



# pyobs Documentation

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## THE OBS CLASS

```
class obs(orig=None, desc='unknown')  
    Class defining an observable
```

### Parameters

- `orig (obs, optional)` – creates a copy of orig
- `desc (str, optional)` – description of the observable

### Examples

```
>>> from pyobs import obs  
>>> a = obs(desc='test')
```

```
add_syst_err(name, err)  
    Add a systematic error to the observable
```

### Parameters

- `name (str)` – label that uniquely identifies the syst. error
- `err (array)` – array with the same dimensions of the observable with the systematic error

### Examples

```
>>> data = [0.198638, 0.403983, 1.215960, 1.607684, 0.199049, ... ]  
>>> vec = pyobs.obs(desc='vector')  
>>> vec.create('A', data, dims=(4,))  
>>> print(vec)  
0.201(13)    0.399(26)    1.199(24)    1.603(47)  
>>> vec.add_syst_err('syst.err', [0.05, 0.05, 0, 0])  
>>> print(vec)  
0.201(52)    0.399(56)    1.199(24)    1.603(47)
```

```
create(ename, data, icnfg=None, rname=None, dims=1, lat=None)  
    Create an observable
```

### Parameters

- `ename (str)` – label of the ensemble
- `data (array, list of arrays)` – the data generated from a single or multiple replica
- `icnfg (array of ints or list of arrays of ints, optional)` – indices of the configurations corresponding to data; if not passed the measurements are assumed to be contiguous

- `rname` (*str or list of str, optional*) – identifier of the replica; if not passed integers from 0 are automatically assigned
- `dims` (*tuple, optional*) – dimensions of the observable, data must be passed accordingly
- `lat` (*list of ints, optional*) – the size of each dimension of the master-field; if passed data is assumed to be obtained from observables measured at different sites and `icnfg` is re-interpreted as the index labeling the sites; if `icnfg` is not passed data is assumed to be contiguous on all sites.

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**Note:** For data and `icnfg` array can mean either a list or a 1-D `numpy.array`. If the observable has already been created, calling `create` again will add a new replica to the same ensemble.

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### Examples

```
>>> data = [0.43, 0.42, ... ] # a scalar observable
>>> a = pyobs.obs(desc='test')
>>> a.create('EnsembleA',data)
```

```
>>> data0 = [0.43,0.42, ... ] # replica 0
>>> data1 = [0.40,0.41, ... ] # replica 1
>>> a = pyobs.obs(desc='test')
>>> a.create('EnsembleA',[data0,data1],rname=['r0','r1'])
```

```
>>> data = [0.43, 0.42, 0.44, ... ]
>>> icnfg= [ 10, 11, 13, ... ]
>>> a = pyobs.obs(desc='test')
>>> a.create('EnsembleA',data,icnfg=icnfg)
```

```
>>> data = [1.0, 2.0, 3.0, 4.0, ... ]
>>> a = pyobs.obs(desc='matrix')
>>> a.create('EnsembleA',data,dims=(2,2))
```

### Examples

```
>>> data = [0.43, 0.42, 0.44, ... ]
>>> lat = [64,32,32,32]
>>> a = pyobs.obs(desc='test-mf')
>>> a.create('EnsembleA',data,lat=lat)
```

```
>>> data = [0.43, 0.42, 0.44, ... ]
>>> idx = [0, 2, 4, 6, ...] # measurements on all even points of time-slice
>>> lat = [32, 32, 32]
>>> a = pyobs.obs(desc='test-mf')
>>> a.create('EnsembleA',data,lat=lat,icnfg=idx)
```

`create_cd(cname, value, covariance)`

Create observables based on covariance matrices

#### Parameters

- `cname` (*str*) – label that uniquely identifies the data set
- `value` (*array*) – central value of the observable; only 1-D arrays are supported
- `covariance` (*array*) – a 2-D covariance matrix; if `covariance` is a 1-D array of same length as `value`, a diagonal covariance matrix is assumed.

## Examples

```
>>> mpi = pyobs.obs(desc='pion masses, charged and neutral')
>>> mpi.create_cd('mpi-pdg18', [139.57061, 134.9770], [0.00023**2, 0.0005**2])
>>> print(mpi)
139.57061(23)    134.97700(50)
```

`error(errinfo={}, plot=False, pfile=None)`

Estimate the error of the observable, by summing in quadrature the systematic errors with the statistical errors computed from all ensembles and master fields.

### Parameters

- `errinfo (dict, optional)` – dictionary containing one instance of the `errinfo` class for each ensemble/master-field. The `errinfo` class provides additional details for the automatic or manual windowing procedure in the Gamma method. If not passed default parameters are assumed.
- `plot (bool, optional)` – if specified a plot is produced, for every element of the observable, and for every ensemble/master-field where the corresponding element has fluctuations. In addition one piechart plot is produced for every element, showing the contributions to the error from the various sources, only if there are multiple sources, ie several ensembles. It is recommended to use the plotting function only for observables with small dimensions.
- `pfile (str, optional)` – if specified all plots produced with the flag `plot` are saved to disk, using `pfile` as base name with an additional suffix.

**Returns** the central value and error of the observable.

**Return type** list of two arrays

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**Note:** By default, the errors are computed with the Gamma method, with the *Stau* parameter equal to 1.5. Additionally the jackknife method can be used by passing the appropriate *errinfo* dictionary with argument *bs* set to a non-zero integer value. For master fields the error is computed using the master-field approach and the automatic windowing procedure requires the additional argument *k* (see main documentation), which by default is zero, but can be specified via the *errinfo* dictionary. Through the *errinfo* dictionary the user can treat every ensemble differently, as explained in the examples below.

---

## Examples

```
>>> obsA = pyobs.obs('obsA')
>>> obsA.create('A', dataA) # create the observable A from ensemble A
>>> [v,e] = obsA.error() # collect central value and error in v,e
>>> einfo = {'A': errinfo(Stau=3.0)} # specify non-standard Stau for ensemble A
>>> [_,e1] = obsA.error(errinfo=einfo)
>>> print(e,e1) # check difference in error estimation
```

```
>>> obsB = pyobs.obs('obsB')
>>> obsB.create('B', dataB) # create the observable B from ensemble B
>>> obsC = obsA * obsB # derived observable with fluctuations from ensembles A,B
>>> einfo = {'A': errinfo(Stau=3.0), 'B': errinfo(W=30)}
>>> [v,e] = obsC.error(errinfo=einfo, plot=True)
```

`error_of_error(errinfo={})`

Returns the error of the error based on the analytic prediction obtained by U. Wolff.

**Parameters** `errinfo (dict, optional)` – see the documentation of the `error` method.

**Returns** the error of the error

**Return type** array

**peek()**

Display a brief summary of the content of the observable, including its memory footprint and requirements (for error computation), its description and ensemble/replica content

### Example

```
>>> obs.peek()
Observable with shape = (1, 4)
- description: vector-test
- size: 82 KB
- mean: [[0.20007161 0.40085252 1.19902686 1.60184989]]
- Ensemble A
  - Replica 0 with mask [0, 1, 2, 3] and ncnfg 500
    temporary additional memory required 0.015 MB
```

**tauint()**

Estimates the integrated autocorrelation time and its error for every ensemble, with the automatic windowing procedure.

## TENSOR MANIPULATIONS

`reshape(x, new_dims)`

Change the shape of the observable

**Parameters**

- `x (obs)` – observables to be reshaped
- `new_dims (tuple)` – the new shape of the observable

**Returns** reshaped observable

**Return type** *obs*

**Notes**

This function acts exclusively on the mean value.

`concatenate(x, y, axis=0)`

Join two arrays along an existing axis

**Parameters**

- `y (x, )` – the two observable to concatenate
- `axis (int, optional)` – the axis along which the observables will be joined.  
Default is 0.

**Returns** the concatenated observable

**Return type** *obs*

**Notes**

If *x* and *y* contain information from separate ensembles, they are merged accordingly by keeping only the minimal amount of data in memory.

`transpose(x, axes=None)`

Transpose a tensor along specific axes. For an array *a* with two axes, gives the matrix transpose.

**Parameters**

- `x (obs)` – input observable
- `axes (tuple or list of ints, optional)` – If specified, it must be a tuple or list which contains a permutation of [0,1,...,N-1] where N is the number of axes of *x*. For more details read the documentation of *numpy.transpose*

**Returns** the transposed observable

**Return type** *obs*

`sort(x, axis=-1)`

Sort a tensor along a specific axis.

**Parameters**

- `x (obs)` – input observable
- `axis (int, optional)` – the axis which is sorted. Default is -1, the
- `axis. (last)` –

**Returns** the sorted observable

**Return type** *obs*

`diag(x)`

Extract the diagonal of 2-D array or construct a diagonal matrix from a 1-D array

**Parameters** `x (obs)` – input observable

**Returns** the diagonally projected or extended observable

**Return type** *obs*

## UNARY OPERATIONS

`sum(x, axis=None)`

Sum of array elements over a given axis.

### Parameters

- `x (obs)` – array with elements to sum
- `axis (None or int or tuple of ints, optional)` – Axis or axes along which a sum is performed. The default, `axis=None`, will sum all elements of the input array.

**Returns** sum along the axis

**Return type** *obs*

### Examples

```
>>> import pyobs
>>> pyobs.sum(a)
>>> pyobs.sum(a,axis=0)
```

`trace(x, offset=0, axis1=0, axis2=1)`

Return the sum along diagonals of the array.

### Parameters

- `x (obs)` – observable whose diagonal elements are taken
- `offset (int, optional)` – offset of the diagonal from the main diagonal; can be both positive and negative. Defaults to 0.
- `axis2 (axis1,)` – axes to be used as the first and second axis of the 2-D sub-arrays whose diagonals are taken; defaults are the first two axes of *x*.

**Returns** the sum of the diagonal elements

**Return type** *obs*

### Notes

If *x* is 2-D, the sum along its diagonal with the given offset is returned, i.e., the sum of elements *x*[*i*,*i*+*offset*] for all *i*. If *x* has more than two dimensions, then the axes specified by *axis1* and *axis2* are used to determine the 2-D sub-arrays whose traces are returned. The shape of the resulting array is the same as that of *x* with *axis1* and *axis2* removed.



### Examples

```
>>> tr = pyobs.trace(mat)
```

$\log(x)$

Return the Natural logarithm element-wise.

**Parameters**  $x$  (obs) – input observable

**Returns** the logarithm of the input observable, element-wise.

**Return type** *obs*

### Examples

```
>>> logA = pyobs.log(obsA)
```

$\exp(x)$

Return the exponential element-wise.

**Parameters**  $x$  (obs) – input observable

**Returns** the exponential of the input observable, element-wise.

**Return type** *obs*

### Examples

```
>>> expA = pyobs.exp(obsA)
```

$\cosh(x)$

Return the Hyperbolic cosine element-wise.

**Parameters**  $x$  (obs) – input observable

**Returns** the hyperbolic cosine of the input observable, element-wise.

**Return type** *obs*

### Examples

```
>>> B = pyobs.cosh(obsA)
```

$\sinh(x)$

Return the Hyperbolic sine element-wise.

**Parameters**  $x$  (obs) – input observable

**Returns** the hyperbolic sine of the input observable, element-wise.

**Return type** *obs*

### Examples

```
>>> B = pyobs.sinh(obsA)
```

`arccosh(x)`

Return the inverse Hyperbolic cosine element-wise.

**Parameters** *x* (*obs*) – input observable

**Returns** the inverse hyperbolic cosine of the input observable, element-wise.

**Return type** *obs*

### Examples

```
>>> B = pyobs.arccosh(obsA)
```

`besselk(v, x)`

Modified Bessel function of the second kind of real order *v*, element-wise.

**Parameters**

- *v* (*float*) – order of the Bessel function
- *x* (*obs*) – real observable where to evaluate the Bessel function

**Returns** the modified bessel function computed for the input observable

**Return type** *obs*

## LINEAR ALGEBRA ROUTINES

`eig(x)`

Computes the eigenvalues and eigenvectors of a square matrix observable. The central values are computed using the *numpy.linalg.eig* routine.

**Parameters** `x (obs)` – a symmetric square matrix (observable) with dimensions  $N \times N$

**Returns** a vector observable with the eigenvalues and a matrix observable whose columns correspond to the eigenvectors

**Return type** list of obs

### Notes

The error on the eigenvectors is based on the assumption that the input matrix is symmetric. If this not respected, the returned eigenvectors will have under or over-estimated errors.

### Examples

```
>>> [w,v] = pyobs.linalg.eig(mat)
>>> for i in range(N):
>>>     # check eigenvalue equation
>>>     print(mat @ v[:,i] - v[:,i] * w[i])
```

`eigLR(x)`

Computes the eigenvalues and the left and right eigenvectors of a square matrix observable. The central values are computed using the *numpy.linalg.eig* routine.

**Parameters** `x (obs)` – a square matrix (observable) with dimensions  $N \times N$ ;

**Returns** a vector observable with the eigenvalues and two matrix observables whose columns correspond to the right and left eigenvectors respectively.

**Return type** list of obs

### Notes

This input matrix is not expected to be symmetric. If it is the usage of *eig* is recommended for better performance.

## Examples

```
>>> [l,v,w] = pyobs.linalg.eigLR(mat)
>>> for i in range(N):
>>>     # check eigenvalue equation
>>>     print(mat @ v[:,i] - v[:,i] * l[i])
>>>     print(w[:,i] @ mat - w[:,i] * l[i])
```

`inv(x)`

Compute the inverse of a square matrix

**Parameters** `x (obs)` – Matrix to be inverted

**Returns** (Multiplicative) inverse of `x`

**Return type** `obs`

## Examples

```
>>> from pyobs.linalg import inv
>>> a = pyobs.obs()
>>> a.create('A',data,dims=(2,2))
>>> ainv = pyobs.inv(a)
```

## Notes

If the number of dimensions is bigger than 2, `x` is treated as a stack of matrices residing in the last two indexes and broadcast accordingly.

`matrix_power(x, a)`

Raises a square symmetric matrix to any non-integer power `a`.

**Parameters**

- `x (obs)` – a symmetric square matrix (observable) with dimensions  $N \times N$
- `a (float)` – the power

**Returns** the matrix raised to the power `a`

**Return type** `obs`

## Notes

The calculation is based on the eigenvalue decomposition of the matrix.

## Examples

```
>>> matsq = pyobs.linalg.matrix_power(mat, 2) # identical to mat @ mat
>>> matsqrt = pyobs.linalg.matrix_power(mat, -0.5)
>>> matsqrt @ mat @ matsqrt # return the identity
```

## THE MFIT CLASS

```
class mfit(x, W, f, df, v='x')
```

Class to perform fits to multiple observables, via the minimization of the  $\chi^2$  function

$$\chi^2 = r^T W r \quad , \quad r_i = y_i - \phi(\{p\}, \{x_i\})$$

with  $\phi$  the model function,  $p_\alpha$  the model parameters ( $\alpha = 1, \dots, N_\alpha$ ) and  $x_i^\mu$  the kinematic coordinates ( $i = 1, \dots, N$  corresponds to the  $i$ -th kinematical point, and  $\mu$  labels the dimensions). The matrix  $W$  defines the metric of the  $\chi^2$  function.

The ideal choice for the matrix  $W$  is the inverse of the covariance matrix, which defines a correlated fit. Instead a more practical choice for cases where a reliable estimate of covariances is not available, is given by the inverse of the diagonal part of the covariance matrix, which instead defines an uncorrelated fit.

### Parameters

- **x** (*array*) – array with the values of the x-axis; 2-D arrays are accepted and the second dimension is interpreted with the index  $\mu$
- **W** (*array*) – 2-D array with the matrix  $W$ ; if a 1-D array is passed, the program interprets it as the inverse of the diagonal entries of the covariance matrix
- **f** (*function*) – callable function or lambda function defining  $\phi$ ; the program assumes  $x_i^\mu$  correspond to the first arguments
- **df** (*function*) – callable function or lambda function returning an array that contains the gradient of  $\phi$ , namely  $\partial\phi(\{p\}, \{x_i\})/\partial p_\alpha$
- **v** (*str, optional*) – a string with the list of variables used in  $f$  as the kinematic coordinates. Default value corresponds to  $x$ , which implies that  $f$  must be defined using  $x$  as first and unique kinematic variable.

### Notes

Once created the class must be called with at least one argument given by the observables corresponding to the data points  $y_i$ . See examples below.

### Examples

```
>>> xax=[1,2,3,4]
>>> f=lambda x,p0,p1: p0 + p1*x
>>> df=lambda x,p0,p1: [1, x]
>>> [y,dy] = yobs1.error()
>>> W=1./dy**2
>>> fit1 = mfit(xax,W,f,df)
>>> pars = fit1(yobs1)
>>> print(pars)
0.925(35)    2.050(19)
```

`eval(xax, pars)`

Evaluates the function on a list of coordinates using the parameters obtained from a  $\chi^2$  minimization.

#### Parameters

- `xax` (*array, list of arrays*) – the coordinates  $x_i^\mu$  where the function must be evaluated. For combined fits, a list of arrays must be passed, one for each fit.
- `pars` (*obs*) – the observable returned by calling this class

#### Returns

**observables corresponding to the functions evaluated** at the coordinates *xax*.

**Return type** *obs*, list of obs

#### Examples

```
>>> fit1 = mfit(xax,W,f,df)
>>> pars = fit1(yobs1)
>>> print(pars)
0.925(35)    2.050(19)
>>> xax = numpy.arange(0,10,0.2)
>>> yeval = fit1.eval(xax, pars)
```

`pars()`

Prints the list of parameters

## 5.1 Additional functionalities

`diff(f, x, dx)`

Utility function to compute the gradient and hessian of a function using symbolic calculus

#### Parameters

- `f` (*string*) – the reference function
- `x` (*string*) – variables that are not differentiated; different variables must be separated by a comma
- `dx` (*string*) – variables that are differentiated; different variables must be separated by a comma

**Returns** (scalar) function *f* lambda : (vector) function of the gradient of *f* lambda : (matrix) function of the hessian of *f*

**Return type** lambda

## Notes

The symbolic manipulation is based on the library *sympy* and the user must follow the *sympy* syntax when passing the argument *f*. The analytic form of the gradient and hessian is automatically printed.

## Examples

```
>>> res = diff('a+b*x','x','a,b') # differentiate wrt to a and b
a + b*x
[1, x]
[[0, 0], [0, 0]]
>>> for i in range(3):
>>>     print(res[i](0.4,1.,2.))
1.8
[1, 0.4]
[[0, 0], [0, 0]]
```

## INDICES AND TABLES

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## PYTHON MODULE INDEX

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