# nctoolkit

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nctoolkit is a comprehensive and computationally efficient Python package for analyzing and post-processing netCDF data.

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# **ONE**

## WHO IS NCTOOLKIT FOR?

Everyone from casual to regular users of netCDF data will find nctoolkit useful. Casual users will appreciate the easy ability to do such as things as matching up point observation data with gridded netCDF data. For expert users, nctoolkit provides the ability to carry out 80-100% of your day to day analysis and post-processing.

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TWO

# WHAT TYPE OF DATA IS NCTOOLKIT DESIGNED FOR?

nctoolkit is designed primarily with climate and oceanic data in mind. If you work with this type of data, nctoolkit can help you do it quickly and efficiently.

CHAPTER
THREE

# WHAT SYSTEMS CAN NCTOOLKIT WORK ON?

nctoolkit requires a Linux or macOS operating system.

**CHAPTER** 

### **FOUR**

### WHAT CAN NCTOOLKIT DO?

The core abilities of nctoolkit include:

- Cropping to geographic regions
- Interactive plotting of data
- Subsetting to specific time periods
- Calculating time averages
- Calculating spatial averages
- · Calculating rolling averages
- Calculating climatologies
- Creating new variables using arithmetic operations
- · Calculating anomalies
- · Horizontally and vertically remapping data
- Calculating the correlations between variables
- · Calculating vertical averages for the likes of oceanic data
- Calculating ensemble averages
- Calculating phenological metrics

nctoolkit is developed as open source software by the Marine Systems Modelling group at Plymouth Marine Laboratory.

### 4.1 Installation

#### 4.1.1 How to install nctoolkit

You will need a Linux or Mac operating system for nctoolkit to work. It will not work on Windows due to system requirements.

nctoolkit is available from the Python Packaging Index. To install nctoolkit using pip:

```
$ pip install numpy
```

\$ pip install nctoolkit

If you already have numpy installed, ignore the first line. This is only included as it will make installing some dependencies smoother. nctoolkit partly relies on cartopy for plotting. This has some additional dependencies, so you may need to follow their guide here to ensure cartopy is installed fully. If you install nctoolkit using conda, you will not need to worry about that.

If you install netoolkit from pypi, you will need to install the system dependencies listed below.

nctoolkit can also be installed using conda, as follows:

```
$ conda install -c conda-forge nctoolkit
```

Note that recent releases are not available for Python 3.8 on macOS on conda. This issue is being investigated at the minute, and will hopefully be resolved shortly. In the meantime, if you are using macOS and Python 3.8, it is best to install using pip.

At present this can be slow due to the time taken to resolve dependency versions. If you run into problems just use pip.

To install the development version from GitHub:

```
$ pip install git+https://github.com/r4ecology/nctoolkit.git
```

### 4.1.2 Plotting issue

An update to a dependency of a dependency has broken plotting in nctoolkit, unless you have ncplot version 0.2.4 installed. If you experience an error related to jinja2, downgrade the package as follows:

```
$ conda install jinja2=3.0.3
$ pip install jinja2==3.0.3
```

Or install the latest version of ncplot:

```
$ conda install ncplot=0.2.4
$ pip install ncplot==0.2.4
```

### 4.1.3 Jupyter notebook issue

A recent update to ipykernel has broken some functionality in jupyter notebooks, with Python not exiting properly when notebooks are restarted or closed. This is resulting in nctoolkit not automatically deleting temporary files at the end of sessions. To fix this just downgrade ipykernel:

```
$ conda install ipykernel=6.9.1
$ pip install ipykernel==6.9.1
```

### 4.1.4 Python dependencies

- Python (3.6 or later)
- numpy (1.14 or later)
- pandas (0.24 or later)
- xarray (0.14 or later)
- netCDF4 (1.53 or later)
- ncplot

### 4.1.5 System dependencies

There are two main system dependencies: Climate Data Operators, and NCO. The easiest way to install them is using conda:

```
$ conda install -c conda-forge cdo
$ conda install -c conda-forge nco
```

CDO is necessary for the package to work. NCO is an optional dependency and does not have to be installed.

If you are working on an Ubuntu system, you should be able to install CDO as follows:

```
$ sudo apt install cdo
```

If you want to install CDO from source, you can use one of the bash scripts available here.

### 4.2 Introduction to nctoolkit

nctoolkit is a multi-purpose tool for analyzing and post-processing netCDF files. It is designed to carry out almost all analysis and post-processing chains, and to do so easily and efficiently. It is designed explicitly with climate change and oceanographic work in mind. Under the hood, it uses Climate Data Operators (CDO), but it operates as a stand-alone package with no knowledge of CDO being required to use it.

Let's look at what it can do using a historical global dataset of sea surface temperature, which you can find here.

The preferred way to import nctoolkit is:

```
[1]: import nctoolkit as nc
nctoolkit is using Climate Data Operators version 1.9.10
```

### 4.2.1 It lets you quickly visualize data

nctoolkit offers plotting functionality that will let you automatically plot data from almost any type of netCDF file. It's as simple as the following, which calculates mean historical sea surface temperature and then plots it:

```
[2]: ds = nc.open_data("sst.mon.mean.nc")
ds.plot()

Data type cannot be displayed: application/javascript, application/vnd.holoviews_load.v0+json

Data type cannot be displayed: application/javascript, application/vnd.holoviews_load.v0+json

Data type cannot be displayed: application/javascript, application/vnd.holoviews_load.v0+json
```

Data type cannot be displayed: application/javascript, application/vnd.holoviews\_load.v0+json

```
[2]: :DynamicMap [time]
    :Overlay
    .Image.I :Image [lon,lat] (sst)
    .Coastline.I :Feature [Longitude,Latitude]
```

### 4.2.2 It lets you calculate spatial averages

Calculating the spatial mean

```
[3]: ds = nc.open_data("sst.mon.mean.nc")
    ds.spatial_mean()
    ds.plot()

[3]: :DynamicMap [variable]
    :Curve [time] (value)
```

### 4.2.3 It lets you do mathematical operations

nctoolkit offers an 'assign' method for performing mathematical operations on variables. This works in a way that will be familiar to users of Pandas. The method is illustrated below in a processing chain that works out how much warmer each part of the ocean is than the global mean.

### 4.2.4 It lets you crop data

We can crop to a specific region using the **crop** method. To get a region covering most of Europe, we could do this:

### 4.2.5 It lets you regrid data

nctoolkit has built-in methods for regridding data to user-specified grids. One of the most useful is to\_latlon. This let's you regrid to a regular latlon grid. You just need to specify the extent of the new grid, the resolution and the regridding method.

```
[6]: ds = nc.open_data("sst.mon.mean.nc")
    ds.to_latlon(lon = [-13, 38], lat = [30, 67], res = 0.5, method = "nn")
    ds.plot()

[6]: :DynamicMap [time]
    :Overlay
    .Image.I :Image [lon,lat] (sst)
    .Coastline.I :Feature [Longitude,Latitude]
```

### 4.2.6 It lets you calculate temporal averages

nctoolkit features a suite of methods, beginning with the letter t, that let you calculate temporal statistics. For example, if we wanted to calculate how much sea surface temperature varies each year, we could do this:

```
[7]: ds = nc.open_data("sst.mon.mean.nc")
    ds.trange("year")
    ds.tmean()
    ds.plot()

[7]: :Overlay
        .Image.I :Image [lon,lat] (sst)
        .Coastline.I :Feature [Longitude,Latitude]
```

### 4.2.7 It lets you calculate anomalies

In an example above we calculated the global mean sea surface temperature every month since 1850. But calculate the anomaly might be more interesting. The code below will calculate the change in global annual mean sea surface temperature since 1850-1969. The window argument let's you calculate it on a rolling basis.

### 4.2.8 It lets you calculate zonal averages

It is easy to calculate zonal averages using nctoolkit. In the example below change in temperature since 1850-1869 in each latitude band is calculated:

```
[9]: ds = nc.open_data("sst.mon.mean.nc")
   ds.annual_anomaly(baseline = [1850, 1869], window= 20)
   ds.zonal_mean()
   ds.plot()

[9]: :QuadMesh [time,lat] (sst)
```

### 4.2.9 Getting started with nctoolkit

To get started with nctoolkit it is best to start *here*, and to consider getting the *cheatsheet*.

### 4.3 News

#### 4.3.1 Release of v0.7.1

Release data: 10th September 2022.

This is a major release with some breaking changes.

The deprecated *select* method has now been removed. Users should now use the *subset* method.

A progress bar will now display when processing large datasets. This will only show when nctoolkit thinks something will take a while. If you want to always show a progress bar for multi-file datasets, you can do this: nc.options(progress = 'on').

#### 4.3.2 Release of v0.6.0

Release date: 15th August 2022.

This is a major release that introduces some breaking changes. All methods that carry out temporal averaging of any sort will now align output times to the right. This applies to methods such as *tmean* and *rolling\_mean*. The internals when *align* = "*left*" option have been modified, as the CDO call was sometimes giving incorrect results.

#### 4.3.3 Release of v0.5.4

This is a minor release on August 10th 2022.

It improves the abilities of temporal methods, giving users the ability to select how they want times in output to be aligned.

For example, if you are calculating a rolling mean, you might want the output times to be the first, middle or final time in the temporal window. This release will add that ability to nctoolkit's temporal methods. Previously nctoolkit used CDO's default methods, and did not allow users to do anything else. By default, output dates will be aligned to the middle.

The *match points* methods were throwing an error when there were non-unique vertical values. This is now fixed.

Some improvements have been made to package internals.

### 4.3.4 Release of v0.5.1

This was a minor release made on 30th June 2022. It includes method enhancements.

The *subset* method now allows negative time slicing.

The set\_missing method is deprecated and replaced with a less ambiguously named as\_missing method.

The *plot* method will no longer show a plot title by default to make things cleaner.

The *vertical\_integration* method now works with multi-file datasets and will not calculate vertical integrations for the thickness variable.

Some improvements have been made to improve error messages, and the *check* method now checks for data type of time.

A new method as\_type has been added for changing data type of individual variables and coordinates.

#### 4.3.5 Release of v0.5.0

This relase was made on 13th June 2022. The match\_points method now allows extrapolation to vertical depths.

#### 4.3.6 Release of v0.4.9

This relase was made on 9th June 2022. The subset method now accepts levels.

#### 4.3.7 Release of v0.4.8

This release improves temporal merging of large datasets. Previously on some systems this would fail on datasets made up of more than 1,000 files due to system limits. Under the hood, nctoolkit now deals with this.

The merge method also now contains a check argument that can be used to speed up merging of large datasets when you know the files can be merged problem-free. Previously, merge always checked if files being merged had the same variables when doing a temporal merge. This can now be switched off if you are confident this does not need to happen.

#### 4.3.8 Release of v0.4.7

Version 0.4.7 was released on June 5th 2022.

This release contained a new method called match\_points that can do matchups with a spatiotemporal dataframe.

#### 4.3.9 Release of v0.4.6

Version 0.4.6 was released on June 3rd 2022.

This release will enhance existing methods.

The select method will be replaced by subset. This behave in the way same way as select, but will also allow users to subset data base on longitude and latitude using the lon and lat as args.

The export methods to\_nc, to\_xarray and to\_dataframe now allow only a subset of the data to be exported. Additional arguments can be sent to the methods, which will then be sent to the subset method.

The new matchpoint methods for matching netCDF and point data have been smoothed out with additional options.

Minor bug fix: The weighted in datasets with recycled regridding weights were not copied properly. This is now fixed.

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### 4.3.10 Release of v0.4.5

Version 0.4.5 was released in late May 2022. This was a minor release that fixed an issue with ds.variables when there were a) many variables and b) CDO version above 2.0.0.

#### 4.3.11 Release of v0.4.4

Version 0.4.4 was released in late May 2022.

This version introduces a new class called *Matchpoint* which will allow automated matchups between netCDF files and point observations in pandas dataframes. This class is created using nc.open\_matchpoint. Matchups are generated by using the add\_data, add\_points, add\_depths, and matchup methods.

For datasets, ds now provides a more informative summary of dataset contents.

The split method now automatically sorts the files, so that they are sorted by date when temporal splitting occurs.

The methods surface, merge\_time and tvariance` have been removed after periods of deprecation. Use top, merge and tvar instead.

#### 4.3.12 Release of v0.4.3

Version 0.4.3 was released in May 2022. This is release with some new methods, improvements to internals some bug fixes. Code written for previous 0.4x versions of nctoolkit will be compatible.

This version will be compatible with CDO versions 2.0.5x.

A new function open\_geotiff will allow GeoTiff files to be opened. This is a wrapper around rioxarray, which will convert the GeoTiff to NetCDF. It will require rioxarray to be installed.

A new method surface\_mask has been added to enable identifying top levels with data in cases when there are missing values in the actual top level.

A new method is\_corrupt has been added. This can identify whether NetCDF files are likely to be corrupt. Under-the hood, methods will now suggest running is\_corrupt when system errors imply the files are corrupt.

The methods to\_xarray and to\_dataframe no long accept the *cdo\_times* argument, as this has essentially been redundant for a few nctoolkit versions.

The plot method now lets users send kwargs to hyplot to make customizations, such as log-scales an option. This will require the latest version of ncplot.

The select method now lets user select days of month, using ds.select(day = 1).

The split method now allows splitting by timestep using split("timestep").

#### 4.3.13 Release of v0.4.2

Version 0.4.2 was released in March 2022.

This is a minor release with a couple of method enhancements. Plots can now be saved to html files using the *out* arguments. The nco\_command method now works over multiple cores when these are set using nc.options.

#### 4.3.14 Release of v0.4.1

Version 0.4.1 was released in March 2022. This is a minor release focusing on improving nctoolkit internals.

A new method, called check is introduced that can be used to troubleshoot data problems and to ensure there are no obvious data issues (such as a lack of CF-compliance).

Users can now access dataset calendars using ds.calendar.

The drop method now lets you remove time steps using the times argument.

The dataset attribute *variables\_detailed* is now removed after being replaced by *contents* in version 0.3.9.

This version will recommend CDO versions greater than 1.9.7, because ensuring nctoolkit compatibility with earlier versions was becoming difficult and likely of little need to users.

Some coding improvements have enhanced the performance of the add, subtract etc. methods.

Bug fixes: The methods multiply etc. failed when datasets did not have time as a dimension in version 0.4.0. This is now fixed. Previously, *ds.contents* always returned None for the number of time steps. Now fixed.

#### 4.3.15 Release of v0.4.0

Version 0.4.0 was released in January 2022. This is a major release that features some breaking changes. Methods for adding, subtracting, multipling and substracting datasets from each other will be enhanced. Until now these methods used a simplistic approach values from matching time steps were added to each other, etc. So if you are subtracting a 12 time step file from a dataset, only the first 12 time steps were subtracted from. However, often this is not what you want. For example, you might want to subtract yearly months from a file which contains monthly values for each year.

This version of nctoolkit updates these methods so that it can figure out what kind of addition etc. it should carry out. For example, if you have a dataset which has monthly values for each year from 1950 to 1999, and use subtract to subtract the values from a file which contains annual means for each year from 1950, it will subtract the annual mean for 1950 from each month in 1950 and the the annual mean for 1951 from each month in 1951, and so on.

Users are now able to specify the numeric precision of datasets using ds.set\_precision. By default uses the underlying netCDF file's data type. This is normally not a problem. However, when the data type is integer, this can cause problems. nc.open\_data has been updated with this issue in mind. It will now warn users when the data type of the netCDF is integer, and it suggested switching to float 'F64' or 'F32'.

The drop method has been enhanced. It now accepts day, month and year as arguments to enable dropping specific time periods. For example ds.drop(month = 2, day = 29) will remove leap days. Code written to use the old drop method will now fail, as keywords are now required.

The method surface has now been renamed top for consistency with bottom. surface is deprecated and will be removed in a few months.

The split method now allows users to split datasets into multiple files by variable.

ds.times now returns a datetime object, not a str as before.

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### 4.3.16 Release of v0.3.9

Version 0.3.9 was released in November 2021. This is minor release focusing on under-the-hood improvements and new methods.

A new method, from\_xarray is added for converting xarray datasets to nctoolkit datasets.

Methods for identifying how many missing values appear in datasets have been added:  $na\_count$  and  $na\_frac$ . These will identify the number or fraction of values that are missing values in each grid cell. The methods operate the same way as the temporal methods. So  $ds.na\_frac$  ("year") will result in what fraction of values are missing values each year.

Methods for better upscaling of datasets will be added: box\_mean, box\_sum, box\_max. This will allow you to upscale to, for example, each 10 by 10 grid box using the mean of that grid box. This is useful for upscaling things like population data where you want the upscaled grid boxes to represent the entirety of the grid box, not the centre.

Improvements to merge have been made. When variables are not included in all files nctoolkit will now only merge those in each file in a multi-file dataset. Previously it threw an error.

Functions for finding the times and months in netCDF files are now available: nc\_years and ``nc\_months`.

The attribute variables\_detailed has been changed to contents. It will also now give the number of time steps available for each variable.

cdo\_command now allows users to specify whether the CDO command used is an ensemble method. Previously methods applied on a file by file basis.

#### 4.3.17 Release of v0.3.8

Version 0.3.8 was released in October 2021. This is a minor release, focusing on under-the-hood improvements and introducing better handling of files with varying vertical layers.

A method, vertical\_integration for calculating vertically integrated totals for netCDF data of the likes of oceanic data, where the vertical levels vary spatially, were introduced. vertical\_mean has been improved and can now calculate vertical mean in cases where the cell thickness varies in space.

merge\_time is deprecated, and its functionality will be incorporated into merge. So, following this release ensemble merging should use merge.

open\_url is now able to handle multiple urls. Previously it could only handle one.

Some under-the-hood improvements have been made to assign to ensure that truth statements do not occassionally throw an error.

#### 4.3.18 Release of v0.3.7

Version 0.3.7 was released in August 2021. This is a minor release.

New mathematical methods for simple operations on variables were added: abs, power, square, sqrt, exp, log and log10. These methods match numpy names.

Bug fixes: assign previously did not work with log10. Now fixed.

compare\_all was deleted after a period of deprecation.

#### 4.3.19 Release of v0.3.6

Version 0.3.6 was released in July 2021. This was a minor release.

New methods ensemble\_var and ensemble\_stdev were introduced for calculating variance and standard deviation across ensembles. The method tvariance will be deprecated and is now renamed tvar for naming consistency.

#### 4.3.20 Release of v0.3.5

Version 0.3.5 was released in May 2021.

This is a minor release focusing on some under-the-hood improvements in performance and a couple of new methods.

It drops support for CDO version 1.9.3, as this is becoming too time-consuming to continue given the increasingly low reward.

A couple of new methods have been added. distribute enables files to be split up spatially into equally sized m by n rectangles. collect is the reverse of distribute. It will collect distributed data into one file.

In prior releases assign calls could not be split over multiple lines. This is now fixed.

There was a bug in previous releases where regrid did not work with multi-file datasets. This was due to the enabling of parallel processing with nctoolkit. The issue is now fixed.

The deprecated methods mutate and assign have now been removed. Variable creation should use assign.

#### 4.3.21 Release of v0.3.4

Version 0.3.3 was released in April 2021.

This was a minor release focusing on performance improvements, removal of deprecated methods and introduction of one new method.

A new method fill\_na has been introduced that allows missing values to be filled with the distanced weighted average.

The methods remove\_variables and cell\_areas have been removed and are replaced permanently by drop and cell\_area.

#### 4.3.22 Release of v0.3.2

Version 0.3.2 was released in March 2021. This was a quick release to fix a bug causing to\_nc to not save output in the base directory.

#### 4.3.23 Release of v0.3.1

Version 0.3.1 was released in March 2021. This is a minor release that includes new methods, under-the-hood improvements and the removal of deprecated methods.

New methods are introduced for identifying the first time step will specific numerical thresholds are first exceeded or fallen below etc: first\_above, first\_below, last\_above and last\_below. The thresholds are either single numbers or can come from a gridded dataset for grid-cell specific thresholds.

Methods to compare a dataset with another dataset or netCDF file have been added: gt and lt, which stand for 'greater than' and 'less than'.

Users are be able to recycle the weights calculated when interpolating data. This can enable much faster interpolation of multiple files with the same grid.

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The temporal methods replaced by tmean etc. have now been removed from the package. So monthly\_mean etc. can no longer be used.

#### 4.3.24 Release of v0.3.0

Version 0.3.0 was released in February 2021. This will be a major release introducing major improvements to the package.

A new method assign is now available for generating new variables. This replaces the mutate and transmute, which were place-holder functions in the early releases of nctoolkit until a proper method for creating variables was put in place. assign operates in the same way as the assign method in Pandas. Users can generate new variables using lambda functions.

A major-change in this release is that evaluation is now lazy by default. The previous default of non-lazy evaluation was designed to make life slightly easier for new users of the package, but it is probably overly annoying for users to have to set evaluation to lazy each time they use the package.

This release features a subtle shift in how datasets work, so that they have consistent list-like properties. Previously, the files in a dataset given by the `current` attribute could be both a str or a list, depending on whether there was one or more files in the dataset. This now always gives a list. As a result datasets in nctoolkit have list-like properties, with `append and remove methods available for adding and removing files. remove is a new method in this release. As before datasets are iterable.

This release will also allow users to run nctoolkit in parallel. Previous releases allowed files in multi-file datasets to be processed in parallel. However, it was not possible to create processing chains and process files in parallel. This is now possible in version thanks to under-the-hood changes in nctoolkit's code base.

Users are now able to add a configuration file, which means global settings do not need to be set in every session or in every script.

#### 4.4 Datasets

#### 4.4.1 Data format requirements

nctoolkit requires NetCDF data that follow the GDT, COARDS or CF Conventions. Its computational backend is CDO, which be able to carry out most operations regardless of whether it is compliant with those conventions. In general, most data producers follow CF-conventions when generating NetCDF files, however if you are unclear if you are working with compliant files you can check here.

### 4.4.2 Opening datasets

There are 3 ways to create a dataset: open\_data, open\_url or open\_thredds.

If the data you want to analyze is available on your computer use open\_data. This will accept either a path to a single file or a list of files. It will also accept wildcards.

If you want to use data that can be downloaded from a url, just use open\_url. This will download the netCDF files to a temporary folder, and it can then be analyzed.

If you want to analyze data that is available from a thredds server or OPeNDAP, then use open\_thredds. The file paths should end with .nc.

#### [1]: import nctoolkit as nc

```
nctoolkit is using Climate Data Operators version 2.0.5
```

If you want to get a quick overview of the contents of a dataset, we can use the contents attribute. This will display a dataframe showing the variables available in the dataset and details about the variable, such as the units and long names. The example below opens a sea-surface temperature dataset and displays the contents.

```
[2]: ds = nc.open_thredds("https://psl.noaa.gov/thredds/dodsC/Datasets/COBE2/sst.mon.ltm.1981-
     →2010.nc")
    ds
[2]: <nctoolkit.DataSet>:
    Number of files: 1
    File contents:
             variable ntimes npoints nlevels
               long_name unit data_type
    0
                                               1 Long Term Mean Monthly Means of Global Sea
                  sst
                           12
                                 64800
     →Surface Temperature degC
                                      F32
                           12
                                                                        count of non-missing_
    1 valid_yr_count
                                 64800
                                              1
     →values used in mean None
                                      I16
```

### 4.4.3 Checking validity of source data

nctoolkit should work out of the box with most NetCDF data. However, it is possibly the format of the data could be incompatible with the system libraries used by nctoolkit or the files could be corrupt. To carry out a general check on the data use the check method as follows:

This will carry out some basic checks on data format compatability. You should install the cfchecker package if you want check to check for CF-compliance.

If you want to check if the files in a dataset are corrupt, the following should tell you. This will simply read and write the data in the source files to a temporary file, which should be sufficient to ensure files are not corrupt.

```
[4]: ds.is_corrupt()
```

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```
[4]: False
```

### 4.4.4 Modifying datasets

If you want to modify a dataset, you just need to use nctoolkit's built in methods. These methods operate directly on the dataset itself. The example below selects the first time step in a sea surface temperature dataset and plots the result.

```
ds = nc.open_thredds("https://psl.noaa.gov/thredds/dodsC/Datasets/COBE2/sst.mon.ltm.1981-2010.nc") ds.select(time = 0) ds.plot()
```

Underlying datasets are temporary files representing the current state of the dataset. We can access this using the current attribute:

```
[5]: ds.current
[5]: ['https://psl.noaa.gov/thredds/dodsC/Datasets/COBE2/sst.mon.ltm.1981-2010.nc']
```

In this case, we have a single temporary file. Any temporary files will be generated and deleted, as needed, so there should be no need to manage them yourself.

### 4.4.5 Lazy evaluation by default

Look at the processing chain below.

What is potentially wrong with this? It carries out four operations, so we absolutely do not want to create temporary file in each step. So instead of evaluating the operations line by line, nctoolkit only evaluates them either when you tell it to or it has to. So in the code example above we have told, nctoolkit what to do to that dataset, but have not told it to actually do any of it.

We can see this if we look at the current state of the dataset. It is still the starting point:

```
[7]: ds.current
[7]: ['https://psl.noaa.gov/thredds/dodsC/Datasets/COBE2/sst.mon.ltm.1981-2010.nc']
```

If we want to evaluate this we can use the run method or methods such as plot that require commands to be evaluated.

```
[8]: ds.run()
ds.current

[8]: ['/tmp/nctoolkitcvbxvolgnctoolkittmp_p_p_7rk.nc']
```

This method chaining ability within nctoolkit comes from Climate Data Operators (CDO), which is the backend computational engine for nctoolkit. nctoolkit does not require you to understand CDO, but if you want to see the underlying CDO commands used, just use the history attribute. In the example, below, you can see that 4 lines of Python code have been converted to a single CDO command.

Then if we run this, we can see the full command used:

```
[10]: ds.run() ds.history
```

If you want to visualize a dataset, you just need to use plot:

→out of range

Data type cannot be displayed: application/javascript, application/vnd.holoviews\_load.v0+json

/local1/data/scratch/rwi/miniconda3/envs/nctoolkit/lib/python3.8/site-packages/nctoolkit/
api.py:706: UserWarning: The variable valid\_yr\_count has integer data type. Consider\_
setting data type to float 'F64' or 'F32' using set\_precision.
/local1/data/scratch/rwi/miniconda3/envs/nctoolkit/lib/python3.8/site-packages/xarray/
coding/times.py:673: SerializationWarning: Unable to decode time axis into full numpy.
datetime64 objects, continuing using cftime.datetime objects instead, reason: dates\_
out of range
/local1/data/scratch/rwi/miniconda3/envs/nctoolkit/lib/python3.8/site-packages/xarray/
core/indexing.py:423: SerializationWarning: Unable to decode time axis into full numpy.
datetime64 objects, continuing using cftime.datetime objects instead, reason: dates\_
out of range
/local1/data/scratch/rwi/miniconda3/envs/nctoolkit/lib/python3.8/site-packages/xarray/
coding/times.py:673: SerializationWarning: Unable to decode time axis into full numpy.
datetime64 objects, continuing using cftime.datetime objects instead, reason:dates\_
datetime64 objects, continuing using cftime.datetime objects instead, reason:dates\_
datetime64 objects, continuing using cftime.datetime objects instead, reason:

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(continued from previous page)

```
/local1/data/scratch/rwi/miniconda3/envs/nctoolkit/lib/python3.8/site-packages/xarray/

→core/indexing.py:423: SerializationWarning: Unable to decode time axis into full numpy.

→datetime64 objects, continuing using cftime.datetime objects instead, reason: dates_out of range

[11]: :DynamicMap [Variable]
    :Overlay
    .Image.I :Image [lon,lat] (sst)
    .Coastline.I :Feature [Longitude,Latitude]
```

### 4.4.6 Method chaining

When you start to use nctoolkit it is important to realize that it does not allow method chaining in the way pandas and xarray do. So the following will not work:

```
[12]: (
          ds
          .tmean()
          .spatial_mean()
          .add(1)
      )
      AttributeError
                                                 Traceback (most recent call last)
      Input In [12], in <cell line: 2>()
            1 (
      ---> 2
            3
                  .tmean()
                   .spatial_mean()
            4
            5
                  .add(1)
            6)
      AttributeError: 'NoneType' object has no attribute 'spatial_mean'
```

This is because this type of method chaining requires the methods to return an object. However, nctoolkit's methods in general do not return objects. Instead they modify them.

You would need to do the following instead:

```
[13]: ds.tmean()
  ds.spatial_mean()
  ds.add(1)
```

### 4.4.7 Dataset attributes

You can find out key information about a dataset using its attributes. If you want to know the variables available in a dataset called ds, we would do:

```
[14]: ds.variables
[14]: ['sst', 'valid_yr_count']
```

If you want more details about the variables, access the contents attribute. This will tell you details such as long names, units, number of time steps etc. for each variable.

```
[15]: ds.contents
[15]:
               variable ntimes npoints nlevels \
                                   64800
                    sst
                              1
                                                1
     1 valid_yr_count
                              1
                                   64800
                                                1
                                                 long_name unit data_type
        Long Term Mean Monthly Means of Global Sea Sur...
                                                            degC
                                                                       F32
     1
                  count of non-missing values used in mean None
                                                                       I16
```

If you want to know the vertical levels available in the dataset, we use the following.

```
[16]: ds.levels
[16]: [0.0]
```

If you want to know the files in a dataset, we would do this. nctoolkit works by generating temporary files, so if you have carried out any operations, this will show a list of temporary files.

```
[17]: ds.current
[17]: ['/tmp/nctoolkitcvbxvolgnctoolkittmp4vxeymsc.nc']
```

If you want to find out what times are in the dataset we do this:

```
[18]: ds.times
[18]: [datetime.datetime(1, 1, 1, 0, 0)]
```

If you want to find out what months are in the dataset:

```
[19]: ds.months
[19]: [1]
```

If you want to find out what years are in the dataset:

We can also access the history of operations carried out on the dataset. This will show the operations carried out by nctoolkit's computational back-end CDO:

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# 4.5 Importing and exporting data

nctoolkit can work with data available on local file systems, urls and over thredds and OPeNDAP.

### 4.5.1 Opening single files and ensembles

If you want to import a single netCDF file as a dataset, do the following:

```
import nctoolkit as nc
ds = nc.open_data(infile)
```

The *open\_data* function can also import multiple files. This can be done in two ways. If we have a list of files we can do the following:

```
import nctoolkit as nc
ds = nc.open_data(file_list)
```

Alternatively, *open\_data* is capable of handling wildcards. So if we have a folder called data, we can import all files in it as follows:

```
import nctoolkit as nc
ds = nc.open_data("data/*.nc")
```

### 4.5.2 Opening files from urls/ftp

If we want to work with a file that is available at a url or ftp, we can use the *open\_url* function. This will start by downloading the file to a temporary folder, so that it can be analysed.

```
import nctoolkit as nc
ds = nc.open_url(www.foo.nc)
```

### 4.5.3 Opening data available over thredds servers or OPeNDAP

If you want to work with data that is available over a thredds server or OPeNDAP, you can use the *open\_thredds* method. This will require that the url ends with ".nc".

```
import nctoolkit as nc
ds = nc.open_thredds(www.foo.nc)
```

### 4.5.4 Exporting datasets

nctoolkit has a number of built in methods for exporting data to netCDF, pandas dataframes and xarray datasets.

### 4.5.5 Save as a netCDF

The method to\_nc lets users export a dataset to a netCDF file. If you want this to be a zipped netCDF file use the zip method before to to\_nc. An example of usage is as follows:

```
ds = nc.open_data(infile)
ds.tmean()
ds.zip()
ds.to_nc(outfile)
```

### 4.5.6 Convert to pandas dataframe

The method to\_dataframe lets users export a dataset to a pandas dataframe.

```
ds = nc.open_data(infile)
ds.tmean()
df = ds.to_dataframe()
```

### 4.5.7 Interacting with xarray datasets

If you want to move between nctoolkit and xarray dataset, you can use from\_xarray and to\_xarray.

The method to\_xarray lets users export a dataset to an xarray dataset. An example of usage is as follows:

```
ds = nc.open_data(infile)
ds.tmean()
xr_ds = ds.to_xarray()
```

If you want to convert an xarray dataset to an nctoolkit dataset, you can just the from\_xarray function, as follows:

### 4.5.8 Exporting subsets of data

If you want to only export a subset of the data you can do this by providing additional args to the to\_nc, to\_xarray and to\_dataframe methods. These args will then be sent to the subset method.

For example, if you only wanted to export the year 2000 to xarray, you would do the following:

```
ds.to\_xarray(year = 2000)
```

Or if you wanted a spatial subset of the data you could do this:

```
ds.to\_xarray(lon = [0, 90], lat = [0, 90])
```

# 4.6 Subsetting data

nctoolkit has many built in methods for subsetting data. The main method is subset. This let's you select specific variables, years, months, seasons and timesteps.

### 4.6.1 Selecting variables

If you want to select specific variables, you would do the following:

```
ds.subset(variables = ["var1", "var2"])
```

If you only want to select one variable, you can do this:

```
ds.subset(variables = "var1")
```

### 4.6.2 Selecting years

If you want to select specific years, you can do the following:

```
ds.subset(years = [2000, 2001])
```

Again, if you want a single year the following will work:

```
ds.subset(years = 2000)
```

The select method allows partial matches for its arguments. So if we want to select the year 2000, the following will work:

```
ds.subset(year = 2000)
```

In this case we can also select a range. So the following will work:

```
ds.subset(years = range(2000, 2010))
```

### 4.6.3 Selecting months

You can select months in the same way as years. The following examples will all do the same thing:

```
ds.subset(months = [1,2,3,4])
ds.subset(months = range(1,5))
ds.subset(mon = [1,2,3,4])
```

#### 4.6.4 Selecting seasons

You can easily select seasons. For example if you wanted to select winter, you would do the following:

```
ds.subset(season = "DJF")
```

### 4.6.5 Selecting timesteps

You can select specific timesteps from a dataset in a similar manner. For example if you wanted to select the first two timesteps in a dataset the following two methods will work:

```
ds.subset(time = [0,1])
ds.subset(time = range(0,2))
```

### 4.6.6 Geographic subsetting

If you want to select a geographic subregion of a dataset, you can use crop. This method will select all data within a specific longitude/latitude box. You just need to supply the minimum longitude and latitude required. In the example below, a dataset is cropped with longitudes between -80 and 90 and latitudes between 50 and 80:

```
ds.crop(lon = [-80, 90], lat = [50, 80])
```

Alternatively, you can use the subset method:

```
ds.subset(lon = [-80, 90], lat = [50, 80])
```

### 4.7 Interpolation

nctoolkit features built in methods for horizontal and vertical interpolation.

### 4.7.1 Horizontal interpolation

We will illustrate how to carry out horizontal interpolation using a global dataset of global SST from NOAA. Find out more information about the datset here.

The data is available using a thredds server. So we will work with the first time step, which looks like this:

```
[1]: import nctoolkit as nc
    ds = nc.open_thredds("https://psl.noaa.gov/thredds/dodsC/Datasets/COBE2/sst.mon.mean.nc")
    ds.select(time = 0)
    ds.plot()
    nctoolkit is using Climate Data Operators version 1.9.10
```

Data type cannot be displayed: application/javascript, application/vnd.holoviews\_load.v0+json

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```
[1]: :Overlay
    .Image.I :Image [lon,lat] (sst)
    .Coastline.I :Feature [Longitude,Latitude]
```

### 4.7.2 Interpolating to a set of coordinates

If you want to regrid a dataset to a specified set of coordinates you can **regrid** and a pandas dataframe. The first column of the dataframe should be the longitudes and the second should be latitudes. The example below regrids a sea-surface temperature dataset to a single location with longitude -30 and latitude 50.

```
[2]: import pandas as pd
    ds = nc.open_thredds("https://psl.noaa.gov/thredds/dodsC/Datasets/COBE2/sst.mon.mean.nc")
    ds.select(timestep = 0)
    coords = pd.DataFrame({"lon":[-30], "lat":[50]})
    ds.regrid(coords)
    ds.to_dataframe()
[2]:
                         lon
                               lat
                                           sst
     time
                ncells
     1850-01-01 0
                       -30.0
                              50.0
                                   10.935501
```

### 4.7.3 Interpolating to a regular Ionlat grid

If you want to interpolate to a regular latlon grid, you can use to\_latlon. lon and lat specify the minimum and maximum longitudes and latitudes, while res, a 2 variable list specifies the resolution. For example, if we wanted to regrid the globe to 0.5 degree north-south by 1 degree east-west resolution, we could do the following:

### 4.7.4 Interpolating to another dataset's grid

If we are working with two datasets and want to put them on a common grid, we can interpolate one onto the other's grid. We can illustate this with a dataset of global sea surface temperature. Let's start by cropping this dataset to the northern hemisphere.

```
[4]: :Overlay
    .Image.I :Image [lon,lat] (sst)
    .Coastline.I :Feature [Longitude,Latitude]
```

Now, we can regrid the original file to this northern hemisphere grid.

This method will also work using netCDF files. So, if you wanted you can also use a path to a netCDF file as the target grid.

### 4.7.5 How to reuse the weights for regridding

Under the hood nctoolkit regrids data by first generating a weights file. There are situations where you will want to be able to re-use these weights. For example, if you are post-processing a large number of files one after the other. To make this easier nctoolkit let's you recycle the regridding info. This let's you interpolate using either regrid or to\_latlon, but keep the regridding data for future use by regrid.

```
[6]: ds = nc.open_thredds("https://psl.noaa.gov/thredds/dodsC/Datasets/COBE2/sst.mon.mean.nc")
    ds.select(timestep = 0)
    ds.to_latlon(lon = [-79.5, 79.5], lat = [-0.75, 89.75], res = [1, 0.5], recycle = True)
    ds.plot()
[6]: :0verlay
        .Image.I
                     :Image
                               [lon, lat]
                                           (sst)
        .Coastline.I :Feature
                                 [Longitude, Latitude]
[7]: ds1 = nc.open_thredds("https://psl.noaa.gov/thredds/dodsC/Datasets/COBE2/sst.mon.mean.nc
    ds1.select(timestep = 0)
    ds1.regrid(ds)
    ds1.plot()
[7]: :Overlay
        .Image.I
                     :Image
                               [lon, lat]
                                           (sst)
        .Coastline.I :Feature
                                 [Longitude, Latitude]
```

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### 4.7.6 Horizontal Resampling

If you want to make data more coarse spatially, just use the resample\_grid method. This will, for example, let you select every 2nd grid grid cell in a north-south and east-west direction. This is illustrated in the example below, where a dataset which has spatial resolution of 1 by 1 degrees is coarsened, so that only every 10th cell is selected in a north-south and east-west. In other words it is now a 10 degrees by 10 degrees dataset.

```
[8]: ds = nc.open_thredds("https://psl.noaa.gov/thredds/dodsC/Datasets/COBE2/sst.mon.mean.nc")
    ds.select(timestep = 0)
    ds.resample_grid(10)
    ds.plot()

[8]: :Overlay
        .Image.I :Image [lon,lat] (sst)
        .Coastline.I :Feature [Longitude,Latitude]
```

### 4.7.7 Spatial Infilling

Some times you will have data with missing values, which you want to replace with a nearby value. nctoolkit handles this situation using the fill\_na method. This uses distance-weighting. You just need to specify the number of nearest-neighbours to use for the weighting. For example, if you simply want to replace missing values with their nearest neighbour, you just set the number to 1, as follows:

```
[9]: ds = nc.open_thredds("https://psl.noaa.gov/thredds/dodsC/Datasets/COBE2/sst.mon.mean.nc")
    ds.select(timestep = 0)
    ds.fill_na(1)
    ds.plot()

[9]: :Overlay
        .Image.I :Image [lon,lat] (sst)
        .Coastline.I :Feature [Longitude,Latitude]
```

### 4.7.8 Vertical interpolation

We can carry out vertical interpolation using the vertical\_interp method. This is particularly useful for oceanic data. This is illustrated below by interpolating depth-resolved ocean temperatures from NOAA's World Ocean Atlas for January to a depth of 500 metres. The vertical\_interp method requires a levels argument, which is sea-depth in this case.

[]:

# 4.8 Plotting

nctoolkit provides automatic plotting of netCDF data in a similar way to the command line tool neview.

If you have a dataset, simply use the plot method to create an interactive plot that matches the data type.

We can illustate this using a sea surface temperature dataset available here.

Let's start by calculating mean sea surface temperature for the year 2000 and plotting it:

```
[1]: import nctoolkit as nc
     ff = "sst.mon.mean.nc"
     ds = nc.open_data(ff)
     ds.select(year = 2000)
     ds.tmean()
     ds.plot()
     nctoolkit is using Climate Data Operators version 1.9.10
       Data type cannot be displayed: application/javascript, application/vnd.holoviews load.v0+json
       Data type cannot be displayed: application/javascript, application/vnd.holoviews_load.v0+json
       Data type cannot be displayed: application/javascript, application/vnd.holoviews_load.v0+json
       Data type cannot be displayed: application/javascript, application/vnd.holoviews_load.v0+json
[1]: :Overlay
         .Image.I
                        :Image
                                   [lon, lat]
                                                 (sst)
         .Coastline.I :Feature
                                     [Longitude, Latitude]
```

We might be interested in the zonal mean. nctoolkit can automatically plot this easily:

```
[2]: ff = "sst.mon.mean.nc"
    ds = nc.open_data(ff)
    ds.select(year = 2000)
    ds.tmean()
    ds.zonal_mean()
    ds.plot()

[2]: :DynamicMap [variable]
    :Curve [lat] (value)
```

nctoolkit can also easily handle heat maps. So, we can easily plot the change in zonal mean over time:

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```
[3]: ff = "sst.mon.mean.nc"
   ds = nc.open_data(ff)
   ds.zonal_mean()
   ds.annual_anomaly(baseline = [1850, 1869], window = 20)
   ds.plot()

[3]: :QuadMesh [time,lat] (sst)
```

In a similar vein, it can automatically handle time series. Below we plot a time series of global mean sea surface temperature since 1850:

```
[4]: ff = "sst.mon.mean.nc"
    ds = nc.open_data(ff)
    ds.spatial_mean()
    ds.plot()

[4]: :DynamicMap [variable]
    :Curve [time] (value)
```

# 4.8.1 Internal: ncplot

Plotting is carried out using the ncplot package. If you come across any errors, please raise an issue here.

This is a package that aims to deliver easy use. Colour scales for heat map default to a diverging blue-to-red pallette when there are positives and negatives and a viridis palette otherwise.

# 4.9 Temporal statistics

nctoolkit has a number of built-in methods for calculating temporal statistics, all of which are prefixed with t: tmean, tmin, tmax, trange, tpercentile, tmedian, tvariance, tstdev and tcumsum.

These methods allow you to quickly calculate temporal statistics over specified time periods using the over argument.

By default the methods calculate the value over all time steps available. For example the following will calculate the temporal mean:

```
import nctoolkit as nc
ds = nc.open_data("sst.mon.mean.nc")
ds.tmean()
```

However, you may want to calculate, for example, an annual average. To do this we use **over**. This is a list which tells the function which time periods to average over. For example, the following will calculate an annual average:

```
ds.tmean(["year"])
```

If you are only averaging over one time period, as above, you can simply use a character string:

```
ds.tmean("year")
```

The possible options for over are "day", "month", "year", and "season". In this case "day" stands for day of year, not day of month.

In the example below we are calculating the maximum value in each month of each year in the dataset.

```
ds.tmax(["month", "year"])
```

# 4.9.1 Calculating rolling averages

nctoolkit has a range of methods to calcate rolling averages: rolling\_mean, rolling\_min, rolling\_max, rolling\_range and rolling\_sum. These methods let you calculate rolling statistics over a specified time window. For example, if you had daily data and you wanted to calculate a rolling weekly mean value, you could do the following:

```
ds.rolling_mean(7)
```

If you wanted to calculated a rolling weekly sum, this would do:

```
ds.rolling_sum(7)
```

# 4.9.2 Calculating anomalies

nctoolkit has two methods for calculating anomalies: annual\_anomaly and monthly\_anomaly. Both methods require you to specify a baseline period to calculate the anomaly against. They require that you specify a baseline period showing the minimum and maximum years of the climatological period to compare against.

So, if you wanted to calculate the annual anomaly compared with a baseline period of 1950-1969, you would do this:

```
ds.annual_anomaly(baseline = [1950, 1969])
```

By default, the annual anomaly is calculated as the absolute difference between the annual mean in a year and the mean across the baseline period. However, in some cases this is not suitable. Instead you might want the relative change. In that case, you would do the following:

```
ds.annual_anomaly(baseline = [1950, 1969], metric = "relative")
```

You can also smooth out the anomalies, so that they are calculated on a rolling basis. The following will calculate the anomaly using a rolling window of 10 years.

```
ds.annual_anomaly(baseline = [1950, 1969], window = 10)
```

Monthly anomalies are calculated in the same way:

```
ds.monthly_anomaly(baseline = [1950, 1969]
```

Here the anomaly is the difference between the value in each month compared with the mean in that month during the baseline period.

# 4.9.3 Calculating climatologies

This means we can easily calculate climatologies. For example the following will calculate a seasonal climatology:

```
ds.tmean("season")
```

These methods allow partial matches for the arguments, which means you do not need to remember the precise argument each time. For example, the following will also calculate a seasonal climatology:

```
ds.tmean("Seas")
```

Calculating a climatological monthly mean would require the following:

```
ds.tmean("month")
```

and daily would be the following:

```
ds.tmean("day")
```

# 4.9.4 Calculating climatologies

This means we can easily calculate climatologies. For example the following will calculate a seasonal climatology:

```
ds.tmean("season")
```

#### 4.9.5 Cumulative sums

We can calculate the cumulative sum as follows:

```
ds.tcumsum()
```

Please note that this can only calculate over all time periods, and does not accept an over argument.

## 4.10 Multi-file datasets

nctoolkit is built to handle multi-file datasets easily and efficiently. Parallel processing of files, ensemble averaging and merging are all easily done.

To create a multi-file dataset, you just need to supply a list of files to open\_data. Alternatively, you can use wild cards. The following will create a multi-file dataset with all of the files in the foo folder:

```
import nctoolkit as nc
ds = nc.open_data("foo/*.nc")
```

Standard nctoolkit methods can then be applied to each file within the ensemble. For example, if we wanted a temporal mean of each file, we would do the following:

```
ds.tmean()
```

Note, to avoid any confusion: this operation will only apply to individual members of the multi-file dataset. We will later discuss ensemble methods such as ensemble\_mean, which let you calculate statistics across the ensemble.

# 4.10.1 Merging multi-file datasets

There are two ways to merge mult-file datasets, time-based and variable-based.

Merging by time is done as follows:

```
ds.merge("time")
```

This will join files together so that their times join up. It should be used when files have the same variables and grids, but distinct times.

The second merging method is joining variables. In this case files should have the same time steps or one file should have at most one time step. This is done as follows:

```
ds.merge("variable")
```

By default, nctoolkit uses variable-based merging.

# 4.10.2 Speeding up multi-file processing

If you have access to multiple cores, it is very easy to ensure files within a multi-file dataset are processed in parallel. Just set the number of cores to be used. In the following case, we set it to 6:

```
nc.options(6)
```

This results in files being processed simultaneously with 6 cores.

If you are working on multi-file datasets, it is almost always much faster to set the number of cores to a high number and carry out operations on the files before merging them using merge and not the other way round.

## 4.10.3 Ensemble statistics

In some cases, you will want to calculate averages etc. across the multi-file dataset. For example, each file in a dataset could be from a different climate model and you might simply the mean value across them. This is very easily done. We can just calculate the ensemble mean as follows:

```
ds.ensemble_mean()
```

This will calculate the mean for each time step. For example, if you have an ensemble which is made of monthly projections of temperature from 20 different climate models, ensemble\_mean will calculate the monthly mean of those 20 models.

Multiple ensemble methods are available: ensemble\_mean, ensemble\_percentile, ensemble\_stdev, ensemble\_var, ensemble\_max, ensemble\_min, ensemble\_range and ensemble\_sum.

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# 4.11 Matchups with point data

A common challenge when working with netCDF data is matching up with point data. This is often difficult because point data is sparse both spatially and temporally, and when working in the ocean this data can be at varying depths. From version 0.4.7 on, nctoolkit includes the ability to match datasets to spatiotemporal dataframes. Here we will provide an overview of how to do this.

# 4.11.1 Matching data at specific locations

First, we will illustrate how matchpoint works for data at specific spatial locations and depths. After this we will deal with different times. The data will be ocean nitrate from NOAA's World Ocean Atlas.

We can download part of it as follows:

This is a subset of the data covering a large part of the North Atlantic, and it has nitrate values from the sea surface to the sea floor.

```
[2]: ds.plot()
```

Data type cannot be displayed: application/javascript, application/vnd.holoviews\_load.v0+json

Data type cannot be displayed: application/javascript, application/vnd.holoviews\_load.v0+json

Data type cannot be displayed: application/javascript, application/vnd.holoviews\_load.v0+json

Data type cannot be displayed: application/javascript, application/vnd.holoviews load.v0+json

/home/robert/miniconda3/envs/notebook/lib/python3.9/site-packages/ncplot/plot.py:181:□

—UserWarning: Warning: xarray could not decode times!

```
[2]: :DynamicMap [depth]
     :Overlay
     .Image.I :Image [lon,lat] (n_an)
     .Coastline.I :Feature [Longitude,Latitude]
```

Now, let's say we had the following dataframe of 4 coordinates and depths. How would we identify the nitrate values using nctoolkit?

```
[3]: import pandas as pd
    df = pd.DataFrame({"lon":[-10, -12, -14, -16], "lat":[45, 50, 53, 55], "depth":[4, 2, 30,
     → 40]})
    df
[3]:
       lon lat
                  depth
       -10
              45
       -12
                      2
    1
              50
    2
       -14
              53
                     30
       -16
                     40
              55
```

Note: if we are matching datasets to dataframes, the dataframe columns must be named one of the following: 'lon', 'lat', 'depth', 'year', 'month' or 'day'.

If we want to match our dataset to this dataframe we use the match\_points method as follows:

```
[4]: ds.match_points(df)
     Depths assumed to be [0.0, 5.0, 10.0, 15.0, 20.0, 25.0, 30.0, 35.0, 40.0, 45.0, 50.0, 55.
     \rightarrow0, 60.0, 65.0, 70.0, 75.0, 80.0, 85.0, 90.0, 95.0, 100.0, 125.0, 150.0, 175.0, 200.0, \Box
     →225.0, 250.0, 275.0, 300.0, 325.0, 350.0, 375.0, 400.0, 425.0, 450.0, 475.0, 500.0, ...
     \rightarrow550.0, 600.0, 650.0, 700.0, 750.0, 800.0]
     All variables will be used
     Points will be matched for all time steps
[4]:
        lon
             lat
                  depth
                              n_an
                                    day
                                         month year
        -10
              45
                      4
                         5.661312
                                     16
                                              1
                                                 1958
                      2 8.932839
       -12
              50
                                     16
                                              1
                                                1958
       -14
              53
                      30
                         8.672163
                                     16
                                              1 1958
        -16
              55
                      40
                         6.973096
                                     16
                                              1
                                                1958
```

We now have the matchups required. The match\_points method returns a pandas dataframe with the desired matchups.

You will get messages from nctoolkit confirming some of the assumptions taken when matching up. In most cases these can be ignored. The only exception is with depths. nctoolkit will derive from these from the dataset, but some times this will not be appropriate. Just keep an eye out for the message and explicitly provide depths if necessary.

# 4.11.2 Spatial matchup approach

The approach taken to matching up data spatially is as follows. First, data is regridded horizontally using bilinear interpolation to the lon/lat pairs provided. If depths are provided the data is than interpolated vertically with 1d interpolation using scipy.

## 4.11.3 Spatiotemporal matchups

We will now illustrate how to do spatiotemporal matchups. This will be done with air temperature from the CMIP6 climate model GFDL-CM4. This is a large file, but it can be downloaded by clicking here. The dataset contains gridded daily air temperature for the earth between 1850 and 1859.

Let's start by matching it up with the following dataframe:

```
[5]: import nctoolkit as nc import pandas as pd (continues on next page)
```

(continued from previous page)

```
df = pd.DataFrame({"lon": [50, 60], "lat": [50, 45], "year":[1850, 1852], "month":[1, 3],
     → "day":[2, 3]})
    df
[5]:
       lon
            lat
                 year
                        month day
        50
                 1850
                                 2
              50
                            1
                 1852
                            3
                                 3
    1
        60
              45
```

This only contains two data points, but for different times. We can match up our dataset as before:

```
\rightarrowchecks = False)
   df_match = ds.match_points(df)
   df_match
   All variables will be used
[6]:
      lon
          lat
                           month
                                day
                   tas
                      year
     50.0
         50.0
              252.836945
                                 2
                      1850
                              1
   1 60.0
         45.0
              271.053040
                      1852
                              3
                                 3
```

As expected, we now have a pandas dataframe with the surface air temperature for the locations and times specified.

The match\_points method works in a similar way to the pandas merge method. So, if we only specified year and month, and ignore day, we would get every day for those years and months, as follows:

```
[7]: df_match = ds.match_points(df.drop(columns = "day"))
    df match
    All variables will be used
[7]:
          lon
                lat
                            tas year month
         50.0
               50.0
    0
                     254.234680
                                 1850
                                            1
                                                 1
                     252.836945
    1
        50.0
               50.0
                                 1850
                                            1
                                                 2
    2
        50.0
               50.0
                    252.467865
                                 1850
                                                 3
                                            1
               50.0
                                                 4
    3
        50.0
                     253.731049
                                 1850
                                            1
                                                 5
    4
        50.0
               50.0
                     245.843506
                                 1850
                                            1
                . . .
                             . . .
                                  . . .
     57
        60.0
              45.0
                    276.231720
                                 1852
                                                27
        60.0
    58
              45.0
                     277.647888
                                 1852
                                            3
                                                28
     59
        60.0
              45.0
                     275.756226
                                  1852
                                            3
                                                29
        60.0 45.0 274.968018 1852
                                                30
    60
                                            3
    61 60.0 45.0 277.621979 1852
                                                31
     [62 rows x 6 columns]
```

We now have each day for the given times.

# 4.11.4 Optional arguments

The match\_points method provided optional arguments that can refine the matchup process. These arguments are variables, tmean, top and nan.

They work as follows. If you only wanted to select a subset of variables you would use variables, as follows:

```
[8]: df_match = ds.match_points(df, variables = "tas")
```

In some cases, you have monthly point data, but your dataset has daily resolution. In this case you might want a monthly mean output. You can do this using the tmean argument:

```
[9]: df = pd.DataFrame({"lon": [50, 60], "lat": [50, 45], "year":[1850, 1852], "month":[1, 3]}
    df_match = ds.match_points(df, tmean = True)
    df_match
    All variables will be used
[9]:
        lon
              lat
                           tas year
                                      month
                                             day
       50.0
              50.0
                   256.112976
                                1850
                                          1
                                              16
    1 60.0
                                          3
             45.0
                   271.545959
                                1852
                                              16
```

This works by applying the dataset tmean method to the dataset with the temporal grouping in df. In this case this is the equivalent of running ds.tmean(["year", "month"]) on the dataset.

When you have a multi-level dataset, but only want the top level, you can set top=True in match\_points. Similarly, if you have a values in the dataset that should be set to missing values, you set them using the nan argument.

# 4.12 Mathematical operations

# 4.12.1 Creating new variables

Variable creation in nctoolkit can be done using the assign method, which works in a similar way to the method available in pandas.

The assign method works using lambda functions. Let's say we have a dataset with a variable 'var' and we simply want to add 10 to it and call the new variable 'new'. We would do the following:

```
ds.assign(new = lambda x: x.var + 10)
```

If you are unfamilar with lambda functions, note that the x after lambda signifies that x represents the dataset in whatever comes after ':', which is the actual equation to evaluate. The *x.var* term is *var* from the dataset.

By default assign keeps the original variables in the dataset. However, we may only want the new variable or variables. In that case you can use the drop argument:

```
ds.assign(new = lambda x: x.var+ 10, drop = True)
```

This results in only one variable.

Note that the assign method uses kwargs for the lambda functions, so drop can be positioned anywhere. So the following will do the same thing

```
ds.assign(new = lambda x: x.var+ 10, drop = True)
ds.assign(drop = True, new = lambda x: x.var+ 10)
```

At present, assign requires that it is written on a single line. So avoid doing something like the following:

```
ds.assign(new = lambda x: x.var+ 10,
drop = True)
```

The *assign* method will evaluate the lambda functions sent to it for each dataset grid cell for each time step. So every part of the lambda function must evaluate to a number. So the following will work:

```
k = 273.15
ds.assign(drop = True, sst_k = lambda x: x.sst + k)
```

However, if you set k to a string or anything other than a number it will throw an error. For example, this will throw an error:

```
k = "273.15"
ds.assign(drop = True, sst_k = lambda x: x.sst + k)
```

# 4.12.2 Applying mathematical functions to dataset variables

As part of your lambda function you can use a number of standard mathematical functions. These all have the same names as those in numpy: abs, floor, ceil, sqrt, exp, log10, sin, cos, tan, arcsin, arccos and arctan.

For example if you wanted to calculate the ceiling of a variable you could do the following:

```
ds.assign(new = lambda x: ceil(x.old))
```

An example of using logs would be the following:

```
ds.assign(new = lambda x: log10(x.old+1))
```

# 4.12.3 Using spatial statistics

The assign method carries out its calculations in each time step, and you can access spatial statistics for each time step when generating new variables. A series of functions are available that have the same names as nctoolkit methods for spatial statistics: spatial\_mean, spatial\_max, spatial\_min, spatial\_sum, vertical\_mean, vertical\_max, vertical\_min, vertical\_sum, zonal\_mean, zonal\_max, zonal\_min and zonal\_sum.

An example of the usefulness of these functions would be if you were working with global temperature data and you wanted to map regions that are warmer than average. You could do this by working out the difference between temperature in one location and the global mean:

```
ds.assign(temp_comp = lambda x: x.temperature - spatial_mean(x.temperature), drop = True)
```

You can also do comparisons. In the above case, we instead might simply want to identify regions that are hotter than the global average. In that case we can simply do this:

```
ds.assign(\texttt{temp\_comp} = \texttt{lambda} \ \texttt{x:} \ \texttt{x.temperature} \ > \ spatial\_\texttt{mean}(\texttt{x.temperature}) \text{,} \ drop = \textbf{True})
```

Let's say we wanted to map regions which are 3 degrees hotter than average. We could that as follows:

```
ds.assign(temp_comp = lambda x: x.temperature > spatial_mean(x.temperature + 3), drop = 

∴True)
```

or like this:

```
ds.assign(temp_comp = lambda x: x.temperature > (spatial_mean(x.temperature)+3), drop =_{\square} True)
```

Logical operators work in the standard Python way. So if we had a dataset with a variable called 'var' and we wanted to find cells with values between 1 and 10, we could do this:

```
ds.assign(one2ten = lambda x: x.var > 1 & x.var < 10)
```

You can process multiple variables at once using assign. Variables will be created in the order given, and variables created by the first lambda function can be used by the next one, and so on. The simple example below shows how this works. First we create a var1, which is temperature plus 1. Then var2, which is var1 plus 1. Finally, we calculate the difference between var1 and var2, and this should be 1 everywhere:

```
ds.assign(var1 = lambda x: x.var + 1, var2 = lambda x: x.var1 + 1, diff = lambda x: x. 

⇒var2 - x.var1)
```

## 4.12.4 Functions that work with nctoolkit variables

The following functions can be used on nctoolkit variables as part of lambda functions.

Function	Description	Example
abs	Absolute value	abs(x.sst)
ceiling	Ceiling of variable	ceiling(x.sst -1)
cell_area	Area of grid-cell (m2)	cell_area(x.var)
cos	Trigonometric cosine of variable	cos(x.var)
day	Day of the month of the variable	day(x.var)
exp	Exponential of variable	exp(x.sst)
floor	Floor of variable	floor(x.sst + 8.2)
hour	Hour of the day of the variable	hour(x.var)
isnan	Is variable a missing value/NA?	isnan(x.var)
latitude	Latitude of the grid cell	latitude(x.var)
level	Vertical level of variable.	level(x.var)
log	Natural log of variable	log10(x.sst + 1)
log10	Base log10 of variable	log10(x.sst + 1)
longitude	Longitude of the grid cell	longitude(x.var)
month	Month of the variable	month(x.var)
sin	Trigonometric sine of variable	sin(x.var)
spatial_max	Spatial max of variable at time-step	<pre>spatial_max(x.var)</pre>
spatial_mean	Spatial mean of variable at time-step	<pre>spatial_mean(x.var)</pre>
spatial_min	Spatial min of variable at time-step	<pre>spatial_min(x.var)</pre>
spatial_sum	Spatial sum of variable at time-step	<pre>spatial_sum(x.var)</pre>
sqrt	Square root of variable	sqrt(x.sst + 273.15)
tan	Trigonometric tangent of variable	tan(x.var)
timestep	Time step of variable. Using Python indexing.	timestep(x.var)
year	Year of the variable	year(x.var)
zonal_max	Zonal max of variable at time-step	zonal_max(x.var)
zonal_mean	Zonal mean of variable at time-step	zonal_mean(x.var)
zonal_min	Zonal min of variable at time-step	zonal_min(x.var)
zonal_sum	Zonal sum of variable at time-step	zonal_sum(x.var)

# 4.12.5 Simple mathematical operations on variables

If you want to do simple operations like adding or subtracting numbers from the variables in datasets you can use the add, subtract, divide and multiply methods. For example if you wanted to add 10 to every variable in a dataset, you would do the following:

```
ds.add(10)
```

If you wanted to multiply everything by 10, you would do this:

```
ds.multiply(10)
```

These methods will also let you use other datasets or netCDF files. So, you could add the values in a dataset data2 to a dataset called data1 as follows:

```
ds1.add(ds2)
```

Please note that this will require that the datasets are structured in a way that the operation makes sense. So each dimension in the datasets will either have to be identical, with the exception of when one dataset has a single value for a dimension. So for example if ds2 above has data covering only 1 timestep, but ds1 has multiple timesteps the data from that single time step will be added to all timesteps in ds1. But if the time steps match, then the data from the first time step in ds2 will be added to the data in the first time step in ds1, and the same will happen with the following time steps.

# 4.12.6 Simple numerical comparisons

If you want to do something as simple as working out whether the values of the variables in a dataset are greater than zero, you can use the compare method. This method accepts a simple comparison formula, which follows Python conventions. For example, if you wanted to figure out if the values in a dataset were greater than zero, you would do the following:

```
ds.compare(">0")
```

If you wanted to know if they were equal to zero you would do this:

```
ds.compare("==0")
```

# 4.13 Adding or subtracting datasets

Often you might want to subtract datasets from each other. This is potentially made complicated as datasets can take different forms. For example, you might want to subtract a dataset which contains annual means from a dataset that contains monthly values. In this case you want to subtract the annual mean from the relevant month in each year. To deal with this problem, nctoolkit offers the methods add, subtract, multiply and divide, which from nctoolkit v0.4.0 onwards can automatically work out the relevant method required for the dataset given.

Let's illustrate this using a dataset of monthly sea surface temperature from 1850 to the present day. In the snippet below, we load the data into a dataset. Then we generate a second which is the annual mean temperature and subtract it from the original dataset:

```
[1]: import nctoolkit as nc
    ds1 = nc.open_data("sst.mon.mean.nc")
    ds2 = nc.open_data("sst.mon.mean.nc")
    (continues on next page)
```

(continued from previous page)

```
ds2.tmean("year")
ds1.subtract(ds2)
nctoolkit is using Climate Data Operators version 1.9.10
Subtracting a yearly time series
```

You can see that nctoolkit has stated that it has subtracted a yearly time series.

If we wanted to subtract the monthly mean, we would do this:

```
[2]: import nctoolkit as nc
ds1 = nc.open_data("sst.mon.mean.nc")
ds2 = nc.open_data("sst.mon.mean.nc")
ds2.tmean("month")
ds1.subtract(ds2)
Subtracting a monthly time series
```

Similarly, if you want to subtract a dataset with only one time step, things will work as expected:

```
[3]: import nctoolkit as nc
  ds1 = nc.open_data("sst.mon.mean.nc")
  ds2 = nc.open_data("sst.mon.mean.nc")
  ds2.tmean()
  ds1.subtract(ds2)

Subtracting a single time step time series
```

Note: these methods require consistency between the datasets. For example, in the code below we are subtracting the annual means from the monthly values, but we have removed the year 2000. So running this code will throw an error.

```
[]: import nctoolkit as nc
    ds1 = nc.open_data("sst.mon.mean.nc")
    ds2 = nc.open_data("sst.mon.mean.nc")
    ds2.drop(year = 2000)
    ds2.tmean("year")
    ds1.subtract(ds2)
```

## 4.13.1 Automatic methods available

At present, the add, subtract divide and multiply methods will be automatically able to handle daily, monthly and yearly dataset. At present, they will not be able to handle hourly datasets or anything finer.

However, it will automatically be able to deal add, subtract, divide or multiply files that either have single time steps or have identical time steps. In this case time step comparisons are unambiguous.

# 4.14 Parallel processing

nctoolkit is written to enable rapid processing and analysis of netCDF files, and this includes the ability to process in parallel. Two methods of parallel processing are available. First is the ability to carry out operations on multi-file datasets in parallel. Second is the ability to define a processing chain in nctoolkit, and then use the multiprocessing package to process files in parallel using that chain.

# 4.14.1 Parallel processing of multi-file datasets

If you have a multi-file dataset, processing the files within it in parallel is easy. All you need to is the following:

```
nc.options(cores = 6)
```

This will tell nctoolkit to process the files in multi-file datasets in parallel and to use 6 cores when doing so. You can, of course, set the number of cores as high as you want. The only thing nctoolkit will do is limit it to the number of cores on your machine.

# 4.14.2 Parallel processing using multiprocessing

A common task is taking a bunch of files in a folder, doing things to them, and then saving a modified version of each file in a new folder. We want to be able to parallelize that, and we can using the multiprocessing package in the usual way.

But first, we need to change the global settings:

```
import nctoolkit as nc
nc.options(parallel = True)
```

This tells nctoolkit that we are about to do something in parallel. This is critical because of the internal workings of nctoolkit. Behind the scenes nctoolkit is constantly creating and deleting temporary files. It manages this process by creating a safe-list, i.e. a list of files in use that should not be deleted. But if you are running in parallel, you are adding to this list in parallel, and this can cause problems. Telling nctoolkit it will be run in parallel tells it to switch to using a type of list that can be safely added to in parallel.

We can use multiprocessing to do the following: take all of the files in folder foo, do a bunch of things to them, then save the results in a new folder:

We start with a function giving a processing chain. There are obviously different ways of doing this, but I like to use a function that takes the input file and output file:

```
def process_chain(infile, outfile):
    ds = nc.open_data(ff)
    ds.assign(tos = lambda x: x.sst + 273.15)
    ds.tmean()
    ds.to_nc(outfile)
```

We now want to loop through all of the files in a folder, apply the function to them and then save the results in a new folder called new:

```
ensemble = nc.create_ensemble("../../data/ensemble")
import multiprocessing
pool = multiprocessing.Pool(3)
for ff in ensemble:
```

(continues on next page)

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```
pool.apply_async(process_chain, [ff, ff.replace("ensemble", "new")])
pool.close()
pool.join()
```

The number 3 in this case signifies that 3 cores are to be used.

Please note that if you are working interactively or in a Jupyter notebook, it is best to reset parallel as follows once you have stopped any parallel processing:

```
nc.options(parallel = False)
```

This is because of the effects of manually terminating commands on multiprocessing lists, which nctoolkit uses when in parallel mode.

# 4.15 Examples

This tutorial runs through a number of example work flows.

# 4.15.1 Global sea surface temperature since 1850

This example analyzes a global sea surface temperature dataset, covering the years since 1850. The data is available from the National Oceanic and Atmospheric Administration (NOAA) here.

We are looking at global sea surface temperature since 1850, so an obvious question is how much the oceans have warmed over this time period. We can use nctoolkit's spatial\_mean method to calculate this:

Once the file is downloaded, we should set it to ff:

```
[1]: import nctoolkit as nc
    ff = "sst.mon.mean.nc"
    nctoolkit is using Climate Data Operators version 1.9.10
```

```
[2]: ds = nc.open_data(ff)
  ds.spatial_mean()
  ds.plot()
```

Data type cannot be displayed: application/javascript, application/vnd.holoviews\_load.v0+json

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```
[2]: :DynamicMap [variable] :Curve [time] (value)
```

We can see a clear temperature rise of about 1 degree Celcius. But this is monthly data, so a bit noisy. We can smooth it out by taking an annual mean. In this case we send "year" to tmean to tell it to calculate the mean for each year:

```
[3]: ds = nc.open_data(ff)
    ds.tmean(["year"])
    ds.spatial_mean()
    ds.plot("sst")

[3]: :DynamicMap [variable]
    :Curve [time] (value)
```

That is getting better. But again, we possibly want a rolling average. We can use the rolling\_mean method to calculate the mean over every 20-year period:

```
[4]: ds = nc.open_data(ff)
    ds.tmean(["year"])
    ds.spatial_mean()
    ds.rolling_mean(20)
    ds.plot("sst")

[4]: :DynamicMap [variable]
    :Curve [time] (value)
```

We'll finish things off by tweaking this so that we can work out how much temperature has increased since the first 20 years in the time period. For this we can use the annual\_anomaly method.

```
[5]: ds = nc.open_data(ff)
  ds.annual_anomaly(baseline = [1850, 1869], window = 20)
  ds.spatial_mean()
  ds.plot("sst")

[5]: :DynamicMap [variable]
    :Curve [time] (value)
```

## 4.15.2 More to come....

## 4.16 Random Data Hacks

nctoolkit features a number of useful methods to tweak data.

# 4.16.1 Shifting time

Sometimes the times in datasets are not quite what we want, and we need some way to adjust time. An example of this is when you are missing a year of data, so want to copy data from the prior year and use it. But first you would need to shift the times in that year forward by a year. You can do this with the shift method. This let's you shift time forward by a specified number of hours, days, months or years. You just need to supply hours, days, months or years as an argument. So, if you wanted to shift time backward by one year, you would do the following:

```
ds.shift(years = -1)
```

If you wanted to shift time forward by 12 hours, this would do it:

```
ds.shift(hours = 12)
```

Note: this method allows partial matches to the arguments, so you could use hour, day, month or year just as easily.

# 4.16.2 Adding cell areas to a dataset

You can add grid cell areas to a dataset as follows:

```
ds.cell_area()
```

By default, this will add the cell area (in square metres) to the dataset. If you want the dataset to only include cell areas you need to set the join argument to False:

```
ds.cell_area(join = False)
```

Of course, this method will only if it is possible to calculate the areas the grid cells.

# 4.16.3 Changing the format of the netCDF files in a dataset

Sometimes you will want to change the format of the files in a dataset. You can do this using the format method. This let's you set the format, with the following options:

- netCDF = "nc1"
- netCDF version 2 (64-bit offset) = "nc2"/"nc"
- netCDF4 (HDF5) = "nc4"
- netCDF4-classi = "nc4c"
- netCDF version 5 (64-bit data) = "nc5"

So, if you want to set the format to netCDF4, you would do the following:

```
ds.format("nc4")
```

# 4.16.4 Getting rid of dimensions with only one value

Sometimes you will have a dataset that has a dimension with only one value, and you might want to get rid of that dimension. For example, you might only have one one timestep and keeping it may have no value. Getting rid of that dimension can be done using the reduce\_dims method. It works as follows:

```
ds.reduce_dims()
```

# 4.16.5 Removing leap days

If you want to remove a leap day from a dataset, just do the following:

```
ds.drop(month = 2, day = 29)
```

# 4.16.6 Renaming variables

If you want to rename variables, you can use the *rename* method. Just provide a dictionary where the keys are the original variable names and the values are the new names. So if you wanted to rename a variable x to y, you would do this:

```
ds.rename({"x":"y"})
```

# 4.17 Global settings

nctoolkit let's you set global settings using options.

# 4.17.1 Setting the number of cores in use

If you are working with ensembles, you will probably to change the number of cores used for processing multiple files. For example, you can process multiple files in parallel using 6 cores as follows.

```
nc.options(cores = 6)
```

# 4.17.2 Setting the temporary directory to use

By default nctoolkit uses the OS's temporary directories when it needs to create temporary files. In most cases this is optimal. Most of the time reading and writing to temporary folders is faster. However, in some cases this may not be a good idea because you may not have enough space in the temporary folder. In this case you can change the directory used for saving temporary files as follows:

```
nc.options(temp_dir = "/foo")
```

# 4.17.3 Turning progress bars on or off

By default, nctoolkit will display a progress bar when it thinks a process will take a long time for a multi-file dataset. If you always want a progress bar to display when calculations are being carried out on multi-file datasets, regardless of their size, you can do the following:

```
nc.options(progress = 'on')
```

If you find the progress bar annoying or distracting, you can just do this:

```
nc.options(progress = 'off')
```

# 4.17.4 Switching off lazy evaluation

By default evaluation in nctoolkit is lazy, so things are only evaluated when they have to be. If you want things to be evaluated each time a method is used, you can do this:

```
nc.options(lazy = False)
```

# 4.17.5 Setting global settings using a configuration file

You may want to set some global settings either permanently or on a project level. You can do this by setting up a configruation file. This should be a plain text file called .nctoolkitrc or nctoolkitrc. It should be placed in one of two locations: your working directory or your home directory. When nctoolkit is imported, it will look first in your working directory and then in your home directory for a file called .nctoolkitrc or nctoolkitrc. It will then use the first it finds to change the global settings from the defaults.

The structure of this file is straightforward. For example, if you wanted to set evaluation to lazy and the number of cores used for processing multi-file datasets, you would the following in your configuration file:

```
lazy : True cores : 6
```

The files roughly follow Python dictionary syntax, with the setting and value separate by:. Note that unless the setting is specified in the file, the defaults will be used. If you do not provide a configuration file, nctoolkit will use the default settings.

## 4.18 Backends

nctoolkit relies on Climate Data Operators (CDO) as its computational backend. This is a high-powered command line tool for manipulating and analyzing climate model data. You can read more about CDO on their website.

nctoolkit is designed as a stand alone package and users will require no understanding of CDO to use it. However, people with knowledge of CDO may want to use the cdo\_command method to use CDO methods directly.

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# 4.18.1 Using CDO commands

If you want to apply a CDO command in nctoolkit, all you need to do is remove the beginning and end, i.e. 'cdo' and the file names.

So, a typical CDO command looks like this:

```
cdo yearmean infile.nc outfile.nc
```

If we wanted to use this in nctoolkit, we would just do this:

```
ds.cdo_command("yearmean")
```

If the CDO command is an ensemble method that takes multiple files as input and produces one, you will need to specify that it is an ensemble method, as follows:

```
ds.cdo_command("ensmean", ensemble = True)
```

# 4.18.2 Using NCO commands

nctoolkit also allows you to apply NCO commands to datasets using the nco\_command method. You just need to remove the two file names from the command you want to apply.

So, the following command:

```
ncks -v kd_490 -d lat,40.0,70.0 -d lon,-20.0,15.0 infile.nc outfile.nc
```

would become:

```
ds.nco_command("ncks -v kd_490 -d lat,40.0,70.0 -d lon,-20.0,15.0")
```

# 4.19 Toubleshooting

If you get errors running nctoolkit these are most likely caused by problems in the data. In some cases these can be fixed. The tips below will point you help you do this.

# 4.19.1 Check data types

Under-the-hood, nctoolkit uses Climate Data Operators (CDO) as its computational engine. By default, CDO uses the data type stored in netCDF files. In most cases, this will not cause any problems. However, some times it will. For example, imagine you want to calculate the fraction of time temperature exceeds 30 degrees, but the data is stored as integer format. In nctoolkit, you could calculate this as follows:

```
ds.assign(temperature = lambda x: x.temperature > 30)
ds.tmean()
```

In theory, this is fine. But, if the data is stored as integer format, you will end up either with 0 or 1 in the data. Instead we want to change the numerical precision of the data. We could do this as follows:

```
ds.set_precision("F64")
ds.assign(temperature = lambda x: x.temperature > 30)
ds.tmean()
```

By default, nctoolkit will warn you if a dataset has integer data types when you open a dataset. But if you want to know what data types each variable has just do the following:

ds.contents

# 4.19.2 How to carry out general checks on a dataset

There is a built in method in nctoolkit for checking if the format of a dataset is problematic. Just do the following:

ds.check()

This will carry out a number of checks. First, it will check if there are any variables with integer data types. Second, it will check if the time dimension is stored as an integer data type, which can potentially cause problems. Third, it will check if files are CF-compliant. Lack of CF-compliance could point towards problems with CDO interpreting the contents of the dataset, and thus problems in nctoolkit. Finally, it will check if the variables in a datset have the same horizontal grids.

# 4.19.3 How to check if a file is corrupt

A common problem with netCDF files is that they can be corrupt. This typically means that parts of the data cannot be accessed. If you want to check if a dataset is corrupt just do the following:

ds.is\_corrupt()

### 4.19.4 How to fix a dataset with coordinates as variables

Sometimes longitude and latitude will be stored as variables in a netCDF file. Ideally they should be coordinates for nctoolkit to work fully. You can fix this using the assign\_coords method as follows:

```
ds.assign_coords(lon_name = "lon", lat_name = "lat")
```

where lon\_name and lat\_name should be the name of the longitude and latitude variables.

## 4.20 API Reference

## 4.20.1 Session options

options(\\*\\*kwargs)

Define session options.

#### nctoolkit.options

nctoolkit.options(\\*\\*kwargs)

Define session options. Set the options in the session. Available options are thread\_safe and lazy. Set thread\_safe = True if hdf5 was built to be thread safe. Set lazy = False if you want methods to evaluate non-lazily Set cores = n, if you want nctoolkit to process the individual files in multi-file datasets in parallel. Note this only applies to multi-file datasets and will not improve performance with single files. Set temp\_dir = "/foo" if you want to change the temporary directory used by nctoolkit to save temporary files. Set = "/foo" if you want to change the temporary directory used by nctoolkit to save temporary files. Set progress to "on" or "off" if you always or never want a progress bar to show when multi-file datasets are processed. This defaults to "auto", i.e. nctoolkit will automatically decide whether to show a progress bar based on the size of the ensemble.

**Parameters** \*\*kwargs – Define options using key, value pairs.

### **Examples**

If you wanted to process the files in multi-file datasets in parallel with 6 cores, do the following:

```
>>> import nctoolkit as nc
>>> nc.options(cores = 6)
```

If you want to set evaluation to always be lazy do the following:

```
>>> nc.options(lazy = True)
```

If you want nctoolkit to store temporary files in a specific directory, do this:

```
>>> nc.options(temp_dir = "/foo")
```

## 4.20.2 Opening/copying data

open_data([x, checks])	Read netCDF data as a DataSet object	
	3	
<pre>open_url([x, ftp_details, wait, file_stop])</pre>	Read netCDF data from a url as a DataSet object	
open_thredds([x, wait, checks])	Read thredds data as a DataSet object	
<pre>open_geotiff([x])</pre>	Read geotiff and convert to nctoolkit dataset	
from_xarray(ds)	Convert an xarray dataset to an nctoolkit dataset This	
	will first save the xarray dataset as a temporary netCDF	
	file.	
DataSet.copy(self)	Make a deep copy of an DataSet object.	

### nctoolkit.open\_data

```
nctoolkit.open_data(x=[], checks=True, \*\*kwargs)
Read netCDF data as a DataSet object
```

#### **Parameters**

• **x** (str or list) – A string or list of netCDF files or a single url. The function will check the files exist. If x is not a list, but an iterable it will be converted to a list. If a \*.nc style wildcard is supplied, open\_data will use all files available. By default an empty dataset is created, ie. using open\_data() will create an empty dataset that can then be expanded using append.

- checks (boolean) Do you want basic checks to ensure cdo can read files? Default to True
- \*\*kwargs (kwargs) Optional arguments for internal use by open\_thredds and open\_url.

## Returns open\_data

Return type nctoolkit.DataSet

## **Examples**

If you want to open a single file as a dataset, do the following:

```
>>> import nctoolkit as nc
>>> ds = nc.open_data("example.nc")
```

If you want to open a list of files as a multi-file dataset, you would do something like this:

```
>>> import nctoolkit as nc
>>> ds = nc.open_data(["file1.nc", "file2.nc", "file3.nc"])
```

If you wanted to open all files in a directory "data" as a multi-file dataset, you can use a wildcard:

```
>>> import nctoolkit as nc
>>> ds = nc.open_data("data/*.nc")
```

### nctoolkit.open url

nctoolkit.open\_url(x=None, ftp\_details=None, wait=None, file\_stop=None)
Read netCDF data from a url as a DataSet object

#### **Parameters**

- **x** (*str*) A string with a url. Prior to processing data will be downloaded to a temp folder.
- **ftp\_details** (*dict*) A dictionary giving the user name and password combination for ftp downloads: {"user":user, "password":pass}
- wait (int) Time to wait, in seconds, for data to download. A minimum of 3 attempts will be made to download the data.
- **file\_stop** (*int*) Time limit, in minutes, for individual attempts at downloading data. This is useful to get around download freezes.

## Returns open\_url

Return type nctoolkit.DataSet

#### **Examples**

If you want to open a file available over a url do the following:

```
>>> import nctoolkit as nc
>>> ds = nc.open_url("htttp:://foo.nc")
```

This will download the file as a temporary folder for use in the dataset.

#### nctoolkit.open thredds

```
nctoolkit.open_thredds(x=None, wait=None, checks=False)
```

Read thredds data as a DataSet object

#### **Parameters**

- $\mathbf{x}$  (str or list) A string or list of threads urls, which must end with .nc.
- **checks** (*boolean*) Do you want to check if data is available over thredds?
- wait (int) Time to wait for threads server to be checked. Limitless if not supplied.

#### Returns open\_thredds

Return type nctoolkit.DataSet

#### **Examples**

If you want to open a file available over threads or opendap, do the following:

```
>>> import nctoolkit as nc
>>> ds = nc.open_thredds("htttp:://foo.nc")
```

# nctoolkit.open\_geotiff

```
nctoolkit.open_geotiff(x=[])
```

Read geotiff and convert to nctoolkit dataset

**Parameters**  $\mathbf{x}(str\ or\ list)$  – A string or list of geotiff files or a single url. This requires rioxarray to be installed.

Returns open\_data

Return type nctoolkit.DataSet

## nctoolkit.from\_xarray

```
nctoolkit.from_xarray(ds)
```

Convert an xarray dataset to an nctoolkit dataset This will first save the xarray dataset as a temporary netCDF file.

**Parameters ds** (xarray dataset) – xarray dataset you want to convert to nctoolkit DataSet.

Returns from\_xarray

Return type nctoolkit.DataSet

## nctoolkit.DataSet.copy

#### DataSet.copy(self)

Make a deep copy of an DataSet object. Note: This will not make disk copies of the temporary files underlying datasets, so it will be disk-space efficient. :returns: **copy** :rtype: nctoolkit DataSet

# 4.20.3 Merging or analyzing multiple datasets

merge(\*datasets[, match])	Merge datasets
<pre>cor_time([x, y])</pre>	Calculate the temporal correlation coefficient between
	two datasets This will calculate the temporal correlation
	coefficient, for each time step, between two datasets.
cor_space([x, y])	Calculate the spatial correlation coefficient between two
	datasets This will calculate the spatial correlation coef-
	ficient, for each time step, between two datasets.

## nctoolkit.merge

#### **Parameters**

- datasets (*kwargs*) Datasets to merge.
- match (list) Temporal matching criteria. This is a list which must be made up of a subset of day, year, month. This checks that the datasets have compatible times. For example, if you want to ensure the datasets have the same years, then use match = ["year"].

#### nctoolkit.cor\_time

### nctoolkit.cor\_time(x=None, y=None)

Calculate the temporal correlation coefficient between two datasets This will calculate the temporal correlation coefficient, for each time step, between two datasets. The datasets must either have the same variables or only have one variable.

#### **Parameters**

- **x** (dataset) First dataset to use
- y (dataset) Second dataset to use

## nctoolkit.cor\_space

#### nctoolkit.cor\_space(x=None, y=None)

Calculate the spatial correlation coefficient between two datasets This will calculate the spatial correlation coefficient, for each time step, between two datasets. The datasets must either have the same variables or only have one variable.

#### **Parameters**

- **x** (dataset) First dataset to use
- y (dataset) Second dataset to use

# 4.20.4 Adding and removing files to a dataset

append		
remove		

# nctoolkit.append

## **Functions**

append(self[, x])	Add new file(s) to a dataset.
remove(self[, x])	Remove file(s) from a dataset

## nctoolkit.remove

# **Functions**

<pre>nc_remove(ff[, deep])</pre>	Method for removing netCDF files.

# 4.20.5 Accessing attributes

DataSet.variables	List variables contained in a dataset
DataSet.contents	Detailed list of variables contained in a dataset.
DataSet.times	List times contained in a dataset
DataSet.years	List years contained in a dataset
DataSet.months	List months contained in a dataset
DataSet.levels	List levels contained in a dataset
DataSet.size	The size of an object This will print the number of files,
	total size, and smallest and largest files in an DataSet
	object.
DataSet.current	The current file or files in the DataSet object
DataSet.history	The history of operations on the DataSet
DataSet.start	The starting file or files of the DataSet object
DataSet.calendar	List calendars of dataset files
DataSet.ncformat	List formats of files contained in a dataset

#### nctoolkit.DataSet.variables

#### property DataSet.variables

List variables contained in a dataset

#### nctoolkit.DataSet.contents

#### property DataSet.contents

Detailed list of variables contained in a dataset. This will only display the variables in the first file of an ensemble.

#### nctoolkit.DataSet.times

#### property DataSet.times

List times contained in a dataset

## nctoolkit.DataSet.years

#### property DataSet.years

List years contained in a dataset

#### nctoolkit.DataSet.months

#### property DataSet.months

List months contained in a dataset

#### nctoolkit.DataSet.levels

## property DataSet.levels

List levels contained in a dataset

## nctoolkit.DataSet.size

## property DataSet.size

The size of an object This will print the number of files, total size, and smallest and largest files in an DataSet object.

#### nctoolkit.DataSet.current

### property DataSet.current

The current file or files in the DataSet object

## nctoolkit.DataSet.history

## property DataSet.history

The history of operations on the DataSet

## nctoolkit.DataSet.start

#### property DataSet.start

The starting file or files of the DataSet object

#### nctoolkit.DataSet.calendar

#### property DataSet.calendar

List calendars of dataset files

#### nctoolkit.DataSet.ncformat

## property DataSet.ncformat

List formats of files contained in a dataset

# 4.20.6 Plotting

DataSet.plot(self[, vars, autoscale, out])

## nctoolkit.DataSet.plot

DataSet.plot(self, vars=None, autoscale=True, out=None, \\*\\*kwargs)

## 4.20.7 Variable modification

DataSet.assign(self[, drop])	Create new variables Existing columns that are re-
	assigned will be overwritten.
DataSet.rename(self, newnames)	Rename variables in a dataset
DataSet.as_missing(self[, value])	Set the missing value for a single number or a range
<pre>DataSet.sum_all(self[, drop])</pre>	Calculate the sum of all variables for each time step

#### nctoolkit.DataSet.assign

DataSet.assign(self, drop=False, \\*\\*kwargs)

Create new variables Existing columns that are re-assigned will be overwritten.

#### **Parameters**

• **drop** (*boo1*) – Set to True if you want existing variables to be removed once the new ones have been created. Defaults to False.

should evaluate to a numeric. New variables are calculated for each grid cell and time step.

• \*\*kwargs (dict of {str: callable}) - New variable names are keywords. All terms in the equation given by the lamda function should evaluate to a numeric. New variables are calculated for each grid cell and time step.

#### **Notes**

Operations are carried out in the order give. So if a new variable is created in the first argument, it can then be used in following arguments.

#### nctoolkit.DataSet.rename

DataSet.rename(self, newnames)

Rename variables in a dataset

**Parameters newnames** (dict) – Dictionary with key-value pairs being original and new variable names

#### **Examples**

If you want to rename a variable x to y, do the following:

```
>>> ds.rename({"x":"y"})
```

## nctoolkit.DataSet.as\_missing

DataSet.as\_missing(self, value=None)

Set the missing value for a single number or a range

**Parameters value** (2 variable list or int/float) – If int/float is provided, the missing value will be set to that. If a list is provided, values between the two values (inclusive) of the list are set to missing.

# nctoolkit.DataSet.sum\_all

DataSet.sum\_all(self, drop=True)

Calculate the sum of all variables for each time step

**Parameters drop** (boolean) – Do you want to keep variables?

## 4.20.8 netCDF file attribute modification

<pre>DataSet.set_longnames(self[, name_dict])</pre>	Set the long names of variables
<pre>DataSet.set_units(self[, unit_dict])</pre>	Set the units for variables

## nctoolkit.DataSet.set\_longnames

DataSet.set\_longnames(self, name\_dict=None)

Set the long names of variables

**Parameters name\_dict** (*dict*) – Dictionary with key, value pairs representing the variable names and their long names

## nctoolkit.DataSet.set\_units

DataSet.set\_units(self, unit\_dict=None)

Set the units for variables

**Parameters unit\_dict** (*dict*) – A dictionary where the key-value pairs are the variables and new units respectively.

## 4.20.9 Vertical/level methods

DataSet.top(self)	Extract the top/surface level from a dataset This extracts
	the first vertical level from each file in a dataset.
DataSet.bottom(self)	Extract the bottom level from a dataset This extracts the
	bottom level from each netCDF file.
<pre>DataSet.vertical_interp(self[, levels])</pre>	Verticaly interpolate a dataset based on given vertical
	levels This is calculated for each time step and grid cell
<pre>DataSet.vertical_mean(self[, thickness,])</pre>	Calculate the depth-averaged mean for each variable
	This is calculated for each time step and grid cell
DataSet.vertical_min(self)	Calculate the vertical minimum of variable values This
	is calculated for each time step and grid cell
DataSet.vertical_max(self)	Calculate the vertical maximum of variable values This
	is calculated for each time step and grid cell
DataSet.vertical_range(self)	Calculate the vertical range of variable values This is cal-
	culated for each time step and grid cell
DataSet.vertical_sum(self)	Calculate the vertical sum of variable values This is cal-
	culated for each time step and grid cell
<pre>DataSet.vertical_integration(self[,])</pre>	Calculate the vertically integrated sum over the water
	column This calculates the sum of the variable multi-
	plied by the cell thickness
	continues on next page

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DataSet.vertical_cumsum(self)	Calculate the vertical sum of variable values This is cal-
	culated for each time step and grid cell
DataSet.invert_levels(self)	Invert the levels of 3D variables This is calculated for
	each time step and grid cell
DataSet.bottom_mask(self)	Create a mask identifying the deepest cell without miss-
	ing values.

## nctoolkit.DataSet.top

#### DataSet.top(self)

Extract the top/surface level from a dataset This extracts the first vertical level from each file in a dataset.

## **Examples**

If you wanted to extract the top vertical level of a dataset, do the following:

```
>>> ds.top()
```

This method is most useful for things like oceanic data, where this method will extract the sea surface.

#### nctoolkit.DataSet.bottom

#### DataSet.bottom(self)

Extract the bottom level from a dataset This extracts the bottom level from each netCDF file. Please note that for ensembles, it uses the first file to derive the index of the bottom level. Use bottom\_mask for files when the bottom cell in netCDF files do not represent the actual bottom.

## **Examples**

If you wanted to extract the bottom vertical level of a dataset, do the following:

```
>>> ds.bottom()
```

This method is most useful for things like oceanic model data, where the bottom cell corresponds to the bottom of the ocean.

## nctoolkit.DataSet.vertical\_interp

## DataSet.vertical\_interp(self, levels=None)

Verticaly interpolate a dataset based on given vertical levels This is calculated for each time step and grid cell

**Parameters levels** (*list*, *int or str*) – list of vertical levels, for example depths for an ocean model, to vertically interpolate to. These must be floats or ints.

## **Examples**

If you wanted to vertically interpolate a dataset to 5 and 10 metres, you would do the following:

```
>>> ds.vertical_interp([5,10])
```

This method is most useful for things like oceanic data, where you need to interpolate to certain depth levels. It will require that vertical levels are the same in every grid cell.

#### nctoolkit.DataSet.vertical\_mean

DataSet.vertical\_mean(self, thickness=None, depth\_range=None)

Calculate the depth-averaged mean for each variable This is calculated for each time step and grid cell

**thickness: str or Dataset** Only use when vertical levels vary in space One of: a variable, in the dataset, which contains the variable thicknesses; a .nc file which contains the thicknesses; or a Dataset that contains the thicknesses. Note: the .nc file or Dataset must only contain one variable.

**depth\_range: list** Only use when vertical levels vary in space Set a depth range if desired. Should be of the form [min depth, max depth].

## **Examples**

If you wanted to vertical mean of every variable in a dataset, you would do this:

```
>>> ds.vertical_mean()
```

This method will calculate the vertical mean weighted by the thickness of each cell. Note that if cell thickness cannot be derived it will just average the values in each vertical cell.

#### nctoolkit.DataSet.vertical min

DataSet.vertical\_min(self)

Calculate the vertical minimum of variable values This is calculated for each time step and grid cell

#### **Examples**

If you wanted to vertical minimum of every variable in a dataset, you would do this:

```
>>> ds.vertical_min()
```

### nctoolkit.DataSet.vertical\_max

DataSet.vertical\_max(self)

Calculate the vertical maximum of variable values This is calculated for each time step and grid cell

## **Examples**

If you wanted to vertical maximum of every variable in a dataset, you would do this:

```
>>> ds.vertical_max()
```

## nctoolkit.DataSet.vertical\_range

#### DataSet.vertical\_range(self)

Calculate the vertical range of variable values This is calculated for each time step and grid cell

## **Examples**

If you wanted to range of values across all vertical levels of every variable in a dataset, you would do this:

```
>>> ds.vertical_range()
```

## nctoolkit.DataSet.vertical\_sum

#### DataSet.vertical\_sum(self)

Calculate the vertical sum of variable values This is calculated for each time step and grid cell

#### **Examples**

If you wanted to sum of values across all vertical levels of every variable in a dataset, you would do this:

```
>>> ds.vertical_sum()
```

## nctoolkit.DataSet.vertical\_integration

DataSet.vertical\_integration(self, thickness=None, depth\_range=None)

Calculate the vertically integrated sum over the water column This calculates the sum of the variable multiplied by the cell thickness

#### **Parameters**

- **thickness** (*str or Dataset*) One of: a variable, in the dataset, which contains the variable thicknesses; a .nc file which contains the thicknesses; or a Dataset that contains the thicknesses. Note: the .nc file or Dataset must only contain one variable.
- **depth\_range** (*list*) Set a depth range if desired. Should be of the form [min\_depth, max\_depth].

## **Examples**

If you wanted to sum of values across all vertical levels of every variable in a dataset, you would do this:

>>> ds.vertical\_sum()

## nctoolkit.DataSet.vertical\_cumsum

#### DataSet.vertical\_cumsum(self)

Calculate the vertical sum of variable values This is calculated for each time step and grid cell

## **Examples**

If you wanted to calculate the cumulative sum of values across all vertical levels of every variable in a dataset, you would do this:

>>> ds.vertical\_sum()

The cumulative sum will be calculated from the first to the last vertical level. For example, in oceanic data it would start at the sea surface.

#### nctoolkit.DataSet.invert levels

## DataSet.invert\_levels(self)

Invert the levels of 3D variables This is calculated for each time step and grid cell

#### **Examples**

If you wanted to invert the vertical levels, you would do this:

>>> ds.invert\_levels()

#### nctoolkit.DataSet.bottom mask

#### DataSet.bottom\_mask(self)

Create a mask identifying the deepest cell without missing values. This converts a dataset to a mask identifying which cell represents the bottom, for example the seabed. 1 identifies the deepest cell with non-missing values. Everything else is 0, or missing. At present this method only uses the first available variable from netCDF files, so it may not be suitable for all data

# 4.20.10 Rolling methods

DataSet.rolling_mean(self[, window, align])	Calculate a rolling mean based on a window
<pre>DataSet.rolling_min(self[, window, align])</pre>	Calculate a rolling minimum based on a window
<pre>DataSet.rolling_max(self[, window, align])</pre>	Calculate a rolling maximum based on a window
<pre>DataSet.rolling_sum(self[, window, align])</pre>	Calculate a rolling sum based on a window
<pre>DataSet.rolling_range(self[, window, align])</pre>	Calculate a rolling range based on a window
<pre>DataSet.rolling_stdev(self[, window, align])</pre>	Calculate a rolling standard deviation based on a window
DataSet.rolling_var(self[, window, align])	Calculate a rolling variance based on a window

#### nctoolkit.DataSet.rolling mean

DataSet.rolling\_mean(self, window=None, align='right')

Calculate a rolling mean based on a window

#### **Parameters**

- window (int) The size of the window for the calculation of the rolling mean
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

## **Examples**

If you wanted to calculate a rolling mean with the mean calculated over every 10 time steps, do the following:

```
>>> ds.rolling_mean(10)
```

## nctoolkit.DataSet.rolling\_min

DataSet.rolling\_min(self, window=None, align='right')

Calculate a rolling minimum based on a window

#### **Parameters**

- window (int) The size of the window for the calculation of the rolling minimum
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

#### **Examples**

If you wanted to calculate a rolling minimum with the minimum calculated over every 10 time steps, do the following:

>>> ds.rolling\_min(10)

#### nctoolkit.DataSet.rolling max

DataSet.rolling\_max(self, window=None, align='right')

Calculate a rolling maximum based on a window

#### **Parameters**

- window (int) The size of the window for the calculation of the rolling maximum
- **align** (str) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

## **Examples**

If you wanted to calculate a rolling maximum with the maximum calculated over every 10 time steps, do the following:

>>> ds.rolling\_max(10)

## nctoolkit.DataSet.rolling\_sum

DataSet.rolling\_sum(self, window=None, align='right')

Calculate a rolling sum based on a window

#### **Parameters**

- window (int) The size of the window for the calculation of the rolling sum
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

#### **Examples**

If you wanted to calculate a rolling sum with the sum calculated over every 10 time steps, do the following:

>>> ds.rolling\_sum(10)

#### nctoolkit.DataSet.rolling\_range

DataSet.rolling\_range(self, window=None, align='right')

Calculate a rolling range based on a window

#### **Parameters**

- window (int) The size of the window for the calculation of the rolling range
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

If you wanted to calculate a rolling range with the range calculated over every 10 time steps, do the following:

```
>>> ds.rolling_range(10)
```

# nctoolkit.DataSet.rolling\_stdev

DataSet.rolling\_stdev(self, window=None, align='right')

Calculate a rolling standard deviation based on a window

#### **Parameters**

- window (int) The size of the window for the calculation of the rolling sum
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

# **Examples**

If you wanted to calculate a rolling standard deviation with the standard deviation calculated over every 10 time steps, do the following:

```
>>> ds.rolling_sum(10)
```

## nctoolkit.DataSet.rolling\_var

DataSet.rolling\_var(self, window=None, align='right')

Calculate a rolling variance based on a window

#### **Parameters**

- window (int) The size of the window for the calculation of the rolling sum
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

# **Examples**

If you wanted to calculate a rolling variance with the variance calculated over every 10 time steps, do the following:

```
>>> ds.rolling_sum(10)
```

# 4.20.11 Evaluation setting

DataSet.run(self)

Run all stored commands in a dataset

### nctoolkit.DataSet.run

DataSet.run(self)

Run all stored commands in a dataset

# **Examples**

If evaluation is lazy and you need to evaluate commands on a dataset, do the following:

>>> ds.run()

# 4.20.12 Cleaning functions

\_

# 4.20.13 Ensemble creation

create\_ensemble([path, recursive])

Generate an ensemble

# nctoolkit.create\_ensemble

nctoolkit.create\_ensemble(path=", recursive=True)

Generate an ensemble

## **Parameters**

- path (str) The directory to search for netCDF files
- **recursive** (*boolean*) True/False depending on whether you want to search the path recursively. Defaults to True.

Returns A list of files

Return type list

If you wanted to recursively find all netCDF files available in a directory "data", you would do this:

```
>>> import nctoolkit as nc
>>> nc.create_ensemble("data")
```

If you wanted to find the files in that directory and ignore subdirectories, you would instead do this:

```
>>> nc.create_ensemble("data", recursive = False)
```

# 4.20.14 Arithemetic methods

DataSet.abs(self)	Method to get the absolute value of variables
<pre>DataSet.add(self[, x, var])</pre>	Add to a dataset This will add a constant, another dataset
	or a netCDF file to the dataset.
DataSet.assign(self[, drop])	Create new variables Existing columns that are re-
	assigned will be overwritten.
DataSet.exp(self)	Method to get the exponential of variables
DataSet.log(self)	Method to get the natural log of variables
DataSet.log10(self)	Method to get the base 10 log of variables
DataSet.multiply(self[, x, var])	Multiply a dataset This will multiply a dataset by a con-
	stant, another dataset or a netCDF file.
DataSet.power(self[, x])	Powers of variables in dataset
DataSet.sqrt(self)	Method to get the square root of variables
DataSet.square(self)	Method to get the square of variables
DataSet.subtract(self[, x, var])	Subtract from a dataset This will subtract a constant, an-
	other dataset or a netCDF file from the dataset.
DataSet.divide(self[, x, var])	Divide the data This will divide the dataset by a constant,
	another dataset or a netCDF file.

### nctoolkit.DataSet.abs

DataSet.abs(self)

Method to get the absolute value of variables

If you wanted to get the absolute value of each variable, you just need do this:

>>> ds.abs()

#### nctoolkit.DataSet.add

DataSet.add(self, x=None, var=None)

Add to a dataset This will add a constant, another dataset or a netCDF file to the dataset. nctoolkit will automatically determine the appropriate comparison required.

#### **Parameters**

- **x**(*int*, *float*, *DataSet or netCDF file*) An int, float, single file dataset or netCDF file to add to the dataset. If a dataset or netCDF file is supplied, this must have only one variable, unless var is provided. The grids must be the same.
- **var** (*str*) A variable in the x to use for the operation

Examples

- -----
- ullet you wanted to add 10 to all variables in a dataset (If) –
- would do the following (you) -
- ds.add(10) (>>>) -
- add the values in a dataset ds2 from a dataset ds1(To)-
- would do the following -
- ds1.add(ds2) (>>>) -
- in the datasets must match. Addition will occur in matching timesteps in ds1 and ds2. If there is only 1 timestep in ds2 (Grids) –
- then -
- data from that timestep will be added to the data in all ds1 time steps.  $(the)\,-\,$
- ullet the data from another netCDF file will work in the same way (Adding) -
- ds1.add("example.nc") (>>>) -

# nctoolkit.DataSet.exp

DataSet.exp(self)

Method to get the exponential of variables

If you wanted to calculate the exponential of a variable, you just need to do this:

```
\Rightarrow > ds.exp(0.5)
```

# nctoolkit.DataSet.log

DataSet.log(self)

Method to get the natural log of variables

# **Examples**

If you wanted to calculate the natural log of each variable, you just need to do this:

```
>>> ds.log()
```

# nctoolkit.DataSet.log10

DataSet.log10(self)

Method to get the base 10 log of variables

# **Examples**

If you wanted to calculate the base 10 log of each variable, you just need to do this:

```
>>> ds.log10()
```

# nctoolkit.DataSet.multiply

DataSet.multiply(self, x=None, var=None)

Multiply a dataset This will multiply a dataset by a constant, another dataset or a netCDF file.

#### **Parameters**

- **x**(*int*, *float*, *DataSet* or *netCDF file*) An int, float, single file dataset or netCDF file to multiply the dataset by. If multiplying by a dataset or single file there must only be a single variable in it, unless var is supplied. The grids must be the same.
- **var** (*str*) A variable in the x to multiply the dataset by

If you wanted to multiply variables in a dataset by 10, you would do the following:

```
>>> ds.multiply(10)
```

To multiply the values in a dataset by the values of variables in dataset ds2, you would do the following:

```
>>> ds1.multiply(ds2)
```

Grids in the datasets must match. Multiplication will occur in matching timesteps in ds1 and ds2. If there is only 1 timestep in ds2, then the data from that timestep in ds2 will multiply the data in all timesteps in ds1.

Multiplying a dataset by the data from another netCDF file will work in the same way:

```
>>> ds.multiply("example.nc")
```

## nctoolkit.DataSet.power

DataSet.power(self, x=None)

Powers of variables in dataset

Parameters x (int, float) - An int or float to take the variables to the power of

## **Examples**

If you wanted to take each variable to the power of 0.5 you would do this:

```
>>> ds.power(0.5)
```

# nctoolkit.DataSet.sqrt

DataSet.sqrt(self)

Method to get the square root of variables

## **Examples**

If you wanted to calculate the square root of each variable, you just need to do this:

```
>>> ds.sqrt()
```

### nctoolkit.DataSet.square

DataSet.square(self)

Method to get the square of variables

If you wanted to calculate the square of each variable, you just need to do this:

>>> ds.power()

#### nctoolkit.DataSet.subtract

DataSet.subtract(self, x=None, var=None)

Subtract from a dataset This will subtract a constant, another dataset or a netCDF file from the dataset.

#### **Parameters**

- **x** (*int*, *float*, *DataSet or netCDF file*) An int, float, single file dataset or netCDF file to subtract from the dataset. If a dataset or netCDF is supplied this must only have one variable, unless var is provided. The grids must be the same.
- **var** (*str*) A variable in the x to use for the operation

## **Examples**

If you wanted to subtract 10 from all variables in a dataset, you would do the following:

```
>>> ds.subtract(10)
```

To substract the values in a dataset ds2 from those in a dataset ds1, you would do the following:

```
>>> ds1.subtract(ds2)
```

Grids in the datasets must match. Division will occur in matching timesteps in ds1 and ds2 if there are matching timesteps. If there is only 1 timestep in ds2, then the data from that timestep in ds2 will be subtracted from the data in all timesteps in ds1.

Subtracting of the data from another netCDF file will work in the same way:

```
>>> ds1.subtract("example.nc")
```

## nctoolkit.DataSet.divide

DataSet.divide(self, x=None, var=None)

Divide the data This will divide the dataset by a constant, another dataset or a netCDF file.

# **Parameters**

- **x** (*int*, *float*, *DataSet or netCDF file*) An int, float, single file dataset or netCDF file to divide the dataset by. If a dataset or netCDF file is supplied, this must have only one variable, unless var is provided. The grids must be the same.
- **var** (*str*) A variable in the x to use for the operation

If you wanted to dividie all variables in a dataset by 20, you would do the following:

>>> ds.divide(10)

To divide values in a dataset by those in the dataset ds2 from a dataset ds1, you would do the following:

>>> ds1.divide(ds2)

Grids in the datasets must match. Division will occur in matching timesteps in ds1 and ds2. If there is only 1 timestep in ds2, then the data from that timestep in ds2 will divided the data in all ds1 time steps.

Adding the data from another netCDF file will work in the same way:

>>> ds.divide("example.nc")

# 4.20.15 Ensemble statistics

<pre>DataSet.ensemble_mean(self[, nco, ignore_time])</pre>	Calculate an ensemble mean
<pre>DataSet.ensemble_min(self[, nco, ignore_time])</pre>	Calculate an ensemble min
<pre>DataSet.ensemble_max(self[, nco, ignore_time])</pre>	Calculate an ensemble maximum
DataSet.ensemble_percentile(self[, p])	Calculate an ensemble percentile This will calculate the
	percentles for each time step in the files.
DataSet.ensemble_range(self)	Calculate an ensemble range The range is calculated for
	each time step; for example, if each file in the ensemble
	has 12 months of data the statistic will be calculated for
	each month.
DataSet.ensemble_stdev(self)	Calculate an ensemble standard deviation
DataSet.ensemble_sum(self)	Calculate an ensemble sum The sum is calculated for
	each time step; for example, if each file in the ensemble
	has 12 months of data the statistic will be calculated for
	each month.
DataSet.ensemble_var(self)	Calculate an ensemble variance

# nctoolkit.DataSet.ensemble\_mean

DataSet.ensemble\_mean(self, nco=False, ignore\_time=False)

Calculate an ensemble mean

#### **Parameters**

- **nco** (*boolean*) Do you want to use NCO for the calculation? Default is False, i.e. CDO is used. Modify default if run time is an issue.
- **ignore\_time** (*boolean*) If True the mean is calculated over all time steps. If False, the ensemble mean is calculated for each time steps; for example, if the ensemble is made up of monthly files the mean for each month will be calculated.

## nctoolkit.DataSet.ensemble min

DataSet.ensemble\_min(self, nco=False, ignore\_time=False)

Calculate an ensemble min

#### **Parameters**

- **nco** (*boolean*) Do you want to use NCO for the calculation? Default is False, i.e. CDO is used. Modify default if run time is an issue.
- **ignore\_time** (*boolean*) If True the min is calculated over all time steps. If False, the ensemble min is calculated for each time steps; for example, if the ensemble is made up of monthly files the min for each month will be calculated.

### nctoolkit.DataSet.ensemble\_max

DataSet.ensemble\_max(self, nco=False, ignore\_time=False)

Calculate an ensemble maximum

#### **Parameters**

- **nco** (*boolean*) Do you want to use NCO for the calculation? Default is False, i.e. CDO is used. Modify default if run time is an issue.
- **ignore\_time** (*boolean*) If True the max is calculated over all time steps. If False, the ensemble max is calculated for each time steps; for example, if the ensemble is made up of monthly files the max for each month will be calculated.

## nctoolkit.DataSet.ensemble percentile

# DataSet.ensemble\_percentile(self, p=None)

Calculate an ensemble percentile This will calculate the percentles for each time step in the files. For example, if you had an ensemble of files where each file included 12 months of data, it would calculate the percentile for each month.

**Parameters p** (*float or int*) – percentile to calculate. 0<=p<=100.

#### nctoolkit.DataSet.ensemble range

### DataSet.ensemble\_range(self)

Calculate an ensemble range The range is calculated for each time step; for example, if each file in the ensemble has 12 months of data the statistic will be calculated for each month.

# nctoolkit.DataSet.ensemble\_stdev

## DataSet.ensemble\_stdev(self)

Calculate an ensemble standard deviation

The ensemble standard deviation is calculated for each time steps; for example, if the ensemble is made up of monthly files the standard deviation for each month will be calculated.

#### nctoolkit.DataSet.ensemble sum

#### DataSet.ensemble\_sum(self)

Calculate an ensemble sum The sum is calculated for each time step; for example, if each file in the ensemble has 12 months of data the statistic will be calculated for each month.

# nctoolkit.DataSet.ensemble\_var

#### DataSet.ensemble\_var(self)

Calculate an ensemble variance

The ensemble variance is calculated for each time steps; for example, if the ensemble is made up of monthly files the standard deviation for each month will be calculated.

# 4.20.16 Subsetting operations

<pre>DataSet.subset(self, \*\*kwargs)</pre>	A method for subsetting datasets to specific variables,
	years, longitudes etc.
DataSet.crop(self[, lon, lat, nco, nco_vars])	Crop to a rectangular longitude and latitude box
DataSet.drop(self, \*\*kwargs)	Remove variables This will remove stated variables from
	files in the dataset.

#### nctoolkit.DataSet.subset

# DataSet.subset(self, \\*\\*kwargs)

A method for subsetting datasets to specific variables, years, longitudes etc. Operations are applied in the order supplied.

Parameters \*kwargs – Possible arguments: variables, years, months, seasons, timesteps, lon, lat

Note: this uses partial matches. So year, month, var etc. will also work

Each kwarg works as follows:

variables [str or list] A variable or list of variables to select. This method will accept wild cards. So using 'var\*' would select all variables beginning with 'var'.

seasons [str] Seasons to select. One of "DJF", "MAM", "JJA", "SON".

days [list, range or int] Days(s) to select.

months [list, range or int] Month(s) to select.

**years** [list,range or int] Years(s) to select. These should be integers

**hours** [list, range or int] Hours(s) to select.

**range** [list] List of the form [date\_min, date\_max], where dates must be datetime objects or strings of the form "DD/MM/YYYY" or "DD-MM-YYYY". Times selected will be on or after date\_min and before date\_max.

**timesteps** [list or int] time step(s) to select. For example, if you wanted the first time step set times=0.

lon: list The longitude range to select. This must be two variables, between -180 and 180.

lat: list The latitude range to select. This must be two variables, between -90 and 90.

**levels** [list] List of the form [min\_level, max\_level]. Levels/depths between the two will be selected

If you want to select a single variable do the following:

```
>>> ds.subset(variable = "var")
```

If you want to select a list of variables, do this:

```
>>> ds.subset(variable = ["var1", "var2"])
```

If you want to select data for January, do the following:

```
>>> ds.subset(month = 1)
```

If you want to select a range of months, do the following:

```
>>> ds.subset(months = range(1, 7))
```

If you want to select a range of years, for example the 2010s, do the following:

```
>>> ds.subset(years = range(2010, 2020))
```

If you want to select the first two timesteps in a dataset, do the following:

```
>>> ds.subset(timesteps = [0,1])
```

## nctoolkit.DataSet.crop

DataSet.**crop**(*self*, *lon=[-180, 180]*, *lat=[-90, 90]*, *nco=False*, *nco\_vars=None*)

Crop to a rectangular longitude and latitude box

#### **Parameters**

- **lon** (*1ist*) The longitude range to select. This must be two variables, between -180 and 180 when nco = False.
- lat (list) The latitude range to select. This must be two variables, between -90 and 90 when nco = False.
- nco (boolean) Do you want this to use NCO for cropping? Defaults to False, and uses CDO. Set to True if you want to call NCO. NCO is typically better at handling very large horizontal grids.
- nco\_vars (str or list) If using NCO, the variables you want to select

## **Examples**

If you wanted to crop a dataset to longitudes between -40 and 30 and latitudes between -10 and 40, you would do the following:

```
>>> ds.crop(lon = [-40, 30], lat = [-10, 40])
```

If you wanted to select only the northern hemisphere, the following will work:

```
>>> ds.crop(lat = [0, 90])
```

## nctoolkit.DataSet.drop

DataSet.drop(self, \\*\\*kwargs)

Remove variables This will remove stated variables from files in the dataset.

#### **Parameters**

• \*kwargs – Possible arguments: var, year, month, day

Note: this uses partial matches. So years, month, variable etc. will also work

- kwarg works as follows (Each) -
- **var** (*str or list*) A variable or list of variables to select. This method will accept wild cards. So using 'var\*' would select all variables beginning with 'var'.
- day (list, range or int) Day(s) to drop.
- month (list, range or int) Month(s) to drop.
- year (list, range or int) Year(s) to drop.
- time (list, range or int) Time steps to to drop. This can include negative indices.

# **Examples**

If you wanted to remove a single variable 'var1' from a dataset data, you would do the following:

```
>>> ds.drop(variable = 'var')
```

If you wanted to remove a list of variables, you would do the following:

```
>>> ds.drop(variable = ['var1', 'var2', 'var2'])
```

If you wanted to remove the 29th Feburary you would do the following:

```
\rightarrow >> ds.drop(month = 2, day = 29)
```

# 4.20.17 Time-based methods

DataSet.set_date(self[, year, month, day,])	Set the date in a dataset You should only do this if you have to fix/change a dataset with a single, not multiple dates.
<pre>DataSet.set_year(self, x)</pre>	Set the year in a dataset
<pre>DataSet.shift(self, \*\*kwargs)</pre>	Shift method.

## nctoolkit.DataSet.set date

DataSet.set\_date(self, year=None, month=None, day=None, base\_year=1900)

Set the date in a dataset You should only do this if you have to fix/change a dataset with a single, not multiple dates.

#### **Parameters**

- **year** (*int*) The year
- month (int) The month
- day (int) The day
- base\_year (int) The base year for time creation in the netCDF. Defaults to 1900.

## nctoolkit.DataSet.set year

```
DataSet.set_year(self, x)
```

Set the year in a dataset

Parameters x (int) – Year to set dataset to

#### nctoolkit.DataSet.shift

DataSet.shift(self, \\*\\*kwargs)

Shift method. A wrapper for shift\_days, shift\_hours Operations are applied in the order supplied.

**Parameters \*kwargs** – hours maps to shift\_hours days maps to shift\_days months maps to shift\_months years maps to shift\_years

Note: this uses partial matches. So hour, day, month, year will also work.

# **Examples**

If you wanted to shift all times back 1 hour, you would do the following:

```
>>> ds.shift(hours = -1)
```

If you wanted to shift all times forward 2 days, you would do the following:

```
>>> ds.shift(days = 2)
```

If you wanted to shift all times forward 6 months, you would do the following:

```
>>> ds.shift(months = 6)
```

If you wanted to shift all times forward 1 year, you would do the following:

```
>>> ds.shift(years = 1)
```

This method will allow partial matches in arguments. So the following will do the same thing:

```
>>> ds.shift(year = 2)
```

```
>>> ds.shift(years = 2)
```

# 4.20.18 Interpolation, matching and resampling methods

DataSet.regrid(self[, grid, method, recycle])	Regrid a dataset to a target grid
DataSet.to_latlon(self[, lon, lat, res,])	Regrid a dataset to a regular latlon grid
<pre>DataSet.match_points(self[, df, variables,])</pre>	Match dataset to a spatiotemporal points dataframe
<pre>DataSet.resample_grid(self[, factor])</pre>	Resample the horizontal grid of a dataset
<pre>DataSet.time_interp(self[, start, end,])</pre>	Temporally interpolate variables based on date range and
	time resolution
<pre>DataSet.timestep_interp(self[, steps])</pre>	Temporally interpolate a dataset to given number of time
	steps between existing time steps
<pre>DataSet.fill_na(self[, n])</pre>	Fill missing values with a distance-weighted average.
<pre>DataSet.box_mean(self[, x, y])</pre>	Calculate the grid box mean for all variables This is per-
	formed for each time step.
<pre>DataSet.box_max(self[, x, y])</pre>	Calculate the grid box max for all variables This is per-
	formed for each time step.
<pre>DataSet.box_min(self[, x, y])</pre>	Calculate the grid box min for all variables This is per-
	formed for each time step.
DataSet.box_sum(self[, x, y])	Calculate the grid box sum for all variables This is per-
	formed for each time step.
DataSet.box_range(self[, x, y])	Calculate the grid box range for all variables This is per-
	formed for each time step.

# nctoolkit.DataSet.regrid

DataSet.**regrid**(self, grid=None, method='bil', recycle=False, \\*\\*kwargs)
Regrid a dataset to a target grid

#### **Parameters**

- **grid** (nctoolkit.DataSet, pandas data frame or netCDF file) The grid to remap to
- **method** (*str*) Remapping method. Defaults to "bil". Methods available are: bilinear "bil"; nearest neighbour "nn" "nearest neighbour" bicubic interpolation "bic" Distance-weighted average "dis" First order conservative remapping "con" Second order conservative remapping "con" Large area fraction remapping "laf"
- **recycle** (*bool*) Set to True if you want to re-use the remapping weights when you are regridding another dataset.
- **kwargs** (*optional method to generate grid*) Instead of supplying a grid using 'grid', you can supply *lon* and *lat*. These must be equally lengthed lists or arrays that will be used to generate the grid. If you want to regrid to a single location you can just supply a float to lon and lat.

#### nctoolkit.DataSet.to latlon

DataSet.to\_latlon(self, lon=None, lat=None, res=None, method='bil', recycle=False)
Regrid a dataset to a regular latlon grid

#### **Parameters**

- lon (1ist) 2 element list giving minimum and maximum longitude of target grid
- lat (list) 2 element list giving minimum and maximum latitude of target grid
- **res** (*float*, *int* or *list*) If float or int given, this will be the horizontal and vertical resolution of the target grid. If 2 element list is given, the first element is the longitudinal resolution and the second is the latitudinal resolution.
- **method** (*str*) Remapping method. Defaults to "bil". Methods available are: bilinear "bil"; nearest neighbour "nn" "nearest neighbour" bicubic interpolation "bic" Distance-weighted average "dis" First order conservative remapping "con" Second order conservative remapping "con" Large area fraction remapping "laf"
- **recycle** (*boo1*) Do you want the grid and weights to be available for recycling and use in regrid? Defaults to False

#### nctoolkit.DataSet.match points

DataSet.match\_points(self, df=None, variables=None, depths=None, tmean=False, top=False, nan=None, regrid='bil', max\_extrap=5, \\*\\*kwargs)

Match dataset to a spatiotemporal points dataframe

#### **Parameters**

- **df** (*pandas DataFrame*) The column names must be made up of a subset of "lon", "lat", "year", "month", "day" and "depth" Pressure (in dbars), named "pressure", can also be used instead of "depth", which will require the optional dependency seawater to be installed.
- **variables** (*str or list*) Str or list of variables. All variables are matched up if this is not supplied. This can include variables generated by assign using kwargs.
- **depths** (nctoolkit DataSet or list) If each cell has different vertical levels, this must be provided as a dataset. If each cell has the same vertical levels, provide it as a list. If this is not supplied nctoolkit will try to figure out what they are. Only required if carrying out vertical matchups.
- **tmean** (*boo1*) Set to True or False, depending on whether you want temporal averaging at the temporal resolution given by df. For example, if you only had months in df, but had daily data in ds, you might want to calculate a daily average in the monthly dataset. This is equivalent to apply *ds.tmean(..)* to the dataset.
- **top** (*boo1*) Set to True if you want only the top/surface level of the dataset to be selected for matching.
- nan (float or list) Value or range of values to set to nan. Defaults to 0. Only required if values in dataset need changed to missing
- **regrid** (*str*) Regridding method. Defaults to "bil". Options available are those in nctoolkit regrid method. "nn" for nearest neighbour.
- max\_extrap (float) Maximum distance for extrapolation. Defaults to 5.
- **kwargs** (*kwargs*) Additional arguments to send to assign

### **Returns matchpoints**

Return type pandas.DataFrame

# nctoolkit.DataSet.resample\_grid

DataSet.resample\_grid(self, factor=None)

Resample the horizontal grid of a dataset

**Parameters factor** (*int*) – The resampling factor. Must be a positive integer. No interpolation occurs. Example: factor of 2 will sample every other grid cell

# **Examples**

If you wanted to select every other grid cell, you could do the following:

>>> ds.resample\_grid(2)

## nctoolkit.DataSet.time\_interp

DataSet.time\_interp(self, start=None, end=None, resolution='monthly')

Temporally interpolate variables based on date range and time resolution

#### **Parameters**

- **start** (*str*) Start date for interpolation. Needs to be of the form YYYY/MM/DD or YYYY-MM-DD.
- **end** (*str*) End date for interpolation. Needs to be of the form YYYY/MM/DD or YYYY-MM-DD. If end is not given interpolation will be to the final available time in the dataset.
- **resolution** (*str*) Time steps used for interpolation. Needs to be "daily", "weekly", "monthly" or "yearly". Defaults to monthly.

### nctoolkit.DataSet.timestep interp

DataSet.timestep\_interp(self, steps=None)

Temporally interpolate a dataset to given number of time steps between existing time steps

**Parameters steps** (*int*) – Number of time steps to interpolate between existing time steps. For example, if you wanted to go from daily to hourly data you would set steps=24.

# nctoolkit.DataSet.fill na

DataSet.**fill\_na**(self, n=1)

Fill missing values with a distance-weighted average. This carries out infilling for each time step and vertical level.

**Parameters n** (int) – Number of nearest neighbours to use. Defaults to 1. To

#### nctoolkit.DataSet.box mean

```
DataSet.box_mean(self, x=1, y=1)
```

Calculate the grid box mean for all variables This is performed for each time step.

#### **Parameters**

- **x** (int) Number of boxes in the x, e.g. east-west direction
- y (int or float) Number of boxes in the y, e.g. north-south direction

### nctoolkit.DataSet.box max

```
DataSet.box_max(self, x=1, y=1)
```

Calculate the grid box max for all variables This is performed for each time step.

#### **Parameters**

- **x** (int) Number of boxes in the x, e.g. east-west direction
- y (int or float) Number of boxes in the y, e.g. north-south direction

### nctoolkit.DataSet.box min

```
DataSet.box_min(self, x=1, y=1)
```

Calculate the grid box min for all variables This is performed for each time step.

#### **Parameters**

- **x** (*int*) Number of boxes in the x, e.g. east-west direction
- y (int or float) Number of boxes in the y, e.g. north-south direction

# nctoolkit.DataSet.box\_sum

```
DataSet.box_sum(self, x=1, y=1)
```

Calculate the grid box sum for all variables This is performed for each time step.

#### **Parameters**

- **x** (int) Number of boxes in the x, e.g. east-west direction
- y (int or float) Number of boxes in the y, e.g. north-south direction

### nctoolkit.DataSet.box\_range

```
DataSet.box_range(self, x=1, y=1)
```

Calculate the grid box range for all variables This is performed for each time step.

#### **Parameters**

- $\mathbf{x}$  (int) Number of boxes in the x, e.g. east-west direction
- y (int or float) Number of boxes in the y, e.g. north-south direction

# 4.20.19 Masking methods

<pre>DataSet.mask_box(self[, lon, lat])</pre>	Mask a lon/lat box
---	--------------------

### nctoolkit.DataSet.mask box

DataSet.mask\_box(self, lon=[-180, 180], lat=[-90, 90])
Mask a lon/lat box

#### **Parameters**

- **lon** (*list*) Longitude range to mask. Must be of the form: [lon\_min, lon\_max]
- lat (list) Latitude range to mask. Must be of the form: [lat\_min, lat\_max]

# 4.20.20 Anomaly methods

DataSet.annual_anomaly(self[, baseline,])	Calculate annual anomalies for each variable based on a baseline period The anomaly is derived by first calculating the climatological annual mean for the given baseline period.
<pre>DataSet.monthly_anomaly(self[, baseline])</pre>	Calculate monthly anomalies based on a baseline period
	The anomaly is derived by first calculating the climato-
	logical monthly mean for the given baseline period.

# nctoolkit.DataSet.annual\_anomaly

DataSet.annual\_anomaly(self, baseline=None, metric='absolute', window=1)

Calculate annual anomalies for each variable based on a baseline period The anomaly is derived by first calculating the climatological annual mean for the given baseline period. Annual means are then calculated for each year and the anomaly is calculated compared with the baseline mean. This will be calculated on a per-file basis in a multi-file dataset.

#### **Parameters**

- baseline (1ist) Baseline years. This needs to be the first and last year of the climatological period. Example: a baseline of [1980,1999] will result in anomalies against the 20 year climatology from 1980 to 1999.
- **metric** (*str*) Set to "absolute" or "relative", depending on whether you want the absolute or relative anomaly to be calculated.
- window (int) A window for the anomaly. By default window = 1, i.e. the annual anomaly is calculated. If, for example, window = 20, the 20 year rolling means will be used to calculate the anomalies.

If you wanted to calculate an annual anomaly where values are compared with the mean for the years 1950-1969, you would do this:

```
>>> ds.annual_anomaly(baseline = [1950, 1969])
```

By default, this results in the absolute difference to be used. If you wanted the anomaly to be calculated relative to the baseline mean, you would do this:

```
>>> ds.annual_anomaly(baseline = [1950, 1969], metric = "relative")
```

You might want to smooth out the anomalies, so that you are looking at rolling averages. In that case you can supply a windows. So if you wanted to calculate the anomaly using a rolling average with a 10 year window, you would do this:

```
>>> ds.annual_anomaly(baseline = [1950, 1969], window = 10)
```

# nctoolkit.DataSet.monthly\_anomaly

## DataSet.monthly\_anomaly(self, baseline=None)

Calculate monthly anomalies based on a baseline period The anomaly is derived by first calculating the climatological monthly mean for the given baseline period. Monthly means are then calculated for each year and the anomaly is calculated compared with the baseline mean. This is calculated separately for each file in a multi-file dataset.

**Parameters baseline** (*list*) – Baseline years. This needs to be the first and last year of the climatological period. Example: a baseline of [1985,2005] will result in anomolies against 20 year climatology from 1986 to 2005.

# **Examples**

If you wanted to calculate a monthly anomaly where values are compared with the climatological monthly mean for the years 1950-1969, you would do this:

```
>>> ds.monthly_anomaly(baseline = [1950, 1969])
```

# 4.20.21 Statistical methods

<pre>DataSet.tmean(self[, over, align])</pre>	Calculate the temporal mean of all variables
DataSet.tmin(self[, over, align])	Calculate the temporal minimum of all variables
<pre>DataSet.tmedian(self[, over, align])</pre>	Calculate the temporal median of all variables
<pre>DataSet.tpercentile(self[, p, over, align])</pre>	Calculate the temporal percentile of all variables
DataSet.tmax(self[, over, align])	Calculate the temporal maximum of all variables
DataSet.tsum(self[, over, align])	Calculate the temporal sum of all variables
DataSet.trange(self[, over, align])	Calculate the temporal range of all variables
DataSet.tstdev(self[, over, align])	Calculate the temporal standard deviation of all vari-
	ables
DataSet.tcumsum(self[, align])	Calculate the temporal cumulative sum of all variables
DataSet.tvar(self[, over, align])	Calculate the temporal variance of all variables
	continues on next page

Table 23 – continued from previous page	Table	23 -	<ul> <li>continued</li> </ul>	from	previous	page
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	unued from previous page
<pre>DataSet.cor_space(self[, var1, var2])</pre>	Calculate the correlation correct between two variables
	in space This is calculated for each time step.
<pre>DataSet.cor_time(self[, var1, var2])</pre>	Calculate the correlation correct in time between two
	variables The correlation is calculated for each grid cell,
	ignoring missing values.
DataSet.spatial_mean(self)	Calculate the area weighted spatial mean for all variables
	This is performed for each time step.
DataSet.spatial_min(self)	Calculate the spatial minimum for all variables This is
• • • • • • • • • • • • • • • • • • • •	performed for each time step.
DataSet.spatial_max(self)	Calculate the spatial maximum for all variables This is
* - ( )	performed for each time step.
<pre>DataSet.spatial_percentile(self[, p])</pre>	Calculate the spatial sum for all variables This is per-
	formed for each time step.
DataSet.spatial_range(self)	Calculate the spatial range for all variables This is per-
2 a cas o c : sp a c 2 a 2 a 1 g c (3 a 1 )	formed for each time step.
DataSet.spatial_sum(self[, by_area])	Calculate the spatial sum for all variables This is per-
	formed for each time step.
DataSet.spatial_stdev(self)	Calculate the spatial range for all variables This is per-
	formed for each time step.
DataSet.spatial_var(self)	Calculate the spatial range for all variables This is per-
	formed for each time step.
DataSet.centre(self[, by, by_area])	Calculate the latitudinal or longitudinal centre for each
=	year/month combination in files.
DataSet.zonal_mean(self)	Calculate the zonal mean for each year/month combina-
	tion in files.
DataSet.zonal_min(self)	Calculate the zonal minimum for each year/month com-
()	bination in files.
DataSet.zonal_max(self)	Calculate the zonal maximum for each year/month com-
2 4 6 4 5 6 7 2 6 1 4 2 1 1 4 1 1 1 1 1 1 1 1 1 1 1 1 1 1	bination in files.
DataSet.zonal_range(self)	Calculate the zonal range for each year/month combina-
2 u c u c c c c c c c c c c c c c c c c	tion in files.
DataSet.meridonial_mean(self)	Calculate the meridonial mean for each year/month com-
parabet mer radirar_mean (son)	bination in files.
DataSet.meridonial_min(self)	Calculate the meridonial minimum for each year/month
2 3 2 3 2 2	combination in files.
DataSet.meridonial_max(self)	Calculate the meridonial maximum for each year/month
z a cas e e i mez z avizaz _man(ben)	combination in files.
DataSet.meridonial_range(self)	Calculate the meridonial range for each year/month
Databet.merraonrar_range(son)	combination in files.
	Comomation in mes.

### nctoolkit.DataSet.tmean

DataSet.tmean(self, over='time', align='right')
Calculate the temporal mean of all variables

#### **Parameters**

- **over** (*str or list*) Time periods to average over. Options are 'year', 'month', 'day'.
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

If you want to calculate mean over all time steps. Do the following:

```
>>> ds.tmean()
```

If you want to calculate the mean for each year in a dataset, do this:

```
>>> ds.tmean("year")
```

If you want to calculate the mean for each month in a dataset, do this:

```
>>> ds.tmean("month")
```

If you want to calculate the mean for each month in each year in a dataset, do this:

```
>>> ds.tmean(["year", "month"])
```

This method will also let you easily calculate climatologies. So, if you wanted to calculate a monthly climatological mean, you would do this:

```
>>> ds.tmean( "month")
```

A daily climatological mean would be the following:

```
>>> ds.tmean( "day")
```

### nctoolkit.DataSet.tmin

DataSet.tmin(self, over='time', align='right')

Calculate the temporal minimum of all variables

## **Parameters**

- **over** (str or list) Time periods to average over. Options are 'year', 'month', 'day'.
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

### **Examples**

If you want to calculate minimum over all time steps. Do the following:

```
>>> ds.tmin()
```

If you want to calculate the minimum for each year in a dataset, do this:

```
>>> ds.tmin("year")
```

If you want to calculate the minimum for each month in a dataset, do this:

```
>>> ds.tmin("month")
```

If you want to calculate the minimum for each month in each year in a dataset, do this:

```
>>> ds.tmin(["year", "month"])
```

This method will also let you easily calculate climatologies. So, if you wanted to calculate a monthly climatological min, you would do this:

```
>>> ds.tmin( "month")
```

A daily climatological minimum would be the following:

```
>>> ds.tmin( "day")
```

### nctoolkit.DataSet.tmedian

DataSet.tmedian(self, over='time', align='right')

Calculate the temporal median of all variables

#### **Parameters**

- over (str or list) Time periods to average over. Options are 'year', 'month', 'day'.
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

# **Examples**

If you want to calculate median over all time steps. Do the following:

```
>>> ds.tmedian()
```

If you want to calculate the median for each year in a dataset, do this:

```
>>> ds.tmedian("year")
```

If you want to calculate the median for each month in a dataset, do this:

```
>>> ds.tmedian("month")
```

If you want to calculate the median for each month in each year in a dataset, do this:

```
>>> ds.tmedian(["year", "month"])
```

This method will also let you easily calculate climatologies. So, if you wanted to calculate a monthly climatological median, you would do this:

```
>>> ds.tmedian( "month")
```

A daily climatological median would be the following:

```
>>> ds.tmedian( "day")
```

# nctoolkit.DataSet.tpercentile

DataSet.**tpercentile**(*self*, *p=None*, *over='time'*, *align='right'*)

Calculate the temporal percentile of all variables

#### **Parameters**

- p (float or int) Percentile to calculate
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

## **Examples**

If you want to calculate the 20th percentile over all time steps. Do the following:

```
>>> ds.tpercentile(20)
```

If you want to calculate the 20th percentile for each year in a dataset, do this:

```
>>> ds.tpercentile(20)
```

### nctoolkit.DataSet.tmax

DataSet.tmax(self, over='time', align='right')

Calculate the temporal maximum of all variables

#### **Parameters**

- over (str or list) Time periods to average over. Options are 'year', 'month', 'day'.
- = **str** (align) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

# **Examples**

If you want to calculate maximum over all time steps. Do the following:

```
>>> ds.tmax()
```

If you want to calculate the maximum for each year in a dataset, do this:

```
>>> ds.tmax("year")
```

If you want to calculate the maximum for each month in a dataset, do this:

```
>>> ds.tmax("month")
```

If you want to calculate the maximum for each month in each year in a dataset, do this:

```
>>> ds.tmax(["year", "month"])
```

This method will also let you easily calculate climatologies. So, if you wanted to calculate a monthly climatological max, you would do this:

```
>>> ds.tmax( "month")
```

A daily climatological maximum would be the following:

```
>>> ds.tmax( "day")
```

#### nctoolkit.DataSet.tsum

DataSet.tsum(self, over='time', align='right')

Calculate the temporal sum of all variables

**Parameters** = str(align) – This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

## nctoolkit.DataSet.trange

DataSet.trange(self, over='time', align='right')

Calculate the temporal range of all variables

#### **Parameters**

- over (str or list) Time periods to average over. Options are 'year', 'month', 'day'.
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

## **Examples**

If you want to calculate range over all time steps. Do the following:

```
>>> ds.trange()
```

If you want to calculate the range for each year in a dataset, do this:

```
>>> ds.trange("year")
```

If you want to calculate the range for each month in a dataset, do this:

```
>>> ds.trange("month")
```

If you want to calculate the range for each month in each year in a dataset, do this:

```
>>> ds.trange(["year", "month"])
```

This method will also let you easily calculate climatologies. So, if you wanted to calculate a monthly climatological range, you would do this:

```
>>> ds.trange( "month")
```

A daily climatological range would be the following:

```
>>> ds.trange( "day")
```

#### nctoolkit.DataSet.tstdev

DataSet.tstdev(self, over='time', align='right')

Calculate the temporal standard deviation of all variables

#### **Parameters**

- over (str or list) Time periods to average over. Options are 'year', 'month', 'day'.
- **align** (str) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

## **Examples**

If you want to calculate standard deviation over all time steps. Do the following:

```
>>> ds.tstdev()
```

If you want to calculate the standard deviation for each year in a dataset, do this:

```
>>> ds.tstdev("year")
```

If you want to calculate the standard deviation for each month in a dataset, do this:

```
>>> ds.tstdev("month")
```

If you want to calculate the standard deviation for each month in each year in a dataset, do this:

```
>>> ds.tstdev(["year", "month"])
```

This method will also let you easily calculate climatologies. So, if you wanted to calculate a monthly climatological var, you would do this:

```
>>> ds.tstdev("month")
```

A daily climatological standard deviation would be the following:

```
>>> ds.tstdev("day")
```

#### nctoolkit.DataSet.tcumsum

DataSet.tcumsum(self, align='right')

Calculate the temporal cumulative sum of all variables

**Parameters align** (str) – This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

If you want to calculate the cumulative sum for all variables over all timesteps, do this:

```
>>> ds.tcumsum()
```

#### nctoolkit.DataSet.tvar

DataSet.tvar(self, over='time', align='right')

Calculate the temporal variance of all variables

#### **Parameters**

- **over** (str or list) Time periods to average over. Options are 'year', 'month', 'day'.
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

# **Examples**

If you want to calculate variance over all time steps. Do the following:

```
>>> ds.tvar()
```

If you want to calculate the variance for each year in a dataset, do this:

```
>>> ds.tvar("year")
```

If you want to calculate the variance for each month in a dataset, do this:

```
>>> ds.tvar("month")
```

If you want to calculate the variance for each month in each year in a dataset, do this:

```
>>> ds.tvar(["year", "month"])
```

This method will also let you easily calculate climatologies. So, if you wanted to calculate a monthly climatological var, you would do this:

```
>>> ds.tvar( "month")
```

A daily climatological variance would be the following:

```
>>> ds.tvar( "day")
```

# nctoolkit.DataSet.cor\_space

```
DataSet.cor_space(self, var1=None, var2=None)
```

Calculate the correlation correct between two variables in space This is calculated for each time step. The correlation coefficient coefficient is calculated using values in all grid cells, ignoring missing values.

## **Parameters**

- var1 (str) The first variable
- var2 (str) The second variable

# **Examples**

If you wanted to calculate the spatial correlation coefficient between variables x and y in a dataset, you would do this:

```
>>> ds.cor_space("x", "y")
```

The correlation coefficient will be calculated for each time step.

## nctoolkit.DataSet.cor time

DataSet.cor\_time(self, var1=None, var2=None)

Calculate the correlation correct in time between two variables The correlation is calculated for each grid cell, ignoring missing values.

#### **Parameters**

- **var1** (*str*) The first variable
- var2 (str) The second variable

# **Examples**

If you wanted to calculate the temporal correlation coefficient between variables x and y in a dataset, you would do this:

```
>>> ds.cor_space("x", "y")
```

The correlation coefficient will be calculated for each grid cell. This method will indicate how temporally correlated variables are in different spatial regions.

# nctoolkit.DataSet.spatial\_mean

# DataSet.spatial\_mean(self)

Calculate the area weighted spatial mean for all variables This is performed for each time step.

If you want to calculate the spatial mean for a dataset, just do the following:

```
>>> ds.spatial_mean()
```

Note that this calculation will calculate the average using weights based on each cell's area. If cell areas cannot be calculated, it will take a straight average, and a warning will say this.

# nctoolkit.DataSet.spatial\_min

### DataSet.spatial\_min(self)

Calculate the spatial minimum for all variables This is performed for each time step.

# **Examples**

If you want to calculate the spatial minimum for a dataset, just do the following:

```
>>> ds.spatial_min()
```

## nctoolkit.DataSet.spatial\_max

# DataSet.spatial\_max(self)

Calculate the spatial maximum for all variables This is performed for each time step.

# **Examples**

If you want to calculate the spatial maximum for a dataset, just do the following:

```
>>> ds.spatial_max()
```

## nctoolkit.DataSet.spatial percentile

## DataSet.spatial\_percentile(self, p=None)

Calculate the spatial sum for all variables This is performed for each time step.

**Parameters p** (int or float) – Percentile to calculate. 0<=p<=100.

### **Examples**

If you want to calculate the median of each variable across space for a dataset, just do the following:

```
>>> ds.spatial_percentile(50)
```

# nctoolkit.DataSet.spatial\_range

#### DataSet.spatial\_range(self)

Calculate the spatial range for all variables This is performed for each time step.

## **Examples**

If you want to calculate the range of each variable across space for a dataset, just do the following:

```
>>> ds.spatial_max()
```

# nctoolkit.DataSet.spatial\_sum

DataSet.**spatial\_sum**(*self*, *by\_area=False*)

Calculate the spatial sum for all variables This is performed for each time step.

**Parameters by\_area** (*boolean*) – Set to True if you want to multiply the values by the grid cell area before summing over space. Default is False.

# **Examples**

If you want to calculate the spatial sum each variable across space for a dataset, just do the following:

```
>>> ds.spatial_sum()
```

By default, this method simply sums up each grid cell value. In some cases this is not suitable. For example, the values in each cell may concentrations or values per square metre etc. In this case multiplying each cell value by the cell area is more suitable. Do the following:

```
>>> ds.spatial_sum(by_area = True)
```

Each cell's value will be multiplied by the area of the cell (in square metres) prior to calculating the spatial sum.

# nctoolkit.DataSet.spatial\_stdev

```
DataSet.spatial_stdev(self)
```

Calculate the spatial range for all variables This is performed for each time step.

## **Examples**

If you want to calculate the range of each variable across space for a dataset, just do the following:

```
>>> ds.spatial_max()
```

# nctoolkit.DataSet.spatial\_var

### DataSet.spatial\_var(self)

Calculate the spatial range for all variables This is performed for each time step.

## **Examples**

If you want to calculate the range of each variable across space for a dataset, just do the following:

>>> ds.spatial\_max()

### nctoolkit.DataSet.centre

DataSet.centre(self, by='latitude', by\_area=False)

Calculate the latitudinal or longitudinal centre for each year/month combination in files. This applies to each file in an ensemble.

#### **Parameters**

- **by** (str) Set to 'latitude' if you want the latitiduinal centre calculated. 'longitude' for longitudinal.
- **by\_area** (*boo1*) If the variable is a value/m2 type variable, set to True, otherwise set to False.

### nctoolkit.DataSet.zonal mean

DataSet.zonal\_mean(self)

Calculate the zonal mean for each year/month combination in files. This applies to each file in an ensemble.

# **Examples**

If you want to calculate the zonal mean for a dataset, do the following:

>>> ds.zonal\_mean()

## nctoolkit.DataSet.zonal\_min

DataSet.zonal\_min(self)

Calculate the zonal minimum for each year/month combination in files. This applies to each file in an ensemble.

## **Examples**

If you want to calculate the zonal minimum for a dataset, do the following:

>>> ds.zonal\_min()

## nctoolkit.DataSet.zonal max

### DataSet.zonal\_max(self)

Calculate the zonal maximum for each year/month combination in files. This applies to each file in an ensemble.

# **Examples**

If you want to calculate the zonal maximum for a dataset, do the following:

```
>>> ds.zonal_max()
```

# nctoolkit.DataSet.zonal\_range

### DataSet.zonal\_range(self)

Calculate the zonal range for each year/month combination in files. This applies to each file in an ensemble.

# **Examples**

If you want to calculate the zonal range for a dataset, do the following:

```
>>> ds.zonal_range()
```

## nctoolkit.DataSet.meridonial\_mean

# DataSet.meridonial\_mean(self)

Calculate the meridonial mean for each year/month combination in files. This applies to each file in an ensemble.

# **Examples**

If you want to calculate the meridonial mean for a dataset, do the following:

```
>>> ds.meridonial_mean()
```

# nctoolkit.DataSet.meridonial\_min

## DataSet.meridonial\_min(self)

Calculate the meridonial minimum for each year/month combination in files. This applies to each file in an ensemble.

If you want to calculate the meridonial minimum for a dataset, do the following:

>>> ds.meridonial\_min()

# nctoolkit.DataSet.meridonial\_max

### DataSet.meridonial\_max(self)

Calculate the meridonial maximum for each year/month combination in files. This applies to each file in an ensemble.

# **Examples**

If you want to calculate the meridonial maximum for a dataset, do the following:

>>> ds.meridonial\_max()

## nctoolkit.DataSet.meridonial range

### DataSet.meridonial\_range(self)

Calculate the meridonial range for each year/month combination in files. This applies to each file in an ensemble.

# **Examples**

If you want to calculate the meridonial range for a dataset, do the following:

>>> ds.meridonial\_max()

# 4.20.22 Merging methods

DataSet.merge(self[, join, match, check])	Merge a multi-file ensemble into a single file 2 methods
	are available.

# nctoolkit.DataSet.merge

DataSet.merge(self, join='variables', match=['year', 'month', 'day'], check=True)

Merge a multi-file ensemble into a single file 2 methods are available. 1) merging files with different variables, but the same time steps. 2) merging files with the same variables, with different times.

#### **Parameters**

- **join** (*str*) This defines the type of merging to carry out. "variables": this will merge by variable, so that an ensemble with different variables, but the same number of time steps is merged to a single file. "time": this will merge files with the same variables, but different times to a single file, into a single file with ordered times. join defaults to "variables", and uses partial matches, so "var" will give variable based merging.
- match (list, str) Optional argument when join = 'variables'. A list or str stating what

must match in the netCDF files. Defaults to year/month/day. This list must be some combination of year/month/day. An error will be thrown if the elements of time in match do not match across all netCDF files. The only exception is if there is a single date file in the ensemble.

• **check** (*boo1*) – By default nctoolkit out checks in case files do not have the same variables etc. Set check to False if you are confident merging will be problem free. If you are unsure if files have the same variables, set check to True to find out. Note: if you do not explicitly provide check and there are more than 30 files in a dataset, checks will be turned off.

# 4.20.23 Splitting methods

<pre>DataSet.split(self[, by])</pre>	Split the dataset Each file in the ensemble will be sepa-
	rated into new files based on the splitting argument.

## nctoolkit.DataSet.split

DataSet.split(self, by=None)

Split the dataset Each file in the ensemble will be separated into new files based on the splitting argument.

**Parameters by** (str) – Available by arguments are 'year', 'month', 'yearmonth', 'season', 'day' 'name', "timestep". year will split files by year, month will split files by month, yearmonth will split files by year and month; season will split files by year, day will split files by day. Using "timestep" will split files by timestep. 'name' will split by variable name

## **Examples**

If you want to split each file into a dataset into a separate files for each year, do the following:

```
>>> ds.split("year")
```

If you wanted to split by month, do the following:

```
>>> ds.split("month")
```

# 4.20.24 Output and formatting methods

<pre>DataSet.to_nc(self, out[, zip, overwrite])</pre>	Save a dataset to a named file This will only work with
	single file datasets.
<pre>DataSet.to_xarray(self[, decode_times])</pre>	Open a dataset as an xarray object
<pre>DataSet.to_dataframe(self[, decode_times])</pre>	Open a dataset as a pandas data frame
DataSet.zip(self)	Zip the dataset This will compress the files within the
	dataset.
DataSet.format(self[, ext])	Zip the dataset This will compress the files within the
	dataset.

## nctoolkit.DataSet.to nc

DataSet.to\_nc(self, out, zip=True, overwrite=False, \\*\\*kwargs)

Save a dataset to a named file This will only work with single file datasets.

#### **Parameters**

- **out** (*str*) Output file name.
- zip (boolean) True/False depending on whether you want to zip the file. Default is True.
- **overwrite** (*boolean*) If out file exists, do you want to overwrite it? Default is False.
- **\*\*kwargs** (*kwargs*) Optional arguments to be sent to subset.

# **Examples**

If you want to export a dataset to a netCDF file, do the following:

```
>>> ds.to_nc("out.nc")
```

By default this file will be zipped. If you do not want it zipped, do this:

```
>>> ds.to_nc("out.nc", zip = False)
```

By default this cannot overwrite files. If the output file exists, do the following:

```
>>> ds.to_nc("out.nc", overwrite = True)
```

If you only want to export a subset of the data, you can use optional arguments that will be sent to subset. For example, if you only wanted the year 2000, you would do this:

```
>>> ds.to_nc("out.nc", year = 2000)
```

## nctoolkit.DataSet.to\_xarray

DataSet.to\_xarray(self, decode\_times=True, \\*\\*kwargs)

Open a dataset as an xarray object

#### **Parameters**

- **decode\_times** (*boolean*) Set to False if you do not want xarray to decode the times. Default is True. If xarray cannot decode times, CDO will be used.
- **\*\*kwargs** (*kwargs*) Optional arguments to be sent to subset.

Returns to\_xarray

Return type xarray.Dataset

If you want to convert a dataset to an xarray dataset, do the following:

```
>>> ds.to_xarray()
```

This will return an xarray dataset.

If you do not want time to be decoded, do the following:

```
>>> ds.to_xarray(decode_times = False)
```

## nctoolkit.DataSet.to dataframe

DataSet.to\_dataframe(self, decode\_times=True, \\*\\*kwargs)

Open a dataset as a pandas data frame

#### **Parameters**

- **decode\_times** (*boolean*) Set to False if you do not want xarray to decode the times prior to conversion to data frame. Default is True.
- **\*\*kwargs** (*kwargs*) Optional arguments to be sent to subset.

Returns to\_dataframe

Return type pandas.DataFrame

# nctoolkit.DataSet.zip

DataSet.zip(self)

Zip the dataset This will compress the files within the dataset. This works lazily.

### **Examples**

If you want to zip the files in a dataset, do the following:

```
>>> ds.zip()
```

This will occur lazily, so will only occur after everything has been evaluated.

## nctoolkit.DataSet.format

DataSet.format(self, ext=None)

Zip the dataset This will compress the files within the dataset. This works lazily.

**Parameters ext** (str) – New format. Must be one of "nc", "nc1", "nc2", "nc4" and "nc5". netCDF = nc1 netCDF version 2 (64-bit offset) = nc2/nc netCDF4 (HDF5) = nc4 netCDF4-classi = nc4c netCDF version 5 (64-bit data) = nc5

# 4.20.25 Miscellaneous methods

DataSet.na_count(self[, over, align])	Calculate the number of missing values
DataSet.na_frac(self[, over, align])	Calculate the number of missing values
DataSet.distribute(self[, m, n])	Split the dataset into multiple evenly sized horizontal
	and vertical new files
DataSet.collect(self)	Collect a dataset that has been split using distribute
DataSet.cell_area(self[, join])	Calculate the area of grid cells.
DataSet.first_above(self[, x])	Identify the time step when a value is first above a thresh-
	old This will do the comparison with either a number, a
	Dataset or a netCDF file.
DataSet.first_below(self[,x])	Identify the time step when a value is first below a thresh-
	old This will do the comparison with either a number, a
	Dataset or a netCDF file.
<pre>DataSet.last_above(self[, x])</pre>	Identify the final time step when a value is above a
	threshold This will do the comparison with either a num-
	ber, a Dataset or a netCDF file.
<pre>DataSet.last_below(self[, x])</pre>	Identify the last time step when a value is below a thresh-
	old This will do the comparison with either a number, a
	Dataset or a netCDF file.
<pre>DataSet.cdo_command(self[, command, ensemble])</pre>	Apply a cdo command
DataSet.nco_command(self[, command, ensemble])	Apply an nco command
DataSet.compare(self[, expression])	Compare all variables to a constant
DataSet.gt(self, x)	Method to calculate if variable in dataset is greater than
	that in another file or dataset This currently only works
	with single file datasets
DataSet.lt(self, x)	Method to calculate if variable in dataset is less than that
	in another file or dataset This currently only works with
	single file datasets
DataSet.reduce_dims(self)	Reduce dimensions of data This will remove any dimen-
	sions with only one value.
<pre>DataSet.reduce_grid(self[, mask])</pre>	Reduce the dataset to non-zero locations in a mask
DataSet.set_precision(self, x)	Set the precision in a dataset
DataSet.check(self)	Check contents of files for common data problems.
DataSet.is_corrupt(self)	Check if files are corrupt
DataSet.fix_nemo_ersem_grid(self)	A quick hack to change the grid file in North West Eu-
	ropean shelf Nemo grids.
DataSet.set_gridtype(self, grid)	Set the grid type.
DataSet.surface_mask(self)	Create a mask identifying the shallowest cell without
	missing values.
DataSet.strip_variables(self[, vars])	Remove any variables, such as bnds etc., from variables.
DataSet.no_leaps(self)	Remove leap years.
DataSet.as_double(self, x)	
<pre>DataSet.as_double(self, x)</pre>	Set a variable/dimension to double This is mostly useful
<pre>DataSet.as_double(self, x)</pre>	Set a variable/dimension to double This is mostly useful for cases when time is stored as an int, but you need a

## nctoolkit.DataSet.na count

DataSet.na\_count(self, over='time', align='right')

Calculate the number of missing values

#### **Parameters**

- **over** (*str or list*) Time periods to to the count over over. Options are 'time', 'year', 'month', 'day'.
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

## nctoolkit.DataSet.na\_frac

DataSet.na\_frac(self, over='time', align='right')

Calculate the number of missing values

#### **Parameters**

- **over** (*str or list*) Time periods to to the count over over. Options are 'time', 'year', 'month', 'day'.
- **align** (*str*) This determines whether the output time is at the left, centre or right hand side of the time window. Options are "left", "centre" and "right"

#### nctoolkit.DataSet.distribute

DataSet.**distribute**(self, m=1, n=1)

Split the dataset into multiple evenly sized horizontal and vertical new files

#### **Parameters**

- m (int) Number of rows
- **n** (int) Number of columns

#### nctoolkit.DataSet.collect

DataSet.collect(self)

Collect a dataset that has been split using distribute

## nctoolkit.DataSet.cell\_area

DataSet.cell\_area(self, join=True)

Calculate the area of grid cells. Area of grid cells is given in square meters.

**Parameters join** (*boolean*) – Set to False if you only want the cell areas to be in the output. join=True adds the areas as a variable to the dataset. Defaults to True.

## **Examples**

If you wanted to add the cell\_areas as a new variable in a dataset, you would do the following:

```
>>> ds.cell_area()
```

If you wanted to replace a dataset with the cell areas of that dataset, you would do the following:

```
>>> ds.cell_area(join = False)
```

## nctoolkit.DataSet.first\_above

## DataSet.first\_above(self, x=None)

Identify the time step when a value is first above a threshold This will do the comparison with either a number, a Dataset or a netCDF file.

**Parameters x** (*int*, *float*, *DataSet or netCDF file*) – An int, float, single file dataset or netCDF file to use for the threshold(s). If comparing with a dataset or single file there must only be a single variable in it. The grids must be the same.

## **Examples**

If you wanted to calculate the first time step where the value in a grid cell goes above 10, you would do the following

```
>>> ds.first_above(10)
```

If you wanted to calculate the first time step where the value in a grid cell goes above that in another dataset, the following will work. Note that both datasets must have the same grid, and can only have single variables. The second dataset can, of course, only have one timestep.

```
>>> ds.first_above(ds1)
```

#### nctoolkit.DataSet.first below

#### DataSet.first\_below(self, x=None)

Identify the time step when a value is first below a threshold This will do the comparison with either a number, a Dataset or a netCDF file.

**Parameters x** (int, float, DataSet or netCDF file) — An int, float, single file dataset or netCDF file to use for the threshold(s). If comparing with a dataset or single file there must only be a single variable in it. The grids must be the same.

## **Examples**

If you wanted to calculate the first time step where the value in a grid cell goes below 10, you would do the following

```
>>> ds.first_below(10)
```

If you wanted to calculate the first time step where the value in a grid cell goes above that in another dataset, the following will work. Note that both datasets must have the same grid, and can only have single variables. The second dataset can, of course, only have one timestep.

```
>>> ds.first_below(ds1)
```

## nctoolkit.DataSet.last above

#### DataSet.last\_above(self, x=None)

Identify the final time step when a value is above a threshold This will do the comparison with either a number, a Dataset or a netCDF file.

**Parameters x** (int, float, DataSet or netCDF file) – An int, float, single file dataset or netCDF file to use for the threshold(s). If comparing with a dataset or single file there must only be a single variable in it. The grids must be the same.

## **Examples**

If you wanted to calculate the last time step where the value in a grid cell is above 10, you would do the following

```
>>> ds.first_above(10)
```

If you wanted to calculate the last time step where the value in a grid cell goes above that in another dataset, the following will work. Note that both datasets must have the same grid, and can only have single variables. The second dataset can, of course, only have one timestep.

```
>>> ds.first_above(ds1)
```

#### nctoolkit.DataSet.last below

## DataSet.last\_below(self, x=None)

Identify the last time step when a value is below a threshold This will do the comparison with either a number, a Dataset or a netCDF file.

**Parameters x** (int, float, DataSet or netCDF file) – An int, float, single file dataset or netCDF file to use for the threshold(s). If comparing with a dataset or single file there must only be a single variable in it. The grids must be the same.

## **Examples**

If you wanted to calculate the last time step where the value in a grid cell is below 10, you would do the following

```
>>> ds.last_below(10)
```

If you wanted to calculate the last time step where the value in a grid cell is above that in another dataset, the following will work. Note that both datasets must have the same grid, and can only have single variables. The second dataset can, of course, only have one timestep.

```
>>> ds.last_below(ds1)
```

#### nctoolkit.DataSet.cdo command

 ${\tt DataSet.{\bf cdo\_command}(\it self, \it command=None, \it ensemble=False)}$ 

Apply a cdo command

#### **Parameters**

- **command** (*string*) cdo command to call. This command must be such that "cdo {command} infile outfile" will run.
- **ensemble** (*boo1*) Is this an ensemble command?

## nctoolkit.DataSet.nco command

 ${\tt DataSet.nco\_command}(\textit{self}, \textit{command=None}, \textit{ensemble=False})$ 

Apply an nco command

#### **Parameters**

- **command** (*string*) nco command to call. This must be of a form such that "nco {command} infile outfile" will run.
- **ensemble** (*boolean*) Set to True if you want the command to take all of the files as input. This is useful for ensemble methods.

## nctoolkit.DataSet.compare

DataSet.compare(self, expression=None)

Compare all variables to a constant

**Parameters expression** (str) – This a regular comparison such as "<0", ">0", "==0"

#### **Examples**

If you wanted to identify grid cells with positive values you would do the following:

```
>>> ds.compare(">0")
```

This will be calculcated for each time step.

If you wanted to identify grid cells with negative values, you would do this

```
>>> ds.compare("<0")
```

## nctoolkit.DataSet.gt

DataSet.gt(self, x)

Method to calculate if variable in dataset is greater than that in another file or dataset This currently only works with single file datasets

Parameters x (str or single file dataset) – File path or nctoolkit dataset

#### nctoolkit.DataSet.lt

DataSet. 1t(self, x)

Method to calculate if variable in dataset is less than that in another file or dataset This currently only works with single file datasets

Parameters x (str or single file dataset) - File path or notoolkit dataset

## nctoolkit.DataSet.reduce\_dims

DataSet.reduce\_dims(self)

Reduce dimensions of data This will remove any dimensions with only one value. For example, if only selecting one vertical level, the vertical dimension will be removed.

#### **Examples**

If you want to remove any dimensions that have only one value, do the following:

```
>>> ds.reduce_dims("out.nc")
```

Note that this will work lazily. This method is most useful when you want to simplify datasets before exporting them to something like a pandas dataframe.

## nctoolkit.DataSet.reduce\_grid

DataSet.reduce\_grid(self, mask=None)

Reduce the dataset to non-zero locations in a mask

**Parameters mask** (str or dataset) – single variable dataset or path to .nc file. The mask must have an identical grid to the dataset.

## nctoolkit.DataSet.set precision

## DataSet.set\_precision(self, x)

Set the precision in a dataset

#### **Parameters**

- **x** (str) The precision. One of 'I8', 'I16', 'I32', 'F32', 'F64'.
- **month** (*int*) The month
- day (int) The day
- base\_year (int) The base year for time creation in the netCDF. Defaults to 1900.

#### nctoolkit.DataSet.check

### DataSet.check(self)

Check contents of files for common data problems.

## nctoolkit.DataSet.is\_corrupt

#### DataSet.is\_corrupt(self)

Check if files are corrupt

## nctoolkit.DataSet.fix\_nemo\_ersem\_grid

#### DataSet.fix\_nemo\_ersem\_grid(self)

A quick hack to change the grid file in North West European shelf Nemo grids.

## nctoolkit.DataSet.set gridtype

```
DataSet.set_gridtype(self, grid)
```

Set the grid type. Only use this if, for example, the grid is "generic" when it should be lonlat.

**Parameters grid** (*str*) – Grid type. Needs to be one of "curvilinear", "unstructured", "dereference", "regular", "regularn" or "lonlat".

## nctoolkit.DataSet.surface\_mask

#### DataSet.**surface\_mask**(self)

Create a mask identifying the shallowest cell without missing values. This converts a dataset to a mask identifying which cell represents top level, for example the sea surface. 1 identifies the shallowest cell with non-missing values. Everything else is 0, or missing. At present this method only uses the first available variable from netCDF files, so it may not be suitable for all data

## nctoolkit.DataSet.strip\_variables

#### DataSet.strip\_variables(self, vars=None)

Remove any variables, such as bnds etc., from variables. This should probably only be done at the end of a processing chain before converting to a dataframe etc., as it is stripping away critical info for netCDF operations.

**Parameters vars** (str or list) – individual or list of variables to select and strip. All variables will be stripped if this is not defined.

## nctoolkit.DataSet.no\_leaps

## DataSet.no\_leaps(self)

Remove leap years. This uses an undocumented CDO feature to remove Feb 29 and sets the calendar to leap year free

## nctoolkit.DataSet.as\_double

## DataSet.as\_double(self, x)

Set a variable/dimension to double This is mostly useful for cases when time is stored as an int, but you need a double

**Parameters x** (list) − A list of variable/dimensions you want to convert to floats

## 4.20.26 Ecological methods

<pre>DataSet.phenology(self[, var, metric, p])</pre>	Calculate phenologies from a dataset Each file in an en-
	semble must only cover a single year, and ideally have
	all days.

## nctoolkit.DataSet.phenology

#### DataSet.phenology(self, var=None, metric=None, p=None)

Calculate phenologies from a dataset Each file in an ensemble must only cover a single year, and ideally have all days. The method assumes datasets have daily resolution.

## **Parameters**

- **var** (*str*) Variable to analyze.
- **metric** (*str*) Must be peak, middle, start or end. Peak is defined as the day of the maximum value. Middle is the day when the cumulative total of the variable first exceeds the cumulative total for the entire year. Start or end is defined as the first day when the cumulative total exceeds a percentile p of the maximum cumulative total.
- **p** (*str*) Percentile to use for start or end.

# 4.21 Package info

This package was created by Robert Wilson at Plymouth Marine Laboratory (PML).

# 4.21.1 Acknowledgements

The current codebase of nctoolkit was developed using funding from the NERC Climate Linked Atlantic Sector Science programme (NE/R015953/1) and a combination of UK Research and Innovation (UKRI) and European Research Council (ERC) funded research projects.

# 4.21.2 Bugs and issues

If you identify bugs or issues with the package please raise an issue at PML's Marine Systems Modelling group's GitHub page here or contact nctoolkit's creator at rwi@pml.ac.uk.

## 4.21.3 Contributions welcome

The package is new, with new features being added each month. There remain a large number of features that could be added, especially for dealing with atmospheric data. If packages users are interested in contributing or suggesting new features they are welcome to raise and issue at the package's GitHub page or contact me.

## 4.22 Cheat sheet

A cheat sheet providing a quick 2-page overview of nctoolkit is available here.

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