GAUSSIAN INTEGRALS: AVERAGES OVER MATRIX COMPONENTS AND THE WICK CONTRACTION

We’ve seen how to evaluate a Gaussian integral with matrices in the exponent:

\[
\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 dx_2 \cdots dx_N e^{-\frac{1}{2} x^T A x + J^T x} = \sqrt{\frac{(2\pi)^N}{\det A}} e^{\frac{1}{2} J^T A^{-1} J} \tag{1}
\]

Using this formula, we can generalize the definition of averages of powers of \(x\) in the single variable integral. That is, we would like to calculate

\[
\langle x_i x_j \ldots x_k x_\ell \rangle \equiv \frac{\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 dx_2 \cdots dx_N x_i x_j \ldots x_k x_\ell e^{-\frac{1}{2} x^T A x} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 dx_2 \ldots dx_N e^{-\frac{1}{2} x^T A x}}{\int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 dx_2 \cdots dx_N e^{-\frac{1}{2} x^T A x}} \tag{2}
\]

From the LHS of (1) we see that this average can be obtained by taking the derivative with respect to \(J_a\) for each subscript \(a\) in the set of \(x_a\)s that we want to average, and then setting \(J = 0\). For example, since \(J^T x = \sum_a x_a J_a\),

\[
\frac{\partial^2}{\partial J_i \partial J_j} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 dx_2 \cdots dx_N e^{-\frac{1}{2} x^T A x + J^T x} = \frac{\partial^2}{\partial J_i \partial J_j} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} dx_1 dx_2 \cdots dx_N x_i x_j e^{-\frac{1}{2} x^T A x + J^T x} \tag{3}
\]

Therefore

\[
\langle x_i x_j \rangle = \frac{\frac{\partial^2}{\partial J_i \partial J_j} \left( \sqrt{\frac{(2\pi)^N}{\det A}} e^{\frac{1}{2} J^T A^{-1} J} \right) \bigg|_{J=0}}{\sqrt{\frac{(2\pi)^N}{\det A}} e^{\frac{1}{2} J^T A^{-1} J} \bigg|_{J=0}} \tag{5}
\]

\[
= \frac{\partial^2}{\partial J_i \partial J_j} \left( e^{\frac{1}{2} J^T A^{-1} J} \right) \bigg|_{J=0} \tag{6}
\]
Working out these derivatives isn’t all that bad, if we do the first few to see how the pattern goes. To make the notation a bit easier, we’ll define the following:

\[ \alpha \equiv e^{\frac{1}{2} J^T A^{-1} J} \]  
\[ a \equiv A^{-1} \]  
\[ \beta_i \equiv A^{-1}_{ik} J_k = a_{ik} J_k \]  
\[ \partial_i \equiv \frac{\partial}{\partial J_i} \]  

with an implied sum over \( k \) in the definition of \( \beta \). Repeated indices within the same term are always summed in what follows.

Taking the first derivative, we get

\[ \partial_k \alpha = \frac{\alpha}{2} \left( a_{kj} J_j + J_i a_{ik} \right) \]  
\[ = \alpha a_{kj} J_j \]  
\[ = \alpha \beta_k \]  

where the second line follows because \( A \) and therefore \( A^{-1} = a \) are both symmetric matrices. Note that \( J = 0 \) implies \( \beta = 0 \) and \( \alpha = 1 \).

In subsequent derivatives, we’ll need the result

\[ \partial_{\ell} \beta_k = \frac{\partial}{\partial J_{\ell}} a_{ik} J_k \]  
\[ = a_{i\ell} \]  

The second derivative is, from 13

\[ \partial_{\ell} \partial_k \alpha = \beta_k \partial_{\ell} \alpha + \alpha \partial_{\ell} \beta_k \]  
\[ = \alpha \beta_k \beta_{\ell} + \alpha a_{\ell k} \]  
\[ = a_{\ell k} = A_{\ell k}^{-1} \text{ (for } J = 0) \]  

Therefore

\[ \langle x_{\ell} x_k \rangle = A_{\ell k}^{-1} \]  

The third derivative is
\[ \partial_m \partial_\ell \partial_k \alpha = (\partial_m \alpha) \beta_k \beta_\ell + \alpha (\partial_m \beta_k) \beta_\ell + \alpha \beta_k (\partial_m \beta_\ell) + (\partial_m \alpha) a_{\ell k} \]  
\[ (20) \]

\[ = \alpha \beta_m \beta_k \beta_\ell + \alpha a_{mk} \beta_\ell + \alpha \beta_k a_{m\ell} + \alpha \beta_m a_{\ell k} \]  
\[ (21) \]

\[ = 0 \text{ (for } J = 0) \]  
\[ (22) \]

The fourth derivative is

\[ \partial_n \partial_m \partial_\ell \partial_k \alpha = \alpha \beta_n \beta_m \beta_k \beta_\ell + \alpha \beta_n a_{mk} \beta_\ell + \alpha \beta_n \beta_k a_{m\ell} + \alpha \beta_m \beta_a a_{\ell k} + \]  
\[ \alpha a_{mk} a_{\ell n} + \alpha a_{kn} a_{m\ell} + \alpha a_{mn} a_{\ell k} \]  
\[ (23) \]

\[ = a_{mk} a_{\ell n} + a_{kn} a_{m\ell} + a_{mn} a_{\ell k} \text{ (for } J = 0) \]  
\[ (24) \]

To see the general pattern for the derivative \( \partial_i \partial_j \ldots \partial_k \partial_\ell \) containing \( N \) factors, note that the first term is always \( \alpha \beta_i \beta_j \ldots \beta_k \beta_\ell \), that is, it contains \( \alpha \) multiplied by all \( N \) possible \( \beta_i \)'s. Then there is a set of terms consisting of \( \alpha \) multiplied by \( N - 2 \) \( \beta_i \)'s and one \( a_{ij} \). The number of these terms is equal to the number of unique permutations of the \( N \) indices, allowing for the symmetry of \( a_{ij} \). For example, in the fourth derivative above, there are 3 unique ways of distributing the 4 indices among a product of form \( a_{ij} \beta_k \beta_\ell \), so there are 3 of these terms.

Next there are terms consisting of \( \alpha \) multiplied by \( N - 4 \) \( \beta_i \)'s and 2 \( a_{ij} \)'s. Again, the number of terms is equal to the number of unique permutations of the \( N \) indices among the factors in each term, allowing for the symmetry of \( a_{ij} \). In the fourth derivative, this gives terms containing zero \( \beta_i \)'s and two \( a_{ij} \)'s, and there are 3 unique ways of distributing 4 indices between the two \( a_{ij} \)'s.

The process continues \( n \) times, where \( n \) is determined by the condition \( N - 2n = 0 \) (for even-order derivatives) or 1 (for odd-order derivatives). For odd-order derivatives, all terms contain at least one factor \( \beta_i \), so all these derivatives are zero when \( J = 0 \). For even-order derivatives, we get

\[ \langle x_i x_j \ldots x_k x_\ell \rangle = \sum_{W, i < \ell} A_{ab}^{-1} \ldots A_{cd}^{-1} \]  
\[ (25) \]

where each term in the sum is a product of \( \frac{N}{2} A_{ij}^{-1} \) elements, and the sum is over all unique permutations of the \( N \) indices distributed amongst these elements. This set of permutations is known as a Wick contraction.

For the case \( N = 1 \), \( \langle x \rangle \) reduces to the single-variable case we considered earlier, where we found that

\[ \langle x^{2n} \rangle = \frac{(2n - 1)!!}{a^n} \]  
\[ (26) \]
Since each term in the Wick sum contributes the same amount $\frac{1}{a^n}$ in this case, there are $(2n - 1)!!$ terms in the sum.

With these rules, we can write down the sixth-order expansion ($N = 2n = 6$), for which there are $(2 \times 3 - 1)!! = 15$ terms in the Wick sum:

$$\langle x_i x_j x_k x_\ell x_m x_n \rangle = a_{ij} a_{k\ell} a_{mn} + a_{ij} a_{km} a_{\ell n} + a_{ij} a_{kn} a_{\ell m} +$$
$$a_{ik} a_{j\ell} a_{mn} + a_{ik} a_{jm} a_{\ell n} + a_{ik} a_{jn} a_{\ell m} +$$
$$a_{i\ell} a_{jk} a_{mn} + a_{i\ell} a_{jm} a_{kn} + a_{i\ell} a_{jn} a_{km} +$$
$$a_{im} a_{jk} a_{\ell n} + a_{im} a_{jl} a_{kn} + a_{im} a_{jn} a_{k\ell} +$$
$$a_{in} a_{jk} a_{\ell m} + a_{in} a_{jl} a_{km} + a_{in} a_{jm} a_{k\ell}$$

(27)

The pattern followed pairs the first two indices $i$ and $j$ in $a_{ij}$, then works out the Wick contraction of the remaining four indices $k, \ell, m, n$ to produce the first 3 terms. Then pair $i$ with $k$ in $a_{ik}$ and work out the Wick contraction of the other four indices $j, \ell, m, n$ to get the next 3 terms and so on. From this process we can also derive the number of terms in a Wick sum of order $N = 2n$. For $N = 2$, there is only one permutation. For $N = 4$, we can pair the first index with any of the 3 remaining indices, leaving 2 indices which as we’ve just seen, have only one permutation. Thus for $N = 4$ the number of permutations is $3 \times 1 = 3$. For $N = 6$, the first index can be paired with any of the 5 remaining indices, leaving 4 other indices which can be permuted in 3 ways, so the number of terms is $5 \times 3 \times 1 = 15$ and so on.