University of Kentucky, Physics 335
Homework #6, Rev. A, due Monday, 2024-10-21

2-d: Gaussian Generator—The χ^2 distribution with $\nu = 2$ degrees of freedom can be used to create a more efficient and accurate Gaussian generator.

a) Integrate joint Gaussian distribution $p(\vec{\chi}) = p_G(z_1)p_G(z_2)$ of the vector $\vec{\chi} = (z_1, z_2) = (\chi \cos\phi, \chi \sin\phi)$ over ϕ in cylindrical coordinates (χ, ϕ) to obtain the χ^2 distribution $p_\chi(u; 2)$ where $u = \chi^2 = \vec{\chi} \cdot \vec{\chi} = {z_1}^2 + {z_2}^2$.

b) Histogram the distribution of $u = {z_1}^2 + {z_2}^2$ into 1000 bins over $0 \le u \le 10$, using 100,000 pairs (z_1, z_2) from 1b) with $n = 100$ again, and plot together with $p_\chi(u; 2)$ from 2a).

c) Working backwards, use the fact that $p_u(x)dx = p_e(u)du$ to determine the function $u(x)$ which transforms the uniform deviate x into u following the exponential distribution $p_e(u) = \frac{1}{2}\exp(-u/2)$ defined on $0 \le u < \infty$.

d) Generate a 100,000 pairs of Gaussian deviates $\vec{\chi} = (z_1, z_2)$ by generating $\chi = \sqrt{u}$ from the exponential deviate u of 2c) and a uniform deviate ϕ in the range $0 \le \phi < 2\pi$, and finally transforming (χ, ϕ) back to rectangular coordinates (z_1, z_2). Histogram both z's in 1000 bins over $-5 \le z < 5$ and plot each together with the normalized Gaussian distribution.

2-d. Gaussian Generator (Reprise)—The general 2-d Gaussian, including both the *variances* σ_x^2, σ_y^2 and *covariance* $\sigma_{xy}^2 = \sigma_{yx}^2$, takes the form $p_G(x_1, x_2) = Ne^{-\chi^2/2}$, where N is the normalization, $\vec{\chi} = \vec{x} - \vec{\mu} = (x_1 - \mu_1, x_2 - \mu_2)$, is the vector of *deviances*, and $\chi^2 = \vec{\chi} \cdot \vec{\chi} = \chi^T W \chi$ is *weighted* by the *metric* $W = \Sigma^{-1}$, which is the inverse of the symmetric *covariance matrix*

$$\Sigma = \begin{pmatrix} \sigma_x^2 & \sigma_{xy}^2 \\ \sigma_{yx}^2 & \sigma_y^2 \end{pmatrix}.$$

If all covariances vanish (for example, in 1-d), this reduces to $\chi^2 = z_1^2 + z_2^2 + \ldots$ of H05, where the variances have been absorbed into $z_i = (x_i - \mu_i)/\sigma_i$, as before. In this case the distribution factorizes into the simple product $p_G(z_1, z_2, \ldots) = p_G(z_1)p_G(z_2)\cdots$ of 1-d Gaussians. Otherwise, one must transform to new variables $\vec{\chi}' = (u_1, u_2, \ldots)$ to perform this factorization.

a) To generate a $p_G(x_1, x_2)$ with covariance, let $u = x + y$ and $v = x - y$ be independent. Generate n =100,000 random points (u, v) centered at $\vec{\mu} = (0, 0)$ with $\sigma_u = 1$ and $\sigma_v = 2$. Draw a *scatter plot* of (x, y). [*bonus*: draw the u and v axes on the same plot]

b) Calculate the means μ_x, μ_y, variances $\sigma_x^2 = \sigma_{xx}^2$, $\sigma_y^2 = \sigma_{yy}^2$, and covariance σ_{xy}^2, where $\sigma_{ij}^2 = \sum(x_i - \mu_i)(x_j - \mu_j)/n$, for $i, j = x, y$. Calculate the *correlation coefficient* $r = \sigma_{xy}^2/\sigma_x\sigma_y$.

c) Derive the distribution $p_G(x, y)$ from $p_G(u)$ and $p_G(v)$ used in a) to determine the covariance matrix Σ and compare with b). [*bonus*: graph the contours $\chi^2 = 1$ and $\chi^2 = 2$ in a)]

d) Plot a 2d histogram of (x, y) and calculate the χ^2 statistic on all bins with greater than 10 entries. What is the likelihood of the these random points following this distribution?

e) [*bonus*: Describe the procedure for generating random pairs (x, y) from a general Gaussian distribution with means $\vec{\mu}$ and covariances Σ. How does this generalize to higher dimension?]

3-d: [*bonus*: The **Maxwell distribution** of the energy of atoms in an ideal gas is just the χ^2 distribution for $\nu = 3$ degrees of freedom because each component of $\vec{v} = (v_x, v_y, v_z)$ is normally distributed according to its Boltzmann factor $p_B(v_x) = e^{-E/kT}$, where $E = v_x^2/2m$, etc.

a) Integrate the 3-d velocity distribution over spherical shells of thickness dv to derive the Maxwell distribution of velocities $p_M(v)$. Use the Gaussian generator of 2d) to generate 100,000 velocities in units of $\sqrt{mkT}$ and histogram them together with a plot of $p_M(v)$.

b) Equivalently, integrate the joint normal distribution $p(\vec{\chi}) = p_G(z_1)p_G(z_2)p_G(z_2)$ over spherical shells of radius du for $u = \vec{\chi} \cdot \vec{\chi}$ in the vector space $\vec{\chi} = (z_1, z_2, z_3)$ to obtain $p_\chi(u; 3)$. Thus, show that the Maxwell energy distribution equals $p_\chi(v^2/mkT; 3)$.

c) Calculate the mode v_{max}, mean $\bar{v}$, and RMS $v_{rms} = \sqrt{\langle v^2 \rangle}$ of the Maxwell velocity distribution. ...

ν-d: [*bonus*: Higher dimensional χ^2 distributions are used to test the consistency of distributions, for example, in labs X03 and X04. Data are least-squares fit to a curve by minimizing a χ^2 function. In this case ν equals the number of Gaussian distributions (for example, the bins you are comparing) minus the number of constraints (for example, the parameters of a distribution or fit function).

a) Using the volume of a ν-dimensional ball $V_\nu(\chi) = \pi^{n/2}\chi^n/\Gamma(n/2+1)$, integrate the ν-d joint Gaussian distribution over hypershells to derive the χ^2 distribution $p_\chi(u; \nu)$. Plot the distribution for $\nu = 1, 2, 3, \ldots, 10$.

b) Show that as $\nu \to \infty$, $p_\chi(u; \nu)$ tends to the Gaussian distribution $p_G(u; \nu; 2\nu)$.]