Probability of false negative results in GSR detection: 
a Bayesian approach

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Abstract

We calculated the probability of obtaining false negative results in GSR detection depending on the resolution setup for sample scanning, in order to quantitatively describe the trade-off between low false negative rates in the detection of characteristic particles and the effort that measurements entail. We built and validated a GSR particle detection model that associates particle size with equipment registers, and we applied it to samples analyzed by a forensic science laboratory. Our results indicate that the probability of a false negative, i.e. a result where all characteristic particles in a sample which go undetected, is below 5% for pixel sizes below $0.32 \mu m$. These results indicate that pixel sizes as great as the double that is commonly used in usual laboratory casework are effective for an initial scanning of a sample as it yields good rates of detection of characteristic particles, which might exponentially reduce laboratory workload.
1 Introduction

Scanning electron microscopy (SEM) is used to characterize the chemical composition of particles to detect gunshot residue (GSR) in samples collected from individuals’ hands. Particle categories as defined by ASTM E1588-17 [1] are:

- particles characteristic of GSR: those with composition PbSbBa;
- particles consistent with GSR: those with composition PbBaCaSi, BaCuSi, SbBa, PbSb, BaAl, PbBa, Pb, Ba and Sb.

Additional elements commonly found in these particle classes include Al, Si, P, S, Cl, K, Ca, Fe, Ni, Cu, Zn, Zr and Sn.

Pioneering work by Woltet et. al. and, more recently, Zeichner et.al. [2, 3] determined that a particle characteristic of GSR is most likely caused by a gunshot. However, over the last few decades, particles of this kind have also been generated by cartridge-operated industrial tools [4], fireworks and car brake linings [5, 6]. Many of the particles analyzed in these studies presented morphological anomalies, among others, which were used to differentiate them from actual GSR particles. Although characteristic particles do not necessarily originate in the use of a firearm, they are extremely rare in the environment [7] and thus still provide strong evidence of gun firing origin.

In 1987, automated search software was first used together with SEM to analyze GSR samples [8, 9]. As key advantages, these tools help bypass the need of a microscopy operator throughout sample scanning and the bias associated with manual particle search, hence allowing standardized and more exhaustive analysis. On the other hand, these techniques do rely on microscope calibration and setup to reach good contrast for particles of high atomic numbers, which could be classified as characteristic through energy-dispersive X-ray spectroscopy (EDS). In these conditions, pixel resolution for sample scanning is selected by the operator. The latest ASTM guidelines of 2020 [10] indicate that particle sizes typically vary between $0.2\mu m^2$ and $7800\mu m^2$ but make neither reference to particle size distribution nor recommendations for magnification or pixel size for analysis.

Characteristic particle size distribution is a fundamental factor in GSR analysis, as it determines the likelihood of false negatives, i.e., characteristic particles in a sample which go undetected. The $0.5\mu m$ and $100\mu m$ equivalent circle diameter, respectively.
The probability of a false negative will depend on both particle size distribution and microscope setup. In this work, we will focus on the association between these aspects from a Bayesian statistics viewpoint.

The use of probability and statistics in forensic analysis has become increasingly widespread in recent decades, especially through the work conducted by Aitken, Taroni, Bozza and Biedermann [11, 12], who used these tools to establish the contribution of forensic analysis techniques from an epistemological and applied perspective. In this work, we will rely on the findings reported by these authors to build models which can calculate the distributions of interest.

Instruments are often thought to make direct measurements of the objects of interest; however, the sizes detected by automated microscopes are actually altered by detection strategies. This work lain the foundations for building and validating a model to describe the measurements of GSR with a microscope. Understanding the trade-off between shortening measurement times and reducing the probability of false negatives is essential to tap on the capacity of forensic laboratories.

2 Materials and methods

2.1 Circular particle model

The microanalysis system† requires the operator to select search parameters, the most critical ones being the threshold value –determined by measuring a reference sample– and the smallest expected particle width. A pixel size is then defined which is usually half the smallest expected particle width, and the system only detects pixels whose signal is above the threshold. Activated pixels correspond to chemical elements with high atomic numbers, which are of special interest in the search for particles containing heavy metals such as those in GSR. With this measurement strategy, a particle with area is not fully registered because partially covered pixels are disregarded. So, instead of $A$, an eroded version of the particle is registered with a seemingly $B$ area.

In this context, we modeled the relationship between real areas $A$ and registers $B$, on the hypothesis of circular particle shape. This representation poses the advantages of being simple, symmetric, descriptive of GSR, and suited to modelling requirements. Particle shape may be disregarded when

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†for instance INCA Energy.
Figure 1: Circular particle size registration. The numbers indicate the area of each particle in unit pixels. The real areas $A$ are different from the registered areas $B$. The values of $B$ are the areas occupied by completely covered pixels and depend on particle location on the grid.

size exceeds pixel area $p_x$, as $B$ will then be a good representation of total area. Instead, when $A \sim p_x$, both particle shape and position on the pixel grid affect registration $B$ (Fig. 1).

Different values of $B$ can be measured, given a particle of area $A$. The set of $B$ results is discrete, finite, and depends on $p_x$ size. Although a single unequivocal value of $B$ cannot be established on the basis of a particle of area $A$, the fact that all positions on the grid are equivalent allows the calculation of $P(B|A)$. However, as $B$ is actually measured in practice, the question arises as to what values of $A$ are feasible. These values can be calculated using Bayes’ theorem.

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)} \propto L(A|B)P(A),$$

(1)

where $L(A|B)$ is known as the likelihood function and equals the expression $P(B|A)$, although analyzed as a function of $A$. Worth pointing out, $L(A|B)$ is not a probability distribution as a function of $A$. On the other hand, $P(A)$ is indeed a probability distribution known as prior probability and represent the degree of certainty about the values that $A$ may take regardless of any other values. When there are no reasons to believe that some values will be more likely than others, this distribution is defined as an improper uniform distribution, i.e., $P(A) \propto 1$.

To calculate $L(A|B)$ we simulated circular particles with uniform area distribution and placed

\[\text{Notation for the probability of measuring } B \text{ given a certain value of } A\

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them homogeneously on a grid. With the results of the simulation, we built the likelihood function \( L(A|B) \) as follows: for each discrete value \( B \), we recorded its frequency for all \( A \) simulated on the grid. This defines \( L(A|B) \) for each possible discrete value \( B \).

2.2 Application to forensic laboratory samples

The quantization introduced by the pixel grid raises the possibility that some GSR particles in the sample may go undetected. This is critical to the analysis of this forensic technique, as false negative results may thus be reported. To quantify such probability in real cases, we applied our study to GSR samples collected and analyzed in a forensic science laboratory.

![Figure 2: Histograms of data recorded for the analysis of GSR samples collected in a forensic microscopy service unit. a) Histogram of areas \( B \) recorded for characteristic particles with \( p_x = 0.16 \). b) Histogram of the number of characteristic particles, \( N \).](image)

The use of real case samples requires a different strategy from that used in the analysis of experimental data obtained in controlled conditions. Only a few parameters (firearm, ammunition, collection time, etc.) can vary in experimental designs. For comparisons to be made with real case scenarios, however, parameters need to be weighted in a way that resembles the frequency they exhibit in practice. This entails extensive experimental work in several different conditions and the analysis of each condition’s relevance. In contrast, using all the real case samples collected at a forensic laboratory harmonizes data so that inferences can be made which are closely linked to everyday practice. We used a set of 1,174 samples collected from hands and analyzed by Policía de Investigación de Rosario (Criminalistics Unit at Rosario Police Department, Santa Fé, Argentina) between 2017 and 2019; at least one characteristic particle was registered in 320 out of the 1,174
samples with a sum of 2069 particles. Analyses were carried out on a Zeiss Evo LS 15 microscope (SEM) and an X-ray spectrometer (EDS) using INCA software for GSR detection. All samples were analyzed with a resolution \( p_x = 0.16 \mu m^2 \). Of particular interest were the distribution of areas \( B \) of characteristic GSR particles and the number of these particles (\( N \)) registered in each sample (see Fig. 2).

### 2.3 Distribution of areas \( A \)

Calculating the probability of false negatives implies determining how many particles, proportionally speaking, may go undetected. To this end, we built a model that describes real particle area \( A \) distribution on the basis of measured values \( B \) (Fig. 3).

\[
\theta = (\mu, \sigma, \nu)
\]

Figure 3: Model diagram for the distribution of areas \( A \) and their registers \( B \). \( A \) is described as having a log-t Student’ distribution dependent on parameters (\( \mu, \sigma, \nu \)). The distribution \( P(B|A, p_x) \) corresponds to the probability of obtaining a recorded value \( B \), given a real size \( A \) and a pixel size \( p_x \).

The distribution of \( A \) must take positive values and be long tailed, as particles may be found of \( 0.1 \mu m^2 \) to more than \( 1000 \mu m^2 \) with non-negligible frequency. A log-t Student’ distribution \( \ell t(\mu, \sigma, \nu) \) was then used because it meets both criteria and only depends on three parameters, \( \mu, \sigma \) and \( \nu \)

\[
\ell t(A|\mu, \sigma, \nu) = \frac{\Gamma((\nu + 1)/2)}{\Gamma(\nu/2)} \frac{1}{\sqrt{\nu \pi \sigma A}} \left[ 1 + \frac{1}{\nu} \left( \frac{\log(A) - \mu}{\sigma} \right)^2 \right]^{-(\nu+1)/2}.
\]

(2)
Parameters $\mu$ and $\sigma$ describe the location and width of the distribution, respectively. Parameter $\nu$ determines the slope of the distribution; the tails will be longer for small values of $\nu$ and shorter for large values of $\nu$, converging on the limit of $\nu \to \infty$ to a log-normal distribution.

The complete modeling scheme consists of a log-$t$ distribution for areas $A$ and $B$ in the representation of circular particle measurement described in Section 2.1. Data were numerically fitted using Python 3.7, whose code consists of a Markov chain Monte Carlo (MCMC) method programmed in STAN and implemented with the CmdStanPy library\footnote{13} [14].

2.4 Probability of a false negative

Using the full probabilistic model, we inferred what size values may be recorded for different pixel sizes. In particular, we aimed to determine the conditions which may render $B = 0$ for all characteristic particles in a sample, i.e., a false negative situation. We calculate this probability as follows:

$$P('\text{false negative}'|p_x) = \sum_{n=1}^{\infty} P(\{\text{all } B = 0\}|p_x) \ P(n)$$

$$= \sum_{n=1}^{\infty} P(B = 0|p_x)^n \ P(n)$$

(3)

where:

$$P(B = 0|p_x) = \int_{0}^{\infty} P(B = 0|A,p_x) \ P(A) \ dA \ .$$

(4)

Here, $P(n)$ is the distribution of the number of characteristic particles per sample estimated with the frequencies observed, and $P(A)$ is the distribution of areas $A$ integrated over the distribution of the parameters inferred (Fig. 2).
3 Results

3.1 Circular particle acquisition model

Under the hypothesis of circular geometry of particles we studied the statistical predictions between $B$ and $A$ which are depicted in Fig. 4.

![Figure 4: Statistical relationship between the real area $A$ and the area $B$ observed. (Top) behavior of the mean value of records $B$ for different values of $A$ in units of $p_x$. (Bottom) behavior of the quotient of the mean value $B$ over $A$ as a function of $A$.](image)

Displaying $L(A|B)$ for different values of $A$ (Fig. 5) we observe that a region exists for $A \neq 0$ with a probability of $B = 0$, that is, some particles as large as $A = 5p_x$ will not be detected. It should be noted that variable $A$ is continuous, while $B$ only takes integer pixel values.
3.2 Validation of the circular acquisition model

To determine whether circular particle shape and the measurement process model are good representations of the size register, we performed successive measurements with different $p_x$ values on the same sample of GSR particles. We experimentally recorded their areas and obtained a distribution of sizes $B$ which varies with $p_x$ but, in belonging to the same sample, is given by the same distribution of sizes $A$.

The smallest pixel value used was close to the maximum resolution of our equipment ($p_x^{\text{min}} = 0.01\mu m^2$). This measurement best described particle morphology in the sample and was used as an approximation of areas $A$ to infer the size distributions registered for larger pixels. To distinguish sizes registered from those inferred, $B$ will remain the notation for values registered and $\hat{B}$ will be used for values predicted by the model with the data of $p_x = 0.01\mu m^2$ as input.
Figure 6 presents the results of measurements for $p_x = (0.01; 0.04; 0.09) \mu m^2$ and inferences $\hat{B}$ for $p_x = (0.04; 0.09) \mu m^2$. As $p_x$ grows, the distributions fall less steeply and the data show oscillation and even gaps for some values. This may be attributed to the fact that values for particles and pixels are commensurable, as mentioned above.

The description we present here thus simultaneously reproduces these data features and validates the hypotheses of circularity and full-pixel registration as a good quantitative representation bridging real areas $A$ with measured areas $B$.

Figure 6: Measurements and inferences made about the size of GSR particles registered with different $p_x$ values, taking the measurements made with $p_x^{\text{min}} = 0.01 \mu m^2$ as the real area. For higher $p_x$ values, the distributions of values $B$ become wider and present gaps. Inferences in this model simultaneously reproduce both data features. The bin size of each plot is scaled to the pixel size so the relative frequencies are comparable.
3.3 Distribution fitting of A

In Fig. 7 we present the fit of the full probabilistic model described in to the complete set of 2069 characteristic GSR particle sizes recorded $B$. The parameter values obtained were: $\mu = 1.53 \pm 0.03$, $\sigma = 1.17 \pm 0.02$ and $\nu = 76 \pm 22$. The model reproduces the data behavior of interest both for small and large particle sizes, with an explained variance $R^2 = 0.91$. Worth highlighting, the purpose of this modeling process is to provide a simple description of the size distribution with few parameters. Caution should be exercised in extrapolating these results to values outside the source data range $(0.16, 1000)\mu m^2$, although this point is beyond the scope of our work.

![Figure 7: Results of the fit of the model described in Section 3.3 superimposed on the distribution of sizes $B$ recorded for characteristic GSR particles. The fitted parameters describing the log-t distribution ($\mu, \sigma, \nu$) are indicated on the plot. Graphic evidence and parameters’ low standard deviation values strongly validate this description.](image)

3.4 Probability of a false negative

Combining the parameters fitted to the distribution of $A$ with the circular particle model, we calculated the probability of obtaining a false negative result in a typical GSR sample by means of a representative particle size distribution (Eq. 3). Fig. 8 shows the behavior of this probability for different values of $p_x$.

As mentioned above, pixel discretization implies that some GSR particles in the sample will inevitably fail to be detected. For this reason, any measurement of particle quantity should be...
expressed in probabilistic terms, and the approach presented here allows to quantify such probability, for example $P(X \text{ characteristic particles} | p_x = 0.16\mu m^2) = 95\%$. The model predicts that only setups extremely close to $p_x = 0$ can guarantee that absolutely all particles are detected. However, these are unattainable standards in everyday practice, which means that false-negative scenarios are indeed plausible and need to be described in a probabilistic manner.

In this context, the numerical results obtained here show that $P(\text{false negative} | p_x)$ is below 7% for $p_x$ values under 0.4$\mu m^2$ and 1.6% for $p_x = 0.16\mu m^2$, the value used in data registration. These values are extremely low, as other factors (such as sample collection time) may entail particle loss in larger proportions [15].

4 Conclusions

The sizes GSR of particles recorded by automated systems $B$ are a statistical representation of real areas $A$. Furthermore, size measurements of the same particle may vary with its location in the sample and the pixel size $p_x$ used in the scan. The size measured is systematically smaller than the $A$ value for each particle, and may thus not be registered when $A$ is close to $p_x$. For these reasons and given that real particle sizes are not directly accessible, false negative results may always arise.
It is in this way that the definition of $p_x$ regulates the probability of obtaining false negative results in the analysis of GSR samples.

In this work, we used GSR particles from 1,174 hand samples collected by the forensic science laboratory of Policía de Investigación de Rosario between 2017 and 2019. These samples’ realistic variability allowed us to extrapolate our results to recommendations for GSR analysis and thus harness the laboratory’s extensive background. While nothing suggests that these results may differ from those of other laboratories, this comparison exceeds the purpose of this analysis. Nevertheless, the authors are open to collaborative work comparing results with other forensic science units.

We used measurements to construct the distribution of areas $A$ of characteristic particles and then calculated the probability of obtaining a false negative result for different pixel sizes. We found a probability of 1.6% for $p_x = 0.16\mu m^2$, which is a high effectiveness rate compared to other factors affecting the technique such as the loss of particles due to collection time. We also found a probability of false negative results below 5% for $p_x$ values between 0.16 and 0.32$\mu m^2$. These results indicate that pixel sizes as great as the double that is commonly used in usual laboratory casework are effective for an initial scanning of a sample as it yields good rates of detection of characteristic particles, which might exponentially reduce laboratory workload. This preliminary work allows the evaluation of the time saving in different scanning strategies and issue recommendations for measurement protocols that optimize microscope usage in forensic laboratories.
References

[1] ASTM-International. *Practice for Gunshot Residue Analysis by Scanning Electron Microscopy/Energy Dispersive X-Ray Spectrometry*. en. Designation: E1588 17 (2017). doi: 10.1520/E1588-17 (Visited on 10/25/2020).

[2] G.M. Wolten et al. “Particle analysis for the detection of gunshot residue. I: Scanning electron microscopy/energy dispersive X-ray characterisation of hand deposits from firing”. en. In: *Journal of Forensic Sciences* 24.2 (1979).

[3] Arie Zeichner and Nadav Levin. “More on the Uniqueness of Gunshot Residue (GSR) Particles”. en. In: *Journal of Forensic Sciences* 42.6 (Nov. 1997), 14255J. issn: 00221198. doi: 10.1520/JFS14255J url: http://www.astm.org/doiLink.cgi?JFS14255J (visited on 08/10/2021).

[4] J.S. Wallace and J. McQuillan. “Discharge Residues from Cartridge-operated Industrial Tools”. en. In: *Journal of the Forensic Science Society* 24.5 (Sept. 1984), pp. 495–508. issn: 00157368. doi: 10.1080/00157368(84)72329-2 url: https://linkinghub.elsevier.com/retrieve/pii/S0015736884723292 (visited on 08/10/2021).

[5] P.V. Mosher et al. “Gunshot Residue-Similar Particles Produced by Fireworks”. en. In: *Canadian Society of Forensic Science Journal* 31.3 (Jan. 1998), pp. 157–168. issn: 0008-5030, 2332-1660. doi: 10.1080/00085030.1998.10757115 url: http://www.tandfonline.com/doi/abs/10.1080/00085030.1998.10757115 (visited on 08/10/2021).

[6] C. Torre et al. “Brake Linings: A Source of Non-GSR Particles Containing Lead, Barium, and Antimony”. en. In: *Journal of Forensic Sciences* 47.3 (May 2002). issn: 00221198. doi: 10.1520/JFS2001093 url: https://www.astm.org/DIGITAL_LIBRARY/JOURNALS/FORENSIC/PAGES/JFS2001093.htm (visited on 08/10/2021).

[7] L Garofano et al. “Gunshot residue Further studies on particles of environmental and occupational origin”. en. In: *Forensic Science International* (1999), p. 21.
[8] Warren L. Tillman. “Automated Gunshot Residue Particle Search and Characterization”. en. In: *Journal of Forensic Sciences* 32.1 (Jan. 1987), 12327J. ISSN: 00221198. DOI: 10.1520/JFS12327J. URL: http://www.astm.org/doiLink.cgi?JFS12327J (visited on 02/11/2019).

[9] T.G. Kee and C. Beck. “Casework assessment of an automated scanning electron microscope/microanalysis system for the detection of firearms discharge particles”. en. In: *Journal of the Forensic Science Society* 27.5 (Sept. 1987), pp. 321–330. ISSN: 00157368. DOI: 10.1016/S0015-7368(87)72771-6. URL: https://linkinghub.elsevier.com/retrieve/pii/S0015736887727716 (visited on 06/07/2022).

[10] ASTM-International. *Standard Practice for Gunshot Residue Analysis by Scanning Electron Microscopy/Energy Dispersive X-Ray Spectrometry*. en. Designation: E1588 20 (2020). DOI: 10.1520/E1588-20.

[11] C. G. G. Aitken. *Statistics and Evaluation of Evidence for Forensic Scientists*. en. Edinburg, UK: John Wiley & Sons, Ltd, 1995. ISBN: 0471955329.

[12] Franco Taroni et al. *Data Analysis in Forensic Science: A Bayesian Decision Perspective*. en. Chichester, UK: John Wiley & Sons, Ltd, Apr. 2010. ISBN: 978-0-470-66508-4 978-0-470-99835-9. DOI: 10.1002/9780470665084 (Visited on 11/04/2020).

[13] Stan Development Team. *Stan Modeling Language Users Guide and Reference Manual*. English. Version Version 2.29. URL: https://mc-stan.org

[14] Stan Development Team. *CmdStanPy*. English. Version Version 1.01. URL: https://mc-stan.org/cmdstanpy/

[15] Bruno Cardinetti et al. “A proposal for statistical evaluation of the detection of gunshot residues on a suspect”. en. In: *Scanning* 28.3 (Dec. 2006), pp. 142–147. ISSN: 01610457, 19328745. DOI: 10.1002/sca.4950280302. URL: https://onlinelibrary.wiley.com/doi/10.1002/sca.4950280302 (visited on 08/10/2021).