

APPENDIX B

GAUSSIAN INTEGRALS

One variable

We begin by evaluating the following Gaussian integral

$$I = \int_{-\infty}^{\infty} \exp\left(-\frac{\lambda}{2}x^2\right) dx.$$

This is easily done by considering the square of the integral, and then changing to polar coordinates:

$$\begin{aligned} I^2 &= \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left(-\frac{\lambda}{2}x^2 - \frac{\lambda}{2}y^2\right) dx dy \\ &= \int_0^{\infty} \int_0^{2\pi} \exp\left(-\frac{\lambda}{2}r^2\right) r dr d\theta \\ &= \pi \int_0^{\infty} \exp\left(-\frac{\lambda}{2}u\right) du \\ &= \frac{2\pi}{\lambda} \end{aligned}$$

where we have changed variables first using $x = r \cos \theta, y = r \sin \theta$ and then using $r^2 = u$. Taking the square root we finally obtain

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

Several variables

Consider the evaluation of the W -dimensional Gaussian integral

$$I_W = \int \exp\left(-\frac{1}{2}\mathbf{w}^T \mathbf{A} \mathbf{w}\right) d\mathbf{w}$$

\mathbf{A} is a $W \times W$ real symmetric matrix, \mathbf{w} is a W -dimensional vector, and integration is over the whole of \mathbf{w} -space. In order to evaluate this integral it is convenient to consider the eigenvector equation for \mathbf{A} in the form

$$\mathbf{A}\mathbf{u}_k = \lambda_k \mathbf{u}_k. \tag{B.5}$$

\mathbf{A} is real and symmetric, we can choose the eigenvectors to form a complete orthonormal set

$$\mathbf{u}_k^T \mathbf{u}_l = \delta_{kl} \tag{B.6}$$

discussed in Appendix A. We can then expand the vector \mathbf{w} as a linear combination of the eigenvectors

$$\mathbf{w} = \sum_{k=1}^W \alpha_k \mathbf{u}_k. \tag{B.7}$$

Integration over the weight values $d\mathbf{w}_1 \dots d\mathbf{w}_W$ can now be replaced by an integration over $d\alpha_1 \dots d\alpha_W$. The Jacobian of this change of variables is given

$$J = \det \left(\frac{\partial w_i}{\partial \alpha_k} \right) = \det (u_{ki}) \tag{B.8}$$

u_{ki} is the i th element of the vector \mathbf{u}_k , and 'det' denotes the determinant. The u_{ki} are also the elements of a matrix \mathbf{U} whose columns are given by the \mathbf{u}_k , which is an orthogonal matrix, i.e. it satisfies $\mathbf{U}^T \mathbf{U} = \mathbf{I}$, since its columns are orthonormal. Thus

$$J^2 = \{\det(\mathbf{U})\}^2 = \det(\mathbf{U}^T) \det(\mathbf{U}) = \det(\mathbf{U}^T \mathbf{U}) = \det(\mathbf{I}) = 1 \tag{B.9}$$

hence $|J| = 1$. Using the orthonormality of the \mathbf{u}_k we have

$$\mathbf{w}^T \mathbf{A} \mathbf{w} = \sum_{k=1}^W \lambda_k \alpha_k^2. \tag{B.10}$$

Various integrals over the α_k now decouple, and so we can write

$$I_W = \prod_{k=1}^W \int_{-\infty}^{\infty} \exp \left(-\frac{\lambda_k \alpha_k^2}{2} \right) d\alpha_k. \tag{B.11}$$

Using the result (B.3) we obtain

$$I_W = \prod_{k=1}^W \left(\frac{2\pi}{\lambda_k} \right)^{1/2}$$

Since the determinant of a matrix is given by the product of its eigenvalues,

$$|\mathbf{A}| = \prod_{k=1}^W \lambda_k,$$

we finally obtain

$$I_W = (2\pi)^{W/2} |\mathbf{A}|^{-1/2}.$$

Inclusion of linear term

In deriving the distribution of network outputs within the Bayesian framework of Exercise 10.2, we need to consider a more general form of the Gaussian distribution which has an additional linear term, of the form

$$I_W = \int \exp \left(-\frac{1}{2} \mathbf{w}^T \mathbf{A} \mathbf{w} + \mathbf{h}^T \mathbf{w} \right) d\mathbf{w}.$$

Again, it is convenient to work in terms of the eigenvectors of \mathbf{A} . We find h_k to be the projections of \mathbf{h} onto the eigenvectors

$$h_k = \mathbf{h}^T \mathbf{u}_k.$$

This again leads to a set of decoupled integrals over the α_k of the form

$$I_W = \prod_{k=1}^W \int_{-\infty}^{\infty} \exp \left(-\frac{\lambda_k \alpha_k^2}{2} + h_k \alpha_k \right) d\alpha_k.$$

Completing the square in the exponent, we have

$$-\frac{\lambda_k \alpha_k^2}{2} + h_k \alpha_k = -\frac{\lambda_k}{2} \left(\alpha_k - \frac{h_k}{\lambda_k} \right)^2 + \frac{h_k^2}{2\lambda_k}.$$

If we now change integration variables to $\tilde{\alpha}_k = \alpha_k - h_k/\lambda_k$, we again obtain a product of integrals which can be evaluated using (B.3) to give

$$I_W = (2\pi)^{W/2} |\mathbf{A}|^{-1/2} \exp \left(\sum_{k=1}^W \frac{h_k^2}{2\lambda_k} \right).$$

we now apply A^{-1} to both sides of (B.5) we see that A^{-1} has the same eigenvectors as A , but with eigenvalues λ_k^{-1} :

$$A^{-1}u_k = \lambda_k^{-1}u_k. \tag{B.20}$$

product of its eigenvalues

using (B.6) and (B.16), we see that

$$h^T A^{-1} h = \sum_k \frac{h_k^2}{\lambda_k}. \tag{B.21}$$

using this result in (B.19) we obtain our final result:

$$I_W = (2\pi)^{W/2} |A|^{-1/2} \exp\left(\frac{1}{2} h^T A^{-1} h\right). \tag{B.22}$$

in the Bayesian framework
form of the Gaussian integrals

w) dw .

vectors of A . We first de

er the α_k of the form

$$v_k \alpha_k) d\alpha_k.$$

$$\left(\frac{v_k}{v_k}\right)^2 + \frac{h_k^2}{2\lambda_k}.$$

$v_k - h_k/\lambda_k$, we again obtain
(B.3) to give

$$\sum_{i=1}^W \left(\frac{h_k^2}{2\lambda_k}\right).$$