
nifti-mrs

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This is the API documentation for the `nifti-mrs` Python package.

Source code is available at https://github.com/wtclarke/nifti_mrs_tools.

NIFTI_MRS

1.1 nifti_mrs.nifti_mrs

Core Nifti-MRS class. For more information on NIFTI-MRS see https://github.com/wtclarke/mrs_nifti_standard

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exception nifti_mrs.nifti_mrs.NIFTIMRS_DimDoesntExist

exception nifti_mrs.nifti_mrs.NotNIFTI_MRS

class nifti_mrs.nifti_mrs.NIFTI_MRS(*args, validate_on_creation=True, **kwargs)

A class to load and represent Nifti-MRS formatted data. Utilises the fsipy Image class and nibabel nifti headers.

Access the underlying fsipy Image object for useful attributes using obj.image.

property header

Returns NIFTI-MRS header object

property ndim

Returns number of dimensions in the NIFTI-MRS object

property shape

Returns the data shape. Singleton dimensions implied by header extension keys are included. Use obj.image.shape to get the shape of the stored data

property dtype

Returns data type

property nifti_mrs_version

Get NIFTI-MRS version string.

set_version_info(major, minor)

Puts mrs_v{major}_{minor} into intent_name

property dwelltime

Return dwelltime in seconds

property spectralwidth

Return spectral width in Hz

property bandwidth

Alias for spectralwidth (Hz)

property nucleus

Returns resonant nucleus string(s) - returns list

property spectrometer_frequency

Central or spectrometer frequency in MHz - returns list

property field_strength

Field strength in tesla. NaN returned if unrecognised nucleus.

getAffine(*args)

Return an affine transformation which can be used to transform coordinates from `from_` to `to`.

Valid values for the `from_` and `to` arguments are:

- `'voxel'`: The voxel coordinate system
- `'world'`: The world coordinate system, as defined by the image `sform/qform`
- `'fsl'`: The FSL coordinate system (scaled voxels, with a left-right flip if the `sform/qform` has a positive determinant)

Parameters

- **from** – Source coordinate system
- **to** – Destination coordinate system

Returns

A numpy array of shape (4, 4)

property worldToVoxMat

Returns a numpy array of shape (4, 4) containing an affine transformation from world coordinates to voxel coordinates.

property voxToWorldMat

Returns a numpy array of shape (4, 4) containing an affine transformation from voxel coordinates to world coordinates.

property hdr_ext

Return MRS JSON header extension object.

add_hdr_field(key, value, doc=None)

Add a field to the header extension

Parameters

- **key** (*str*) – Field key
- **value** – Value of field to add
- **doc** (*optional*, *str*) – Use to convey meaning of user-defined header value.

remove_hdr_field(key)

Remove a field from the header extension

Parameters

- **key** (*str*) – Key to remove

property file**property filename**

Name of file object was generated from. Returns empty string if N/A.

property dim_tags

Return the three higher dimension tags

dim_position(dim_tag)

Return position of dim if it exists.

set_dim_tag(dim, tag, info=None, header=None)

Set or update the dim_N, dim_N_info, and dim_N_header fields

Tag must be one of the standard-defined tags (e.g. DIM_DYN)

Parameters

- **dim** (*str* or *int*) – The existing dim tag or python dimension index (i.e. N-1)
- **tag** (*str*) – New tag
- **info** (*str*) – New info string
- **header** (*dict*) – dict containing the dimension headers

copy(remove_dim=None)

Return a copy of this image, optionally with a dimension removed.

Parameters

remove_dim (*str* or *int*, *optional*) – dimension index (4, 5, 6) or tag to remove. Takes first index. Defaults to None/no removal

Returns

Copy of object

Return type

NIFTI_MRS

remove_dim(remove_dim)

Return a copy of this image with a dimension removed. (Intuitive wrapper of copy function with remove_dim.)

Parameters

remove_dim (*str* or *int*, *optional*) – dimension index (4, 5, 6) or tag to remove. Takes first index. Defaults to None/no removal

Returns

Copy of object

Return type

NIFTI_MRS

save(filepath)

Save NIFTI-MRS to file

Parameters

filepath (*str* or *pathlib.Path*) – Name and path of save location

iterate_over_dims(dim=None, iterate_over_space=False, reduce_dim_index=False, voxel_index=None)

Return generator to iterate over all indices or one dimension (and FID).

Parameters

- **dim** (*str* or *int*, *optional*) – None, dimension index (4, 5, 6) or tag. None iterates over all indices. Defaults to None

- **iterate_over_space** (*bool, optional*) – If True also iterate over spatial dimension, defaults to False
- **reduce_dim_index** (*bool, optional*) – If True the returned slice index will have the selected dimension removed. Defaults to False.
- **voxel_index** (*slice or tuple, optional*) – slice or tuple of first three spatial dimensions., defaults to None

Returns

yeilds array of sliced data

Return type

np.array

Returns

data location slice object.

Return type

slice

iterate_over_spatial()

Iterate over spatial voxels yeilding a data array the shape of the FID and any higher dimensions + index.

Yield

Complex FID data with any higher dimensions. Index to data.

Return type

tuple

dynamic_hdr_vals()

Return representations of the dynamic header values

Returns

List of dicts containing labelled header parameters

Returns

List of tuples containing header values

Returns

Flattened numpy array for each generated spectrum containing header values

plot(*display_dim=None, ppmlim=None, plot_avg=False, mask=None, legend=True*)

1.2 nifti_mrs.create_nmrs

Generate new NIfTI-MRS objects and files from data blocks.

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nifti_mrs.create_nmrs.gen_nifti_mrs(*data, dwelltime, spec_freq, nucleus='1H', affine=None, dim_tags=[None, None, None], nifti_version=2, no_conj=False*)

Generate NIfTI-MRS from data and required metadata

Parameters

- **data** (*numpy.array*) – Complex-typed numpy array of at least 4 dimensions (max 7)
- **dwelltime** (*float*) – Spectral (4th dimension) dwelltime in seconds
- **spec_freq** (*float*) – Spectrometer Frequency in MHz
- **nucleus** (*str, optional*) – Resonant Nucleus string (e.g. 1H, 31P, 2H), defaults to '1H'

- **affine** (*numpy.array, optional*) – 4x4 orientation/position affine, defaults to None which will use default (scaled identity).
- **dim_tags** (*list, optional*) – List of dimension tags (e.g. DIM_DYN), defaults to [None, None, None]
- **nifti_version** (*int, optional*) – Version of NIfTI header format, defaults to 2
- **no_conj** (*bool, optional*) – If true stops conjugation of data on creation, defaults to False

Returns

NIFTI-MRS object

Return type

nifti_mrs.nifti_mrs.NIFTI_MRS

```
nifti_mrs.create_nmrs.gen_nifti_mrs_hdr_ext(data, dwelltime, hdr_ext, affine=None, nifti_version=2,
                                             no_conj=False)
```

Generate NIFTI-MRS from data and header extension object

Parameters

- **data** (*numpy.array*) – Complex-typed numpy array of at least 4 dimensions (max 7)
- **dwelltime** (*float*) – Spectral (4th dimension) dwelltime in seconds
- **hdr_ext** (*nifti_mrs.hdr_ext.Hdr_Ext*) – Populated NIFTI-MRS header extension
- **affine** (*numpy.array, optional*) – 4x4 orientation/position affine, defaults to None which will use default (scaled identity).
- **dim_tags** (*list, optional*) – List of dimension tags (e.g. DIM_DYN), defaults to [None, None, None]
- **nifti_version** (*int, optional*) – Version of NIfTI header format, defaults to 2
- **no_conj** (*bool, optional*) – If true stops conjugation of data on creation, defaults to False

Returns

NIFTI-MRS object

Return type

nifti_mrs.nifti_mrs.NIFTI_MRS

1.3 nifti_mrs.definitions

Translate the JSON definitions of NIFTI-MRS standard meta data and dimension tags to python usable formats.

Type fields should either be generic python types: float, int, str or a tuple indicating an array type and element type : (list, float) or (list, str)

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```
nifti_mrs.definitions.field_def
```

alias of HeaderExtensionField

```
nifti_mrs.definitions.translate_definitions(obj)
```

Translate the JSON defined object to python dicts with python types

1.4 nifti_mrs.validator

exception `nifti_mrs.validator.Error`

Base class for other exceptions

exception `nifti_mrs.validator.headerExtensionError`

Raised if problems with header extension are found.

exception `nifti_mrs.validator.niftiHeaderError`

Raised if problems with nifti header are found.

exception `nifti_mrs.validator.niftiDataError`

Raised if problems with nifti data are found.

`nifti_mrs.validator.validate_nifti_mrs(nifti_mrs)`

Validate a full NIFTI MRS image.

`nifti_mrs.validator.validate_nifti_data(nifti_img_data)`

Validate the data inside a nibabel nifti image 1. Check data is complex 2. Check number of dimensions is at least 4 but less than 8.

`nifti_mrs.validator.validate_nifti_header(nifti_header)`

Validate the header of a nibabel nifti image Check data type is complex Check orientation data. - How? TO DO
Check dwell time Check intent name

`nifti_mrs.validator.validate_hdr_ext(header_ex, dimension_sizes, data_dimensions=None)`

Validate the header extension 1. Check that it is json formatted string. 2. Check that it contains the required meta-data 3. Check that it contains any required dimension information. 4. Check that standard-defined data is of correct type.

Parameters

- **header_ex** (*str*) – NIFTI-MRS header extensions as a json deserialisable string
- **dimension_sizes** (*tuple of ints*) – Size of the NIFTI-MRS dimensions
- **data_dimensions** (*int, optional*) – Total number of data dimensions in corresponding nifti-mrs data, defaults to None When None the dimensions are inferred from the tags and size

`nifti_mrs.validator.check_type(value, json_type)`

Checks that values is of type json_type json_type may be a tuple to handle array types e.g. (list, str) indicates a list of strings.

`nifti_mrs.validator.validate_spectralwidth(header_ex, dwelltime)`

If a SpectralWidth field is present, check that it matches the dwell time

Dwell time is stored in pixdim[4].

Parameters

- **header_ex** (*str*) – NIFTI-MRS header extensions as a json deserialisable string
- **dwelltime** (*float*) – Dwell time as stored in pixdim[4] to check against any SpectralWidth definition. In seconds.

1.5 nifti_mrs.hdr_ext

class nifti_mrs.hdr_ext.Hdr_Ext(*spec_frequency, resonant_nucleus, dimensions=None*)

Class to hold meta data stored in a NIFTI MRS header extension. Required fields must be passed to initialise, Default dimension information automatically generated, but may be modified by set_dim_info method. Standard defined meta-data and user-defined data can be added using set_standard_def and set_user_def respectively.

classmethod from_header_ext(*hdr_ext_dict*)

Create a Hdr_Ext object from a json string deserialised into a python dict

Parameters

hdr_ext_dict (*dict*) – header extension as a dict.

Returns

Class object

Return type

Hdr_Ext

property ndim

Returns the number of dimensions implied by the 'dim_{5,6,7}' tags

set_dim_info(*dim, tag, info=None, hdr=None*)

Set information associated with the optional, higher data dimensions.

Parameters

- **dim** (*str or int*) – May be (0,1,2) or (“5th”, “6th”, “7th”)
- **tag** (*str*) – Must be one of the defined dimension tag strings. E.g. DIM_DYN or None
- **info** (*str, optional*) – Optional, free-form for documentation, defaults to None
- **hdr** (*dict, optional*) – Dict containing relevant header value names and values. Defaults to None

remove_dim_info(*dim*)

Set a dimension’s information to None

Parameters

dim (*str or int*) – 0,1,2 or “5th”, “6th”, “7th”

set_standard_def(*key, value*)

Add a single standard-defined bit of meta-data to the object.

set_user_def(*key, value, doc*)

Add user-defined metadata keys to the header extension. add keys and values one at a time using key, value and doc.

remove_standard_def(*key*)

Remove key from list of standard defined key-value pairs

Parameters

key (*str*) – Key name

remove_user_def(*key*)

Remove key from list of user defined key-value pairs

Parameters

key (*str*) – Key name

to_dict()

Generate dictionary representation from properties.

property **current_keys**

to_json()

copy()

1.6 nifti_mrs.tools.misc

Miscellaneous tools for NIFTI-MRS

Author: Will Clarke <william.clarke@ndcn.ox.ac.uk> Copyright (C) 2021 University of Oxford

nifti_mrs.tools.misc.conjugate(nmrs: *NIFTI_MRS*) → *NIFTI_MRS*

Conjugate a nifti-mrs object.

Parameters

nmrs (*NIFTI_MRS*) – NIFTI_MRS object to conjugate

Returns

Conjugated NIFTI_MRS

Return type

NIFTI_MRS

1.7 nifti_mrs.tools.reshape

Tools for reshaping the higher dimensions of NIFTI-MRS

Author: Will Clarke <william.clarke@ndcn.ox.ac.uk> Copyright (C) 2021 University of Oxford

nifti_mrs.tools.reshape.reshape(nmrs: *NIFTI_MRS*, reshape: *tuple[int, ...]*, d5: *str | None = None*, d6: *str | None = None*, d7: *str | None = None*) → *NIFTI_MRS*

Reshape the higher dimensions (5-7) of an nifti-mrs file. Uses numpy reshape syntax to reshape. Use -1 for automatic sizing.

If the dimension exists after reshaping a tag is required. If None is passed but one already exists no change will be made. If no value exists then an exception will be raised.

Parameters

- **nmrs** (*NIFTI_MRS*) – Input NIFTI-MRS file
- **reshape** (*tuple*) – Tuple of target sizes in style of numpy.reshape, higher dimensions only.
- **d5** (*str*, *optional*) – Dimension tag to set dim_5, defaults to None
- **d6** (*str*, *optional*) – Dimension tag to set dim_6, defaults to None
- **d7** (*str*, *optional*) – Dimension tag to set dim_7, defaults to None

nifti_mrs.tools.reshape.remove_dim(nmrs: *NIFTI_MRS*, remove_dim: *str | int*) → *NIFTI_MRS*

Removes a specified dimension from a NIFTI_MRS object and returns a copy of the so modified NIFTI_MRS.

Parameters

- **nmrs** (*NIFTI_MRS*) – Input nifti_mrs object from which to remove dim
- **remove_dim** (*str | int*) – dimension index (4, 5, 6) or tag to remove. Takes first index.

Returns

A NIFTI_MRS object with dimensionality reduced

Return type

NIFTI_MRS

1.8 nifti_mrs.tools.split_merge

Tools for merging and splitting the dimensions of NIFTI-MRS

Author: Will Clarke <william.clarke@ndcn.ox.ac.uk> Copyright (C) 2021 University of Oxford

`nifti_mrs.tools.split_merge.split(nmrs: NIFTI_MRS, dimension: str | int, index_or_indices: int | list[int]) → tuple[NIFTI_MRS, NIFTI_MRS]`

Splits, or extracts indices from, a specified dimension of a NIFTI_MRS object. Output is two NIFTI_MRS objects. Header information preserved.

Parameters

- **nmrs** (*fsl_mrs.core.nifti_mrs.NIFTI_MRS*) – Input nifti_mrs object to split
- **dimension** (*str* or *int*) – Dimension along which to split. Dimension tag or one of 4, 5, 6 (for 0-indexed 5th, 6th, and 7th)
- **index_or_indices** (*int* or *[int]*) – Single integer index to split after, or list of integer indices to insert into second array. E.g. '0' will place the first index into the first output and 1 -> N in the second. '[1, 5, 10]' will place 1, 5 and 10 into the second output and all other will remain in the first.

Returns

Two NIFTI_MRS object containing the split files

Return type

tuple[*NIFTI_MRS*, *NIFTI_MRS*]

`nifti_mrs.tools.split_merge.merge(array_of_nmrs: list[NIFTI_MRS] | tuple[NIFTI_MRS, ...], dimension: str | int) → NIFTI_MRS`

Concatenate NIFTI-MRS objects along specified higher dimension

Parameters

- **array_of_nmrs** (*tuple* or *list of fsl_mrs.core.nifti_mrs.NIFTI_MRS*) – Array of NIFTI-MRS objects to concatenate
- **dimension** (*int* or *str*) – Dimension along which to concatenate. Dimension tag or one of 4, 5, 6 (for 0-indexed 5th, 6th, and 7th).

Returns

Concatenated NIFTI-MRS object

Return type

fsl_mrs.core.nifti_mrs.NIFTI_MRS

1.9 nifti_mrs.utils

Utility functions for Nifti-MRS utilities

Author: Will Clarke <william.clarke@ndcn.ox.ac.uk> Copyright (C) 2021 University of Oxford

exception `nifti_mrs.utils.NIFTI_MRSIncompatible`

`nifti_mrs.utils.modify_hdr_ext(new_hdr_ext, nifti_header)`

Generate a new NIFTI header with a modified header extension. New header is a copy of the one passed

Parameters

- **new_hdr_ext** (*Hdr_Ext object*) – Modified header extension
- **nifti_header** (*nibabel.nifti2.Nifti2Header*) – NIFTI header

Returns

Copied header with modified hdr extension

Return type

`nibabel.nifti2.Nifti2Header`

`nifti_mrs.utils.check_type(in_format)`

Return type of header: long (list) or short (dict)

Parameters

in_format (*list or dict*) – Value of header key

Returns

'long' or 'short'

Return type

str

`nifti_mrs.utils.dim_n_header_short_to_long(in_format, elements)`

`nifti_mrs.utils.dim_n_header_long_to_short(in_format)`

MRS_TOOLS

The command-line tool for manipulation of NIFTI-MRS files.

usage: mrs_tools [-h] [-v] {info,vis,merge,split,reorder,conjugate} ...

NIFTI-MRS (Magnetic Resonance Spectroscopy) tools

optional arguments:

-h, --help	show this help message and exit
-v, --version	show program's version number and exit

subcommands:

Available tools

{info, vis, merge, split, reorder, conjugate}

2.1 info

Information about the NIFTI-MRS file.

usage: mrs_tools info [-h] FILE or list of FILEs [FILE or list of FILEs ...]

positional arguments:

FILE or list of FILEs
NIFTI MRS file(s)

optional arguments:

-h, --help	show this help message and exit
-------------------	---------------------------------

2.2 vis

Quick visualisation of a NIFTI-MRS file or FSL-MRS basis set.

usage: mrs_tools vis [-h] [--ppmlim LOW HIGH] [--mask MASK] [--save SAVE] [--display_dim DISPLAY_DIM] [--no_mean] FILE or DIR

positional arguments:

FILE or DIR
NIFTI file or directory of basis sets

optional arguments:

-h, --help	show this help message and exit
--ppmlim LOW-HIGH	limit the fit to a freq range (default=(.2,4.2))

--mask MASK	Mask for MRSI
--save SAVE	Save fig to path
--display_dim	DISPLAY_DIM. A NIFTI-MRS tag. Do not average across this dimension.
--no_mean	Do not plot the mean signal line in the case of multiple spectra.

2.3 merge

Merge NIFTI-MRS along higher dimensions.

```
usage: mrs_tools merge [-h] --files FILES [FILES ...] --dim DIM [--newaxis] [--output OUTPUT] [--filename FILENAME]
```

optional arguments:

-h, --help	show this help message and exit
--newaxis	Join files along a new axis (tag specified by <code>--dim</code>).
--output OUTPUT	output folder (defaults to current directory)
--filename FILENAME	Override output file name.

required arguments:

--files FILES [FILES ...]	List of files to merge
--dim DIM	NIFTI-MRS dimension tag to merge across.

2.4 split

Split NIFTI-MRS along higher dimensions.

```
usage: mrs_tools split [-h] --file FILE --dim DIM (--indices INDICES [INDICES ...] | --index INDEX) [--output OUTPUT] [--filename FILENAME]
```

optional arguments:

-h, --help	show this help message and exit
--indices INDICES [INDICES ...]	List of indices to extract into second file. All indices are zero-indexed.
--index INDEX	Index to split at (split after index, zero-indexed).
--output OUTPUT	output folder (defaults to current directory)
--filename FILENAME	Override output file names.

required arguments:

--file FILE	File to split
--dim DIM	NIFTI-MRS dimension tag to split across.

2.5 reorder

Reorder higher dimensions of NIFTI-MRS.

```
usage: mrs_tools reorder [-h] --file FILE --dim_order DIM_ORDER [DIM_ORDER ...] [--output OUTPUT] [--filename FILENAME]
```

optional arguments:

- h, --help** show this help message and exit
- output OUTPUT** output folder (defaults to current directory)
- filename FILENAME** Override output file names.

required arguments:

- file FILE** File to reorder
- dim_order DIM_ORDER [DIM_ORDER ...]**
NIFTI-MRS dimension tags in desired order. Enter as strings (min:1, max:3). Can create singleton dimension at end.

2.6 reshape

Reshapes the higher dimensions of a NIFTI-MRS file.

usage: `mrs_tools reshape [-h] --file FILE --shape SHAPE [SHAPE ...] [--d5 D5] [--d6 D6] [--d7 D7] [--output OUTPUT] [--filename FILENAME]`

optional arguments:

- h, --help** show this help message and exit
- d5 D5** 5th dimension tag (e.g. DIM_DYN).
- d6 D6** 6th dimension tag (e.g. DIM_DYN).
- d7 D7** 7th dimension tag (e.g. DIM_DYN).
- output OUTPUT** output folder (defaults to current directory)
- filename FILENAME** Override output file names.

required arguments:

- file FILE** File to reshape
- shape SHAPE [SHAPE ...]**
Numpy-like target shape. Enter as integers, -1 is used for any. Only enter shape for higher (5th-7th) dimensions.

2.7 conjugate

Conjugate data to correct phase/frequency convention in a NIFTI-MRS file.

usage: `mrs_tools conjugate [-h] --file FILE [--output OUTPUT] [--filename FILENAME]`

optional arguments:

- h, --help** show this help message and exit
- output OUTPUT** output folder (defaults to current directory)
- filename FILENAME** Override output file names.

required arguments:

- file FILE** File to conjugate

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