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Algebraic method of Calculating the Moment Generating Function in Gaussian Multiple Distribution

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Abstract

The method of calculating the moment generating function in multiple gaussian distribution having correlations among variables, is given. The derivation is obtained from the investigation of the meanings of the integration of gaussian distribution, one of which is algebraic and the other is geometrical. The method of calculating is equivalent to obtaining a solution of simultaneous equations. The formula obtained is applicable to the calculation of the configurational partition function of ternary solutions.

1. Introduction and formulation of the problem

It is well known that the moment genrating function (m. g. f.) is very important and convenient in order to obtain moments and correations of all types of orders. Especially it is of considerable use to obtain m. g. f. of multiple gaussian distribution, because it is a familiar function to us in various problem. Conseaquently it seems quite valuable that we derive algebraically the formula of calculating m. g. f. in multiple gaussian distribution, although it is known that it has been derived already by other methods.

The following formula is well known and may be seen in almost every table of integrations:

$$M(2\beta)\equiv C_1\int_{-\infty}^{\infty} e^{-\lambda x^2}e^{2\beta x}dx=e^{\beta^2/\lambda} \tag{1}$$

together with

$$C_1=(\pi/\lambda)^{-1/2} \tag{2}$$

where C_1 is the normalization factor. Let us consider the meaning of this integration. In carrying out the integration (1) for practial purposes we rewrite it as follows:

$$C_1\int_{-\infty}^{\infty}\exp\left\{-\lambda\left(x-\frac{\beta}{\lambda}\right)^2+\lambda\left(\frac{\beta}{\lambda}\right)^2\right\}dx=\exp\left(\frac{\beta^2}{\lambda}\right) \tag{3}$$

where the following formula it used:

$$\int_{-\infty}^{\infty} e^{-\lambda x^2}dx=\left(\frac{\pi}{\lambda}\right)^{1/2}. \tag{4}$$

This result that the integration (3) is equivalent to making a square term of integration variable in exponent and putting it into zero, if we omit the coefficient C_1 temporarily. In addition, making the square term in exponent zero is to obtain the average value of gaussian distribution:

$$\lambda x=\beta \tag{5}$$

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that is, to get the abscissa of the top of gassian distribution, geometrically. Substituting the average value in place of the variable x into the first exponent on the left side of (1) and changing the sign, we have the correct results of the integration. This is the principle of derivating m. g. f. in a gaussian distribution.

Extending (1) to multiple gaussian distribution, we have the following m. g. f. :

$$W(2\beta)=C_n\int_{-\infty}^{\infty}\cdots\int \exp\left(-\sum_{i,j}^{n}\lambda_{ij}x_ix_j\right)\exp\left(2\sum_i\beta_ix_i\right)\prod_i dx_i$$
$$=\exp\left(\sum_{i,j}\alpha_{ij}\beta_i\beta_i\right) \tag{6}$$

where matrices $\lambda=\{\lambda_{ij}\}$ and $\lambda^{-1}=\{\alpha_{ij}\}$ are defined.

2. An example having two variables

Especially, in the case of two variables, the problem is to derive the following equation :

$$C_2\int_{-\infty}^{\infty}\int \exp(-\lambda_{11}x_1^2-\lambda_{22}x_2^2-2\lambda_{12}x_1x_2)\cdot\exp 2(\beta_1x_1+\beta_2x_2)dx_1dx_2$$
$$=\exp(\alpha_{11}\beta_1^2+\alpha_{22}\beta_2^2+2\alpha_{12}\beta_1\beta_2). \tag{7}$$

Firstly, differentiating the function in exponent by x_1 and x_2, in order to obtain the mean values, we have

$$\left.\begin{array}{l}\lambda_{11}x_1+\lambda_{12}x_2=\beta_1\\ \lambda_{21}x_1+\lambda_{22}x_2=\beta_2\end{array}\right\} \tag{8}$$

together with

$$\lambda_{12}=\lambda_{21}.$$

On defining a matrix,

$$\lambda=\begin{pmatrix}\lambda_{11} & \lambda_{12}\\ \lambda_{21} & \lambda_{22}\end{pmatrix} \tag{9}$$

we have

$$\lambda\begin{pmatrix}x_1\\ x_2\end{pmatrix}=\begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix}. \tag{10}$$

When we write this with adequate vectors, we have

$$\lambda\mathbf{x}=\beta \tag{10'}$$

formally in accord with (5). On solving (10) we have

$$\begin{pmatrix}x_1\\ x_2\end{pmatrix}=\lambda^{-1}\begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix}=\begin{pmatrix}\alpha_{11} & \alpha_{12}\\ \alpha_{21} & \alpha_{22}\end{pmatrix}\begin{pmatrix}\beta_1\\ \beta_2\end{pmatrix} \tag{11}$$

where we put

$$\lambda^{-1}=\begin{pmatrix}\alpha_{11} & \alpha_{12}\\ \alpha_{21} & \alpha_{22}\end{pmatrix},\qquad \alpha_{12}=\alpha_{21}.$$

When we substitute (11) into the first exponent on the left side of (7), we have the following result :

$$\exp\{\lambda_{11}(\alpha_{11}\beta_1+\alpha_{12}\beta_2)^2+\lambda_{22}(\alpha_{21}\beta_1+\alpha_{22}\beta_2)^2$$
$$+2\lambda_{12}(\alpha_{11}\beta_1+\alpha_{12}\beta_2)(\alpha_{21}\beta_1+\alpha_{22}\beta_2)\}. \tag{12}$$

This leads to the final expression :

$$\exp(\alpha_{11}\beta_1^2+\alpha_{22}\beta_2^2+2\alpha_{12}\beta_1\beta_2). \tag{13}$$

Thus (7) is proved.

In order to write down this expression correctly, we make use of the following correspondence of matrices with fringes of x_i and β_i.

$$\begin{array}{c} \\ x_1 \\ x_2 \end{array}\!\!\begin{array}{c} x_1 \quad x_2 \\ \begin{pmatrix} \lambda_{11} & \lambda_{12} \\ \lambda_{21} & \lambda_{22} \end{pmatrix} \end{array} \longleftrightarrow \begin{array}{c} \\ \beta_1 \\ \beta_2 \end{array}\!\!\begin{array}{c} \beta_1 \quad \beta_2 \\ \begin{pmatrix} \alpha_{11} & \alpha_{12} \\ \alpha_{21} & \alpha_{22} \end{pmatrix} \end{array} \tag{14}$$

The coefficient C_2 is given by

$$|\lambda|^{1/2}/(\pi^{1/2}\pi^{1/2}) \tag{15}$$

on the analogy of (2).

As known, on carrying out the integration of (7) having $\beta_i=0$ for practical purposes we write as follows

$$\iint \exp(-\lambda_{11}x_1^2-\lambda_{22}x_2^2-2\lambda_{12}x_1x_2)dx_1dx_2$$

$$=\iint \exp\left\{-\lambda_{11}\left(x_1+\frac{\lambda_{12}}{\lambda_{11}}x_2\right)^2-\left(\lambda_{22}-\frac{\lambda_{12}^2}{\lambda_{11}}\right)x_2^2\right\}dx_1dx_2.$$

On integrating by x_1 at the first time, we have the coefficient $\pi^{1/2}/\lambda_{11}^{1/2}$ and next integrating by x_2, we have $\pi^{1/2}\Big/\left(\lambda_{22}-\frac{\lambda_{12}^2}{\lambda_{11}}\right)^{1/2}$. Bringing them together, we have

$$(\pi^{1/2})^2/(\lambda_{11}\lambda_{22}-\lambda_{12}^2)^{1/2}. \tag{16}$$

The reciprocal of this is the normalization factor C_2, which agrees with (15).

The inner part of parentheses of the denominator of (16) is also obtained by neglecting x_1 from (8) having $\beta_i=0$, that is

$$(\lambda_{12}^2-\lambda_{11}\lambda_{22})x_2=0. \tag{17}$$

Thus we have the following statement:

> Integrating a gaussian distribution step by step through x_1 and x_2 is equivalent to obtaining the solution by eliminating variables step by step from simultaneous equations.

In order to derive the final result (13) by practical integration, we may write the part in the exponent as follows

$$-\lambda_{11}\left(x_1+\frac{\lambda_{12}x_2-\beta_1}{\lambda_{11}}\right)^2-\left(\lambda_{22}-\frac{\lambda_{12}^2}{\lambda_{11}}\right)\left\{x_2+\frac{\left(\frac{\lambda_{12}\beta_1}{\lambda_{11}}-\beta_2\right)^2}{\left(\lambda_{22}-\frac{\lambda_{12}^2}{\lambda_{11}}\right)}\right\}^2+\frac{\beta_1^2}{\lambda_{11}}+\frac{\left(\frac{\lambda_{12}\beta_1}{\lambda_{11}}-\beta^2\right)^2}{\left(\lambda_{22}-\frac{\lambda_{12}^2}{\lambda_{11}}\right)}. \tag{18}$$

After the integration of the function having (18) in the exponent, we have

$$\exp\left\{\frac{\beta_1^2}{\lambda_{11}}+\frac{\left(\frac{\lambda_{12}\beta_1}{\lambda_{11}}-\beta_2\right)^2}{\left(\lambda_{22}-\frac{\lambda_{12}^2}{\lambda_{11}}\right)}\right\}$$

which leads to (13).

3. The general gaussian multiple distribution

As may be seen the principle and method of deriving m. g. f. in the example of two variables above, we may find the proof of the problem (6). By analogy with (7), on differentiating the function in exponent by x_i, we have the following simultaneous equations:

$$\left.\begin{array}{l} \lambda_{11}x_1+\lambda_{12}x_2+\ \dots\ +\lambda_{1n}x_n=\beta_1 \\ \lambda_{21}x_1+\lambda_{22}x_2+\ \dots\ +\lambda_{2n}x_n=\beta_2 \\ \cdots\cdots \\ \lambda_{n1}x_1+\lambda_{n2}x_2+\ \dots\ +\lambda_{nn}x_n=\beta_n \end{array}\right\} \tag{19}$$

On introducing the matrix λ

$$\lambda=\begin{pmatrix}\lambda_{11}\lambda_{12}\ldots\lambda_{1n}\\ \lambda_{21}\lambda_{22}\ldots\lambda_{2n}\\ \cdots\cdots\\ \lambda_{n1}\lambda_{n2}\ldots\lambda_{nn}\end{pmatrix}, \tag{20}$$

we have

$$\lambda\begin{pmatrix}x_1\\ x_2\\ \vdots\\ x_n\end{pmatrix}=\begin{pmatrix}\beta_1\\ \beta^2\\ \vdots\\ \beta_n\end{pmatrix}. \tag{21}$$

This leads to the vector expression:

$$\lambda\mathbf{x}=\beta \tag{21'}$$

which agrees formally with (5). Therefore the normalization factor is

$$C_n=|\lambda|^{1/2}/(\pi^{1/2})^n. \tag{22}$$

When we substitute x_i from (21) into the first exponent of (6) having changed the sign, we have

$$M(2\beta)\equiv\exp\{\sum_{i,j}\lambda_{ij}(\sum_k\alpha_{ik}\beta_k)(\sum_e{}_{je}\beta_e)\} \tag{23}$$

wher $\alpha_{ij}'s$ are elements of the inverse of the matrix (20). Let us sum with j. Then we have

$$\sum_{i,e}\lambda_{ij}\alpha_{ie}\quad =1,\text{ if } i=e$$
$$=\text{zero, otherwise.}$$

Therefore we have

$$M(2\beta)\equiv\exp\sum_{e,k}\alpha_{e,k}\beta_k\beta_e. \tag{24}$$

m. g. f. of three variables appears in the calculation of configurational partition function of ternary system[1].

Reference

1) M. Onodera, J. Phys. Soc. Japan 37, 24(1974).