

RichValues

– Python Library –

User Guide

Andrés Megías Toledano
Centre for Astrobiology (CAB), Madrid

Version 1.2
February 2023

Index

1. Introduction	3
2. Installation	3
3. Formatting style for representing rich values	4
4. Creation of rich values	4
4.1. Individual rich values	4
4.1.1. Function rich_value	5
4.1.2. Class RichValue	5
4.1.3. Operations with rich values	8
4.2. Arrays of rich values	10
4.2.1. NumPy arrays	10
4.2.2. Function rich_array	10
4.2.3. Class RichArray	11
4.2.4. Operations with arrays of rich values	13
4.3. Tables of rich values	15
4.3.1. Pandas dataframes	15
4.3.2. Function rich_dataframe	15
4.3.3. Class RichDataFrame	16
4.3.4. Operations with rich tables of rich values	17
5. Importing and exporting of rich values	18
5.1. Importing	18
5.2. Exporting	18
6. Plotting rich values	19
7. Making fits with rich values	20
8. Changing the default parameters	24

9. Mathematical basis of operations with rich values	26
9.1. Centered values	26
9.1.1. Normal distribution	27
9.1.2. Bounded normal distribution	27
9.1.3. Mirrored lognormal distribution	28
9.2. Upper/lower limits and finite intervals	28
9.3. Summary	29
10. Additional useful functions	29
10.1. Rounding numbers	29
10.2. Creating distributions	31
10.3. Evaluating distributions	32
Citation of the library	33
Useful links	33
Credits	34
License	34

1. Introduction

The library RichValues is a Python 3 library whose purpose is to manage numeric values with uncertainties and upper/lower limits, which we will call *rich values*.¹ With it, one can easily import rich values written in plain text documents in an easily readable format, operate with them propagating the uncertainties automatically, and export them in the same formatting style as the import. It also supports finite intervals of values.

For example, to represent the value $(6.3 \pm 0.4) \cdot 10^3$, we could write `6.3 +/- 0.4 e3`, and for the upper limit $< 1.2 \cdot 10^5$ we could write `< 1.2 e5`. Then these text strings would be parsed as Python objects containing all the necessary information to describe the rich value, and they will be displayed in the screen in the same formatting style. The main way to do so is to write the text string between simple quotation marks and write it inside the function `rich_value`; for example, `rich_value('6.3 +/- 0.4 e3')`. Then, we could make arithmetic operations between them and other rich values or even usual numbers, like addition, subtraction, multiplication, and division.

2. Installation

RichValues works in Python 3. It requires the libraries NumPy, Pandas, SciPy and Matplotlib. This library is published in GitHub:

<https://github.com/andresmegias/richvalues> .

In order to install it, you can use the Python Package Installer (PyPI), running from the terminal the following command:

```
pip3 install richvalues .
```

You can also use the Conda package installer, running instead the following command:

```
conda install richvalues -c richvalues .
```

Alternatively, you can install the library manually in your computer. To do so, you have to download the file `richvalues.py` and copy it to one of the Python system paths. To display the list of all these paths, you can run Python (for example, from the terminal, writing `python3`), and run the two following commands:

```
import sys
sys.path
```

For example, for MacOS, if you did not install Conda one of these paths would be:

```
/Users/<user>/Library/Python/<3.x>/lib/python/site-packages ,
```

with `<user>` being your username and `<3.x>` your exact Python version.

Now, RichValues can be used in a Python script like any other library, with the name `richvalues`. Therefore, to import it you would write:

```
import richvalues .
```

1. Like *rich text* for text with information about the font type, size, weight, etc.

You can also use an abbreviation for the library name, like `rv`:

```
import richvalues as rv .
```

In the following examples of code, we will consider that we already imported `RichValues` with this abbreviation. We will also use the abbreviations `np` and `pd` for the libraries `NumPy` and `Pandas`, respectively.

3. Formatting style for representing rich values

The `RichValues` library uses a specific formatting style to represent the different kinds of rich values with plain text. This is the way in which they are displayed in the screen and in which they can be imported and exported. It can also be used to create rich values within a script. Below are the rules for this formatting style:

- If the value has no uncertainty, just put the number.
- If it has uncertainty, you can join the central value and the uncertainty with `+/-` or `+-`, using blank spaces if you want; for example: `5.2 +/- 0.4`.
- If it has a lower and an upper uncertainty, you should write the lower uncertainty just after the central value preceded by `-`, and then write the upper uncertainty preceded by `+`, using blank spaces if you want; for example: `5.2 -0.3+0.4`.
- If you want to use scientific notation (exponential notation with decimal base), for the central value and the uncertainty (or uncertainties), you just have to write an `e`, separated by a blank space from the numbers and followed by the exponent argument; for example: `5.2 -0.3+0.4 e-3`.
- If you want to specify an upper or lower limit, just write `<` or `>` before the value (without uncertainty), putting a blank space if you want; for example: `< 5.2 e2`.
- If you want to specify the domain of the value, that is, the minimum and maximum values that the magnitude corresponding to this value could take, you have to write it between brackets, using the text `inf` to represent infinity; for example: `5.2 -0.3+0.4 e3 [0,inf]`. By default (that is, if it is not specified), the domain is all the real numbers, that is: `[-inf,inf]`.
- If you wanted to specify a finite interval of values, you should write the edges of the interval separated by two hyphens (`--`), without uncertainties; for example: `9 e3 -- 62 e3`.

4. Creation of rich values

With the library `RichValues`, we can create individual rich values and use them in tuples, lists, dictionaries, etc., but we can also create arrays –based on `NumPy` arrays– and tables –based on `Pandas` dataframes.

4.1. Individual rich values

There are mainly two ways to create a single rich value: with the function `rich_value` and with the class `RichValue`, being the first one the easiest way.

4.1.1. Function `rich_value`

It can also be called with the shortened name `rval`. Below are the arguments of this function, although the first one is the only required:

- **text.** Text string representing the rich value, using the formatting style explained in section 3.
- **domain.** List containing the edges of the domain of the rich value, that is, the minimum and maximum values that the magnitude corresponding to this array could take. By default, it is the domain showed in the input text string, but if it is not specified it will be $(-\infty, \infty)$.²

The default values for these arguments, and for most of the arguments of the following functions, can be modified as explained in section 7.

Below is a simple example of how we would create two different rich values:³

```
x = rv.rich_value('5.2 +/- 0.3')
y = rv.rich_value('2.1 -0.4+0.5')
```

In this way, we have created a Python object of class `RichValue`. These objects will be displayed on screen with the previous formatting style except for the domain, which will be hidden. For example:

```
[in]    rv.rich_value('0.327 -0.12+0.18 [-1,1]')
[out]   0.33-0.12+0.18
```

Instead of doing this, we could have defined our rich value directly with the class `RichValue`.

4.1.2. Class `RichValue`

This is the main class of the library. The other classes and most of the functions are built around it.

Arguments

Below are the arguments of this Python class, being the first one the only required one:

- **main.** Main value of the rich value, that is, central value or value of the upper/lower limit.
- **unc.** Uncertainty associated with the central value. If two values are given, they would be the lower and upper uncertainties, respectively. By default it is 0.
- **is_lolim.** Logical variable that determines if the rich value is a lower limit. By default it is False.
- **is_uplim.** Logical variable that determines if the rich value is an upper limit. By default it is False.
- **is_range.** Logical variable that determines if the rich value is actually a constant range of values.⁴ By default it is False.

2. The NumPy object `inf` is used to represent infinity.

3. Using the shortened name, of the function, we could create a rich value as: `x = rv.rval('5.2 +/- 0.3')`.

4. This can be specified instead with the argument `center`, putting the edges of the interval as a list.

- **domain.** List containing the edges of the domain of all the entries of the rich array, that is, the minimum and maximum values that the magnitude corresponding to this array could take. By default, it is `[-np.inf, np.inf]`.⁵

As an example, below is a code to create the same rich values as in the examples of the previous section:

```
x = rv.RichValue(5.2, 0.3)
y = rv.RichValue(2.1, [0.4,0.5], domain=[0,np.inf])
z = rv.RichValue(0.327, [0.12,0.18], domain=[-1,1])
```

Instance variables

All of the arguments of the `RichValue` class correspond to instance variables with the same name.⁶ To access to them, you should write a dot after the name of the rich value Python variable and then the name of the instance variable. For example, to access to the instance variable `main` of a certain rich value `x`, you would write `x.main`. You can modify these variables if you want to modify the rich value. Additionally, there are other two instance variables for this class:

- **num_sf.** Number of significant figures to use for displaying the elements of the rich array, taking into account the uncertainties. By default it is the number of scientific figures used in the rich value represented by the input text string.⁷
- **min_exp.** Minimum exponent in absolute value to be used for displaying the rich value in scientific notation. By default it is 4.

These two instance variables determine how the rich value is displayed on screen, and also how it will be exported into a plain text file. You can also tweak an additional visualization option changing the value of the default parameter `limit` for extra significant figure (see section 8).

Methods

The `RichValue` class have several methods.⁸ Some of them just provide additional information on the rich value but others are more complex and can be used to modify the rich value. Below is the list of all of them with their arguments between brackets:

- **is_lim(self).** Logical variable that is `True` if the rich value is an upper/lower limit.
- **is_interv(self).** Logical variable that is `True` if the rich value is a finite interval of values or an upper/lower limit. It is the opposite as the result of `is_centr(self)`.
- **is_centr(self).** Logical variable that is `True` if the rich value is a centered value, with a central value and uncertainties. It is the opposite as the result of `is_interv(self)`.
- **center(self).** If the rich value is a centered value, it returns the main value (that is, the central value); if not, it returns `NaN` (`np.nan`).⁵ This can be useful when using Mat-

5. Assuming that the library NumPy was imported with the abbreviation `np` (`import numpy as np`).

6. An instance variable is a variable contained by an object of a certain class.

7. If there is no uncertainty, the number will be showed with an additional significant figure.

8. A method is a function that can be called within an object of a certain class.

plotlib's function `errorbar`.⁹

- **unc_eb**(self). Uncertainties of the rich value as a list with shape (2, 1), so that it can be easily used with Matplotlib's function `errorbar`.⁹
- **rel_unc**(self).¹⁰ Relative uncertainties of the rich value.
- **signal_noise**(self).¹¹ Signal-to-noise ratios (S/N) of the rich value, which are the inverses of the relative uncertainties.
- **ampl**(self). Distances between the central value and the bounds of the domain, which we call *amplitudes*.
- **rel_ampl**(self). Distances between the central value and the bounds of the domain divided by the uncertainties (*relative amplitudes*). They are a measure of the normality of the PDF associated with the rich value.
- **prop_factor**(self). It returns the minimum value of the signal-to-noise ratios and the relative amplitudes of the rich value. This value will be used to determine the use or not of a fast approximation to calculate the uncertainty propagation when applying a function to the rich value, in case that the normality is high enough.
- **interval**(self, sigmas). If the rich value is a central value with uncertainties, it returns the interval defined by the central values plus and minus sigma times the corresponding uncertainties (by default, sigmas = 3.0). If the rich value is a constant interval of values or an upper/lower limit, it returns the interval of values that defines the rich value (which can include infinity as one of the edges).
- **latex**(self, dollars, mult_symbol). It returns a text string of a LaTeX code representing the rich value, using `mult_symbol` as the multiplication symbol in scientific notation (by default, `mult_symbol = \\cdot`).¹² The logical variable `dollars`, which is True by default, determines if the text string is enclosed with dollar symbols (\$) or not.
- **set_lims_factor**(self, factor). If the rich value is an upper/lower limit, the uncertainty instance variable (`unc`) will be replaced as the central value divided by the factor (by default, `factor = 4.0`). This can be useful when plotting upper/lower limits with the function `errorbar` from the library Matplotlib.
- **pdf**(self, x). It applies the probability density function (PDF) associated with the rich value to the given array `x`, returning the resulting array.
- **sample**(self, N). It returns a sample of size `N` of the distribution associated with the rich value, whose corresponding PDF can be explored with the previous method, `pdf`. By default, `N` is equal to the 10 000.

9. You can instead use the function `errorbar` within this library (see section 6).

10. The arguments `self` means that the method has to be called within an object of this class, but it is not actually written when calling the method; for example: if `x` is a rich value, to call the method `rel_unc` we should write `x.rel_unc()`.

11. The arguments `self` means that the method has to be called within an object of this class, but it is not actually written when calling the method; for example: if `x` is a rich value, to call the method `rel_unc` we should write `x.rel_unc()`.

12. In Python, two backslashes are needed in order to display just one in a text string.

- **function**(self, function, **kwargs). It applies the given function (function) to the rich value. Additional arguments can be passed (kwargs), which are the arguments of the function function with_rich_values (see next section).

The last methods allows to apply a function to the rich value and therefore to obtain a new one. Next section explains how to make operations with rich values.

4.1.3. Operations with rich values

The RichValue class has special methods for the basic arithmetic operations: addition, subtraction, multiplication, division, and power. Therefore, you can just use the arithmetic operators (+, -, *, /, **) to combine a rich value with another rich value or with a usual number. The uncertainties will be propagated automatically, and the condition of an upper/lower limit (or even a finite interval) will be taken into account to obtain the final result. For example:

```
[in]    x = rv.rich_value('5.2 +/- 0.3')
[in]    y = rv.rich_value('2.1 -0.4+0.5')
[in]    x + y
[out]   7.3-0.5+0.6

[in]    x = rv.rich_value('< 5.2 [0,inf]')
[in]    x + 3
[out]   3.0 -- 8.2

[in]    x = rv.rich_value('5.2 +/- 0.3')
[in]    x**2
[out]   27+/-3
```

At this point, there is one thing that must be taken into account. Every rich value variable present in a mathematical expression will be treated by Python as an independent variable, even if there is one variable repeated in the expression. Therefore, in that case you may not get the desired result. For example, $x \times x$ is not equal to x^2 , as in the first case Python will treat each x as independent from the other x . In any case, if the relative uncertainties are small, the differences will be mainly in the uncertainties. For example:

```
[in]    x = rv.rich_value('5.20 +/- 0.30')
[in]    print(x*x, x**2)
[out]   27.0-2.1+2.3  27+/-3

[in]    x = rv.rich_value('3.60 +/- 0.40')
[in]    print(x+x, 2*x)
[out]   7.2+/-0.6  7.2+/-0.8
```

In case you cannot simplify your expression so that it only contains each variable once, you can use the function `function_with_rich_values`, where you can also write the mathematical expression you want to compute, and this time each repeated variable will be treated as it. Also, if you want to apply more than two or three operations and the uncertainties are relatively high, it will be faster and more precise to use `function_with_rich_values`.

Function `function_with_rich_values`

Using this function one can compute any expression involving rich values. It can also be

called with the shortened name function. Below is the full list of its arguments, although only the two first ones are mandatory:

- **function.** Python function to be applied to the given rich values. If its expression is short, it can be defined within the list of arguments using a lambda function.¹³ The output of the given Python function can be a single value or several ones.
- **args.** List with the input rich values, in the same order as the arguments of the given function.
- **unc_function.** Python function used to approximate the uncertainties in case that analytic uncertainty propagation can be applied. The arguments should be the central values first and then the uncertainties, with the same order as in the input function.¹⁴ If it is not specified, the analytic uncertainty propagation will never be used.
- **is_vectorizable.** Logical variable that states if the given Python function is vectorizable, that is, if it can be applied to NumPy arrays. If so, computation time will decrease considerably. By default it is False.
- **len_samples.** Size of the samples of the arguments that will be drawn for calculating the final distribution applying the input function. The default is the square root of the number of arguments times the default sample size (10 000).
- **domain.** Domain of the result. If the given function returns several outputs, it can be a list of the domains of the different outputs. If this variable is not specified, the domain of the output (or domains) will be estimated automatically.
- **sigmas.** Threshold to use approximate uncertainty propagation. The value is the minimum of the signal-to-noise ratios and the distances to the bounds of the domain relative to the uncertainties. By default it is 20.0.
- **consider_ranges.** Logical variable that determines if the final distribution can be interpreted as a constant range of values; if not, it will be treated as a rich value with a central value and uncertainties. By default it is True.
- **use_sigma_combs.** Logical variable that determines if the calculation of the uncertainties is optimized when approximate uncertainty propagation can be performed but there is no uncertainty function provided. It performs combinations of the central value plus and minus the uncertainties for every argument and applies the function, taking the minimum and maximum of the resulting values as bounds to compute the uncertainties. By default it is False, as it is not fully tested for more than one argument.
- **lims_fraction.** In case the resulting value is an upper/lower limit, this factor is used to calculate the limit. It can take values from 0 to 1, and the closest it is to 1, the closest the resulting limit will be to the function applied to the central/limit value of the argu-

13. A lambda function is defined in the following way: first you write lambda followed by a blank space; now, you write the arguments of the function with any desired letter and separated by commas, ending with a colon, and followed optionally by a blank space; finally, you write the mathematical expression of the function using the same letters you used before. For example: `lambda a,b: a+b`.

14. For example: `lambda a,b,da,db: da+db`.

ments. By default it is 0.1.

- **num_reps_lims.** Number of repetitions of the sampling done in the cases of having an upper/lower limit for better estimating its value. By default it is 4. Greater values are recommended if `lims_fraction` is greater than 0.1.

Let's see a short example of the use of this function.

```
[in] x = rv.rich_value('5.2 +/- 0.3')
[in] y = rv.rich_value('2.1 -0.4+0.5')
[in] rv.function_with_rich_values(lambda a,b: a+b, [x,y])
[out] 7.3-0.5+0.6
```

That would be it.¹⁵ As you can see, the basic use of this function is quite simple. If the given function has to return several outputs, the code would be very similar.

```
[in] rv.function_with_rich_values(lambda a,b: (a+b,a-b), [x,y])
[out] (7.3-0.5+0.6, 3.1-0.6+0.5)
```

4.2. Arrays of rich values

There are three ways to create arrays of rich values within this library: using just NumPy arrays containing rich values, using the function `rich_array`, or using directly the class `RichArray`. We will call these arrays *rich arrays*.

4.2.1. NumPy arrays

Using the functions from the library NumPy (like the function `array`), one can create arrays whose elements are rich values (of class `RichValue`). Below is a simple example of a creation of an array of rich values using the NumPy function `array` and the two ways of creating rich values mentioned in section 2.1.¹⁶

```
import numpy as np
u = np.array([rv.rich_value('1.21 +/- 0.14'), rv.rich_value('< 4')])
u = np.array([rv.RichValue(1.21, 0.14), rv.RichValue(4, is_uplim=True)])
```

With this method, we do not need any additional functions or classes more than those of NumPy. However, we recommend using one of the two other ways of creating arrays of rich values, as they are simpler and more flexible.

4.2.2. Function `rich_array`

It can also be called with the shortened name `rarray`. Below are the arguments of this function, although the first one is the only required:

- **array.** It should be a list, an array or similar. The elements of the input argument can be either a rich value (of class `RichValue`) or a text string representing a rich value, that is, with the formatting style explained in section 3.
- **domain.** List containing the edges of the domain to be set to the entries of the rich array, that is, the minimum and maximum values that the magnitude corresponding to

15. Using the shortened name of the function, the third line would be: `rv.function(lambda a,b: a+b, [x,y])`.

16. For the rest of code examples, we will assume that we imported NumPy as `np` (`import numpy as np`).

this array could take. By default, the domain of each entry of the rich value will be preserved.

For example, the creation of the same array as in the previous example would be:¹⁷

```
u = rv.rich_array(['1.21 +/- 0.14', '< 4'])
```

In this way, we create an object of class `RichArray`, which is basically the NumPy class `ndarray` with some additional features. Alternatively, we could have created the rich value directly using the class `RichArray`.

4.2.3. Class `RichArray`

This class is inherited from the class `ndarray` from NumPy. An object of this class is basically a NumPy array but with some additional instance variables and methods. It is useful when you already have an array with the central values of a certain variable and another array with the corresponding uncertainties.

Arguments

Below are the arguments of this Python class, being the first element the only required:

- **mains**. Array of central values.
- **uncs**. Array of lower and upper uncertainties associated with the central values. By default, it is an array of 0 values.
- **are_lolims**. Array of logical variables that indicate if each central value is actually a lower limit. By default, it is an array of False values.
- **are_uplims**. Array of logical variables that indicate if each central value is actually an upper limit. By default, it is an array of False values.
- **are_ranges**. Array of logical variables that indicate if each central value is actually a finite interval or an upper/lower limit. By default, it is an array of False values.

Additionally, you can specify the arguments `domain`, `num_sf`, `min_exp`, `len_sample`, and `allow_log_scale`, to set these `RichValue` properties to all the elements of the rich array.

As an example, below is a code to create the same rich array as in the previous section:

```
u = rv.RichArray([1.21,4], [0.14,0], are_uplims=[False,True])
```

Instance variables

The `RichArray` class does not have any instance variable. Instead, you can use some of the methods to access to some of the properties of the entries of the rich array.

Methods

The `RichArray` class have several proper methods. Some of them just provide additional information on the rich array but others are more complex and can be used to modify it. Below is the list of all of them with their arguments between brackets:

- **mains**(self). Central values of the elements of the rich array.
- **uncs**(self). Uncertainties of each element of the rich array.

17. With the shortened name of the function, it would be: `u = rv.rarray(['1.21 +/- 0.14', '< 4'])`.

- **are_lolims**(self). Array of logical variables that describe if each element of the rich array is a lower limit.
- **are_uplims**(self). Array of logical variables that describe if each element of the rich array is an upper limit.
- **are_ranges**(self). Array of logical variables that describe if each element of the rich array is a constant range of values.
- **are_intervs**(self). Array of logical variables that describe if each element of the rich array is a constant range of values or an upper/lower limit.
- **rel_uncs**(self). Relative uncertainties of each element of the rich array.
- **signals_noises**(self). Signal-to-noise ratios (SN) for each element of the rich array.
- **ampls**(self). Distances between the central value and the bounds of the domain (which we call *amplitudes*), for each element of the rich array.
- **rel_ampls**(self). Distances between the central value and the bounds of the domain divided by the uncertainties, for each element of the rich array (*relative uncertainties*).
- **prop_factors**(self). Array with the result of the RichValue method `normality(self)` for each entry of the rich array; by default, `sigmas = 3.0`.
- **intervals**(self, sigmas). Array with the result of the RichValue method `interval(self, sigmas)` for each entry of the rich array; by default, `sigmas = 3.0`.
- **latex**(self, dollars, mult_symbol). Array of text strings of a LaTeX code representing each entry of the rich array, using `mult_symbol` as the multiplication symbol in scientific notation (by default, `mult_symbol = \\cdot`). The logical variable `dollars`, which is True by default, determines if the text string is enclosed with dollar symbols (\$) or not.
- **set_params**(self, params). It modifies the parameters of the entries of the rich array specified in the `params` variable (`domain`, `num_sf` or `min_exp`), which must be a dictionary containing entries with the name of each variable to be set and the corresponding desired values.
- **set_lims_factor**(self, factor). For each element of the rich array, if the rich value is an upper/lower limit, the uncertainty instance variable (`unc`) will be defined as the central value divided by the factor (by default, `factor = 4.0`). If two values are provided in the variable `factor`, the first one will be user for lower limits and the second one for upper limits. This can be useful when plotting upper/lower limits with Matplotlib's function `errorbar`.
- **sample**(self, len_sample). For each entry of the rich array, it returns a sample of size `len_sample` of the distribution associated with the corresponding rich value. By default, `len_sample` is 10 000.
- **function**(self, function, **kwargs). It applies the given function (`function`) to every element of the rich array. Additional arguments can be passed (`**kwargs`), which are the arguments of the function `function` with `rich_arrays` (see next section).

The last method allows to apply a function to the rich array and therefore to obtain a new one. See next section for more details on making operations with rich arrays.

There is one important thing that must be taken into account regarding the inherited methods from NumPy arrays. When using an inherited method which is not exclusive from the RichArray class, the resulting object may loose all the instance variables and methods proper of the RichArray class, depending on the method. In this case you should convert the resulting array to a rich array using the function `rich_array`. This is not necessary for slicing nor for the methods `transpose`, `reshape`, `flatten`, and `ravel`.

4.2.4. Operations with arrays of rich values

The RichArray class has special methods for the basic arithmetic operations: addition, subtraction, multiplication, division, and power. Therefore, you can just use the arithmetic operators (+, -, *, /, **) to combine a rich array with another rich array, another rich value or a usual number. The uncertainties will be propagated automatically, and the condition of an upper/lower limit (or even a finite interval) will be taken into account to obtain the final result. For example:

```
[in]    u = rv.rich_array(['1.2 +/- 0.4', '5.8 +/-0.9'])
[in]    v = rv.rich_array(['8 +/- 3', '< 21'])
[in]    u * v
[out]   RichArray([10+/-5, < 150], dtype=object)

[in]    u = rv.rich_array(['1.2 +/- 0.4', '5.8 +/-0.9'])
[in]    u + rich_value(2.0 +/- 0.3)
[out]   RichArray([3.2+/-0.5, 7.8+/-0.9], dtype=object)
```

If instead of working with objects of class RichArray you work with NumPy arrays (class ndarray) whose elements are rich values (class RichValue), you can perform this kind of operations as well, as the class RichValue also have methods for them, as explained in section 2.1.3.

However, similar to what happens with the class RichValue, if in the mathematical expression one rich array appears more than once, it will not be treated as the same variable appearing twice but as two independent variables. Therefore, for those cases, you should use the function `function_with_rich_arrays`, which is like `function_with_rich_values` but for rich arrays. If instead of obtaining a rich array as an output you would like to obtain just one rich value, you can use `function_with_rich_values` with the elements of the input rich arrays as arguments. Additionally, there is another function that you can use to apply a custom mean to a rich array, called `rich_fmean`. This three ways are explained below.

Function `function_with_rich_arrays`

Using this function one can compute any expression involving rich arrays, which can be element by element or not. This function can also be called with the shortened name `array_function`. Its arguments are the same as `function_with_rich_values` plus an additional argument, `elementwise`. Below are the most important ones:

- **function.** Python function to be applied to the given rich arrays. If the function is not

to be applied element-wise, the given Python function can return several numeric values. Therefore, the output itself can be a new array. However, the output could not be consisted of several arrays.

- **args.** List with the input rich arrays, in the same order as the arguments of the given function.
- **len_samples.** Size of the samples of the elements of the arguments that will be drawn for calculating the final distribution applying the input function. The default is the square root of the number of arguments times the default sample size (10 000).
- **elementwise.** Logical variable that states if the given Python function has to be applied element-wise for each of the elements of the input rich arrays.

Let's see some examples of the use of this function.

```
[in]    u = rv.rich_array(['1.2 +/- 0.4', '5.8 +/-0.9'])
[in]    v = rv.rich_array(['8 +/- 3', '< 21'])
[in]    rv.function_with_rich_arrays(lambda a,b: a*b, [u,v])
[out]   RichArray([9-4+5, < 150], dtype=object)
```

That would be it. In this case, the product of two NumPy arrays is defined element-wise, so it is not necessary to specify that the given function has to be applied element by element. The usage for a function which is not element-wise, like the scalar product, would be the same.

```
[in]    rv.function_with_rich_arrays(np.dot, [u,v])
[out]   < 160
```

Finally, we can also apply a function that returns a new array as an output, like the cross product.

```
[in]    u = rv.rich_array(['3.0 +/- 0.4', '2.1 +/- 0.3', '0.0 +/-0.3'])
[in]    v = rv.rich_array(['6.4 +/- 0.8', '-3.6 +/- 0.4', '0.0 +/-0.2'])
[in]    rv.function_with_rich_arrays(np.cross, [u,v])
[out]   RichArray([0-1.2+1.1, 0+/-2.0, -24+/-3], dtype=object)
```

Function rich_fmean

This function applies a generalized quasi-arithmetic mean (or f -mean) along all the elements of the input array, which can be a rich array.¹⁸ To use it, you have to specify the function to be used for the mean and its inverse. Below is the list of its arguments:

- **array.** Input array to apply the mean.
- **function.** Function that defines the mean. By default, it is the identity (which corresponds to the arithmetic mean).
- **inverse_function.** Inverse of the function that defines the mean. By default, it is the identity (which corresponds to the arithmetic mean).
- **weights.** Weights to be applied to the values of the input array. By default, they are equal weights.

18. If f is a function with an inverse function f^{-1} , $\{x_i\}$ is a set of input numbers, and w_i are a set of weights for the input numbers, the generalized f -mean of $\{x_i\}$ is: $\langle x \rangle = f^{-1}\left(\frac{1}{\sum_i w_i} \sum_i w_i f(x_i)\right)$.

- **weight_function.** Function to be applied to the weights before normalization. By default, it is the identity (no operation is applied).

Besides these arguments, you can write more arguments of the function `function_with_rich_arrays` (or, equivalently, of `function_with_rich_values`).

Let's see an example of the use of this function for calculating the arithmetic mean.

```
[in]    u = rv.rich_array(['1.2 +/- 0.4', '5.8 +/-0.9'])
[in]    rv.rich_fmean(u)
[out]   3.5+/-0.5
```

And now, the same example but with the geometric mean.

```
[in]    u = rv.rich_array(['1.2 +/- 0.4', '5.8 +/-0.9'],
domain=[0,np.inf])
[in]    rv.rich_fmean(u, function=np.log, inverse_function=np.exp)
[out]   2.6+/-0.5
```

4.3. Tables of rich values

With this library one can also create tables of rich values, that is, groups of rich values labeled with a column name and an index. This is done using Pandas dataframes, so we will call this objects *rich dataframes*. There are three ways of creating this kind of object: with Pandas dataframes, with the function `rich_dataframe`, and with the class `RichDataFrame`.

4.3.1. Pandas dataframes

Using the library Pandas, one can create dataframes whose elements are rich values (of class `RichValue`). Below is a simple example of a creation of a dataframe of rich values using the Pandas class `DataFrame`.¹⁹

```
import pandas as pd
arr = rv.rich_array([[ '2.1+/-0.3', '3.4+/-0.4', '<4'], [ '5', '<6', '8+/-1']])
df = pd.DataFrame(arr, columns=['a','b','c'])
```

We could have created the dataframe from a Python dictionary as well.²⁰

```
dic = {'a': rich_array(['2.1+/-0.3', '5']),
      'b': rich_array(['3.4+/-0.4', '<6']),
      'c': rich_array(['<4', '8+/-1'])}
df = pd.DataFrame(dic)
```

With this method, we do not need any additional functions or classes more than those of Pandas. However, we recommend using one of the two other ways of creating dataframes of rich values, as they are simpler and are more flexible.

4.3.2. Function `rich_dataframe`

It can also be called with the shortened name `rich_df`. Below are the arguments of this func-

19. For the rest of code examples, we will assume that we imported Pandas as `pd` (`import pandas as pd`).

20. A Python dictionary is an object than includes several variables identified by a keyword. To create one, you have to write the pair of keywords and variables (name of the keyword, a colon, and the variable) separated by commas, and all of this enclosed by keys; for example: `d = {'a': 1, 'b': 2}`.

tion, although the first one is the only required:

- **df.** It should be a dataframe, whose elements can be either a rich value (of class RichValue) or a text string representing a rich value, that is, with the formatting style explained in section 2.1.1.
- **domains.** Dictionary containing, for each column, the domain of its elements, that is, the minimum and maximum values that the magnitude corresponding to each column could take. By default, for each column, it will be the value for the first entry if it is a rich value, and if not, the original domain of each rich value will be preserved.

As an example, below is a code to create a simple dataframe from either an array-like list or a dictionary, as in the previous section.

```
arr = [['2.1+/-0.3', '3.4+/-0.4', '<4'], ['5', '<6', '8+/-1']]
df = rv.rich_dataframe(arr, columns=['a', 'b', 'c'])
dic = {'a': ['2.1+/-0.3', '5'], 'b': ['3.4+/-0.4', '<6'], 'c': ['<4', '8+/-1']}
df = rv.rich_dataframe(dic)
```

As you can see, this method is easier and faster than the one of the previous section. Also, if any element of the input list/array/dictionary for creating the dataframe is a non-numeric text string, it will be preserved to the final rich dataframe. In this way, we create an object of class RichDataFrame, which is basically the Pandas class DataFrame with some additional features. Alternatively, we could have created the rich dataframe using the class RichDataFrame, although it is always easier and more practical to use the function rich_dataframe.

4.3.3. Class RichDataFrame

This class is inherited from the class DataFrame from Pandas. An object of this class is basically a Pandas dataframe but with some additional methods.

Argument

The only argument required for this class is a dataframe containing rich values. It cannot have entries with text strings representing rich values; in that case, the function rich_dataframe should be applied to the input dataframe before calling the class RichDataFrame.

Methods

The RichDataFrame class has all the DataFrame methods that allow to modify its values, and also has some additional methods exclusive of the RichDataFrame class. Below is the list of all of these additional methods:

- **get_params(self).** It returns a dictionary of dictionaries, each of them containing the value of each of the RichValue parameters (domain, num_sf or min_exp) used for each column of the dataframe.
- **set_params(self, params).** It modifies the parameters of each entry of the specified parameters in the params variable, containing entries with the name of the variables to be modified (domain, num_sf and min_exp). The value of each entry must be another dictionary containing one entry for each column of the dataframe that will be modified,

with the corresponding desired value.

- **latex**(self, return_df, row_sep, dollars, mult_symbol). If return_df = True, it returns a dataframe of text strings of a LaTeX code representing each entry of the original dataframe, using mult_symbol as the multiplication symbol in scientific notation (by default, mult_symbol = `\\cdot`). Instead, if return_df = False (by default), it returns a text strings in LaTeX formatting style representing the content of a table, using row_sep as the text that indicates the end of a row (by default, row_sep = `\\tabularnewline`). The logical variable dollars, which is True by default, determines if the text string is enclosed with dollar symbols (\$) or not.
- **set_lims_factor**(self, limits_factors). For each element of each column of the dataframe, if the rich value is an upper/lower limit, the uncertainty instance variable (unc) will be replaced as the central value divided by the factor specified for each column by the variable limits_factors (by default, it is 4.0 for every column). If two values are provided in the variable for a certain column, the first one will be user for lower limits and the second one for upper limits. This can be useful when plotting upper/lower limits with Matplotlib's function errorbar.
- **new_column**(self, function, columns, **kwargs). It returns a new column of type rich array obtained applying the given function (function) to the specified columns (columns) of the dataframe. The rest of the arguments (**kwargs) are the same as in function_with_rich_values.
- **new_row**(self, function, rows, **kwargs). It returns a new row obtained applying the given function (function) to the specified rows (rows) of the dataframe. The rest of the arguments (**kwargs) are the same as in function_with_rich_values.

The last method allows to apply a function to the rich dataframe and obtain a new column or row, which can then be added to the dataframe.

4.3.4. Operations with rich tables of rich values

The class RichDataFrame has special methods for the basic arithmetic operations: addition, subtraction, multiplication, division, and power. Therefore, you can just use the arithmetic operators (+, -, *, /, **) to combine a rich dataframe with another rich dataframe, another rich value or a usual number. The uncertainties will be propagated automatically, and the condition of an upper/lower limit (or even a finite interval) will be taken into account to obtain the final result. Note that this will only work if all the entries of the dataframe are numeric.

Similar to what happens with the classes RichValue and RichArray, if in the mathematical expression one rich dataframe variable appears more than once, it will not be treated as the same variable appearing twice but as two independent variables. Therefore, for those cases, you should use the methods create_column and create_rows. These methods are also useful if you want to make operations with the data within the dataframe.

Below is an example of how to create a new column in a dataframe combining its columns with the method create_column.

```
dic = {'a': ['6.4+/-0.5','8'], 'b': ['3.4+/-0.4','<6'], 'c': ['4','8+/-1']}
df = rv.rich_dataframe(dic, domain=[0,np.inf])
new_column = df.create_column(lambda a,b,c: a/b+c, ['a','b','c'])
df['d'] = new_column
```

5. Importing and exporting of rich values

The importing and exporting of rich values is very simple.

5.1. Importing

For the importing from a plain text file, you can write text strings representing rich values, with the formatting style explained in section 2.1.1. Then, any function that can import text strings will be fine, like NumPy's `loadtxt` or Pandas' `read_csv`. For example, below is a simple table from a file in `.csv` that could be imported into a rich dataframe.

Source \ Molecule	HCCCN	CH3CN
L1517B	5.16+/-0.03 e13	2.1+/-0.3 e11
L1498	1.6+/-0.3 e13	< 8.3 e10
L1544	1.0+/-0.3 e14	1.5+/-0.2 e11
B1-a	4.2+/-1.2 e12	4.9+/-1.1 e11
B1-c	4.2+/-3.4 e12	3.5+/-0.6 e11
SVS 4-5	1.1+/-0.3 e13	5.2+/-0.9 e11
GM Aur	1.9-0.4+0.4 e13	2.1-0.1+0.2 e12
As 209	2.9-0.5+0.5 e13	1.7-0.2+0.2 e12
HD 163296	7.3-1.9+2.5 e13	2.3-0.2+0.2 e12
MWC 480	7.8-2.7+3.9 e13	3.5-0.2+0.2 e12
# (units: /cm2)		
46P	< 0.003	0.017+/-0.001
67P	0.0004	0.0059
# (units: % /H2O)		

It contains the abundances of two molecules (HCCCN and CH₃CN) in different astronomical objects. Assuming that the file is named `table.csv`, we could import the data as:

```
df = pd.read_csv(table.csv, index_col=0, comment='#')
df = rv.rich_dataframe(df, domain=[0,np.inf])
```

As the abundances can only be positive, we specified a domain of `[0, np.inf]`; alternatively, we could have specified the domain in the first entry of each numeric column, as the function `rich_dataframe` will take, for each column, the domain of the first rich value as the domain of the whole column; that is, we should have written `5.16+/-0.03 e13 [0,inf]` and `2.1+/-0.3 e13 [0,inf]` as the first value of the columns labeled as HCCCN and CH₃CN, respectively. The result of the importing will be a rich dataframe whose indexes are the first original column of the table in the `.csv` file, and with two columns with numeric values named HCCCN and CH₃CN.

5.2. Exporting

For the exporting of a variable containing rich values to a plain text file, you can use any function that can export text strings, like NumPy's `savetxt` or Pandas' `to_csv` (which is a

method for the class DataFrame). For example, below is a code for adding a new column to the example table of the previous section as the ratio between the two numeric columns, and exporting it to a .csv file.

```
df['ratio'] = df['HCCCN'] / df['CH3CN']
df.to_csv(table-ratio.csv)
```

And the resulting file would look like the table below.

Source \ Molecule	HCCCN	CH3CN	ratio
L1517B	5.16+/-0.03 e13	2.1+/-0.3 e11	240-30+40
L1498	1.6+/-0.3 e13	< 8 e10	> 100
L1544	1.0+/-0.3 e14	1.50+/-0.20 e11	670-210+230
B1-a	4.2+/-1.2 e12	4.9+/-1.1 e11	8-3+4
B1-c	4+/-3 e12	3.5+/-0.6 e11	12-9+11
SVS 4-5	1.1+/-0.3 e13	5.2+/-0.9 e11	21-6+8
GM Aur	1.9+/-0.4 e13	2.10-0.10+0.20 e12	8.9-1.9+2.0
As 209	2.9+/-0.5 e13	1.70+/-0.20 e12	17-3+4
HD 163296	7.3-1.9+2.5 e13	2.30+/-0.20 e12	32-8+11
MWC 480	8-3+4 e13	3.50+/-0.20 e12	22-8+11
46P	< 3 e-3	1.70+/-0.10 e-2	< 0.21
67P	4.0 e-4	5.9 e-3	0.068

We lost the comments (starting with #) of the original table, but we could actually have added it adding to the dataframe a row with the comment as the index and an empty string ('') as the value for each column. Or, alternatively, we could just add the comments directly to the resulting .csv file.

6. Plotting rich values

In order to easily plot arrays or lists of rich values, this library offers the function `errorbar`, which is basically an implementation of Matplotlib's `errorbar` function.

Function `errorbar`

It accepts arrays of rich values (which can be rich arrays or not) as inputs, as well as all the keyword arguments of Matplotlib's same-name function. Here are the specific arguments of this function:

- **x.** Array of rich values that will be plotted on the horizontal axis.
- **y.** Array of rich values that will be plotted on the vertical axis.
- **lims_factor.** List containing the two factors that define the sizes of the arrows for displaying the upper and lower limits, respectively (the bigger the factor, the smaller the arrow will be). It can be just one value, that will be used for both limits. This is an optional argument; by default the factors will be calculated automatically.

The rest of the arguments are the keyword arguments for Matplotlib's `errorbar` function.²¹ As an output, it returns the same object as in Matplotlib: an `ErrorbarContainer` object. Therefore, additional functions like `xlabel`, `xlim`, `title`, etc, can be used to tweak the appearance of the plot; and working with axes objects is also supported.

21. See Matplotlib's documentation: https://matplotlib.org/stable/api/_as_gen/matplotlib.pyplot.errorbar.html.

Values with a central value and uncertainties will be plotted as points with error bars; upper/lower limits will be plotted as a point (the limit value) and an arrow; and constant ranges of values will be plotted as just an error bar with no point. By default, the color of the points will be gray, and the color of the error bars and arrows will be black.

Let's see a quick example of how to use this function. Consider the following table containing two columns of rich values (split in two halves for a better visualization):

x	y	x	y
< 16	7 +/- 4	19.0 +/- 1.1	49 +/- 3
1.6 +/- 0.5	16 +/- 4	21.1 +/- 0.8	53 +/- 5
2.0 +/- 1.2	11.7 +/- 2.5	21.1 +/- 0.9	52 +/- 4
4.5 +/- 0.8	22 +/- 5	21.4 +/- 0.8	50 +/- 4
8.6 +/- 0.9	29 +/- 5	21.9 +/- 1.3	49 +/- 3
8.8 +/- 0.7	29.8 +/- 2.2	23.9 +/- 1.1	< 100
9.4 +/- 1.3	30 +/- 3	29.8 +/- 0.9	72 +/- 4
12.0 +/- 0.4	32.3 +/- 2.4	31.1 +/- 0.8	71.2 +/- 2.4
13.2 +/- 0.6	38 +/- 3	33.9 +/- 1.1	84 +/- 3
13.3 +/- 1.0	37 +/- 4	35.0 +/- 0.7	84 +/- 3
13.6 +/- 0.3	41 +/- 4	35.1 +/- 0.9	76 +/- 5
14.9 +/- 0.8	43 +/- 4	38.4 +/- 0.9	96 +/- 3
16.1 +/- 0.8	45 +/- 3	39.2 +/- 1.0	79 +/- 4
16.4 +/- 0.9	43.3 +/- 2.1	39.4 +/- 1.1	86 +/- 4
17.2 +/- 0.4	47 +/- 4	42.5 +/- 1.1	60 -- 105

Supposing that this table is stored in a .csv file named table.csv, we could import it with Panda's read_csv function, and then just plot both columns with errorbar.

```
import pandas as pd
import matplotlib.pyplot as plt
df = pd.read_csv('table.csv')
df = rv.rich_dataframe(df)
plt.figure(1, figsize=(7,4))
rv.errorbar(df['x'], df['y'])
plt.xlim(left=0)
```

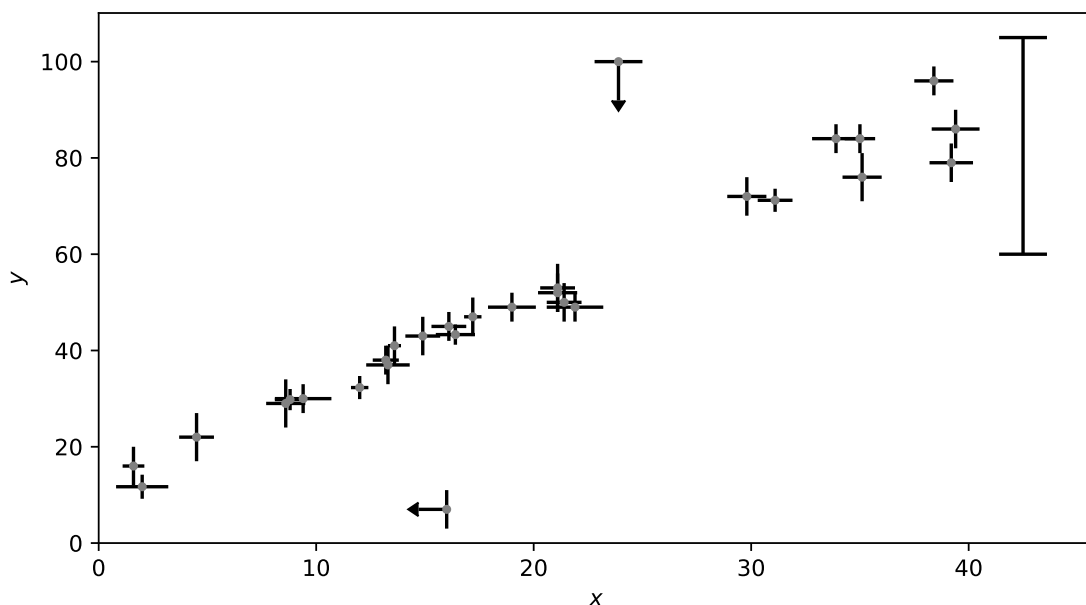


Figure 1. Plot of the example data shown in the table above using the function errorbar.

```
plt.ylim(bottom=0)
plt.xlabel('$x$')
plt.ylabel('$y$')
plt.tight_layout()
```

7. Making fits with rich values

Performing a fit of a set of rich values to a given model can be easily done with some functions included in this library: `point_fit` and `curve_fit`.

They rely on SciPy's function `minimize`, which will minimize a loss (error) function between several samples of the input rich values and the predictions given by the model function; by default, the loss function will be the mean squared error (MSE).

In order to take into account for the status of rich value of the input (presence of uncertainties, upper/lower limits, and/or constant range of values), and also to obtain the fitted parameters as rich values (obtaining a central value and uncertainties in most cases), the optimization process would be repeated in several iterations. In each one, one value will be sampled for each input rich value and the fit will be performed with these values. Therefore, the result would be a distribution of values for each parameter of the model function, which will be represented with a rich value for each of them.

Function `point_fit`

It makes a fit of an input set of rich values, \vec{y} , with respect to a given function, $f(\vec{\theta})$, that depends on a certain set of parameters, $\vec{\theta}$, and that makes a prediction of the input rich values, $\vec{y}' = f(\vec{\theta})$.²²

Below are the arguments of this function:

- **y.** Set of rich values that will be used to fit the model function. It can be a list or array of rich values or a rich array itself.
- **function.** Python function whose parameters will be optimized with respect to the given rich values. If it returns more than one output, the number of outputs must match the number of input points.
- **guess.** List containing a starting value for each of the parameters of the given function ($\vec{\theta}$). These values will be used to start the optimization process.
- **num_samples.** Number of different samples of the input rich values that will be drawn. It will be the number of times that the fit will be performed to obtain a distribution of values for each parameter. By default, it is 3000.
- **loss.** Python function that defines the error between a sample of a rich value and a numeric prediction of it. The function to be minimized will be the mean error between the samples of the input rich values and the predictions of the model function. By default, it is the squared error, so when applied to the whole set of points it is the mean squared error (MSE).

22. Both the input rich values, \vec{y} , and the model parameters, $\vec{\theta}$, can have just one element. However, to obtain a unique solution the number of parameters should be less or equal than the number of input rich values.

- **lim_loss_factor.** Factor to enlarge the loss if the rich value is not a centered value and the prediction falls outside the interval of possible values of the rich value. By default it is 4.

Besides, additional keyword arguments from SciPy's function `minimize` can be specified.

The output of the function will be a Python dictionary containing the results of the optimization process. Its entries are the following:

- **parameters.** List containing the fitted parameters ($\vec{\theta}$) as rich values.
- **samples.** Array containing the samples of the fitted parameters used to compute the rich values.
- **loss.** Array containing the loss corresponding of each group of fitted parameters in the `samples` entry.
- **fails.** Number of times that the fit failed, for the iterations among the different samples (the total number of iterations is equal to `num_samples`).

Let's see a quick example of how to use this function. Consider the following set of rich values: $(5.8 \pm 0.6, 2.2 \pm 0.4, 0.43 \pm 0.08)$. Now suppose that we know that these three values can be modeled with the function $f(a,b) = (a^2 + b, a^2 - b, 2b/a^2)$. We need to make a first guess of the parameters, which, by trial and error, could be something like $a = 2.0, b = 1.2$.²³ Then, the fitting would be quite simple.

```
[in] y = rv.rich_array(['5.4 +/- 0.6', '2.6 +/-0.4', '0.83 +/- 0.08'])
[in] function = lambda a,b: (a**2 + b, a**2 - b, 2*b / a**2)
[in] result = rv.point_fit(y, function, guess=[2.0,1.2])
[in] result['parameters']
[out] [2.00+/-0.09, 1.4+/-0.3]
```

The optimization should take just a few seconds.

Function `curve_fit`

It makes a fit of two arrays of rich values, \vec{x} and \vec{y} , treating the second one as dependent of the first, and given a function that converts the independent variable into the dependent one. That is, it performs a fit of \vec{y} over \vec{x} with respect to a model function $f(x, \vec{\theta})$, that depends on the dependent variable, x , and a certain set of parameters, $\vec{\theta}$, and that applied to a sample of the input array \vec{x} returns an array \vec{y}' , which are the predictions of the input array \vec{y} .²⁴

In order to compute the loss, only the rich values of \vec{x} that are not intervals (that is, they have a central value and uncertainties, even if they are zero) are sampled to then make the predictions of \vec{y} . Then, the loss between a sample of \vec{y} and its predictions, \vec{y}' , is computed. Finally, it is checked that the rich values of \vec{x} that are actually intervals are consistent with the current model.

Below are the arguments of this function:

23. Actually, in this simple case we can derive an analytical solution for the parameters, but that will not be the case in general.

24. Both the input rich values, \vec{y} , and the model parameters, $\vec{\theta}$, can have just one element. However, to obtain a unique solution the number of parameters should be less or equal than the number of input rich values.

- **x**. Input array of rich values corresponding to the independent variable.
- **y**. Input array of rich values corresponding to the dependent variable.
- **function**. Python function whose parameters will be optimized with respect to the given rich values. Its first argument has to be the independent variable (x), and then the parameters of the model ($\vec{\theta}$).
- **guess**. List containing an starting value for each of the parameters of the given function ($\vec{\theta}$). These values will be used to start the optimization process.
- **num_samples**. Number of different samples of the input rich values that will be drawn. It will be the number of times that the fit will be performed to obtain a distribution of values for each parameter. By default, it is 3000.
- **loss**. Python function that defines the error between a rich value and a prediction of it. The function to be minimized will be the mean error between the input rich values and the predictions of the model function. By default, it is the squared error (as explained at the beginning of the section).
- **lim_loss_factor**. Factor to enlarge the loss if the rich value is not a centered value and the prediction falls outside the interval of possible values of the rich value. By default it is 4.

Besides, additional keyword arguments from SciPy's function `minimize` can be specified.

The output of the function will be a Python dictionary containing the results of the optimization process, like with the function `point_fit`. Its entries are the following:

- **parameters**. List containing the fitted parameters ($\vec{\theta}$) as rich values.
- **samples**. Array containing the samples of the fitted parameters used to compute the rich values.
- **loss**. Array containing the loss corresponding of each group of fitted parameters in the samples entry.
- **fails**. Number of times that the fit failed, for the iterations among the different samples (the total number of iterations is equal to `num_samples`).

Now, let's see an example of the use of this function. Consider the same data than in figure 1 (section 6). It seems that the data follow a linear trend. Therefore, a linear function could be used to model it: $f(x; m, b) = m \cdot x + b$, with m being the slope and b the offset. We will use the values $(m, b) = (2.0, 10.0)$ as a first guess done by eye. Again, we suppose that the input data are stored in a file named `table.csv`.

```
[in] import pandas as pd
[in] df = pd.read_csv('table.csv')
[in] df = rv.rich_dataframe(df)
[in] function = lambda x,m,b: m*x + b
[in] result = rv.curve_fit(df['x'], df['y'], function, guess=[2.,10.])
[in] result['parameters']
[out] [1.94+/-0.07, 12.0+/-1.5]
```

The optimization process should take a few moments, less than a minute in any case. Using

the samples entry from the output dictionary, we can plot a sample of the fitted models and also the median model (that is, the one with the median slope and median offset), as in figure 2. The code to obtain such a plot can be seen in the example script `linearfit.py`, in the examples folder of the GitHub repository.²⁵

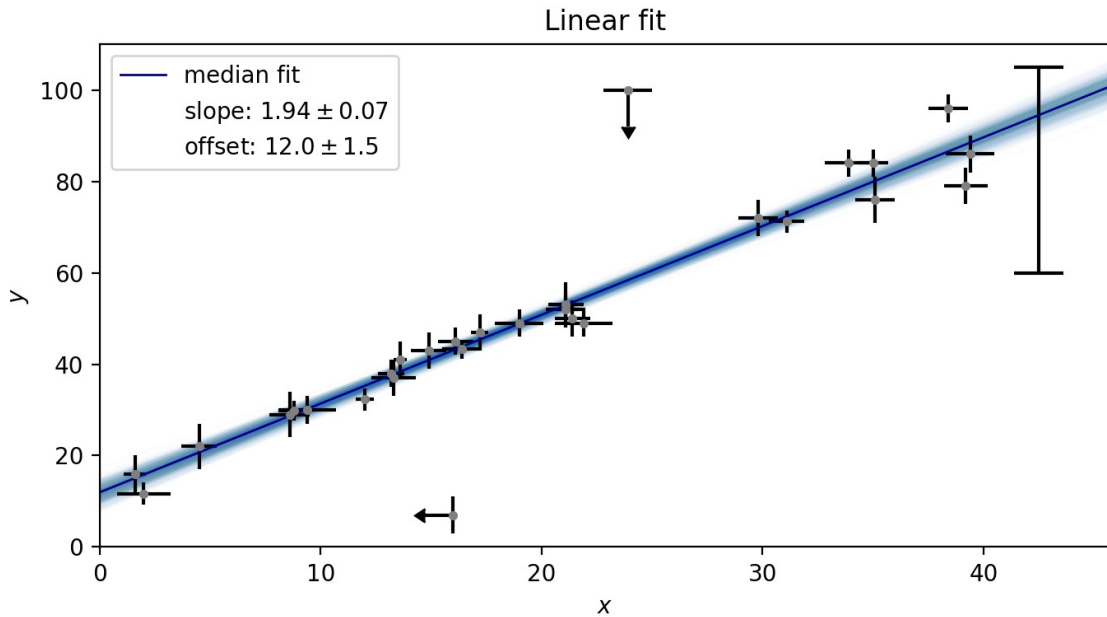


Figure 1. Plot of the example data shown in the table from section 6 (figure 1) and the linear fit performed in the code above. To see the exact code to display the fit, see footnote 29.

8. Changing the default parameters

Most of the default parameters of the functions and classes of this library can be modified through the variable `defaultparams`. This is a Python dictionary containing the values of the default variables with a specific name. Below is a list with all the parameter names, the corresponding variable names used in the library and their description:

- **domain.** Domain of the rich values, that is, the minimum and maximum values that the variables associated with the rich values can take. By default it is all the real numbers, that is, `[-np.inf, np.inf]`.
- **size of samples.** Size of the sample of the distribution associated with the rich value used to estimate the uncertainty propagation (usually `len_samples`). By default it is 10^4 , that is, 10000.
- **number of significant figures.** Number of significant figures to display the rich values (usually `num_sf`).²⁶ By default it is 1.
- **minimum exponent for scientific notation.** Minimum exponent used to display the number in scientific notation (usually `min_exp`). By default it is 4.
- **limit for extra significant figure.** If the significand/mantissa²⁷ of the uncertainty of the rich value (if it is a centered value) or its main value (if it is an upper/lower limit, or

25. <https://github.com/andresmegias/richvalues>.

26. If there is no uncertainty, the number will be showed with an additional significant figure.

27. The number multiplying the decimal power.

an edge of an interval) is lower than this limit number, the rich value will be displayed with an additional significant figure. By default it is 2.5, and it is called `lim_for_extra_sf` in some functions. If you want that limit to be excluded from the extra significant figure, you can define this variable as your limit minus a tiny number; for example: `2.5 - 1e-15`.

- **sigmas to define upper/lower limits.** If a rich value with a central value and uncertainties has one bound of its 1σ interval which surpasses one of the domain edges, the rich value will be reconsidered as an upper/lower limit. Then, the main value will be the original central value minus/plus this parameter times the lower/upper uncertainty.
- **sigmas to use approximate uncertainty propagation.** This value defines when to apply the analytic approximation for uncertainty propagation in the operations with rich values. If the minimum value of the set of the signal-to-noise ratios plus the relative amplitudes is greater than this value, the approximation will be applied instead of creating samples from the distributions associated with the rich values, hence reducing the computation time. By default it is 20.0, and it is called `sigmas` in some functions.
- **use 1-sigma combinations to approximate uncertainty propagation.** Logical variable (usually called `use_sigma_combs`) that determines if the propagation of uncertainties is approximated with the use of the corresponding function applied to the central value plus and minus its uncertainties. By default it is `False`.
- **fraction of the central value for upper/lower limits.** Variable used in `function_with_rich_values` with the name `lims_fraction`. In case the rich value resulting of applying the corresponding function is an upper/lower limit, this factor is used to calculate the limit. It can take values from 0 to 1, and the closest it is to 1, the closest the resulting limit will be to the function applied to the central/limit value of the arguments. By default it is 0.1.
- **number of repetitions to estimate upper/lower limits.** Variable used in `function_with_rich_values` with the name `num_reps`. It is the number of repetitions of the sampling done in the cases of having an upper/lower limit for better estimating its value. By default it is 4. Greater values are recommended if fraction of the central value for upper/lower limits is greater than 0.1.
- **decimal exponent to define zero.** When performing operations and creating samples from distributions, any number lower in absolute value than the decimal power of this value will be considered as 0. By default it is -90.0.
- **decimal exponent to define infinity.** When performing operations and creating samples from distributions, any number lower in absolute value than the decimal power of this value will be considered as ∞ . By default it is 90.0.
- **multiplication symbol for scientific notation in LaTeX.** Symbol to be used when displaying a value in scientific notation in LaTeX mathematical mode for the multiplication of the significand/mantissa and the decimal power. By default it is `\cdot`.²⁸

28. In Python, two backslashes are needed in order to display just one in a text string.

Therefore, for changing any of the default parameters, we have to modify the corresponding entry of the dictionary `defaultparams`. For example:

```
defaultparams['limit for extra significant figure'] = 2.0
```

9. Mathematical basis of operations with rich values

Here is explained the algorithm used to make the operations between rich values, that is, to apply a certain function f to a group of rich values. Let's consider a group of n rich values x_i , which can be a value with a central value μ_i and lower and upper uncertainties $(\sigma_{i1}, \sigma_{i2})$, an upper/lower limit, or even a finite interval. Each rich value has a probability density function (PDF) associated with it, depending on the properties of the rich value.

As each rich value has a PDF, for each of them we can draw a sample of a large number of values (which we choose to be $m \approx 10^4 n$), obtaining a set of n distributions $\{x_i\}$; or, grouped different, we have m groups of n values, each group containing a specific value of each variable x_i . Then, we can apply the function f to each of the m groups of values, obtaining a new distribution of values, $\{f(\{x_i\})\}$. Lastly, we have to determine if the distribution is localized around a certain value, in which case it would represent a rich value with a central value and lower and upper uncertainties, of it is more sparse, in which case it would be an upper/lower limit or a finite interval.

In the following subsections we will see the different PDFs used for each kind of rich value. As for the exact algorithm of detecting the type of rich value that corresponds to the final distribution, it is not explained, but it can be inspected in the source code of the function `evaluate_distr`.

9.1. Centered values

Let's consider a group of n variables x_i , with central values μ_i and uncertainties σ_i . This means that the probability density function (PDF) of the variable x_i is centered around μ_i with a width of the order of σ_i , so that the 1σ confidence interval (which includes 68.27 % of the distribution) is $(\mu_i - \sigma_i, \mu_i + \sigma_i)$. We define the left and right amplitudes, a_1 and a_2 , as the distances between the limits of the domain and the median, that is, $a_j = |b_j - \mu|$ for $j = 1, 2$. Now, as these amplitudes can be different, we will split our desired PDF in two halves, one for $x < \mu$ and other for $x \geq \mu$. Then, we will use an amplitude a as a reference, which must be greater than the uncertainty, $a > \sigma$.

To propagate the uncertainties through a function f applied to the variables $\{x_i\}$, we can draw a sample of a large number of values ($\approx 10^4 n$) of each variable x_i , apply the function to each of the elements of the samples, and then obtain a central value and an uncertainty for the resulting distribution. To do so, we need two things: an appropriate PDF for converting each variable x_i to a distribution of values, and a proper method to obtain a central value and an uncertainty from the resulting distribution. For the last task, we can use the mean or the median as the central value,²⁹ and the 1σ confidence interval (68.27 %) to obtain the lower

29. We prefer to use the median, as it is more robust to outliers.

and upper uncertainty (with respect to the central value). As for the PDF, it will depend of the domain of the variable.

We will define our PDFs for the case of a variable x with a central value μ and an uncertainty σ , building the final PDF with two halves with amplitude $a = a_j$, $j = 1, 2$. In case we had lower and upper uncertainties, σ_1 and σ_2 , we should just replace σ by σ_1 for the left half of the PDF and by σ_2 for the right half. This construction of the final PDF by two halves creates a discontinuity in the median, which is noticeable if any of the two relative amplitudes (a_j / σ_j) is relatively small (high uncertainty) and both of them are considerably different. Ideally, this discontinuity should not appear; however, as long as we do not have a PDF that can directly accept the parameters $(\mu, \sigma_1, \sigma_2, a_1, a_2)$, this procedure can be considered a good approximation.

9.1.1. Normal distribution

If the domain of the variable x is $(-\infty, \infty)$, a proper function is the well-known gaussian function:

$$f(x) = \frac{1}{\tau^{1/2} \sigma} \exp\left(-\frac{1}{2} \left(\frac{x - \mu}{\sigma}\right)^2\right),$$

with $\tau \equiv 2\pi$.³⁰ This would lead to a normal distribution.

9.1.2. Bounded normal distribution

If the domain of the variable is not $(-\infty, \infty)$, the normal distribution would be incorrect. Therefore, we have to use another function as the PDF.

Let's suppose a domain (b_1, b_2) . If the amplitude is quite greater than the uncertainty, $a \gg \sigma$, a good PDF would be just the normal distribution truncated to the domain (b_1, b_2) . However, for amplitudes closer to the uncertainty, it would be clearly incorrect, as the truncation shifts the median of the distribution and modifies the confidence intervals, and thus the uncertainties.

To fix this, we make the following variable change:

$$x - \mu \rightarrow \tilde{x} - \mu \equiv \frac{4}{\tau} a \tan\left(\frac{\tau}{4} \frac{x - \mu}{a}\right).$$

Using this new variable \tilde{x} with a normal distribution, we are able to compress the original domain of $(-\infty, \infty)$ to $(-a, a)$. However, we get two disadvantages. Firstly, the normalization constant is now different, and second, the relation between the parameter of the standard deviation of the original normal distribution and the 1σ confidence interval (from which we define the uncertainty, σ) is now different; therefore, we should rename the standard deviation of the original normal distribution to s , which we will call *width*.

The first change is not a problem, as the PDF will be normalized computationally for each case. As for the second one, we can characterize computationally the relation between σ and s . It happens that s/σ decreases with a/σ , having $s/\sigma \simeq 2.65$ when $a/\sigma = 2$ and $s/\sigma \rightarrow 1$

30. See <https://tauday.com>.

when $a/\sigma \rightarrow \infty$. We have then a relation between the width, the uncertainty and the amplitude, that is, $s = s(\sigma, a)$.

Therefore, the resulting PDF, which we will call *bounded gaussian function*, would be the following:

$$f(x) \propto \exp\left(-\frac{1}{2} \left(\frac{\frac{4}{\tau} a \tan\left(\frac{\tau}{4} \frac{x-\mu}{a}\right)}{s(\sigma, a)} \right)^2\right),$$

which would led to a *bounded normal distribution* (see figure 1). However, it happens that s/σ increases quasi-exponentially as a/σ approaches a minimum value of ~ 1.47 . Moreover, the numeric relation $s(\sigma, a)$ starts to be incorrect if $a/\sigma \lesssim 1.7$ due to the increasing dispersion in s . Therefore, we must use another PDF for the cases in which $a/\sigma \lesssim 1.7$. Actually, for that limit case the shape of this PDF is almost that of a uniform distribution between $-a$ and a . We can model this PDF as a trapezoidal function with a rectangular core and triangles in the edges. Doing so, one can easily demonstrate that this kind of PDF would only work if a/σ is greater than the inverse of the integrated area corresponding to the 1σ confidence interval (~ 0.683); that is, $a/\sigma \gtrsim 1.46$, which is consistent with the found behaviors of the calculated relationship $s(\sigma, a)$. In order to be conservative and for the sake of simplicity, the bounded normal will only be used for $a \geq 2\sigma$. Note that for $a \gg \sigma$, this PDF tends to a gaussian, which is a good behaviour.

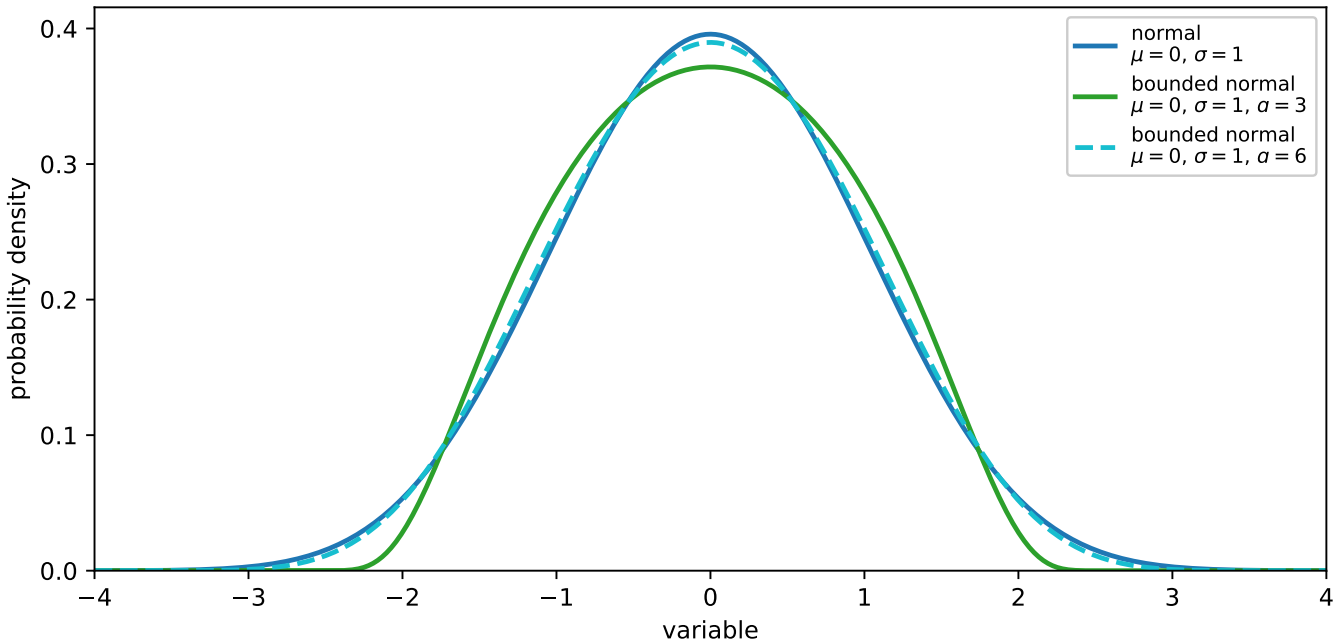


Figure 1. Probability density functions for a normal distribution and two bounded normal distributions.

9.1.3. Mirrored lognormal distribution

Finally, for $\sigma < a < 2\sigma$, we use a *mirrored log-gaussian function*:

$$f(x) = \frac{1}{\tau^{1/2} \ln(1 - \sigma/a)} \frac{1}{|x - (\mu - a)|} \exp\left(-\frac{1}{2} \left(\frac{|x - (\mu - a)| - \ln(a)}{\ln(1 - \sigma/a)} \right)^2\right),$$

which is a lognormal function shifted and mirrored, and which would led to a *mirrored log-*

normal distribution (see figure 2). This PDF meets our requirements: the median is equal to μ and the uncertainty associated with the 1σ interval is σ . It may seem that the shape of the function is not good, as its median is not equal to its maximum. However, there is no way to avoid this if the domain is too small. We could think about using a trapezoidal function, like discussed in the previous section, but we showed that this would only work for $a/\sigma \gtrsim 1.46$. Therefore, the PDF should have some kind of central dip, like in the mirrored lognormal distribution. Although ideally we would like to have a continuous function for all the possible values of $a/\sigma \geq 1$ (for example, a continuous transition between the bounded gaussian and the mirrored log-gaussian), for the moment this can be considered a good approximation to that ideal situation.

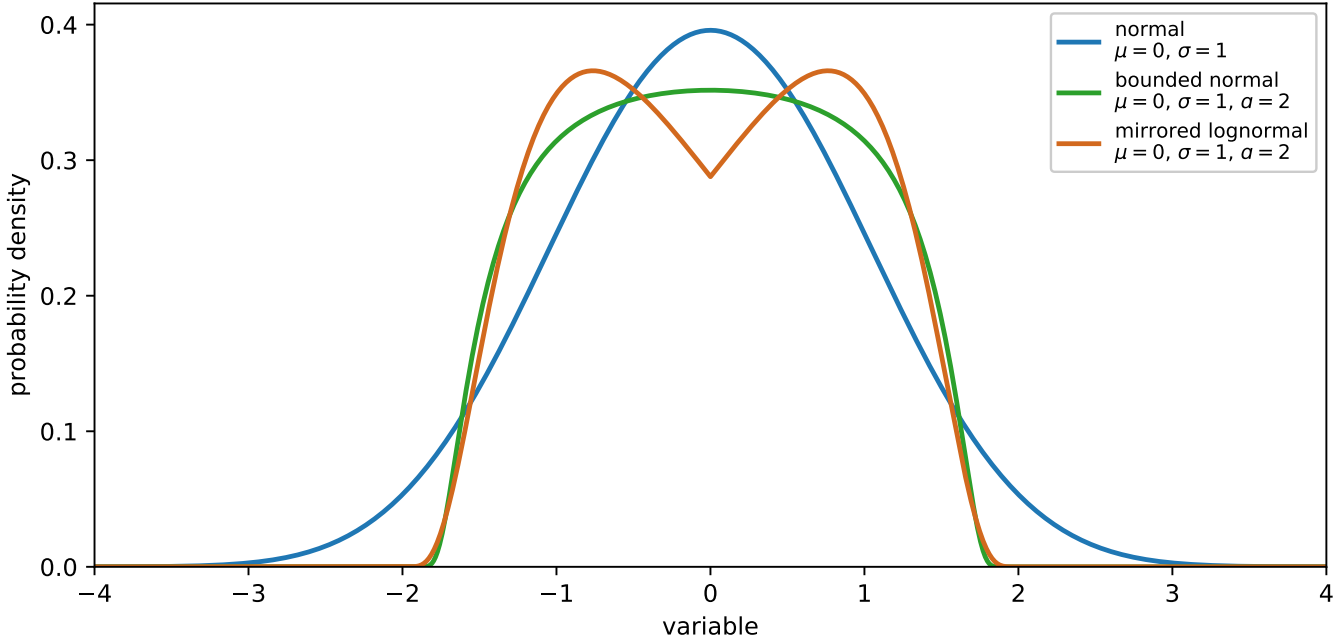


Figure 4. Probability density functions for a normal distribution, a bounded normal distribution and a mirrored lognormal distribution.

9.2. Upper/lower limits and finite intervals

Lastly, we should also address the case of a variable with an upper/lower limit or even a finite interval. Let's consider an interval (x_1, x_2) , which may be finite or infinite (and which can represent an upper/lower limit). If it is finite, we choose a uniform distribution between x_1 and x_2 as the corresponding PDF, with finite thresholds for 0, which we set to $\pm 10^{-90}$. But if it is infinite, we choose a symmetric loguniform distribution with finite thresholds for 0 and $\pm \infty$, which we set to $\pm 10^{-90}$ and $\pm 10^{90}$. For example, for an interval of $(-100, \infty)$, we would build a sample $\{x_-\}$ from a uniform distribution between -90 and 2 and a sample $\{x_+\}$ from a uniform distribution between -90 and 90 . Our final distribution would be the joining of the samples of $\{-10^{\{x_-\}}\}$ and $\{10^{\{x_+\}}\}$.

9.3. Summary

To sum up, if we have a set of variables x_i with central values μ_i and uncertainties σ_1, σ_2 we first build distributions $\{x_i\}$ using the mentioned PDFs. Then, we apply the function to the

distributions, $f(\{x_i\})$, obtaining a new distribution. Finally, we use an algorithm to detect if the distribution corresponds to an interval (that can be an upper/lower limit) or a defined value with uncertainties, and derive the corresponding parameters.

10. Additional useful functions

Besides the functions explained throughout this document, the RichValues libraries uses some additional functions to work. This section contains explanations of most of them, as they may be of interest.

10.1. Rounding numbers

The following functions are used for displaying the rich values with the correct number of significant figures, rounding the numbers accordingly to the type of rich value and, if existent, its uncertainties.

Function `round_sf`

If rounds the given number to the given number of significant figures. The arguments are:

- **x**. Input number.
- **n**. Number of significant figures. The default is 1.
- **min_exp**. Minimum exponent to display the number in scientific notation. The default is 4.
- **lim_for_extra_sf**. If the significand/mantissa of the number is lower than this limit value, the number will be displayed with an additional significant figure. By default it is 2.5.

Function `round_sf_unc`

If rounds the given value and uncertainty to the given number of significant figures. The arguments are:

- **x**. Input value.
- **dx**. Uncertainty of the input value.
- **n**. Number of significant figures. The default is 1.
- **min_exp**. Minimum exponent to display the numbers in scientific notation. The default is 4.
- **lim_for_extra_sf**. If the significand/mantissa of the uncertainty is lower than this limit value, the numbers will be displayed with an additional significant figure. By default it is 2.5.

Function `round_sf_uncs`

If rounds the given value and uncertainties to the given number of significant figures. The arguments are:

- **x**. Input value.
- **dx**. List containing the lower and upper uncertainties of the input value.

- **n.** Number of significant figures. The default is 1.
- **min_exp.** Minimum exponent to display the numbers in scientific notation. The default is 4.
- **lim_for_extra_sf.** If the significand/mantissa of the lower uncertainty is lower than this limit value, the number will be displayed with an additional significant figure. By default it is 2.5.

10.2. Creating distributions

The following functions are used for creating the distributions associated with the rich values.

Function `bounded_gaussian`

It applies the bounded gaussian function defined in section 7.1.2, which is the probability density function (PDF) of a bounded gaussian distribution. The arguments are:

- **x.** Input array of values to apply the function.
- **m.** Median of the curve. By default it is 0.
- **s.** Width of the curve (similar to the standard deviation). By default it is 1.
- **a.** Amplitude of the curve (distance from the median to the domain edges). By default it is 10.
- **norm.** Logical variable that determines if the resulting curve is normalized. By default it is False.

Function `mirrored_loggaussian`

It applies the mirrored log-gaussian function defined in section 7.1.3, which is the probability density function (PDF) of a mirrored lognormal distribution. The arguments are:

- **x.** Input array of values to apply the function.
- **m.** Median of the curve. By default it is 0.
- **s.** Width of the curve (similar to the standard deviation). By default it is 1.
- **a.** Amplitude of the curve (distance from the median to the domain edges). By default it is 10.
- **norm.** Logical variable that determines if the resulting curve is normalized. By default it is False.

Function `sample_from_pdf`

It draws a sample from the distribution specified with the given probability density function (PDF). The arguments are:

- **pdf.** Input PDF of the distribution.
- **size.** Size of the sample.
- **low.** Minimum of the input values for the PDF.
- **high.** Maximum of the input values for the PDF.

Additionally, you can use any of the keyword arguments of the input PDF.³¹

loguniform_distribution

It draws a sample from a lognormal distribution, with finite thresholds for 0 and $\pm\infty$.

- **low**. Minimum of the input values for the PDF. By default it is -1.
- **high**. Maximum of the input values for the PDF. By default it is 1.
- **size**. Size of the sample. By default it is 1.
- **zero_log**. Decimal logarithm of the minimum value in absolute value that can be returned. By default it is -90.0.
- **infinity_log**. Decimal logarithm of the maximum absolute in absolute value that can be returned. By default it is 90.0.

distr_with_rich_values

It creates a distribution resulting from applying the given function to the given rich values, which will be represented by their corresponding distributions.

- **function**. Function to be applied to the input rich values.
- **args**. Input rich value arguments.
- **len_samples**. Size of the samples of the arguments. By default, it is the square root of the number of arguments times the default sample size (10 000).

10.3. Evaluating distributions

The following functions are used for evaluating distributions of numbers in order to interpret them as rich values.

Function center_and_uncs

It returns the central value and uncertainties of the given distribution.

- **distr**. Input distribution of numbers.
- **function**. Function used to define the central value. By default, it is the median, calculated with `np.median`.
- **interval**. Confidence interval, in percent, used to define the uncertainties. The default is the 1σ confidence interval ($\sim 68.27\%$), that is, 68.27.
- **fraction**. Fraction of the input distribution (centered in the calculated central value) used to compute the uncertainties. By default, it is 1.0.

Function evaluate_distr

It interprets the given distribution as a rich value.

- **distr**. Input distribution of numbers.
- **domain**. Domain of the result, in case it is already known. By default it is $(-\infty, \infty)$.

31. Keyword arguments are arguments that have a default value. For example, in `bounded_gaussian` and `symmetric_loggaussian`, the arguments `m`, `s`, and `a` are keyword arguments.

- **zero_log.** Decimal logarithm of the threshold in absolute value for ± 0 , used to calculate the resulting domain and the range of the resulting distribution. By default it is -90.0.
- **infinity_log.** Decimal logarithm of the threshold in absolute value for $\pm \infty$, used to calculate the resulting domain and the range of the resulting distribution. By default it is 90.0.

Optionally, you can specify most of the keyword arguments of `function_with_rich_values`: `function`, `args`, `len_samples`, `is_function_vectorizable`, `lims_fraction`, and `num_reps_lims`. If so, the estimation of the rich value could be a bit better.

Citation of the library

If you use RichValues for your work, it would be great if you cite it. You can put the link to the GitHub repository, where this user guide can also be downloaded:

<https://github.com/andresmegias/richvalues> .

If you use RichValues for scientific research, you can cite the paper in the following link, in whose appendix the library is introduced:

<https://ui.adsabs.harvard.edu/abs/2023MNRAS.519.1601M/abstract> .

Useful links

The following links may be of interest:

- **Python.**
<https://www.python.org/>
- **Python's standard library.**
<https://docs.python.org/3/library/>
- **NumPy.**
<https://numpy.org/>
- **Pandas.**
<https://pandas.pydata.org/>
- **SciPy.**
<https://scipy.org/>
- **Matplotlib.**
<https://matplotlib.org/>

Credits

This software has been developed at the Centre for Astrobiology (*Centro de Astrobiología*, CAB), in Madrid (Spain), within the group of Chemical Complexity in the Interstellar Medium and Star Formation (Department of Astrophysics).

Coding and testing

Andrés Megías Toledano

Testing

Álvaro López Gallifa

Discussion

Jacobo Aguirre Araujo

Eva Herrero Cisneros

License

The library RichValues is published under a BSD 3-Clause “New” or “Revised” License.

Copyright © 2022 - Andrés Megías Toledano (<https://www.github.com/andresmegias>)

Redistribution and use in source and binary forms, with or without modification, are permitted provided that the following conditions are met:

1. Redistributions of source code must retain the above copyright notice, this list of conditions and the following disclaimer.
2. Redistributions in binary form must reproduce the above copyright notice, this list of conditions and the following disclaimer in the documentation and/or other materials provided with the distribution.
3. The name of the author may not be used to endorse or promote products derived from this software without specific prior written permission.

This software is provided by the author “as is” and any express or implied warranties, including, but not limited to, the implied warranties of merchantability and fitness for a particular purpose are disclaimed. In no event shall the author be liable for any direct, indirect, incidental, special, exemplary, or consequential damages (including, but not limited to, procurement of substitute goods or services; loss of use, data, or profits; or business interruption) however caused and on any theory of liability, whether in contract, strict liability, or tort (including negligence or otherwise) arising in any way out of the use of this software, even if advised of the possibility of such damage.