Problems: Gaussian random variables and a little bit of linear algebra

ISSYP 2016

1. *Simulating Gaussian random variables.* A question which sometimes arises is how to simulate a Gaussian random variable in N dimensions, assuming the existence of an algorithm for randomly simulating a one-dimensional Gaussian.[1] In this problem we will study this question in the case $N = 2$.

   (a) Consider a 2-component Gaussian random variable X_i, with mean $\bar{X}_i = 0$ assumed for simplicity, and covariance matrix

$$C_{ij} = \langle X_i X_j \rangle = \begin{pmatrix} C_{11} & C_{12} \\ C_{12} & C_{22} \end{pmatrix} \tag{1}$$

   Suppose we simulate independent one-dimensional Gaussian random numbers u_1, u_2 with variance $\sigma^2 = 1$. Show that if we define:

$$\begin{aligned} X_1 &= \sqrt{C_{11}}\,u_1 \\ X_2 &= \frac{C_{12}}{\sqrt{C_{11}}}u_1 + \sqrt{C_{22} - \frac{C_{12}^2}{C_{11}}}\,u_2 \end{aligned} \tag{2}$$

   then $\langle X_i X_j \rangle = C_{ij}$. This is one algorithm for simulating a two-dimensional Gaussian.

   (b) More generally, show that a linear transformation of the form $X_i = A_{ij} u_j$ gives covariance matrix $\langle X_i X_j \rangle = C_{ij}$ if and only if $C_{ij} = A_{ik} A_{jk}$.[2]

   (c) If you're comfortable with computer programming then try coding this up! For a specific choice of covariance matrix, say $C_{11} = 2$, $C_{12} = 1$, and $C_{22} = 3$, try making random realizations of X_i using Eq. (2), and verify that the averages $\langle X_i X_j \rangle$ converge to C_{ij} in the limit of many realizations.

2. *2-by-2 matrix inversion.* Consider a general 2-by-2 matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \tag{3}$$

   Show that the matrix elements of the inverse matrix

$$A^{-1} = \begin{pmatrix} A_{11}^{-1} & A_{12}^{-1} \\ A_{21}^{-1} & A_{22}^{-1} \end{pmatrix} \tag{4}$$

   are given explicitly by

$$\begin{aligned} A_{11}^{-1} &= \frac{A_{22}}{A_{11}A_{22} - A_{12}A_{21}} \\ A_{12}^{-1} &= -\frac{A_{12}}{A_{11}A_{22} - A_{12}A_{21}} \\ A_{21}^{-1} &= -\frac{A_{21}}{A_{11}A_{22} - A_{12}A_{21}} \\ A_{22}^{-1} &= \frac{A_{11}}{A_{11}A_{22} - A_{12}A_{21}} \end{aligned} \tag{5}$$

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[1] All modern programming lanugages have this built in. For example, in python you can get a Gaussian random number with `numpy.random.standard_normal()`.

[2] If this equation holds then we say that A is a "matrix square root" of C. Thus the problem of simulating multivariate Gaussian random numbers is linked to the problem of finding matrix square roots (which turn out to be non-unique). The coefficients given in Eq. (2) are one choice of matrix square root in the 2-by-2 case.

A brute force approach is to show that the defining condition for the inverse matrix, namely $A_{ij}A^{-1}_{jk} = \delta_{ik}$, holds for all four choices of indices i, k. If you have taken some linear algebra, you may know some machinery which is more efficient than the brute force approach – if so then feel free to use it!

3. *Gaussian integrals.* In this problem, you can assume that:

$$\int_{-\infty}^{\infty} dx\, e^{-x^2} = \sqrt{\pi} \tag{6}$$

(If you're curious how this is shown, there is a famous trick which is explained in the appendix!)

(a) By change of variable show that

$$\int_{-\infty}^{\infty} dx\, e^{-ax^2} = \sqrt{\pi} a^{-1/2} \tag{7}$$

where $a > 0$ is a real number.

(b) Now show that

$$\int_{-\infty}^{\infty} dx\, x^2 e^{-ax^2} = \frac{\sqrt{\pi}}{2} a^{-3/2} \tag{8}$$

using one of two possible approaches. One way is to group the integrand on the LHS as $(x)(xe^{-ax^2})$ and use integration by parts. The second way is to differentiate both sides of Eq. (7) with respect to a.

(c) Using the previous results show that the Gaussian probability distribution in one variable

$$p(x) = \frac{1}{(2\pi)^{1/2}\sigma} \exp\left(-\frac{x^2}{2\sigma^2}\right) \tag{9}$$

is correctly normalized (i.e. $\int p(x) = 1$) with variance σ^2 (i.e. $\int x^2 p(x) = \sigma^2$), as implicitly assumed in the lecture.

(d) Can you generalize part (b) to give a formula for $\int x^N e^{-ax^2}$, where N is a positive integer?

Appendix A: A famous trick for calculating $\int_{-\infty}^{\infty} dx e^{-x^2}$

As far as I know, the following strange trick is the only way of doing the integral! You'll need to have studied a little bit of multivariate calculus, in particular changing variables from Cartesian to polar coordinates in a 2D integral. Define:

$$I = \int_{-\infty}^{\infty} dx\, e^{-x^2} \tag{A1}$$

We can write I^2 as a 2D integral over the (x, y) plane.

$$\begin{aligned} I^2 &= \left(\int_{-\infty}^{\infty} dx\, e^{-x^2}\right)\left(\int_{-\infty}^{\infty} dy\, e^{-y^2}\right) \\ &= \int\int dx\, dy\, e^{-x^2-y^2} \end{aligned} \tag{A2}$$

This doesn't appear to be making progress, but if we now change variables to polar coordinates (r, θ), then we can do the integral! (In the steps below, we integrate over θ first and then r.)

$$\begin{aligned} I^2 &= \int dr\, d\theta\, r e^{-r^2} \\ &= 2\pi \int_0^{\infty} dr\, r e^{-r^2} \\ &= 2\pi \left(\frac{1}{2}\right) \end{aligned} \tag{A3}$$

Note that the extra factor of r we picked up in the change of variables to polar coordinates is what allows us to do the integral. Taking the square root on both sides we now get $I = \sqrt{\pi}$ as desired.