Subject: Re: wavelength calibration
Posted by ameigs on Tue, 23 Feb 2010 17:07:51 GMT
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On 20 Feb, 05:38, sid <gunvicsi...@gmail.com> wrote:
> Hi,
> Please give some tips and suggesions on wavelength calibration for
> spectral data
> regards
> sid

Where is the spectra from? What type of instrument and do you have measurements of the dispersion as a function of instrument wavelength (and probably how it varies across your detector for a given setting) or a theoretical prediction for the dispersion of the instrument.

Steps:
1) Measure the dispersion accurately; ideally across the entire range for which you wish to use the instrument. In the visible (assuming), using various light sources (Ne, He, Hg, Ar, Xe pen-ray lamps are convenient), take as many different wavelength settings as you can that have at least 1 pair of lines from the lamps (more pairs equals better result for the variation across the detector at a given setting). Fit the line pairs (Gaussian, centroid, whatever, to determine the line centers on the detector in "pixel" space. Then the sometimes hard part; identify these lines. Once you are reasonably sure of the identifications, plot wavelength of the lines (from the wavelength table you id'ed the line with) versus "pixel" for a particular instrument setting (wavelength). If this is a straight line (and you have a few pairs) then you're lucky and have a non-varying dispersion across the detector for that setting. Assuming near linear curve at all settings, then plot the slope of the line (nm/pixel) of each setting versus the instrumental wavelength setting. This will give you a good central (ie center of the detector) dispersion versus instrument setting curve which you can then either use appropriate interpolation, polynomial/spline fitting or best, fit the theoretical dispersion formula to this (nice for Czerney-Turner spectrometers). With this curve, then you can go on to step two.
2) Apply the dispersion along with the central dispersion to your pixel data (wave[p] = wave0[p0] + (p-p0)*dispersion[wave0]). This is your first guess. Now try to match up your line peaks to the wavelength tables (NIST, etc). p0 is the center pixel of your detector, wave0 is the instrument setting, dispersion[wave0] is the dispersion from you nice curve from 1 at wave0. You may find that you need to adjust p0.