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The role of Poisson's binomial distribution in the analysis of TEM images

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ABSTRACT

Frank's observation that a TEM bright-field image acquired under non-stationary conditions can be modeled by the time integral of the standard TEM image model [J. Frank, Nachweis von objektbewegungen im lichtoptis- chen diffraktogramm von elektronenmikroskopischen auf- nahmen, Optik 30 (2) (1969) 171–180.] is re-derived here using counting statistics based on Poisson's binomial distribution. The approach yields a statistical image model that is suitable for image analysis and simulation.
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1. Introduction

As is argued in the companion paper [1], there is a need for a new generation of high-throughput transmission electron microscopes (TEMs) designed to autonomously extract information from specimens. Such TEMs will operate under the feedback control principle, which consists of a two-step cycle: (i) The parameters of interest (e.g., defocus, specimen position) are measured from acquired images and compared to their desired reference values; (ii) the observed differences (if any) are corrected by commanding relevant actuators (e.g., the objective lens or the specimen holder). The feedback cycle is executed repeatedly at constant rate. In a high-throughput TEM, this cycle has a very short period and must, therefore, be executed when the microscope is not yet stable [1]. As a consequence, both the specimen position and the microscope's optical parameters may vary noticeably during the image acquisition period. The effect of parameter variations during TEM bright-field (TEM-BF) image acquisition has been studied before. For instance, the effect of linear specimen motion was addressed in [2], and the effect of linear defocus variation was analyzed in [1]. In both cases, the analysis was based on Frank's observation that TEM-BF images acquired under these conditions can be represented by the time integral of the standard stationary image model [3] (Frank's observation stemmed from the properties of the photographic emulsions used to record TEM images [4]).

In the present note, Frank's observation is re-derived using counting statistics based on Poisson's binomial (PB) distribution [5]. Our approach is a generalization of that in [6] and, thus, is well suited to model digitally acquired TEM images. This approach leads to a statistical TEM-BF image model whose statistics can be computed exactly or, under certain conditions, approximated by those of a Poisson distribution. Moreover, the model is suitable for both image analysis and simulation.

The rest of the paper is organized as follows. Section 2 summarizes the properties of the PB distribution. The statistical model of TEM-BF images with time varying parameters is derived in Section 3 and, finally, Section 4 presents our conclusions.

2. On Poisson's binomial distribution

It is well known (see, e.g., [7]) that the binomial distribution describes the statistics of the number "successes" in a finite set of independent Bernoulli trials (i.e., success/fail experiments such as a coin toss) that have identical probability distributions. More specifically, let the random variables[1] $\boldsymbol{x}_l \in \{0,1\}$, $l=1,\ldots,N$, represent the outcomes of $N \geq 1$ independent trials (i.e., $\boldsymbol{x}_l = 1$ if the l-th trial is a success and $\boldsymbol{x}_l = 0$ if it is a failure), and let them be identically distributed (i.e., $\mathrm{P}\{\boldsymbol{x}_l = 1\} = p$ for all $l = 1,\ldots,N$). Then, the number of successes in the N trials is given by the random variable $\boldsymbol{S} \triangleq \sum_{l=1}^{N} \boldsymbol{x}_l$, which is Bernoulli distributed. That is, $\boldsymbol{S}$ has an associated probability mass function, $\mathcal{B}(k)$, given by

$$\mathcal{B}(k) = \mathrm{P}\{\boldsymbol{S} = k\} = \binom{N}{k} p^k (1-p)^{N-k}, \quad (1)$$

$k = 0,\ldots,N$. When two or more trials do *not* have the same distribution, the statistics of $\boldsymbol{S}$ are described by the more general

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[1] Random variables are denoted here in italic, bold-faced fonts.

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Poisson's binomial distribution, with associated probability mass function $\mathcal{P}(k)$. To derive a correspondence rule for $\mathcal{P}(k)$ similar to that in (1), let p_l represent the success probability of the l-th trial (i.e., $\mathrm{P}\{\boldsymbol{x}_l=1\}=p_l$, $l=1,\ldots,N$). Next, let $\mathcal{F}_k$ denote the collection of k-elements subsets of $\{1,\ldots,N\}$. That is [5]

$$\mathcal{F}_k=\{A : A\subseteq\{1,\ldots,N\},|A|=k\},$$

where $k=0,\ldots,N$ ($\mathcal{F}_0$ is the empty set) and $|A|$ denotes the number of elements in A. The sets in $\mathcal{F}_k$ identify the different ways (combinations) in which k successes can happen in the N (non-identical) trials. For instance, if $N=5$ and $k=3$, then $A=\{1,2,3\}\in\mathcal{F}_3$ denotes that one possibility to have three successes in five trials is to have a success at trials 1, 2 and 3 and a failure at trials 4 and 5. With these considerations it is easy to show that

$$\mathcal{P}(k)=\mathrm{P}\{\boldsymbol{S}=k\}=\sum_{A\in\mathcal{F}_k}\left(\prod_{l\in A}p_l\right)\left(\prod_{j\in A^c}(1-p_j)\right), \tag{2}$$

$k=0,\ldots,N$, where $A^c\triangleq\{1,\ldots,N\}\backslash A$ is the complement of A with respect to $\{1,\ldots,N\}$. For instance, if $N=5$ then for $k=3$, the summation in (2) has 10 terms (there are $\binom{5}{3}=10$ ways to get three successes in five trials) and

$$\mathcal{P}(3)=p_1p_2p_3(1-p_4)(1-p_5)+\cdots+p_3p_4p_5(1-p_1)(1-p_2).$$

It follows from its definition that the mean and variance of $\boldsymbol{S}$ are given, respectively, by

$$\mathbf{E}\{\boldsymbol{S}\}=\sum_{l=1}^{N}p_l$$

and

$$\mathrm{Var}\{\boldsymbol{S}\}\triangleq\mathbf{E}\{\boldsymbol{S}^2\}-\mathbf{E}\{\boldsymbol{S}\}^2 =\sum_{l=1}^{N}p_l(1-p_l)=N\overline{p}(1-\overline{p})-Ns_p^2, \tag{3}$$

where $\mathbf{E}\{\cdot\}$ denotes expected value, and $\overline{p}=(1/N)\sum_{l=1}^{N}p_l$ and $s_p^2=(1/N)\sum_{l=1}^{N}(p_l-\overline{p})^2$ denote, respectively, the mean and the variance of the set of success probabilities $\{p_1,\ldots,p_N\}$ (see [5]). Note from (3) that $\mathrm{Var}\{\boldsymbol{S}\}$ attains its largest value when all p_l are equal (i.e., when $p_l=p$ for all $l=1,\ldots,N$), in which case $\mathcal{P}$ and $\mathcal{B}$ coincide (i.e., $\mathcal{B}$ is a particular case of $\mathcal{P}$).

PB-distributed random variables, such as $\boldsymbol{S}$, can be simulated either by directly using the probability mass function in (2) or by approximating it by a Poisson distribution. In the former case, the probability masses, $\mathcal{P}(k)$, must first be computed for all $k=0,\ldots,N$. This can be done using either iterative or discrete Fourier transform (DFT) methods (see, respectively, [8,9]). The DFT method can be faster and simpler to use, specially if $N+1$ is a power of 2, in which case the fast Fourier transform algorithm [10] can be used to compute the DFT. This approach requires one to first compute the coefficients ρ_l, $l=0,\ldots,N$, given by

$$\rho_l=\frac{1}{N+1}\prod_{j=1}^{N}\left(p_j\left(\exp\left(\frac{\imath2\pi l}{N+1}\right)-1\right)+1\right)$$

($\imath=\sqrt{-1}$), and then use them to compute the probability masses as follows [9]:

$$\mathcal{P}(k)=\sum_{l=0}^{N}\left(\rho_l\exp\left(\frac{-\imath2\pi kl}{N+1}\right)\right)$$

for all $k=0,\ldots,N$. That is, $[\mathcal{P}(0),\ldots,\mathcal{P}(N)]=DFT([\rho_0,\ldots,\rho_N])$ [10].

On the other hand, when the probabilities p_l, $l=1,\ldots,N$, are small it is simpler to instead simulate $\hat{\boldsymbol{S}}$, a Poisson-distributed random variable with mean $\lambda=\mathbf{E}\{\hat{\boldsymbol{S}}\}=\mathrm{Var}\{\hat{\boldsymbol{S}}\}=\sum_{l=1}^{N}p_l$. The error introduced by this approximation is small, since the "distance" between $\boldsymbol{S}$ and $\hat{\boldsymbol{S}}$, in terms of their cumulative probabilities, is bounded from above. That is, [11,12]

$$\sup_{u\in\mathbb{R}}\left|\mathrm{P}\{\boldsymbol{S}\leq u\}-\mathrm{P}\{\hat{\boldsymbol{S}}\leq u\}\right|\leq 9\max\{p_1,\ldots,p_N\}$$

(sharper bounds are possible, see [13]). Further note that $\mathbf{E}\{\boldsymbol{S}\}=\mathbf{E}\{\hat{\boldsymbol{S}}\}$ and that $\mathrm{Var}\{\hat{\boldsymbol{S}}\}(1-\max\{p_1,\ldots,p_N\})\leq\mathrm{Var}\{\boldsymbol{S}\}\leq\mathrm{Var}\{\hat{\boldsymbol{S}}\}$ $(1-\min\{p_1,\ldots,p_N\})$. Thus, the quality of the approximation depends only on the size of the success probabilities and not on the number of trials (i.e., this is not an asymptotic approximation).

These concepts are applied to model TEM-BF images acquired under time-varying conditions next.

3. Statistical modeling of TEM-BF images with time-varying parameters

Consider the continuous-space TEM-BF image model, $I(r)=|\phi(r)*h(r)|^2$, where $r=(x,y)$ denotes position in the image plane, $\phi(r)$ is the specimen's transmittance function, $*$ denotes convolution over r, and $h(r)$ is the microscope's point spread function [14]. It describes the image projected at the microscope's phosphorous screen, under the assumption of a stationary specimen and constant optical parameters. When the specimen is not stationary (i.e., when it drifts) and/or when the optical parameters change over time, this model can be extended as follows

$$I(r,t)=|\phi(r-d(t))*h(r,t)|^2, \tag{4}$$

where $t\geq0$ denotes time and the function $d(t)\in\mathbb{R}^2$ represents the specimen's drift path. $h(r,t)$ is the time-varying point spread function given by

$$h(r,t)=\mathfrak{F}^{-1}\{A(q)E(q)\exp(\imath\chi(q,t))\}, \tag{5}$$

where $\mathfrak{F}$ denotes the Fourier transform over r, $q=(u,v)$ denotes position in the spatial frequency plane, $A(q)$ is the aperture function, $E(q)$ is the envelope function[2] that describes effects such as temporal incoherence (see [2,14]), and $\chi(q,t)$ is the time-varying aberration function. In [3], Frank stated that under these conditions the model of a *photographically* recorded image, $I_{bf}(r)$, is given by

$$I_{bf}(r)=\int_{t_o}^{t_o+T}I(r,t)\,dt, \tag{6}$$

where t_o is the moment the recording starts and T is the duration of the integration (or recording) period.

The goal here is to re-derive this expression for TEM-BF images recorded using an ideal electron counting detector. The latter is assumed to be a grid of back-to-back, finite-size, electron detection cells that output the number of electrons that hit them during a fixed integration (or counting) period (the consequences of employing more realistic detector models such as those in [15,16] will be considered elsewhere). Thus, the (i,j)-th pixel in an image produced by such a detector is given by the electron count of the (i,j)-th detector cell. Using the same reasoning as in [14, Section 3.7.6], it will be assumed, with small approximation error that the electrons hit the detector one at a time and at regular intervals (this is clearly an idealization that simplifies the analysis and does not alter its conclusions). In mathematical terms, the electrons hit the detector at discrete times $t_l=t_o+(l-1)\Delta t\in[t_o,t_o+T]$, $l=1,\ldots,N_e$, where t_o is the time the first electron hits the detector, Δt is the time between electrons (without loss of

[2] The envelop function $E(q)$ is assumed to be time-independent. This is the case when, for instance, there is no spatial incoherence [14], or when the time-dependent envelopes are dominated by time-independent ones.

generality, it is assumed that $T=N_e\Delta t$), and $N_e=6.241\times10^{18} i_b T$ is the total number of electrons that hit the detector during the integration period (i_b is the beam current). At the end of this period, the electron count of the (i,j)-th detector cell, $\boldsymbol{I}_{bf}(i,j)$, indicates the number of those N_e electrons that hit the (i,j)-th detector cell. Clearly (see Section 2), $\boldsymbol{I}_{bf}(i,j)$ can be interpreted as the number of successes in N_e independent, but not necessarily identically distributed, Bernoulli trials. Each trial consists in observing whether a particular electron hits the (i,j)-th detector cell and is modeled by a random variable, $\boldsymbol{x}_l$, with success (or hit) probability, $\mathrm{P}\{\boldsymbol{x}_l=1\}=p_{ij}(t_l)$, given by

$$p_{ij}(t_l)=\frac{\iint_{R_{ij}} I(r,t_l)\,dr}{\iint_{\mathbb{R}^2} I(r,t_l)\,dr}, \tag{7}$$

where R_{ij} is the area of the continuous-space image that is projected into the (i,j)-th detector cell. Thus, $\boldsymbol{I}_{bf}(i,j)=\sum_{l=1}^{N_e}\boldsymbol{x}_l$, so it follows from Section 2 that the detector cell electron counts are PB-distributed random variables. This allows one to re-derive (6) using an asymptotic approximation approach. To do so, first note that in (7), $I(r,t_l)$ was interpreted, after normalization by $\iint_{\mathbb{R}^2} I(r,t_l)\,dr$, as a probability density function over the image plane [17–19]. Further note that the normalization factor, $\iint_{\mathbb{R}^2} I(r,t_l)\,dr$, is time-independent. To see this, note from (4), (5) and Rayleigh's Theorem [10] that

$$\begin{aligned}\iint_{\mathbb{R}^2} I(r,t_l)\,dr &= \iint_{\mathbb{R}^2} \left|\phi(r-d(t_l))*h(r,t_l)\right|^2 dr\\ &= \iint_{\mathbb{R}^2} \left|e^{-2\pi\imath q\cdot d(t_l)}\Phi(q)A(q)E(q)e^{\imath\chi(q,t_l)}\right|^2 dq\\ &= \iint_{\mathbb{R}^2} \left|\Phi(q)A(q)E(q)\right|^2 dq\\ &\triangleq (\alpha_d)^{-1},\end{aligned}$$

with $\Phi(q)\triangleq\mathfrak{F}\{\phi(r)\}$. Thus in (7)

$$p_{ij}(t_l)=\alpha_d\iint_{R_{ij}} I(r,t_l)\,dr, \quad \forall t_l, l=1,\ldots,N_e. \tag{8}$$

Next, note that

$$\mathbf{E}\left\{\frac{\boldsymbol{I}_{bf}(i,j)}{N_e}\right\}=\frac{\sum_{l=1}^{N_e} p_{ij}(t_l)}{N_e}.$$

Also, since $p(1-p)\le 1/4$ for $p\in[0,1]$, note from (3) that

$$\mathrm{Var}\left\{\frac{\boldsymbol{I}_{bf}(i,j)}{N_e}\right\}=\frac{\sum_{l=1}^{N_e} p_{ij}(t_l)(1-p_{ij}(t_l))}{(N_e)^2}\le\frac{1}{4N_e},$$

so it follows from Chebyshev's inequality [7] that

$$\mathrm{P}\left\{\left|\frac{\boldsymbol{I}_{bf}(i,j)}{N_e}-\mathbf{E}\left\{\frac{\boldsymbol{I}_{bf}(i,j)}{N_e}\right\}\right|\ge\varepsilon\right\}\le\frac{\mathrm{Var}\left\{\frac{\boldsymbol{I}_{bf}(i,j)}{N_e}\right\}}{\varepsilon^2}\le\frac{1}{4\varepsilon^2 N_e}. \tag{9}$$

Thus, the probability that $\boldsymbol{I}_{bf}(i,j)/N_e$ deviates from its mean more than ε is generally small ($N_e\approx10^9$ for a typical integration time of $T=0.1$ s) and decreases for larger N_e (i.e., for larger integration periods or beam currents) as expected. Thus, for large N_e, (9) implies that all the realizations of $\boldsymbol{I}_{bf}(i,j)/N_e$ lie close to its expected value, so (see (8))

$$\begin{aligned}\boldsymbol{I}_{bf}(i,j) &\approx \sum_{l=1}^{N_e} p_{ij}(t_l)=N_e\frac{\sum_{l=1}^{N_e} p_{ij}(t_l)\Delta t}{T}\\ &=\frac{N_e}{T}\int_{t_o}^{t_o+T} p_{ij}(t)dt\\ &=\frac{N_e}{T}\iint_{R_{ij}}\int_{t_o}^{t_o+T}\alpha_d I(r,t)\,dt\,dr,\end{aligned} \tag{10}$$

where the second equality is obtained by noticing that the time integral is well approximated by its Reimann sum when the integrant is continuous and Δt is small, as is the case here. Thus, for larger N_e, this expression shows that a pixel in a TEM-BF image recorded with an ideal electron counting detector can be treated as a deterministic quantity that is proportional to the time integral of a particular region of the continuous-space image model (4). That is,

$$\boldsymbol{I}_{bf}(i,j)\propto\iint_{R_{ij}}\int_{t_o}^{t_o+T} I(r,t)\,dt\,dr$$

($\propto$ denotes proportionality). This expression is the sought-after equivalent of (6) for digitally acquired (ideal) TEM-BF images.

Note that if the optical parameters are constant and the specimen is stationary, $I(r,t)$ becomes independent of t (i.e., $I(r,t)=I(r)$). In such case (10) implies that

$$\boldsymbol{I}_{bf}(i,j)\approx N_e\alpha_d\iint_{R_{ij}} I(r)\,dr, \tag{11}$$

which agrees with the standard interpretation of digitally recorded TEM-BF images as discretized versions of (the projected) continuous-space TEM-BF images. It is important to remark that to make the approximations in (10) and (11) valid for detector cells with low probability of being hit by the electrons, larger N_e values are needed. For instance, suppose that in (9) the expected value of $\boldsymbol{I}_{bf}(i,j)/N_e$ is 0.01. Thus, if one wants to limit the probability of $\boldsymbol{I}_{bf}(i,j)/N_e$ differing from its mean by 10% to be less than 0.001, then $N_e\ge250\times10^6$. This in turn implies that, for a 1024×1024 pixels detector, the average number of electrons hitting a detector cell exceeds 230, which is clearly a high average.

For smaller N_e values (i.e., smaller beam currents or shorter integration times) the approximations in (10) and (11) are less valid, since the realizations of $\boldsymbol{I}_{bf}(i,j)$ display greater statistical variability. In such cases, Frank's deterministic model (6) is no longer appropriate. Instead, each detector cell count, $\boldsymbol{I}_{bf}(i,j)$, should be treated as a PB-distributed random variable. Moreover, to simplify its analysis and simulation, the detector cell count could also be approximated by a Poisson-distributed random variable with *mean* electron count, λ_{ij}, given by the right-hand-side of (10). That is,

$$\lambda_{ij}\triangleq\mathbf{E}\{\boldsymbol{I}_{bf}(i,j)\}=\frac{N_e}{T}\iint_{R_{ij}}\int_{t_o}^{t_o+T}\alpha_d I(r,t)\,dt\,dr$$

and

$$\mathrm{P}\{\boldsymbol{I}_{bf}(i,j)=k\}=\frac{\lambda_{ij}^k e^{-\lambda_{ij}}}{k!}, \quad k=0,\ldots,N_e.$$

This approximation is specially attractive when the hit probabilities are small (see Section 2) and leads to the so-called Poisson "noise" model. The latter, under time-invariant hit probability conditions, has been successfully used for image analysis purposes before [6,18,19].

Finally, note that the counting statistic analysis presented in this section remains valid even if $E(q)$ is allowed to be time-dependent (see footnote 2). In such case, however, α_d would no longer be a time-independent constant, so the right-hand-side of (10) should no longer be interpreted as the discretized version of (6). Instead, images should be interpreted as the discretization of the time integral of $\alpha_d(t)I(r,t)$. That is,

$$\boldsymbol{I}_{bf}(i,j)\propto\iint_{R_{ij}}\int_{t_o}^{t_o+T}\alpha_d(t)I(r,t)\,dt\,dr,$$

with $\alpha_d(t)=\iint_{\mathbb{R}^2} I(r,t)\,dr$.

4. Conclusions

Frank's observation that practical TEM bright-field images can be modeled by the time integral of the standard TEM image model has been re-derived, under mild assumptions using counting statistics, a technique that is well suited to model digitally acquired TEM images. It was shown that the electron counts produced by an ideal camera (i.e., one that behaves as an ideal electron counting detector) can be statistically modeled by random variables with Poisson's binomial distribution, yielding a statistical image model that is amenable to both analysis and simulation.

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