Optimal Bayesian Spectral Fitting of Near-Gaussian Lines with Gauss-Hermite Functions

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Background and Overview

HIREX and such

Gauss-Hermite Functions

The (Probabilist's) Hermite polynomials are an orthogonal set of polynomials under a Gaussian weight function, e.g. satisfying

$$\int_{-\infty}^{\infty} He_m(x) He_n(x) e^{-x^2/2}\,\mathrm{d}x \equiv \langle He_m, He_n \rangle = \sqrt{2\pi}\, n! \delta_{nm} \tag{1}$$

The first few and their plots of the Hermite function $He_n(x)e^{-x^2/2}$ are shown below

$$\begin{aligned} He_0(x) &= 1 \\ He_1(x) &= x \\ He_2(x) &= x^2 - 1 \end{aligned} \tag{2}$$

Note that for example, the 0th Hermite function is simply a Gaussian.

Gauss-Hermite Functions and Moments

Given a function $h(x)\exp\left(-x^2/2\right) = \left[\sum_j a_j He_j(x)\right]\exp\left(-x^2/2\right)$, the first few (unnormalized) moments are very easy to calculate:

$$\begin{aligned} M_0 = \int_{-\infty}^{\infty} 1 \cdot \sum_j a_j He_j(x)\exp\left(-x^2/2\right) = \langle 1, h\rangle = \sqrt{2\pi}a_0 \\ M_1 = \langle x, h\rangle = \sqrt{2\pi}a_1 \\ M_2 = \left\langle x^2, h\right\rangle = Aa_0 + Ba_2 \end{aligned} \tag{3}$$

Note that the higher order Hermite functions are not involved with the moment calculations at all

Chi-Squared Minimization of Near-Gaussian Lines

Fitting of spectral lines typically involves minimizing χ^2, which from the Bayesian perspective, is finding the maximum a posteriori (MAP) estimate of a given set of photon counts

$$\hat{\theta} = \underset{\theta}{\text{argmin}} \left[\sum_i \frac{(f_i(\theta) - N_i)^2}{N_i} \right] \equiv \underset{\theta}{\text{argmin}} \left[\chi^2(\theta, \{N_i\}) \right] \tag{4}$$

If $\mu(N_i) = C + (A_0 + A(x_i))e^{-x_i^2/2}$, $f_i = \hat{C} + h(\theta, x_i)e^{-x_i^2/2}$, where $x_i \equiv (\lambda_i - \lambda_c)/s$ and $A_0 \gg C, A$, then

$$E[\chi^2] \approx \sum_i \frac{(h(\theta, x_i) - (A_0 + A(x_i))^2 e^{-x^2}}{A_0 e^{-x^2/2}} \tag{5}$$

$$\approx \sum_i D \left[(h(\theta, x_i) - (A_0 + A(x_i)))^2 e^{-x^2/2} \right] \tag{6}$$

$$\approx \langle h(\theta) - (A_0 + A), h(\theta) - (A_0 + A) \rangle \tag{7}$$

Orthogonal Projection onto Hermite Basis

$$E[\chi^2] \approx \langle h(\theta) - (A_0 + A), h(\theta) - (A_0 + A) \rangle \tag{8}$$

- This is a least squares minimization with a generalized inner product. The Hermite polynomials form an orthogonal basis for this inner product.
- If $h(\theta)$ is a sum of Hermite polynomials, then the solution is given by an orthogonal projection of $A_0 + A$ onto its component Hermite polynomials.
- For calculating moments, it doesn't even matter if convergence is bad! The polynomials are orthogonal!

Fitting Actual Data

- To extend to multiple lines, approximate the sum over multiple regions - multiple approximately orthogonal Hermite basis sets
- Need to find $x_i = (\lambda_i - \lambda_0)/s$ - assume the lowest order center and scale parameters are the same for all lines
- Perform nonlinear optimization

Analytic Calculation of Error – TODO

Approximating the output error as Gaussian (see the corner plots), can perform propagation of error:

$$\Sigma^{\theta} = J\Sigma^{N} J^{T} \tag{9}$$

How to calculate this though, it's a nonlinear optimization? Key is that for fixed λ_0, s then the Hermite polynomial coefficients are the result of an orthogonal projection of the vector N (i.e. a linear operation), so that part is easy. To calculate $\frac{\partial s}{\partial N}$, note that $\theta(\lambda_0, s, \{a_j\})$ calculate the pullback of ds onto V and then project N onto the resulting vector space.