

PyClimate 1.2: Python tools for the climate variability analysis

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1 Change Log

- Version 1.2–December, 2002.
 1. Corrected bugs
 - (a) In module `bpcca.py`, if the second field was not two-dimensional, the program crashed. It is already corrected.
 - (b) The last character in the last line of a file could be missed by `readdat.py` if the last line did not end in a new line. It is corrected now.
 2. Added a netCDF iterator. This is an object which reads a list of filenames (all of the COARDS-compliant netCDF type) and is able to iterate through all the records in the list of files. It has methods like `__len__` and `__getitem__` and `getfield()`, to handle the iterator and the fields inside. It is a cheap version of `ncrcat`. Its main interest is that under some systems (Linux, for instance), files larger than 2 Gb may produce errors in the filesystem. This way, they may be processed as smaller chunks and, still, give the user the impression of a single object that can be traversed by means of a single iteration.
 3. Huge dataset EOFs (`hdseofs.py`)

Is a version of the EOF computing-code for huge datasets. Instead of performing the SVD of the data matrix, like `svdeofs.py` does, it simply iterates once or twice over the dataset, depending on the type instantiated. It builds the covariance matrix and performs a SVD of it. Then, after iterating once more over the dataset, it can compute the PCs. Other bells and whistles, like Monte Carlo tests and the North test or an automatic shape/unshape mechanism of the eigenvectors or even the possibility of the call of an external SVD solver (not the one in `LapackLite`) are also included. It is useful for Gigabyte-sized data, as these problems are difficult to solve by the previously available EOF-solver (`svdeofs.py`) due to memory constraints. In order to efficiently manage the memory, it uses the "memory-managing" versions of `Numeric.add()`, `Numeric.reduce()` and so on. However, it is slower than the previous version of the routines and should only be used when the dataset is very big.

4. Monte Carlo test for the Barnett-Preisendorfer version of the CCA

We have added a new Monte carlo test on the congruence coefficient of canonical correlation patterns of random subsamples of the canonical correlation analysis of fields by means of the Barnett-Preisendorfer approach.

5. Search of analogs for downscaling purposes

We perform the search in the PCA space as well as in the CCA space, too. Mathematical details can be found in (Fernandez and Saenz, under revision).

6. Array of numerical histograms (NHArray)

A special module has been written in C to allow the use of arrays of numerical histograms for Monte Carlo tests. It is much faster than the iteration over a multivariate distribution of univariate histograms as those available in Scientific.Statistics.

7. svdeofs.py

A new object-oriented front end to the EOFs computation. Some methods have been added, for instance, take a look in the manual at `reconstructedField`, `unreconstructedField`, `projectField`

8. Cleaner name spaces

We have removed ALMOST all the imports of the kind `from XXXX import *` This means, basically, that our code is cleaner and that it will not (hopefully) corrupt your name spaces, but it means more requirements on your code as well. It can also create some incompatibilities with older versions of PyClimate. However, in order to leave the user name space cleaner, we have adhered to these stricter requirements.

The next script:

```
from pyclimate.ncstruct import *
onc=create_bare_COARDS(
    "XXX.nc",
    None, None, arange(0., 377.6, 2.5), None
)
```

would work in PyClimate 1.1, but it will crash in PyClimate 1.2. It worked before because `Numeric` was in your name space because `pyclimate.ncstruct` imported it and functions such as `'arange'` were automatically in your name space. Under PyClimate 1.2, this is no longer true.

To make the script run under PyClimate 1.2, you must add line of code to import `Numeric` yourself

```
from pyclimate.ncstruct import *
from Numeric import * # Add this line
onc=create_bare_COARDS(
    "XXX.nc",
    None, None, Numeric.arange(0., 377.6, 2.5), None
)
```

In particular, versions 1.1 and 1.2 of PyClimate allow the user to call equally `pyclimate.readdat`, `pyclimate.writedat` and `pyclimate.asciidat`. This is an obsolescent feature. In a couple of versions (about twenty years in the

future), `pyclimate.asciidat` will be the only way to access all these functions and `pyclimate.readdat` and `pyclimate.writedat` will disappear.

9. Statistical tests added to `tools.py`

Two new functions are available in the module `pyclimate.tools`. `'ttest'` performs a t-Student test on the difference of means and `'fctest'` performs a F-test on the difference of variances.

10. `writedat.py` `formatstring` argument has changed a bit

Blank spaces are managed by the `writedat` function, there's no need to worry about them in the `'formatstring'` argument.

- Version 1.1.1–July, 2001.

1. Re-Corrected bugs.

- (a) `readdat.py` bug on comments is now *really* corrected

2. The main reason for this release are the changes in python 2.1 which cause some of our modules to crash. Namely, comparisons like `if a==None` have had to be rewritten as `if not a`. The affected modules are `readdat`, `ncstruct` and `LanczosFilter`.

- Version 1.1–June, 2001.

1. Corrected bugs.

- (a) Previous version of `svdEOFs()` used a denominator of (N-1) to compute the variance, whilst the data sets were standardized using the sample variance (N) in the denominator. Thus, PCs were actually scaled by the factor $\sqrt{(N-1)/N}$ and eigenvalues (variances) by a factor $(N-1)/N$. We are using N in all denominators in this version.

- (b) `readdat.py` is able to handle comments like `#Variance of XXX` (without blank between the # and `Variance`), which caused a crash in previous versions.

2. To be able to run properly under Python 2.n, all exception strings have been removed and converted to exception classes. All the exceptions are instances of a root class (`PyClimateException`) which can be printed with a very comprehensive message via the `__str__` method. The exceptions have an alternative method `GetExceptionValue()`, which returns the most important data relevant to each exception.

3. The differential operators have been extended. They can work using periodic and non periodic boundary conditions in the longitudinal direction. For latitudes, the previous approach (backward and forward second order finite difference schemes) is used at the borders. In the current version, they are able to work using 3D (Z,lat,lon) and 4D (time,Z,lat,lon) fields arranged according to COARDS conventions, not just 2D fields, like in `PyClimate 1.0`. This allows to compute the operation for all the records in a data set (if it fits into memory) or for all the levels in a record at a time.

4. A new module `writedat.py` provides simple functions to write arrays in a way that can be directly inverted by `readdat.py`. Both modules (`writedat.py` and `readdat.py`) have been included into `asciidat.py`, although they can still be called independently for backward compatibility.

5. A new module `bpcca.py` provides Canonical Correlation Analysis with an EOF prefiltering (Barnett–Preisendorfer approach).
 6. Easier interface for the routines which compute EOFs and the SVD decomposition of coupled fields. The input data sets can be arbitrarily shaped, with the only precondition that the leading axis is the time dimension. The fields are automatically reshaped inside the routines before returning. Similarly, the eigenvectors and singular vectors are automatically reshaped to the original shape before returning to the caller. Some simple functions have added to these modules (`svd.py` and `svdeofs.py`).
 7. A new function `getcoefcorrelations()` has been added to `svd.py` to get the correlations of paired SVD expansion coefficients.
 8. A new function `pcseriescorrelation()` has been added to the module `svdeofs.py` to get the correlation patterns between each principal component and the original field.
 9. New versions of the manual and the tests cover the previously described changes.
 10. We have slowly started to provide `__doc__` strings to SOME (very few, yet) of the routines.
 11. New function `create_bare_COARDS()` to create the bare minimum of a COARDS compliant netCDF file in `ncstruct.py`.
- Version 1.0–October, 2000.
 1. Improved tests. They are more accurate, reliable, informative, comprehensive and use less disk space.
 2. The package compiles using `distutils`. This feature has been checked on FreeBSD, Linux and OSF platforms.
 3. Some minor typos corrected in the documentation.
 4. Added `KPDF.c`, a extension module to estimate univariate and multivariate kernel–based probability density functions.
 5. Added a class to compute the vertical component of the curl and the divergence of an horizontal vectorial field in `diffoperators.py`.
 6. `DCDFLIB.C` is currently distributed with the package.
 7. `KZFilter.py` has been converted into a general purpose `LinearFilter.py` which holds the basic operations of any linear filter. There are two different subclasses currently, the Lanczos filter [5] and the previous Kolmogorov–Zurbenko filter, `KZFilter.py`.

2 Installation

2.1 Download

The package is freely available from the official website <http://www.pyclimate.org> as a tar.gz source file. Even though full backward compatibility is kept when possible, previous releases of the package are also available from the website.

2.2 Prerequisites

Many of the functions developed in this package have been built over other freely distributed packages and libraries. So, before installing this package, the next software is needed:

- **Python** interpreter itself, freely available at:
<http://www.python.org>
- The Numeric extensions to **Python**, freely available at:
<http://sourceforge.net/projects/numpy>
- Konrad Hinsen's **Scientific Python**, available at:
<http://starship.python.net/crew/~hinsen>
- The **netCDF** library, freely available at:
<http://www.unidata.ucar.edu>

Versions prior to **PyClimate 1.0** required **DCDFLIB.C 1.1** library, too, which is freely available at: http://odin.mdacc.tmc.edu/anonftp/page_3.html. The current version of the package distributes the source and documentation of this library to ease the installation of **PyClimate**. In case the original C files of some of the extensions were edited, D. Beazley's **SWIG** (<http://www.swig.org>) will be needed to create the **Python** interface to the C routines. The **SWIG** source files (*.i) are distributed in the subdirectory `swig`.

2.3 Compilation

Since version 1.0 **pyclimate** is distributed using `distutils`. Thanks to Alberto García for his help in setting up the `setup.py` script. After downloading the file `PyClimate-1.0.tar.gz`, you should decompress, untar and install it. The UNIX commands needed are:

```
gunzip PyClimate-1.0.tar.gz
tar xf PyClimate-1.0.tar
```

After these steps, go into the main directory of **pyclimate** and a typical installation command is:

- For a general installation (root password required):
`python setup.py install`
- For a private installation:
`python setup.py install --home=~`

In this last case, you will have to set manually the value of the environmental variable `PYTHONPATH` to be able to access **pyclimate**. The script `pyclimatetest.py` in the `test` directory runs a test that covers many of the routines in the package (see subsection 2.4).

2.4 Test

After installing the package, a user may be interested in knowing if it is working properly. There is a script which makes extensive use of the functions in **pyclimate** in

the subdirectory `test`. This script (`pyclimatetest.py`) compares the results obtained after the installation with the ones obtained and checked during the development and extensive checking of the package. Thus, `python pyclimatetest.py` runs the tests and compares the output with the data stored in file `reference.cdf`. The output of the script is quite informative. Here is shown a excerpt of the output:

```
XG_44_44 |hgt_eofs      | : 1.00e-00 dG:-1.11022e-16
  G_45_45 |hgt_eofs      | : 1.00e+00 dG: 2.22045e-16
  G_46_46 |hgt_eofs      | : 1.00e+00 dG: 0.00000e+00
XG_47_47 |hgt_eofs      | : 1.00e-00 dG:-1.11022e-16
  RMS Error |hgt_lambdas   | : 0.00e+00
```

The first character of each file may be a blank (no difference detected) or a X, in which case, a difference has been detected. Most often, these differences are not important, and they are simply due to the fact that the control used is of the type `if rms!=0.0):`, which is not accurate enough. The second column shows which is the measure used to evaluate the differences. Usually, RMS errors are used, but congruence coefficients ($G_{i,i}$) are also used to evaluate errors in EOFs (and related quantities, like PCs, expansion coefficients for SVD analysis or heterogeneous and homogeneous correlation maps) due to the fact that both \mathbf{x} and $-\mathbf{x}$ are valid solutions of the eigenvalue problem. The third column states the name of the netCDF variable which holds the reference data and the fourth column shows the value of the error measure (RMS or congruence coefficient). For the special case of congruence coefficients, a last column (dG) shows the difference $1 - |g_{i,i}|$ to let the user know the real difference for those lines with a X as the first character.

The new tests in version 1.1 have increased the size of `reference.cdf` to 1.6 Mb. Therefore, it is not currently distributed with `pyclimate`, and the distribution still fits in a floppy disk (or two, if you download the reference file and `gzip -9` it first). The test script can retrieve the file from the URL, and, additionally, the file can always be downloaded from the primary WEB server <http://www.pyclimate.org>. `python pyclimatetest.py -g` forces the retrieval of the reference file from its URL.

`python pyclimatetest.py` will usually be called without command line arguments, and it performs the comparisons. However, if a user detects that with her hardware or software she is getting different results (for instance, phases in EOFs) and she prefers to have her own `reference.cdf` file, she can use the command line option `-o` to overwrite the reference file. It is not advisable to do this unless the correctness of **pyclimate** has been examined at least once after the primary installation in that platform.

2.5 Examples

The previous manual included some examples on the use of the code. However, we have removed those examples from the current version of the manual to save some trees. They can be found at the directory `examples` of the distribution, and you can print them, if you don't mind using paper. Another different source of information on the use of the package can be found in the `pyclimatetest.py` file, which covers most of the functions in the package, using real-life data sets.

3 IO functions

3.1 ASCII files: `asciidat.py`

3.1.1 `readdat.py`

The main goal of file `readdat.py` is to provide a set of functions to handle IO from ASCII files. The ASCII files must be written in the way `gnuplot` files are, but not all of the `gnuplot`-compliant files are readable. Each row in the file is a row of the output data. Lines whose first token is a `#` are comments for these functions. No comments are allowed at the tail of a line. Empty lines are allowed, but they are discarded and not used to separate datasets in the file. Better support for these features exists in other packages for **Python**, like M. Haggerty's **Gnuplot** or the IO functions in K. Hinsen's **Scientific Python**. The interest of this file is that it allows to read files with complex numbers and other data types, a feature that is not supported by the mentioned files. Complex numbers are written as: `real,imag,imag` or `real,` in the input file, with no blank spaces (nor tabs) separating the members of a complex number. Examples of use of these routines can be found in file `exiofuncs.py`

Function: `def readdat(fname,typecode=None)`

Reads all the data in the file `fname` and returns a bidimensional NumPy array of the same shape as the data in the original array and with a `typecode` given as `Float64` by default (`Complex64` in case there were complex elements in the file). If the parameter `typecode` is explicitly assigned, the output array is coerced to that type. If the file to be read contains only one row or column of data the returned array is one-dimensional.

Function: `def readcol(fname,col=1,typecode=None)`

In this case, the `col`-eth column is read and returned as a one dimensional NumPy array. The numbering of columns is not according to **Python**'s scheme, but to `gnuplot`'s one instead, that is, from 1 to N. The type coercion works as in the previous function.

Function: `def readcols(fname,cols=[1],typecode=None)`

Similar to `readcol`, but reads from the file `fname` and returns a n -dimensional NumPy array, where n is the length of the sequence object `cols`. The type coercion works as in the previous two functions. The columns are returned in the same order as they appear in `cols`.

Function: `def read1Ddat(fname,typecode=None)`

Similar to `readdat`, but even if the ASCII file has several columns they are read row by row as a 1D array. This allows to read files with an unequal number of columns in each row.

Function: `def readstdin(typecode=None)`

Similar to `readdat`, but reads from the standard input. Allows to pipe your python script to the output of another program.

3.1.2 `writedat.py`

As a `readdat.py` related tool is provided `writedat.py`. A NumPy array can be directly written in a way that can be recovered with `readdat.py`. This provides an easy way to pass arrays from one program to another with human readable intermediate files.

Function: `def writedat(fname, matrix, header="", formatstring="%g")`

The name of the file to be created is passed as the first argument `fname`. If the file already exists it will be overwritten without prompting. One and two-dimensional arrays can be written and they are passed as the second argument `matrix` to the function. All

other arguments are optional. A header can be specified, but the user must take care of writing a # at the beginning of each line. Finally, the output format can be controlled by passing a format string. The default format string is "%g".

3.2 netCDF files

To access netCDF files, **pyclimate** uses the excellent netCDF package in K. Hinsen's **Scientific Python**. Two special functions have been built on top of K. Hinsen's interface to make the use of structured netCDF files easier, and they are included in the file `ncstruct.py`.

Function: `def nccopystruct(name,inc,dims,vars,varcontents)`

This function replicates the structure of a Conventions-compliant netCDF file (see COARDS conventions <http://www.unidata.ucar.edu>). These conventions usually imply the definition of a set of variables like latitude, longitude or vertical level and some auxiliary attributes like units or the numbers assigned to the missing values or scale and offset values for packing. This function helps in the creation of structured output files from an input dataset without having to individually copy ALL of the global attributes, auxiliary variables and their attributes. In case a `history` attribute existed, it is updated with the date and the name and arguments of the calling program. The function returns a netCDF file object ready to be used. This function opens the existing netCDF file with the 'w' flag, overwriting any existing file with the same name. Parameter **name** is the name of the output datafile to be created. **inc** is the input NetCDF file whose structure is to be replicated. **dims** is a sequence of dimensions of the input datafile which are to be copied onto the output datafile. **vars** is a sequence of variables to be copied onto the output datafile without copying the contents, just the declaration, type, structure and comments. **varcontents** is a sequence of variables in the parameter **vars** whose structure and contents are to be copied from the input dataset. The function `exiofuncsnc.py` shows examples of use of this function.

Function: `create_bare_COARDS(ncname, tdat=None, zdat=None, latdat=None, londat=None)`

This function creates a bare-minimum COARDS-compliant netCDF file. **ncname** is the name of the output file that is being created. **tdat** is `None` or a tuple with first element the NumPy array of items to be held (`None` for a record variable) and with second element in the tuple the units attribute of the created time variable. If **tdat** is `None`, no time variable nor dimension will be created. **zdat** is a tuple with two elements. The first one is the NumPy array of vertical levels. The second one is the units attribute of the vertical levels. If **zdata** is `None`, no vertical dimension is created. **latdat** is a NumPy array of latitudes. The units attribute is always set to "degrees.north". If this parameter is `None`, no latitudinal dimension is created. **londat** is a NumPy array of longitudes. The units attribute is set to "degrees.east". If this parameter is `None`, no zonal dimension is created.

From PyClimate 1.2 on, a new module to handle NetCDF files has been added: `nciterator.py`. It allows to access multiple NetCDF files containing the same variable for different times (e. g. the NCEP distributes the data in a NetCDF file per year) transparently, not caring about in which file is the record you want to read.

Class: `nciterator`

Method: `nciterator.__init__(self, namelist, tvarname)`

Default constructor. **namelist** is a list with the name of the files to include in the iterator. **tvarname** is the NetCDF variable name (it must exist in all files in **namelist**).

Method: nciterator._len_(self)

Return the total number of records.

Method: nciterator.getfield(self, varname, irec)

Returns a NumPy array with the variable **varname** corresponding to the global record **irec**. Particularly, asking for **varname="time"** the time positioning of the record can be obtained.

Method: nciterator.getncitem(self, irec)

Locates the NetCDF file which contains the global record **irec** and returns it as an open NetCDFFile object.

Method: nciterator.getncrec(self, irec, inc)

Returns the local record of the NetCDFFile **inc** corresponding to the global record **irec**

4 Time handling routines

One of the problems that researchers in climate analysis are usually faced to is the need to position their observations accurately in time. The file `JDTIME.py` provides some functions to face this problem. It does not intend to provide a complete set of date handling routines. In particular, all the computations assume UTC time-zone and no DST functions are included (M.A. Lemburg's **mxDate** provides some of these extra features). `JDTIME.py` allows fast, accurate and easy date processing from **Python** without the need of extra packages. A very interesting feature is the possibility of easily using monthly intervals by means of the function `monthllystep()`, computed from the definition of a tropical year with the same value used in Unidata's `udunits.dat`, so that the time values created this way can be correctly read and interpreted by the SDF interface in plotting programs as GrADS. The date arithmetic is carried out by means of Julian Days stored as double precision (Float64) numbers. Conversion functions to date structures are provided by means of a C extension based on astronomical algorithms [6]. The file `exjdtime.py` provides some examples of the use of these functions. The algorithm does not support dates before the start of the Gregorian calendar (1582-10-15). In particular, this means that you can not properly recover dates from some of the NCEP Reanalysis netCDF files, which start at 1-1-1, a date not included in the Gregorian calendar.

Class: JDTime

Integer members: **year, month, day, hour, minute.**

Double member: **second.**

The previous members can be directly accessed from **Python**.

Function: def date2jd(jdt)

From a `JDTime` structure **jdt**, get the Julian Day number as a double.

Function: def jd2date(jd,jdt)

Given a Julian Day **jd**, get the broken date structure **jdt**.

Function: def monthllystep()

Return the number of Julian Days in a month, that is, number of tropical days per year (365.242198781) divided by twelve. This provides adequate accuracy for dates during the instrumental part of the climate record. However, this approach poses a problem because of the truncation problem that appears due to the different length of the months. When using this approximation, some months are longer than others and this means that one of the time steps may be in the first day of one month and the last step on the last day of the same month (if month is longer than 30.43 days). To avoid this truncation problem, the origin should be set to day 15th of the starting month. This

way, for every record, the first two fields of the date structure (year and month) will be adequately resolved by `jd2date()`. This can be easily explained with the next example, and its output.

```
from pyclimate.JDTimeHandler import *
from pyclimate.JDTime import *

a=JDTimeHandler("hours since 1958-01-01")
b=JDTimeHandler("hours since 1958-01-15")
mstep=monthllystep()*24
print mstep," in hours = ",mstep/24.," days"
print a.getdatefields(0.0,3)
print b.getdatefields(0.0,3)
print a.getdatefields(0.0+mstep,3)," Still in January"
print b.getdatefields(0.0+mstep,3)," In February"
```

```
730.484397562  in hours =  30.4368498984  days
[1958, 1, 1]
[1958, 1, 15]
[1958, 1, 31]  Still in January
[1958, 2, 14]  In February
```

There is a second file that allows the handling of COARDS compliant time variables in netCDF files, `JDTimeHandler.py`.

Class: JDTimeHandler

Function: def __init__(self,units)

The creator parses a COARDS-type units attribute of the netCDF *time* variable (ex: *hours since 1958-01-01 0:0*) and computes the offset and the scale factor to get Julian Days from the netCDF *time* variable for each record.

Function: def getdatefields(self,tvalue,listlen=6)

This method scales the value of **tvalue** using the scaling factor corresponding to the *units* attribute and adds the offset computed from the units attribute, getting the Julian Day corresponding to the time coordinate **tvalue**. The Julian Day value is used to create a broken date structure, and its values (year,month,day,hour,minute,second) are returned as a list, with as many members as those requested by **listlen**.

Function: def gettimevalue(self,datefields,listlen=6)

This function is the inverse of the previous one. It creates a Julian Day from the values in the list **datefields** (as many values as the value of **listlen**), computes the offset from the origin of coordinates and scales the value to the units corresponding to the *units* attribute of the *time* variable used to create the instance of this class. Due to some truncations which appear during the floating point operations, this function is only accurate to about 12 significant figures. So, if you are creating a netCDF file from scratch, it is more accurate and fast just to add equal time intervals using a fixed time step from record to record.

5 Distribution functions

DCDFLIB.C 1.1 is a library of C Routines for Cumulative Distribution Functions developed by Barry W. Brown, James Lovato and Kathy Russell, Department of Biomathematics, The University of Texas, M.D. Anderson Cancer Center. The library allows

the determination of cumulative distribution functions, inverses, and the parameters of the following statistical distributions: Beta, Binomial, χ^2 , Noncentral χ^2 , F , Noncentral F , Gamma, Negative Binomial, Normal, Poisson, Student's t and Noncentral t . The file `pydcdflib.py` provides access to this library from **Python**. For each one of these distributions, a class has been created that wraps the parameters in the call to the functions of this routine and some C functions that wrap the original C calls to make them available to the **Python** interpreter. The same names have been used in the wrapping of the parameters, so that the original documentation of the **DCDFLIB.C** library is valid for each of the classes in this **Python** extension. The class is passed to a function with the same name of the original one (with `py` prepended to the name of the wrapper function). The fields of each class are updated by the wrapper functions. The code of the original C library is untouched. Examples on the use of these wrappers can be obtained from the `testDCDFLIB.py` script in the source directory of the distribution and from the enclosed `exdcdflib.py` file. There is an error when computing the parameters for the F distribution using the value `which=3`. This seems to be linked to the properties of the F distribution and, in case it were a bug, it also exists in the original **DCDFLIB.C**, as the same problem appears using the C file `testF.c`, provided in the source directory. The documentation of the original DCDFLIB.C library is distributed within the `doc` subdirectory of the distribution.

6 Simple multivariate statistical tools

The main goal of file `mvarstatools.py` is to provide some routines that are being used by others like `svdeofs.py`. However, some of them may be interesting by themselves, and they are thus documented in this section.

Function: def center(dataset)

Given an input multivariate dataset with arbitrary dimensions x_t (with the restriction that first dimension is time), this function returns the centered dataset $\tilde{x}_t = x_t - \mu$, with μ the sample average $\mu = \frac{\sum_t x_t}{N}$.

Function: def standardize(dataset)

Given an input multivariate dataset with arbitrary dimensions x_t (with the restriction that first dimension is time), this function returns the standardized dataset $\hat{x}_t = \frac{x_t - \mu}{\sigma_x}$, with σ_x the sample standard deviation $\sigma_x = \sqrt{\frac{\sum_t (x_t - \mu)^2}{N}}$.

Function: def covariancematrix(X,Y)

Given two input datasets X and Y , with first dimension time and second dimension space, this function returns the S-mode covariance matrix $S = \frac{(X - \bar{X})^T (Y - \bar{Y})}{N}$.

Function: def correlationmatrix(X,Y)

Given two input datasets X and Y , with first dimension time and second dimension space, this function returns the S-mode correlation matrix $S = \frac{x^T y}{N}$ from the standardized x and y datasets.

Function: def detrend(dataset,tvalues,order=1)

From the **univariate** time series **dataset**, this function returns a tuple (**detrended,trend-coefs**). The trend is computed adjusting by means of linear least squares a polynomial $x(t) = \sum_{i=0}^M a_i t^i$ to the data, where M is **order**. The tuple holds the detrended time series as the first member and the trend coefficients a_i as the second element of the tuple.

Function: def congruence(pattern1,pattern2)

Given two spatial patterns **pattern1** (\vec{e}_1) and **pattern2** (\vec{e}_2), this function returns the congruence coefficient $g_{1,2} = \frac{\vec{e}_1 \cdot \vec{e}_2}{|\vec{e}_1| |\vec{e}_2|}$ [3, 14].

7 EOF analysis

A subroutine is provided in the file `svdeofs.py` to perform the decomposition of a dataset in its spatial eigenvectors (Empirical Orthogonal Functions, EOFs), the fraction of variance explained by each mode and its temporal expansion coefficients [12, 16] (PCs). One of the problems of this technique in climatological analysis is the singularity of covariance matrices when the number of spatial degrees of freedom is bigger than the number of temporal samples. To avoid this problem, the routine is based on the SVD decomposition of the data matrix $X = [x_{ij}]$. For this implementation, $i = 1 \dots N$ means a temporal sample and $j = 1 \dots M$ a grid point or observing site. Corrections derived from quadrature or area factors [2, 11] must be applied prior to this routine. There is an example on the use of these function in file `exsvdeofs.py`.

Since version 1.1, the input data set may be arbitrarily shaped, with the only restriction that the leading axis must be the time axis.

NEW: Since version 1.2, the EOF analysis has been re-implemented using objects to avoid giving redundant information to the functions of the module. Please, refer to a previous version of the manual to get information about the previous syntax (which is already available for backward compatibility).

Class: SVDEOFs

Method: SVDEOFs.__init__(self, dataset)

Given a two dimensional dataset $N \times M$ as described above, this constructor computes $\mathbf{Z}, \Lambda, \mathbf{E}$. $\mathbf{Z} = [z_1 | \dots | z_L]$ is a $N \times L$ matrix, where each column z_k is a vector of length N and is the k -th PC of the field. Each element λ_k in the one dimensional array Λ , is the variance accounted for by the k -th component. Finally, the matrix $\mathbf{E} = [\mathbf{e}_1 | \dots | \mathbf{e}_L]$ has as columns each of the eigenvectors (EOFs) of the dataset. The maximum number of EOFs (L) will be $\min(M, N)$, depending on the rank of the data matrix. The input dataset is centered (mean removed) inside the routine.

Method: SVDEOFs.eofs(self, pccscaling=0)

Returns the empirical orthogonal functions. From version 1.1 `pyclimate` supports multidimensional **dataset** provided that the first dimension keeps being the temporal one. In that case the EOFs are returned stored as *generalized columns* (ie: they can be recovered as $E[\dots, eof_number]$ instead of $E[:, eof_number]$) and their spatial shape is that of the original field. This approach is backwards compatible with previous versions but is more flexible for the user. If the **pccscaling** is set to 0 the output eigenvalues are scaled as variances, the PCs z_k are scaled so that their variance is the variance accounted for by each component, and the eigenvectors are orthonormal, i.e. $\langle z_k, z_j \rangle = \delta_{kj} \lambda_j$, $\mathbf{e}_k \cdot \mathbf{e}_j = \delta_{kj}$. If the **pccscaling** is set to 1 the output PCs have unit variance and the eigenvectors are no longer orthonormal but just orthogonal.

Method: SVDEOFs.pcs(self, pccscaling=0)

Return the principal components of the field. See the previous method for the behavior induced by a **pccscaling** different from the default (0).

Method: SVDEOFs.eigenvalues(self)

The decreasing variances associated to each EOF.

Method: SVDEOFs.eofsAsCorrelation(self)

Return the EOFs scaled as the correlation of the PC with the original field. It uses the

formula:

$$\text{Corr}(z_i, X_j) = \frac{\sigma(z_i)}{\sigma(X_j)} E_{ij}$$

where X_j is the time series at the j -th site. The correlation fields of the original time series with each PC are returned as *generalized columns*.

Method: SVDEOFs.eofsAsExplainedVariance(self)

Return the EOFs scaled as fraction of explained variance of the original field

Method: SVDEOFs.varianceFraction(self)

Returns the fraction of variance $f_i = \lambda_i / \sum_{k=1}^L \lambda_k$ associated to each of the eigenvalues.

Method: SVDEOFs.northTest(self)

Tests the degeneracy of eigenvalues according to $\delta\lambda_i \approx \frac{\sqrt{2}\lambda_i}{\sqrt{N}}$. It returns the array of values $\Delta\lambda = \{\delta\lambda_i\}$. In case that for a pair of eigenvalues $\lambda_i - \delta\lambda_i \approx \lambda_{i+1} + \delta\lambda_{i+1}$, both members of the pair should be maintained or removed simultaneously in the factorization [11].

Method: SVDEOFs.bartlettTest(self)

Test the hypothesis that the last $p - k$ eigenvalues are equal by means of the statistic [9]:

$$\chi^2 = -\nu \sum_{j=k+1}^p \ln(\lambda_j) + \nu(p - k) \ln \left[\frac{\sum_{i=k+1}^p \lambda_i}{p - k} \right] \quad (1)$$

It is distributed as a χ^2 with $\frac{1}{2}(p - k + 1)(p - k + 2)$ degrees of freedom. ν is the degrees of freedom of the covariance matrix. The function returns a tuple of arrays (each of them one item shorter than Λ), (χ_i, p_{χ_i}) . The first element of the tuple is an array with the values of χ^2 obtained from eqn (1), while the second element holds their probabilities. This test is usually too liberal and tends to overfactor [9].

Method: SVDEOFs.MCTest(self, subsamples, length, neofs=None)

This function tests, by means of a Monte Carlo test [3], the stability of the EOFs to temporal subsampling of the original dataset. This method builds several **subsamples** choosing the records in the original dataset at random. The subsamples are of length **length**, which must be smaller than the length of the original dataset. The function returns a Numeric array of shape $(\text{subsamples}, \text{neofs})$ which holds the congruence coefficients of the master (whole sample) and perturbed (subsample) eigenvectors for each subsample and eigenvector.

Method: SVDEOFs.projectField(self, neofs, X=None)

Projects a field **X** onto the neofs leading EOFs returning its coordinates in the EOF-space

Method: SVDEOFs.reconstructedField(self, neofs)

Reconstructs the original field using **neofs** EOFs

Method: SVDEOFs.unreconstructedField(self, neofs, X=None)

Returns the part of the field NOT reconstructed by neofs EOFs. **neofs** is the number of EOFs for reconstructing the field. **X** is the field to try to reconstruct. Defaults to the data field used to derive the EOFs.

Method: SVDEOFs.totalAnomalyVariance(self)

The total variance associated to the field of anomalies

From PyClimate 1.2 on, there is another module dedicated to Principal Component Analysis: `hdseofs.py`. It is intended for **huge data sets** and minimizes the use of memory sacrificing execution speed with one or two python cycles (these are made in

C in the module `svdeofs.py`). It is object oriented and can perform the calculations in two different ways.

Class: SIHDSEOFs

Method: SIHDSEOFs.__init__(self, iterator, tcode='d', therecords=None, corrmatrix=0)

Constructor for the single iteration approach. The dataset to decompose (**iterator** can be any indexable object (e. g. list, Numpy array, a NetCDF iterator, ...)). Some records can be skipped by passing explicitly the sequence **therecords** desired to enter the calculation. This approach allows to calculate correlation matrix based EOFs.

Class: DIHDSEOFs

Method: DIHDSEOFs.__init__(self, iterator, tcode='d', therecords=None, corrmatrix=0)

Constructor for the double iteration approach. All arguments of the constructor are used like the **SIHDSEOFs** ones.

Class: HDSEOFs

Mother class for both huge data set EOFs constructors. Do not instantiate, use **SIHDSEOFs** or **DIHDSEOFs**, instead.

Method: HDSEOFs.Eigenvectors(self, Neofs, pscaling=0, svdsolver=LA.singular_value_decomposition)

EOFs, the eigenvectors of the covariance (correlation) matrix. **Neofs** is the number of EOFs to return. **pscaling** is the kind of PC scaling. Defaults to 0, orthonormal EOFs. Set this parameter to 1 to obtain variance carrying orthogonal EOFs. The routine to perform the SVD underlying decomposition (**svdsolver**) can be selected. Defaults to LinearAlgebra's `singular_value_decomposition`.

Method: HDSEOFs.PCs(self, Neofs, iterator, irecord, pscaling=0)

Principal components. The number of desired components **Neofs**, the **iterator** to project onto to obtain the PCs (usually the one used to derive the EOFs) and the **irecord** of the component to get must be passed to this method. The **pscaling** can also be selected.

Method: WholePCs (self, Neofs, iterator, pscaling=0)

Same as **HDSEOFs.PCs** but asks for all the records returning the whole PCs instead of each record at a time.

Method: HDSEOFs.Eigenvalues(self, svdsolver=LA.singular_value_decomposition)

Eigenvalues of the covariance (correlation) matrix

Method: HDSEOFs.MCTest(self, Neofs, iterator, subsamples, length)

Monte Carlo test on the congruence. Works just as the **SVDEOFs** version.

Method: HDSEOFs.NorthTest(self)

North error bars. Works just as the **SVDEOFs** version.

Method: HDSEOFs.ScatteringMeasure(self)

Returns the covariance or correlation matrix depending on the constructor

Method: HDSEOFs.VarianceFraction(self, svdfunc=LA.singular_value_decomposition)

Total variance fraction accounted for each principal mode

Method: HDSEOFs.Average(self)

Time average of the original field

8 SVD of coupled datasets

The SVD decomposition of the covariance matrix of two datasets is one of the simplest, yet powerful, method to analyze the linear relationship between two coupled geophysical datasets [1, 4, 10, 16]. Some functions that implement most of the computations

usually needed for this analysis are provided in the file `svd.py`. One example on the use of these functions is in the file `testsvd.py`.

Function: def svd(xfield,yfield)

Given two fields X (**xfield**) and Y (**yfield**), defined as in section 7 (first dimension of the array is the temporal one), this function returns the SVD decomposition of their covariance matrix $C_{xy} = \frac{X^T Y}{N}$. It returns a tuple of three arrays U , Σ and V . Each column \mathbf{u}_i holds the i -eth singular vector of the left (X) field. Same convention is followed by the ordering of elements in V . Σ is a one-dimensional array which holds the singular values σ_i . The singular vectors are orthonormal ($\mathbf{u}_i \cdot \mathbf{u}_j = \mathbf{v}_i \cdot \mathbf{v}_j = \delta_{ij}$) and can be used to linearly project each of the fields to define the expansion coefficients $p_i(t) = x(t) \cdot \mathbf{u}_i$ and $q_i(t) = y(t) \cdot \mathbf{v}_i$ whose covariance is the same as the singular value associated to that mode $\langle p_i, q_i \rangle = \sigma_i$. The datasets are centered (sample mean is removed) inside the function prior to the SVD computation. **NEW:** Since version 1.1, the data sets may have arbitrary dimensions, but the leading one must be time.

As in the case of EOF decomposition the fields can also be entered as more-than-two-dimensional arrays and the returned matrices will be accordingly reshaped to avoid the user to care about the internal use of two-dimensional matrices. The SVD patterns are returned as *generalized columns* in the sense described in the EOF section.

Function: def getcoefs(data,svectors)

Given a dataset **data** (X or Y) and the corresponding set of singular vectors (U or V) returned by `svd()`, this function returns the expansion coefficients (p_i or q_i) up to the order stated by the evaluation of `svectors.shape[-1]`). This, in fact, means truncating the representation of the field at this number. This same approach is used in the next two routines. The output Numeric arrays hold the coefficients in each column. That is, the expansion coefficients associated to the i -eth singular vector are: `coefs[:,i]`.

Function: def getcoefcorrelations(scoefs,zcoefs)

Given the left and right SVD expansion coefficients returns a one-dimensional array containing the paired correlation of the corresponding coefficients.

Function: def homogeneousmaps(data,svectors)

From the input dataset **data** and the array **svectors**, returns an array with as many homogeneous correlation maps ($\langle X, \mathbf{u}_i \rangle$ or $\langle Y, \mathbf{v}_i \rangle$) as ending subarrays (singular vectors) are in **svectors**. Each subarray `themaps[... ,imap]` is the `imap`-eth map.

Function: def heterogeneousmaps(xdata,ycoefs)

From the input dataset **xdata** and the array of expansion coefficients **ycoefs**, it returns an array with as many heterogeneous correlation maps ($\langle Y, p_k \rangle$ or $\langle X, q_k \rangle$) as columns (expansion coefficients) are in **ycoefs**. The ordering of the maps is as described in previous routine.

Function: def SCF(sigmas)

This function returns the squared covariance fraction associated to each singular value,

$$scf_k = \frac{\sigma_k^2}{\sum_k \sigma_k^2}$$

from the array Σ returned by `svd()`.

Function: def CSCF(sigmas)

This function returns the cumulative squared covariance fraction associated to a set of singular values,

$$cscf_k = \sum_{i=0}^k \frac{\sigma_i^2}{\sum_k \sigma_k^2}$$

from the array Σ returned by `svd()`.

Function: def makemctest(Um,Vm,ldata,rdata,itime,ielems)

This function performs a Monte Carlo test on the stability of the left singular vectors **Um** and the right singular vectors **Vm** obtained from `svd()` or truncated to the

leading ones ($U_m.shape[-1]==V_m.shape[-1]$). It computes **itimes** simultaneous subsamples (**ielems** long each) of each datafield **ldata**, **rdata**, and evaluates the congruence coefficient of the master singular vectors to those derived from the subsamples. It returns a tuple of Numerical Python arrays (**ucoeffs**, **vcoeffs**) which hold the congruence coefficient for each sample and each U/V master singular vector ($ucoeffs.shape=(itimes, U_m.shape[-1])$). **ielems** must be smaller than $len(ldata)$.

9 CCA (Canonical Correlation Analysis)

Canonical correlation analysis can be performed by `bpcca.py`. This technique gets the pattern decomposition of two fields such that the correlation between the temporal coefficients of paired patterns is maximum. The Barnett and Preisendorfer [1] approach has been implemented. In this approach an EOF prefiltering is performed and the CCA is carried out in EOF-coordinates. The user never deals with these coordinates but can customize some features of the EOF decomposition.

The results are scaled for the canonical expansion coefficients to have unit variance. If the columns of A and B are the canonical expansion coefficients and P and Q are the canonical patterns, the fields S and Z can be partially (due to the EOF prefiltering) recovered as:

$$\begin{aligned}\tilde{S} &= AP^T \\ \tilde{Z} &= BQ^T\end{aligned}$$

The internal calculus are carried out by means of singular value decomposition of the principal component cross covariance matrix.

Class: BPCCA

Method: BPCCA.__init__(leftfield, rightfield, retainedeofs=None)

Given two two-dimensional datasets this constructor performs the CCA decomposition of the fields. **leftfield** and **rightfield** are the left and right fields respectively. The user can specify the number of EOFs to be retained in each field as a tuple **retainedeofs**. If no **retainedeofs** is specified 70% rule is used: EOFs are retained until a 70% of the variance is explained.

Method: BPCCA.leftPatterns()

This method returns an array which columns are the left (those associated to the **leftfield**) canonical patterns.

Method: BPCCA.rightPatterns()

Idem for the right patterns.

Method: BPCCA.leftExpCoeffs()

This method returns an array which columns are the left (those associated to the **leftfield**) canonical expansion coefficients.

Method: BPCCA.rightExpCoeffs()

Idem for the right coefficients.

Method: BPCCA.correlation()

Gives the ordered canonical correlations of the expansion coefficients as an array.

Method: BPCCA.varianceFractions()

Returns a tuple containing the variance fraction explained by each canonical pattern. The first element of the tuple is the array of fractions corresponding to the left field. The second one is that of the right field.

Method: BPCA.leftAdjointPatterns(self)

Returns (along the last dimension) the left adjoint canonical patterns

Method: BPCA.rightAdjointPatterns(self)

Returns (along the last dimension) the right adjoint canonical patterns

Method: BPCA.EOFspaceLeftPatterns(self)

Returns the left canonical patterns in EOF coordinates

Method: BPCA.EOFspaceRightPatterns(self)

Returns the right canonical patterns in EOF coordinates

Method: BPCA.reconstructedFields(self, nccps)

Reconstructs the original fields with the desired number (**nccps**) of canonical patterns.

Method: BPCA.MCTest(self, subsamples, length)

Monte Carlo test for the temporal stability of the canonical patterns. The number of Monte Carlo **subsamples** to take and the **length** of each subsample (obviously less than the total number of time records) must be provided. Returns a tuple with the left and right NumPy arrays containing in each row the congruence coefficient of each subsample obtained patterns with those obtained for the whole dataset.

Method: BPCA.MCTestCorrelation(self, samples)

Monte Carlo test for the significance of the canonical correlations. The input data are randomly temporally disordered and CCA is performed obtaining a distribution of canonical correlations due to non actually correlated fields (but inherently with the same probability distribution as the original ones) **samples** is the number of Monte Carlo subsamples to take. Returns a Numpy array which columns are the different canonical correlations for each MC run.

The BPCA object provides the following accessible attributes. They are only supposed to be accessible for obtaining additional info, altering their values could be dangerous:

BPCA.sPCA Is s SVDEOFs object with the PCA analysis of the left field.

BPCA.zPCA Idem for right field.

10 Multivariate linear filters: `LinearFilter.py`

Filters are used in climate analysis to attenuate components of irrelevant frequencies from a broadband signal and to select the frequencies of interest for the problem under consideration. The simplest of these filters are the linear filters and two of them are provided: the Kolmogorov-Zurbenko filter and the Lanczos filter. In the current version, the filter does not handle missing values.

Both of them filter the data by weighting the input with coefficients a_k that depend on the filter:

$$y_t = \sum_{k=-n}^n a_k x_{k+t}$$

This common part of the computation is carried out by subclassing the `LinearFilter` class.

Class: LinearFilter

Method: LinearFilter.getfiltered(ifield)

Given an input field, the function returns the filtered data corresponding to each input record. This function must be called in an iterative way. The filter has been implemented with performance in mind, so that, in order to avoid several iterations through a possibly long dataset, it iterates just once, performing a multivariate filtering to each

record. This makes that during the initialization phase, the internal running buffer must be initialized (filled) until valid values can be obtained. During the initialization phase of the filter, this function returns `None`. After the internal buffer is ready, the function returns valid filtered fields until the user arrives at the final record of the iteration.

Method: `LinearFilter.reset()`

This method resets the linear filter so that it is able to start computing with a data set of a different shape avoiding the creation of a new instance of the class.

10.1 KZ filter: `KZFilter.py`

The Kolmogorov–Zurbenko digital filter is a very simple but powerful digital filter. Its features are documented elsewhere [7, 13].

Class: `KZFilter`

Method: `KZFilter.__init__(self, points, iterations, lowpass=1)`

Default (and only) constructor. **points** is an odd integer representing the number of points in the moving average, while **iterations** is an integer representing the number of times that the average is iterated to get a better damping of the secondary maximums. When the flag **lowpass** is false, the filter instance works as a high-pass filter.

Method: `KZFilter.getcoefs(self)`

This function returns the coefficients that are being used in the filter.

Method: `KZFilter.cutofffrequency()`

Returns the approximate cutoff frequency of the filter.

10.2 Lanczos filter: `LanczosFilter.py`

The Lanczos filter is another very common filter and its mathematical properties and the algorithms for the compilation of the coefficients can be found for instance at [5].

Class: `LanczosFilter`

Method: `LanczosFilter.__init__(self, filtertype='bp', fc1=0.0, fc2=0.5, n=None)`

Default constructor. **filtertype** specifies if the filter is low ('lp'), high ('hp') or band ('bp') pass. The cut-off frequencies for the bandpass case are set in **fc1** and **fc2**. If the **filtertype** is set to 'lp' or 'hp' both cut-off frequencies must be equal. Band-pass filter will be assumed if the frequencies are different, regardless you have specified other type of filter!

The number of different coefficients to be calculated is set with the parameter **n**. Even though it has a default value that is appropriate in the band-pass case, it is strongly recommended not to use the default value in any other case (high-pass or low-pass) [5].

Method: `LanczosFilter.getcoefs(self)`

As in section 10.1 this function returns the coefficients that are being used in the filter.

11 Differential operators: `diffoperators.py`

Some routines to compute differential operators on the sphere specially suited for climate analysis are provided. By now, they only process regular latitude–longitude grids. The operators make the computations by means of centered differences, except at the borders, where they use backward or forward differences. Periodic boundary conditions are supported in the zonal axis. All the operators assume that the input fields are organized according to the COARDS scheme ([latindex, lonindex]), with other dimensions (time, vertical level) prepending the latitude and longitude axis of the arrays.

Class: HGRADIENT

Method: HGRADIENT.__init__(self,lats,lons,asdegrees=1,PBlon=0)

This is the constructor for the horizontal gradient calculator. **lats** is a NumPy array which holds the latitudes corresponding to the grid points, **lons** holds the longitudes of the grid points and if the optional parameter **asdegrees** is set to true, it means that the input angular variables are expressed as degrees, not radians. **PBlon** is true if periodic boundary conditions are to be applied in the longitudinal axis. In this case, second order centered differences are used in the whole zonal domain.

Method: HGRADIENT.hgradient(self,hfield,R=6.37e6)

Given as input the horizontal field **hfield** (Φ), get as a result a tuple which holds the zonal and meridional components of the gradient on the sphere ($\frac{1}{R \cos \varphi} \frac{\partial \Phi}{\partial \lambda}, \frac{1}{R} \frac{\partial \Phi}{\partial \varphi}$). **R** is assigned by default the radius of the Earth.

Class: HDIVERGENCE

Method: HDIVERGENCE.__init__(self,lats,lons,asdegrees=1,PBlon=0)

Default constructor, with parameters defined as for the gradient operator.

Method: HDIVERGENCE.hdivergence(u,v,R=6.37e6)

From the zonal (**u**) and meridional (**v**) components of a vectorial field, find the horizontal divergence $\frac{1}{R \cos \varphi} \left[\frac{\partial u}{\partial \lambda} + \frac{\partial (v \cos \varphi)}{\partial \varphi} \right]$. The function returns a bidimensional array with the divergence field.

Class: VCURL

Method: VCURL.__init__(self,lats,lons,asdegrees=1,PBlon=0)

Default constructor, with parameters defined as for the gradient operator.

Method: VCURL.vcurl(u,v,R=6.37e6)

From the zonal (**u**) and meridional (**v**) components of a vectorial field, find the vertical component of the curl operator on the sphere, $\frac{1}{R \cos \varphi} \left[\frac{\partial v}{\partial \lambda} - \frac{\partial (u \cos \varphi)}{\partial \varphi} \right]$. The function returns a scalar field with the vertical component of the curl of the vectorial field.

12 Multivariate and Univariate Kernel based Probability Density Function Estimation: KPDF . c

Histograms are useful and simple estimators for the Probability Density Function (PDF) associated with physical or modelling experiments. However, the estimation of PDFs by means of histograms presents some drawbacks like the instability to the selection of the bins (bin number and bin origin) or the lack of derivability. Thus, it has been proposed [15] the use of a kernel based approach to the estimation of the PDF. This module provides functions to perform univariate and multivariate PDF estimation. The relevant equations for this module are (2) for univariate density estimation and (3) for multivariate series.

$$f(x) = \frac{1}{nh} \sum_{i=1}^n K \left(\frac{x - X_i}{h} \right), \quad (2)$$

$$f(\mathbf{x}) = \frac{\det S^{-\frac{1}{2}}}{nh^d} \sum_{i=1}^n K \left(h^{-2} (\mathbf{x} - \mathbf{X}_i)^T S^{-1} (\mathbf{x} - \mathbf{X}_i) \right), \quad (3)$$

with n the number of points, h a scalar which holds the bandwidth used in the estimation, X_i and \mathbf{X}_i the experimental points, x and \mathbf{x} the points where the PDF is being estimated, K is the function used as the kernel and S is the scaling matrix which can optionally be used in the multivariate estimators, usually, the covariance matrix.

Function: def UPDFEpanechnikov(edata,gdata,h)

Returns a NumPy array with the PDF associated to the experimental data **edata** evaluated at points **gdata** (NumPy array, too) using a bandwidth **h**. For this and next functions, **edata** and **gdata** must be NumPy arrays and the function returns a NumPy array of typecode Float64. The kernel used in the estimation is a Epanechnikov one. It raises `TypeError` if **edata** or **gdata** is not a 1-D NumPy array It raises `MemoryError` if it is unable to allocate the returned array or some temporal arrays which are needed as working space.

Function: def UPDFBiweight(edata,gdata,h)

Same as the previous function, but use a biweight kernel, instead (S86, Table 3.1). It raises `TypeError` if **edata** or **gdata** is not a 1-D NumPy array It raises `MemoryError` if it is unable to allocate the returned array or some temporal arrays which are internally needed as working space.

Function: def UPDFTriangular(edata,gdata,h)

Same as the previous function, but using a triangular kernel function (see S86, Table 3.1) It raises `TypeError` if **edata** or **gdata** is not a 1-D NumPy array It raises `MemoryError` if it is unable to allocate the returned array or some temporal arrays which are internally needed as working space.

Function: def UPDFOptimumBandwidth(edata)

Get an approximation to the optimum bandwidth by means of equation 3.28 (S86). Unless there is a better suggestion, it can be a good starting point. **edata** is, as previously, a NumPy array (internally works as Float64). It raises `ValueError` if **edata** is not a source sequence.

Function: def MPDFEpanechnikov(edata,gdata,h,Sm1=None,K=0.0)

Given a multidimensional (dimension $p \in [2, 3]$ currently) experimental data set **edata** (NumPy array), evaluate the PDF at each p -dimensional point in the NumPy array **gdata**, using a radially symmetric bandwidth h . The optional parameter **Sm1** is a $p \times p$ matrix (NumPy array, too) which can be used to scale each of the directions in the **edata** and **gdata** arrays. Usually, the inverse of the covariance matrix of **edata** is a good selection for this parameter. It can also be `None`, in which case, no scaling is applied to the directions in the p -dimensional space. **K** is a renormalizing constant which must be computed according to the scaling defined by **Sm1**. If the inverse of the covariance matrix is selected as **Sm1** and the square root of the determinant of the covariance matrix is input as **K**, then, a Fukunaga estimator is being used in the estimation (S86, Eq. 4.7). This function uses a multidimensional Epanechnikov kernel (S86, Eq. 4.4) for the estimation. It raises `ValueError` if **edata** or **gdata** are not NumPy arrays. It raises `TypeError` if **h** is not a number. It raises `ValueError` if the dimensionality of the data sets **edata** and **gdata** is not correct because they exceed the implemented capability, they are not "compatible" (for instance, one is 2-D and the other one 3-D), or the scaling matrix is not of the adequate range ($p \times p$).

Function: def MPDFGaussian(edata,gdata,h, Sm1=None, K=0.0)

Same as MPDFEpanechnikov, but using a Gaussian multivariate kernel (S86, Eq. 4.3). It raises `ValueError` if **edata** or **gdata** are not NumPy arrays. It raises `TypeError` if **h** is not a number. It raises `ValueError` if the dimensionality of the data sets **edata** and **gdata** is not correct because they exceed the implemented capability, they are not "compatible" (for instance, one is 2-D and the other one 3-D), or the scaling matrix is not of the adequate range ($p \times p$).

Function: def MPDFOptimumBandwidth(edata)

Provides a first guess to the optimum bandwidth (S86, Eq. 4.14). It raises `ValueError` if **edata** is not a source sequence or if its dimensions exceed current capabilities.

Function: def MPDF2DGrid2Array(xdata,ydata,fastestdim=0)

This function returns an array of shape $(\text{len}(xdata)*\text{len}(ydata), 2)$ which holds in a linear fashion the grid defined by arrays **xdata** and **ydata**. The optional parameter **fastestdim** allows the selection of the dimension which grows faster (outer one by default) or inner one if it is non zero.

This functionality can be obtained by means of other standard Python techniques, like using complex calls to `replicate()`, `concatenate()` and `map()`, or the new feature of *List comprehension* in Python 2.0. However, this function is much more efficient.

Function: def MPDF3DGrid2Array(xdata,ydata,zdata,fastestdim=0)

This function is similar to `MPDF2DGrd2Array` in the sense that it returns an array shaped like $(\text{len}(xdata)*\text{len}(ydata)*\text{len}(zdata), 3)$ which holds in a linear fashion the grid defined by arrays **xdata**, **ydata** and **zdata**. The optional parameter **fastestdim** allows the selection of the dimension which grows faster (outer one by default) or inner one if it is non zero.

13 Analog search

The module `analog.py` allows to search for analogs in a data array. As usual, the first dimension of the arrays are supposed to run in time, and given a spatial base pattern the module searches the time record of the data most similar to the base pattern. The similitude can be measured in a principal component truncated space or in a canonical correlation one. For details see [8].

Class: EOFANALOG

Method: EOFANALOG.__init__(self, dataset, neofs=None, pccaling=1)

This is the constructor for a PCA-space search. A NumPy array with the library **dataset** (time is first dimension) must be provided. **neofs** is the number of EOFs to retain. This sets the degrees of freedom of the search space. Defaults to the number of EOFs accounting for a 70% of the total variance. The **pccaling** of the EOFs can also be set. 0 means orthonormal EOFs (Mahalanobis distance). 1 means standardized PCs (spherized search space). Defaults to 1.

Method: EOFANALOG.getCoords(self, field)

Returns the coordinates of **field** in the PCA space.

Class: CCAANALOG

Method: CCAANALOG.__init__(self, dataset, theotherdataset, neofs=None, spherized=1)

This is the constructor for a CCA-space search. Again, a NumPy array with the library **dataset** (time is first dimension) must be provided. But, besides, **theotherdataset** has to be passed to the constructor to perform the CCA analysis and obtain predictand related analogs. This is actually the target field to be reconstructed by the analogs. **neofs** is in this case a tuple with the number of EOFs to retain in each field in the PCA prefilter for the CCA. This sets the degrees of freedom of the search space (these are the minimum of this tuple). Defaults to the number of EOFs accounting for a 70% of the total variance in each field. **spherized** is a bit (0 or 1, yes or not) indicating if the search is performed in an spherized space (1) or an inverse correlation scaled one (0). Default: 1

Method: EOFANALOG.getCoords(self, field)

Returns the coordinates of **field** in the CCA space.

Class: ANALOGSelector

Method: ANALOGSelector.__init__(self, ANALOGobj, patterns, smoothing=1, weightexp=2.0, report='')

This is the constructor for an **ANALOGSelector** object. This object is able to select the analogs of a series of base **patterns** in a library which is specified by an **ANALOGobj** created by instantiating an **EOFANALOG** or **CCAANALOG** object. The **smoothing** allows to search more than one analog for each base case and average them weighting with the inverse distance to the base case raised to the **weightexp** power. If a filename is specified in the **report** optional argument, a detailed report of the search is written on that file.

Method: returnAverage(self, field=None)

Returns the simple average reconstructed field (NOT weighted, even though you had specified explicitly a **weightexp**). The optional argument **field** is to reconstruct the analogs in a field different from the library dataset. The first axis dimension must match that of the library dataset.

Method: returnAnalog(self, field=None)

Returns the single analog (**smoothing=1**) reconstructed field. The output is exactly the same as that of the method `returnAverage()` It's just a notation matter. There is no need to use this specific method for the case `smoothing=1` if you are, for instance, into a loop over several smoothing factors.

Method: returnWeightedAverage(self, field=None)

Returns the weighted average reconstructed field. The optional argument **field** is to reconstruct the analogs in a field different from the library dataset. The first axis dimension must match that of the library dataset.

14 Efficient array of numeric histogramas: **NHArray.py**

`NHArray.py` is a python wrapper for a module internally written in C which provides multivariate histograms. The module allows to perform a Monte Carlo test in a point-wise way, returning integrated probabilities from the histograms. It is implemented as a class.

Class: NHArray

Method: NHArray.__init__(self, xl, xu, nbins, elems)

Constructor for the `NHArray` class The lower (**xl**) and upper (**xu**) limits for the histograms must be provided along with the number of bins (**nbins**). Number of histograms to be hold simultaneously has also to be specified through the parameter **elems**.

Method: NHArray.Update(self, field)

Adds a new multidimensional item **field** to the histogram.

Method: NHArray.GetDeltaX(self)

Returns the increment per bin given the lower and upper limits specified and the number of bins.

Method: NHArray.GetRange(self, prob)

Returns the range leaving an area **prob** in each tail of the of the histogram

15 Other links

There are other packages that can be combined with **Python**, **pyclimate**, and the other packages that have been mentioned previously and which allow to easily build

powerful data analysis tools and programs. To name a few, for graphics, for instance, there exists the possibility of using **DISLIN** (<http://www.linmpi.mpg.de/dislin/>), free for some platforms. There is another set of statistical functions by G. Strangman (http://www.nmr.mgh.harvard.edu/Neural_Systems_Group/gary/python.html). A complete repository of **Python** programs can be found at the official WEB server (<http://www.python.org>) or Starship, (<http://starship.python.net>) the server for the community of **Python** contributors and developers.

Special mention deserve two other **Python** packages designed to work with climate data. One of them is CDAT, developed by the Lawrence Livermore National Laboratory (<http://sourceforge.net/projects/cdat>), and the other one is mtaCDF, developed at the Institut für Meereskunde, Kiel (<http://www.ifm.uni-kiel.de/to/sfb460/b3/Products/mtaCDF.html>).

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