Maximum Likelihood Spectral Fitting: the Batchelor Spectrum

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Abstract

We have developed a simple technique for fitting spectra that is applicable to any problem of adjusting a theoretical spectral form to fit observations. All one needs is a functional form for the theoretical spectrum, and an estimate for the instrumental noise spectrum. The method, based on direct application of the Maximum Likelihood approach, has several advantages over other fitting techniques:

1. It is unbiased in comparison with other least-squares or cost function-based approaches.

2. It is insensitive to dips and wiggles in the spectrum. This is because the range of wavenumbers used in the fit does not vary, and the built-in noise model tells the routine to ignore the spectrum as it gets down towards the noise level.

3. Error bars. There is a theoretical estimate for the variance of the fitted parameters, based on how broad or narrow the likelihood function is in the vicinity of its peak.

4. We calculate statistical quantities that indicate how well the observed spectrum fits the theoretical form. This is extremely useful in automating analysis software, to get the computer to automatically flag "bad" fits.

The method is demonstrated using data from SCAMP (Self-Contained Autonomous Microstructure Profiler), a free-falling temperature microstructure profiler. Maximum Likelihood fits to the Batchelor spectrum are compared to the SCAMP-generated fits and other least-squares techniques, and also tested against pseudo-data generated by Monte-Carlo techniques.

Pseudo-code outlines for the spectral fit routines are given.