An Iterative Solution to an Inverse Problem in Spectrometry

Sascha Eichstädt[1], Franko Schmähling[1], Gerd Wübbeler[1], Udo Krüger[2] and Clemens Elster[1]

[1]*Physikalisch-Technische Bundesanstalt, Braunschweig and Berlin, Germany*
[2]*TechnoTeam Bildverarbeitung GmbH, Ilmenau, Germany*

ABSTRACT

In radiometry and photometry spectral power distributions are measured using array spectrometers and monochromators. The observed output of these devices can be modeled as the convolution of the spectrum of the source with the instrument's line spread function, i.e. as the result of a Fredholm integral equation of the first kind. The kernel function of this Fredholm integral equation is inferred from calibration measurements. The goal is to reconstruct the spectrum of the source from the observed spectrum. This task constitutes an ill-posed inverse problem [1].

One approach to this inverse problem popular in the field of spectrometry is based on local polynomial approximations [2]. The method can be seen as an extension of the classical method of Stearns [3]. However, the local polynomial approximation method has been demonstrated to be very sensitive to measurement noise. We present an alternative iterative approach based on an adaption of the Richardson-Lucy method which has been shown to be superior to classical approaches in this field [4, 5].

The Richardson-Lucy method originates from image processing and guarantees non-negative estimates provided that the initial estimate and the kernel function are non-negative. The method can be shown to converge to the inverse of the Fredholm equation. However, due to the ill-posedness of the estimation problem this results in an unbounded amplification of measurement noise and is thus undesirable. Hence, a premature stopping of the iterations as a means of regularization is typically employed. To this end, we propose an automatic stopping criterion based on the curvature of the estimation progress which proves to be both efficient and robust [4].

We assess the proposed method in terms of an extensive simulation study as well as by its application to measurement data. We also compare the results to those obtained by the classical approach in spectrometry, and we finally give some guidance as to the choice of method in that field.

Keywords: spectrometry, deconvolution, Richardson-Lucy, bandpass correction, inverse problem, regularization

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