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An Application of Negative Powers of Poisson Numbers in Crystallography

Julian Henn*

Bayreuth, Germany

Abstract

The formerly introduced negative integer powers [Henn (2012). *ActaCryst*. A 68, 703--704] are applied to a crystallographic problem. The formal notation is slightly changed in order to simplify and unify the formal appearance. The purpose of this publication is to generalize the formalism from negative integer powers to negative real-valued powers with the help of a generalized hypergeometric function. The application demonstrates that the formalism works successfully. For all powers, the expectation values approach zero for small values of the Poisson parameter λ, whereas the solutions known from the literature, that all use a truncated and renormalized probability density function, approach one in this case. The truncation of the probability density function from the literature leads to a wrong result in the application.

Keywords

Poisson Distribution, Negative Powers, Hypergeometric Function, Generalized Hypergeometric Function

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1. Introduction

Exact representations and approximations (Chao & Strawderman, 1972; Gupta, 1979; Henn, 2012; Hu *et al.*, 2014; Jones & Zhigljavsky, 2004; Phillips & Zhigljavsky, 2014; Tiku, 1964) of negative moments as well as fractional (positive) moments (Dremin, 1994) of the Poisson distribution have attracted considerable interest through a long period of time. These moments play an important role in different fields like for example mixed Poisson distributions and life testing problems as well as multi-centre clinical trials and neutron- and X-ray diffraction experiments and their applications. Also non-integer moments are relevant; consider for example the crystallographic agreement factor R_1; it can be predicted for a set of observations under the assumption that no background signals occur and that the variance of the individual reflections is caused solely by the Poisson distribution inherent to the beam of arbitrary high stability and is given by $R_1 = \frac{1}{2}\frac{1}{\left\langle I_o^{1/2}\right\rangle}$ (Henn, 2010) with the observed intensity I_o. Recently, all integer positive and negative moments of a Poisson random number were expressed in a consistent and unified way with the help of the hypergeometric function (Henn, 2012). In the present work this is applied to a crystallographic problem. In Henn, 2012, the notation is not as simple as possible. The change of notation into a formally appealing, unified and simple form is presented here, also. With this change of notation, the range of applicability is also extended from integer powers to real-valued powers. This again involves the hypergeometric function. To allow for non-integer powers, however, the hypergeometric function has to be modified such that it also allows for non-integer powers of Pochhammer symbols.

The deeper mathematical implications of the formalism including a substantiation of the derivation of the equations are passed to future work. Instead, the focus is here on a crystallographic problem that remains unsolved, when negative powers show the accepted, but in this context wrong

* Corresponding author
E-mail address: Julian.Henn@uni-bayreuth.de

asymptotic behaviour of approaching one for λ approaching zero.

2. Formalism

The hypergeometric function ${}_pF_q$ of degree *p* in the upper index *a* and of degree *q* in the lower index *b* is given by

$${}_pF_{q\,b_1,\ldots,b_q}^{\;a_1,\ldots,a_p}(\lambda)=\sum_{k=0}^{\infty}\frac{(a_1)_k(a_2)_k\ldots(a_p)_k}{(b_1)_k(b_2)_k\ldots(b_q)_k}\frac{\lambda^k}{k!} \quad (1)$$

with the Pochhammer symbols (rising factorials)

$$(a)_k=\frac{\Gamma(a+k)}{\Gamma(a)}. \quad (2)$$

To allow for powers $s_1,\ldots,s_p$ and $t_1,\ldots,t_q$ of the Pochhammer symbols it is defined:

$${}_pF_{q\,b_1,\ldots,b_q;t_1,\ldots,t_q}^{\;a_1,\ldots,a_p;s_1,\ldots,s_p}(\lambda)=\sum_{k=0}^{\infty}\frac{((a_1)_k)^{s_1}((a_2)_k)^{s_2}\ldots((a_p)_k)^{s_p}}{((b_1)_k)^{t_1}((b_2)_k)^{t_2}\ldots((b_q)_k)^{t_q}}\frac{\lambda^k}{k!}, \quad (3)$$

where the powers of the individual Pochhammer symbols are denoted after the upper and lower indices after a separation with a semicolon on the left hand side of eq. (3). To the best of the author's knowledge, this function is not known in the literature. With this notation, and with the usual normalization condition,

$$\sum_{x=0}^{\infty}p(x)=1, \quad (4)$$

$$p(X=x)=e^{-\lambda}\frac{\lambda^x}{x!}, \quad (5)$$

the expectation value $\langle X^m\rangle$ of any positive and negative real power $m\in\Re^*$ (this denotes $\{m|m\in\Re,m\neq 0\}$) of a Poisson random variable X that can assume values $x\in\{0,1,2,3,\ldots\}$ can be written in the simple form:

$$\langle X^m\rangle:=\lambda e^{-\lambda}\,{}_1F_{11;m-1}^{2;m-1}(\lambda), \quad (6)$$

where the discontinuity in the range of definition is closed by the normalization condition

$$\langle X^m\rangle\big|_{m=0}=1. \quad (7)$$

This ensures the validity of $\langle X^1\rangle=\lambda$ in (6), as for *m* = 1 the modified hypergeometric function reduces to the exponential function ${}_1F_{11;0}^{2;0}(\lambda)=e^{\lambda}$ (Henn, 2012).

The modified hypergeometric function is obviously even more general than the already very powerful ordinary hypergeometric function. From this new freedom, however, only little use is made as the upper (a_1= 2) and lower (b_1= 1) indices as well as $s_1\equiv t_1:=m-1$ are already specified in the present context. It may be expected that the investigation of this function will lead to many more connections and applications, but this is not the topic of the present work. The definition (3) allows for smooth changes in the parameter *m*. As a consequence, the expectation values of all real positive and negative powers can be written in the unified and simple way as indicated in equation (6).

The right hand side of (6) exists for all $m\in\Re^*$ and $\lambda>0$ and converges to a well defined value as each of the factors is well defined and finite.

2.1. Consistency with Known Results

The definition (6) reproduces the well-known expectation values of positive integer powers $\langle X\rangle=\lambda$, $\langle X^2\rangle=\lambda^2+\lambda$, $\langle X^3\rangle=\lambda^3+3\lambda^2+\lambda$, etc.. It additionally allows for the calculation of negative powers with Poissonian probability of the single events. This is important, because the probability of the event of detecting zero, one, two,... particles in a given period of time is solely determined by the process the particles originate from and must not be altered when expectation values of negative powers are calculated.

The definition (6) is also in accordance with a well-known differential equation from the literature (see *e.g.* Haight, 1967):

$$\langle X^{m+1}\rangle=\lambda\left(1+\frac{d}{dx}\right)\langle X^m\rangle, \quad (8)$$

(see supplementary material).

2.2. Properties

By simple algebraic manipulations it is seen that (6) may be rewritten in the form

$$\langle X^m\rangle=\sum_{x=1}^{\infty}x^m p(x), m\in\Re^* \quad (9)$$

with $p(x)$ given by (5) (see supplementary material). This is the way in which (6) was constructed. Eq.(9) is the usual definition of the expectation values but with a shifted lower index. This result is in contrast to the standard textbook definition, where the *probabilities* are changed *via* exclusion of the value zero and renormalization. In the present approach the probabilities are unaltered. This shift in the lower summation index from zero to one does numerically not affect the expectation values for positive real valued powers, whereas it allows for the meaningful definition of negative powers from events described by Poisson statistics.

Positive and negative powers are here treated exactly in the same way, in contrast to the literature, where negative powers are treated with a renormalized probability density function (Chao, 1972, Gupta, 1979; Jones, 2004; Tiku, 1964).

As a consequence, the expectation values of all (and not only positive) powers $m \in \Re^*$ approach zero for small values of λ; $\lim_{\substack{\lambda \to 0 \\ \lambda > 0}} \langle X^m \rangle = 0$ and all of them (and not only the positive ones) start linearly in λ: $\lim_{\substack{\lambda << 1 \\ \lambda > 0}} \langle X^m \rangle = \lambda$ This is again in contrast to expectation values of negative powers that work with a truncated and renormalized probability density function with renormalization factor $(1-e^{-\lambda})^{-1}$. In those cases, the limiting value for λ approaching zero is one. At a sufficiently large value of λ, however, both expectation values are numerically indistinguishable as the renormalization factor approaches unity (see Fig. 1).

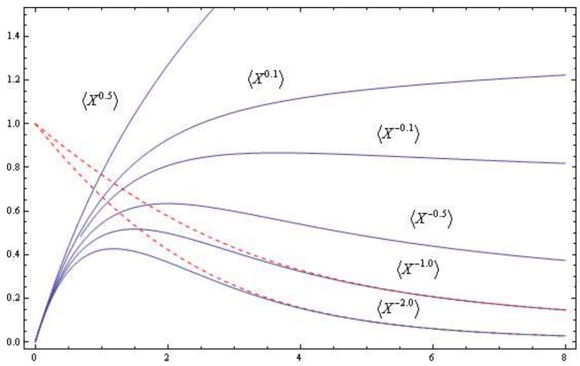

Fig. 1. Expectation values (ordinate) for different powers *m* as a function of λ (abscissa). The red dashed lines correspond to the first two negative moments of the truncated Poisson distribution from the literature (see *e.g.* Chao, 1972).

In the present approach each negative power, when considered as a function of the parameter λ, has a maximum value, because zero is approached for both λ going to zero and to infinity. The maximum values of the first ten negative integer powers are given in Table 1. The expectation values for some powers are plotted in Fig. 1 as a function of λ in a range starting from close to 0 and 8.

Table 1. Maximum values of the first ten negative integer powers and corresponding value of λ, at which the maximum occurs.

m	max $\langle X^{-m} \rangle$	λ
1	0.51735	1.5029
2	0.42724	1.1831
3	0.39450	1.0787
4	0.38043	1.0362
5	0.37395	1.0172
6	0.37085	1.0083
7	0.36935	1.0041
8	0.36861	1.0020
9	0.36824	1.0010
10	0.36806	1.0005
∞	1/e	1

3. Applications

In Schwarzenbach *et al.* (1989) a formula is given, which is also discussed in Blessing (1997) for the calculation of an external variance from *n* multiply observed or equivalent intensities, denoted with y_i, $i = 1,\ldots, n$, with suitable chosen weights *w*. The case is discussed in which the weights are chosen to be the inverse squared experimental error estimates, $w = 1/\sigma^2(y_i)$:

$$\sigma^2_{ext} = \frac{n}{\sum_{i=1}^{n} \frac{1}{\sigma^2(y_i)}} \tag{10}$$

This choice tacitly excludes the case $\sigma^2(y_i) = 0$ which appears in the case of one or many zero intensity observations $y_j = 0$. This case of pure Poisson signals is going to be discussed here. The Poisson process allows for the intensity observations y_i being positive integer numbers or zero. The experimental error estimate is equal to the observed intensity: $\sigma^2(y_i) = y_i$ including the value zero for zero intensity observations. The calculation of the external variance is in this case defined to be the inverse expectation value of the inverse intensity:

$$\sigma^2_{ext} = \frac{1}{\left\langle \frac{1}{y_i} \right\rangle} \tag{11}$$

Fig. 2 shows a plot of (11) in the limit of infinite large data sets for a range $0.01 \le \lambda \le 8$. It is larger than λ for λ< 2, equal to λ at λ = 2, and smaller than λ for λ > 2 with an asymptotic difference of one.

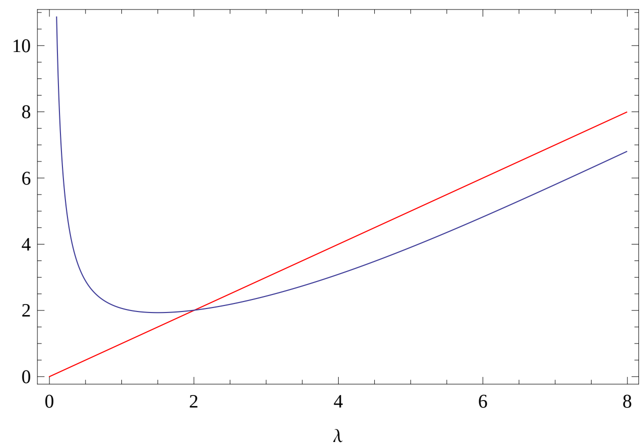

Fig. 2. Expectation values (ordinate) according to eq. (11) as a function of λ (abscissa). For a comparison the Poisson variance λ is also given (red line).

In the case of only zero variance observations the resulting external variance approaches infinity. This just expresses the fact that for λ approaching zero $\left\langle \frac{1}{y_i} \right\rangle$ approaches also zero (see Fig. 1).

Please note that the calculation of the expectation value eq. (11) with a renormalized Poisson distribution that is confined to positive values $x > 0$ leads to wrong results, as the particles of the beam follow a Poisson distribution and not a truncated Poisson distribution.

4. Conclusion

The expectation values for all positive and negative real powers $m \in \Re^*$ of a Poisson distribution with parameter λ can be written in the unified and simple way as indicated in (6).The solutions obtained with (6) are for an infinite large set of Poisson random numbers identical to the definition (9) with (5). The probability density function (5), is not altered, however, in the summation (9) the value $x = 0$ is omitted, which makes no difference for positive powers and allows for the meaningful definition of negative powers. The expectation values for negative powers known from literature show a discontinuity in the definition of the probability density function which is different for positive and negative powers. This reflects in the differing limiting behaviour of these expectation values for λ approaching zero. This limit jumps from zero for positive powers to one for the power zero, where it remains also for negative powers. In the present work, however, the probability density function is the same, full Poisson probability density function for positive and negative powers. Expectation values of all powers approach zero for λ approaching zero. The discontinuity is now in the range of validity of $m \in \Re^*$, where the power zero has to be excluded. This discontinuity in the range of definition is closed by the normalization condition (4).

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