Modular Toolkit for Data Processing (MDP)

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

Tutorial

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Modular toolkit for Data Processing (MDP) is a Python library to perform data processing. Already implemented algorithms include: Principal Component Analysis (PCA), Independent Component Analysis (ICA), Slow Feature Analysis (SFA), and Growing Neural Gas (GNG).

MDP supports the most common numerical extensions to Python and the `symeig` package (a Python wrapper for the LAPACK functions to solve the standard and generalized eigenvalue problems for symmetric (hermitian) positive definite matrices). MDP also includes `graph` (a lightweight package to handle graphs).

When used together with `SciPy` (the scientific Python library) and `symeig`, MDP gives to the scientific programmer the full power of well-known C and FORTRAN data processing libraries. MDP helps the programmer to exploit Python object oriented design with C and FORTRAN efficiency.

MDP has been written for 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 side together with the reusability of the implemented nodes could make it also a valid educational tool.

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, typecode='f')
```

MDP is of course much more than this: it allows to combine different algorithms and other data processing elements (nodes) into data processing sequences (flows). Moreover, it provides a framework that makes the implementation of new algorithms easy and intuitive.

This is a guide to basic and some more advanced features of the MDP library.

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.

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Nodes

A node is the basic unit in MDP and it represents a data processing element, like for example a learning algorithm, a filter, a visualization step etc. Each node can have a training phase, 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). MDP is designed to make the implementation of new algorithms easy and intuitive, for example by setting automatically input and output dimension and by casting the data to match the typecode (e.g. float or double precision) of the internal structures. Most of the nodes were designed to be applied to arbitrarily long sets of data: the internal structures can be updated successively by sending chunks of the input 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). Already implemented nodes include Principal Component Analysis (PCA), Independent Component Analysis (ICA), Slow Feature Analysis (SFA), and Growing Neural Gas Network.

Node Creation

Nodes can be obtained by creating an instance of the node class. Each node is characterized by an input dimension, that corresponds to the dimensionality of the input vectors, an output dimension, and a typecode, which determines the typecode of the internal structures and of the output signal. These three attributes are inherited from the input data if left unspecified. Input dimension and typecode can usually be specified when an instance of the node class is created. The constructor of each node class can require other task-specific arguments.

Some examples of node creation:

- Create a node that performs Principal Component Analysis (PCA) whose input dimension and typecode 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, typecode='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, typecode='None')
```

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

```
>>> pcanode3 = mdp.nodes.PCANode(typecode = 'f')
>>> pcanode3
PCANode(input_dim=None, output_dim=None, typecode='f')
```

  You can obtain a list of the typecodes supported by a node by calling its `get_supported_typecodes` method:

```
>>> pcanode3.get_supported_typecodes()
['f', 'd']
```

- A PolynomialExpansionNode expands its input in the space of polynomals 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. This can be done during a training phase by calling the `train` method.

Some examples of node training:

- Create some random data and update the internal structures (i.e. mean and covariance matrix) of the PCANode:

```
>>> x = mdp.numx_rand.random((100, 25))  # 25 variables, 100 observa-
tions
>>> pcanode1.train(x)
```

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

```
>>> pcanode1
PCANode(input_dim=25, output_dim=None, typecode='d')
```

- 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 Generators section):

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

- Some nodes don't need to be trained:

```
>>> expnode.is_trainable()
0
```

Trying to train them anyway would raise an exception:

```
>>> x = mdp.numx_rand.random((100, 5))
>>> expnode.train(x)
Traceback (most recent call last):
File "<stdin>", line 1, in ?
File "...", line 190, in train
  raise IsNotTrainableException, "This node is not trainable."
mdp.signal_node.IsNotTrainableException: This node is not trainable.
```

- The training phase ends when the `stop_training`, `execute`, or `inverse` method are called. For example we can stop the training of the PCANode (at this point the principal components are computed):

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

It is now possible to access the trained internal data

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

Node Execution

After the training phase 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)
```

Node Inversion

If the operation computed by the node is invertible, it is possible to compute the inverse transformation:

- Given the output data, compute the inverse projection to the input space for the PCA node:

  ```
  >>> pcanode1.is_invertible()
  1
  >>> x = pcanode1.inverse(y_pca)
  ```

- The expansion node in not invertible:

  ```
  >>> expnode.is_invertible()
  0
  ```

  Trying to compute the inverse would raise an exception:

  ```
  >>> expnode.inverse(y_exp)
  Traceback (most recent call last):
  File "<stdin>", line 1, in ?
  File "...", line 252, in inverse
    raise IsNotInvertibleException, "This node is not invertible."
  mdp.signal_node.IsNotInvertibleException: This node is not invertible.
  ```

Writing your own nodes: subclassing SignalNode

MDP tries to make it easy to write new data processing elements that fit with the existing elements. To expand the MDP library of implemented nodes with your own nodes you can subclass the SignalNode class, overriding some of the methods according to your needs. We'll see in the following some examples:

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

  Define the class as a subclass of SignalNode:

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

  This node cannot be trained. To define this, one has to overwrite the `is_trainable` method to return 0:

  ```
  ...     def is_trainable(self): return 0
  ```

  Execute has in principle only to multiply x by 2

  ```
  ...     def execute(self, x):
  ```

  However, we must first call the method of the parent class that performs some tests, for example to make sure that `x` has the right rank and dimensionality:

  ```
  ...         super(TimesTwoNode, self).execute(x)
  ```

  Each subclass has to handle the typecode defined by the user or inherited by the input data, and make sure that internal structures are stored consistently. This often means that input data has to be cast. SignalNode contains a helper function that casts the array only if necessary:

  ```
  ...         x = self._refcast(x)
  ```

  Finally we can compute the result. Note that we have to cast the scalar to be sure that if we use some of the numeric extension (e.g. `Numeric`), the result of the multiplication is not upcasted Use the internal helper function to do so:

```
...         return self._scast(2)*x
```

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

```
...     def inverse(self, y):
```

As in execute, we first have to call the parent class and cast the input vector and the scalar:

```
...         super(TimesTwoNode, self).inverse(y)
...         return self._refcast(y/self._scast(2))
...
>>>
```

The same definition without comments:

```
>>> class TimesTwoNode(mdp.SignalNode):
...     def is_trainable(self): return 0
...     def execute(self, x):
...         super(TimesTwoNode, self).execute(x)
...         x = self._refcast(x)
...         return self._scast(2)*x
...     def inverse(self, y):
...         super(TimesTwoNode, self).inverse(y)
...         return self._refcast(y/self._scast(2))
...
>>>
```

Test the new node:

```
>>> node = TimesTwoNode(typecode = 'i')
>>> 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 at the instance's creation

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

We redefine the init method to take the power as first argument. In general one should always give the possibility to set the typecode 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, typecode=None):
```

Initialize the parent class:

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

Store the power:

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

`PowerNode` is not trainable...

```
...     def is_trainable(self): return 0
```

... nor invertible:

```
...     def is_invertible(self): return 0
```

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

```
...     def get_supported_typecodes(self):
...         return ['f', 'd']
```

The `execute` method:

```
...     def execute(self, x):
...         super(PowerNode, self).execute(x)
...         return self._refcast(x**self._scast(self.power))
...
>>>
```

The same definition without comments:

```
>>> class PowerNode(mdp.SignalNode):
...     def __init__(self, power, input_dim=None, typecode=None):
...         super(PowerNode, self).__init__(input_dim=input_dim, type-
code=typecode)
...         self.power = power
...     def is_trainable(self): return 0
...     def is_invertible(self): return 0
...     def get_supported_typecodes(self):
...         return ['f', 'd']
...     def execute(self, x):
...         super(PowerNode, self).execute(x)
...         return self._refcast(x**self._scast(self.power))
...
>>>
```

Test the new node

```
>>> node = PowerNode(3)
>>> x = mdp.numx.array([[1.0, 2.0, 3.0]])
>>> y = node.execute(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.SignalNode):
...     def __init__(self, input_dim=None, typecode=None):
...         super(MeanFreeNode, self).__init__(input_dim=input_dim,
...                                            typecode=typecode)
```

Mean of the input data. We initialize it to None since we still don't know how large is an input vector:

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

Number of training points:

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

The `train` method receives the input data:

```
...     def train(self, x):
...         super(MeanFreeNode, self).train(x)
...         x = self._refcast(x)
```

Initialize the mean vector with the right size and typecode if necessary:

```
...         if self.avg is None:
...             self.avg = mdp.numx.zeros(self.get_input_dim(),
...                                       typecode=self.get_typecode())
```

Update the mean with the sum of the new data:

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

Count the number of points processed:

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

The `stop_training` function is called when the training phase is over:

```
...     def stop_training(self):
...         super(MeanFreeNode, self).stop_training()
```

When the training is over, divide the sum of the training data by the number of training vectors to obtain the mean:

```
...         self.avg /= self._scast(self.tlen)
```

The `execute` and `inverse` methods:

```
...     def execute(self, x):
...         super(MeanFreeNode, self).execute(x)
...         return self._refcast(x - self.avg)
...     def inverse(self, y):
...         super(MeanFreeNode, self).inverse(y)
...         return self._refcast(y + self.avg)
...
>>>
```

The same definition without comments:

```
>>> class MeanFreeNode(mdp.SignalNode):
...     def __init__(self, input_dim=None, typecode=None):
...           su-
per(MeanFreeNode, self).__init__(input_dim=input_dim,
...                                            typecode=typecode)
...         self.avg = None
...         self.tlen = 0
...     def train(self, x):
...        super(MeanFreeNode, self).train(x)
...        x = self._refcast(x)
...        if self.avg is None:
...        self.avg = mdp.numx.zeros(self.get_input_dim(),
...                                  typecode=self.get_typecode())
```

```
...         self.avg += sum(x, 0)
...         self.tlen += x.shape[0]
...     def stop_training(self):
...         super(MeanFreeNode, self).stop_training()
...         self.avg /= self._scast(self.tlen)
...     def execute(self, x):
...         super(MeanFreeNode, self).execute(x)
...         return self._refcast(x - self.avg)
...     def inverse(self, y):
...         super(MeanFreeNode, self).inverse(y)
...         return self._refcast(y + self.avg)
...
>>>
```

Test the new node:

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

- In our last example we'll define a node that repeats its input twice, returning an input that has twice as many dimensions:

  ```
  >>> class TwiceNode(mdp.SignalNode):
  ...     def is_trainable(self): return 0
  ...     def is_invertible(self): return 0
  ```

  When `SignalNode` inherits the input and output dimension from the input data, it calls the `_set_default_inputdim` and `_set_default_outputdim` functions. Here we overwrite the `_set_default_outputdi` to set the output dimension to be twice the input dimension:

  ```
  ...     def _set_default_outputdim(self, nvariables):
  ...         self._output_dim = 2*nvariables
  ```

  The `execute` method:

  ```
  ...     def execute(self, x):
  ...         super(TwiceNode, self).execute(x)
  ...         x = self._refcast(x)
  ...         return mdp.numx.concatenate((x, x),1)
  ...
  >>>
  ```

  The same definition without comments:

  ```
  >>> class TwiceNode(mdp.SignalNode):
  ...     def is_trainable(self): return 0
  ...     def is_invertible(self): return 0
  ...     def _set_default_outputdim(self, nvariables):
  ...         self._output_dim = 2*nvariables
  ...     def execute(self, x):
  ...         super(TwiceNode, self).execute(x)
  ```

```
...         x = self._refcast(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 consists in an acyclic graph of nodes (currently only node sequences are implemented). The data is sent to an input node and is successively processed by the following nodes on the graph. The general flow implementation automatizes the training, execution, and inverse execution (if defined) of the whole graph. 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 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 creation, training and execution

Suppose we have an input signal with an high number of dimensions, on which we would like to perform ICA. To make the problem affordable, we first need to reduce its dimensionality with PCA. Finally, we would like to visualize the data sequence at the beginning and after each step.

We could start by quickly defining a node to visualize the data (see the Writing your own nodes: subclassing SignalNode section for details on subclassing `SignalNode`). For visualization we use in the following a generic `plot` function that the user will have to link to the plotting package he has installed. If you have `SciPy` you could for example define:

```
>>> plot = scipy.gplt.plot
>>> class VisualizeNode(mdp.SignalNode):
...     def is_trainable(self): return 0
...     def is_invertible(self): return 0
...     def execute(self, x):
...         mdp.SignalNode.execute(self,x)
...         self._refcast(x)
...         plot(x)
...         return x
>>>
```

Generate some input signal randomly (which makes the example useless, but it's just for illustration...). Generate a signal with 20 dimensions and 1000 observations:

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

Rescale x to have zero mean and unit variance:

```
>>> inp = (inp - mdp.utils.mean(inp,0))/mdp.utils.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 linearly the input signals:

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

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

  1. Visualize the input data:

     ```
     >>> plot(x)
     ```

  2. Perform PCA:

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

  3. Visualize data after PCA:

     ```
     >>> plot(out1)
     ```

  4. Perform ICA using CuBICA algorithm:

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

  5. Visualize data after ICA:

     ```
     >>> plot(out2)
     ```

- ... or we could use flows, the recommended way:

  ```
  >>> flow = mdp.SimpleFlow([VisualizeNode(),
  ...                        mdp.nodes.PCANode(output_dim=5),
  ...                        VisualizeNode(),
  ...                        mdp.nodes.CuBICANode(),
  ...                        VisualizeNode()])
  ...
  >>> flow.train(x)
  >>> out = flow.execute(x)
  ```

  You will probably get some warnings here. This is expected, see the section about Generators to learn more about that, for the moment you can simply ignore them.

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

```
>>> cov = mdp.utils.amax(abs(mdp.utils.cov(inp[:,:5],out)))
>>> print cov
[ 0.99324451  0.99724133  0.99247439  0.99049607  0.994309  ]
```

Flow inversion

Flows can be inverted by calling their inverse function. In this case, however, the flow contains non-invertible nodes, and trying to invert it would raise an exception. To overcome this we simply get a slice of the flow instance with the invertible nodes. Note that a slice of a flow instance returns a new instance containing references to the corresponding nodes. Reconstruct the mix inverting the flow:

```
>>> rec = flow[1::2].inverse(out)
```

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

```
>>> cov = mdp.utils.amax(abs(mdp.utils.cov(x/mdp.utils.std(x,0),
...                                         rec/mdp.utils.std(rec,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

We have seen that we can get flow slices. Actually flows are Python container type objects, very much like lists, i.e. you can loop through them:

```
>>> for node in flow:
...     print repr(node)
...
VisualizeNode(input_dim=20, output_dim=20, typecode='d')
PCANode(input_dim=20, output_dim=5, typecode='d')
VisualizeNode(input_dim=5, output_dim=5, typecode='d')
CuBICANode(input_dim=5, output_dim=5, typecode='d')
VisualizeNode(input_dim=5, output_dim=5, typecode='d')
>>>
```

You can `pop`, `insert` and `append` nodes like you would do with lists:

```
>>> len(flow)
5
>>> nodetoberemoved = flow.pop(-1)
>>> nodetoberemoved
VisualizeNode(input_dim=5, output_dim=5, typecode='d')
>>> len(flow)
4
```

Finally, you can concatenate flows:

```
>>> dummyflow = flow[3:].copy()
>>> longflow = flow + dummyflow
>>> len(longflow)
5
```

The returned flow is always consistent, i.e. input and output dimensions of successive nodes always match. If you try to create an inconsistent flow you'll get an error:

```
>>> flow
SimpleFlow([VisualizeNode(input_dim=20, output_dim=20, typecode='d'),
            PCANode(input_dim=20, output_dim=5, typecode='d'),
```

```
              VisualizeNode(input_dim=5, output_dim=5, typecode='d'),
              CuBICANode(input_dim=5, output_dim=5, typecode='d')])
>>> flow.pop(1)
Traceback (most recent call last):
  File "<stdin>", line 1, in ?
  [...]
ValueError: dimensions mismatch: 20 != 5
```

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

Switch on crash recovery:

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

Attempt to train the flow:

```
>>> flow.train([[None]])
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 put the dump:

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

Generators

A generator is a Python iterator introduced in Python 2.2 that returns a value after each call and can be used for example in `for` loops. See http://linuxgazette.net/100/pramode.html for an introduction, and http://www.python.org/peps/pep-0255.html for a complete description.

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

```
>>> BogusNode = mdp.IdentityNode
>>> class BogusNode2(mdp.IdentityNode):
...     """This node does nothing. but it's not trainable and not invert-
ible.
...     """
...     def is_trainable(self): return 0
...     def is_invertible(self): return 0
...
>>>
```

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 `ProgressBar` to get progress information.

```
>>> def gen_data(blocks):
...     progressbar = mdp.utils.ProgressBar(0,blocks)
...     progressbar.update(0)
...     for i in xrange(blocks):
...         block_x = mdp.utils.atleast_2d(mdp.numx.arange(2,1001,2))
...         block_y = mdp.utils.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]))
...         progressbar.update(i+1)
...         yield block
...     print '\n'
...     return
...
>>>
```

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

```
>>> flow = mdp.SimpleFlow([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 generators. 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 (IdentityNode)
[===================================100%==================================>]

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

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

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

```
>>> flow = mdp.SimpleFlow([BogusNode(),BogusNode()])
>>> block_x = mdp.utils.atleast_2d(mdp.numx.arange(2,1001,2))
>>> block_y = mdp.utils.atleast_2d(mdp.numx.arange(1,1001,2))
```

```
>>> sin-
gle_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 generator for the non-trainable nodes:

```
>>> flow = mdp.SimpleFlow([BogusNode2(),BogusNode()], verbose=1)
>>> flow.train([None,gen_data(5000)])
Training node #0 (BogusNode2)
Training finished
Training node #1 (IdentityNode)
[===================================100%==================================>]

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

If in this case you try the one-shot training you'll get two warnings like the following ones:

```
>>> flow = mdp.SimpleFlow([BogusNode2(),BogusNode()], verbose=1)
>>> flow.train(single_block)
Training node #0 (BogusNode2)
/.../linear_flows.py:94: MDPWarning:
! Node 0 in not trainable
You probably need a 'None' generator for this node. Continuing anyway.
  warnings.warn(wrnstr, mdp.MDPWarning)
Training finished
Training node #1 (IdentityNode)
Training finished
Close the training phase of the last node
```

You can get rid of this warning either by doing what the warning asks you, namely use the generator syntax and provide a None generator for the non-trainable nodes, or by switching off MDP warnings altogether:

```
>>> import warnings
>>> warnings.filterwarnings("ignore",'.*',mdp.MDPWarning)
>>> flow = mdp.SimpleFlow([BogusNode2(),BogusNode()], verbose=1)
>>> flow.train(single_block)
Training node #0 (BogusNode2)
Training finished
Training node #1 (IdentityNode)
Training finished
Close the training phase of the last node
```

To switch on MDPWarnings again:

```
>>> warnings.filterwarnings("always",'.*',mdp.MDPWarning)
```

Generators can be used also for execution (and inversion):

```
>>> flow = mdp.SimpleFlow([BogusNode(),BogusNode()], verbose=1)
>>> flow.train([gen_data(1), gen_data(1)])
Training node #0 (BogusNode2)
Training finished
Training node #1 (IdentityNode)
```

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

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 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
...     return
...
>>>
```

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 maxi-
mum (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, typecode='d')
```

Don't forget to clean the rubbish:

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

A real life example (Logistic maps)

We show an application of Slow Feature Analysis to the analysis of non-stationary time series. We consider a chaotic time series generated by the logistic map based on the logistic equation (a demographic model of the population biomass of species in the presence of limiting factors such as food supply or disease), and extract the slowly varying parameter that is hidden behind the 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, http://arxiv.org/abs/cond-mat/0312317

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.utils.linspace(0,1,10000,endpoint=0) # time axis 1s, sampler-
ate 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')
```

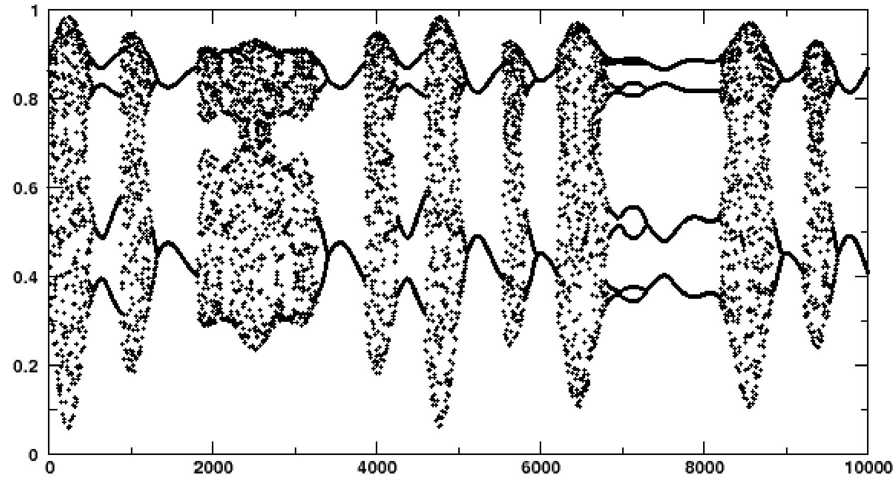
Fix the initial condition:

```
>>> 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:



Define a flow to perform SFA in the space of polynomials of degree 3. We need a node that embeds the time-series in a 10 dimensional space, where different variables correspond to time-delayed copies of the original time-series: the `TimeFramesNode(10)`. Then we need a node that expands the new signal in the space of polynomials of degree 3: the `PolynomialExpansionNode(3)`. Finally we perform SFA onto the expanded signal and keep the slowest feature: `SFANode(output_dim=1)`. We also measure the *slowness* of the input time-series and of the slow feature obtained by SFA. Therefore we put at the beginning and at the end of the sequence an *analysis node* that computes the *eta-value* (a measure of slowness) of its input (see docs for the definition of eta-value): the `EtaComputerNode()`:

```
>>> sequence = [mdp.nodes.EtaComputerNode(),
...             mdp.nodes.TimeFramesNode(10),
...             mdp.nodes.PolynomialExpansionNode(3),
...             mdp.nodes.SFANode(output_dim=1),
...             mdp.nodes.EtaComputerNode()]
...
>>>
>>> flow = mdp.SimpleFlow(sequence, verbose=1)
```

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.execute(series)
```

The slow feautre 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.utils.mean(dforce,0))/mdp.utils.std(dforce,0)
```

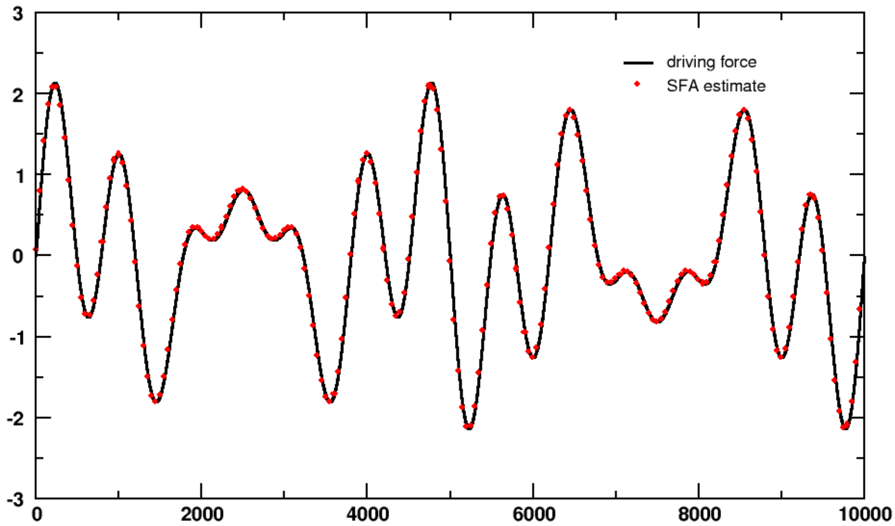
Print covariance between the rescaled driving force and the slow feature. Note that embedding the time-series with 10 time frames leads to a time-series with 9 observations less:

```
>>> mdp.utils.cov(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 `resc_dforce` together with `slow` and see that they match perfectly:



Another real life example (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, 1644375755)
```

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 circumfer-
ence."""
...     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)
  ```

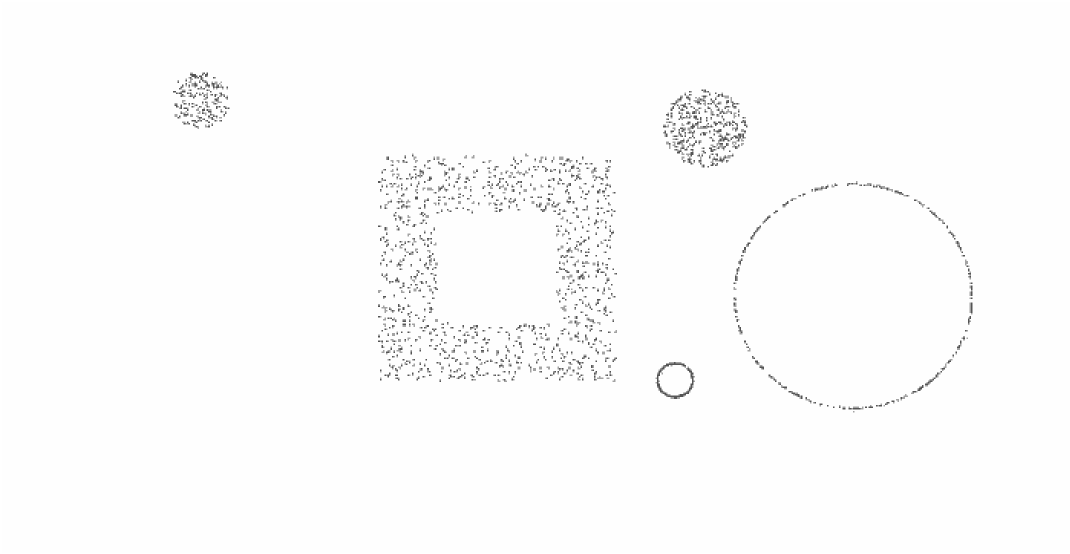
- Rectangles:

  ```
  >>> 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]))
```

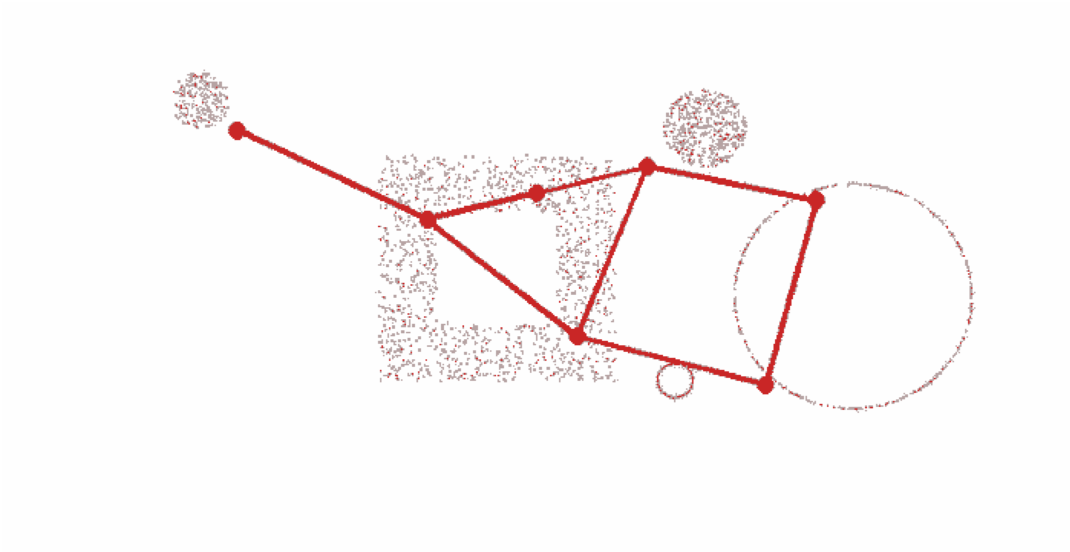
If you have a plotting package `x` should look like this:



Create a GrowingNeuralGasNode and train it:

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

The initial distribution of nodes is randomly chosen:

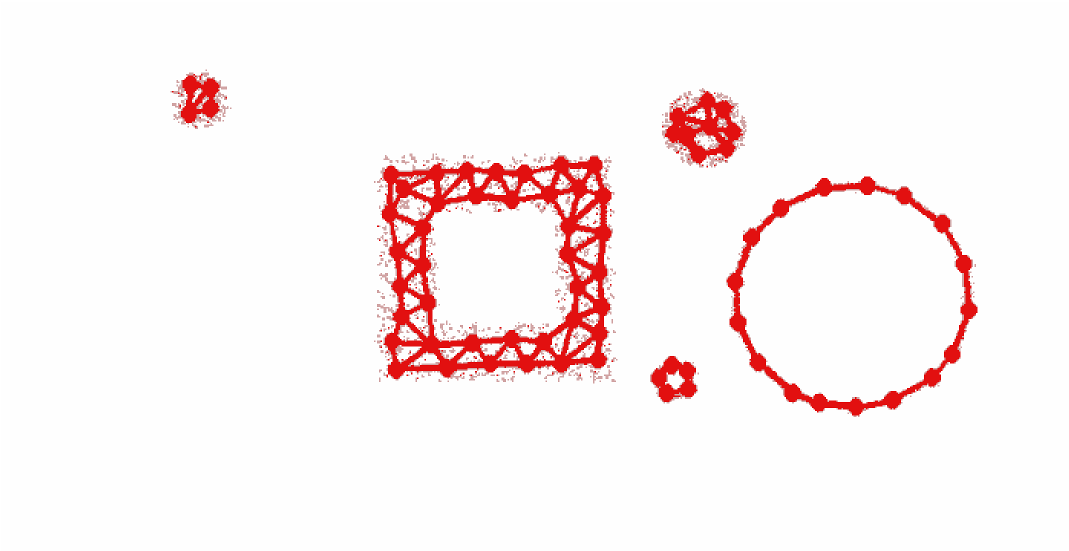


The training is performed in small chunks in order to visualize the evolution of the graph:

```
>>> 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())
5
```

To Do

In this last section we want to give you an overview about our plans for the development of MDP:

- Add more data processing algorithms.
- Extend the linear flows to handle general acyclic graphs of nodes.
- Actual use of the graph structure will be possible only in presence of an easy and intuitive GUI :)
- Wait for a good guy who wants to contribute a `CovarianceMatrix` class that uses some of the fancy sum algorithms to avoid round off errors when adding many numbers.

A final remark

If you want to contribute some code or a new algorithm, please do not hesitate to submit it!

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