A new discrete calculus of variations and its applications in statistical physics

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For a discrete function \( f(x) \) on a discrete set, the finite difference can be either forward and backward. However, we observe that if \( f(x) \) is a sum of two functions \( f(x) = f_1(x) + f_2(x) \) defined on the discrete set, the first order difference of \( \Delta f(x) \) is equivocal for we may have \( \Delta^f f_1(x) + \Delta^b f_2(x) \) where \( \Delta^f \) and \( \Delta^b \) denotes the forward and backward difference respectively. Thus, the first order variation equation for this function \( f(x) \) gives many solutions which include both true and false one. A proper formalism of the discrete calculus of variations is proposed to single out the true one in its own right. Thus the first order variation equation leads to many solutions which can not be all true. By the true solution, we mean that it can be forward, backward, central, and even more complicated combinations of these differences, so that the first order variation equation leads to many solutions which can not be all true. The advantage and peculiarity of our formalism are explicitly illustrated by the derivation of the Bose distribution.

Keywords: statistical distribution, discrete calculus of variations, most probable distribution

Introduction The method of most probable distribution (MPD) is the most common way used to derive various statistical distributions in mathematics, physics, chemistry, materials science and computational science, etc. The original data are usually discrete rather than continuous, so we must be able to deal with the differences, difference quotients and sums of discrete functions, instead of the differentials, derivatives and integrations of the continuous functions. However, we immediately run into a problem: For a discrete function that has extremals, the difference can be forward, backward, central, and even more complicated combinations of these differences, so that the first order variation equation leads to many solutions which can not be all true. The true solution, we mean that it is realistic or physical. There has been no satisfactory procedure to single out the true one in its own right. Thus the derivation of the exact form of the distribution functions for Boltzmann, Bose and Fermi system obtained from the MPD has been an open problem for nearly one century. In present work, I report a discrete calculus of variations to solve this problem.

A new discrete calculus of variations Let us first define an individual function (IF) \( f(x) \) of variable \( x \) on an interval \( C \), which amounts to that the exponential of the function \( f(x) \) as \( \exp f(x) \) can not be further factorized. We can therefore define the sum of two IFs \( f(x) = f_1(x) + f_2(x) \), and the sum of many IFs. Secondly we define the unidirectional differences of the IF \( f(x) \), which means that when taking the finite differences of different orders for the function \( f(x) \), we take forward or backward differences in all first, second, and higher order variation. For instance, the forward directional differences of the IF \( f(x) \) are \( (\Delta^f f(x) = f(x+h) - f(x), (h > 0) \), \( (\Delta^f)^2 f(x) = f(x+2h) - f(x+h) - (f(x+h) - f(x)) = f(x+2h) - 2f(x+h) + f(x), \) and so forth; and the backward unidirectional differences of the IF \( f(x) \) are \( (\Delta^b f(x) = f(x) - f(x-k), (k > 0) \), \( (\Delta^b)^2 f(x) = f(x) - f(x-k) - (f(x-k) - f(x-2k)) = f(x) - 2f(x-k) + f(x-2k), \) and so forth. Thus, the forward directional difference quotients are \( (\Delta^f f(x)) / h, (\Delta^f)^2 f(x) / (h^2), \ldots \); and similarly, the backward directional difference quotients are \( (\Delta^b f(x)) / k, (\Delta^b)^2 f(x) / (k^2), \ldots \). Specially for \( h = 1 \), we have \( (\Delta^f)^i f(x) / h = (\Delta^f)^i f(x) \), \( (i = 1, 2, 3, \ldots) \); and similarly for \( k = 1 \), we have \( (\Delta^b)^i f(x) / k = (\Delta^b)^i f(x) \). The unidirectional differences are similar to the treatment of the parameter \( \lambda \) \( \in \mathbb{R} \) in the usual calculus of variation in which for the given variational parameter \( \lambda \), we must keep using this parameter \( \lambda \) in all orders of variations. However, the different point of the new procedure is that, once \( f(x) = f_1(x) + f_2(x) \), \( \Delta f \) does mean four combinations: \( (\Delta^f) f_1(x) + (\Delta^f) f_2(x), \) \( (\Delta^f) f_1(x) + (\Delta^b) f_2(x), \) \( (\Delta^b) f_1(x) + (\Delta^f) f_2(x), \) and \( (\Delta^b) f_1(x) + (\Delta^b) f_2(x), \) which can be simply named by 1f2f, 1f2b, 1b2f and 1b2b, respectively. Moreover, the second order variations are must be taken unidirectionally, so \( \Delta^2 f \) for the combination 1f2f, 1f2b, 1b2f and 1b2b gives, \( (\Delta^2) f_1(x) + (\Delta^2) f_2(x), \) \( (\Delta^2) f_1(x) + (\Delta^2) f_2(x), \) \( (\Delta^2) f_1(x) + (\Delta^2) f_2(x), \) \( (\Delta^2) f_1(x) + (\Delta^2) f_2(x), \) respectively.

The problem is formulated in the following. We at first deal with a discrete IF \( \Psi(n) \) defined, for convenience, on the interval of semi-positive integers \( n \in \mathbb{Z}^+ \), which has the local maxima and minima, subject to some equality constraints \( \psi = (\psi_1, \psi_2, \psi_3, \ldots) = 0 \). For finding the local maxima and minima of the function \( \Psi(n) \), we construct a
functional $\Phi$,

$$\Phi = \Psi \{ n \} + \alpha \cdot \psi,$$

where $\alpha = (\alpha_1, \alpha_2, \alpha_3, \ldots)$ are Lagrange multipliers each of which $\alpha_i$ accompanies a constraint condition $\psi_i = 0$. The local maxima and minima satisfy,

$$\delta \Phi = 0.$$  \hspace{1cm} (2)

Since the discreteness of the function $\Psi (n)$, the smallest finite change of $n$ is $\Delta n = 1$, and we have accordingly two differences (or difference quotients) of the function $\Psi \{ n \}$ in the following: \(\delta^i \Psi \{ n \}/\delta n = \Psi \{ n + 1 \} - \Psi \{ n \}\) and \(\delta^i \Psi \{ n \}/\delta n = \Psi \{ n - 1 \} - \Psi \{ n \}\) for the forward difference and \(\delta^b \Psi \{ n \}/\delta n = \Psi \{ n \} - \Psi \{ n - 1 \}\) for the backward difference. In consequence, each of two relations $n^\mu = n^\mu (\alpha)$ ($\mu = 1, 2$) solves the equation \(\delta \Phi = 0\), constituting the solution pool which contains both spurious and true one. Then how to single out the true one?

Assuming that all relations $n^\mu = n^\mu (\alpha)$ in the solution pool have different values of the second order differences in the sense of the \textit{unidirectional differences} of $\Psi \{ n \}$, and further assuming that $n^1 = n^1 (\alpha)$ is obtained from the forward difference variation as \(\delta^i \Psi \{ n \} + \alpha \cdot \delta^i \psi \{ n \} = 0\), the another solution $n^2 = n^2 (\alpha)$ must then be obtained from the backward difference variation as \(\delta^b \Psi \{ n \} + \alpha \cdot \delta^b \psi \{ n \} = 0\). To discriminate the difference between $n^1 (\alpha)$ or $n^2 (\alpha)$, we examine \(\delta^i \Psi \{ n \}^2 \{ n \}\) and \(\delta^b \Psi \{ n \}^2 \{ n \}\). Thus, it is reasonable to conjecture that if \(\delta^i \Psi \{ n \}^2 \{ n \}\) or \(\delta^b \Psi \{ n \}^2 \{ n \}\) are noninteracting, indistinguishable particles confined to a space of volume $V$ and sharing a given energy $E$. Let $\varepsilon_1$ denote the energy of $i$-th level and $\varepsilon_1 < \varepsilon_2 < \varepsilon_3 < \ldots$, and $q_i$ denote the degeneracy of the level. In a particular situation, we may have $n_1$ particles in the first level $\varepsilon_1$, $n_2$ particles

\textit{Five immediate comments follow. 1. The new procedure is essentially a method of MPD, and importantly during all derivation steps, no one requires that the variable $n$ be very large. 2. In the new procedure, the correct solution differ; and the former refers to its solving the first order equation \(\delta \Phi = 0\) and the latter refers to its maximizing the second order variations. 3. Once there are degenerate solutions which have no difference up to second differences, higher order differences must be invoked. 4. The new procedure can be easily generalized for the \textit{discrete function} $\Psi (n)$ that is the sum of more IFs. 5. If the constraint function $\psi$ is nonlinear in $n$, which is beyond the scope of current studies, the problem must be treated on the case-by-case base.}

\textit{We will simply call the new procedure of the discrete calculus of variations the \textit{IF method}. In the following, I will illustrate the IF method with a detailed derivation of the exact form of the Bose distribution, and slightly discuss the Boltzmann and Fermi distribution.}

\textit{IF method for the Bose system} Considering a system of $N$ noninteracting, indistinguishable particles confined to a space of volume $V$ and sharing a given energy $E$. Let $\varepsilon_i$ denote the energy of $i$-th level and $\varepsilon_1 < \varepsilon_2 < \varepsilon_3 < \ldots$, and $q_i$ denote the degeneracy of the level. In a particular situation, we may have $n_1$ particles in the first level $\varepsilon_1$, $n_2$ particles
in the second level $\varepsilon_2$, and so on, defining a distribution set $\{n_i\}$. The number of the distinct microstates in set $\{n_i\}$ is then given by,

$$\Omega \{n_i\} = \prod_i \frac{(n_i + g_i - 1)!}{n_i!(g_i - 1)!}. \quad (5)$$

The Bose functional $f$ is,

$$f = \sum_i (\ln(n_i + g_i - 1)! - \ln n_i! - \ln(g_i - 1)! - \alpha \left( \sum_i n_i - N \right) - \beta \left( \sum_i n_i\varepsilon_i - E \right). \quad (6)$$

The variational $\delta f$ is,

$$\delta f = \sum_i \left\{ \delta \ln(n_i + g_i - 1)! - \delta \ln n_i! \right\} - \delta n_i (\alpha + \beta\varepsilon_i)$$

$$= \sum_i \delta n_i \left\{ \frac{\delta \ln(n_i + g_i - 1)!}{\delta n_i} - \frac{\delta \ln n_i!}{\delta n_i} - (\alpha + \beta\varepsilon_i) \right\}. \quad (7)$$

Since the independence of variables $n_i$, $\delta f = 0$ leads to,

$$\frac{\delta \ln(n_i + g_i - 1)!}{\delta n_i} - \frac{\delta \ln n_i!}{\delta n_i} - (\alpha + \beta\varepsilon_i) = 0. \quad (8)$$

Thus, there are essentially two IFs $\Psi_1 = \ln(n_i + g_i - 1)!$ and $\Psi_2 = \ln n_i!$. For $\ln(n_i + g_i - 1)!$ and $\ln n_i!$, the smallest forward and backward differences are given in Table I. Four combinations constructing $\delta \ln(n_i + g_i - 1)!/\delta n_i - \delta \ln n_i!/\delta n_i$ are summarized in Table II. Accordingly, we have four solutions presented in Table III, and all satisfy $\delta f = 0$. These distributions are mutually different when $n_i \sim 1$, though all of them converge to the same one when $n_i \gg 1$,

$$n_i \approx \frac{g_i}{e^{\alpha + \beta\varepsilon_i} - 1}. \quad (9)$$

The second order variations of $\delta^2 \ln \Omega \{n_i\}$ for the four solutions are explicitly shown in the Table IV. In order

**TABLE I:** The smallest forward/backward difference of $\Psi_1 = \ln(n_i + g_i - 1)!$ and $\Psi_2 = \ln n_i!$.

|        | $\Psi_1 = \ln(n_i + g_i - 1)!$ | $\Psi_2 = \ln n_i!$ |
|--------|-------------------------------|----------------------|
| forward | $\ln(n_i + g_i)$              | $\ln(n_i + 1)$       |
| backward| $\ln(n_i + g_i - 1)$          | $\ln(n_i)$           |

**TABLE II:** The column and row give the forward/backward differences for $\Psi_1 = \ln(n_i + g_i - 1)!$ and $\Psi_2 = \ln n_i!$, respectively, and we list the results of four combinations $\Delta \ln(n_i + g_i - 1)! - \Delta \ln n_i!$.

|        | $\Psi_2$ forward | $\Psi_2$ backward |
|--------|------------------|-------------------|
| $\Psi_1$ forward | $\ln(n_i + g_i) - \ln(n_i + 1)$ for 1f2f | $\ln(n_i + g_i) - \ln n_i$ for 1f2b |
| $\Psi_1$ backward | $\ln(n_i + g_i - 1) - \ln(n_i + 1)$ for 1b2f | $\ln(n_i + g_i - 1) - \ln n_i$ for 1b2b |

**TABLE III:** Four solutions

|        | $\Psi_2$ forward | $\Psi_2$ backward |
|--------|------------------|-------------------|
| $\Psi_1$ forward | $\ln(n_i + g_i)$ for 1f2f | $\ln(n_i + g_i)$ for 1f2b |
| $\Psi_1$ backward | $\ln(n_i + g_i - 1)$ for 1b2f | $\ln(n_i + g_i - 1)$ for 1b2b |
TABLE IV: The column and row give the forward/backward finite differences for $\ln(n_i + g_i - 1)!$ and $\ln n_i!$, respectively, and then forming $\Delta^2 \ln(n_i + g_i - 1)! - \Delta^2 \ln n_i!$ accordingly.

| $\Psi_1$ forward | $\Psi_2$ forward | $\Psi_1$ backward | $\Psi_2$ backward |
|------------------|------------------|------------------|------------------|
| $\ln\left(\frac{n_i + g_i}{n_i - 1}\right)$ for 1f2f | $\ln\left(\frac{n_i + g_i}{n_i - 1}\right)$ for 1f2b | $\ln\left(\frac{n_i + g_i}{n_i - 1}\right)$ for 1b2f | $\ln\left(\frac{n_i + g_i}{n_i - 1}\right)$ for 1b2b |

To eliminate the spurious solutions, we examine which one is the largest in magnitude. It is easily to verify that one combination 1f2b is the only right one for we have,

$$\frac{n_i}{n_i - 1} \frac{n_i + g_i}{n_i + g_i + 1} - \frac{n_i}{n_i - 1} \frac{n_i + g_i - 2}{n_i + g_i - 1} = \frac{n_i}{n_i - 1} \left(\frac{2}{n_i + g_i - 1}\right) > 0, \quad (n_i > 1)$$

(10a)

$$\frac{n_i}{n_i - 1} \frac{n_i + g_i}{n_i + g_i + 1} - \frac{n_i}{n_i - 1} \frac{n_i + 2}{n_i + 1} \frac{n_i + g_i}{n_i + g_i + 1} = \frac{n_i}{n_i - 1} \left(\frac{n_i + g_i - 1}{n_i + g_i + 1}\right) > 0, \quad (n_i > 1)$$

(10b)

$$\frac{n_i}{n_i - 1} \frac{n_i + g_i}{n_i + g_i + 1} - \frac{n_i}{n_i - 1} \frac{n_i + 2 g_i n_i - 2 - g_i + g_i^2}{(n_i + g_i)^2 - 1} > 0, \quad (n_i > 1).$$

(10c)

To note that once $n_i = 0$, and $n_i = 1$, we need to directly invoke the expression for 1f2b in Table IV and the $|\ln(n_i/(n_i - 1)| \to \infty$, and in final we obtain the Bose distribution,

$$n_i = \frac{g_i}{e^\alpha + \beta g_i - 1}.$$  

(11)

Two remarks follow. 1. We can follow the similar manner to present detailed derivations for Boltzmann and Fermi distribution. For the Boltzmann distribution, there is essentially one IF and the true solution comes from backward difference; and for the Fermi distribution there are essentially two IFs and the true solution comes from the combination 1b2b. 2. Our procedure puts no requirement on the total number of particle $N$ that be very large. Within the grand ensemble theory, we can easily show the Bose distribution to be given by with $g_i = 1$,

$$n_i = \frac{1}{e^\alpha + \beta g_i - 1} + \frac{1 + N}{e^{(\alpha + \beta g_i)(1+N)} - 1}.$$  

(12)

It differs from ours (11) by an additional term depending on $N$.

Conclusions and discussions In contrast to the continuous calculus of variations, the discrete one possesses some peculiarities. The function in it can not be treated in the uniformly forward or backward difference, but must exhaust all mathematical possibilities. All possible solutions determined by the first order variation equation include both true and false one. Each of the solutions has its own second order variation and the true solution takes the largest value in magnitude. The application of the procedure to the statistical distributions is successful, giving results identical to those obtained from the grand ensemble theory. However, the ensemble theory is valid only when the total number of particle in the system is large. Our approach does not suffer from such a limitation.

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