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# A Polynomial Curve Fitting Method for Baseline Drift Correction in the Chromatographic Analysis of Hydrocarbons in Environmental Samples

Mauro Mecozzi<sup>a, \*</sup><sup>a</sup>Laboratory of Chemometrics and Environmental Application, Via di Castel Romano 100, 00128 Rome, Italy

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## Abstract

In this paper we describe an algorithm for removing the baseline drift often observed in GC and HPLC plots of complex environmental samples which causes reduction of the analytical accuracy of peak area measurements. The proposed method determines the real baseline (i.e. baseline modeling) directly on the chromatographic plot of each analyzed sample and then substrate it to the analytical time series signals of the chromatogram, so reducing instrumental noise and then improving analytical accuracy. The proposed algorithm, based on a polynomial fitting estimation of the baseline, has been applied to the GC analysis of the hydrocarbon content in marine sediments.

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## 1. Introduction

Chromatographic techniques are widely diffused in all the applications of environmental monitoring due to the possibility of analyzing complex matter samples in automated way. However in some specific analytical cases such as those related to the gas chromatographic determination of the hydrocarbon content in marine sediments, an evident baseline drift is still present even after the blank (i.e. solvent) subtraction (Fig. 1). That is because the baseline drift is a random effect depending on several casual and not reproducible variables

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\* Corresponding author. Tel.: +30-06-50073287;

E-mail address: [mauro.mecozzi@isprambiente.it](mailto:mauro.mecozzi@isprambiente.it); [mauromecozzi2004@libero.it](mailto:mauromecozzi2004@libero.it).

which can produce  $k$ -different baseline shapes in  $k$ -sequential chromatographic analysis [1]. So the blank subtraction procedure could not be reliable to solve the baseline drift problems and to allow the accurate quantification of the chromatographic peaks. For this reason, many papers propose different methods of signal processing for modeling and then correcting baseline drifts in chromatographic analysis [1-4]. In this paper, we propose a curve fitting method for baseline correction. This method consists of modeling the baseline by means of a polynomial curve where the identification of the optimized polynomial grade is performed by the F-Snedekok test [5]. The method has been tested for the GC analysis of total hydrocarbon content in marine sediments by means of a previous method [6].

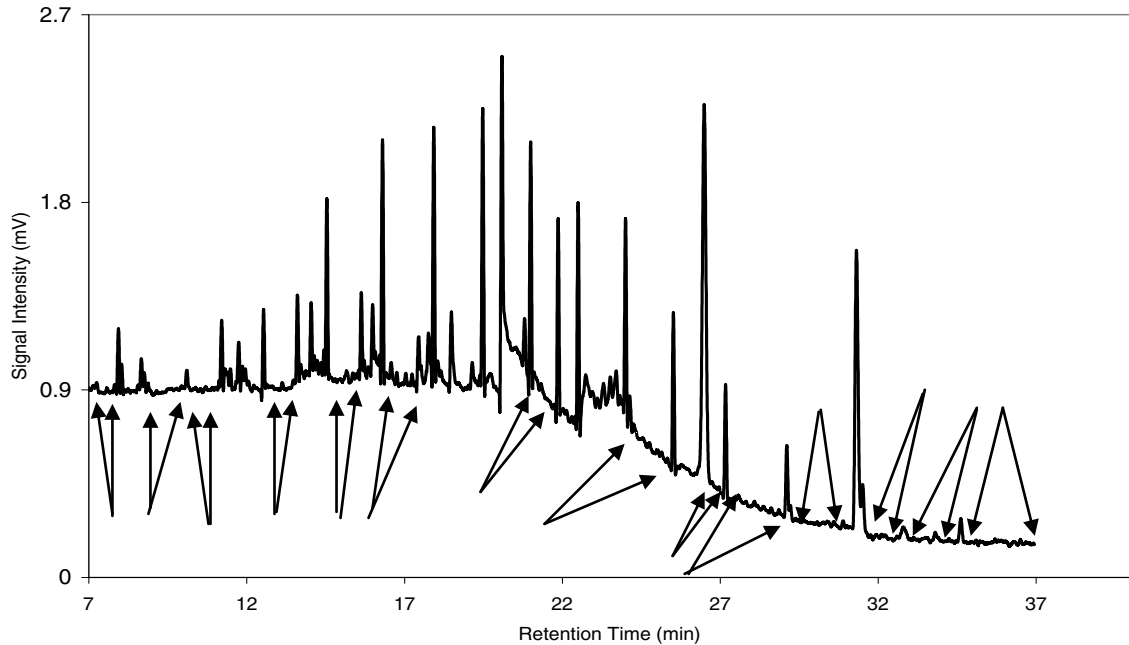


Fig. 1. Example of an evident baseline drift in the GC analysis of hydrocarbons in a marine sediment sample, already submitted to blank subtraction. Each couple of arrows show a time range where the absence of significant peaks makes it suitable for baseline estimation

## 2. Basic theory of the proposed algorithm

The chromatographic plot of a baseline consists of a  $z$ -number of  $y_j$ ,  $x_j$  values;  $y$  and  $x$  are the signal intensity and the acquisition (i.e. retention) time respectively with  $1 < j < z$ . The  $y$  signals represent a continuous and derivable series in the  $x_1$ - $x_z$  time range and according to these characteristics the  $y = f(x)$  relationship can be described according to the Taylor series [7] as

$$y = \sum_{k=0}^z (x-x_0)^k f^{(k)}(x_0)/k! + R_z(x) \quad (1)$$

where  $x_j \leq x_0 \leq x_z$ ,  $f^{(k)}$  is the order of the derivative of the  $f(x)$  function,  $n$  is the polynomial degree and  $R_z(x)$  are the residuals (i.e. differences) among the original  $f(x)$  values and the  $f(x)$  values determined according to Eq. 1. So, on the basis of Eq.1 we can suppose the existence of a polynomial relationship between  $y$  and  $x$

$$y = a_1 * x_j + a_2 * x_j^2 + a_3 * x_j^3 + \dots + a_n * x_j^n + a_0 \quad 1 < j < i \quad (2)$$

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