nifti-mrs

Release 1.3.3

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CONTENTS:

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

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

CHAPTER
ONE

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 fslpy Image class and nibabel nifti headers.

Access the underlying fslpy 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*

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

<a>

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*)

> 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*, *reshape*, *d5=None*, *d6=None*, *d7=None*)

> 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

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*, *dimension*, *index_or_indices*)

> 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**
> > fsl_mrs.core.nifti_mrs.NIFTI_MRS

`nifti_mrs.tools.split_merge.`**`merge`**(*array_of_nmrs*, *dimension*)

> 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 –dim).
--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

PYTHON MODULE INDEX

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