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PAPER

CRIMINALISTICS

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Bayesian Adaptive Approach to Estimating Sample Sizes for Seizures of Illicit Drugs*,†

ABSTRACT: A considerable amount of discussion can be found in the forensics literature about the issue of using statistical sampling to obtain for chemical analyses an appropriate subset of units from a police seizure suspected to contain illicit material. Use of the Bayesian paradigm has been suggested as the most suitable statistical approach to solving the question of how large a sample needs to be to ensure legally and practically acceptable purposes. Here, we introduce a hypergeometric sampling model combined with a specific prior distribution for the homogeneity of the seizure, where a parameter for the analyst's expectation of homogeneity (α) is included. Our results show how an adaptive approach to sampling can minimize the practical efforts needed in the laboratory analyses, as the model allows the scientist to decide sequentially how to proceed, while maintaining a sufficiently high confidence in the conclusions.

KEYWORDS: forensic science, drug sampling, Bayesian approach, adaptive sampling

A common issue in forensic practices is to estimate an adequate size for a subset of units randomly sampled from a police seizure suspected to contain illicit material, such as illicit drugs (ecstasy, lysergic acid diethylamide [LSD], etc). The subset is typically exposed to laboratory inspection based on chemical analyses to estimate the presence of illicit material in the individual units, and conclusions are then drawn about the characteristics of the whole seizure. It has become widely understood that the Bayesian statistical paradigm might provide the most suitable approach to solving the question of how large a sample needs to be taken from the seizure for both legally and practically acceptable purposes (1–3). For earlier approaches to estimating the sample size, see for example, (4–7), and for a general discussion on the statistical issues related to evidence, see (8,9). Aitken (1) considered the problem using a binomial sampling model approximation, which boils down to the question of choosing an appropriate beta prior distribution to represent the *a priori* expectation of the seizure properties. As the sampling is always in practice performed without replacement from a finite population of units, the correct sampling model equals the hypergeometric distribution, which was used by Coulson et al. (3) to estimate the sample size. Their formulation of the problem included the *a priori* element in terms of a set of hypotheses corresponding to ratios of the number of units containing illicit material to the number of those lacking it. Given that an analyst specifies his/her *a priori* beliefs about the seizure properties, both approaches can be readily applied to estimate a suitable sample size for the units to be analyzed. The earlier statistical approaches to estimating the sample size as specified previously are concerned either with the exact number of units in the seizure containing illicit material (or their fraction), or with a statement in terms of a lower boundary for the probability that the seizure contains at least a given fraction of units with illicit material. However, here we formulate the problem instead in terms of sequential hypotheses. The reason for approaching the sample size estimation problem in this manner is that probabilistic characterization of both the available expert knowledge and sampling uncertainty can then be coherently united using Bayesian statistics. Without clearly defined hypotheses and their prior probabilities, it is not possible to use the rules of probability calculus to derive strictly normative decision tools for estimating the sample size. The first hypothesis represents the claim that the seizure is homogeneous, that is, all units contain illicit material. We show that a prior probability distribution can be readily derived for such a model using formal arguments in Bayesian statistical theory. Under such a prior, an analyst can specify any suitable lower bound on level of confidence or degree of belief in the claim of homogeneity of the seizure, which then enables derivation of an expression for the sample size needed to reach the bound if the sample proves to contain only units with illicit material. However, if the first hypothesis is rejected on the basis of the sample actually drawn, that is, at least a single unit lacks illicit material, then a second hypothesis can be formulated. Results from the chemical analyses performed on the sampled subset of the seizure provide information from which a predictive probability distribution can be derived for any quantity of interest for the whole seizure. Typically, the second hypothesis would correspond to a claim that the seizure contains at least a certain number of units with illicit material, to be further utilized by prosecutors in a legal process. If

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the claim is already associated with a sufficiently high predictive probability from the prosecutors' perspective, no further sampling would be necessary. On the other hand, if the sample information is insufficient to reach the conclusive probability for such a claim, the predictive probability distribution can be utilized to derive an expression for the expected gain obtained by sampling and analyzing any particular number of further units from the seizure. Our formulation thus gives raise to an adaptive sampling strategy where savings in the practical inspection efforts can be reached.

First-Stage Sample

Usually, in the situation where a dichotomous property of units in a finite population is investigated, the correct sampling model equals the hypergeometric distribution. Unfortunately, this approach involves some complications when used for forensic purposes unless special care is taken when formulating the prior probability distribution for the unknowns in the model (see Appendix, Section 1.1). Here, we show that choosing initial sample size using a hypothesis-driven parameterization supplies us with the required results. We formulate the initial hypothesis as a dichotomous statement about whether the seizure is homogeneous or not, that is, whether it contains only positive units. The theoretical arguments given in the study by Bernardo and Smith (2) show how a specific prior probability distribution can be derived for the hypothesis that claims homogeneity of the seizure. Here, we modify their approach slightly to arrive at a prior probability distribution that can incorporate analyst's opinion regarding how likely the homogeneity of the seizure is *a priori* (this quantity is denoted by α, see Appendix Section 1.2 for mathematical details). Let N denote the total size of the seizure and n the size of a random sample without replacement from the population of N units. By Eq. (15) in the Appendix, we obtain the posterior probability of homogeneity, given any particular sample, and thus, a sufficiently large sample size n for a given pair (N, α) is obtained by choosing the smallest value which yields at least as high posterior probability as a preestablished threshold β, say 0.95. In Table 1, derived sample sizes are given considering three different values of α (0.75, 0.90, and 0.95) and population size N taking values in the set (10, 10,000). The obtained sample sizes are the minimum values of n that ensure a threshold value of 0.95. More specifically, consider, for example $N = 50$ and $\alpha = 0.75$, where α reflects the expert's expectation about the homogeneity of the seizure. Then, the sample size required to reach the threshold level 0.95 is $n = 5$. In a typical situation encountered in a forensics laboratory, all sampled units from a seizure are positive (contain illicit material), and thus, no further sampling is necessary based on the hypergeometric model derived in the Appendix. However, when at least one unit out of n is negative, then we have to estimate the lower bound (denoted with u_q) of the number of units containing illicit material and compare it with the number M of positive units that the prosecutors wish to claim to exist in the seizure. If $u_q \geq M$, the sample information indicates that no further sampling is necessary to reach sufficient level of probability in the conclusion that the seizure contains at least M units with illicit material, as u_q can be reported for legal purposes. However, if $u_q < M$, then further sampling may be needed if the prosecutors prefer to claim a high fraction of positive units in the seizure. The mathematical details are fully explained in Section 1.3 of the Appendix. As an example of this first-stage sample, let us consider an initial seizure of $N = 5000$, a fixed preestimated threshold $\beta = 0.95$ and let us set the analyst's expectation α to 0.75. According to Eq. (15) in the Appendix, a sample of size $n = 6$ is enough to reach the desired threshold. If in our sample of six units only four contain illicit material, then the first hypothesis of homogeneity of the initial seizure must be rejected. Further, according to Eqs (17) and (18) in the Appendix, a lower bound, denoted u_q, of the number of units containing illicit material in the initial seizure, can be calculated. In this example, we obtain $u_q = 1707$. Consequently, if the prosecutor wishes to claim a higher fraction of positive units, then it is necessary to proceed with a second-stage sample from the seizure.

TABLE 1—*Sample size required, for every* N *in* (10, 10,000) *to ensure a threshold value of* 0.95.

Alpha	Sample Size
0.75	6
0.9	2
0.95	1

Second-Stage Sample

Let θ denote the total number of units with illicit material in the remainder of the seizure N-n after the first-stage sample. Presume now that n_2 additional samples would be taken from the seizure from which the n units were earlier removed. Assuming that x_2 units from the second sample contain illicit material, Eq. (19) in the Appendix gives the likelihood of obtaining x_2 positive units in the future sample of n_2 units conditional on any particular value of θ. The expected gain in terms of claiming seizure properties from n_2 future samples can now be expressed in terms of the predictive expectation of the lower bound U_q, in which the uncertainty about both x_2 and θ is appropriately taken into account (Eq. [22] in the Appendix). This quantity reveals the conditional expected value for how large a number of units with illicit material could be claimed to be present in the seizure with probability q if n_2 additional samples were taken. The conditional expectation captures the information present in the initial sample of n units and transforms that into a prediction for future samples. In Table 2, we illustrate the particular value of information gain arising from specific combinations of the parameters in the sampling design. As we did already in the previous example, we consider an initial sample size of six units and assume that only four of them contain illicit drug. The table presents results for the combination of three levels of *a priori* uncertainty (0.9, 0.95, 0.99) with three different levels of initial population size (1000, 5000, and 10,000). The expected bounds for the number of illicit units in the population are derived for a

TABLE 2—*Information gain obtained with initial sample size* n = 6 *and assuming* x = 4, *when considering three different seizure sizes and three levels of* a priori *uncertainty*.

	N		
	1000	5000	10,000
0.9			
$n = 6$	405	2020	4039
$n_2 = 2$	430	2148	4295
$n_2 = 3$	440	2198	4395
0.95			
$n = 6$	342	1707	3413
$n_2 = 2$	374	1867	3733
$n_2 = 3$	386	1929	3858
$n = 6$	237	1183	2364
0.99			
$n_2 = 2$	276	1380	2759
$n_2 = 3$	292	1459	2918

second-stage samples consisting of two and three units, respectively. Hence, by drawing from an initial seizure of 5000 units, a sample of size 6, four of which contain illicit drug, allows us to claim that with a probability of 0.95, there are at least 1707 units of drugs in the seizure. If this quantity is not sufficient under the legal perspective, then sampling three more units will yield the expected claim that with a probability of 0.95 there are at least 1929 units of drug in the initial population. The analytically explicit characteristics of the predictive model allow one to develop the sampling strategy into a fully adaptive form. Given the fact that the chemical analyses of samples from multiple seizures are typically performed at the same time using a number of mass spectrometers, it would be a practical strategy to analyze the second-stage samples sequentially. This would allow the decision as to whether to analyze any additional samples to depend on a revision of the predictive probabilities in light of the results for the initially analyzed samples among the total of n_2 second-stage samples. As the bounds derived previously are based on the expectation of the gain from future data, they can be sequentially revised after each test result (positive or negative) arrives from the chemical analysis. This is performed by an update of the posterior distribution (Eq. [17]), which in turn implies a change in the predictive distribution of the future samples. A sought level of claim M may thus be obtained earlier, that is, with fewer additional samples, than anticipated by the expectation of the initial predictive distribution obtained from the first-stage sample.

Discussion

The drug sampling problem is a daily issue in most forensic laboratories, and estimating the optimal sample size is fundamental to ensure a legally acceptable procedure. As usual in the forensic field, there are two opposite needs in the context: producing reliable results without spending too much money and time. A well-trained forensic scientist usually needs just to have a look at the seizure to know what he/she is dealing with. It is important to utilize such expertise in the sampling process to save resources, while still being at the same time conservative. Our method, which is purely Bayesian, enables this and jointly with an adaptive sampling approach, allows the scientist/expert to decide sequentially how to proceed. The first-stage sample size is estimated on the basis of a hypergeometric model but using a parameterization where the scientist's opinion based on experience, denoted by α, is considered. If all the sampled units are positive, no further sampling is required to draw conclusions about the content of the seizure and Eq. (15) in the Appendix will provide the posterior probability of seizure homogeneity. If some of the sampled units are not positive, then further sampling may be needed if prosecutors wish to claim a particular amount M of positive material in the seizure. More specifically, when the number of positive test results x is smaller than the initial sample size n, Eq. (17) in the Appendix provides a new posterior probability from which it is possible to calculate the lower bound u_q (defined formally in Eq. [18]). If $u_q \geq M$, the sampling procedure can be terminated as already shown earlier. If, on the other hand, $u_q < M$, then additional sample is required and the expected gain obtained by sampling n_2 units from the population can be assessed. In practice, a forensic expert/scientist can estimate the number of additional units to be sampled to reach the required level M, and to use resources optimally, analyze sequentially a single unit at a time. Thus, after the first additional unit, denoted by z_1, has been sampled and analyzed, the posterior probability $p(\theta|x, z_1)$ can be revised. Then, if $U_q(z_1) \geq M$, the sampling procedure terminates and no more units are needed. Otherwise, further units must be analyzed, and the procedure can be repeated in an equivalent manner. This procedure is schematically represented in Fig. 1. Our adaptive sampling model provides a resource-saving approach while still being simultaneously legally sound, because

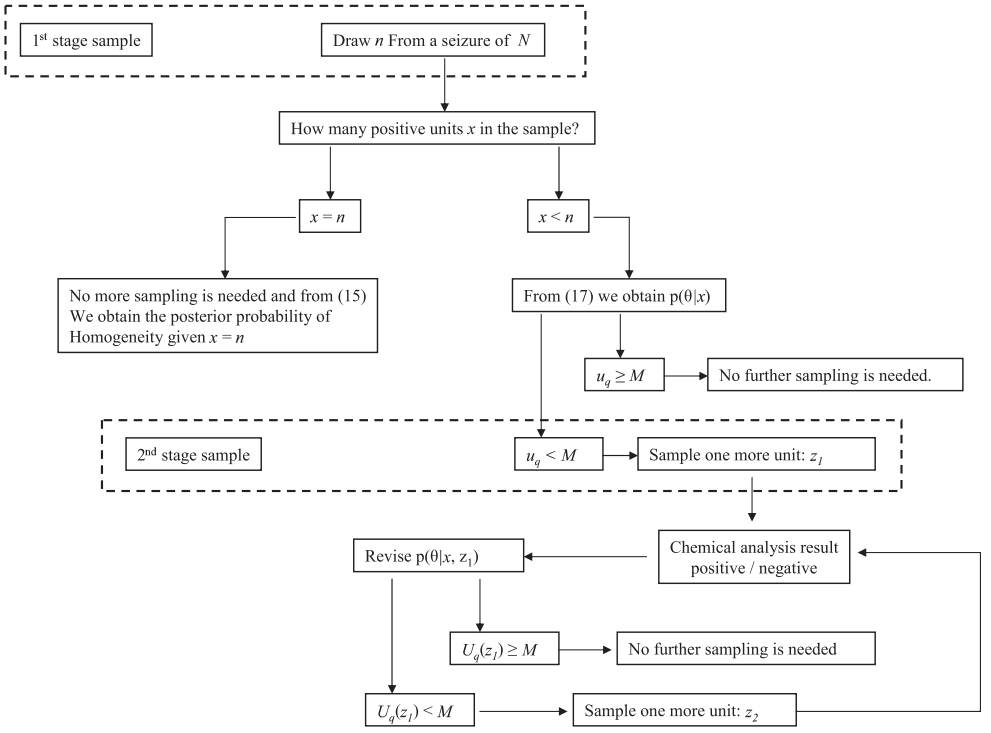

FIG. 1—*Adaptive drug sampling procedure flow chart.*

even for high values of the expert's prior expectation α, a completely innocent suspect will not be harmed because all findings will then be negative. It is worth noticing that for large seizures, a binomial sampling model based on the assumption of infinite population size would provide a feasible approximation to the hypergeometric model. However, because the approach derived here is generally applicable to any seizure size without numerical complications, there is no need to use an approximate likelihood in place of the correct sampling model.

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Appendix

1. Estimating Sample Sizes Using Hypergeometric Distribution

1.1 A Hypergeometric Model—In the situation where a dichotomous property of units in a finite population is investigated using random sampling of units without replacement, the correct sampling model equals the hypergeometric distribution. The hypergeometric model can be defined as

$$p(x|\theta) = \frac{\binom{\theta}{x}\binom{N-\theta}{n-x}}{\binom{N}{n}} \tag{1}$$

where N is the total size of the population (here seizure size), θ is the number of units possessing a property of interest (here, presence of illicit material in the unit), and x is the number of units possessing the property of interest in a randomly chosen sample of size n from the population. The above probability stems from a combinatorial evaluation of the possible configurations of a random sample without replacement. Subsequently, we refer to x and $n - x$ as the number of positive and negative units, respectively, on the basis of results from the chemical analyses, the sample is subjected to. Assume now that $x = n$, then, given the sample information it is known that $n \le \theta \le N$, and the posterior distribution of θ can be written as:

$$p(\theta|x) = \frac{p(x|\theta)p(\theta)}{\sum_{\theta=n}^{N} p(x|\theta = r)p(\theta)} \tag{2}$$

where $p(\theta = r)$, $r = 0, \ldots, N$, specifies the prior probabilities for θ, representing the analyst's uncertainty about the number of units in the seizure containing illicit material. The general inference procedure for the hypergeometric model based on a uniform prior distribution discussed in Bernardo and Smith (2), that is, $p(\theta = r) = 1/(N + 1)$, $r = 0, \ldots, N$, is particularly illuminating in the present context. Assuming all n tested units are positive, the posterior probability of homogeneity of the seizure $\theta = N$ can be written as

$$\begin{aligned} p(\theta = N|x = n) &= \frac{p(x = n|\theta = N)\frac{1}{N+1}}{\sum_{r=n}^{N} p(x = n|\theta = r)\frac{1}{N+1}} \\ &= \frac{\binom{N}{n}}{\sum_{r=n}^{N}\binom{r}{n}\binom{N-r}{n-n}} \end{aligned} \tag{3}$$

Then, by the following general equality

$$\sum_{r=0}^{N}\binom{r}{l}\binom{N-r}{m} = \binom{N+1}{l+m+1} \tag{4}$$

where $l + m = n$ is the sample size for the hypergeometric model and l stands for the number of sampled positive units, and as $\binom{r}{l} = 0$, $r<l$, the posterior probability simplifies to:

$$\begin{aligned} p(\theta = N|x = n) &= \frac{\binom{N}{n}}{\binom{N+1}{n+1}} \\ &= \frac{N!}{n!(N-n)!}\frac{(n+1)!(N+1-n-1)!}{(N+1)!} \\ &= \frac{n+1}{N+1} \end{aligned} \tag{5}$$

Thus, use of the uniform prior would imply that conclusive probabilities for the seizure homogeneity could be obtained only from very large samples, which is obviously not desirable. The actual reason for this behavior of the inferences is that the homogeneity is assigned the smaller probability *a priori*, the larger the size of the total population.

1.2 Choosing Initial Sample Size Using a Hypothesis-Driven Parameterization

We formulate the initial hypothesis as a dichotomous statement about whether the seizure is homogeneous or not, that is, whether it contains only positive units. The theoretical arguments given in Bernardo and Smith (2) show how a specific prior probability distribution can be derived for the hypothesis that claims homogeneity of the seizure. Here, we modify their approach slightly to arrive at a prior probability distribution that can incorporate analyst's opinion regarding how likely the homogeneity of the seizure is *a priori*.

Our prior distribution is derived using a re-parameterization of the hypergeometric distribution. Corresponding to the first hypothesis, we are primarily interested in the dichotomous parameter:

$$\phi = \begin{cases} 1, \text{ if } \theta = N \\ 0, \text{ if } \theta \neq N \end{cases} \quad (6)$$

Define now θ as (ϕ, λ), such that

$$\lambda = \begin{cases} 1, \text{ if } \theta = N \\ \theta, \text{ if } \theta \neq N \end{cases} \quad (7)$$

and define the following prior distribution for the new parameters:

$$p(\phi = 0) = 1 - \alpha \quad (8)$$

$$p(\phi = 1) = \alpha \quad (9)$$

$$p(\lambda = 1 | \phi = 1) = 1 \quad (10)$$

$$p(\lambda = r | \phi = 0) = \frac{1}{N},\ r = 0,\ 1, \ldots,\ N - 1 \quad (11)$$

The probability α represents an analyst's expectation of the homogeneity of the seizure. The above construct implies the following prior for θ:

$$p(\theta) = \begin{cases} \alpha, \text{ if } \theta = N \\ \frac{1-\alpha}{N}, \text{ if } \theta \neq N \end{cases} \quad (12)$$

The reference posterior probability of seizure homogeneity then equals:

$$p(\theta = N | x = n) = \frac{\alpha \binom{N}{n}}{\frac{(1-\alpha)}{N}\left[\binom{N+1}{n+1} - \binom{N}{n}\right] + \alpha \binom{N}{n}} \quad (13)$$

By utilizing the equality

$$\binom{N+1}{n+1} - \binom{N}{n} = \binom{N}{n+1} \quad (14)$$

we obtain the following expression for the posterior probability:

$$p(\theta = N | x = n) = \frac{\alpha \frac{N!}{n!(N-n)!}}{\frac{(1-\alpha)N!}{N(n+1)!(N-n-1)!} + \alpha \frac{N!}{n!(N-n)!}} \quad (15)$$

$$= \frac{\frac{\alpha}{N-n}}{\frac{\alpha}{N-n} + \frac{1-\alpha}{N(n+1)}} \quad (16)$$

It can be shown that when n grows, $p(\theta = N | x = n) \to 1$, which is a desirable property of the inference process.

1.3 Choosing the Number of Eventual Additional Samples

In a typical situation encountered in a forensics laboratory, all sampled units from a seizure are positive, and thus, no further sampling is necessary based on the hypergeometric formulation derived earlier. However, when at least one unit out of n is negative, further sampling may be needed if the prosecutors prefer to claim a high fraction of positive units in the seizure. In probabilistic terms, when $x < n$, the posterior probability of the homogeneity hypothesis $\theta = N$ becomes zero. Correspondingly, the posterior probabilities of other values of θ become in general modified and can be written as:

$$p(\theta | x) = \begin{cases} = \frac{p(x|\theta)p(\theta)}{\sum_{r=x}^{N-(n-x)} p(x|\theta)p(\theta)} = \frac{\binom{\theta}{x}\binom{N-\theta}{n-x}}{\sum_{r=x}^{N-(n-x)} \binom{\theta}{x}\binom{N-\theta}{n-x}}, r = x, \ldots, N-(n-x) \\ = 0, \text{otherwise} \end{cases} \quad (17)$$

Any question about θ can then be readily answered in terms of these probabilities. In particular, let $M < N$ be the number of units containing illicit material that the prosecutors wish to claim to exist in the seizure with a high probability, such that it can be utilized as evidence in a legal process. Boundary of the upper tail area of the posterior distribution (Eq. [17]), say u_q, defines a useful lower bound on the number of units containing illicit material on the basis of the sample of n units with x positive among them. For any probability $q \in (0, 1)$, the boundary can be defined as

$$u_q = \arg\max_r \sum_{\theta=r}^{N-(n-x)} p(\theta | x) \geq q,\ q \in (0,\ 1) \quad (18)$$

Typically, one might use a large value of q, such as 0.99.

If $u_q \geq M$, the sample information indicates that no further sampling is necessary to reach sufficient level of probability in the conclusion that the seizure contains at least M units with illicit material, as u_q can be reported for legal purposes. However, if $u_q < M$, an analyst could assess the gain expected to be obtained from further sampling of units from the seizure to be analyzed. Such gains can be calculated using the predictive distribution of the future samples based on Eq. (17). Presume that n_2 additional samples would be taken from the seizure from which the n units were earlier removed. The posterior distribution of θ for the modified population is then obtained by the simple one-to-one mapping of the earlier elements $x, \ldots, N - (n - x)$ into $0, \ldots, N - n$, resulting from removal of the initial sample. Denote this posterior by $p^*(\theta \mid x)$. Conditional on any particular value of θ, the likelihood of obtaining x_2 positive units in the future sample of n_2 units equals

$$p(x_2 | \theta) = \frac{\binom{\theta}{x_2}\binom{N-n-\theta}{n_2-x_2}}{\binom{N-n}{n_2}},\ x_2 = 0, \ldots,\ n_2 \quad (19)$$

If x_2 positive units were actually obtained, the corresponding predictive bound for the total original seizure becomes

$$U_q(x_2) = x + \arg\max_r \sum_{\theta=x_2}^{N-n} p(\theta|x_2) \geq q,\ q \in (0,\ 1) \tag{20}$$

where the posterior $p(\theta \mid x_2)$ equals

$$p(\theta|x_2) = \frac{\dfrac{\binom{\theta}{x_2}\binom{N-n-\theta}{n_2-x_2}}{\binom{N-n}{n_2}} p^*(\theta|x)}{\sum_{\theta=0}^{N-n} \dfrac{\binom{\theta}{x_2}\binom{N-n-\theta}{n_2-x_2}}{\binom{N-n}{n_2}} p^*(\theta|x)} = \frac{\binom{\theta}{x_2}\binom{N-n-\theta}{n_2-x_2} p^*(\theta|x)}{\sum_{\theta=x_2}^{N-n} \binom{\theta}{x_2}\binom{N-n-\theta}{n_2-x_2} p^*(\theta|x)} \tag{21}$$

Notice that the predictive bound $U_q\ (x_2)$ is a random variable as it depends on the yet unobserved future sample. The expected gain in terms of claiming seizure properties from n_2 future samples can now be expressed in terms of the predictive expectation of the lower bound, in which the uncertainty about the x_2 and θ is appropriately taken into account:

$$U_q = \sum_{\theta=0}^{N-n} \sum_{x_2=0}^{n_2} U_q(x_2) p(x_2|\theta) p^*(\theta|x) \tag{22}$$

This quantity reveals the conditional expected value for how large a number of units with illicit material could be claimed to be present in the seizure with probability q if n_2 additional samples were taken. The conditional expectation captures the information present in the initial sample of n units and transforms that into a prediction for future samples.