Probability models of chance fluctuations in spectra of astronomical sources with applications to X-ray absorption lines

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ABSTRACT
The search for faint emission or absorption lines in astronomical spectra has received considerable attention in recent years, especially in the X-ray wavelength range. These features usually appear as a deficit or excess of counts in a single-resolution element of the detector, and as such they are referred to as unresolved fluctuations. The general problem under investigation is the probability of occurrence of chance fluctuations. A quantitative answer is necessary to determine whether detected fluctuations are a real (astronomical, in this case) signal, or if they can be attributed to chance. This application note provides a new comprehensive method to answer this question as function of the instrument’s resolution, the wavelength coverage of the spectrum, the number of fluctuations of interest, and the confidence level chosen. The method is based on the binomial distribution and addresses also the probability of multiple simultaneous fluctuations. A critical aspect of the model is the a priori knowledge of the location of possible fluctuations, which significantly affects the probability of detection. In fact, a wider wavelength range for the ‘blind’ search of possible fluctuations results in a larger number of ‘tries’ for the detection of a fluctuation, lowering the overall significance of a specific feature. The method is illustrated with a case study and examples using X-ray data.

1. Introduction
The wavelength distribution of radiation from astronomical sources, commonly referred to as spectrum, is a fundamental tool for astronomy. In particular, it is common to search for emission or absorption features as a fluctuation above or below a well-characterized baseline emission level, or continuum, in the spectrum. Such features may originate from a number of astrophysical phenomena, such as emission or absorption lines, and carry valuable information on the emitting source or the intervening interstellar and intergalactic medium between the source and the observer. Often these features are sufficiently weak that it is necessary to study whether they may be simply a random fluctuation due to noise in the spectrum, rather than a real feature of astronomical origin.
Figure 1. A portion of the Chandra X-ray spectrum of PG 1116+215, from [4]. Two sets of data points correspond to two spectra collected by the same instrument, caused by incoming photons being dispersed in opposite directions on the detector (± 1 order). The line was identified by [4] as a Kα line from O VIII, red-shifted by \( z = 0.0911 \). Arrow marks the position of the \( z = 0.0928 \) O VIII Kα line, discussed in detail in Section 6.

This paper focuses on a new comprehensive method to establish when one or multiple spectral features are statistically significant. Although the methods presented in this paper can be applied to any spectrum, examples and applications are from X-ray absorption lines in the spectra of distant astronomical sources that have recently appeared in the literature [3,4,17]. This introductory section first provides a review of basic concepts of spectroscopy, then a review of current methods and the need for a new approach are presented.

1.1. Spectra of astronomical sources

This paper considers unresolved features, defined as fluctuations with a wavelength extent that is smaller than the resolution of the instrument. The resolution of the instrument is characterized by a full-width at half maximum (FWHM) of the response to a narrow (or impulse) function. For example, current-generation X-ray instruments such as the RGS on board XMM-Newton and the LETG on board Chandra have a resolution of order \( \sigma_\lambda \sim 50 \text{ mÅ} \), meaning that an intrinsically narrow spectral feature will be spread over a wavelength range of about 50 mÅ, purely by instrumental effects. An unresolved feature is intended to be confined to approximately one or two resolution elements, depending on binning of the data. Figure 1 shows a portion of the X-ray spectrum of an extragalactic source (PG 1116+215), obtained with the Chandra satellite. The spectrum is binned to a size of 50 mÅ, approximately the size of the resolution of the instrument. The apparent absorption feature near 20.7 Å is the type of fluctuations of interest, and it will discussed in more detail as part of the case study of Section 6. The aim of this paper is to provide a statistical method to determine whether such features are a real (astronomical) signal, or whether they are due to random fluctuations in the spectrum.

An example of spectral lines is given by the O VII Kα absorption line from the interstellar or intergalactic medium, often occurring in the spectrum of a background quasar.
The rest wavelength of this line is \( \lambda_0 = 21.60 \, \text{Å} \), and the O VII ion (i.e. a six-times ionized oxygen atom) is abundant at temperatures of order \( T = 10^6 \, \text{K} \), characteristic of a certain phase of the interstellar and intergalactic media [14,21]. Another example is the O VIII K\( \alpha \) absorption line, with rest wavelength \( \lambda_0 = 18.97 \, \text{Å} \), abundant at higher temperatures than O VII. Much attention has been given in the recent literature to the detection of such absorption lines using X-ray spectra [e.g. 4,9,10,16,18,22]. The spectrum of Figure 1 is an excerpt from [4], where a detection of O VIII was claimed. In Section 2.3 is explained how a line from an astronomical source, such as that of Figure 1, can be shifted from its rest wavelength.

Spectral lines are not infinitely sharp impulse functions. Lines are always broadened by a number of atomic and astrophysical phenomena that provide the line with a specific line profile, even without accounting for the broadening due to the instrumental resolution. A typical source of broadening is the temperature of the plasma responsible for the line, with a typical thermal velocity dispersion for O VII lines of order 50—100 km s\(^{-1}\). Such velocity dispersion is simply given by the fact that plasma particles at a given temperature have velocities given by a Maxwellian distribution. The relationship

\[
\lambda = \lambda_0 \left(1 + \frac{v}{c}\right)
\]

describes the Doppler wavelength shift caused by a radial velocity \( v \), assumed non-relativistic (\( v \ll c \), where \( c \) is the speed of light). A typical radial velocity \( v = 100 \, \text{km s}^{-1} \) corresponds to a wavelength dispersion \( \Delta \lambda \simeq 7 \, \text{mÅ} \) around the nominal O VII K\( \alpha \) wavelength \( \lambda_0 = 21.6 \, \text{Å} \). Therefore, the line profile cannot be resolved by the available X-ray instruments with a resolution of \( \sigma_\lambda \sim 50 \, \text{mÅ} \), and the fluctuation will appear as a deficit of counts in one or perhaps two (depending on binning of data) resolution elements of extent \( \sigma_\lambda \). This situation is typical of X-ray emission and absorption lines in the spectra of bright X-ray sources such as quasars. Different considerations would be used when analyzing **resolved** features, i.e. those that can be detected in several resolution elements, as is typically the case for visible or far-ultraviolet (FUV) lines detected by instruments with better spectral resolution [e.g. 20]. Such extended and resolved features are not considered in this paper.

### 1.2. Current methods to estimate the significance of fluctuations in astronomy and their challenges

The significance of detection of unresolved fluctuations, e.g. faint absorption or emission lines, has received considerable attention in astrophysics in recent years. In particular, this is true for the emerging field of X-ray spectroscopy, where the detectors have a much lower spectral resolution than the more traditional and developed optical or infra-red astronomy fields. Such emission or absorption lines will appear as fluctuations in a single-resolution element, thus making the discussion of Section 1.1 relevant. This section describes current methods to assess the significance of faint and unresolved absorption lines in X-ray astronomy. The aim is to highlight the progress in statistical methods in this field and the need for a more comprehensive framework, which will be described in Sections 2–4.
The standard method to assess the significance of a fluctuation in the spectrum of an astronomical source is that of simply determining the signal-to-noise ratio of the fluctuation, relative to a suitable reference level. In the case of a fluctuation described by a Gaussian statistic, i.e. in the high-count approximation of the Poisson counting statistic, the significance or signal-to-noise ratio

\[
S/N = \frac{\text{measured fluctuation}}{\text{error in the measured fluctuation}}
\]

measures the number of standard deviations of the fluctuation from the reference level. For example, a value of \(S/N = 3\) implies a null hypothesis probability of 0.3% of finding such a deviation by chance. This probability is used to determine whether a feature is real or not. This is the method used, for example, by [18], and it is accurate only if one has an \textit{a priori} reason to expect a fluctuation in the specific spectral bin (i.e. at the wavelength) where it was detected.

Random fluctuation can, however, occur at \textit{any} of the bins available in the spectrum. To improve on the earlier method, [16] explicitly introduced the concept of ‘\textit{number of redshift trials}’; that is to say, to account for the fact that there are many resolution elements in the spectrum where the feature could appear. In Section 5, it will be shown that the method of [16] is in fact an approximation to the more general method that will be presented in the following sections. In [10], it is also discussed the need to account for the number of possible resolution elements, although there was no detailed explanation of their method to assess the statistical significance of the absorption lines.

A method to establish the joint significance of several absorption line features was also discussed in [18]. Having tentatively identified a set of negative fluctuations at specific wavelengths as possible absorption lines from various elements, the authors use an \textit{F}-test to determine whether the additional model that describes the intensity of the absorption lines is significant. This method is accurate only under the conditions that all fluctuations are expected \textit{a priori} at the wavelengths at which they were detected.

The main challenge in the estimation of the statistical significance of fluctuations is the lack of a general framework with a rigorous statistical and probabilistic foundation. The aim of this paper is to provide such general framework to study the statistical significance of one or several fluctuations (e.g. unresolved absorption lines), whether they appear at predetermined wavelengths or randomly (i.e. during a blind search). Such comprehensive framework has not appeared thus far in the refereed literature. It will be shown that some of the methods presented earlier in the literature, such as the number of redshift trials of [16], can be obtained as an approximation of the methods presented in this paper.

\section*{2. Methodology I: Statement of the statistical problem}

The general question of interest is that of how many fluctuations of a given significance are expected in a spectrum purely because of random errors in the measurements. This section presents first a definition of fluctuations in the context of astronomical spectra and the associated probability models. Then a discussion follows on how \textit{priors} can be used to reduce the portion of wavelength space that can be searched for such fluctuations. These two aspects are then incorporated in the statistical models presented in Sections 3–4.
2.1. Definition of fluctuations

A fluctuation can be defined as the deviation of detected counts, or an equivalent quantity such as flux, from a true underlying model of the source,

\[ \Delta K = K - K_{\text{model}}, \]

where \( K \) is the number of counts detected in the resolution element, and \( K_{\text{model}} \) is the number of counts predicted by the model in that bin, e.g. from a fit to the continuum of the astronomical source in a broader wavelength range. The statistical significance of the number \( \Delta K \) depends on the properties of both random variables \( K \) and \( K_{\text{model}} \).

The null hypothesis is that the random variable (or measurement) \( K \) is drawn from the same distribution as \( K_{\text{model}} \), i.e. that the underlying model is an accurate description of the measurement \( K \). As such, the expectation or mean of \( \Delta K \) must be zero, under the null hypothesis. The probability distribution function of \( \Delta K \) (e.g. Gaussian or other) and therefore its variance and confidence intervals depend on the nature of the fluctuations.

Before probability models for \( \Delta K \) are discussed in the following section, a note on Equation (1). Although the equation describes the fluctuation of a given spectral bin, it does incorporate information from the entire spectrum, since all bins are used to fit the continuum and thus determine the probability distribution of \( K_{\text{model}} \). For example, if the model of the continuum is a power-law, uncertainties in the parameters of this model (normalization and index) depend on the statistical fluctuation of all data points used in the fit, with larger fluctuations among data points leading to larger errors in \( K_{\text{model}} \). As a result, information about all other spectral bins and their fluctuations are in fact incorporated in the assessment of \( \Delta K \) for a specific bin.

2.2. Probability models for \( \Delta K \) fluctuations

A general reference for the modeling of the random variable \( \Delta K \) is [2] or any other textbook on the general theory of probability [e.g. 19]. Recall the definition of a fluctuation as the variable \( \Delta K = K - K_{\text{model}} \), where

- \( K \): Number of counts or flux detected in a resolution element
- \( K_{\text{model}} \): Number of counts or flux predicted in a resolution element.

Given that the flux is typically in units of counts (or energy) per unit time and area, and that area and time are known exactly, the properties of \( K \) are those of a counting variable. In most cases, this means that \( K \) is Poisson distributed. When the number of counts exceeds approximately 20, the Poisson distribution is accurately approximated by a Gaussian of same mean and standard deviation [see, e.g. chapter 3.4 of 2]. A central confidence interval for either a Gaussian or Poisson variable can be constructed using Tables 1 and 2, where \( K = n \) is the number of detected counts. In particular, confidence intervals for Poisson variables are obtained using the Gehrels approximation [12], also described in [2]. For example, a 68.3% confidence interval for a Gaussian variable is a range of \( \pm 1\sigma \) around its mean, and a 68.3% confidence interval on for Poisson variable with \( n = 10 \) is the range from 6.90 to 14.28, using the \( S = 1 \) case of Table 2. The Poisson parameter \( S \) is used to relate Gaussian confidence intervals to the non-symmetric Poisson confidence intervals, as explained in [2].
### Table 1. Confidence intervals for Gaussian variables.

| Gaussian Interval | Enclosed Probability | Poisson S |
|-------------------|----------------------|----------|
| ±0.68σ           | 0.50                 | 0.68     |
| ±1σ              | 0.683                | 1        |
| ±1.65σ           | 0.90                 | 1.65     |
| ±2σ              | 0.955                | 2        |
| ±3σ              | 0.997                | 3        |
| ±4σ              | 0.99994              | 4        |

### Table 2. Confidence intervals for Poisson variables. The Poisson S parameter corresponds to the number of Gaussian standard deviations (reproduced from [2]).

| Counts | Poisson S parameter | Lower limit | Enclosed Probability | Upper limit | Enclosed Probability |
|--------|---------------------|-------------|----------------------|-------------|----------------------|
|        |                     | 0.841       | 0.977                | 0.999       | 0.841                |
| 1      |                     | 1           | 0.01                 | 2           | 3.32                 |
| 2      |                     | 0.71        | 0.21                 | 3           | 4.66                 |
| 3      |                     | 1.37        | 0.58                 | 1           | 5.94                 |
| 4      |                     | 2.09        | 1.04                 | 0.03        | 7.18                 |
| 5      |                     | 2.85        | 1.57                 | 0.75        | 8.40                 |
| 10     |                     | 6.00        | 4.71                 | 3.04        | 14.28                |
| 20     |                     | 15.57       | 12.04                | 9.16        | 25.56                |

The continuum model is typically obtained from a fit to the spectrum over a large wavelength range. The variance of $K_{\text{model}}$ is often much smaller than that of the fluctuation $K$, because of the wider baseline of data used for its determination. When the model is known accurately, the probability model of $\Delta K$ is just that of $K$. In this case, Tables 1 and 2 are sufficient to model the fluctuation. Another case that is easily treatable is that of Gaussian $K$ and Gaussian $K_{\text{model}}$; assuming independence between the two variables, $\Delta K$ remains Gaussian with a variance equal to the sum of the two variances.

In astronomy, the fluctuation $\Delta K$ is often modeled directly during the spectral fit using available software. A characteristic example is described in [4], where the continuum is modeled via a power-law component and the absorption line as a Gaussian profile with known central wavelength and width, and with variable depth. In this case, the depth of the Gaussian profile is the parameter that describes the fluctuation $\Delta K$, since it is proportional to the number of counts in the absorption line. The probability distribution function of $\Delta K$ is generally unavailable, except for the simply cases described earlier in this section. The modeling of the difference between counting variables has also received attention in other fields, such as econometrics [8]. One of the challenges of finding the probability distribution function of $\Delta K$ is the fact that the joint distribution of $K$ and $K_{\text{model}}$ is unknown (as is the correlation between them). Therefore, it is in general not possible to know exactly the distribution function of $\Delta K$. This limitation can be circumvented by using an approach that establishes the confidence interval for $\Delta K$, without knowing its probability distribution function. This method is described in the following.

The confidence level of $\Delta K$ is calculated by the analysis software using the $\chi^2_{\text{min}}$ statistic (or, alternatively, the Cash statistic $C$, if $K$ is in the low-count regime), by varying the parameter of interest until $\chi^2$ or $C$ is increased from its minimum by a prescribed amount (e.g. by $+1$ for a 68% confidence interval on the parameter, or $+2.7$ for a 90% confidence interval, as
explained in [2]). During this procedure the other parameters, in particular those describing the continuum, are also adjusted, and the result is a confidence level on the parameter of interest, in this case $\Delta K$, that accounts for variability of the other parameters. This $\Delta \chi^2$ method of analysis is the standard method used in X-ray spectral analysis [e.g. 13], and it provides a confidence interval for $\Delta K$ at the desired probability level. The method does away with the need to study $K$ and $K_{\text{model}}$ separately, and it provides a convenient way to describe the statistical properties of $\Delta K$ directly. In general, $\Delta K$ is not Gaussian distributed, and one needs not know its distribution. The method, however, does provide a confidence interval (e.g. at 68%, 90% or any other level of probability), and this information is sufficient to make an assessment of its statistical significance.

For convenience, this note uses the number of equivalent standard deviations of a Gaussian distribution to describe the probability and confidence intervals of $\Delta K$, e.g. a confidence interval with probability 68% corresponds to a $\pm 1\sigma$ interval.

### 2.3. Choice of wavelength range for the search of fluctuations and the effects of redshift

In general, a spectrum is between two wavelengths $\lambda_1$ and $\lambda_2$ and with of resolution $\sigma_\lambda$. The total number of independent resolution elements $N$ in the spectrum can be therefore calculated via

$$N = \frac{\Delta \lambda}{\sigma_\lambda}, \quad (2)$$

where $\Delta \lambda = \lambda_2 - \lambda_1$ is the wavelength range covered by the observation. Both quantities in the equation above can be expressed in units of Angstrom (Å) or, equivalently, meters. The number $N$ represents the number of opportunities for one fluctuation to appear in the spectrum, given the instrumental resolution. For example, a spectrum of $\Delta \lambda = 1$ Å range with resolution $\sigma_\lambda = 50$ mÅ results in $N = 20$ opportunities for a fluctuation to present itself. This is true only if there is no a priori reason to expect a fluctuation in a smaller sub-set of the wavelength range covered by the spectrum.

Since fluctuations of interest to this paper are unresolved emission or absorption lines, it is necessary to examine in more detail at what wavelength(s) such lines can be detected. In general, the wavelength of a given spectral line is known with great accuracy, as determined by the appropriate (and often quite complicated) quantum mechanical calculation [e.g. 11]. For example, the O VII Kα line is found at $\lambda_0 = 21.60$ Å. Therefore, if one is interested in the detection of an unresolved fluctuation corresponding to this line, there is just $N = 1$ opportunity to detect this fluctuation, and that is given by the resolution element that includes the $\lambda_0 = 21.60$ Å wavelength.

This situation is complicated by the fact that astronomical lines can be shifted from their theoretical rest wavelengths by Doppler (i.e. velocity) effects or by the expansion of the universe, the latter causing a relative velocity between source and observer similar to the usual Doppler effect. In both cases, the observer has a different velocity relative to the source, and this difference in velocity results in a line of rest wavelength $\lambda_0$ being now detected at a new wavelength of

$$\lambda_1 = \lambda_0 (1 + z)$$
where \( z = v/c \) is the so-called redshift of the source, and \( v \) is the associated relative velocity between source and observer, when \( v \ll c \). The reason for the term redshift is that the expansion of the universe causes any distant source to move away from Earth with a positive velocity (\( v > 0 \) and \( z > 0 \)), leading to a shift of visible radiation towards longer wavelengths (\( \lambda_1 > \lambda_0 \)), i.e. towards the red portion of the spectrum. Incidentally, the redshift is also a measure of the distance of a source, since the expansion of the universe causes farther sources to move faster, i.e. with higher \( z \), away from Earth, according to Hubble’s law.

The redshift of the source can have the following implications for the detection of fluctuations:

(a) If the redshift \( z \) is known, then the fluctuation will be expected at a different wavelength, yet still in a single-resolution element. In this case, it is still true that \( N = 1 \). For example, this is the case if one has an a priori knowledge of the location (and therefore redshift) of the astrophysical plasma responsible for the absorption line. One example of this situation is the quasar \( X \) Comae, studied in \([4]\). The quasar has a known source in its foreground, the Coma cluster of galaxies at \( z = 0.0231 \). Therefore, an absorption line from O VII will now occur exactly at \( \lambda_1 = \lambda_0(1 + 0.0231) = 22.10 \text{ Å} \), instead of its rest wavelength of \( \lambda_0 = 21.60 \text{ Å} \). There is no wavelength uncertainty here in the search for such absorption line.

(b) When there is no exact knowledge of the location of the source of emission or absorption, the redshift dependence of the observed wavelength widens the possible range of wavelengths for the search of fluctuations. A typical example is that of quasars used to study absorption lines between the redshift of the source (\( z_S \)) and the observer (by definition at \( z = 0 \)). In this case, the interval of redshifts between \( 0 \) and \( z_S (\Delta z = z_S) \) corresponds to a continuous wavelength range from \( \lambda_0 \) to \( \lambda_0(1 + \Delta z) \), i.e. a wavelength range of size \( \lambda_0 \Delta z \). In this situation, the number of independent opportunities to detect a feature is

\[
N = \frac{\lambda_0 \Delta z}{\sigma_\lambda}.
\]

In a more general situation, one may have a prior knowledge that an absorber may be between redshifts \( z_a \geq 0 \) and \( z_b \leq z_S \), resulting in the use of \( \Delta z = z_b - z_a > 0 \) as the range of redshifts allowed in the search. For example, this situation was applicable to the study of an extragalactic source in \([10]\). A given line can now appear in several resolution elements, simple because of uncertainties in its location and therefore redshift.

In summary, although the rest wavelength of a line is known with accuracy, the observed wavelength may have a continuous distribution because of its redshift dependence. The priors on the location of possible lines therefore determine the range of wavelengths to use in the search, and therefore the number of opportunities \( N \), according to Equation (3).

### 3. Methodology II: Statistical model for the probability of at least one fluctuation

This section describes a general model to determine the probability of occurrence of at least one fluctuation. As is usually the case in probability and statistics, it is necessary to
first state as accurately as possible the question of interest. The question initially posed is simply:

**Question:** What is the probability of occurrence of one chance fluctuation with significance \( \geq n\sigma \)?

The phrase ‘significance \( \geq n\sigma \)’ is meant as the probability associated with exceeding a value of \( \pm n \) standard deviations of a Gaussian distribution. For example, a \( \geq 3\sigma \) fluctuation corresponds to a null hypothesis probability of \( p = 0.003 \) or 0.3% (Table 1). The model is presented and discussed in Section 3.1, then methods of application are presented in Section 3.2.

### 3.1. Development of the model

The model for the probability of an unresolved fluctuation has three components:

1. First step is the evaluation of the number of available tries, \( N \), as discussed in Section 2.3. The equations presented in that section can be used to evaluate the number \( N \), according to the situation at hand.
2. Second, one needs to establish a level of significance for the fluctuation. A fluctuation of significance \( \geq n\sigma \), say \( n = 3 \), means that there is a probability \( p \), in this example \( p = 0.003 \) or 0.3%, of occurrence of one such fluctuation at this this level of probability. This step assumes that there is interest in both positive and negative fluctuations, i.e. the null hypothesis is two-sided. If \( \Delta K \) is not Gaussian, the appropriate distribution must be used to determine the probability of interest \( p \), as described in Section 2.1.
3. The binomial distribution is used to describe the probability of occurrence of one such fluctuation out of \( N \) possible tries, via

   \[
   P(1) = \binom{N}{1}pq^{N-1} = Npq^{N-1}
   \]

   where \( p \) is the null hypothesis probability for the occurrence of a fluctuation, and \( q = 1 - p \) is the probability of the complementary event, i.e. the non-occurrence of such fluctuation. For example, according to Equation (4) and for \( N = 20 \), one \( \geq 1\sigma \) fluctuation \( (p = 0.32) \) has just a 0.4% probability of occurring one time, and one \( \geq 2\sigma \) fluctuation \( (p = 0.045) \) has a 38% probability of occurring one time, according to Equation (4). At first, this example seems counter-intuitive, as one might expect that a lower-significance fluctuation would be more likely than a higher-significance fluctuation. However, Equation (4) only calculates the occurrence of exactly one such fluctuation. Surely, one expects more than one \( \geq 1\sigma \) fluctuations in a spectrum, especially over a wide wavelength coverage, as shown in Figure 2.

   This observation leads to a reformulation of the original question to include the statement of *at least one* instead of *exactly one* fluctuation. Therefore the statistically interesting question becomes:

**Question:** What is the probability of occurrence of at least one chance fluctuation with significance \( \geq n\sigma \)?
Figure 2. (Left) Probability of occurrence of number of fluctuations, for three representative values of probability $p$ and fixed $N = 20$. (Right) Cumulative distribution functions for the same distributions as in the left panel. Each dot represents the probability of at least that number of fluctuations, or larger.

Table 3. Cumulative probabilities $P$ of having at least one fluctuation as function of probability $p$ and number of resolution elements $N$.

| $p$  | Confidence | $N = 5$ | $N = 10$ | $N = 20$ | $N = 40$ | $N = 60$ | $N = 100$ | $N = 300$ | $N = 1000$ |
|------|------------|---------|----------|----------|----------|----------|-----------|-----------|------------|
| 0.32 | $\pm 1\sigma$ | 0.8546 | 0.9789 | 0.9996   | 1.0      | 1.0      | 1.0       | 1.0       | 1.0        |
| 0.1  | $\pm 1.6\sigma$ | 0.4095 | 0.6513 | 0.8784   | 0.9852   | 0.9982   | 1.0       | 1.0       | 1.0        |
| 0.045| $\pm 2\sigma$  | 0.2056 | 0.3690 | 0.6018   | 0.8415   | 0.9369   | 0.9900    | 1.0       | 1.0        |
| 0.01 | $\pm 2.6\sigma$ | 0.0490 | 0.0956 | 0.1821   | 0.3310   | 0.4528   | 0.6340    | 0.9510    | 1.0        |
| 0.003| $\pm 3\sigma$  | 0.0149 | 0.0296 | 0.0583   | 0.1132   | 0.1650   | 0.2595    | 0.5940    | 0.9504     |
| 0.001| $\pm 3.2\sigma$ | 0.0050 | 0.0100 | 0.0198   | 0.0392   | 0.0583   | 0.0952    | 0.2593    | 0.6323     |
| 0.0001| $\pm 3.9\sigma$ | 0.0005 | 0.0010 | 0.0020   | 0.0040   | 0.0060   | 0.0100    | 0.0296    | 0.0952     |
| 0.000064| $\pm 4\sigma$ | 0.0003 | 0.0006 | 0.0013   | 0.0025   | 0.0038   | 0.0063    | 0.0187    | 0.0611     |
| 0.000006| $\pm 4.5\sigma$ | 0.0000 | 0.0001 | 0.0001   | 0.0002   | 0.0004   | 0.0006    | 0.0018    | 0.0060     |

This probability is given by

$$P = \sum_{i=1}^{N} P(i), \quad (5)$$

where

$$P(i) = \binom{N}{i} p^i q^{N-i}. \quad (6)$$

The cumulative probability $P$ of having at least one fluctuation is now a monotonic function of the individual probability $p$, which is in turn a monotonic function of the number $n$ of Gaussian standard deviations to be exceeded by the fluctuation. In other words, Equation (5) ensures a meaningful null hypothesis probability, i.e. the null hypothesis probability $P$ of at least one fluctuation is monotonically decreasing as $p$ decreases (for same $N$, see Table 3). According to the Equation (5) (which replaces Equation (4)) and Table 3, for $N = 20$, at least one $\geq 1\sigma$ fluctuation has now a $\sim 99.9\%$ (versus 0.4\% of exactly one fluctuation), and at least one $\geq 2\sigma$ fluctuation has a $\sim 60\%$ probability (versus 38\% of exactly one fluctuation). An illustration of the binomial probabilities of Equation (6) is shown in Figure 2.

The cumulative probability $P$ of at least one chance fluctuation is a function of both $N$ and $p$, and it is shown for two representative values of $p$ in Figure 3 as function of $N$. For
example, there is approximately a 6% probability of having at least one $\geq 3\sigma$ fluctuation in $N = 20$ resolutions elements. Probabilities of having at least one fluctuation are also summarized in Table 3. This table will guide the data analyst to choose the proper significance level $p$ of unresolved features of interest. For a search with $N = 100$ resolution elements, one expects at least one fluctuation that exceeds the $2\sigma$ level with 99% probability. This is to say, there is a near certainty that there will be at least one fluctuation at this level simply by chance, according to the uncertainties in the measurements. At the $3\sigma$ level, this probability is still approximately 26%, and at the $4\sigma$ level it is reduced to just 0.6%. In a blind search for fluctuations with $N = 100$ resolution elements, an analyst would therefore need to identify a fluctuation with at least (approximately) $4\sigma$ significance, according to Table 3.

### 3.2. Methods of application of the model

Consider finding one $\geq 3\sigma$ fluctuation in a spectrum with 100 resolution elements during a blind search in which the feature can equally well appear in any of the resolution elements. Such feature should be assigned a chance probability of 26%. Alternatively, one can say that there is a 26% probability that such feature is not real and it is caused by randomness in the measurements. This effectively means that even a $3\sigma$ fluctuation cannot be trusted with great confidence, if it is the result of a search with such large number of opportunities for detection. A careful analyst will not claim this detection as real. With 100 resolution elements available, an individual $\geq 4\sigma$ detection results in a cumulative null hypothesis probability of $p = 0.0063$, i.e. there is less than a 1% chance of such fluctuation being caused by randomness in the measurements. It would appear reasonable to claim such a detection as real.

In general there are two types of application of the model for one unresolved fluctuation:

(a) The search for a line of known wavelength and in a fixed redshift range.

This is the case, for example, of the search for a O VII $K\beta$ absorption line, with rest wavelength of $\lambda_0 = 21.60\,\text{Å}$. The relevant equation for $N$ is Equation (3), with $z_a$ and $z_b$ corresponding to the range of redshift where the line is expected. Notice that even when one expects a line at a specific location, e.g. due by a line-of-sight cluster of known redshift, one should still include a redshift range to allow for errors in the measurements of the
redshift. This redshift error may be small, and in that case the equation will yield \( N \leq 1 \), which should be interpreted as \( N = 1 \).

(b) The search for a new line of unknown wavelength.

This is the case when a fluctuation appears at a wavelength that is not consistent with any known lines. In this case, the burden in the calculation of the appropriate value of \( N \) is that of excluding all redshift ranges where all known lines may appear. Having established the range \( \Delta \lambda \) where no known lines are present (or a union of several such ranges), the number of independent tries for the detection of an unknown line will be given by Equation (2). For example, there has recently been a claim of detection of a new emission line due to the presence of dark matter during a blind search of X-ray spectra of galaxy clusters \([6]\). In this work, the authors calculate the number of resolution elements available in the search, correctly excluding a portion of the spectrum where several known lines are known to be present.

4. Methodology III: Statistical model for the probability of at least more than one fluctuation

Another situation of practical interest is the search for more than one unresolved features in the same spectrum. This section extends the model presented in Section 3 to the case of several fluctuations.

4.1. Model for more than one fluctuation

In this case, the statistical question of interest becomes:

**Question:** What is the probability of occurrence of at least \( m \geq 2 \) fluctuations with significance \( \geq n \sigma \)?

The number of trials \( N \) is calculated following the same steps as in Section 3. The question can be answered by a straightforward modification of Equation (5):

\[
P_m = \sum_{i=m}^{N} P(i),
\]

(7)

to account for the fact that \( m \geq 2 \) fluctuations are the new null hypothesis. The model for more than one fluctuation is therefore a simple extension of the model for just one fluctuation. Tables of probabilities for the cases of \( m = 2 \) and \( m = 3 \) are reported, respectively, in Tables 4 and 5. For example, the probability of at least \( m = 3 \) random fluctuations at \( \geq 2\sigma \) for \( N = 10 \) is 0.86% (Table 5), it is 7.2% for at least \( m = 2 \) fluctuations (Table 4) and 36.9% for at least one fluctuation (Table 3).

It is important to notice that this model considers \( m \) fluctuations with the same minimum statistical significance \( n \sigma \). This is typically a reasonable assumption, when performing a blind search for lines of unknown intensity.

4.2. Methods of application of the \( m \geq 2 \) model

There are three main applications of this model:
Table 4. Cumulative probability $P$ of having at least two fluctuations as function of confidence (or probability) level $p$, and number of resolution elements (or tries) $N$.

| Confidence $p$ | $N = 2$ | $N = 5$ | $N = 10$ | $N = 20$ | $N = 40$ | $N = 60$ | $N = 100$ | $N = 300$ | $N = 1000$ |
|---------------|---------|---------|----------|----------|----------|----------|----------|----------|----------|
| 0.32          | 0.1024  | 0.5125  | 0.8794   | 0.9953   | 1.0000   | 1.0000   | 1.0000   | 1.0000   | 1.0000   |
| 0.1           | 0.0100  | 0.0815  | 0.2639   | 0.6083   | 0.9195   | 0.9862   | 0.9997   | 1.0000   | 1.0000   |
| 0.045         | 0.0020  | 0.0185  | 0.0717   | 0.2266   | 0.5426   | 0.7584   | 0.9428   | 1.0000   | 1.0000   |
| 0.01          | 0.0001  | 0.0010  | 0.0043   | 0.0169   | 0.0607   | 0.1212   | 0.2642   | 0.8024   | 0.9995   |
| 0.003         | 0.0000  | 0.0000  | 0.0004   | 0.0016   | 0.0065   | 0.0142   | 0.0367   | 0.2275   | 0.8013   |
| 0.001         | 0.0000  | 0.0000  | 0.0000   | 0.0002   | 0.0008   | 0.0017   | 0.0046   | 0.0369   | 0.2642   |
| 0.0001        | 0.0000  | 0.0000  | 0.0000   | 0.0000   | 0.0000   | 0.0000   | 0.0004   | 0.0047   | 0.2642   |

Table 5. Cumulative probability $P$ of having at least three fluctuations as function of confidence (or probability) level $p$, and number of resolution elements (or tries) $N$.

| Confidence $p$ | $N = 3$ | $N = 5$ | $N = 10$ | $N = 20$ | $N = 40$ | $N = 60$ | $N = 100$ | $N = 300$ | $N = 1000$ |
|---------------|---------|---------|----------|----------|----------|----------|----------|----------|----------|
| 0.32          | 0.0328  | 0.1905  | 0.6687   | 0.9765   | 1.0000   | 1.0000   | 1.0000   | 1.0000   | 1.0000   |
| 0.1           | 0.0010  | 0.0086  | 0.0702   | 0.3231   | 0.7772   | 0.9470   | 0.9981   | 1.0000   | 1.0000   |
| 0.045         | 0.0001  | 0.0009  | 0.0086   | 0.0586   | 0.2681   | 0.5103   | 0.8328   | 0.9999   | 1.0000   |
| 0.01          | 0.0000  | 0.0000  | 0.0001   | 0.0010   | 0.0075   | 0.0224   | 0.0794   | 0.5779   | 0.9973   |
| 0.003         | 0.0000  | 0.0000  | 0.0000   | 0.0002   | 0.0008   | 0.0035   | 0.0626   | 0.5771   | 0.9973   |
| 0.001         | 0.0000  | 0.0000  | 0.0000   | 0.0000   | 0.0000   | 0.0002   | 0.0036   | 0.0802   | 0.9973   |

(a) The search for $m \geq 2$ lines of fixed relative distance.

Consider the case of a plasma with fixed thermodynamical properties, such as fixed temperature and density. Radiative transfer codes can predict the occurrence of several absorption lines at specified wavelengths, optionally also with specified line intensity ratios. For example, a hot plasma may have both O VII and O VIII Kα lines, respectively, at 21.60 and 18.97 Å in the rest frame, with a specified ratio of intensity that depends on temperature. Another example is that of Lyman-α and Lyman-β lines from the same ion, which occur at prescribed wavelengths and intensity for all ions. The relative location and intensity of the lines is fixed and therefore they should be considered as part of a single spectral feature, spread over the appropriate wavelength range. In this case, the relevant model becomes that of Section 3 for just one fluctuation.

The problem therefore shifts to determining the desired combined significance $p$ for the two (or more) lines. For example, consider two lines of identical intensity detected at a significance of $3\sigma$ each. If the lines are detected independently, then the combined significance of two $3\sigma$ lines is obtained by quadrature addition, leading to a $4.2\sigma$ significance (this is true only if fluctuations have the same intensity or counts). This is equivalent to a re-binning of the data such that the two features would appear in the same bin (i.e. counts in the two bins are added). The probability of chance detection of two such lines can be therefore calculated using the $p$ value that corresponds to the combined significance of $4.2\sigma$.

The next step is the calculation of the number of trials $N$. Same considerations as discussed in Section 3 apply. If lines are at a fixed wavelength, and fixed redshift, then typically $N = 1$. In the example above of two $3\sigma$ lines, the chance probability is just that of a $4.2\sigma$ fluctuation, which is less than 0.01%. If there is a range of redshifts to be considered, then
one would use Equation (3) with \( \Delta z \) corresponding to a range of wavelengths that covers all lines under consideration and use the number \( N \) of tries in the calculation of the probability.

This case applies when fitting a spectrum to a model for several lines, for example, as done by [15] to model absorption lines from various elements at the same temperature. Since all lines are related, typically the only free parameter in the fit is the intensity of one of the lines (or an equivalent parameter), with other lines having intensities linked to that of the reference line. All lines contribute to the statistical significance of detection of this one-parameter model.

(b) The search for \( m \geq 2 \) lines at unknown relative distance.

This case applies to the search of lines with known wavelengths in the rest frame, but whose redshifts are unknown and thus the lines do not have fixed distance from one another, as in case (a). This case is applicable to the blind search for, e.g. several O VII K\( \alpha \) lines without having priors on redshifts, as recently done in a paper claiming the detection of the missing baryons via X-ray spectroscopy [17]. We illustrate the application of this method to three typical situations, (1) one in which \( m = 2 \) absorption lines have been detected, (2) with an analysis on the results of [17], and (3) an example for \( m = 3 \).

(1) For \( m = 2 \) and \( N = 100 \) tries, there is a null hypothesis probability of \( P = 0.037 \) or 3.7% that two \( \geq 3 \sigma \) fluctuations occur, as given by Table 4. One would conclude that it is possible that these two detected fluctuations are random, and neither should be claimed as real. But if there were only \( N = 20 \) tries or resolution elements, then the probability would drop to 0.16%. One would conclude that the two fluctuations are unlikely due to randomness, and at least one is real. If only one fluctuation had been detected instead of two, Table 3 indicates that for \( N = 20 \) tries there is a 5.8% null hypothesis probability that the signal is due to a random fluctuation. So, that fluctuation would not be claimed as real. Therefore, as expected, the simultaneous detection of two fluctuations is a much more statistically significant result than a single fluctuation, and the models presented in this paper permit a quantitative comparison between the two cases.

(2) In [17] is reported the detection of two redshifted O VII lines in the line of sight towards a distant X-ray bright source. The importance of this result is that it indicates the discovery of hitherto missing baryonic matter, possibly closing a long-standing mystery in modern cosmology [7]. The finding of this paper is that two O VII K\( \alpha \) lines have been identified, respectively, at \( z = 0.355 \) with significance 3.7–4.2 \( \sigma \) (the range indicates uncertainties in the data analysis) and \( z = 0.434 \) with significance 4.1–4.7 \( \sigma \). Given the wavelength range of the blind search, the authors indicated that there were approximately \( N \simeq 400 \) resolution elements, having excluded regions of known artifacts or unrelated lines from the search. The authors conducted their own analysis to account for the redshift trials in the blind search, based on Monte Carlo simulations, and concluded that these lines remain significant even after accounting for the number of redshift trials. These lines lend themselves to an analysis of their significance using the methods presented in this paper. For \( m = 2 \) (two lines detected) with significance \( \geq 3.9 \sigma \) (using a reasonable approximation of the results in [17]) or \( p = 1 \times 10^{-4} \), Table 4 indicates a cumulative null hypothesis probability of \( \sim 0.04\% \). Clearly, these two detections cannot be given to random fluctuations, even after accounting for the number of available resolution elements, thus confirming the conclusion obtained by the authors based on their Monte Carlo simulations. At least one of these two lines must be a real astrophysics signal. Had only one line (instead of two) been
detected with significance $\geq 3.9\sigma$, then Table 3 for $N = 300$ would indicate a null hypothesis probability of 3%. In this case, one would be much less confident to claim the detection of that lone line.

(3) For $m = 3$ and $N = 100$ tries, there is a large probability of at least three $\geq 2\sigma$ fluctuations (83.3%). An analyst finding three such fluctuations in a blind search should therefore assume that these are chance fluctuations. Not so for $\geq 3\sigma$ fluctuations, since there is now just a 0.35% probability of these simultaneous occurrences being caused by chance fluctuations. In this case, it is still possible that perhaps one of the three fluctuations is caused by random effects. Yet, the simultaneous occurrence of three fluctuations is unlikely to be caused by randomness, so that at least one or two of those fluctuations are likely to be real. The same arguments can be repeated for any value of $m$, and tables equivalent to Table 5 can be constructed from Equation (7).

(c) The search for $m \geq 2$ lines of both known and unknown relative distance.

This is probably the most common occurrence in X-ray astronomy. Typical X-ray sources have a handful of $z = 0$ absorption lines (originating from the Galaxy) that are often detected with high significance, on occasion accompanied by few faint absorption-line features that occur at random wavelengths. This was the case for the source in [17] presented above in case (b), where the two $z > 0$ absorption lines were accompanied by several stronger absorption lines from Galactic material (such as O VII, O I, and many more ions). In such cases, it is customary to first identify and model the lines at fixed wavelength, and then proceed with the blind search of additional lines as described in case (b). The modeling of bright lines at expected wavelengths, such as O VII at 21.6 Å, is also needed to provide an accurate model for the continuum, prior to the search for fainter lines. When the blind search commences, the wavelength range to be searched, and the associated number of resolution elements, is reduced to exclude the range where the fixed-wavelength lines were previously identified. This procedure was in fact followed by [17] and for the source in the case study of Section 6 [4]. In so doing, the fluctuations corresponding to expected features are incorporated in the search for new features.

5. Methodology IV: The approximate $pN$ method

A common and simplified method to deal with the number of resolution elements in blind searches is that of [16], also implemented by [4] and others. For the detection of one feature, the null hypothesis probability $p$ of detection (e.g. $p = 0.003$ for a $3\sigma$ detection) is simply multiplied by the number of resolution elements $N$,

$$P = pN$$

to obtain the cumulative probability $P$ of the null hypothesis. This empirical equation is intended to provide the probability of detection of one feature, adjusted for the number of possible detection opportunities or resolution elements.

This probability can be shown to be a good approximation to Equation (4) when $p \ll 1$ and $N$ is not too large. The main drawback of this approximation is that it does not ensure the property of $P \leq 1$, which is one of the fundamental axioms of the theory of probability. Therefore, it is preferable to use Equation (4) to address the probability of detection of exactly one unresolved feature or Equation (5) for at least one unresolved
feature. Another limitation is that this simple method does not calculate the probability of at least one fluctuation, but that of exactly one fluctuation.

It is useful to investigate when this simplified pN method can be used in place of Equation (5), to approximate the probability of detection of at least one fluctuation with individual significance p, out of N tries. For this purpose, the probability of having at least one fluctuation of significance p can be expanded as a sum,

\[ P(\geq 1) = npq^{N-1} + \frac{N(N-1)}{2}p^2q^{N-2} + \cdots + \binom{N}{i}p^iq^{N-i} + \cdots (i \leq N). \]

For the approximation to hold, one needs to ensure that there is a much smaller probability of two fluctuations than just one fluctuation. This means that:

\[ \frac{N(N-1)}{2}p^2q^{N-2} \ll npq^{N-1} \]

If p is small, \( p \ll 1 \), this condition becomes

\[ pN \ll 2. \quad (8) \]

The condition of \( p \ll 1 \) is quite reasonable, since the analyst usually seeks fluctuations with a small null hypothesis probability in the first place. The resulting condition given by Equation (8) is somewhat more constraining. This condition can be rephrased by saying that, for a given confidence level p, the number of tries must be small enough to satisfy the inequality; alternatively, for a give number of tries n, the individual level of probability p must be small enough to satisfy the condition. For example, in Table 3, all the entries for the first line do not satisfy this criterion, while the entries in the last line do satisfy the criterion.

Next, one also needs to ensure that the probability of more than two fluctuations are likewise negligible, compared to the probability of one fluctuation. This condition can be enforced by requiring that

\[ P(i + 1) \ll P(i), \quad \text{for } i \geq 2 \]

Using the binomial distribution for the probability \( P(i) \), it is easy to show that this condition becomes

\[ pN \ll (i + 1). \]

This condition for \( i \geq 2 \) is automatically satisfied if Equation (8) applies, therefore the only conditions for the applicability of the approximate pN method are:

\[ p \ll 1 \quad \text{and} \quad pN \ll 2. \]

This means that there are many situations in which this simplified method can be used, in place of the more general method described by Equation 5. In those cases, the use of the pN method is justified and it leads to a simpler method of analysis. The accuracy of the pN approximation can be calculated as function of the values of p and N (see Table 6).

6. Application: A case study from the Bonamente et al. (2016) absorption lines in the quasar PG 1116+215

The methods of analysis of fluctuations described in Sections 3–5 are illustrated using the X-ray data of [4] for the astronomical source PG 1116+215.
Table 6. Absolute and percent errors in the use of the pqN approximation for the cumulative probabilities P of having at least one fluctuation as function of p and N. Exact probabilities P are in Table 3.

| p     | Confidence Equiv. σ | N = 5  | N = 10 | N = 20 | N = 40 | N = 60 | N = 100 | N = 300 | N = 1000 |
|-------|---------------------|--------|--------|--------|--------|--------|---------|---------|----------|
| 0.003 | ±3σ                 | 0.0001 | 0.0004 | 0.0017 | 0.0068 | 0.0150 | 0.0405  | 0.3060  | 2.0496   |
|       | (0.60%)             | (1.36%)| (2.88%)| (5.97%)| (9.12%)| (15.60%)| (51.52%)| (215.64%)|
| 0.001 | ±3.2σ               | 0.0000 | 0.0000 | 0.002 | 0.0008 | 0.0017 | 0.0048  | 0.0407  | 0.3677   |
|       | (0.20%)             | (0.45%)| (0.95%)| (1.96%)| (2.98%)| (5.03%)| (15.70%)| (58.15%)|
| 0.0001| ±3.9σ               | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000  | 0.0004  | 0.0048   |
|       | (0.02%)             | (0.05%)| (0.10%)| (0.20%)| (0.30%)| (0.50%)| (1.50%) | (5.08%) |
| 0.00064| ±4σ                 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000  | 0.0002  | 0.0019   |
|       | (0.01%)             | (0.03%)| (0.06%)| (0.12%)| (0.19%)| (0.31%)| (0.94%) | (3.18%) |
| 0.000064| ±4.5σ               | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000 | 0.0000  | 0.0000  | 0.0000   |
|       | (0.00%)             | (0.00%)| (0.01%)| (0.01%)| (0.02%)| (0.03%)| (0.09%) | (0.30%) |

Table 7. Measurement of features in the Chandra spectrum of PG1116+215, reproduced from [4].

| Line ID | Redshift | Flux ΔK (10−6 phot cm−2 s−1) | Significance (ΔK/σK) |
|---------|----------|------------------------------|-----------------------|
| O VII Kα | 0.041    | −7.7 ± 7.2                   | −1.1                  |
| O VII Kα | 0.059    | 7.4 ± 8.9                    | +0.8                  |
| O VII Kα | 0.0911 ± 0.0004 | −11.0 ± 7.5                | −1.5                  |
| O VII Kα | 0.1337   | −3.1 ± 8.6                   | −0.4                  |
| O VII Kα | 0.1385   | 39.1 ± 11.1                  | +3.6                  |
| O VIII Kα | 0.1734  | 8.4 ± 10.1                   | +0.8                  |
| O VIII Kα | 0.041    | −6.8 ± 6.8                   | −1.0                  |
| O VIII Kα | 0.059    | −2.5 ± 7.3                   | −0.3                  |
| O VIII Kα | 0.0911 ± 0.0004 | −31.4 ± 6.0               | −5.2                  |
| O VIII Kα | 0.1337   | −2.2 ± 8.3                   | −0.3                  |
| O VIII Kα | 0.1385   | —                            | —                     |
| O VIII Kα | 0.1734   | 1.4 ± 8.9                    | +0.2                  |

6.1. Description of the data

An X-ray spectrum of the quasar PG 1116+215 was analyzed in search of two extragalactic absorption lines, the Kα lines from O VII and O VIII, respectively with a rest wavelength of λ₀ = 21.60 and 18.97 Å. The search was performed in the neighborhood of 6 different fixed redshifts, chosen from prior knowledge of related absorption lines in the far-ultraviolet portion of the spectrum [20]. This resulted in a total of 12 possible redshift intervals searched for the presence of absorption lines. The resolution of the X-ray spectra (σλ ∼ 50 mÅ) are larger than the width of the lines (dλ ∼ 10 mÅ), therefore absorption lines would appear as unresolved fluctuations.

The search was intended to detect lines originating from a possible warm-hot intergalactic medium (WHIM) along the sight line towards PG 1116+215. This WHIM is assumed to be hot enough so that oxygen is ionized in the form of O VII (six-times ionized) and O VIII (seven-times ionized) ions. Main results from the [4] paper are reported in Table 7. Of the 12 possible lines, O VIII at z = 0.1385 falls at the same wavelength as O VII at z = 0 (not shown in table), which may originate in the Galaxy. Therefore, only N = 11 redshift intervals were useful for the search of extragalactic WHIM.

The redshifts of the lines were fixed at the values indicated by the FUV data, in the initial spectral analysis. In the case of the only ≥ 3σ absorption line detected (O VIII at
z = 0.0928), the redshift was subsequently left free to adjust itself to have a more accurate measurement, given the initial tentative detection. The best-fit redshift of O VIII at z = 0.0911 is consistent with the fixed value initially used, and the effect of such redshift adjustment is described in Section 6.4.

6.2. Detection of an absorption line from the WHIM towards PG 1116+215

The first point in the analysis of the spectrum is to establish the statistical significance required for a fluctuation to be detected at a given confidence level.

**Question:** What significance is required to claim the detection of any one of the 11 possible absorption lines, i.e. to detect the WHIM towards PG 1116+215?

In this case, the analyst would be satisfied with a detection at any redshift. With this information, the number of resolution elements is needed. As discussed in the previous section, there were a total of twelve possible resolution elements (six for O VII and six for O VIII). Since one red-shifted line corresponded to another z = 0 line (which was not interesting for this search), the total number of z > 0 lines searched is reduced to N = 11. Notice that the redshift of the absorption lines was fixed at values set by independent data (in this case, from FUV observations). Therefore, each red-shifted absorption line only had one opportunity to be detected, at the exact wavelength specified by the rest energy and the redshift.

Next, the level of significance of the to-be-detected feature needs to be determined. This means deciding on a cumulative null hypothesis probability P and the associated individual probability p. If one desires an overall probability of detection of 99% (or, in terms of equivalent Gaussian standard deviations, ~ 2.6σ), then the null hypothesis probability is P = 0.01. For N = 11 tries, this means that any individual feature will require an associated confidence according to Table 3 (approximating to N = 10) of p = 0.001 (in terms of equivalent Gaussian standard deviations, ~ 3.3σ).

If one chooses a confidence level corresponding to a 3σ fluctuation (P = 0.003 or 99.7% confidence level), then the individual level of significance would have to rise to p ≃ 0.0003 for 10 resolution elements, corresponding to the requirement of an individual ~ 3.6σ Gaussian fluctuation. The choice of confidence level is largely a matter of personal preference and best practices in the field of study. In the following, the 3σ threshold of detection is used.

**Answer:** An individual ≥ 3.6σ feature can be claimed as a detection at the 3σ or 99.7% level, for the given number of tries (N = 11).

Therefore, any feature detected at an individual significance that is lower than the desired p (in this example, 3.6σ), should be regarded as chance fluctuations, at the 99.7% confidence level.

The next point in the analysis is the determination of the presence of significant features.

**Question:** Are there any statistically significant detections of the 11 possible absorption lines in [4]?
For this purpose, one needs the statistical significance of each absorption feature. In [4], these numbers were reported in their Table 3 (reproduced in Table 7), along with the signal-to-noise ratio of each feature, calculated using the $\Delta \chi^2_{\text{min}}$ method described in Section 2.2. In that analysis, two features stood out: an emission feature at an individual significance level of 3.5\(\sigma\) (or \(p = 0.0005\)) and an absorption feature at a significance of 5.2\(\sigma\), the latter at a redshift of \(z = 0.0911\). The absorption feature is significant at the cumulative \(P\) level of 3\(\sigma\), while the emission feature drops just below the threshold (which would require an individual detection \(\geq 3.6\sigma\)).

**Answer:** The \(z = 0.0911\) absorption feature is the only feature detected at a statistical significance \(\geq 99.7\%\).

Although only indirectly related to the question at hand, it is useful to also discuss the possible emission feature. The availability of \(N = 11\) tries means that there is a cumulative probability \(P \simeq 0.005\) or 0.5\% of having one such fluctuation by chance. This level of probability corresponds to an equivalent confidence level of 2.8\(\sigma\). In other words, the emission feature falls below the 3\(\sigma\) threshold of probability, once the number of possible resolution elements or tries is accounted for. This is an indication that this feature may in fact be a random fluctuation, in line with the observation that there is no immediate plausible explanation for its presence, as also discussed in [4].

It is useful to discuss whether the approximate \(pN\) method of Section 5 is applicable to the detected absorption line. The calculation of the cumulative significance for the absorption feature in the original publication used the approximate \(pN\) method and resulted in an estimated cumulative significance level of \(\sim 4.6\sigma\). Following the discussion of Section 5, the validity of the \(pN\) approximation can be easily verified. For an individual 5.2\(\sigma\) detection, \(p \approx 0.0000002\) (Table 8). Therefore, for \(N \approx 10\), it is clear that \(pN \ll 2\), and the \(pN\) approximation is guaranteed to give an accurate estimate of the cumulative probability \(P\). Under these circumstances, there is no need to use the full calculation according to Equation (5), and the \(pN\) approximation will suffice.

The arbitrariness in the choice of the confidence level makes it such many analysts choose a probability level *a posteriori*, i.e. after having calculated the individual significances of any fluctuations and the number of resolution elements. For example, for these data, it was a logical choice to set a cumulative detection threshold of 3\(\sigma\) or 99.7\%, such that the ‘undesirable’ emission feature becomes attributable to chance, while the ‘desirable’ absorption feature remains significant. This posterior logic has certainly a place in the overall analysis, given that an analyst may have additional information of the nature of the fluctuations, besides its pure statistical significance.

**6.3. Detection of the specific O VIII absorption line at \(z = 0.0911\)**

Another question that can be posed in general terms is:

**Question:** What significance is required to claim the detection of O VIII at \(z = 0.0911\)?

In this case, there is only one resolution element where this absorption feature can be, and therefore the (cumulative) null hypothesis probability associated with this question is
Table 8. Values $A$ of two-sided integral of standard Gaussian within $\pm \sigma$ of mean and corresponding null hypothesis probability $p = 1 - A$. Values are obtained using Python math libraries and are reported with eight digits of decimal precision.

| $\sigma$ | $A$       | $p$       | $\sigma$ | $A$       | $p$       |
|---------|-----------|-----------|---------|-----------|-----------|
| 0       | 0.07965567| 0.92034433| 3       | 0.9973002 | 0.0026998 |
| 0.1     | 0.15851942| 0.84148058| 3.1     | 0.99806479| 0.00193521|
| 0.2     | 0.23582284| 0.76417716| 3.2     | 0.99862572| 0.00137428|
| 0.3     | 0.31084348| 0.68915652| 3.3     | 0.99903315| 0.00096685|
| 0.4     | 0.38292492| 0.61707508| 3.4     | 0.99932614| 0.00067386|
| 0.5     | 0.45149376| 0.54850624| 3.5     | 0.99953474| 0.00046526|
| 0.6     | 0.5160727 | 0.4839273 | 3.6     | 0.99968178| 0.00031822|
| 0.7     | 0.5762892 | 0.4237108 | 3.7     | 0.9997944 | 0.0002156 |
| 0.8     | 0.63187975| 0.36812025| 3.8     | 0.99990381| 0.00009619|
| 0.9     | 0.68268949| 0.31731051| 3.9     | 0.99993634| 0.00006334|
| 1       | 0.7286678 | 0.27133212| 4.0     | 0.99995868| 0.00004132|
| 1.1     | 0.76986066| 0.23013934| 4.1     | 0.99997331| 0.00002669|
| 1.2     | 0.80639903| 0.19360997| 4.2     | 0.99998829| 0.00001708|
| 1.3     | 0.83846668| 0.16151332| 4.3     | 0.99998917| 0.00001083|
| 1.4     | 0.8663856 | 0.1336144 | 4.4     | 0.9999932 | 0.00000668|
| 1.5     | 0.89040142| 0.10959858| 4.5     | 0.99999578| 0.00000422|
| 1.6     | 0.91086907| 0.08913093| 4.6     | 0.99999794| 0.0000026 |
| 1.7     | 0.92813936| 0.07186064| 4.7     | 0.99999841| 0.00000159|
| 1.8     | 0.94256688| 0.05743312| 4.8     | 0.99999904| 0.00000096|
| 1.9     | 0.95449974| 0.04550026| 4.9     | 0.99999943| 0.00000057|
| 2       | 0.96427116| 0.03572884| 5.0     | 0.99999966| 0.00000034|
| 2.1     | 0.9721931 | 0.0278069 | 5.1     | 0.9999998 | 0.0000002 |
| 2.2     | 0.97855178| 0.02144822| 5.2     | 0.99999988| 0.00000012|
| 2.3     | 0.98360493| 0.01639507| 5.3     | 0.99999993| 0.00000007|
| 2.4     | 0.98758067| 0.01241933| 5.4     | 0.99999999| 0.00000004|
| 2.5     | 0.99067762| 0.00932238| 5.5     | 0.99999999| 0.00000002|
| 2.6     | 0.99306605| 0.00693395| 5.6     | 0.99999999| 0.00000001|
| 2.7     | 0.99488974| 0.00511026| 5.7     | 0.99999999| 0.00000001|
| 2.8     | 0.99626837| 0.00373163| 5.8     | 0.99999999| 0.00000001|
| 2.9     | 0.99626837| 0.00373163| 5.9     | 0.99999999| 0.00000001|

equal to the significance of the individual detection, since $N = 1$. If a threshold of $3 \sigma$ or 99.7% is set, so long as the data have a fluctuation $\geq 3\sigma$ at that wavelength, the detection can be claimed as real. No allowance for other possibilities of detection has to be made, since the total number of tries or resolution elements is just $N = 1$. A similar question can be phrased for any of the 11 lines of Table 7.

In principle, this is a perfectly valid question, with a perfectly valid and simple answer. However, the analyst needs to justify why such redshift and absorption line was chosen a priori to formulate the question, i.e. before performing the analysis. There must be a compelling reason why the redshift $z = 0.0911$ and the specific line were chosen, i.e. a reason that makes that redshift unique, to make this question meaningful. Otherwise, the question would appear to be unmotivated, or rather motivated only by the desire to increase the significance of its detection by ignoring all possible opportunities of detection of equivalent features at different redshifts, as in Section 6.2.

Answer: A 3 $\sigma$ significance for the line is required for a 3 $\sigma$ detection, assuming just one resolution element in the search.

A follow-up question is applicable to the specific situation of [4]:

Question: What is the significance of detection of the $z = 0.0911$ O VIII absorption feature of [4]?
In the case of [4], there was no compelling reason indicating that the $z = 0.0911$ redshift was special. In other words, the analysis of the source PG 1116+215 and of foreground structures did not indicate any reasons why that redshift would be a unique candidate for an O VIII absorption line from the WHIM. This means that it would be appropriate to allow for $N = 11$ opportunities to detect any absorption lines, as discussed in Section 6.2. Instead of reporting the significance of detection of the $z = 0.0911$ O VIII absorption line at its individual level of significance of 5.2$\sigma$ (or a null hypothesis probability of $p \simeq 0.000002$), as claimed in the abstract of that paper, it would be more accurate to lower the reported significance of detection according to

$$P = pN \simeq 0.000002$$

which is approximately the probability corresponding to a $\sim 4.7\sigma$ deviation, according to Table 8. This level of significance remains very high, but there may be other situations where a marginal detection becomes not significant when the proper number of tries is accounted.

**Answer:** Accounting for $N = 11$ resolution elements in the search, the line is significant at the $\sim 4.7\sigma$ level ($p \simeq 2 \times 10^{-5}$).

### 6.4. Re-analysis of probabilities allowing an error in the redshift

This case study also lends itself to other considerations that are worth discussing in more detail. The search for absorption lines was initially performed at the exact redshifts indicated by the FUV data of [20]. At these fixed redshifts, the significance of the only absorption line detected at an individual significance $\geq 3\sigma$ was O VIII at the FUV redshift of $z = 0.0928$ (with negligible error), detected with a significance of $3.7\sigma$. For this line, the analysis was refined by allowing the redshift to vary around its nominal FUV value. Reason for this refinement in the analysis is that several sources of error may give rise to a slight change in wavelength between the FUV and X-ray observations. The significance rose to 5.2$\sigma$ when a free redshift was allowed and measured in an amount of $z = 0.0911 \pm 0.0004 \pm 0.0005$ [as reported in 4]. This is the redshift used earlier in this section.

The double error-bar notation is used to identify two sources of error, the first due to the so-called statistical sources (primarily counting statistics) and the second due to the systematic sources (primarily the accuracy of the wavelength scale in the detector, as also discussed in [4]). First of all, it is not clear how the two sources of errors should be added, namely whether in quadrature or linearly, or in a different manner. A quadrature addition would be appropriate if the variable of interest (the fluctuation $\Delta K$) can be thought of as a sum $\Delta K = K_1 + K_2$, where $K_1$ is the measurement of the fluctuation and $K_2$ is a random variable with zero mean, representing the systematic error. Further, the systematic error must be uncorrelated to the measurement for the quadrature addition to apply. This is likely to be the case, since it is assumed that the same systematic error applies regardless of the value of the measurement $K_1$. A quadrature addition of the errors would then be summarized as $z = 0.0911 \pm 0.0007$, showing that this X-ray redshift is within 3 standard deviations of the FUV redshift $z = 0.0928$, as the z-score of the difference is $-2.4$. This criterion can be used to say that the two redshifts are statistically consistent, at the $3\sigma$ level.
This statistical consistency can be used to say that the proper value for the measurement of the fluctuation has a significance of 5.2σ, corresponding to the adjusted redshift. This was the argument used in [4], based on the fact that (a) the initial search at the fixed FUV redshift yielded a ≥ 3σ fluctuation and that (b) knowledge of the detectors allows a slight adjustment.

It is necessary to investigate the effect of a redshift error in more detail. To begin with:

**Question:** How is the total number of tries N affected by an uncertainty in redshift in the search for the WHIM absorption lines?

This allowance for an ‘adjustment’ of the redshift requires a correction to the total number of tries or resolution elements N available in the search. If one allows a range of ±3σ around the nominal FUV redshift (where the standard deviation σ is from the X-ray measurements themselves), then each line may have more than just one resolution element where it can be detected. It was assumed for simplicity that there is a redshift range of σz = ±(3 × 0.0007) where each line can be detected, around the nominal redshift and therefore the nominal wavelength. This redshift range corresponds to a wavelength range of

\[ \Delta \lambda = 2\lambda_0 \sigma_z = 91 \text{ mÅ} \]

for the \( \lambda_0 = 21.6 \) Å O VII line (a similar value apply for the O VIII lines), where \( \sigma_z = 0.0021 \), and the factor of 2 is used to account for positive and negative adjustments. This redshift range (91 mÅ) is approximately twice the size of the resolution element (\( \sigma_\lambda = 50 \text{ mÅ} \)), and therefore it is reasonable to assume that there are two resolution elements where each line has an opportunity to be detected, not just one. Following this argument, one can now say that there was a total of \( N = 22 \) (and not \( N = 11 \) as assumed so far) resolution elements in the search – surely, this same procedure would have been applied to any of the 11 possible lines, had they been detected.

**Answer:** Using a redshift range of \( \sim 90 \) mÅ around each line with a resolution of 50 mÅ, the number of resolution elements doubles to \( N = 22 \).

Finally, we can restate an earlier question, accounting for errors in the redshift:

**Question:** What is the significance of detection of the \( z = 0.0911 \) O VIII absorption feature of [4], accounting for errors in the redshift?

For \( N = 22 \), an individual detection at the 5.2σ level (\( p \approx 0.0000002 \)) corresponds to a cumulative null hypothesis probability of approximately \( P = pN \approx 0.000004 \), where one can use the approximate \( pN \) method since \( pN \) is very small. Such value of \( pN \) corresponds to a \( \approx 4.6 \sigma \) fluctuation, i.e. an individual 5.2σ detection remains very significant also for the increased value of \( N = 22 \). Although in this case study this correction did not affect the result, in general it is important to allow errors in the redshifts to calculate the correct \( N \) and the corresponding cumulative probability \( P \). Marginal detections may become not significant when the proper number of tries is accounted.

**Answer:** Allowing for the redshift uncertainty, the significance is reduced from 4.7σ to 4.6σ.
6.5. Probability of detection of both O VII K\(\alpha\) and O VII K\(\beta\) or other pairs of lines

Having established that the O VIII K\(\alpha\) line is statistically significant, [4] proceeded to seek the presence of the associated K\(\beta\) line, caused by a related atomic transition in the same ion. If O VIII K\(\alpha\) is detected, the weaker K\(\beta\) line must also present. The K\(\beta\) line is located at 16.00 Å in the rest frame, therefore at a fixed distance from the K\(\alpha\) line, and with a prescribed ratio of intensities.

**Question:** Is the O VIII K\(\beta\) absorption line at \(z = 0.0911\) in [4] statistically significant?

The method to detect the O VIII K\(\beta\) was to add another one-parameter model for this line at the prescribed wavelength, corresponding to the same redshift as for the K\(\alpha\) line. The parameter is proportional to the intensity of the line or number of counts in the line. At the wavelength of the O VIII K\(\beta\) line, the spectrum had a deficit of counts corresponding to a negative fluctuation with a flux of \(-13.6 \pm 5.6\) (in same units as Table 7), therefore with 2.4\(\sigma\) significance.

The analysis of [4] can be used to address the question at hand. Given that the search for O VIII K\(\beta\) commenced after the detection of K\(\alpha\) was established, this new search surely has only one possibility of detection (\(N = 1\)). Therefore, the 2.4\(\sigma\) significance can be taken at face value and say that the K\(\beta\) line is not detected at the 3\(\sigma\) (or 99.7%) level, but just at the 2.4\(\sigma\) or 98.4% level. There is a 1.6% chance that this detection is spurious.

**Answer:** The O VIII K\(\beta\) absorption line is not statistically significant, at the 3\(\sigma\) level.

This independent modeling of the K\(\alpha\) and K\(\beta\) lines, however, misses the fact that the relative intensity of the two lines is prescribed.

**Question:** Is the combined detection of O VIII K\(\alpha\) and K\(\beta\) at \(z = 0.0911\) in [4] statistically significant?

In [4], no effort was made to describe the joint probability of detecting both O VIII K\(\alpha\) and K\(\beta\). A simple way to find this probability would have been to link the intensities of the two lines and use a one-parameter model for the joint \(\Delta K\), as explained in case (a) of Section 4.2. This is certainly the most direct way to assess the significance of two lines that are at a fixed distance and with a prescribed ratio of intensities.

Based on the data of [4], the closest one can come to provide a quantitative answer to this question is to combine the individual K\(\alpha\) and K\(\beta\) detections, for a total flux deficit of \(-45.0 \pm 8.2\) or a 5.5\(\sigma\) detection. The usual error propagation formula \(\sigma_{1,2}^2 = \sigma_1^2 + \sigma_2^2\) was used to add the errors [e.g. 1,2]. Given that O VIII K\(\alpha\) was already detected at any reasonable level of significance, clearly the combination of the two is also significant.

**Answer:** Yes, because the significance is driven by the O VIII K\(\alpha\) line.

An independent model for two lines of interest is justified when the intensities of two lines are not linked, as explained in case (b) of Section 4.2. For example:

**Question:** Is oxygen (either O VII or O VIII) significantly detected at \(z = 0.041\) in the spectrum of PG 1116+215?
The relative intensity of O VII and O VIII can have any value, since it is a function of the unknown temperature. Therefore, independent models for the two lines are necessary. According to Table 7, there is a 1.1σ detection of O VII and a 1.0σ detection of O VIII, i.e. neither line is significantly detected individually. It is assumed that there is an a priori reason to seek oxygen at that specific redshift, so that the redshift for the search is fixed. Therefore, one seeks fluctuations in two possible resolution elements (\(N = 2\)), at the two wavelengths of redshifted O VII and O VIII. Following this assumption, the question can be re-stated as: what is the chance probability of two 1σ fluctuations (or \(p = 0.32\)) out of the two possible tries? According to Table 4, there is a 10% chance probability of two 1σ fluctuations out of \(N = 2\) tries. Therefore, one could conclude that oxygen is detected at the 90% confidence level. Usually this confidence level is considered too low to claim a conclusive detection. The main point of this example is to illustrate how to use the model of Section 4 (and Tables 4–5) for multiple fluctuations.

Answer: No, the individual 1.1 and 1.0σ detections do not combine to an overall significant detection of oxygen at that redshift.

In the absence of this method for multiple fluctuations, one could have answered the question by combining the signals at the two wavelengths. The combined O VII and O VIII signal at \(z = 0.041\) is calculated as \(\Delta K_{1,2} = -14.5 \pm 9.9\) using the numbers from Table 7. This corresponds to a \(\sim 1.5\sigma\) detection with a null hypothesis probability of \(\sim 13\%\).

Notice how the answer based on the method described in Section 4 differs from that based on the approximate method of combining the two independent fluctuations. The differences between the two methods are even more significant for a larger number of fluctuations. Consider as an example three identical 1σ fluctuations that can occur in \(N = 3\) resolution elements. According to a simple combination of the signals, one would obtain a \(\sqrt{3} = 1.7\sigma\) fluctuation, with a null hypothesis of 9%. However, the calculation based on the method of Section 4 results in a null hypothesis probability of just 3%, according to Table 5. The method for multiple fluctuations described in this paper can therefore be quite useful for assessing the combined statistical significance of the combination of low-significance features.

7. Conclusions

This paper addressed the probability of occurrence of unresolved fluctuations, such as absorption and emission lines in astronomical spectra, with the goal of determining whether observed features are statistically significant or simply due to chance fluctuations based on the noise in the data. The proposed method generalizes and significantly expands the current best-practices methods of analysis used in the field.

The statistical modeling is based on a binomial probability distribution for the fluctuations. The calculation of chance probability of fluctuations depend on the number of independent resolution elements and the probability level for the fluctuations. This note provides tables and formulas that will aid the analyst in deciding what is a reasonable confidence level to accept detected fluctuations.
The paper is complemented by a case study based on the X-ray data of [4]. The case study highlights the application of the model and other practical aspects in the search for unresolved fluctuations in astronomical spectra, such as the use of a priori assumptions on the location of fluctuations and their impact on the probability of detection.

Notes

1. Å indicates Angstrom, a unit of measure of distance equivalent to $10^{-10}$ m.
2. The profile can be alternatively described by a Lorentz or Voigt profile, and all conclusions will apply to any profile used. The choice of Gaussian parameterization for the line profile is completely unrelated to the Gaussian distribution for any of the model parameters.

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