*32nd EPS Conference on Plasma Phys. Tarragona, 27 June - 1 July 2005 ECA Vol.**29C**, P-5.087 (2005)*

Bayesian Modelling of Spectrometer Systems

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Abstract

For complex measurement systems, modelling of uncertainties and their influence on extracted physical parameters requires the use of probability theory beyond simple linear error propagation of statistical uncertainties. In this paper we describe a model for the analysis of spectrometer data, where uncertainties in addition to photon count statistics, such as instrument function, dispersion and intensity calibration, are taken into account by a comprehensive modelling of the whole measurement process.

1. Introduction

To increase accuracy of inferred plasma parameters, alleviate inconsistency problems between diagnostics, and facilitate integrated analysis [1,2] of measurements, individual diagnostic models need to pay more principled attention to inherent systematic as well as statistical uncertainties in the instrument and measurement procedures. This paper describes a model for extraction of physics parameters from spectrometer data, where uncertainty in auxiliary models of instrument function, dispersion and intensity calibration are incorporated by joining these models together with the spectral model. In section 2 expressions for detector response functions are derived which rely on models of instrument function, dispersion and intensity calibration defined in section 3. In section 4 this is brought together in a joint model.

2. Detector Response

For a monochromatic light source, the response on the detector (which we here assume is a row of pixels on a CCD chip, or a measurement binned into a single row of pixels) is proportional to the normalised instrument function

$$\nu(p - p^0(\lambda)). \tag{1}$$

The position of this function on the detector is given by

$$p^0(\lambda) = p^{ref} + \int_{\lambda^{ref}}^{\lambda} \frac{1}{\omega(\lambda)} d\lambda \tag{2}$$

where p^{ref} is the pixel position of some chosen reference point of the instrument function corresponding to monochromatic light of wavelength λ^{ref}. $\omega(\lambda)$ is the dispersion (nm/pixel) curve of the spectrometer. For light with spectral radiance $s(\lambda)$ the detector response for a wavelength interval $d\lambda$, centred on λ will then be

$$dr(p) = \nu(p - p^0(\lambda))s(\lambda)c_p(\lambda)Td\lambda \tag{3}$$

counts per pixel. Here T is the exposure time and $c_p(\lambda)$ is the calibration coefficient for pixel p, relating detected counts to radiance. Summing contributions from all wavelengths then gives:

$$r(p) = T\int_0^\infty \nu(p - p^0(\lambda))s(\lambda)c_p(\lambda)d\lambda \qquad (4)$$

counts per pixel. For the expected number of counts for a specific pixel, this will give:

$$d_p = T\int_0^\infty s(\lambda)c_p(\lambda)\int_{p-\frac{1}{2}}^{p+\frac{1}{2}} \nu(p - p^0(\lambda))dpd\lambda \qquad (5)$$

If the instrument function is broad the integral over a pixel could be replaced by the central value of that pixel. If kept, this integral enables the accommodation also of narrow instrument functions.

For a given spectrum s(λ), the likelihood of the observed counts is, assuming normal approximation of the photon statistics with standard deviation equal to $\sigma_p = \sqrt{d_p g}$, (g being the gain, or number of electrons per count; for a more sophisticated model of the CCD noise see [3])

$$p(\{d_p^*\} \mid \boldsymbol{k}^s, \boldsymbol{k}^\nu, \boldsymbol{k}^\omega, \boldsymbol{k}^c) = \prod_{p=0}^{N_{pix}-1} \frac{1}{\sqrt{2\pi}\sigma_p}\exp(-\frac{(d_p - d_p^*)^2}{2\sigma_p^2}) \qquad (6)$$

where d_p^* is the observed number of counts for pixel p. $\boldsymbol{k}^s, \boldsymbol{k}^\nu, \boldsymbol{k}^\omega, \boldsymbol{k}^c$ are vectors of free parameters for the spectral model, instrument function, dispersion relationship, and intensity calibration respectively. The expression (6) will thus depend through expression (5) on the free parameters not only of the given spectral model s(λ), but also on the internal model of the instrument function through the parameterisation of (1), the dispersion function through (2), and calibration functions through the calibration constants in (3). The positioning of a spectrum on the chip is here always done through the p^{ref} / λ^{ref} pair in the instrument function position (2), where normally p^{ref} is free while λ^{ref} is an arbitrary constant and does not need to be related to a specific line.

3. Inclusion of instrument function, dispersion and intensity calibration

The data from a specific spectrum will certainly not give much information on the instrument function, dispersion relationship and intensity calibration parameters in (6), so the separate measurement of these quantities must also be incorporated into the model. For the calibration factors, we have used a simple model based on the assumption that the largest source of uncertainty is a shift of the calibration lamp curve, caused by systematic uncertainties of the irradiance and reflectance of the standard lamp used to calibrate the calibration lamp, together with nonlinearity of detectors/amplifiers:

$$\Phi^{lamp,tab} = r^c\Phi^{lamp} \qquad (7)$$

where $\Phi^{lamp,tab}$ is the tabulated, wavelength dependent radiance of the calibration lamp, and Φ^{lamp} the underlying true value, with r^c being a nuisance parameter having a normal prior distribution with mean one and a standard deviation equal to the stated error of the calibration lamp radiance. For long exposure times during calibration measurements, the photon noise can be made negligibly small, and the calibration factors, as here defined, will be directly given by

$$c_p(\lambda_i) = \frac{d_p^c}{T_{p,i}^c \Delta\lambda_p \Phi^{lamp}(\lambda_i)}, \tag{8}$$

being measured for each pixel *p* at a number of wavelenghts λ_i.
For the instrument function, a parameterisation of (1), specific to the instrument, is used (e.g. box function, sum of Gaussians etc.). Using (5) with $s(\lambda) = \Phi^\nu \delta(\lambda^\nu - \lambda)$, λ^ν being the wavelength of the light used, the expression for the expected number of counts for pixel *p* of an instrument function measurement is

$$d_p^\nu = T^\upsilon c_p(\lambda^\nu)\Phi^\nu \int_{p-\frac{1}{2}}^{p+\frac{1}{2}} \nu(p)dp \tag{9}$$

The integral over a pixel is neccessary only for instrument functions that are narrow or have a detailed structure. The likelihood for the instrument function data is

$$p(\{d_p^{\nu*}\} \mid \boldsymbol{k}^\nu, \boldsymbol{k}^c) = \prod_{p=1}^{N_{pix}} \frac{1}{\sqrt{2\pi}\sigma_p} \exp\left(-\frac{(d_p^\nu - d_p^{\nu*})^2}{2\sigma_p^2}\right) \tag{10}$$

conditioned on the free parameters of the instrument function model, and intensity calibration model.
The spectrometer dispersion is measured by using a number of line pairs with known wavelengths. From the pixel distance between such line pairs, the dispersion relationship $\omega(\lambda)$ in (2) can be inferred:

$$\omega(\lambda) = \frac{L}{mfn_g}\left(\sqrt{\cos^2\varphi - \left(\frac{mn_g\lambda}{2}\right)^2} - \frac{1}{2}mn_g\lambda\tan\varphi\right) \tag{11}$$

where *L* is the size of a pixel, *m* the grating order, n_g the number of grooves per mm of the grating. The focal length *f* and angle φ between the normal to the grating in 0^{th} order position and the entrance mirror, are usually the free dispersion model parameters fitted to the data [4]. In this case the expected measurements will be

$$\Delta p_i = \int_{\lambda_i^1}^{\lambda_i^2} \frac{1}{\omega(\lambda)} d\lambda \tag{12}$$

where Δp_i is the measured pixel distance between the two lines with wavelengths λ^1 and λ^2. The corresponding likelihood is

$$p(\{\Delta p_i^* \mid \boldsymbol{k}^\omega) = \prod_{i=1}^{N_{pairs}} \frac{1}{\sqrt{2\pi}\sigma_i} \exp(-\frac{(\Delta p_i - \Delta p_i^*)^2}{2\sigma_i^2} \qquad (13)$$

4. Joint Model

The joint likelihood for the data from the actual spectrum, instrument function, dispersion measurement and intensity calibration will now be

$$p(\{d_p^*\},\{d_p^{\nu *}\},\{\Delta p_i^*\} \mid \boldsymbol{k}^s,\boldsymbol{k}^\nu,\boldsymbol{k}^\omega,\boldsymbol{k}^c) = p(\{d_p^*\} \mid \boldsymbol{k}^s,\boldsymbol{k}^\nu,\boldsymbol{k}^\omega,\boldsymbol{k}^c)\, p(\{d_p^{\nu *}\} \mid \boldsymbol{k}^\nu,\boldsymbol{k}^c)\, p(\{\Delta p_i^* \mid \boldsymbol{k}^\omega) \qquad (14)$$

The joint posterior for all free parameters of the model is then (with $D = \{\{d_p^*\},\{d_p^{\nu *}\},\{\Delta p_i^*\}\}$)

$$p(\boldsymbol{k}^s,\boldsymbol{k}^\nu,\boldsymbol{k}^\omega,\boldsymbol{k}^c \mid D) = \frac{p(D \mid \boldsymbol{k}^s,\boldsymbol{k}^\nu,\boldsymbol{k}^\omega,\boldsymbol{k}^c)\, p(\boldsymbol{k}^s,\boldsymbol{k}^\nu,\boldsymbol{k}^\omega,\boldsymbol{k}^c)}{p(D)} \qquad (15)$$

The inference of the spectral features is then done by marginalizing over the nuisance parameters we are not interested in:

$$p(\boldsymbol{k}^s \mid D) = \iint_{\ldots} p(\boldsymbol{k}^s,\boldsymbol{k}^\nu,\boldsymbol{k}^\omega,\boldsymbol{k}^c \mid D) d\boldsymbol{k}^\nu d\boldsymbol{k}^\omega d\boldsymbol{k}^c \qquad (16)$$

Normally we are interested in posteriors for single elements in the vector $\boldsymbol{k}^s$ giving directly the probability distributions for specific spectral features with all uncertainties in the joint system taken into account through the integral (16).
Practically, the integral (16) is carried out through Markov Chain Monte Carlo (MCMC) sampling from the posterior (15). A numerically faster method is to approximate (15) with a multivariate normal distribution centred at the maximum of the posterior distribution (15) and then carrying out the marginalization integrals (16) directly.
The number of extra free parameters that has to be introduced in order to take into account the error sources we have been describing, is about 7 for a gaussian instrument function, which is not excessive, considering that spectra can easily have many times that number of free parameters.

5. References

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