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Gaussian quadratic form integrals and multivariable approximation of exponential integrals

1.1 Motivation

In [1] eq. I.2.20 is the approximation

$$\int d\mathbf{q} e^{-f(\mathbf{q})/\hbar} \approx e^{-f(\mathbf{a})/\hbar} \sqrt{\frac{2\pi\hbar}{\det f''(\mathbf{a})}}, \tag{1.1}$$

where $[f''(\mathbf{a})]_{ij} \equiv \partial^2 f/\partial q_i \partial q_j \big|_{\mathbf{q}=\mathbf{a}}$. Here $\mathbf{a}$ is assumed to be an extremum of f. This follows from a generalization of the Gaussian integral result. Let's derive both in detail.

1.2 Guts

First, to second order, let's expand $f(\mathbf{q})$ around a min or max at $\mathbf{q} = \mathbf{a}$. The usual trick, presuming that one doesn't remember the form of this generalized Taylor expansion, is to expand $g(t) = f(\mathbf{a} + t\mathbf{q})$ around $t = 0$, then evaluate at $t = 1$. We have

$$g'(t) = \sum_i \frac{\partial f(\mathbf{a} + t\mathbf{q})}{\partial (a_i + t q_i)} \frac{d(a_i + t q_i)}{dt} = \sum_i q_i \frac{\partial f(\mathbf{a} + t\mathbf{q})}{\partial (a_i + t q_i)} = \mathbf{q} \cdot \left(\boldsymbol{\nabla}_{\mathbf{q}} f(\mathbf{q}) \big|_{\mathbf{q}=\mathbf{a}+t\mathbf{q}} \right). \tag{1.2}$$

The second derivative is

$$g''(t) = \sum_{ij} q_i q_j \frac{\partial}{\partial (a_j + t q_j)} \frac{\partial f(\mathbf{a} + t\mathbf{q})}{\partial (a_i + t q_i)}, \tag{1.3}$$

This gives

$$\begin{aligned} g'(0) &= \mathbf{q} \cdot \boldsymbol{\nabla}_{\mathbf{q}} f(\mathbf{q}) = \sum_i q_i \partial q_i f(\mathbf{q}) \\ g''(0) &= \left(\mathbf{q} \cdot \boldsymbol{\nabla}_{\mathbf{q}} \right)^2 f(\mathbf{q}) = \sum_{ij} q_i q_j \partial q_i \partial q_j f(\mathbf{q}). \end{aligned} \tag{1.4}$$

Putting these together, we have to second order in t is

$$f(\mathbf{a}+t\mathbf{q}) \approx f(\mathbf{a}) + \sum_i q_i \partial q_i f(\mathbf{q}) \frac{t^1}{1!} + \sum_{ij} q_i q_j \partial q_i \partial q_j f(\mathbf{q}) \frac{t^2}{2!}, \tag{1.5}$$

or

$$f(\mathbf{a}+\mathbf{q}) \approx f(\mathbf{a}) + \sum_i q_i \left(\frac{\partial f}{\partial q_i} \right)\bigg|_{\mathbf{a}} + \frac{1}{2} \sum_{ij} q_i q_j \left(\frac{\partial^2 f}{\partial q_i \partial q_j} \right)\bigg|_{\mathbf{a}}. \tag{1.6}$$

We can put the terms up to second order in a nice tidy matrix forms

$$\mathbf{b} = \left(\boldsymbol{\nabla}_{\mathbf{q}} f \right)\big|_{\mathbf{a}} \tag{1.7a}$$

$$A = \left[\left(\tfrac{\partial^2 f}{\partial q_i \partial q_j} \right)\Big|_{\mathbf{a}} \right]_{ij}. \tag{1.7b}$$

Note that eq. (1.7b) is a real symmetric matrix, and can thus be reduced to diagonal form by an orthonormal transformation. Putting the pieces together, we have

$$f(\mathbf{a}+\mathbf{q}) \approx f(\mathbf{a}) + \mathbf{q}^{\mathrm{T}}\mathbf{b} + \frac{1}{2}\mathbf{q}^{\mathrm{T}} A \mathbf{q}. \tag{1.8}$$

Integrating this, we have

$$\int dq_1 dq_2 \cdots dq_N \exp\left(-\left(f(\mathbf{a}) + \mathbf{q}^{\mathrm{T}}\mathbf{b} + \frac{1}{2}\mathbf{q}^{\mathrm{T}} A \mathbf{q} \right) \right) = e^{-f(\mathbf{a})} \int dq_1 dq_2 \cdots dq_N \exp\left(-\mathbf{q}^{\mathrm{T}}\mathbf{b} - \frac{1}{2}\mathbf{q}^{\mathrm{T}} A \mathbf{q} \right). \tag{1.9}$$

Employing an orthonormal change of variables to diagonalizae the matrix

$$A = O^{\mathrm{T}} D O, \tag{1.10}$$

and $\mathbf{r} = O\mathbf{q}$, or $r_i = O_{ik} q_k$, the volume element after transformation is

$$\begin{aligned} dr_1 dr_2 \cdots dr_N &= \frac{\partial(r_1, r_2, \cdots, r_N)}{\partial(q_1, q_2, \cdots, q_N)} dq_1 dq_2 \cdots dq_N \\ &= \begin{vmatrix} O_{11} & O_{12} & \cdots & O_{1N} \\ O_{21} & O_{22} & \cdots & O_{2N} \\ \vdots & \vdots & \vdots & \vdots \\ O_{N1} & O_{N2} & \cdots & O_{NN} \end{vmatrix} dq_1 dq_2 \cdots dq_N \\ &= (\det O) dq_1 dq_2 \cdots dq_N \\ &= dq_1 dq_2 \cdots dq_N \end{aligned} \tag{1.11}$$

Our integral is

$$\begin{aligned}
&e^{-f(\mathbf{a})} \int dq_1 dq_2 \cdots dq_N \exp\left(-\mathbf{q}^{\mathrm{T}}\mathbf{b} - \frac{1}{2}\mathbf{q}^{\mathrm{T}} A \mathbf{q}\right) \\
&= e^{-f(\mathbf{a})} \int dr_1 dr_2 \cdots dr_N \exp\left(-\mathbf{q}^{\mathrm{T}} O^{\mathrm{T}} O \mathbf{b} - \frac{1}{2}\mathbf{q}^{\mathrm{T}} O^{\mathrm{T}} D O \mathbf{q}\right) \\
&= e^{-f(\mathbf{a})} \int dr_1 dr_2 \cdots dr_N \exp\left(-\mathbf{r}^{\mathrm{T}} (O\mathbf{b}) - \frac{1}{2}\mathbf{r}^{\mathrm{T}} D \mathbf{r}\right) \\
&= e^{-f(\mathbf{a})} \int dr_1 e^{-\frac{1}{2} r_1^2 \lambda_1 - r_1 (O\mathbf{b})_1} \int dr_2 e^{-\frac{1}{2} r_2^2 \lambda_2 - r_2 (O\mathbf{b})_2} \cdots \int dr_N e^{-\frac{1}{2} r_N^2 \lambda_N - r_N (O\mathbf{b})_N}.
\end{aligned} \tag{1.12}$$

We now have products of terms that are of the regular Gaussian form. One such iintegral is

$$\int e^{-ax^2/2+Jx} = \int \exp\left(-\frac{1}{2}\left(\left(\sqrt{a}x - J/\sqrt{a}\right)^2 - \left(J/\sqrt{a}\right)^2\right)\right) = e^{J^2/2a}\sqrt{2\pi \int_0^\infty r dr e^{-ar^2/2}} \tag{1.13}$$

This is just

$$\int e^{-ax^2/2+Jx} = e^{J^2/2a}\sqrt{\frac{2\pi}{a}}. \tag{1.14}$$

Applying this to the integral of interest, writing $m_i = (O\mathbf{b})_i$

$$\begin{aligned}
&e^{-f(\mathbf{a})} \int dq_1 dq_2 \cdots dq_N \exp\left(-\mathbf{q}^{\mathrm{T}}\mathbf{b} - \frac{1}{2}\mathbf{q}^{\mathrm{T}} A \mathbf{q}\right) \\
&\qquad = e^{-f(\mathbf{a})} e^{-m_1^2/2\lambda_1}\sqrt{\frac{2\pi}{\lambda_1}} e^{-m_2^2/2\lambda_2}\sqrt{\frac{2\pi}{\lambda_2}} \cdots e^{-m_N^2/2\lambda_N}\sqrt{\frac{2\pi}{\lambda_N}} \\
&\qquad = e^{-f(\mathbf{a})}\sqrt{\frac{2\pi}{\det A}} \exp\left(-\frac{1}{2}\left(-m_1^2/\lambda_1 - m_2^2/\lambda_2 \cdots - m_N^2/\lambda_N\right)\right).
\end{aligned} \tag{1.15}$$

This last exponential argument can be put into matrix form

$$-m_1^2/\lambda_1 - m_2^2/\lambda_2 \cdots - m_N^2/\lambda_N = (O\mathbf{b})^{\mathrm{T}} D^{-1} O\mathbf{b} = \mathbf{b}^{\mathrm{T}} O^{\mathrm{T}} D^{-1} O \mathbf{b} = \mathbf{b}^{\mathrm{T}} A^{-1}\mathbf{b}, \tag{1.16}$$

Finally, referring back to eq. (1.7), we have

$$\int d\mathbf{q} e^{-f(\mathbf{q})} \approx e^{-f(\mathbf{a})}\sqrt{\frac{2\pi}{\det A}} e^{-\mathbf{b}^{\mathrm{T}} A^{-1}\mathbf{b}/2}. \tag{1.17}$$

Observe that we can recover eq. (1.1) by noting that $\mathbf{b} = 0$ for that system was assumed (i.e. $\mathbf{a}$ was an extremum point), and by noting that the determinant scales with $1/\hbar$ since it just contains the second partials.

An afterword on notational sugar: We didn't need it, but it seems worth noting that we can write the Taylor expansion of eq. (1.8) in operator form as

$$f(\mathbf{a} + \mathbf{q}) = \sum_{k=0}^{\infty} \frac{1}{k!}\left(\mathbf{q} \cdot \boldsymbol{\nabla}_{\mathbf{q}'}\right)^k f(\mathbf{q}')\Big|_{\mathbf{q}'=\mathbf{a}} = e^{\mathbf{q}\cdot\boldsymbol{\nabla}_{\mathbf{q}'}} f(\mathbf{q}')\Big|_{\mathbf{q}'=\mathbf{a}}. \tag{1.18}$$

Bibliography

[1] A. Zee. *Quantum field theory in a nutshell*. Universities Press, 2005. 1.1