Draft: May 7, 2003

# Spectral Data Models


Jonathan McDowell and Steve Lowe

*(SAO)*

jcm@cfa.harvard.edu


## Contents

# 1. Types of spectra

## 1.1. What is a spectrum?

By spectrum, I mean the intensity of radiation as a function of a photon spectral coordinate (wavelength, frequency, energy, etc.), corrected or not for various instrumental effects. I want to distinguish between a spectrum in the theoretical sense, the energy output versus e.g. frequency $F(\nu)$, and a spectral dataset in the observer's sense of 'taking a spectrum', which maps such a spectrum onto an instrument in often complicated ways (echelle spectra, long slit spectra on an imaging detector, etc.). Spectral datasets often have the unpleasant property that three axes (celestial coordinates and the spectral coordinate) have been projected onto two instrument coordinates, introducing degeneracy in the data. In this document I will describe spectra (the idealized $F(\nu)$) rather than spectral datasets, but keeping in mind the complications introduced by those datasets - for instance, long slit spectra force us to immediately consider arrays of spectra as a function of a single positional coordinate.

The fundamental spectrum as discussed above is clearly a special case of a one-dimensional histogram, and so will share metadata with other such cases (notably, lightcurve). In turn, the one dimensional histogram is a special case of the n-dimensional data array and so will share some metadata with concepts such as the image.

We want to include spectral energy distributions (SEDs), which are typical combinations of individual photometry points and continuous spectral arrays. There are three possible approaches:

- consider photometry and spectra to be different types of object; an SED has N photometry points and M spectra with a total of m samples in them.
- consider each point in a spectrum to have the same metadata as a photometry point, and ignore the fact that the samples in the spectrum are more related to each other than they are to the photometry values. Then an SED has N+m spectral values, with no further substructure.
- consider photometry points to be a special case of a spectrum with m=1 sample each. Then an SED has (N+M) spectra with a total of (N+m) samples, N of the spectra having only 1 sample.

- As above, but allowing related photometry points to be grouped into a single spectrum. Here 'related' means taken at closely the same time, with correlated errors, so that colors are better determined than absolute fluxes.

I propose the last approach since it lets us share metadata for a given spectrum (e.g. slit size) and minimizes the different kinds of software object. In this approach, an SED consists of an array of the spectrum objects described in this document, all applying to the same astronomical object.

### 1.2. What is not a spectrum?

I am not talking here about other kinds of spectrum:

- (I) Other kinds of observable as a function of the photon coordinate: e.g. the percentage polarization versus wavelength, or the extinction coefficient versus wavelength. However, these cases are closely related.
- (II) Cases in which the spectral coordinate is a frequency or wavelength of a massless particle other than a photon: e.g. gravitational wave spectrum; or where the coordinate is that of a massive particle, e.g. electron energy distribution in a radio jet, or cosmic ray spectrum. These cases may also reuse much of the present formalism, but some thought will be required.
- (III) Cases in which the spectral coordinate is a frequency which is not a particle property: e.g. power spectrum of variability, power spectrum of CMB density fluctuations, or tenure probability versus frequency of paper publication. These cases require rather different treatment and come under 'general histogram'.

## 2. Basic properties of a spectrum

The basic spectrum $F(p)$ gives the **value** of an **observable** F as a function of a **spectral coordinate** p.

The properties of the **value** will be those of a generic **quantity**, and will include at least uncertainties and a unit.

The spectral coordinate can be any parameter related to photon energy: energy, wavelength, wavenumber or frequency. In addition, velocity (relative to some reference frequency) is also used; and the coordinate may be a transformation of any of these other parameters - the base 10 logarithm of frequency or wavelength is a common example when plotting spectral data covering more than a decade of linear coordinate. The spectral coordinate can also be an uncalibrated (or indirectly calibrated) instrumental channel (e.g. pulse height bin in X-ray astronomy). The values of the coordinate may be equally spaced (a binned spectrum) or arbitrarily spaced.

The observable can be photon number or energy, either at the source or at the observer and either at a point or per unit solid angle on the sky, either in linear units or some logarithmic form (typically magnitudes). For example, in CGS/astro units,

- $F(\nu)$ [erg cm$^{-2}$ s$^{-1}$ Hz$^{-1}$] vs $\nu$, the flux density (photon energy per unit frequency interval per unit time and unit area at the detector).
- $\nu F(\nu)$ [erg cm$^{-2}$ s$^{-1}$] vs $\log(\nu)$, the flux density per logarithmic interval (photon energy per unit logarithmic frequency interval per unit time and unit area at the detector).
- $L(\lambda)$ [erg s$^{-1}\AA^{-1}$] vs $\lambda$, the luminosity versus wavelength (photon energy per unit time per unit wavelength interval isotropically emitted at the source).
- $S(\lambda)$ [erg cm$^{-2}$ s$^{-1}\AA^{-1}$ arcsec$^{-2}$] vs $\lambda$, the surface brightness (photon energy per unit time per unit wavelength per unit area at the detector per unit solid angle on the sky, for diffuse emission).
- $N(E)$ [photon cm$^{-2}$ s$^{-1}$ keV$^{-1}$] vs $E$ (keV), the number of photons (as opposed to $F(E) = E * N(E)$) per unit energy interval per unit time per unit area, etc. In high energy astronomy, we often use the number of photons rather than their total energy, since counting statistics are important.

### 2.1. Spectral parameter cases

Here I describe the various spectral parameters and their relationships.

| Parameter | FITS code | Symbol | Usual unit |
|---|---|---|---|
| Frequency | FREQ | $\nu$ | Hz |
| Energy | ENER | $E$ | keV |
| Wavelength | WAVE | $\lambda$ | $\AA$, $\mu m$ |
| Wavenumber | WAVN | $k$ | $\mathrm{cm}^{-1}$ |
| Velocity | VELO | $v$ | km/s |
| Beta | BETA | $\beta$ | - |
| Redshift | ZOPT | $z$ | - |
| Log Freq | FREQ-LOG | $\log(\nu)$ | |
| Log Wavelength | WAVE-LOG | $\log(\lambda)$ | |
| Channel | - | $p$ | bin |

We have (following Greisen et al)

$$h\nu = E = hc/\lambda = hck$$

and for velocities relative to $\lambda_0$ (FITS RESTWAV)

$$\lambda = \lambda_0(1+z)$$

and

$$v/c = \beta = \frac{1 - \lambda_0^2/\lambda^2}{1 + \lambda_0^2/\lambda^2}$$

or

$$v = c\left(\frac{(1+z)^2 - 1}{(1+z)^2 + 1}\right)$$

Greisen et al also define the 'radio velocity' $V$

$$V = cz/(1+z)$$

and the 'optical velocity'

$$Z = cz$$

but typically these are used only when the difference between them and the true velocity is not important, and we propose they be regarded as inaccurate attempts to represent the true velocity.

Greisen et al also treat wavelengths measured in air as a different parameter, while we will treat it as a different frame or as a correction (TBD).

### 2.2. Errors

Associated with any spectral data point is uncertainty information. When assembling spectral energy distributions from diverse sources, we must support:

- Statistical errors on the data points which are present in the relative point to point errors within a spectrum
- Systematic errors (e.g. in calibrating the zero points) which also contribute to relative errors within a spectrum
- Systematic errors which only contribute to the absolute errors and to the errors made comparing two spectra. Thus, we may have a 'spectrum' consisting of two photometry points B and V, and the B-V color may be much better determined than B and V alone.
- Correct handling of upper limits is very important in SED work, since the upper limits frequently provide critical scientific constraints.

## 3. Complications

### 3.1. Finite spectral resolution and leaks

All instruments and observing conditions are imperfect, and this introduces errors in the flux scale (calibration, background, stability) and in the spectral scale (finite resolution). In high energy astronomy, and particularly so in past decades, the spectral resolution has been very poor and the data have been heavily oversampled with respect to the resolution. This has led to an approach in which the data have been kept in instrumental units, and model spectra have been folded through instrumental simulators for comparison with the results. The jargon of X-ray astronomy obscures commonalities with other wavebands; one may summarize the process as

$$F(\lambda_o) = \frac{hc}{\lambda_o}\frac{N(\lambda_o)}{\Delta t} = \int_0^\infty d\lambda F(\lambda)\frac{\lambda}{\lambda_o}A(\lambda)R(\lambda,\lambda_o)$$

(note to X-ray aficionados: here I ignore the time variation of A and R due to motion of the detector relative to the sky).

Here, $\lambda_o$ is the instrumental wavelength, $\lambda$ is the true wavelength, $F(\lambda)$ is the usual flux which we divide by the photon energy $hc/\lambda$ to get photon number per area per time, and N are the instrumental counts. $A(\lambda)d\lambda = A(E)dE$ is the quantum efficiency over some energy interval multiplied by the detector geometric area, and R is the line spread function expressing the finite spectral resolution. In high energy astronomy we emphasize the non-diagonality of R by expressing the instrumental wavelength as an integer 'pulse channel' rather than labelling it in spectral coordinate units.

If R is nearly the unit diagonal matrix, we can invert the equation and get

$$F(\lambda_o) = \frac{hc}{\lambda_o}\frac{N(\lambda_o)}{A(\lambda_o)}$$

the usual 'fluxed spectrum', where the difference between $\lambda_o$ and $\lambda$ is seen as a smearing of line features due to the finite spectral resolution. However, in some instruments (not only X-ray!) R has significant off-diagonal elements which can cause 'instrumental features' or 'leaks' far from the nominal wavelength of the photons which are actually causing them.

Most data will be presented in the instrumental space (corrected for sensitivity but not resolution). Sometimes data will be spectrally deconvolved, and sometimes it will be simulated or model data in true spectral coordinate space. We need separate flags in the data to denote whether the data is simulated or observed, and whether it is smeared by the instrumental resolution or not. (Or, we could just set resolution to 0 if it is deconvolved, but that seems prone to trouble).

### 3.2. Coordinate frames

For spectra, some critical metadata are the parameters defining the spectral coordinate and its frame. See Greisen et al 2003 for discussions of air and vacuum wavelengths, and topocentric, geocentric, heliocentric, source and other frames (for instance, spectra of quasars in their rest frame). See Rots 2003 for proposed metadata for coordinate frames.

Although it would be nice to be compatible with the new FITS WCS, I am reluctant to consider the difference between 'air wavelength' and 'vacuum wavelength' as being the same kind as the difference between wavelength and frequency, but different from the difference between observed wavelength and heliocentric wavelength - it seems much closer to the second than the first, although perhaps comparable to the difference between wavelength and instrumental channel.

### 3.3. Orders

When the spectrum is obtained by a dispersive device, multiple dispersion orders are often present in the data. The spectrum may represent a single order, in which case it is important to record which one, or the coaddition of several orders (usually involving rebinning, and rendering uncertainty estimates and other calibrations more problematic), or it may be contaminating with overlapping orders (which can be thought of as a non-diagonal (banded) R in the discussion above).

If the spectrum has been extracted from an imaging device, we should retain some form of information about the parameters of that extraction.

### 3.4. Groups of spectra

One common case is the 1-dimensional spatial ordering mentioned in the context of long slit spectra. We want to be able to access these as a set of spectra versus position, sharing some set of calibration information (wavelength calibration may be the same; sky background spectrum may be shared).

Another common case is a time resolved spectrum, which again may have shared calibration data for its component spectra.

### 3.5. Data quality

Examples of data quality problems are: known instrumental features; bad pixels; reseau marks and saturation (e.g. IUE spectra). We may have a quality value for the whole spectrum as well as for individual pixels.

## 4. A data model for spectra

Here we propose attributes for a spectral model, named in a vaguely UCD-like syntax.

### 4.1. Top level data attributes

All of these top level attributes except for EXTRACT should be present in the general N-dimensional DATA object.

- SPECTRUM - generalization of N-dimensional DATA object
- SPECTRUM_NAXES = 1 (by definition)
- SPECTRUM_AXIS[1] - Axis object to describe spectral parameter
- SPECTRUM_VALUE - Quantity object to describe observable
- SPECTRUM_CURATION - Curation metadata object
- SPECTRUM_OBS - Observation data model object
- SPECTRUM_QUALITY - Overall quality object for spectrum. Should include flag for whether spectrum is fluxed or relative, or whether it is saturated, or whether it has multiple order contamination.
- SPECTRUM_EXTRACT - spectral extraction object (spectrum-specific)

### 4.2. Quantity object

The quantity object will be fully modelled elsewhere but has at least

- VALUE_NAME - observable name, e.g. FLUX_DENSITY_WAVE, NUMBER_FLUX_DENSITY_E, etc.
- VALUE_UNIT - e.g. Jy, mag.
- VALUE_FRAME - frame for flux value, e.g. PHOT_SYS = JOHNSON[B] or FLUX_SYS = CASA_RADIO77.
- VALUE_VALUES
- VALUE_ERR - include support for upper limit
- VALUE_ERR_UNIT - e.g. mJy

- VALUE_RES_FUNC - line spread function (1D resolution function). Can be a single value.
- VALUE_QE - quantum efficiency function.

In addition, the object will have a content descriptor field (possibly a UCD) which implicitly points to a physical semantics object; As we will argue (Lowe 2003 in prep.) the key semantic information for astronomical concepts resides in the algorithms used to transform between different representations (e.g. coordinate frames) of the concept.

### 4.3. Axis object

The Axis object is a specialization of the quantity object. It has

- AXIS_NAME - spectral parameter name, e.g. FREQ, LOG10_WAVE, etc.
- AXIS_UNIT - e.g. A, GHz, TeV
- AXIS_FRAME - frame for spectral parameter, e.g. HELIOCENTRIC, OBS, SOURCE
- AXIS_VALUES_CENTER - enumerated values of the independent variable, if present
- AXIS_VALUES_START - left edge of bin
- AXIS_VALUES_STOP - right edge of bin

(Note that the bins may not be touching, so listing the edges of the bin may be required). There are some unresolved problems in handling sampled (as opposed to binned) data, and these will be addressed in a future document (Rots 2003b in preparation).

In addition it may have

- AXIS_SIZE - number of samples
- AXIS_START - start value of axis
- AXIS_STOP - stop value of axis
- AXIS_STEP - sample size, if fixed (in which case VALUES can be omitted)
- AXIS_FRAMEZERO - zero point in wavelength or frequency for velocity axes. (should be made consistent with Space-Time Coordinates approach)

### 4.4. Extraction object

This should contain parameters such as extraction slit size and spectral order number.

### 4.5. Observation object

This will be modelled seperately. It will include a coverage object which allows you to extract at least

- COV_SPATIAL_REGION
- COV_SPATIAL_APERTURE (approx angular size of extraction region)
- COV_TIME_START
- COV_TIME_STOP
- COV_TIME_TOTAL_EFF (effective exposure time)
- COV_WAVE_START, ..._STOP - in this case, same as AXIS_START, AXIS_STOP

## References

Greisen et al 2003, http://www.aoc.nrao.edu/ egreisen/scs.ps

Bushko 2003, http://www.ivoa.net/forum/dm/0034.htm

Rots 2003, http://hea-www.harvard.edu/ arots/nvometa/stc.pdf