A simple maximization technique for statistical mechanics expressions

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A frequent task in a statistical mechanics course is maximization (or minimization) of a product (or quotient) of factorials and exponentials. For the sake of illustration, we shall use the example

\[ P_n = \binom{N}{n} \left( \frac{2N}{N+n} \right) e^{-\epsilon n}, \]

where the brackets denote binomial coefficients, \( \epsilon \) and \( N \) are constants, and \( 0 \leq n < N \).

The standard maximization procedure, used by the textbooks known to us, gets rid of the factorials by means of Stirling's approximation and then equates the first derivative to zero. (See Refs. 1–5 as a representative sampling of the books that deal with this task.) For an undergraduate, this procedure is obscure, cumbersome, and tedious. Even for simpler cases than example (1), the very copying of every intermediate expression from the blackboard may require of the order of a minute. (Similar concerns were expressed by Burns and Brown.)

The technique we propose here exploits the fact that, while it is hard to express the factorial function in an analytically manageable fashion, its recursion relation is very simple. (This same feature is exploited, in a somewhat similar context, by Bent. \(^4\)) Thus, for the case of example (1), the ratio \( P_n/P_{n-1} \) is just

\[ G(n) = \frac{P_n}{P_{n-1}} = \frac{(N-n+1)^2 e^{-\epsilon}}{n(N+n)}, \]

where \( G \) is used as shorthand. In the usual case, \( N \) is huge and, close to the maximum (to be found \( a \ posteriori \)), \( n \) and \( N - n \) are huge too (extensive quantities). Therefore, we can drop the 1 in the numerator. Note that if the factorials enter the expression for \( P_n \) within binomial coefficients, then \( G(n) \) contains the same number of extensive factors \( (n, N+n, N-n, \text{etc.}) \) in the numerator and in the denominator. Therefore, when quantities of the order of unity are neglected relative to \( N \) or \( n \), we can divide every extensive factor by \( N \) and obtain in general that \( G \) is a function of the ratio \( n/N \) rather than a function of \( n \) and \( N \) separately. \( \epsilon \) is usually positive and not necessarily large.

The criterion for maximization we propose is as follows. Let there be a maximum at \( n = n^* \) and let us study the be-
havior of \( G \) as \( n \) increases, bearing in mind that \( P_n \) is positive in its entire range of definition. While \( n \) is approaching \( \bar{n} \), \( P_n \) increases and therefore \( G > 1 \); while \( n \) is departing from \( \bar{n} \), \( P_n \) decreases and \( G < 1 \). At the maximum,

\[
G(\bar{n}) = 1. \tag{3}
\]

As in the standard procedure, it should be understood that, strictly speaking, the actual value of \( \bar{n} \) is not the real number that solves (3), but rather one of its neighboring integers; however, differences in \( n \) of the order of 1 are irrelevant in the “thermodynamic limit” \( N \gg 1 \). The connection of the present method with the conventional approach can be seen by noting that Eq. (3) is equivalent to the vanishing of the first derivative in the expansion \( P_{n-1} \approx P_n - dP/\bar{n} \). (We thank the referee for this observation.) Clearly, Eq. (3) provides a criterion for minima, too.

Note that (3) is a polynomial rather than a transcendental equation of the sort encountered in the standard procedure. For the case of example (1), after dropping the 1 in expression (2), it has the solutions

\[
\bar{n} = \frac{1 - 2e^{-\epsilon} + \sqrt{1 + 8e^{-2\epsilon}}}{2(1 - e^{-2\epsilon})}. \tag{4}
\]

Note that only solutions giving \( \bar{n} \) in the range \([0,N]\) and also satisfying \( (N - \bar{n}) \gg 1 \) should be considered. Unless \( |\epsilon| \gg 1 \), the result (4) confirms the ansatz that \( \bar{n} \) and \( N - \bar{n} \) are of the order of magnitude of \( N \).

Once \( \bar{n} \) is known, the next task is usually to determine whether it corresponds to a maximum or a minimum, and the width of the distribution \( P_\bar{n} \). In more general terms, what we want to do is to characterize the distribution \( P_\bar{n} \) by telling how much smaller \( P_{\bar{n}+\Delta n} \) is than \( P_\bar{n} \) (i.e., we want to evaluate the ratio \( P_{\bar{n}+\Delta n}/P_\bar{n} \) for any given distance \( \Delta n \) from the maximum. The interesting values of \( \Delta n \) are those for which \( P_{\bar{n}+\Delta n} \) is both appreciably different from \( P_\bar{n} \) and from zero. We shall see \textit{a posteriori} that this is the case for \( \Delta n = 0[ N^{1/2}] \).

Let us first expand the logarithm of \( G(n) \) with respect to \( n \) for \( n \approx \bar{n} \):

\[
\log G(n + l) = \frac{d}{dn} \log G|_{n} + 0[l^2] = al + 0[l^2], \tag{6}
\]

where \( a \) is used as shorthand. If we assume that \( G \) depends only on the ratio \( n/N \), then \( d^2 \log G/\bar{n}^2 \) contains a factor \( N^{-2} \) and the correction term will, in fact, be of the order of \( l^2/N^2 \). Since \( \bar{n} \) and the expression for \( G \) are known, \( a \) is known too. If \( a > 0 \), then \( \bar{n} \) is a minimum; if \( a < 0 \), then \( \bar{n} \) is a maximum. In the case of example (1)

\[
a = -\left( \frac{2}{N - \bar{n}} + \frac{1}{\bar{n}} + \frac{1}{N + \bar{n}} \right). \tag{7}
\]

When considering a situation in which (5) is obeyed, the correction term in (6) is of order \( N^{-1} \) for any \( l \) in the range \([-|\Delta n|,|\Delta n|]\). This permits to neglect that correction and express \( P_{\bar{n}+\Delta n}/P_\bar{n} \) as

\[
\frac{P_{n+\Delta n}}{P_n} = \prod_{i=1}^{\Delta n} G(n + i) \approx \exp \left( a \Delta n \sum_{i=1}^{\Delta n} l \right) \approx \exp \left( a(\Delta n)^2 \right). \tag{8}
\]

(In the last step we have used \( \Delta n \gg 1 \).) This is the familiar expression which is usually obtained by the standard procedure. We see from here that in order to have \( P_{\bar{n}+\Delta n} \) both appreciably different from \( P_n \) and from zero, \( \Delta n \) has to be of the order \( |a|^{-1/2} \). For \( a \) of the order of \( 1/N \), this implies Eq. (5).

As a final remark, we point out that the present method is by no means restricted to a single variable. If instead of \( P_n \) we had, say, an expression \( P_{n_1,n_2,n_3} \) that depends on three variables \( n_1,n_2,n_3 \), then the condition for a maximum (or a minimum, or a saddle point) would be the system of equations

\[
\frac{P_{n_1,n_2,n_3}}{P_{n_1-1,n_2,n_3}} = \frac{P_{n_1,n_2-1,n_3}}{P_{n_1,n_2,n_3-1}} = \frac{P_{n_1,n_2,n_3}}{P_{n_1,n_2,n_3-1}} = 1. \tag{9}
\]

\(^{a}\)On leave of absence from Oranim, Tivon 36910, Israel.


\(^{c}\)T. I. Hill, \textit{An Introduction to Statistical Thermodynamics} (Addison-Wesley, Reading, MA, 1960).


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A new scientific truth does not triumph by convincing its opponents and making them see the light, but rather because its opponents eventually die, and a new generation grows up that is familiar with it.