# Managing Uncertainty in Spectra for Fuzzy Classification

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**Abstract.** The study presented in this paper addresses uncertainties that arise in spectral measurement and analysis. These uncertainties can be dealt by means of fuzzy classification, but on order to achieve high quality results, it is necessary to manage and compute them beforehand. Previous research has typically only addressed uncertainty per wavelength in spectra, without considering the total uncertainty across the spectrum and in the analysis. This paper presents a method for managing and calculating uncertainties throughout the entire process and integrating them into a fuzzy pattern classifier. The approach is based on the Guide to the Expression of Uncertainty in Measurement and extended by our own methodology to manage uncertainty in spectra including the construction of a fuzzy pattern classifier. An example from UV/Vis spectroscopy illustrates the practical applicability of the methods presented.

**Keywords:** Uncertainty Management, Fuzzy Classification, Spectra Analysis.

## 1 Introduction

In the natural sciences, analyzing and interpreting data involves dealing with measurement uncertainties that can arise from various sources, such as instrument accuracy, environmental conditions, or human error. To draw sound conclusions from the data, it is crucial to provide a clear description or classification of these uncertainties. When evaluating spectra and other complex measurements, uncertainties can often be high due to the need to consider multiple variables and parameters. To address these uncertainties, fuzzy classification techniques can be utilized. Fuzzy logic, introduced by Zadeh [1], has been applied in various real-world applications, including monitoring, fault diagnosis, decision support, and control [2]. Most of these methods rely on a fuzzy membership function, which provides flexibility [3, 4]. Neuro-fuzzy systems, fuzzy reinforcement learning, and fuzzy pattern classification are successfully used in various areas such as signal processing applications and automation systems [5, 6], analysis of pollutants in water [7], neural statements, and medical diagnostics [3, 8]. However, many approaches use fixed parameters, such as 2 %, to describe the extent of functions and account for uncertainties without calculating the exact uncertainties. To ensure precision and accuracy, it is important to adopt an approach based on international standards, such as the international Guide to the Expression of Uncertainty in Measurement (GUM) [9], when calculating measurement uncertainties. This article first discusses the

calculation of measurement uncertainties based on the GUM guidelines to provide a solid basis for analysis. It then shows how these uncertainties can be integrated into a fuzzy classifier to provide robust and accurate data analysis. The paper is organized as follows: Sect. 2 describes other work on uncertainty management in spectral analysis. Sect. 3 presents the methodological approach with description or calculation of uncertainties and the theoretical structure of a fuzzy classification. Sect. 4 illustrates the methodology with an example from UV/Vis spectroscopy, and Sect. 5 concludes with a short discussion and summary.

## 2 Related Work

Recording and evaluating spectra is a common practice in various fields. However, the uncertainty in this area has not been extensively researched. The research work managing uncertainties is widely scattered across various fields of application. For instance, Reginatto managed the uncertainty of neutron energy spectra using Bayesian parameters [10]. However, the parameterized spectrum is assumed to be the sum of a Gaussian and a small, smooth background term. In the chapter "Uncertainties in Spectral Color Measurement" by Gardner, the author considers the spectral measurement process and its uncertainty components that influence the calculated color values [11]. However, the author only considers the measurement process. There it is important to note that color measurements on a sample can vary due to different illumination and viewing conditions, as well as non-uniformities. Schinke et al. provide a guideline for implementing and evaluating spectral stray light corrections [12]. The uncertainty analysis is based on a Monte-Carlo approach. The corrected signal/standard uncertainty for each wavelength is the final result. González et al. also describe a methodology for evaluating uncertainties of UV spectra using Monte-Carlo [13]. Verma et al. quantified the uncertainties in metal K-edge X-ray absorption near-edge structure (XANES) spectra using deep neural networks [14]. The analysis successfully predicted the spectra, but only recorded the extended standard uncertainty per wavelength or per energy, not over the entire spectrum, in all three cases mentioned.

## 3 Methods

This section presents a list of methods used, organized according to the topics covered in this paper. The computational basis for uncertainty detection and a possible approach to describe it for spectra are shown. The possible structure of a fuzzy classification with a membership function is then described.

### 3.1 Uncertainty Management

The identification of uncertainties in spectra can be divided into three main parts: Firstly, each individual intensity in the spectrum is examined to determine which variables or standard uncertainties influence it. Secondly, the total standard uncertainty

across the spectrum is calculated. Finally, the standard uncertainties of the evaluation method are quantified, and the expanded uncertainty is calculated for all parts together. In Part 1, the individually recorded intensity points in the spectrum are mainly influenced by the environmental conditions, the experimental setup, the excitation source, the spectrometer, and physical uncertainties. First, a model equation is set up with the measured variables *Y* and the influencing variables *X*.

$$\begin{bmatrix} Y_1 \\ \dots \\ Y_n \end{bmatrix} = f \begin{pmatrix} X_{1,1} & \cdots & X_{n,i} \\ \vdots & \ddots & \vdots \\ X_{n,1} & \cdots & X_{n,i} \end{pmatrix} \tag{1}$$

The GUM describes the exact procedure for calculating the standard uncertainty $u_c$ for each influencing variable *x*. In some cases, a Monte-Carlo distribution can be used. It is crucial to note that most input variables in the spectrum are correlated, and therefore the combined standard uncertainty $u_c^2(y_n)$ per intensity is calculated using a specific equation [9].

$$\mathrm{u_c^2(y_n)} = \sum_{\mathrm{i=1}}^{\mathrm{N}} \left(\frac{\delta \mathrm{f}}{\delta \mathrm{x_i}}\right)^2 \cdot \mathrm{u^2(x_i)} + 2 \sum_{\mathrm{i=1}}^{\mathrm{N}} \sum_{\mathrm{j=1}}^{\mathrm{N}} \frac{\delta \mathrm{f}}{\delta \mathrm{x_i}} \cdot \frac{\delta \mathrm{f}}{\delta \mathrm{x_j}} \cdot \frac{\mathrm{u(x_i, x_j)}}{\mathrm{u(x_i) \cdot u(x_j)}} \tag{2}$$

If there is no correlation of the influencing variables, the combined standard uncertainty $u_c^2(y_n)$ is calculated differently.

$$u_c^2(y_n) = \sum_{i=1}^{N} \left(\frac{\delta f}{\delta x_i}\right)^2 \cdot u^2(x_i) \tag{3}$$

In Part 2, the standard uncertainties per intensity value are provided. As the spectrum cannot be represented by an analytical function, we use an area calculation and the Monte-Carlo method, as described in GUM Supplement 1 [15]. The Monte-Carlo analysis involves repeating the calculation of the deviations of the area, as outlined in Section 2, with all input variables randomly varied in each iteration according to their probability distribution. For a large enough number of iterations, the uncertainty is derived directly from the distribution of the Monte-Carlo results, which vary depending on the influencing variables. To calculate the area $F_{u_c}$ between the standard uncertainties over the x-axis range (λ-range), follow these steps.

$$F_{u_c} = \int_{\lambda_1}^{\lambda_n} \sum_{n=1}^{N} u_n \frac{d\lambda}{du_n} - \int_{\lambda_1}^{\lambda_n} \sum_{n=1}^{N} -u_n \frac{d\lambda}{du_n} \tag{4}$$

The Monte-Carlo method is utilized to determine the standard uncertainty of the complete spectrum. The values of the target variable $F = f(x_{1r}, \dots, x_{nr})$ for *r = 1, ..., m* are calculated using the realizations obtained in this way. The values are then sorted in ascending order to obtain their empirical distribution function. The standard uncertainty $u_y(F)$ is calculated as follows:

$$u_{y_{Spektrum}}(F) = \sqrt{\frac{1}{m-1}\sum_{r=1}^{m}(y_r - \bar{y})^2} \tag{5}$$

Where $y_r$ is the r-th value of the target variable and $\bar{y}$ is the average of the target variable. After this calculation, the combined standard uncertainty of the complete spectrum is available. The calculation presented here represents an average method. If a worst-case method is required, the highest standard uncertainty could be employed in this instance.

In Part 3, the standard uncertainty of the evaluation method for the spectra is calculated. To evaluate the spectra with the fuzzy classification, feature extraction is necessary. We propose generating a mathematical description of the spectra and using it for evaluation. To begin, a reference spectrum is calculated for a known concentration by using a mathematical description. This involves iteratively determining the Gaussian parameters (*a, b*, and *c*) for Gaussian functions g by identifying the local maxima within the absorption spectrum *A* or the difference spectrum $y_{Diff}$. The iterative process always recalculates the difference spectrum by subtracting the newly calculated functions from the Gaussian functions of the absorption spectrum or the previously calculated difference spectrum.

$$G = a \cdot e^{-\frac{(x-b)^2}{2 \cdot c^2}} \tag{6}$$

$$\begin{bmatrix} a_1 & b_1 & c_1 \\ \vdots & \vdots & \vdots \\ a_i & b_i & c_i \end{bmatrix} = \begin{cases} max\left(y_{Diff,i}(height_i,\, position_i,\, width_i)\right), & y_{Diff,i} > 0 \\ max\left(-y_{Diff,i}(-height_i,\, position_i,\, width_i)\right), & y_{Diff,i} < 0 \end{cases} \tag{7}$$

The Gaussian parameters for the difference spectrum $y_{Diff,i}$ are determined iteratively by subtracting the calculated Gaussian functions from the absorption spectrum until there are no more maxima or the difference between the spectra is almost zero.

$$y_{Diff,i} = A - \begin{bmatrix} a_1 \\ \vdots \\ a_i \end{bmatrix} \cdot e^{-\frac{\left(x-\begin{bmatrix} b_1 \\ \vdots \\ b_i \end{bmatrix}\right)^2}{2 \cdot \begin{bmatrix} c_1 \\ \vdots \\ c_i \end{bmatrix}^2}} \tag{8}$$

The absorption spectrum is mathematically described by an overall function $A_{ref,i}$, which is composed of Gaussian functions. The resulting Gaussian parameters are then used in the Gaussian functions.

$$A_{ref,i} = z \cdot \left( \sum_{i=1}^{max\, y_{Diff,i}=0} a_i \cdot e^{-\frac{(x-b_i)^2}{2 \cdot {c_i}^2}} \right) \tag{9}$$

The reference spectrum is fitted to other spectra to calculate the $R^2$ and z-parameters. $R^2$ is used to determine if the existing spectrum matches the calculated spectrum. The z-parameter indicates the drift over the entire spectrum, with higher values indicating higher concentrations or energy of the influencing medium. These two features will be

used to construct the fuzzy classifier. To calculate the standard uncertainty, we once again utilize the Monte-Carlo method and calculate the distribution of the respective parameters using m random numbers in each case. As the evaluation method is not correlated with the recording of the spectra, we can calculate the combined standard uncertainty using simple error propagation, as shown in equation (3). After that the characteristics are available with a total combined standard uncertainty. The expanded uncertainty $U$ can be calculated, which specifies a range around the measurement result that can be expected to cover a large proportion of the distribution of values that can be assigned to the measured variable $Y$.

$$U = k \cdot u_{c_{Ges}} \tag{10}$$

At the end of the uncertainty management, the features are presented with an expanded measurement uncertainty and can be integrated into the fuzzy pattern classifier.

### 3.2 Modelling of Fuzzy Classifications

In fuzzy classification, a clear distinction is made between a learning phase and a working phase. The learning phase involves creating a fuzzy classification model in a multidimensional feature space. Object data sets are initially divided into distinct groups based on their features. This classification can be achieved through cluster analysis or an expert-based approach. These distinct groups are then transformed into fuzzy groups. This section describes the use of a fuzzy pattern classification method, specifically the fuzzy pattern classification method developed by Bocklisch and colleagues [16, 17]. The AIZERMAN membership function is used to describe each group in the one- or multidimensional feature space. This function is a highly flexible parametric potential function type. This potential function was selected for its capacity to facilitate flexible modelling and to accommodate a range of phenomena, including asymmetric data distribution.

$$\mu(x) = \begin{cases} \dfrac{a}{1 + \left(\frac{1}{b_l} - 1\right) \cdot \left(\frac{|\,x_0 - x|}{c_l}\right)^{d_l}}, & x < x_0 \\ \dfrac{a}{1 + \left(\frac{1}{b_r} - 1\right) \cdot \left(\frac{|x\ -\ x_0|}{c_r}\right)^{d_r}}, & x \geq x_0 \end{cases} \tag{11}$$

The unimodal function has a maximum membership value at point $x_0$, which is also known as the representative value of the set. Each of the left and right branches of the function has a set of parameters $b$, $c$, and $d$. The extent of the fuzzy set, which describes the uncertainty of the measurement, is given by $cl > 0$ and $cr > 0$. The fuzziness is parameterized by $b_l$ and $b_r \in [0,1]$, as well as $d_l$ and $d_r \in [2, \infty]$. The objects are unified into one-dimensional sets and then transformed into multidimensional fuzzy pattern classes using an N-fold compensatory Hamacher cut operator [18].

$$\cap_{Ham}^{N} \mu_i = \frac{1}{\frac{1}{N}\sum_{i=1}^{N}\frac{1}{\mu_i}} \tag{12}$$

During the subsequent work phase, the fuzzy pattern classifier reads unknown objects resulting from the learning phase. Membership values are then calculated for each class to determine the assignment of the objects with the highest membership value.

# 4 Example

Absorption spectra recorded using UV/Vis spectroscopy are used as an example. The exact experimental setup and the recording process of the spectra are described in Goblirsch et al [19]. A total of 30 water and 30 compound spectra were recorded. The water was obtained from distilled water, and the substance spectra were recorded using the standard Rhodamine B (Merck, Darmstadt, Germany) at a concentration of 1 mg $L^{-1}$.

## 4.1 Calculation and Management of Uncertainties for Intensity Values, Spectrum, and Characteristics

In Part 1, Figure 1 displays all variables that affect the recording of individual intensities. The aperture calculation is wavelength-dependent, which is why the standard uncertainty for the absorption value is calculated for each wavelength. For instance, the calculation for the wavelength 374.77 nm is described here. The calculation for other wavelengths follows the same procedure, but with different input values.

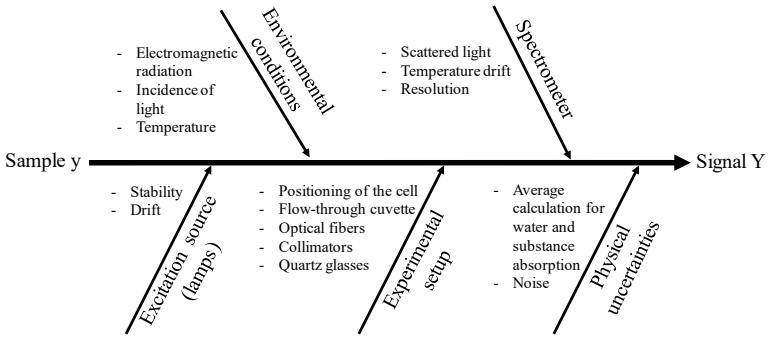


**Fig. 1.** Cause-effect diagram for measuring the spectrum with all influencing variables.

The absorption A is calculated using equation (13),

$$A = I_0 - I \tag{13}$$

with $I_0$ representing the intensity values of water absorption and $I$ representing the intensity of substance absorption. The mean values $x$ and standard uncertainties $u$ (here calculated like the standard deviation, see type A calculation in the GUM) of the 30 recorded measurements can be calculated using standard equations and are given in the following table for a wavelength of 374.77 nm.

**Table 1.** Overview of the mean values and standard uncertainties of the measured spectra

| Average of the water intensity values ($x_{I0}$) | Standard uncertainty of water intensity values ($u_{I0}$) | Average of the substance intensity values ($x_I$) | Standard uncertainty of the intensity values ($u_I$) |
|---|---|---|---|
| 8145.8 | 0.8539 % | 7735.5 | 0.4270 % |

The uncertainties of the experimental setup affect both $I_0$ and $I$ equally and are therefore reduced by the absorption calculation. However, other factors that vary with each measurement cannot be similarly reduced. The influence of ambient conditions is highly dependent on the situation, which is constantly changing, and difficult to quantify. For instance, temperature has a significant impact on the measurement, particularly on the spectrometer. The following section provides a detailed explanation or calculation of this uncertainty. Other environmental conditions are not considered at this point and will be addressed later in the fuzzy classifier. It is important to note that scattered light has a significant impact on spectroscopy. Scattered light refers to light that is deflected by particles in the water sample in various directions instead of passing directly through the sample. The data sheet of the spectrometer specifies a standard uncertainty of 1 % for this. The instrument's ability to resolve fine details in the spectrum is measured by its resolution, which is specified as 1.5 nm in the data sheet. To calculate the uncertainty, we generated a normal distribution for the wavelength using the Monte-Carlo method with 1000 random numbers (refer to Figure 2). The standard uncertainty for the intensity value at the wavelength 374.77 nm is 0.1327 %. Figure 2b shows the calculated standard uncertainties for the other intensity values.

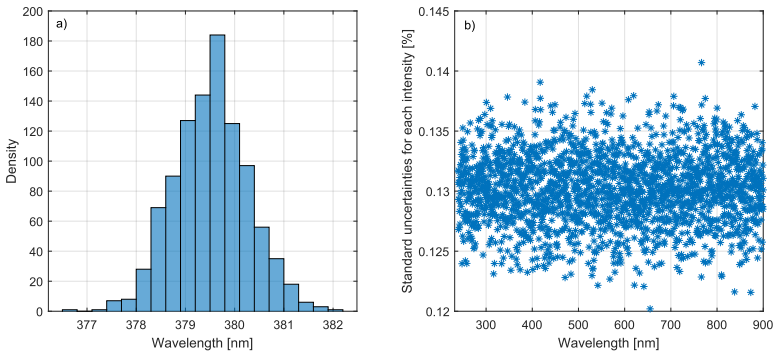


**Fig. 2.** a) Distribution of the resolution of the spectrometer calculated with Monte-Carlo as an example for the value at 374.77 nm and b) calculated standard uncertainties over the complete spectrum for the resolution using Monte-Carlo.

The influence of temperature on the spectrometer is of considerable importance, as higher temperatures can lead to an overall higher intensity of the measured signals. In order to study the effect of temperature on the spectrometer, measurements were taken over a period of 8 hours in a temperature chamber that can be used to maintain a constant temperature. First, the temperature was set at 10 degrees and a spectrum was recorded every 2 minutes. The measurement process was then repeated for temperatures

of 20, 30, and 40 degrees. For the 374.77 nm wavelength, there is a clear relationship between temperature and intensity. The deviation per degree gives a standard uncertainty of 4.95 % per 1 degree. The temperature was measured when the spectra were recorded and varies between 28.60 and 28.80 degrees. In total, there is a temperature difference of 0.2 degrees during the measurement, so the standard uncertainty during the measurement is 0.9915 %.

According to the data sheet, the drift of the lamps has an influence or standard uncertainty of 0.25 %. Regarding stability, the data sheet states a standard uncertainty of 0.1 %. To achieve an optimal signal-to-noise ratio, an average of 10 spectra is formed during the absorbance measurement. The standard deviation was calculated for each intensity value of 10 individually recorded spectra to determine the resulting standard uncertainty. This is done for both water and substance absorption (see figure 3a and 3b). For the wavelength 374.7721 nm, the standard uncertainty is 1.8944 % for water absorption and 1.1157 % for substance absorption. To determine the noise, the spectrum was first considered after the appropriate filter and the standard uncertainty was calculated as 0.05 %.

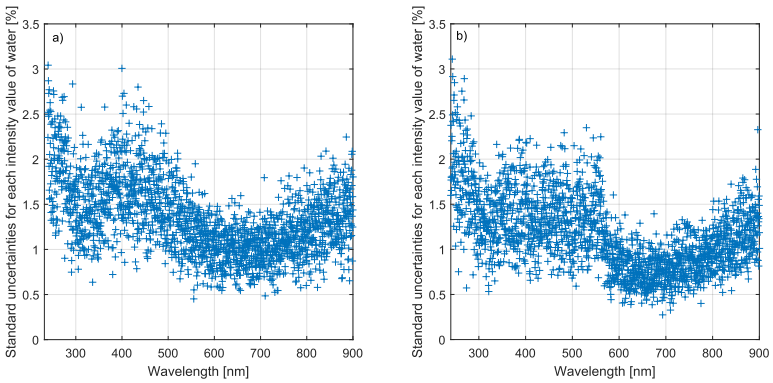


**Fig. 3.** Standard uncertainties caused by the average calculation when a) recording the water spectra and b) when recording the substance spectra.

Since the pure water absorption correlates with the intensity absorption of the substance, the combined standard uncertainty must be calculated according to equation (2). Figure 4a shows the final calculated spectrum with the combined standard uncertainty per intensity. The combined standard uncertainty has been increased only for the plot by a factor of 3 with plus and minus values for clarity. For comparison, the exact plus and minus combined standard uncertainty for each intensity value is shown in Figure 4b.

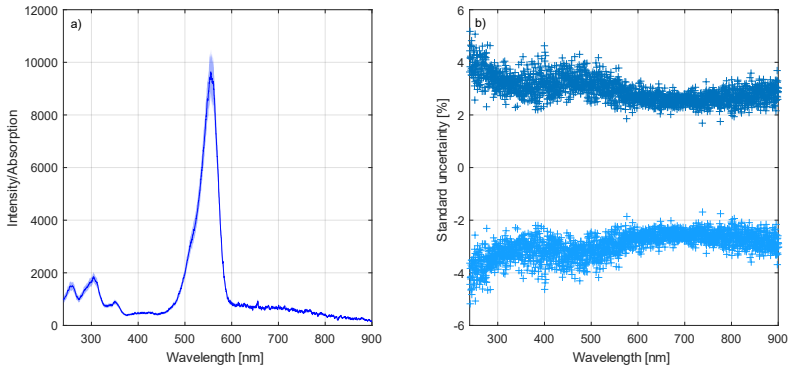


**Fig. 4.** Combined standard uncertainty a) in the absorption spectrum with optical magnification by 3 and b) independent of the absorption values.

For part 2, the recording of the standard uncertainty for the whole spectrum, the area between the combined standard uncertainties per intensity value over the wavelength range is 11814.37 and was determined according to equation (4). The Monte-Carlo method is used to calculate the standard uncertainty of the entire spectrum more accurately. For this purpose, 10,000 random realizations of the input variables are selected. According to the normal distributions chosen for the input variables, the m realizations were performed on a computer. The values of the output variable $F = f(x_{1r}, \dots, x_{nr})$ for $r = 1, \dots, m$ are calculated from the realizations obtained in this way. By sorting the values in ascending order, their empirical distribution function is obtained. The standard uncertainty $u_y(F)$ is calculated according to equation (5). The distribution for the spectrum calculated here using the Monte-Carlo method is shown in Figure 5. These calculations result in a combined standard uncertainty for the entire spectrum of ±2.9481 %.

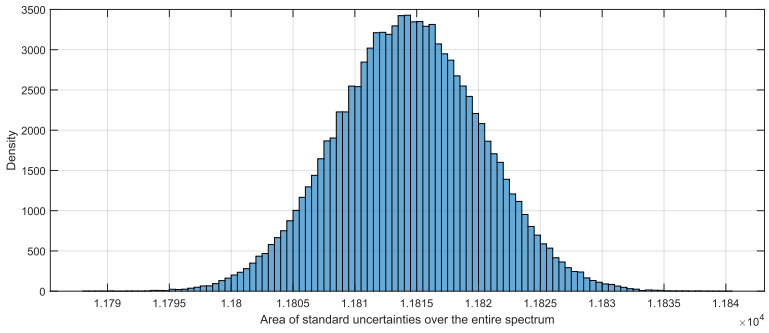


**Fig. 5.** Probability density of the area of standard uncertainties over the spectrum calculated by the Monte-Carlo Method.

In part 3, the standard uncertainties are recorded for each feature in the evaluation method. The reference spectrum is fitted with an $R^2$ of 0.9992 and has a z-parameter of

0.9892. Accordingly, the standard uncertainties of the reference spectrum are for $R^2$ = 0.008 % and for the z-parameter = 0.108, which corresponds to 1.09 %. The reference spectrum is now fitted to other spectra to calculate the $R^2$ and z-parameters. To obtain the average uncertainty, 30 absorption spectra were fitted and the corresponding $R^2$ and z parameters were calculated. To determine the standard uncertainty, the Monte-Carlo method was used again, and the distribution of each parameter was calculated using 10,000 random numbers (see figure 6). The overall result is a standard uncertainty of 0.0012 % for $R^2$ and a standard uncertainty of 0.6534 % for the z-parameter.

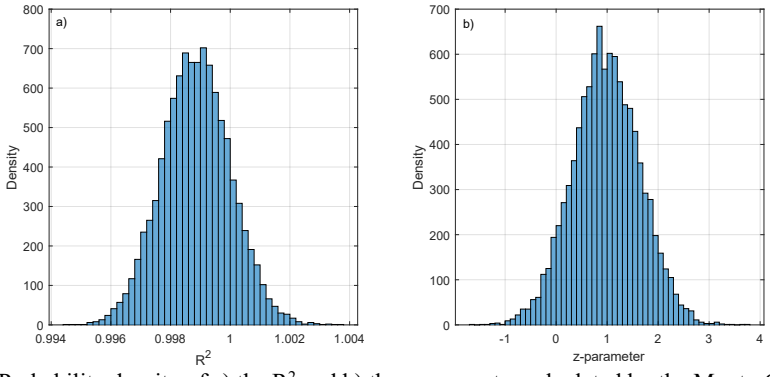


**Fig. 6.** Probability density of a) the $R^2$ and b) the z-parameter calculated by the Monte-Carlo method for evaluating the spectra.

To calculate the combined standard uncertainty from the standard uncertainties of the spectrum, reference spectrum and feature extraction, error propagation is used again. The features $R^2$ were calculated as 0.9989 and z-Parameter as 0.9935 as expected values. The reference spectrum correlates with the feature extraction because the reference spectrum is used for the feature extraction and therefore must be calculated according to Equation (2). This results in a combined standard uncertainty $u_{c_{Auswertung}}(R^2)$ of 0.1267 % for the evaluation of $R^2$ and a combined standard uncertainty $u_{c_{Auswertung}}(z)$ of 1.9481 % for the evaluation of the z parameter. These must now be offset against the standard uncertainty of the spectrum. This time there is no correlation, so the error propagation according to equation (3) can be performed for each parameter. This gives a combined standard uncertainty of $u_{c_{Ges}}(R^2)$ is 2.9508 % for the feature $R^2$ and a combined standard uncertainty of $u_{c_{Ges}}(z)$ is 3.5336 % for the feature z parameter. To calculate the expanded uncertainty, equation (10) is used and a factor of 2 is selected for k so that the value of the measurement variable normally lies within the assigned coverage interval with a probability of approximately 95 %. The overall result is now the expanded uncertainty for the feature $R^2$ with $U_{R^2}$ is 5.9016 % and the feature z-parameter with $U_z$ is 7.0672 %.

### 4.2 Structure of the Fuzzy Pattern Classifier

The calculated expanded uncertainties can now be integrated into the fuzzy classification. For better description and comparison, an additional data set with 30 rhodamine B spectra at a concentration of 0.5 mg $L^{-1}$ was recorded. In a first step, the two feature parameters $R^2$ and z are calculated from all spectra and grouped. This is followed by a fuzzy description and classification, where the calculated measurement uncertainty can be integrated for each feature. The structure of the fuzzy pattern classifier is as described above and explained in detail in [3, 20]. In the example, single linkage clustering and normalized ($a$ = 1), symmetric membership functions with $b_{l/r}$ = 0.5, $d_{l/r}$ = 2 were used to model fuzzy objects. These parameters are frequently recommended in the literature for the construction of normalized multivariate membership functions, as they have been empirically demonstrated to be a reasonable choice in practice. Figure 7 shows the final fuzzy pattern classifier.

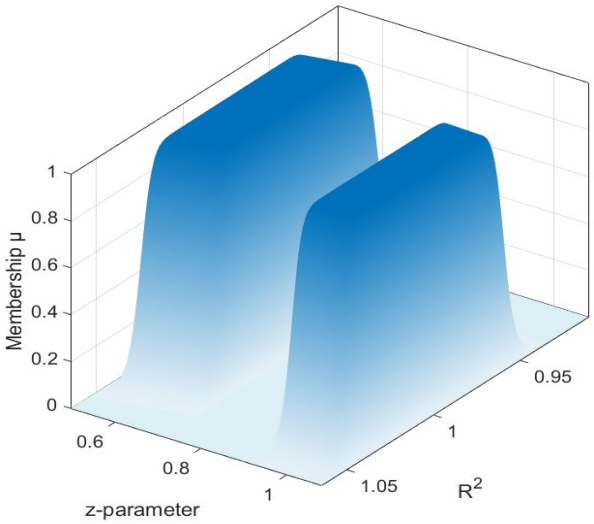


**Fig. 7.** Two-dimensional fuzzy pattern classifier including the calculated uncertainties.

This classifier now forms the basis for the work phase in which unknown data can be read in and assigned to a class. Incorporating uncertainties or vagueness enables a more realistic and flexible description of the data.

## 5 Discussion and Conclusion

The presented method showed how the uncertainties of spectra can be recorded and calculated for fuzzy classification. The calculations were based on the guidelines of the GUM. Because measured Spectra are recorded as discrete values and not as analytical functions, the Monte-Carlo method was used. This allowed uncertainties to be

expressed even for complex spectra. The calculation of uncertainties according to the GUM guidelines undoubtedly represents an important step in managing and quantifying uncertainties in spectrum analysis. However, it should be noted that this method may not fully account for all influences, especially those due to environmental conditions. In addition, a simplification was made in summarizing the uncertainties across the spectrum by calculating the area over all standard uncertainties, although these may differ across the spectral range. Despite these limitations, the calculated expanded uncertainty has been successfully integrated into a fuzzy classification. This integration of the calculated uncertainties allows a better and more realistic consideration of the real spectra in the evaluation and thus contributes to more reliable results. However, it remains important to further refine the uncertainty calculation methods and to align the classes more explicitly with the calculated uncertainties to allow a more precise characterization of the measurement uncertainties. The method was tested using absorption spectra as an example, and the expanded measurement uncertainty for the entire spectrum and the evaluation method were successfully calculated. This expanded uncertainty was then integrated into a fuzzy pattern classifier, which allows spectra to be evaluated considering the uncertainties. This approach opens new possibilities for the precise and reliable evaluation of spectra in various application areas.

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