WrightTools documentation

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1 Introduction

WrightTools is a python package for processing and viewing data. WrightTools is designed to be used in python scripts. For the purpose of this document, we will assume that WrightTools is imported with the alias wt: import WrightTools as wt.

include overview of package structure

As a living software package with evolving capabilities, detailed documentation of WrightTools here is neither easy nor useful. For specific usage notes look to the docstrings in WrightTools itself. This document is meant to provide a coarse-grained description of the entire package. It also describes design philosophies and best-practices when using WrightTools.

2 Data

The Data class is an incredibly general class capable of representing any rectangular dataset. It fills two important roles within WrightTools:

- 1. Data defines a single format to represent the results almost any measurement or simulation.
- 2. Data provides a suite of methods for data manipulation.

Almost every capability of WrightTools relies upon Data to some extent. Data can be thought of as the glue that holds the entire Wright group software stack together.

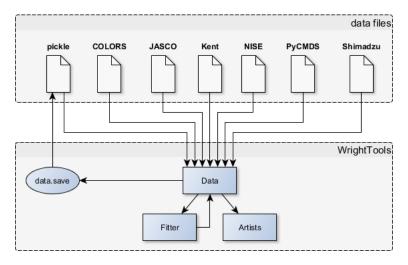


Figure 1: Data is the gateway to WrightTools.

Figure 1 represents WrightTools accepting data from a variety of sources and formats. Data objects are typically not created directly through Data.__init__ like most python classes. Instead, Data objects are created from files through a series of custom 'from_file' methods found in the data.py module. By creating separate methods, WrightTools can allow for easy Data creation from many different file formats. More details on Data creation can be found in Section 2.2. Once created, regardless of origin, the Data object is ready to be used by other classes in WrightTools, such as artists and Fitter.

2.1 Structure & Properties

The heart of Data are the numpy.ndarrays that contain the numbers themselves. Everything else is, in some sense, decoration. The arrays are not attributes of Data itself, rather they are attributes of the closely related wt.data.Axis and wt.data.Channel classes. Data contains lists of Axises and Channels. To understand the basic structure of Data, then, one must first understand the structure of Axis and Channel.

Axes are the *coordinates* of points in a dataset. Since all datasets are rectangular, axes are always one-dimensional. wt.data.Axis is the class that contains these coordinates and their properties.

points numpy.ndarray of axis coordinates

name the 'python-friendly' name

units the current units of the axis

convert method to convert axis units

label_seed list of subscript strings for label

get_label method to get formated label string

Table 1: The most important attributes and methods of the wt.data.Axis class.

values numpy.ndarray of dataset values the 'python-friendly' name name method to invert values invert maximum zmin minimum zmax null value znull signed bool flag for signed data method to enforce scaling such that znull to zmax spans 0-1 normalize method to remove values outside of a certain range clip

Table 2: The most important attributes and methods of the wt.data.Channel class.

Table 1 highlights the most important attributes and methods of Axis. Axes may be regular or differential.

Channels are the values in a dataset. A Data instance may contain many channels, since each coordinate may have multiple recorded values e.g. signal, pyro1, and pyro2. wt.data.Channel is the class that contains these values and their properties. Table 2 highlights the most important attributes and methods of Channel. The signed flag of Channel changes how other parts of WrightTools interact with the dataset. For example, an artist may choose to use a different colorbar if a dataset is signed. Allowing the 'null value' of a dataset to be non-zero is an important feature of WrightTools. When possible, developers should anticipate non-zero znulls. Also note that Channel.values may contain NaNs. When manipulating the values array directly, it is best practices to use Channel._update() to force the flags and attributes of the object to correspond to the new values.

The Data object has two primary attributes: axes, a list of Axis objects, and channels, a list of Channel objects. axes contains exactly one Axis object for each dimension of the dataset. The order of axes matters, so that the nth member of axes contains the coordinates along the nth dimension of the dataset. The order of channels is arbitrary. It is typical for code in WrightTools to assume that the most important channel is first. In addition to members of lists, Data dynamically sets the Axis and Channel objects it contains as attributes of itself according to the names of those objects. This means that users have two choices when accessing axes and channels. For example, consider an axis w1 located in dimension 0. To access this axis' points, one may go via the list: data.axes[0].points or directly data.w1.points. A consequence of this feature is that Axis and Channel object names must be unique to the Data container. Beyond the two main lists, Data is primarily a long series of methods that operate on the dataset it contains. Table 3 highlights the 'structural' attributes and methods of Data. There are many other attributes and methods of

```
axes
                  list of the contained Axis objects
      channels
                  list of the contained Channel objects
                  the 'python-friendly' name
           name
                  powerful method for accessing lower-dimensional slice(s)
           chop
                  method for splitting dataset at axis coordinate(s)
          split
     transpose
                  method to change order of dimensions in dataset
                  method for getting deep copy
           сору
                  method for flipping order of coordinates within an axis
           flip
                  method to map dataset onto new coordinates using interpolation
      map_axis
                  method to remove a channel
remove_channel
bring_to_front
                  method to bring a channel to the front of channels
```

Table 3: The most important attributes and methods of the wt.data.Data class.

Data, most of which will be talked about in specific context elsewhere in this document.

2.2 Instantiation

The creation of a Data object from a raw file or other source may be a very different process depending on the dataset's origin. It is not reasonable to handle all details for all datastreams directly in wt.data.Data.__init__. Instead, Data objects are typically created using a wt.data.from_X method. These methods accept any relevant parameters and return an instantiated Data object. wt.data.from_X methods have been written for all of the commonly-used file formats in the Wright Group.

The details of importing from each source are unique, but there is a common theme:

- 1. Recognize axes of scan
- 2. Grid raw data onto scan axes
- 3. Assemble Data instance

2.2.1 Direct

Direct instantiation of Data is easy, if you start with your dataset as regular arrays in python.

2.2.2 PyCMDS

PyCMDS was developed from the start to work well with WrightTools. One of the most important products of that design is the rich system of headers that PyCMDS .data files posses, making the step of scan axis recognition trivial...

2.2.3 COLORS and Kent

2.3 Manipulation

chop, slice, join etc

2.4 Scaling & Normalization

2.4.1 dOD

Transient absorption data is most usefully viewed in dOD units, but it is naturally recorded in dI and I. The dOD method of Data does the necessary transformation. Conveniently, absolute OD cancels out such that dI and I are all that is needed to calculate dOD.

$$dOD = -\log_{10}\left(\frac{I+dI}{I_0}\right) + \log_{10}\left(\frac{I}{I_0}\right) \tag{1}$$

$$= -(\log_{10}(I+dI) - \log_{10}(I_0)) + (\log_{10}(I) - \log_{10}(I_0))$$
 (2)

$$= \log_{10}(I) - \log_{10}(I + dI) \tag{3}$$

$$= -\log_{10}\left(\frac{I+dI}{I}\right) \tag{4}$$

Here I_0 is the probe intensity before the sample, I is the probe intensity after the sample without pump, and dI is the change in probe intensity caused by the pump.

There are a few instrumental considerations when measuring I and dI:

- 1. Typically it is most convenient to measure I as the average probe intensity for all shots (with and without pump). This is a good approximation as long as $dI \ll I$.
- 2. dI is defined as the total change in intensity. Boxcar averagers in active background subtraction mode return one half of the total change. The dOD method has a kwarg 'method' that can be used to appropriately take this factor of two into account. PyCMDS takes this factor into account in shots processing.

3 Artists

The artists module contains a variety of tools, all related to visualizing data. It contains two workhorse classes: wt.artists.mpl_2D and wt.artists.mpl_1D, which generate general visualizations of 2D and 1D slices of data objects. It also contains a series of specialized artists.

3.1 Colormaps

Figure 3 shows the RGB components of WrightTools' default colormap for single-signed data. This colormap is a custom implementation of the 'cubehelix' color scheme developed by Green [1]. The parameters were chosen to keep the colormap perceptual while closely matching the traditional Wright group colormap (wt.artists.colormaps['wright']). The colormap is slightly distorted in luminosity for aesthetic purposes.

WrightTools colormaps CMRmap cubehelix default experimental earth gnuplot2 greenscale greyscale invisible isoluminant isoluminant2 isoluminant3 ncar paried prism rainbow seismic signed signed_old skyebar skyebar_d skyebar_i spectral

Figure 2: WrightTools colormaps as of version 1.5.0.

wright

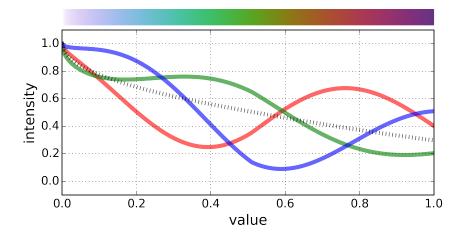


Figure 3: WrightTools default colormap RGB components.

4 Fit

The fit module provides tools for fitting data. It contains a series of Function objects, which handle the actual minimization routines given a dataset. These can be used outside of WrightTools. For example, given xi and yi as 1D arrays:

The fit module also contains a class made to send data through fitting operations: wt.fit.Fitter. Like in WrightTools artists, Fitter will take high dimensionality data and iterate over the dimensions higher than the ones being addressed.

5 Tuning

The tuning module provides tools for interacting with for optical parametric amplifier (OPA) tuning curves. It defines a main class, wt.tuning.curve.Curve, which is capable of representing tuning curves from multiple kinds of OPA. The tuning module also contains a series of modules and methods that accomplish certain specialized data processing tasks related to OPA tuning.

5.1 OPA Tuning Curves

OPA tuning curves are arrays of motor positions corresponding to parametric output colors. Wright-Tools offers an object-type to represent and manipulate OPA tuning curve arrays.

5.1.1 The Curve Class

The Curve class is made to contain OPA tuning curve data for any kind of OPA. By representing curves from different OPA hardware in the same format, WrightTools consolidates common tuning curve manipulations. Curve is a lot like the wt.data.Data class:

- 1. Curve is a container for other objects in this case instances of the wt.tuning.curve.Motor class.
- 2. Curve objects are not meant to be instantiated directly. Instead they are returned by the 'from' methods of the wt.tuning.curve module.

OPA tuning curves are often defined in 'stages' where each stage accomplishes an additional parametric conversion on the light supplied by the previous stage. For example, a 'base' OPA may supply pump and signal to a mixing crystal to be added together again to sum frequency signal. The sum frequency may then go on again to be doubled in another mixing process and so on. Each stage has its own tuning curve. To accommodate this structure Curve objects may be 'nested' inside of themselves, such that each curve refers to its own attribute curve.subcurve to get the motor positions for the previous stage.

Curve objects have some useful methods for visualizing and working with tuning curve arrays.

discuss interpolation

Curve objects also serve as a convenient backend for OPA hardware in PyCMDS...

curve.get_motor_positions returns a numpy array with shape (motor count, color count)...

5.2 TOPAS-C Motortune Processing

Traveling-wave Optical Parametric Amplifier of White-light Continuum (TOPAS-C) is an automated OPA made by Light Conversion. In TOPAS-C, four motors are used in the creation of

discuss map axes, plot, save, offset

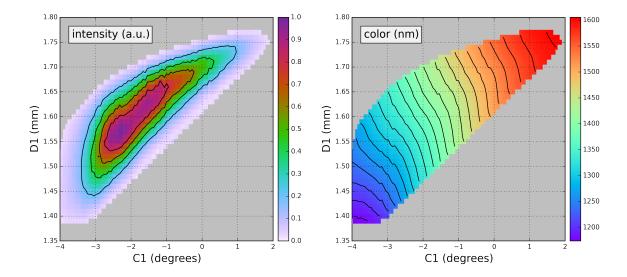


Figure 4: OPA output intensity and color as a function of C1 and D1. Measured on OPA1 (serial number 10743) 2016/01/13. Plotted pixels correspond directly to actual measured OPA outputs. The OPA output was measured using an array detector and fit to a single Gaussian lineshape. Grey pixels gave bad fits and were therefore filtered out. A small number of fits within the body of good data did fail and were filled in using bi-cubic interpolation. Data taken with PyCMDS MOTORTUNE module.

signal and idler. These can be divided into subcategories of 'preamp' and 'poweramp', each containing two motors. After signal and idler are generated, additional motorized crystals, 'mixers', can be used to upconvert or downconvert the base colors. This allows TOPAS-C to achieve a huge dynamic range of output colors, from ultraviolet to mid-infrared.z

WrightTools contains a processing method for each parametric process used in the Wright group TOPAS-C. Each of these methods is described in this section.

5.2.1 Signal Preamp

In the TOPAS-C preamp white light is mixed non-colinearly with a small amount of pump to generate signal and idler. The signal output is angularly isolated and sent on to seed parametric output in a second crystal (the poweramp).

Two motors are used to control preamp output: Crystal 1 (C1) controls the angle of the mixing crystal and Delay 1 (D1) controls the delay between white light and pump in the mixing crystal. White light in TOPAS-C is intentionally chirped, so that D1 influences color by choosing a portion of the white light spectrum to overlap with pump. Since phase matching controlled by C1 angle also influences preamp output color, both motors influence color and intensity of preamp output. The measured dependence of output intensity and color on C1 and D1 positions is shown in Figure 4.

The correlation between motor position, color, and intensity present special challenges to tuning

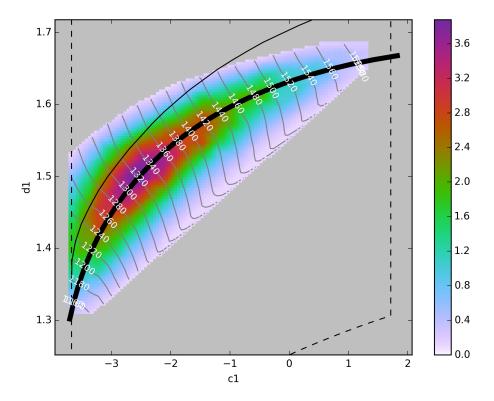


Figure 5:

TOPAS-C preamp...

To address this, WrightTools groups contours of constant color together and fits each contour to a Gaussian. This is shown in Figure 5.

In the final step, WrightTools passes the resulting tune points through a univariate spline to ensure smoothness and attempt to extend the curve outwards. In principle a polynomial fit could be used, but in practice splines are more robust to poor behavior at the edges of the tuning curve, where polynomials may oscillate wildly (Runge's phenomenon).

5.2.2 Signal Poweramp

5.3 OPA800 Motortune Processing

OPA800

MOTORTUNE [w1, w1_Delay_1, wa] 2016.01.12 14_48_42.data

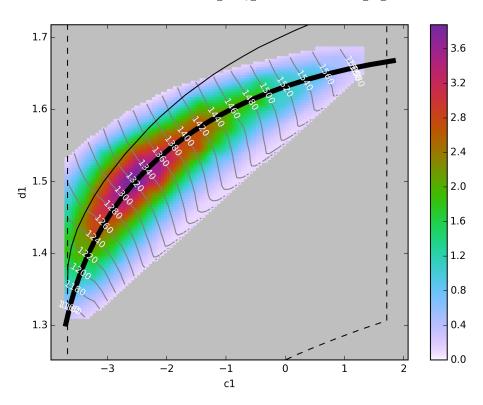


Figure 6:

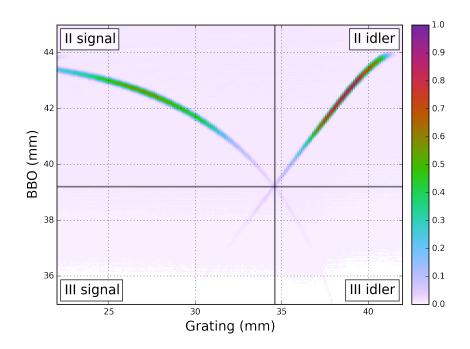


Figure 7: OPA800 (OPA2) signal and idler as measured by pyro. Data recorded 2015/10/15. Four quadrants are labeled with type and seed identification. Data taken with PyCMDS MOTORTUNE module.

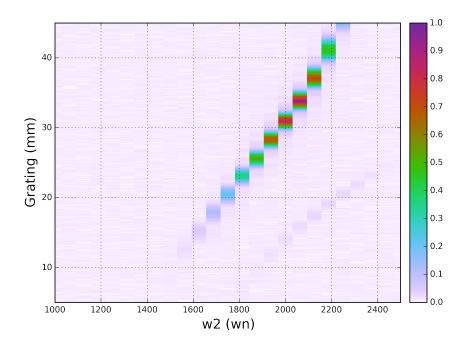


Figure 8: OPA800 (OPA2) DFG as measured by pyro. Data recorded 2015/10/16. Data taken with PyCMDS MOTORTUNE module.

- 5.3.1 Signal & Idler
- 5.4 CoSet

6 Diagrams

The diagrams module provides specialized artists and tools for creating diagrams commonly used to describe CMDS experiments.

References

[1] D. a. Green. "A colour scheme for the display of astronomical intensity images". In: *Bulletin of the Astronomical Society of India* 39.2 (2011), pp. 289–295. ISSN: 03049523. arXiv: 1108.5083.