can replace `node1` in the above example with a `FlowNode`:

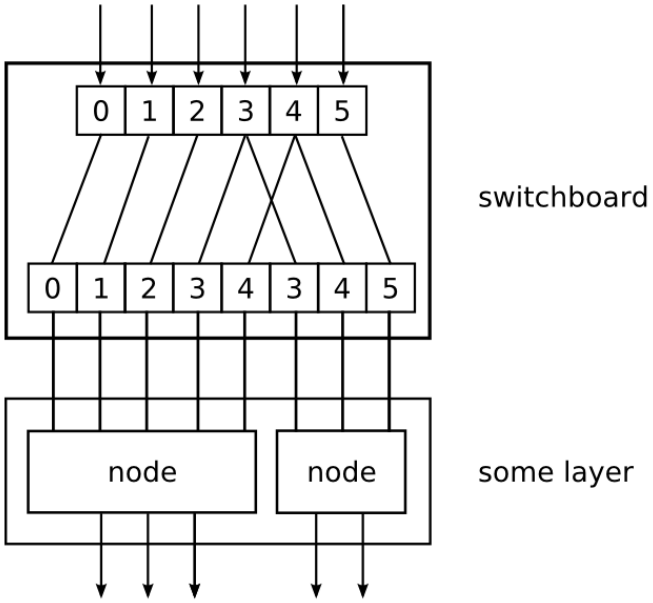
```
>>> node1_1 = mdp.nodes.PCANode(input_dim=100, output_dim=50)
>>> node1_2 = mdp.nodes.SFANode(input_dim=50, output_dim=10)
>>> node1_flow = mdp.Flow([node1_1, node1_2])
>>> node1 = mdp.hinet.FlowNode(node1_flow)
>>> layer = mdp.hinet.Layer([node1, node2])
>>> layer
Layer(input_dim=200, output_dim=30, dtype=None)
```

in this example `node1` has two training phases (one for each internal node). Therefore `layer` now has two training phases as well and behaves like any other node with two training phases. By combining and nesting `FlowNode` and `Layer`, it is thus possible to build complex node structures.

- When implementing networks one might have to route different parts of the data to different nodes in a layer in complex ways. This is done by the `Switchboard` node, which can handle such the routing. A `Switchboard` is initialized with a 1-D Array with one entry for each output connection, containing the corresponding index of the input connection that it receives its input from, e.g.:

```
>>> switchboard = mdp.hinet.Switchboard(input_dim=6, connections=[0,1,2,3,4,3,4,5])
>>> switchboard
Switchboard(input_dim=3, output_dim=2, dtype=None)
>>> x = mdp.numx.array([[2,4,6,8,10,12]])
>>> switchboard.execute(x)
array([[ 2,  4,  6,  8, 10,  8, 10, 12]])
```

The switchboard can then be followed by a layer that splits the routed input to the appropriate nodes, as illustrated in following picture:



By combining layers with switchboards one can realize any feed-forward network topology. Defining the switchboard routing manually can be quite tedious. One way to automatize this is by defining switchboard subclasses for special routing situations. The `Rectangular2dSwitchboard` class is one such example and will be briefly described in a later example.

HTML representation

Since hierarchical networks can be quite complicated, `hinet` includes the class `HiNetHTMLTranslator` that translates an MDP flow into a graphical visualization in an HTML file. We also provide the helper function `show_flow` which creates a complete HTML file with the flow visualization in it and opens it in your standard browser.

```
>>> mdp.hinet.show_flow(flow)
```

To integrate the HTML representation into your own custom HTML file you can take a look at `show_flow` to learn the usage of `HiNetHTMLTranslator`. You can also specify custom translations for node types via the extension mechanism (e.g to define which parameters are displayed). Note that `HiNetHTMLTranslator` is derived from `HiNetTranslator` which is the base class for general flow translations and is for example also used in the `parallel` package (to translate a flow into a parallel version).

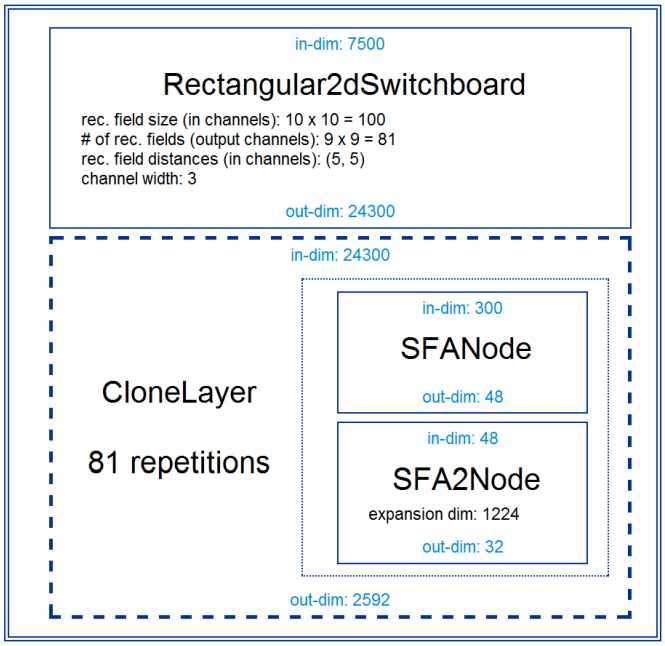
Example application (2-D image data)

As promised we now present a more complicated example. We define the lowest layer for some kind of image processing system. The input data is assumed to consist of image sequences, with each image having a size of 50 by 50 pixels. We take color images, so after converting the images to one dimensional numpy arrays each pixel corresponds to three numeric values in the array, which the values just next to each other (one for each color channel).

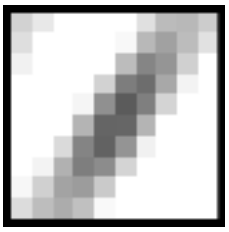
The processing layer consists of many parallel units, which only see a small image region with a size of 10 by 10 pixels. These so called receptive fields cover the whole image and have an overlap of five pixels. Note that the image data is represented as an 1-D array. Therefore we need the `Rectangular2dSwitchboard` class to correctly route the data for each receptive field to the corresponding unit in the following layer. We also call the switchboard output for a single receptive field an output channel and the three RGB values for a single pixel form an input channel. Each processing unit is a flow consisting of an `SFANode` (to somewhat reduce the dimensionality) that is followed by an `SFA2Node`. Since we assume that the statistics are similar in each receptive filed we actually use the same nodes for each receptive field. Therefore we use a `CloneLayer` instead of the standard `Layer`. Here is the actual code:

```
>>> switchboard = mdp.hinet.Rectangular2dSwitchboard(x_in_channels=50,
...                                                  y_in_channels=50,
...                                                  x_field_channels=10,
...                                                  y_field_channels=10,
...                                                  x_field_spacing=5,
...                                                  y_field_spacing=5,
...                                                  in_channel_dim=3)
>>> sfa_dim = 48
>>> sfa_node = mdp.nodes.SFANode(input_dim=switchboard.out_channel_dim,
...                              output_dim=sfa_dim)
>>> sfa2_dim = 32
>>> sfa2_node = mdp.nodes.SFA2Node(input_dim=sfa_dim,
...                                output_dim=sfa2_dim)
>>> flownode = mdp.hinet.FlowNode(mdp.Flow([sfa_node, sfa2_node]))
>>> sfa_layer = mdp.hinet.CloneLayer(flownode,
...                                  n_nodes=switchboard.output_channels)
>>> flow = mdp.Flow([switchboard, sfa_layer])
```

The HTML representation of the the constructed flow looks like this in your browser:



Now one can train this flow for example with image sequences from a movie. After the training phase one can compute the image pattern that produces the highest response in a given output coordinate (use `mdp.utils.QuadraticForm`). One such optimal image pattern may look like this (only a grayscale version is shown):



So the network units have developed some kind of primitive line detector. More on this topic can be found in: Berkes, P. and Wiskott, L., *Slow feature analysis yields a rich repertoire of complex cell properties*. Journal of Vision, 5(6):579-602.

One could also add more layers on top of this first layer to do more complicated stuff. Note that the `in_channel_dim` in the next `Rectangular2dSwitchboard` would be 32, since this is the output dimension of one unit in the `CloneLayer` (instead of 3 in the first switchboard, corresponding to the three RGB colors).

Parallelization

The `parallel` package adds the ability to parallelize the training and execution of MPD flows. This package is split into two decoupled parts:

- The first part consists of a parallel extension of the familiar MDP structures of nodes and flows. The first basic building block is the extension class `ParallelExtensionNode` for nodes which can be trained in a parallelized way. It adds the `fork` and `join` methods. When providing a parallel extension for custom node classes you should provide `_fork` and `_join`. Secondly there is the `ParallelFlow` class, which internally splits the training or execution into tasks which can then be processed in parallel.
- The second part consists of the schedulers. A scheduler takes tasks and processes them in a more or less parallel way (e.g. in multiple Python processes). A scheduler deals with the more technical aspects of the parallelization, but does not need to know anything about nodes and flows.

Basic Examples

In the following example we parallelize a simple `Flow` consisting of PCA and quadratic SFA, so that it makes use of two cores on a modern CPU:

```
>>> node1 = mdp.nodes.PCANode(input_dim=100, output_dim=10)
>>> node2 = mdp.nodes.SFA2Node(input_dim=10, output_dim=10)
>>> parallel_flow = mdp.parallel.ParallelFlow([node1, node2])
>>> n_data_chunks = 2
>>> data_iterables = [[mdp.numx_rand.random((200, 100))
...                    for _ in range(n_data_chunks)]
...                    for _ in range(2)]
>>> scheduler = mdp.parallel.ProcessScheduler(n_processes=2)
>>> parallel_flow.train(data_iterables, scheduler=scheduler)
>>> scheduler.shutdown()
```

So only two additional lines were needed to parallelize the training of the flow. All one has to do is use a `ParallelFlow` insttead of the normal `Flow` and provide a scheduler. Note that the `shutdown` method should be always called at the end to make sure that the threads and processes used by the scheduler are cleaned up properly. So one should better put the `shutdown` call into a safer try/finally statement:

```
>>> try:
...     parallel_flow.train(data_iterables, scheduler=scheduler)
... finally:
...     scheduler.shutdown()
...
```

Scheduler

A scheduler is an instance of one of the scheduler classes we provide. They are all derived from the `Scheduler` base class. Apart from the base class we currently only provide the `ProcessScheduler` which distributes the incoming tasks over multiple Python processes (circumventing the global interpreter lock). There is also experimental support for the Parallel Python library in the `mdp.parallel.pp_support` package.

The first important method of the scheduler class is `add_task`. This method takes two arguments: `data` and `task_callable`, which can be a function or an object with a `__call__` method. The return value of the

task_callable is the result of the task. If task_callable is None then the last provided task_callable will be used. This splitting into callable and data makes it possible to implement caching of the task_callable in the scheduler and its workers (caching is turned on by default in the ProcessScheduler). To further influence caching you can also derive from the TaskCallable class, which has a fork to generate new callables when the cached callable must be preserved. For MDP training and execution there already are corresponding TaskCallable classes which are automatically used, so normally there is no need to worry about this.

After submitting all the tasks with add_task you can then call the get_results method. This method returns all the task results, normally in a list. If there are open tasks in the scheduler get_results will wait until all the tasks are finished. You can also check the status of the scheduler by looking at the n_open_tasks property, which tells you the number of open tasks. After using the scheduler you should always call the shutdown method, otherwise you might get error messages from not properly closed processes.

Internally an instance of the base class mdp.parallel.ResultContainer is used for the storage of the results in the scheduler. By providing your own result container to the scheduler you modify the storage. For example the default result container is an instance of OrderedResultContainer

Parallel Nodes

If you want to parallelize your own nodes you have to provide parallel extensions for them. The ParallelExtensionNode base class has the new template methods fork and join. fork should return a new node instance. This new instance can then be trained somewhere else (e.g. in a different process) with the usual train method. Afterwards one calls join on the original node, with the forked node as the argument. This is effectively the same as calling train directly on the original node.

When writing your own parallel node extension you should only overwrite the _fork and _join methods, which are automatically called by fork and join. The fork and join take care of the standard node attributes like the dimensions. You should also look at the source code of a parallel node like ParallelPCANode to get a better idea of how to parallelize nodes.

Currently we provide the following parallel nodes: ParallelPCANode, ParallelWhiteningNode, ParallelSFANode, ParallelSFA2Node, ParallelFDANode, ParallelHistogramNode, ParallelAdaptiveCutoffNode, ParallelFlowNode, ParallelLayer, ParallelCloneLayer (the last three are derived from the hinet package).

Parallel Flows

As shown earlier in the example a parallel flow implements the parallel training (and execution) using a provided scheduler. The scheduler is simply provided as an additional argument for the train or execute method of the parallel flow. If no scheduler is provided the parallel flow behaves just like a normal flow.

You can also do the parallel training in a customized way by manually fetching tasks and assigning them to a scheduler. However, this should rarely be required.

Classifier nodes

New in MDP 2.6 is the ClassifierNode base class which offers a simple interface for creating classification tasks. Usually, one does not want to use the classification output in a flow but extract this information independently. Most classification nodes will therefore simply return the identity function on execute; all classification work is done with the new methods label, prob and rank.

As a first example, we will use the GaussianClassifierNode.

```
>>> gc = mdp.nodes.GaussianClassifierNode()
>>> gc.train(mdp.numx_rand.random((50, 3)), +1)
>>> gc.train(mdp.numx_rand.random((50, 3)) - 0.8, -1)
```

We have trained the node and assigned the labels +1 and -1 to the sample points. Note that in this simple case we don't need to give a label to each individual point, when only a single label is given, it is assigned to the whole batch of features. However, it is also possible to use the more explicit form:

```
>>> gc.train(mdp.numx_rand.random((50, 3)), [+1] * 50)
```

We can then retrieve the most probable labels for some testing data,

```
>>> test_data = mdp.numx.array([[0.1, 0.2, 0.1], [-0.1, -0.2, -0.1]])
>>> gc.label(test_data)
[1, -1]
```

and also get the probability for each label.

```
>>> gc.prob(test_data)
[{-1: 0.21013407927789607, 1: 0.78986592072210393},
 {-1: 0.99911458988539714, 1: 0.00088541011460285866}]
```

Finally, it is possible to get the ranking of the labels, starting with the likeliest.

```
>>> gc.rank(test_data)
[[1, -1], [-1, 1]]
```

New nodes should inherit from `ClassifierNode` and implement the `_label` and `_prob` methods. The public `rank` method will be created automatically from `prob`.

Real life examples

Logistic maps

In this section we show a complete example of MDP usage in a machine learning application, and use non-linear Slow Feature Analysis for processing of non-stationary time series. We consider a chaotic time series derived by a logistic map (a demographic model of the population biomass of species in the presence of limiting factors such as food supply or disease) that is non-stationary in the sense that the underlying parameter is not fixed but is varying smoothly in time.

The goal is to extract the slowly varying parameter that is hidden in the observed time series. This example reproduces some of the results reported in Laurenz Wiskott, *Estimating Driving Forces of Nonstationary Time Series with Slow Feature Analysis*. arXiv.org e-Print archive.

Generate the slowly varying driving force, a combination of three sine waves (freqs: 5, 11, 13 Hz), and define a function to generate the logistic map

```
>>> p2 = mdp.numx.pi*2
>>> t = mdp.numx.linspace(0,1,10000,endpoint=0) # time axis 1s, samplerate 10KHz
>>> dforce = mdp.numx.sin(p2*5*t) + mdp.numx.sin(p2*11*t) + mdp.numx.sin(p2*13*t)
>>> def logistic_map(x,r):
...     return r*x*(1-x)
...
>>>
```

Note that we define `series` to be a two-dimensional array. Inputs to MDP must be two-dimensional arrays with variables on columns and observations on rows. In this case we have only one variable:

```
>>> series = mdp.numx.zeros((10000,1),'d')
```

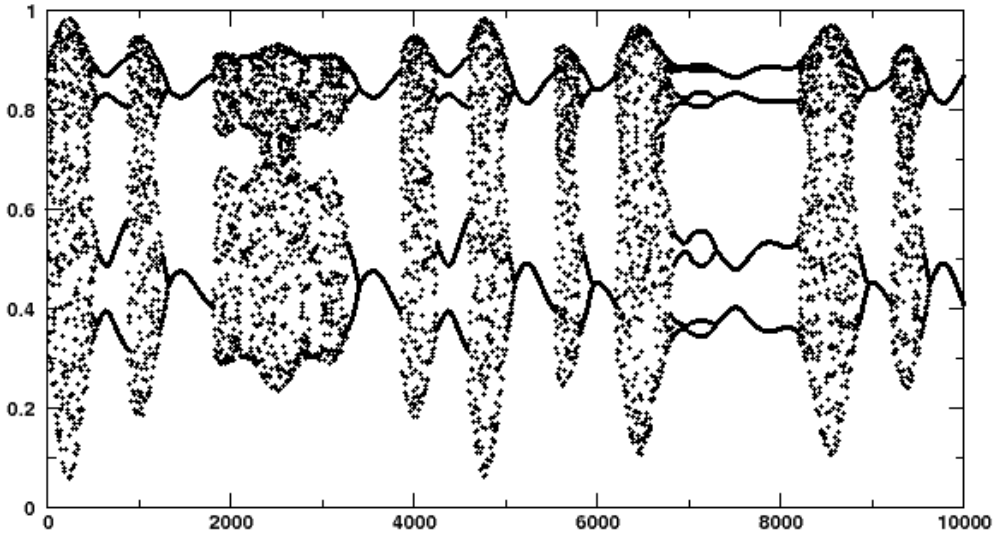
Fix the initial condition:

```
>>> series[0] = 0.6
```

Generate the time series using the logistic equation. The driving force modifies the logistic equation parameter `r`:

```
>>> for i in range(1,10000):
...     series[i] = logistic_map(series[i-1],3.6+0.13*dforce[i])
...
>>>
```

If you have a plotting package `series` should look like this:



To reconstruct the underlying parameter, we define a `Flow` to perform SFA in the space of polynomials of degree 3. We first use a node that embeds the 1-dimensional time series in a 10 dimensional space using a sliding temporal window of size 10 (`TimeFramesNode(10)`). Second, we expand the signal in the space of polynomials of degree 3 using a `PolynomialExpansionNode(3)`. Finally, we perform SFA on the expanded signal and keep the slowest feature using the `SFANode(output_dim=1)`.

In order to measure the slowness of the input time series before and after processing, we put at the beginning and at the end of the node sequence a node that computes the eta-value (a measure of slowness) of its input (`EtaComputerNode()`):

```
>>> flow = (mdp.nodes.EtaComputerNode() +
...          mdp.nodes.TimeFramesNode(10) +
...          mdp.nodes.PolynomialExpansionNode(3) +
...          mdp.nodes.SFANode(output_dim=1) +
...          mdp.nodes.EtaComputerNode() )
...
>>>
```

Since the time series is short enough to be kept in memory we don't need to define generators and we can feed the flow directly with the whole signal:

```
>>> flow.train(series)
```

Since the second and the third nodes are not trainable we are going to get two warnings (`Training Interrupted`). We can safely ignore them. Execute the flow to get the slow feature

```
>>> slow = flow(series)
```

The slow feature should match the driving force up to a scaling factor, a constant offset and the sign. To allow a comparison we rescale the driving force to have zero mean and unit variance:

```
>>> resc_dforce = (dforce - mdp.numx.mean(dforce,0))/mdp.numx.std(dforce,0)
```

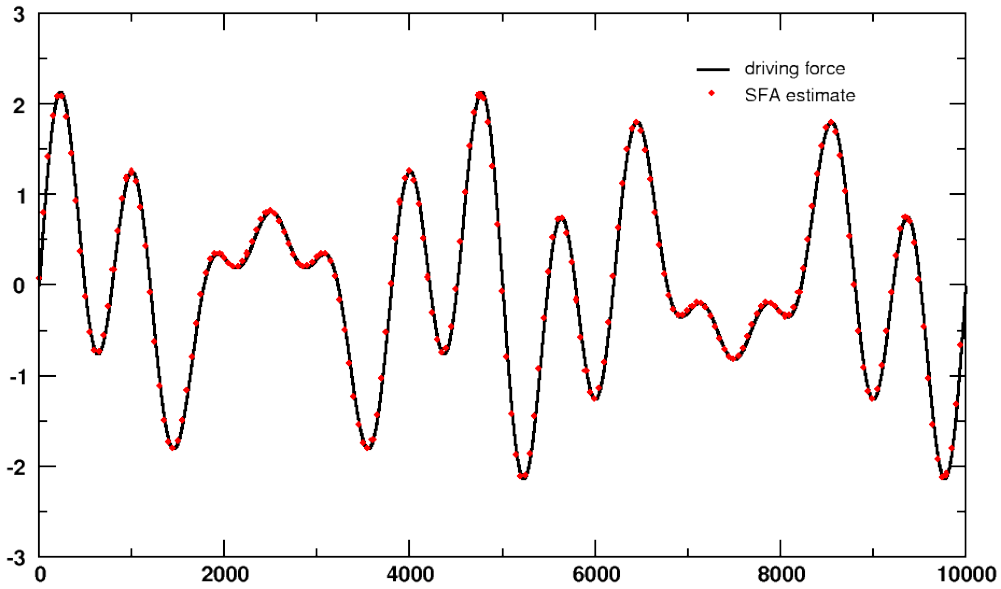
Print covariance between the rescaled driving force and the slow feature. Note that embedding the time series with 10 time frames leads to a time series with 9 observations less:

```
>>> mdp.utils.cov2(resc_dforce[:-9],slow)
0.99992501533859179
```

Print the *eta-values* of the chaotic time series and of the slow feature

```
>>> print 'Eta value (time series): ', flow[0].get_eta(t=10000)
Eta value (time series):  [ 3002.53380245]
>>> print 'Eta value (slow feature): ', flow[-1].get_eta(t=9996)
Eta value (slow feature):  [ 10.2185087]
```

If you have a plotting package you could plot the real driving force is plotted together with the driving force estimated by SFA and see that they match perfectly:



Growing neural gas

We generate uniformly distributed random data points confined on different 2-D geometrical objects. The Growing Neural Gas Node builds a graph with the same topological structure.

Fix the random seed to obtain reproducible results:

```
>>> mdp.numx_rand.seed(1266090063)
```

Some functions to generate uniform probability distributions on different geometrical objects:

```
>>> def uniform(min_, max_, dims):
...     """Return a random number between min_ and max_ ."""
...     return mdp.numx_rand.random(dims)*(max_-min_)+min_
...
>>> def circumference_distr(center, radius, n):
...     """Return n random points uniformly distributed on a circumference."""
...     phi = uniform(0, 2*mdp.numx.pi, (n,1))
...     x = radius*mdp.numx.cos(phi)+center[0]
...     y = radius*mdp.numx.sin(phi)+center[1]
...     return mdp.numx.concatenate((x,y), axis=1)
...
>>> def circle_distr(center, radius, n):
...     """Return n random points uniformly distributed on a circle."""
...     phi = uniform(0, 2*mdp.numx.pi, (n,1))
...     sqrt_r = mdp.numx.sqrt(uniform(0, radius*radius, (n,1)))
...     x = sqrt_r*mdp.numx.cos(phi)+center[0]
...     y = sqrt_r*mdp.numx.sin(phi)+center[1]
...     return mdp.numx.concatenate((x,y), axis=1)
...
>>> def rectangle_distr(center, w, h, n):
...     """Return n random points uniformly distributed on a rectangle."""
...     x = uniform(-w/2., w/2., (n,1))+center[0]
...     y = uniform(-h/2., h/2., (n,1))+center[1]
...     return mdp.numx.concatenate((x,y), axis=1)
...
>>> N = 2000
```

Explicitly collect random points from some distributions:

- Circumferences:

```
>>> cf1 = circumference_distr([6,-0.5], 2, N)
>>> cf2 = circumference_distr([3,-2], 0.3, N)
```

- Circles:

```
>>> cl1 = circle_distr([-5,3], 0.5, N/2)
>>> cl2 = circle_distr([3.5,2.5], 0.7, N)
```

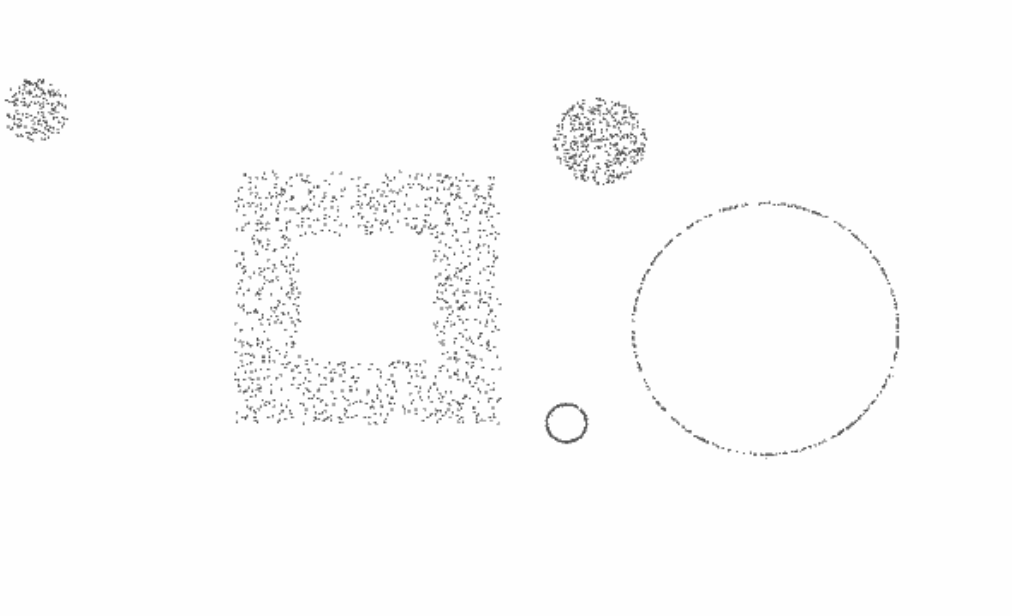
- Rectangles:

```
>>> r1 = rectangle_distr([-1.5,0], 1, 4, N)
>>> r2 = rectangle_distr([+1.5,0], 1, 4, N)
>>> r3 = rectangle_distr([0,+1.5], 2, 1, N/2)
>>> r4 = rectangle_distr([0,-1.5], 2, 1, N/2)
```

Shuffle the points to make the statistics stationary

```
>>> x = mdp.numx.concatenate([cf1, cf2, cl1, cl2, r1,r2,r3,r4], axis=0)
>>> x = mdp.numx.take(x,mdp.numx_rand.permutation(x.shape[0]), axis=0)
```

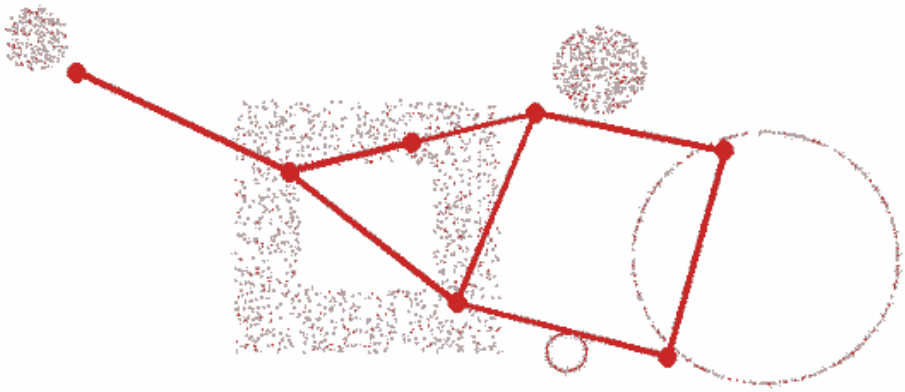
If you have a plotting package `x` should look like this:



Create a `GrowingNeuralGasNode` and train it:

```
>>> gng = mdp.nodes.GrowingNeuralGasNode(max_nodes=75)
```

The initial distribution of nodes is randomly chosen:

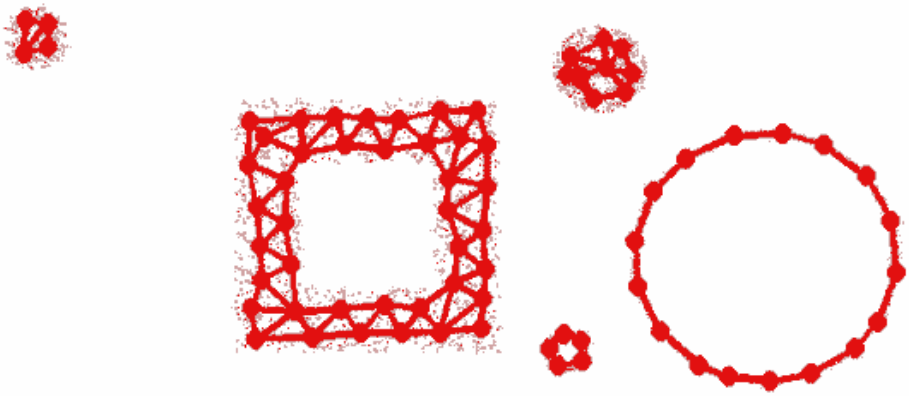


The training is performed in small chunks in order to visualize the evolution of the graph:

```
>>> STEP = 500
>>> for i in range(0,x.shape[0],STEP):
...     gng.train(x[i:i+STEP])
...     # [...] plotting instructions
...
>>> gng.stop_training()
```

See here the animation of training.

Visualizing the neural gas network, we'll see that it is adapted to the topological structure of the data distribution:

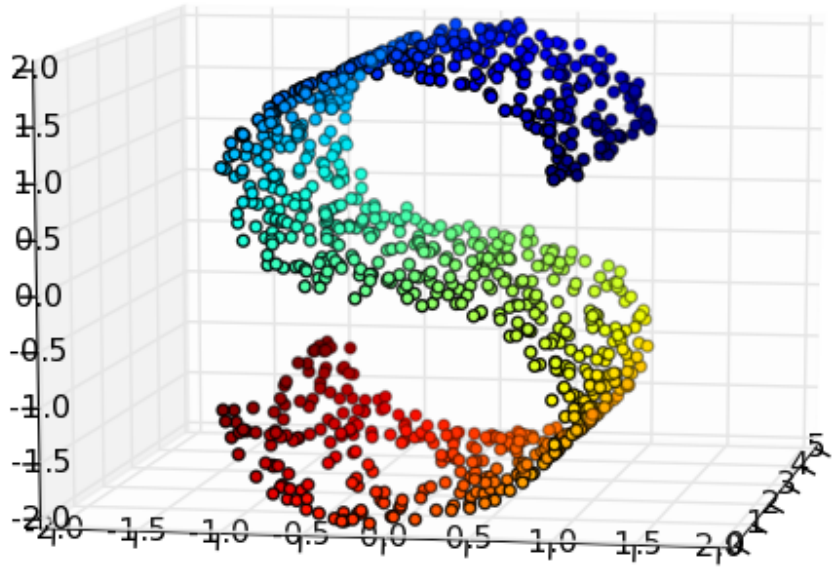


Calculate the number of connected components:

```
>>> n_obj = len(gng.graph.connected_components())
>>> print n_obj
5
```

Locally linear embedding

Locally linear embedding (LLE) approximates the input data with a low-dimensional surface and reduces its dimensionality by learning a mapping to the surface. Here we consider data generated randomly on an S-shaped 2D surface embedded in a 3D space:



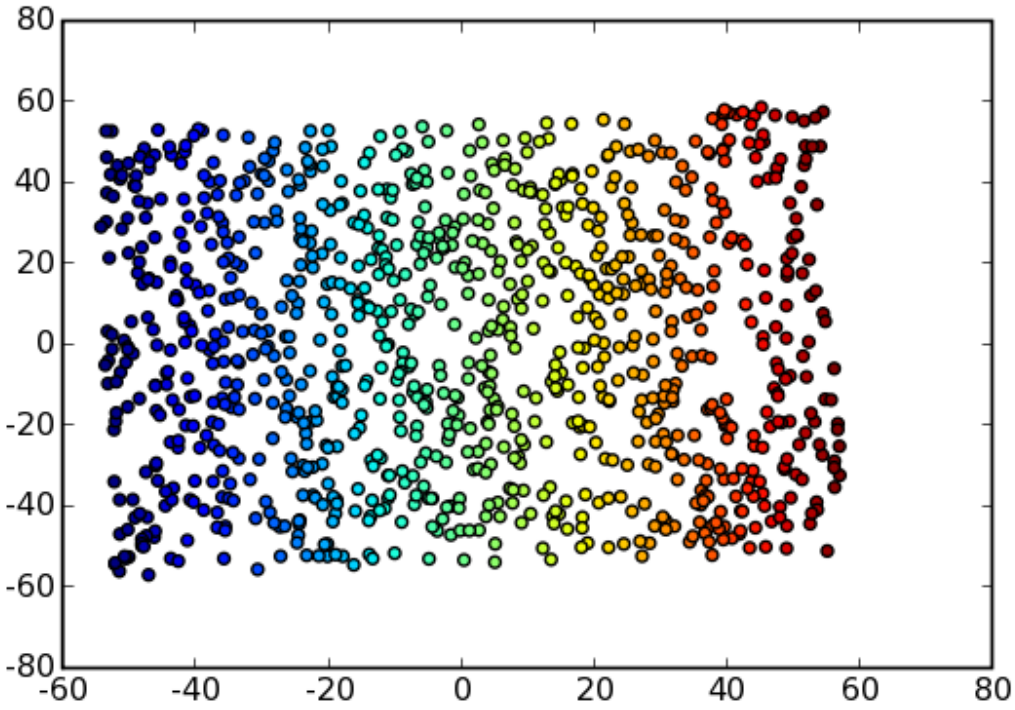
The surface is defined by the function

```
>>> def s_distr(npoints, hole=False):
...     """Return a 3D S-shaped surface. If hole is True, the surface has
...     a hole in the middle."""
...     t = mdp.numx_rand.random(npoints)
...     y = mdp.numx_rand.random(npoints)*5.
...     theta = 3.*mdp.numx.pi*(t-0.5)
...     x = mdp.numx.sin(theta)
...     z = mdp.numx.sign(theta)*(mdp.numx.cos(theta) - 1.)
...     if hole:
...         indices = mdp.numx.where(((0.3>t) | (0.7<t)) | ((1.>y) | (4.<y)))
...         return x[indices], y[indices], z[indices], t[indices]
...     else:
...         return x, y, z, t
```

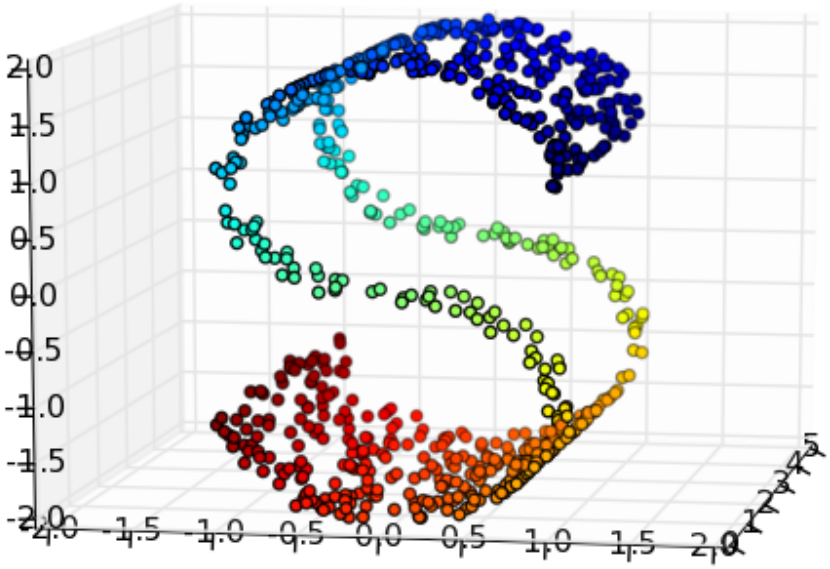
We generate 1000 points on this surface, then define an LLENode with parameters k=15 (number of neighbors) and output_dim=2 (the number of dimensions of the reduced representation), then train and execute the node to obtain the projected data:

```
>>> n, k = 1000, 15
>>> x, y, z, t = s_distr(n, hole=False)
>>> data = mdp.numx.array([x,y,z]).T
>>> lle_projected_data = mdp.nodes.LLENode(k, output_dim=2)(data)
```

The projected data forms a nice parametric representation of the S-shaped surface:



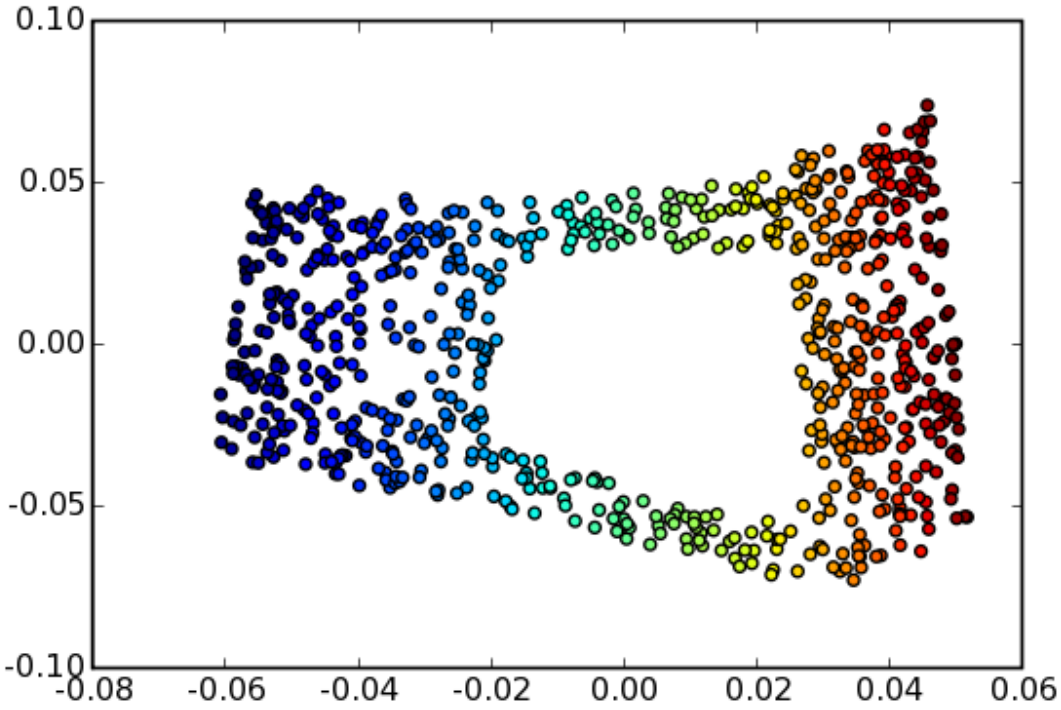
The problem becomes more difficult if the surface has a hole in the middle:



In this case, the LLE algorithm has some difficulty finding the correct representation. The lines

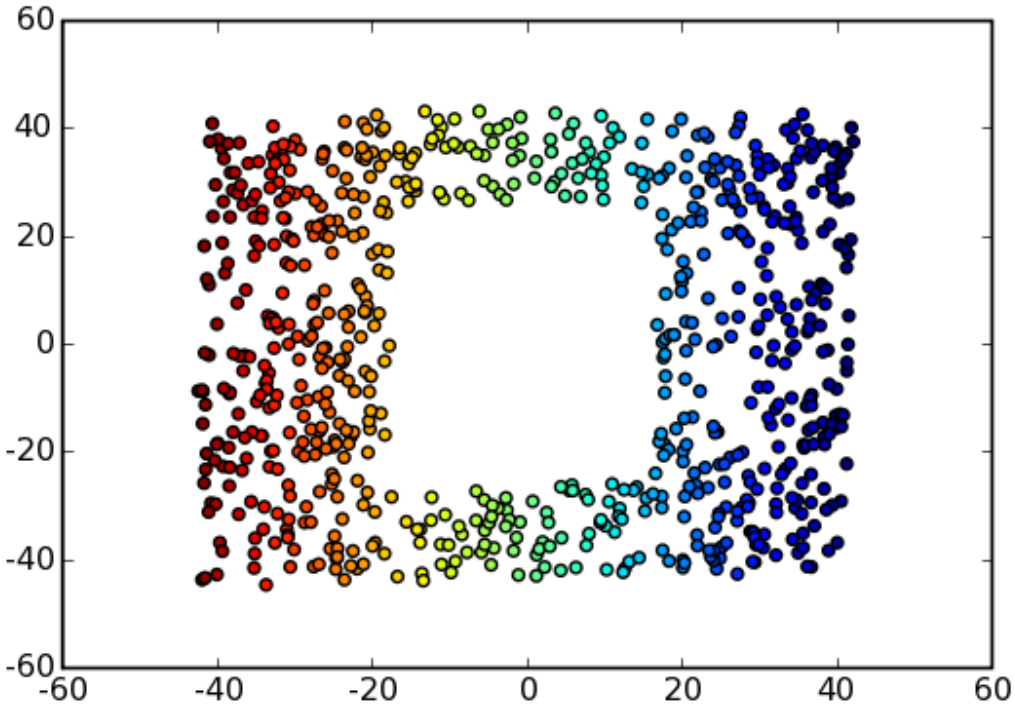
```
>>> x, y, z, t = s_distr(n, hole=True)
>>> data = mdp.numx.array([x,y,z]).T
>>> lle_projected_data = mdp.nodes.LLENode(k, output_dim=2)(data)
```

return a distorted mapping:



The Hessian LLE Node takes the local curvature of the surface into account, and is able to find a better representation:

```
>>> hlle_projected_data = mdp.nodes.HLLENode(k, output_dim=2)(data)
```



Node List

Here is the complete list of implemented nodes. Refer to the API for the full documentation and interface description.

- **AdaptiveCutoffNode** Works like the *HistogramNode*. The cutoff bounds are then chosen such that a given fraction of the training data would have been clipped.

- **CuBICANode** Perform Independent Component Analysis using the CuBICA algorithm.
  Reference: Blaschke, T. and Wiskott, L. (2003). *CuBICA: Independent Component Analysis by Simultaneous Third- and Fourth-Order Cumulant Diagonalization*. IEEE Transactions on Signal Processing, 52(5), pp. 1250-1256. More information about ICA can be found among others in Hyvarinen A., Karhunen J., Oja E. (2001). *Independent Component Analysis*, Wiley.
- **CutoffNode** Clip the data at the specified upper and lower bounds.
- **DiscreteHopfieldClassifier** Learns discrete patterns and can retrieve them again even when they are slightly distorted.
- **EtaComputerNode** Compute the eta values of the normalized training data. The delta value of a signal is a measure of its temporal variation, and is defined as the mean of the derivative squared, i.e. `delta(x) = mean(dx/dt(t)^2)`. `delta(x)` is zero if 'x' is a constant signal, and increases if the temporal variation of the signal is bigger. The eta value is a more intuitive measure of temporal variation, defined as `eta(x) = T/(2*pi) * sqrt(delta(x))`. If 'x' is a signal of length 'T' which consists of a sine function that accomplishes exactly 'N' oscillations, then `eta(x) = N`.
  Reference: Wiskott, L. and Sejnowski, T.J. (2002). *Slow Feature Analysis: Unsupervised Learning of Invariances*, Neural Computation, 14(4):715-770.
- **FANode** Perform Factor Analysis. The current implementation should be most efficient for long data sets: the sufficient statistics are collected in the training phase, and all EM-cycles are performed at its end. More information about Factor Analysis can be found in Max Welling's classnotes in the chapter "Linear Models".
- **FastICANode** Perform Independent Component Analysis using the FastICA algorithm.
  Reference: Aapo Hyvarinen (1999). *Fast and Robust Fixed-Point Algorithms for Independent Component Analysis*, IEEE Transactions on Neural Networks, 10(3):626-634. More information about ICA can be found among others in Hyvarinen A., Karhunen J., Oja E. (2001). *Independent Component Analysis*, Wiley.
- **FDANode** Perform a (generalized) Fisher Discriminant Analysis of its input. It is a supervised node that implements FDA using a generalized eigenvalue approach.
  More information on Fisher Discriminant Analysis can be found for example in C. Bishop, *Neural Networks for Pattern Recognition*, Oxford Press, pp. 105-112.
- **GaussianClassifierNode** Perform a supervised Gaussian classification. Given a set of labelled data, the node fits a gaussian distribution to each class.
- **GrowingNeuralGasNode** Learn the topological structure of the input data by building a corresponding graph approximation.
  More information about the Growing Neural Gas algorithm can be found in B. Fritzke, *A Growing Neural Gas Network Learns Topologies*, in G. Tesauro, D. S. Touretzky, and T. K. Leen (editors), *Advances in Neural Information Processing Systems 7*, pages 625-632. MIT Press, Cambridge MA, 1995.
- **HistogramNode** Store a fraction of the incoming data during training. This data can then be used to analyse the histogram of the data.
- **HitParadeNode** Collect the first 'n' local maxima and minima of the training signal which are separated by a minimum gap 'd'.
- **HLLENode** Original code contributed by Jake VanderPlas.
  Perform a Hessian Locally Linear Embedding analysis on the data.
  Implementation based on algorithm outlined in David L. Donoho and Carrie Grimes, *Hessian Eigenmaps: new locally linear embedding techniques for high-dimensional data*, Proceedings of the National Academy of Sciences 100(10):5591-5596 (2003).
- **ISFANode** Perform Independent Slow Feature Analysis on the input data.
  More information about ISFA can be found in: Blaschke, T. , Zito, T., and Wiskott, L. *Independent Slow Feature Analysis and Nonlinear Blind Source Separation.* Neural Computation 19(4):994-1021 (2007).
- **JADENode** Original code contributed by Gabriel Beckers.
  Perform Independent Component Analysis using the JADE algorithm.
  References: Cardoso, J.-F, and Souloumiac, A. *Blind beamforming for non Gaussian signals.* Radar and Signal Processing, IEE Proceedings F, 140(6): 362-370 (1993), and Cardoso, J.-F. *High-order contrasts for independent component analysis.* Neural Computation, 11(1): 157-192 (1999). More information about ICA can be found among others in Hyvarinen A., Karhunen J., Oja E. (2001). *Independent Component Analysis*, Wiley.

- **KMeansClassifier** Employs K-Means Clustering for a given number of centroids.
- **LibSVMClassifier** The LibSVMClassifier class acts as a wrapper around the LibSVM library for support vector machines, which needs to be installed as a python module. The software can be found here: http://www.csie.ntu.edu.tw/~cjlin/libsvm/

  Warning: Because it is a new addition to MDP, the LibSVMClassifier should be used with caution. Also, the interface might have some flaws. Any hints or bug reports are very welcome.

  See also, Chih-Chung Chang and Chih-Jen Lin, *LIBSVM : a library for support vector machines* (2001).
- **LinearRegressionNode** Compute least-square, multivariate linear regression on the input data.
- **LLENode** Original code contributed by Jake VanderPlas.

  Perform a Locally Linear Embedding analysis on the data.

  Based on the algorithm outlined in *An Introduction to Locally Linear Embedding* by L. Saul and S. Roweis, using improvements suggested in *Locally Linear Embedding for Classification* by D. deRidder and R.P.W. Duin.

  References: Sam Roweis and Lawrence Saul, *Nonlinear dimensionality reduction by locally linear embedding*, Science 290(5500):2323-2326, 2000.
- **NIPALSNode** Original code contributed by Michael Schmuker, Susanne Lezius, and Farzad Farkhooi.

  Perform Principal Component Analysis using the NIPALS algorithm. This algorithm is particularyl useful if you have more variable than observations, or in general when the number of variables is huge and calculating a full covariance matrix may be unfeasable. It's also more efficient of the standard PCANode if you expect the number of significant principal components to be a small. In this case setting output_dim to be a certain fraction of the total variance, say 90%, may be of some help.

  Reference for NIPALS (Nonlinear Iterative Partial Least Squares): Wold, H. *Nonlinear estimation by iterative least squares procedures.* in David, F. (Editor), Research Papers in Statistics, Wiley, New York, pp 411-444 (1966).

  More information about Principal Component Analysis, a.k.a. discrete Karhunen-Loeve transform can be found among others in I.T. Jolliffe, *Principal Component Analysis*, Springer-Verlag (1986).
- **NoiseNode** Original code contributed by Mathias Franzius.

  Inject multiplicative or additive noise into the input data.
- **PCANode** Filter the input data throug the most significatives of its principal components.

  More information about Principal Component Analysis, a.k.a. discrete Karhunen-Loeve transform can be found among others in I.T. Jolliffe, *Principal Component Analysis*, Springer-Verlag (1986).
- **PerceptronClassifier** Trains a single binary perceptron with multiple inputs.
- **PolynomialExpansionNode** Perform expansion in a polynomial space.
- **QuadraticExpansionNode** Perform expansion in the space formed by all linear and quadratic monomials
- **RBMNode** Implementation of a Restricted Boltzmann Machine.

  For more information on RBMs, see Geoffrey E. Hinton (2007) Boltzmann machine. Scholarpedia, 2(5):1668
- **RBMWithLabelsNode** Implementation of a Restricted Boltzmann Machine with softmax labels.

  For more information on RBMs, see Geoffrey E. Hinton (2007) Boltzmann machine Scholarpedia, 2(5):1668

  Hinton, G. E, Osindero, S., and Teh, Y. W. *A fast learning algorithm for deep belief nets*, Neural Computation, 18:1527-1554 (2006).
- **ShogunSVMClassifier** The ShogunSVMClassifier class works as a wrapper class for accessing the SHOGUN machine learning toolbox. We use the python_modular wrapper to access SHOGUN and SHOGUN must not be older than version 0.9. **Warning**: Because it is a new addition to MDP, the ShogunSVM-Classifier should be used with caution. Also, the interface might have some flaws. Any hints or bug reports are very welcome.

  Most of the kernel machines and linear classifiers of shogun should work with this class.

  For exact information about data formats which SHOGUN can accept, see http://www.shogun-toolbox.org/

  S. Sonnenburg, G. Raetsch, C. Schaefer and B. Schoelkopf, *Large Scale Multiple Kernel Learning*, Journal of Machine Learning Research, 7:1531-1565 (2006).

- **SFANode** Extract the slowly varying components from the input data.

  More information about Slow Feature Analysis can be found in Wiskott, L. and Sejnowski, T.J., *Slow Feature Analysis: Unsupervised Learning of Invariances*, Neural Computation, 14(4):715-770 (2002).

- **SFA2Node** Get an input signal, expand it in the space of inhomogeneous polynomials of degree 2 and extract its slowly varying components. The `get_quadratic_form` method returns the input-output function of one of the learned unit as a `mdp.utils.QuadraticForm` object.

  More information about Slow Feature Analysis can be found in Wiskott, L. and Sejnowski, T.J., *Slow Feature Analysis: Unsupervised Learning of Invariances*, Neural Computation, 14(4):715-770 (2002).

- **SimpleMarkovClassifier** Learns the probability with which a label is assigned to a label.

- **TDSEPNode** Perform Independent Component Analysis using the TDSEP algorithm. Note that TDSEP, as implemented in this Node, is an online algorithm, i.e. it is suited to be trained on huge data sets, provided that the training is done sending small chunks of data for each time.

  Reference: Ziehe, Andreas and Muller, Klaus-Robert (1998). *TDSEP an efficient algorithm for blind separation using time structure.* in Niklasson, L, Boden, M, and Ziemke, T (Editors), Proc. 8th Int. Conf. Artificial Neural Networks (ICANN 1998).

- **TimeFramesNode** Copy delayed version of the input signal on the space dimensions.

```
For example, for time_frames=3 and gap=2:

[ X(1) Y(1)        [ X(1) Y(1) X(3) Y(3) X(5) Y(5)
  X(2) Y(2)          X(2) Y(2) X(4) Y(4) X(6) Y(6)
  X(3) Y(3)   -->    X(3) Y(3) X(5) Y(5) X(7) Y(7)
  X(4) Y(4)          X(4) Y(4) X(6) Y(6) X(8) Y(8)
  X(5) Y(5)          ...  ...  ...  ...  ...  ... ]
  X(6) Y(6)
  X(7) Y(7)
  X(8) Y(8)
  ...  ...  ]
```

- **WhiteningNode** 'Whiten' the input data by filtering it through the most significatives of its principal components. All output signals have zero mean, unit variance and are decorrelated.

- **XSFANode** Perform Non-linear Blind Source Separation using Slow Feature Analysis. This node is designed to iteratively extract statistically independent sources from (in principle) arbitrary invertible nonlinear mixtures. The method relies on temporal correlations in the sources and consists of a combination of nonlinear SFA and a projection algorithm. More details can be found in the reference given below (once it's published).

  More information about XSFA can be found in: Sprekeler, H., Zito, T., and Wiskott, L. (2009). *An Extension of Slow Feature Analysis for Nonlinear Blind Source Separation.* Journal of Machine Learning Research, submitted

> **Didn't you find what you were looking for?**
> If you want to contribute some code or a new algorithm, please do not hesitate to submit it!

Additional utilities

MDP offers some additional utilities of general interest in the `mdp.utils` module. Refer to the API for the full documentation and interface description.

CovarianceMatrix This class stores an empirical covariance matrix that can be updated incrementally. A call to the `fix` method returns the current state of the covariance matrix, the average and the number of observations, and resets the internal data.

Note that the internal sum is a standard `__add__` operation. We are not using any of the fancy sum algorithms to avoid round off errors when adding many numbers. If you want to contribute a `CovarianceMatrix` class that uses such algorithms we would be happy to include it in MDP. For a start see the Python recipe by Raymond Hettinger. For a review about floating point arithmetic and its pitfalls see this interesting article.

DelayCovarianceMatrix This class stores an empirical covariance matrix between the signal and time delayed signal that can be updated incrementally.

MultipleCovarianceMatrices Container class for multiple covariance matrices to easily execute operations on all matrices at the same time.

dig_node(node) Crawl recursively an MDP `Node` looking for arrays. Return (dictionary, string), where the dictionary is: { attribute_name: (size_in_bytes, array_reference)} and string is a nice string representation of it.

get_node_size(node) Get 'node' total byte-size using `cPickle` with protocol=2. (The byte-size is related the memory needed by the node).

progressinfo(sequence, length, style, custom) A fully configurable text-mode progress info box tailored to the command-line die-hards. To get a progress info box for your loops use it like this:

```
>>> for i in progressinfo(sequence):
...     do_something(i)
```

You can also use it with generators, files or any other iterable object, but in this case you have to specify the total length of the sequence:

```
>>> for line in progressinfo(open_file, nlines):
...     do_something(line)
```

A few examples of the available layouts:

```
[==================================73%=============>..................]
```

Progress: 67%[=======================================>]

23% [02:01:28] - [00:12:37]

QuadraticForm Define an inhomogeneous quadratic form as `1/2 x'Hx + f'x + c`. This class implements the quadratic form analysis methods presented in: Berkes, P. and Wiskott, L. On the analysis and interpretation of inhomogeneous quadratic forms as receptive fields. *Neural Computation*, 18(8): 1868-1895. (2006).

refcast(array, dtype) Cast the array to 'dtype' only if necessary, otherwise return a reference.

rotate(mat, angle, columns, units) Rotate in-place a NxM data matrix in the plane defined by the 'columns' when observation are stored on rows. Observations are rotated counterclockwise. This corresponds to the following matrix-multiplication for each data-point (unchanged elements omitted):

```
[  cos(angle) -sin(angle)     [ x_i ]
   sin(angle)  cos(angle) ] * [ x_j ]
```

random_rot(dim, dtype) Return a random rotation matrix, drawn from the Haar distribution (the only uniform distribution on SO(n)). The algorithm is described in the paper Stewart, G.W., *The efficient generation of random orthogonal matrices with an application to condition estimators*, SIAM Journal on Numerical Analysis, 17(3), pp. 403-409, 1980. For more information see this Wikipedia entry.

symrand(dim_or_eigv, dtype) Return a random symmetric (Hermitian) matrix with eigenvalues uniformly distributed on (0,1].

HTML Slideshows

The `mdp.utils` module contains some classes and helper function to display animated results in a Webbrowser. This works by creating an HTML file with embedded JavaScript code, which dynamically loads image files (the images contain the content that you want to animate and can for example be created with matplotlib). MDP internally uses the open source Templete templating libray, written by David Bau.

The easiest way to create a slideshow it to use one of these two helper function:

show_image_slideshow(filenames, image_size, filename=None, title=None, **kwargs) Write the slideshow into a HTML file, open it in the browser and return the file name. `filenames` is a list of the images files that you want to display in the slideshow. `image_size` is a 2-tuple containing the width and height at which the images should be displayed. There are also a couple of additional arguments, which are documented in the docstring.

image_slideshow(filenames, image_size, title=None, **kwargs) This function is similar to `show_image_slideshow`, but it simply returns the slideshow HTML code (including the JavaScript code) which you can then embed into your own HTML file. Note that the default slideshow CSS code is not included, but it can be accessed in `mdp.utils.IMAGE_SLIDESHOW_STYLE`.

Note that there are also two demos for slideshows in the `mdp\demo` folder.

Graph module

MDP contains `mdp.graph`, a lightweight package to handle directed graphs.

Graph Represent a directed graph. This class contains several methods to create graph structures and manipulate them, among which

- `add_tree`**: Add a tree to the graph.** The tree is specified with a nested list of tuple, in a LISP-like notation. The values specified in the list become the values of the single nodes. Return an equivalent nested list with the nodes instead of the values.
  Example:
- `topological_sort`: Perform a topological sort of the nodes.
- `dfs`, `undirected_dfs`: Perform Depth First sort.
- `bfs`, `undirected_bfs`: Perform Breadth First sort.
- `connected_components`**: Return a list of lists containing** the nodes of all connected components of the graph.
- `is_weakly_connected`: Return True if the graph is weakly connected.

GraphEdge Represent a graph edge and all information attached to it.

GraphNode Represent a graph node and all information attached to it.

recursive_map(func, seq) Apply a function recursively on a sequence and all subsequences.

recursive_reduce(func, seq, *argv) Apply `reduce(func, seq)` recursively to a sequence and all its subsequences.

BiMDP

BiMDP defines a framework for more general flow sequences, involving top-down processes (e.g. for error back-propagation) and loops. So the *bi* in BiMDP primarily stands for *bidirectional*. It also adds a couple of other features, like a standartized way to transport additional data, and a HTML based flow inspection utility. Because BiMDP is a rather large addition and changes a few things compared to standard MDP it is not included in `mdp` but must be imported seperately as `bimdp` (BiMDP is included in the standard MDP installation):

```
>>> import bimdp
```

Warning: BiMDP is a new addition to MDP, so currently it should be considered as beta-stage software. Even though it already went through long testing and several refactoring rounds it is still not as mature and polished as the rest of MDP. This also means that your bug findings or suggestions for improvement will be very valuable. The API of BiMDP should be pretty stable now, we don't expect any fundamental breakages in the future.

Here is a brief summary of the most important new features in BiMDP:

- Nodes can specify other nodes as jump targets, where the execution or training will be continued. It is now possible to use loops or backpropagation, in contrast to the strictly linear execution of a normal MDP flow. This is enabled by the new `BiFlow` class. The new `BiNode` base class adds a `node_id` string attribute, which can be used to target a node.

  The complexities of arbitrary data flows are evenly split up between `BiNode` and `BiFlow`: Nodes specify their data and target using a standartized interface, which is then interpreted by the flow (somewhat like a very primitive domain specific language). The alternative approach would have been to use specialised flow classes or container nodes for each use case, which ultimately comes down to a design decision. Of course you can (and should) still take that route if for some reson BiMDP is not an adequate solution for your problem.

- In addition to the standard array data, nodes can transport more data in a message dictionary (these are really just standard Python dictionaries, so they are `dict` instances). The new `BiNode` base class provides functionality to make this as convenient as possible.

- An interactive HTML-based inspection for flow training and execution is available. This allows you to step through your flow for debugging or add custom visualizations to analyse what is going on.

- BiMDP supports and extends the `hinet` and the `parallel` packages from MDP. BiMDP in general is compatible with MDP, so you can use standard MDP nodes in a `BiFlow`. You can also use `BiNode` instances in a standard MDP flow, as long as you don't use certain BiMDP features.

The structure of BiMDP closely follows that of MDP, so there are submodules `bimdp.nodes`, `bimdp.parallel`, and `bimdp.hinet`. The module `bimdp.nodes` contains `BiNode` versions of nearly all MDP nodes. For example `bimdp.nodes.PCABiNode` is derived from both `BiNode` and `mdp.nodes.PCANode`.

There are currently two examples available in the `mdp-examples` repository, which demonstrate how BiMDP can be used. The first example `backpropagation` is a simple multilayer perceptron, using backpropagation for learning. The second example `binetdbn` is a proof-of-concept implementation of a deep belief network.

Finally note that this tutorial is intended to serve as an introduction, covering all the basic aspects of BiMDP. For more detailed specifications have a look at the docstrings.

Targets, id's and Messages

The return value of the `execute` method in a normal MDP node is restricted to a single 2d array. A BiMDP `BiNode` on the other hand can optionally return a tuple containing an additional message dictionary and a target value. So in general the return value is a tuple `(x, msg, target)`, where `x` is a the usual 2d array. Alternatively a `BiNode` is also allowed to return only the array `x` or a 2-tuple `(x, msg)` (specifying no target value). Unless stated otherwise the last entry in the tuple should not be `None`, but all the other values are allowed to be `None` (so if you specify a target then `msg` can be `None`, and even `x` can be `None`).

The `msg` message is a normal Python dictionary. You can use it to transport any data that does not fit into the `x` 2d data array. Nodes can take data from to the message and add data to it. The message is propagated along with the `x` data. If a normal MDP node is contained in a `BiFlow` then the message is simply passed around it. A `BiNode` can freely decide how to interact with the message (see the BiNode section for more information).

The target value is either a string or a number. The number is the relative position of the target node in the flow, so a target value of 1 corresponds to the following node, while -1 is the previous node. The `BiNode` base class also allows the specification of a `node_id` string in the `__init__` method. This string can then be used as a target value.

The `node_id` string is also useful to access nodes in a `BiFlow` instance. The standard MDP `Flow` class already implements standard Python container methods, so `flow[2]` will return the third node in the flow. `BiFlow` in addition enables you to use the `node_id` to index nodes in the flow, just like for a dictionary. Here is a simple example:

```
>>> pca_node = bimdp.nodes.PCABiNode(node_id="pca")
>>> biflow = bimdp.BiFlow([pca_node])
>>> biflow["pca"]
PCABiNode(input_dim=None, output_dim=None, dtype=None, node_id="pca")
```

BiFlow

The `BiFlow` class mostly works in the same way as the normal `Flow` class. We already mentioned several of the new features, like support for targets, messages, and retrieving nodes based on their `node_id`. Appart from that the only major difference is the way in which you can provide additional arguments for nodes. For example the `FDANode` in MDP requires class labels in addition to the data array (telling the node to which class each data point belongs). In the `Flow` class the additional data (the class labels) is provided by the same iterable as the data. In a `BiFlow` this is no longer allowed, since this functionality is provided by the more general message mechanism. In addition to the `data_iterables` keyword argument there is a new `msg_iterables` argument, to provide iterables for the message dictionary. The structure of the `msg_iterables` argument must be the same as that of `data_iterables`, but instead of yielding arrays it should yield dictionaries (containing the additional data values with the corresponding keys). Here is an example:

```
>>> samples = mdp.numx_rand.random((100,10))
>>> labels = mdp.numx.arange(100)
>>> flow = bimdp.BiFlow([mdp.nodes.PCANode(), bimdp.nodes.FDABiNode()])
>>> flow.train([[samples],[samples]], [None,[{"cl": labels}]])
```

The `_train` method of `FDANode` requires the `cl` argument, so this is used as the key value. Note that we have to use the `BiNode` version of `FDANode`, called `FDABiNode` (alomost every MDP node has a `BiNode` version following this naming scheme). The `BiNode` class provides the `cl` value from the message to the `_train` method.

In a normal `Flow` the additional arguments can only be given to the node which is currently in training. This limitation does not apply to a `BiFlow`, where the message can be accessed by all nodes (more on this later). Message iterators can also be used during execution, via the `msg_iterable` argument in `BiFlow.execute`. Of course messages can be also returned by `BiFlow.execute`, so the return value has the form `(y, msg)`. If iterables are used then the `BiFlow` not only concatenates the `y` result arrays, but also tries to join the `msg` dictionaries into a single one. Arrays in the `msg` will be concatenated, for all other types the plus operator is used.

The train method of BiFlow also has an additional argument called stop_messages, which can be used to provide message iterables for stop_training. The execute method on the other hand has an argument target_iterable, which can be used to specify the initial target in the flow execution.

BiNode

We now want to give an overview of the BiNode API, which is mostly an extension of the Node API. First we take a look at the possible return values of a BiNode and briefly explain their meaning:

execute x or (x, msg) or (x, msg, target). Normal execution continues, directly jumping to the target if one is specified.

train

- None terminates training.
- x or (x, msg) or (x, msg, target). Means that execution is continued and that this node will be reached again to terminate training. If x is None and no target is specified then the remaining msg is dropped (so it is not required to 'clear' the message manually in _train for custom nodes to terminate training).

stop_training, stop_message

- None terminates the stop_message propagation.
- (msg, target). If no target is specified then the remaining msg is dropped (terminates the propagation).

Of course all these methods also accept messages. Compared to Node methods they have a new msg argument. The target part on the other hand is only used by the BiFlow.

As you can see from train, the training does not always stop when the training node is reached. Instead it is possible to continue with the execution to come back later. For example this is used in the backpropagation example (in the MDP examples repository). There is also a new stop_training result option. If stop_training returns a result then the BiFlow enters a mode where it propagates the result based on the given target by calling stop_message. This can be used to propagate results from the node training or to prepare nodes for their upcoming training.

Some of these new options might be confusing at first. However, you can simply ignore those that you don't need and concentrate on the features that are useful for your current project. For example you could use messages without ever worrying about targets.

There are also three more additions to the BiNode API:

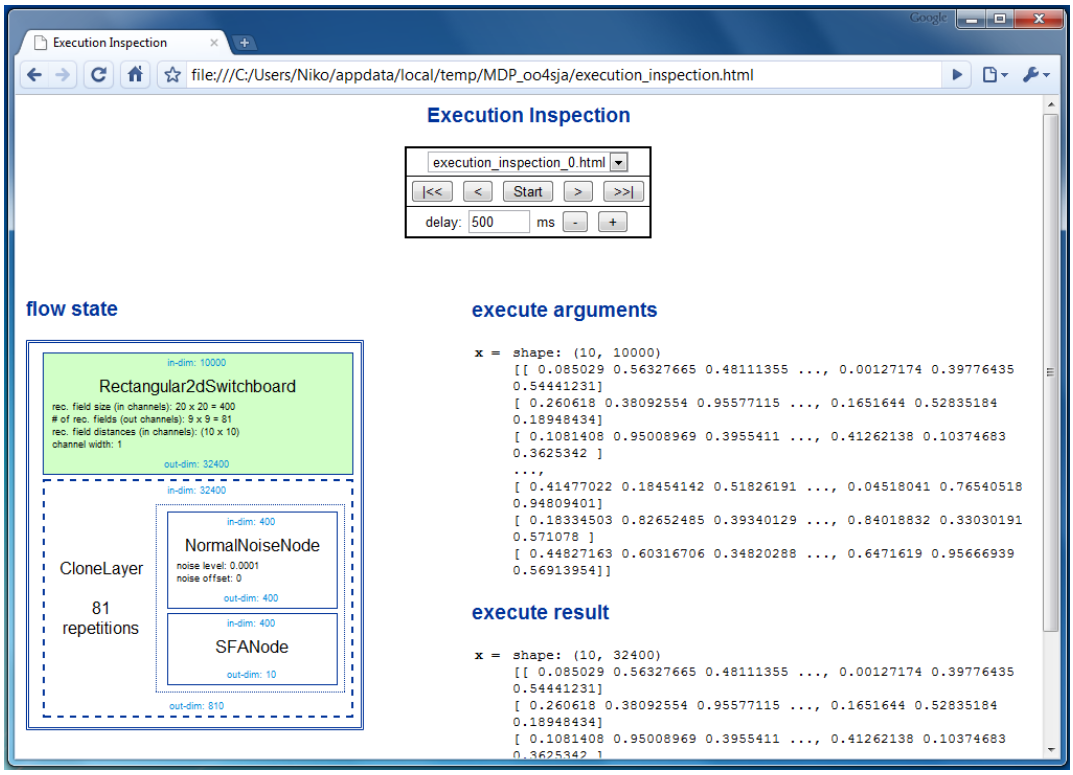
node_id This is a read-only property, which returns the node id (which is None if it wasn't specified). The __init__ method of a BiNode generally accepts a node_id keyword argument to set this value.

bi_reset This method is called by the BiFlow before and after training and execution (and the stop_training / stop_message propagation). It can be overriden by derived classes to reset internal state variables.

is_bi_training This method is similar to the is_training method of standard MDP nodes. It can be used to signal that a node is doing some data gathering. A node might for example do perform training during the normal execute (e.g., a neural network might adjust internal weights while it is already returning results). Generally this method isn't that important, but the ParallelBiFlow uses it to determine if nodes can simply be copied or must be forked

Inspection

Using jumps and messages can result in complex data flows. Therefore BiMDP offers some convenient inspection capabilites to help with debugging and analyzing what is going on. This functionality is based on the static HTML view from the mdp.hinet module. Instead of a static view of the flow you get an animated slideshow of the flow training or execution. An example is provided in bimdp/test/demo_hinet_inspection.py. You can simply call bimdp.show_execution(flow, data) instead of the normal flow.execute(data). This will automatically perform the inspection and open it in your webbrowser. Similar functionality is available for training. Just call bimdp.show_execution(flow, data_iterables), which will perform training as in flow.train(data_iterables). Have a look at the docstrings to learn about additional options.



The BiMDP inspection is also useful to visualize the data processing that is happening inside a flow. This is especially handy if you are trying to build or understand new algorithms and want to know what is going on. Therefore we made it very easy to customize the HTML views in the inspection. One simple example is provided in `bimdp/test/demo_custom_inspection.py`, where we use matplotlib to plot the data and present it inside the HTML view. Note that `bimdp.show_training` and `bimdp.show_execution` are just helper functions. If you need more flexibility you can directly access the machinery below (but this is rather messy and hardly ever needed).

Extending BiNode and Message Handling

As in the `Node` class any derived `BiNode` classes should not directly overwrite the public `execute` or `train` methods but instead the private versions with an underscore in front (for training you can of course also overwrite `_get_train_seq`). In addtion to the dimensionality checks performed on `x` by the `Node` class this enables a couple of message handling features. This also applies to the new `_stop_message` method. On the other hand `bi_reset` and `is_bi_training` can be directly overwritten (like `is_training` in `Node`), there are no private methods for these.

The automatic message handling is a major feature in `BiNode` and relies on the dynamic nature of Python. In the `FDABiNode` and `BiFlow` example we have alrady seen how a value from the message is automatically passed to the `_train` method, because the key of the value is also the name of a keyword argument.

Public methods like `execute` in `BiNode` accept not only a data array `x`, but also a message dictionary `msg`. When given a message they perform introspection to determine the arguments for the corresponding private methods (like `_train`). If there is a matching key for an argument in the message then the value is provided as a keyword argument. It remains in the dictionary and can therefore be used by other nodes in the flow as well.

A private method like `_train` has the same return options as the public `train` method, so one can for example return a tupple `(x, msg)`. The `msg` in the return value from `_train` is then used by `train` to update the original `msg`. Thereby `_train` can overwrite or add new values to the message. There are also some special features ("magic") to make handling messages more convenient:

- You can use message keys of the form `node_id->argument_key` to address parts of the message to a specific node. When the node with the corresponding id is reached then the value is not only provided as an argument, but the key is also deleted from the message. If the argument_key is not an argument of the method then the whole key is simply erased.

- If a private method like `_train` has a keyword argument called `msg` then the complete message is provided. The message from the return value replaces the original message in this case. For example this makes it possible to delete parts of the message (instead of just updating them with new values).

- The key `"method"` is treated in a special way. Instead of calling the standard private method like `_train` (or `_execute`, depending on the called public method) the "method" value will be used as the method name, with an underscore in front. For example the message `{"method": "classify"}` has the effect that

a method `_classify` will be called. Note that this feature can be combined with the extension mechanism, when methods are added at runtime.

- The key `"target"` is treated in a special way. If the called private method does not return a target value (e.g., if it just returned `x`) then the `"target"` value is used as target return value (e.g, instead of `x` the return value of `execute` would then have the form `x, None, target`).
- If the key "method" has the value `inverse` then, as expected, the `_inverse` method is called. However, additionally the checks from `inverse` are run on the data array. If `_inverse` does not return a target value then the target -1 is returned. So with the message `{"method": "inverse"}` one can execute a `BiFlow` in inverse node (note that one also has to provide the last node in the flow as the initial target to the flow).
- This is more of a `BiFlow` feature, but the target value specified in `bimdp.EXIT_TARGET` (currently set to `"exit"`) causes `BiFlow` to terminate the execution and to return the last return value.
- To make it possible to call `execute` and `inverse` via `stop_message` there is some magic going on if these are specified via the `"method"` key: In addition to the normal automatic extraction of the `"x"` key from the message the array output of the node is also stored back as `"x"` in the message (overwriting the previous value). Additionally the target is given a default value of 1 or -1 (so setting the `"method"` value is sufficient for normal execution or inverse during the `stop_message` phase).

Of course all these features can be combined, or can be ignored when they are not needed.

HiNet in BiMDP

BiMDP is mostly compatibel with the hierarchical networks introduced in `mdp.hinet`. For the full BiMDP functionality it is of required to use the BiMDP versions of the the building blocks.

The `bimdp.hinet` module provides a `BiFlowNode` class, which is offers the same functionality as a `FlowNode` but with the added capability of handling messages, targets, and all other BiMDP concepts.

There is also a new `BiSwitchboard` base class, which is able to deal with messages. Arrays present in the message are mapped with the switchboard routing if the second axis matches the switchboard dimension (this works for both execute and inverse).

Finally there is a `CloneBiLayer` class, which is the BiMDP version of the `CloneLayer` class in `mdp.hinet`. To support all the features of BiMDP some significant functionality has been added to this class. The most important new aspect is the `use_copies` property. If it is set to `True` then multiple deep copies are used instead of just a reference to the same node. This makes it possible to use internal variables in a node that persist while the node is left and later reentered. You can set this property as often as you like (note that there is of course some overhead for the deep copying). You can also set the `use_copies` property via the message mechanism by simply adding a `"use_copies"` key with the required boolean value. The `CloneBiLayer` class also looks for this key in outgoing messages (so it can be send by nodes inside the layer).

Parallel in BiMDP

The parallelisation capabilites introduced in `mdp.parallel` can be used for BiMDP. The `bimdp.parallel` module provides a `ParallelBiFlow` class which can be used like the normal `ParallelFlow`. No changes to schedulers are required.

The most important difference between the parallelization in standard MDP and BiMDP is that BiNodes can signal via the `is_bi_training` method wether they should be forked instead of the usual deep copy. Unlike the `is_training` method there can be multiple nodes for which `is_bi_training` returns `True`. All these forked nodes are joined after the exectuion or training.

Note that a `ParallelBiFlow` uses a special callable class. So if you want to use a custom callable you will have to make a few modifications (compared to the standard callable class used by `ParallFlow`).

Classifiers in BiMDP

BiMDP introduces a special `BiClassifier` base class for the new `Classifier` nodes in MDP. This makes it possible to fully use classifiers in a normal `BiFlow`. Just like for normal nodes the BiMDP versions of the classifier are available in `bimdp.nodes` (the SVM classifiers are currently not available by default, but it is possible to manually derive a `BiClassifier` version of them).

The `BiClassifier` class makes it possible to provide the training labels via the message mechanism (simply store the labels with a `"labels"` key in the `msg` dict). It is also possible to transport the classification results in the outgoing message. The `_execute` method of a `BiClassifier` has three keyword arguments called `return_labels`, `return_ranks`, and `return_probs`. These can be set via the message mechanism. If for example `return_labels` is set to `True` then `execute` will call the `label` method from the classifier node and store the result in the outgoing

message (under the key `"labels"`). The `return_labels` argument (and the other two) can also be set to a string value, which is then used as a prefix for the `"labels"` key in the outgoing message (e.g., to target this information at a specific node in the flow).

Future Development

MDP is currently maintained by a core team of 4 developers, but it is open to user contributions. Users have already contributed some of the nodes, and more contributions are currently being reviewed for inclusion in future releases of the package. The package development can be followed online on the public git code repositories or cloned with:

```
git clone git://mdp-toolkit.git.sourceforge.net/gitroot/mdp-toolkit/mdp-toolkit
git clone git://mdp-toolkit.git.sourceforge.net/gitroot/mdp-toolkit/docs
git clone git://mdp-toolkit.git.sourceforge.net/gitroot/mdp-toolkit/examples
git clone git://mdp-toolkit.git.sourceforge.net/gitroot/mdp-toolkit/contrib
```

Questions, bug reports, and feature requests are typically handled by the user mailing list

Contributors

In this final section we want to thank all users who have contributed code and bug reports to the MDP project. Strictly in alphabetical order:

- Gabriel Beckers
- Sven Dähne
- Alberto Escalante
- Farzad Farkhooi
- Mathias Franzius
- Michael Hanke
- Konrad Hinsen
- Christian Hinze
- Samuel John
- Susanne Lezius
- Michael Schmuker
- Benjamin Schrauwen
- Henning Sprekeler
- Jake VanderPlas