

Univariate Normal distribution

In general, it has two parameters, μ and σ (mean and standard deviation). A special case is **standardized** Normal distribution, with the mean of 0 and standard deviation equal to 1. Any general X can be converted to standardized Z by

$$Z = \frac{X - \mu}{\sigma}$$

and reverse

$$X = \sigma Z + \mu$$

It is usually a lot easier to deal with Z , and then convert the results to X .

We should recall that in general, if $X \in \mathcal{N}(\mu, \sigma)$, then

$$aX + b \in \mathcal{N}(a\mu + b, |a|\sigma) \quad (1)$$

where a and b are constants.

The probability density function (PDF from now on) of Z and X is

$$f_Z(z) = \frac{\exp(-\frac{z^2}{2})}{\sqrt{2\pi}}$$
$$f_X(x) = \frac{\exp(-\frac{(x-\mu)^2}{2\sigma^2})}{\sqrt{2\pi}\sigma}$$

respectively.

Similarly, the moment generating function (MGF) is

$$M_z(t) = \exp\left(\frac{t^2}{2}\right)$$
$$M_x(t) = e^{\mu t} \cdot M_z(\sigma t) = \exp\left(\frac{\sigma^2 t^2}{2} + \mu t\right)$$

Bivariate Normal distribution

Again, we consider two versions, the general (X and Y) and standardized (Z_1 and Z_2). The general distribution is defined by 5 parameters (the individual means and variances, plus the correlation coefficient ρ), the standardized version has only one, namely ρ .

The two joint (bivariate) PDF's are

$$f_{zz}(z_1, z_2) = \frac{\exp\left(-\frac{z_1^2 + z_2^2 - 2\rho z_1 z_2}{2(1-\rho^2)}\right)}{2\pi\sqrt{1-\rho^2}}$$
$$f_{xy}(x, y) = \frac{\exp\left(-\frac{\left(\frac{x-\mu_1}{\sigma_1}\right)^2 + \left(\frac{y-\mu_2}{\sigma_2}\right)^2 - 2\rho\left(\frac{x-\mu_1}{\sigma_1}\right)\left(\frac{y-\mu_2}{\sigma_2}\right)}{2(1-\rho^2)}\right)}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}}$$

for the standardized and general case, respectively.

Similarly, the joint MGFs are

$$\begin{aligned} M_{zz}(t_1, t_2) &= \exp\left(\frac{t_1^2 + t_2^2 + 2\rho t_1 t_2}{2}\right) \\ M_{xy}(t_1, t_2) &= e^{\mu_1 t_1 + \mu_2 t_2} \cdot M_{zz}(\sigma_1 t_1, \sigma_2 t_2) = \\ &= \exp\left(\frac{\sigma_1^2 t_1^2 + \sigma_2^2 t_2^2 + 2\rho\sigma_1\sigma_2 t_1 t_2}{2} + \mu_1 t_1 + \mu_2 t_2\right) \end{aligned}$$

We should remember that a joint MGF enables us to find joint simple moments of the distribution by

$$\mathbb{E}(X^n Y^m) = \left. \frac{\partial^{(n+m)} M_{xy}(t_1, t_2)}{\partial t_1^n \partial t_2^m} \right|_{t_1=t_2=0}$$

Also, we can easily find the MGF of a **marginal** distribution of X by setting $t_2 = 0$. This tells us immediately that both Z_1 and Z_2 are standardized Normal.

But now, there is one extra issue to investigate:

Conditional distribution of $Z_1 \mid Z_2 = \mathbf{z}_2$ (using boldface implies that \mathbf{z}_2 is no longer variable, but is assumed to have one specific 'observed' value).

To find the corresponding (univariate!) PDF, we have to do this:

$$\frac{f_{zz}(z_1, \mathbf{z}_2)}{f_z(\mathbf{z}_2)} = \frac{\exp\left(-\frac{z_1^2 + \mathbf{z}_2^2 - 2\rho z_1 \mathbf{z}_2}{2(1-\rho^2)}\right)}{2\pi\sqrt{1-\rho^2}} \div \frac{\exp\left(-\frac{\mathbf{z}_2^2}{2}\right)}{\sqrt{2\pi}} = \frac{\exp\left(-\frac{(z_1 - \rho\mathbf{z}_2)^2}{2(1-\rho^2)}\right)}{\sqrt{2\pi}\sqrt{1-\rho^2}}$$

by simple algebra. The result can be identified as $\mathcal{N}(\rho\mathbf{z}_2, \sqrt{1-\rho^2})$, i.e. Normal, with mean of $\rho\mathbf{z}_2$ and standard deviation equal to $\sqrt{1-\rho^2}$ (smaller than what it was marginally, i.e. before we observed Z_2). Note that many textbooks use this notation, but put variance in place of standard deviation.

How do we utilize this result to find the conditional distribution of X given that Y has been observed to have a value of \mathbf{y} . Well, we could use the same procedure, but the algebra would get a lot more messier, or we can do this:

We already know that the conditional distribution of $\frac{X-\mu_1}{\sigma_1} \mid \frac{Y-\mu_2}{\sigma_2} = \frac{\mathbf{y}-\mu_2}{\sigma_2}$ is $\mathcal{N}\left(\rho\frac{\mathbf{y}-\mu_2}{\sigma_2}, \sqrt{1-\rho^2}\right)$. So we have the conditional distribution of $\frac{X-\mu_1}{\sigma_1} \mid Y = \mathbf{y}$ (which is clearly the same thing). Now, using (1), which holds conditionally as well, we find that the conditional distribution of $X \mid Y = \mathbf{y}$ is

$$\mathcal{N}\left(\mu_1 + \sigma_1\rho\frac{\mathbf{y}-\mu_2}{\sigma_2}, \sigma_1\sqrt{1-\rho^2}\right)$$

Multivariate Normal Distribution

Consider N independent, standardized, Normally distributed random vari-

ables. Their joint PDF is

$$\begin{aligned} f(z_1, z_2, \dots, z_N) &= (2\pi)^{-N/2} \cdot \exp\left(-\frac{\sum_{i=1}^N z_i^2}{2}\right) \\ &\equiv (2\pi)^{-N/2} \cdot \exp\left(-\frac{\mathbf{z}^T \mathbf{z}}{2}\right) \end{aligned}$$

Corresponding MGF

$$\exp\left(\frac{\sum_{i=1}^N t_i^2}{2}\right) \equiv \exp\left(\frac{\mathbf{t}^T \mathbf{t}}{2}\right)$$

The following linear transformation

$$\mathbf{X} = \mathbb{B} \mathbf{Z} + \boldsymbol{\mu}$$

where \mathbb{B} is an arbitrary (regular) N by N matrix, defines a new set of N random variables having a *general* Normal distribution.

The corresponding PDF is

$$\begin{aligned} &\frac{|\det(\mathbb{B}^{-1})|}{\sqrt{(2\pi)^N}} \exp\left(-\frac{(\mathbf{x} - \boldsymbol{\mu})^T (\mathbb{B}^{-1})^T \mathbb{B}^{-1} (\mathbf{x} - \boldsymbol{\mu})}{2}\right) \\ &= \frac{1}{\sqrt{(2\pi)^N \det(\mathbb{V})}} \exp\left(-\frac{(\mathbf{x} - \boldsymbol{\mu})^T \mathbb{V}^{-1} (\mathbf{x} - \boldsymbol{\mu})}{2}\right) \end{aligned}$$

since $\mathbf{Z} = \mathbb{B}^{-1}(\mathbf{X} - \boldsymbol{\mu})$, which further implies that

$$\begin{aligned} &(\mathbf{X} - \boldsymbol{\mu})^T (\mathbb{B}^{-1})^T \mathbb{B}^{-1} (\mathbf{X} - \boldsymbol{\mu}) \\ &= (\mathbf{X} - \boldsymbol{\mu})^T (\mathbb{B} \mathbb{B}^T)^{-1} (\mathbf{X} - \boldsymbol{\mu}) \\ &= (\mathbf{X} - \boldsymbol{\mu})^T \mathbb{V}^{-1} (\mathbf{X} - \boldsymbol{\mu}) \end{aligned}$$

which must thus have the χ_N^2 distribution.

The corresponding MGF is

$$\begin{aligned} &\mathbb{E} \left\{ \exp \left[\mathbf{t}^T (\mathbb{B} \mathbf{Z} + \boldsymbol{\mu}) \right] \right\} \\ &= \exp(\mathbf{t}^T \boldsymbol{\mu}) \cdot \exp\left(\frac{\mathbf{t}^T \mathbb{B} \mathbb{B}^T \mathbf{t}}{2}\right) \\ &= \exp(\mathbf{t}^T \boldsymbol{\mu}) \cdot \exp\left(\frac{\mathbf{t}^T \mathbb{V} \mathbf{t}}{2}\right) \end{aligned}$$

where $\mathbb{V} \equiv \mathbb{B} \mathbb{B}^T$ is the corresponding variance-covariance matrix (must be symmetric and positive definite). This shows each marginal distribution remains Normal, without a change in the corresponding $\boldsymbol{\mu}$ and \mathbb{V} elements.

Note that there are many different \mathbb{B} 's resulting in the same \mathbb{V} .

To generate a set of normally distributed random variables having a given variance-covariance matrix \mathbb{V} requires us to solve for the corresponding \mathbb{B} (Maple provides us with \mathbf{Z} only, when typing: `stats[random,normald](20)`). There is infinitely many such \mathbb{B} matrices, one of them (easy to construct) is lower triangular.

Partial correlation coefficient

The variance-covariance matrix can be converted into the correlation matrix:

$$\mathbb{C}_{ij} \equiv \frac{\mathbb{V}_{ij}}{\sqrt{\mathbb{V}_{ii} \cdot \mathbb{V}_{jj}}}$$

The main diagonal elements of \mathbb{C} are all equal to 1 (the correlation of X_i with itself).

Suppose we have three normally distributed random variables with a given variance-covariance matrix. The conditional distribution of X_2 and X_3 given that $X_1 = \underline{x}_1$ has a correlation coefficient independent of the value of \underline{x}_1 . It is called the **partial correlation coefficient**, and denoted $\rho_{23|1}$. Let us find its value in terms of the ordinary correlation coefficients..

Any correlation coefficient is independent of scaling. We can thus choose the three X 's to be standardized (but *not* independent), having the following 3-D PDF:

$$\frac{1}{\sqrt{(2\pi)^3 \det(\mathbb{C})}} \cdot \exp\left(-\frac{\mathbf{z}^T \mathbb{C}^{-1} \mathbf{z}}{2}\right)$$

where

$$\mathbb{C} = \begin{bmatrix} 1 & \rho_{12} & \rho_{13} \\ \rho_{12} & 1 & \rho_{23} \\ \rho_{13} & \rho_{23} & 1 \end{bmatrix}$$

Since the marginal PDF of z_1 is

$$\frac{1}{\sqrt{2\pi}} \cdot \exp\left(-\frac{z_1^2}{2}\right)$$

the conditional PDF we need is

$$\frac{1}{\sqrt{(2\pi)^2 \det(\mathbb{C})}} \cdot \exp\left(-\frac{\mathbf{z}^T \mathbb{C}^{-1} \mathbf{z} - z_1^2}{2}\right)$$

The information about the five parameters of the corresponding bi-variate dis-

tribution is in

$$\begin{aligned} \mathbf{z}^T \mathbf{C}^{-1} \mathbf{z} - z_1^2 = & \frac{\left(\frac{z_2 - \rho_{12} z_1}{\sqrt{1 - \rho_{12}^2}} \right)^2 + \left(\frac{z_3 - \rho_{13} z_1}{\sqrt{1 - \rho_{13}^2}} \right)^2}{1 - \left(\frac{\rho_{23} - \rho_{12} \rho_{13}}{\sqrt{1 - \rho_{12}^2} \sqrt{1 - \rho_{13}^2}} \right)^2} \\ & - 2 \frac{\rho_{23} - \rho_{12} \rho_{13}}{\sqrt{1 - \rho_{12}^2} \sqrt{1 - \rho_{13}^2}} \left(\frac{z_2 - \rho_{12} z_1}{\sqrt{1 - \rho_{12}^2}} \right) \left(\frac{z_3 - \rho_{13} z_1}{\sqrt{1 - \rho_{13}^2}} \right) \end{aligned}$$

which, in terms of the two conditional means and standard deviations agrees with what we know from MATH 2F81. The extra parameter is our partial correlation coefficient

$$\rho_{23|1} = \frac{\rho_{23} - \rho_{12} \cdot \rho_{13}}{\sqrt{1 - \rho_{12}^2} \sqrt{1 - \rho_{13}^2}}$$

or

$$\rho_{ij|k} = \frac{\rho_{ij} - \rho_{ik} \cdot \rho_{jk}}{\sqrt{1 - \rho_{ik}^2} \sqrt{1 - \rho_{jk}^2}}$$

in general.

To get the conditional mean, standard deviation and correlation coefficient given more than one X has been observed, one can 'iterate' in the following manner:

$$\begin{aligned} \mu_{i|K\ell} &= \mu_{i|K} + \sigma_{i|K} \rho_{i\ell|K} \frac{\bar{x}_\ell - \mu_{\ell|K}}{\sigma_{\ell|K}} \\ \sigma_{i|K\ell} &= \sigma_{i|K} \sqrt{1 - \rho_{i\ell|K}^2} \\ \rho_{ij|K\ell} &= \frac{\rho_{ij|K} - \rho_{i\ell|K} \cdot \rho_{j\ell|K}}{\sqrt{1 - \rho_{i\ell|K}^2} \sqrt{1 - \rho_{j\ell|K}^2}} \end{aligned}$$

etc., where K now represents any number of indices (corresponding to the already observed X 's).

A more direct way to find these is presented in the following section.

General conditional distribution:

When the N variables are partitioned into two subsets, say $\mathbf{X}_{(1)}$ and $\mathbf{X}_{(2)}$, with means $\boldsymbol{\mu}_{(1)}$ and $\boldsymbol{\mu}_{(2)}$, and the variance-covariance matrix

$$\begin{bmatrix} \mathbb{V}_{11} & \mathbb{V}_{12} \\ \mathbb{V}_{21} & \mathbb{V}_{22} \end{bmatrix}$$

whose inverse is

$$\mathbb{A} = \begin{bmatrix} (\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})^{-1} & -(\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})^{-1} \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \\ -(\mathbb{V}_{22} - \mathbb{V}_{21} \mathbb{V}_{11}^{-1} \mathbb{V}_{12})^{-1} \mathbb{V}_{21} \mathbb{V}_{11}^{-1} & (\mathbb{V}_{22} - \mathbb{V}_{21} \mathbb{V}_{11}^{-1} \mathbb{V}_{12})^{-1} \end{bmatrix}$$

The conditional PDF of $\mathbf{X}_{(1)}$ given $\mathbf{X}_{(2)} = \underline{\mathbf{x}}_{(2)}$ is obviously

$$\frac{1}{\sqrt{(2\pi)^N \det(\mathbb{V})}} \exp\left(-\frac{(\mathbf{x} - \boldsymbol{\mu})^T \mathbb{V}^{-1} (\mathbf{x} - \boldsymbol{\mu})}{2}\right) \div$$

$$\frac{1}{\sqrt{(2\pi)^{N_2} \det(\mathbb{V}_{22})}} \exp\left(-\frac{(\underline{\mathbf{x}}_{(2)} - \boldsymbol{\mu}_{(2)})^T \mathbb{V}_{22}^{-1} (\underline{\mathbf{x}}_{(2)} - \boldsymbol{\mu}_{(2)})}{2}\right)$$

i.e. still Normal. To get the resulting (conditional) variance-covariance matrix, all we need to do is to invert the corresponding block of \mathbb{A} , getting

$$\mathbb{V}_{(1,2)} \equiv \mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21}$$

Similarly, the conditional mean (say $\boldsymbol{\mu}_{(1|2)}$) is found based on

$$-\mathbf{x}_{(1)}^T \mathbb{V}_{(1|2)}^{-1} \boldsymbol{\mu}_{(1|2)} = -\mathbf{x}_{(1)}^T (\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})^{-1} \boldsymbol{\mu}_{(1)} -$$

$$\mathbf{x}_{(1)}^T (\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})^{-1} \mathbb{V}_{12} \mathbb{V}_{22}^{-1} (\underline{\mathbf{x}}_{(2)} - \boldsymbol{\mu}_{(2)})$$

It equals

$$\boldsymbol{\mu}_{(1|2)} = \boldsymbol{\mu}_{(1)} + \mathbb{V}_{12} \mathbb{V}_{22}^{-1} (\underline{\mathbf{x}}_{(2)} - \boldsymbol{\mu}_{(2)})$$

Proof:

$$[\mathbf{x}_{(1)} - \boldsymbol{\mu}_{(1)} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} (\underline{\mathbf{x}}_{(2)} - \boldsymbol{\mu}_{(2)})]^T (\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})^{-1} [\mathbf{x}_{(1)} - \boldsymbol{\mu}_{(1)} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} (\underline{\mathbf{x}}_{(2)} - \boldsymbol{\mu}_{(2)})]$$

$$= (\mathbf{x}_{(1)} - \boldsymbol{\mu}_{(1)})^T (\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})^{-1} (\mathbf{x}_{(1)} - \boldsymbol{\mu}_{(1)})$$

$$- (\underline{\mathbf{x}}_{(2)} - \boldsymbol{\mu}_{(2)})^T \mathbb{V}_{22}^{-1} \mathbb{V}_{21} (\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})^{-1} (\mathbf{x}_{(1)} - \boldsymbol{\mu}_{(1)})$$

$$- (\mathbf{x}_{(1)} - \boldsymbol{\mu}_{(1)})^T (\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})^{-1} \mathbb{V}_{12} \mathbb{V}_{22}^{-1} (\underline{\mathbf{x}}_{(2)} - \boldsymbol{\mu}_{(2)})$$

$$+ (\underline{\mathbf{x}}_{(2)} - \boldsymbol{\mu}_{(2)})^T \mathbb{V}_{22}^{-1} \mathbb{V}_{21} (\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})^{-1} \mathbb{V}_{12} \mathbb{V}_{22}^{-1} (\underline{\mathbf{x}}_{(2)} - \boldsymbol{\mu}_{(2)})$$

Since

$$\mathbb{V}_{21} (\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})^{-1} \equiv \mathbb{V}_{22} (\mathbb{V}_{22} - \mathbb{V}_{21} \mathbb{V}_{11}^{-1} \mathbb{V}_{12})^{-1} \mathbb{V}_{21} \mathbb{V}_{11}^{-1}$$

the last matrix equals

$$(\mathbb{V}_{22} - \mathbb{V}_{21} \mathbb{V}_{11}^{-1} \mathbb{V}_{12})^{-1} \mathbb{V}_{21} \mathbb{V}_{11}^{-1} \mathbb{V}_{12} \mathbb{V}_{22}^{-1}$$

$$= (\mathbb{V}_{22} - \mathbb{V}_{21} \mathbb{V}_{11}^{-1} \mathbb{V}_{12})^{-1} (\mathbb{V}_{21} \mathbb{V}_{11}^{-1} \mathbb{V}_{12} - \mathbb{V}_{22} + \mathbb{V}_{22}) \mathbb{V}_{22}^{-1}$$

$$= (\mathbb{V}_{22} - \mathbb{V}_{21} \mathbb{V}_{11}^{-1} \mathbb{V}_{12})^{-1} - \mathbb{V}_{22}^{-1}$$

in full agreement with the conditional PDF quoted above.

Finally, to show that $\det(\mathbb{V}) \div \det(\mathbb{V}_{22}) = \det(\mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21})$, take the determinant of each side of

$$\begin{bmatrix} \mathbb{I} & -\mathbb{V}_{12} \mathbb{V}_{22}^{-1} \\ \mathbb{O} & \mathbb{V}_{22}^{-1} \end{bmatrix} \begin{bmatrix} \mathbb{V}_{11} & \mathbb{V}_{12} \\ \mathbb{V}_{21} & \mathbb{V}_{22} \end{bmatrix} = \begin{bmatrix} \mathbb{V}_{11} - \mathbb{V}_{12} \mathbb{V}_{22}^{-1} \mathbb{V}_{21} & \mathbb{O} \\ \mathbb{V}_{22}^{-1} \mathbb{V}_{21} & \mathbb{I} \end{bmatrix}$$

Estimating μ , ρ and ρ

The standard method of finding good **estimators** of distribution parameters is called **Maximum Likelihood (ML)** technique. We will demonstrate it on the general Normal bivariate case.

First, take the natural logarithm of the PDF of a random independent sample of n pairs of X and Y observations (product of individual PDFs), namely

$$\begin{aligned} & \ln \prod_{i=1}^n \frac{\exp\left(-\frac{(\frac{x_i-\mu_1}{\sigma_1})^2 + (\frac{y_i-\mu_2}{\sigma_2})^2 - 2\rho(\frac{x_i-\mu_1}{\sigma_1})(\frac{y_i-\mu_2}{\sigma_2})}{2(1-\rho^2)}\right)}{2\pi\sigma_1\sigma_2\sqrt{1-\rho^2}} \\ &= -\frac{\sum_{i=1}^n \left[\left(\frac{x_i-\mu_1}{\sigma_1}\right)^2 + \left(\frac{y_i-\mu_2}{\sigma_2}\right)^2 - 2\rho\left(\frac{x_i-\mu_1}{\sigma_1}\right)\left(\frac{y_i-\mu_2}{\sigma_2}\right) \right]}{2(1-\rho^2)} \\ & \quad -n \ln(2\pi) - n \ln \sigma_1 - n \ln \sigma_2 - \frac{n}{2} \ln(1-\rho^2) \end{aligned}$$

Then, replace the x_i and y_i variables by the actual sample values (switch to boldface), and maximize this expression with respect to the $\mu_1, \mu_2, \sigma_1, \sigma_2$ and ρ parameters (by setting the corresponding derivatives equal to zero):

$$\begin{aligned} & \sum_{i=1}^n \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1}\right) - \rho \sum_{i=1}^n \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2}\right) = 0 \\ & \sum_{i=1}^n \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2}\right) - \rho \sum_{i=1}^n \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1}\right) = 0 \\ & \frac{1}{\sigma_1^3} \sum_{i=1}^n (\mathbf{x}_i - \mu_1)^2 - \frac{\rho}{\sigma_1^2} \sum_{i=1}^n (\mathbf{x}_i - \mu_1) \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2}\right) = \frac{n}{\sigma_1} (1 - \rho^2) \\ & \frac{1}{\sigma_2^3} \sum_{i=1}^n (\mathbf{y}_i - \mu_2)^2 - \frac{\rho}{\sigma_2^2} \sum_{i=1}^n (\mathbf{y}_i - \mu_2) \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1}\right) = \frac{n}{\sigma_2} (1 - \rho^2) \\ & \frac{1}{1-\rho^2} \sum_{i=1}^n \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1}\right) \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2}\right) - \frac{\rho}{(1-\rho^2)^2} \\ & \cdot \sum_{i=1}^n \left[\left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1}\right)^2 + \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2}\right)^2 - 2\rho \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1}\right) \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2}\right) \right] \\ & = -\frac{n\rho}{(1-\rho^2)} \end{aligned}$$

The first two equations are solved by making both $\sum_{i=1}^n (\mathbf{x}_i - \mu_1)$ and $\sum_{i=1}^n (\mathbf{y}_i - \mu_2)$ equal to zero, which means

$$\hat{\mu}_1 = \frac{\sum_{i=1}^n \mathbf{x}_i}{n} \equiv \bar{\mathbf{x}}$$

$$\hat{\mu}_2 = \frac{\sum_{i=1}^n \mathbf{y}_i}{n} \equiv \bar{\mathbf{y}}$$

(the usual sample means).

The next three equations can be re-written as

$$\begin{aligned} \sum_{i=1}^n \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1} \right)^2 - \rho \sum_{i=1}^n \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1} \right) \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2} \right) &= n(1 - \rho^2) \\ \sum_{i=1}^n \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2} \right)^2 - \rho \sum_{i=1}^n \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1} \right) \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2} \right) &= n(1 - \rho^2) \\ (1 - \rho^2) \sum_{i=1}^n \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1} \right) \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2} \right) - \\ - \rho \sum_{i=1}^n \left[\left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1} \right)^2 + \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2} \right)^2 - 2\rho \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1} \right) \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2} \right) \right] & \\ = -n\rho(1 - \rho^2) & \end{aligned}$$

Using the first two equations, the second term of the last equation can be simplified to $-2\rho n(1 - \rho^2)$. The last equation thus reads

$$(1 - \rho^2) \sum_{i=1}^n \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1} \right) \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2} \right) = n\rho(1 - \rho^2)$$

which implies

$$\rho = \frac{\sum_{i=1}^n (\mathbf{x}_i - \mu_1)(\mathbf{y}_i - \mu_2)}{n \sigma_1 \sigma_2}$$

Substituting this for the second term of the first two equations makes the second term read $-n\rho^2$. Cancelling with the corresponding term on the right hand side yields

$$\begin{aligned} \sum_{i=1}^n \left(\frac{\mathbf{x}_i - \mu_1}{\sigma_1} \right)^2 &= n \\ \sum_{i=1}^n \left(\frac{\mathbf{y}_i - \mu_2}{\sigma_2} \right)^2 &= n \end{aligned}$$

and the following final estimators:

$$\begin{aligned} \hat{\sigma}_1 &= \sqrt{\frac{\sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})^2}{n}} \\ \hat{\sigma}_2 &= \sqrt{\frac{\sum_{i=1}^n (\mathbf{y}_i - \bar{\mathbf{y}})^2}{n}} \end{aligned}$$

and

$$\hat{\rho} = \frac{\sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})(\mathbf{y}_i - \bar{\mathbf{y}})}{\sqrt{\sum_{i=1}^n (\mathbf{x}_i - \bar{\mathbf{x}})^2 \cdot \sum_{i=1}^n (\mathbf{y}_i - \bar{\mathbf{y}})^2}}$$

(sample correlation coefficient), more commonly denoted r .

We know that \bar{X} , \bar{Y} , $\frac{\sum_{i=1}^n (X_i - \bar{X})^2}{\sigma_1^2}$ and $\frac{\sum_{i=1}^n (Y_i - \bar{Y})^2}{\sigma_2^2}$ have simple distributions, the distribution of r is a lot more complicated; this is its PDF:

$$\frac{(n-2) \cdot \Gamma(n-1) \cdot (1-\rho^2)^{\frac{n-1}{2}}}{\sqrt{2\pi} \cdot \Gamma(n-\frac{1}{2})} \cdot \frac{(1-r^2)^{\frac{n}{2}-2}}{(1-\rho r)^{n-\frac{3}{2}}} \cdot F(\frac{1}{2}, \frac{1}{2}; n-\frac{1}{2}; \frac{1+\rho r}{2})$$

where F is the hypergeometric function defined by

$$F(a, b; c; x) = 1 + \frac{a \cdot b}{c \cdot 1!} x + \frac{a(a+1) \cdot b(b+1)}{c(c+1) \cdot 2!} x^2 + \frac{a(a+1)(a+2) \cdot b(b+1)(b+2)}{c(c+1)(c+2) \cdot 3!} x^3 + \dots$$

This result is due to Hotelling (1953).

The corresponding expected value of r is

$$\frac{\rho \Gamma(\frac{n}{2})^2}{\Gamma(\frac{n-1}{2})\Gamma(\frac{n+1}{2})} F(\frac{1}{2}, \frac{1}{2}; \frac{n+1}{2}; \rho^2)$$

so the estimator is clearly biased. Expanded in powers of $\frac{1}{n}$, this becomes

$$\rho - \frac{\rho(1-\rho^2)}{2n} - \frac{3\rho(1-\rho^2)(1+3\rho^2)}{8n^2} \dots$$

One finds that the distribution of $\operatorname{arctanh}(r)$ converges to Normal distribution a lot faster (it has a smaller bias, and a lot smaller skewness).

To derive this PDF, we first need some formulas concerning

n dimensional sphere

of radius r is defined as the following set

$$x_1^2 + x_2^2 + \dots + x_n^2 \leq r^2$$

Its volume $V_n(r) = r^n V_n(1)$ and surface area $S_n(r)$ are clearly related by

$$S_n(r) = \frac{dV_n(r)}{dr} = nr^{n-1} V_n(1) = r^{n-1} S_n(1)$$

It is easier to find S_n from

$$\pi^{n/2} = \int \dots \int \exp(-x_1^2 - x_2^2 - \dots - x_n^2) dx_1 dx_2 \dots dx_n =$$

$$\begin{aligned} S_n(1) \int_0^\infty r^{n-1} \exp(-r^2) dr &= \\ \frac{S_n(1)}{2} \int_0^\infty y^{n/2-1} \exp(-y) dy &= \frac{S_n(1)}{2} \Gamma\left(\frac{n}{2}\right) \end{aligned}$$

which implies that

$$S_n(1) = \frac{2\pi^{n/2}}{\Gamma\left(\frac{n}{2}\right)}$$

$$S_n(r) = \frac{2\pi^{n/2}r^{n-1}}{\Gamma\left(\frac{n}{2}\right)}$$

and

$$V_n(r) = \frac{2\pi^{n/2}r^n}{n\Gamma\left(\frac{n}{2}\right)}$$

Sample from standardized bi-variate Normal distribution

has a PDF given by

$$(2\pi)^{-n}(1-\rho^2)^{-n/2} \exp\left(-\frac{\sum(x_i^2 + y_i^2 - 2\rho x_i y_i)}{2(1-\rho^2)}\right) dx_1 \dots dy_n =$$

$$(2\pi)^{-n}(1-\rho^2)^{-n/2} \cdot$$

$$\exp\left(-\frac{n(s_1^2 + \bar{x}^2 + s_2^2 + \bar{y}^2 - 2\rho r s_1 s_2 - 2\rho \bar{x} \bar{y})}{2(1-\rho^2)}\right) dx_1 \dots dy_n$$

where

$$\bar{x} = \frac{\sum x_i}{n} \quad \bar{y} = \frac{\sum y_i}{n}$$

$$s_1^2 = \frac{\sum (x_i - \bar{x})^2}{n} \quad s_2^2 = \frac{\sum (y_i - \bar{y})^2}{n}$$

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{n s_1 s_2}$$

All we have to do now is to figure out the volume of the $2n$ dimensional region filled by taking each of the five quantities s_1 , s_2 , \bar{x} , \bar{y} and r , and increasing them by ds_1 , ds_2 , $d\bar{x}$, $d\bar{y}$ and dr respectively.

We know that

$$\frac{\sum x_i}{\sqrt{n}} = \sqrt{n}\bar{x}$$

is a plane in the 'first' n dimensions (the x -space), going through $(\bar{x}, \bar{x}, \dots, \bar{x})$ and having $\frac{(1, 1, \dots, 1)}{\sqrt{n}}$ as normal. Similarly

$$\sum (x_i - \bar{x})^2 = n s_1^2$$

is an n dimensional sphere centered on $(\bar{x}, \bar{x}, \dots, \bar{x})$, with the radius of $s_1 \sqrt{n}$. The plane cuts the sphere in 'the middle', thus creating (the corresponding cross section) an $n - 1$ dimensional sphere, whose surface is

$$\frac{2\pi^{(n-1)/2} s_1^{n-2} n^{(n-2)/2}}{\Gamma\left(\frac{n-1}{2}\right)}$$

This needs to be further multiplied (since the $\sqrt{n}ds_1$ and $\sqrt{n}d\bar{x}$ directions are perpendicular) by $n d\bar{x} ds_1$.

Similar argument can be made in the y space, except now we need to keep the $(y_1 - \bar{y}, y_2 - \bar{y}, \dots, y_n - \bar{y})$ vector at a fixed angle to $(x_1 - \bar{x}, x_2 - \bar{x}, \dots, x_n - \bar{x})$, an angle whose cos is r . This reduces the $n - 1$ dimensional spherical surface of radius $s_2\sqrt{n}$ to an $n - 2$ dimensional spherical surface of radius $s_2\sqrt{n(1 - r^2)}$. This then contributes

$$\frac{2\pi^{(n-2)/2}s_1^{n-3}n^{(n-3)/2}(1-r^2)^{(n-3)/2}}{\Gamma\left(\frac{n-2}{2}\right)}n d\bar{y} ds_2 \frac{s_2\sqrt{n}}{\sqrt{1-r^2}}dr$$

So now we have

$$\frac{n^n(1-r^2)^{(n-4)/2}s_1^{n-2}s_2^{n-2}}{2^{n-2}\pi^{3/2}(1-\rho^2)^{n/2}\Gamma\left(\frac{n-1}{2}\right)\Gamma\left(\frac{n-2}{2}\right)} \cdot \exp\left(-\frac{n(s_1^2 + \bar{x}^2 + s_2^2 + \bar{y}^2 - 2\rho r s_1 s_2 - 2\rho\bar{x}\bar{y})}{2(1-\rho^2)}\right) d\bar{x}d\bar{y}ds_1ds_2dr$$

(R. A. Fisher, 1915).

The $d\bar{x}d\bar{y}$ integration (separable, from $-\infty$ to ∞ each) can be carried out easily, yielding

$$\frac{n^{n-1}(1-r^2)^{(n-4)/2}s_1^{n-2}s_1^{n-2}}{\pi(1-\rho^2)^{(n-1)/2}(n-3)!} \cdot \exp\left(-\frac{n(s_1^2 + s_2^2 - 2\rho r s_1 s_2)}{2(1-\rho^2)}\right) ds_1 ds_2 dr$$

(we have also replaced $2^{n-3}\Gamma\left(\frac{n-1}{2}\right)\Gamma\left(\frac{n-2}{2}\right)$ by $(n-3)!\sqrt{\pi}$).

To integrate over s_1 and s_2 , we realize that the $s_1 > s_2$ and $s_1 < s_2$ regions must contribute the same amount (the function is $s_1 \leftrightarrow s_2$ symmetric), so we multiply the integrand by 2 and integrate over the latter.

Introducing the following one-to-one transformation (ξ goes from 0 to ∞ , η from 1 to infinity):

$$\begin{aligned} \xi &= s_1 s_2 \\ \eta &= \frac{1}{2} \left(\frac{s_1}{s_2} + \frac{s_2}{s_1} \right) = \frac{s_1^2 + s_2^2}{2s_1 s_2} \end{aligned}$$

whose Jacobian is

$$\det \left[\begin{array}{cc} \frac{s_2}{\frac{1}{2} \left(\frac{1}{s_2} - \frac{s_2}{s_1^2} \right)} & \frac{s_1}{\frac{1}{2} \left(\frac{1}{s_1} - \frac{s_1}{s_2^2} \right)} \end{array} \right] = \left(\frac{s_2}{s_1} - \frac{s_1}{s_2} \right) = 2\sqrt{\eta^2 - 1}$$

results in

$$\frac{n^{n-1}(1-r^2)^{(n-4)/2}\xi^{n-2}}{\pi(1-\rho^2)^{(n-1)/2}(n-3)!} \exp\left(-\frac{n(\eta - \rho r)\xi}{1-\rho^2}\right) \frac{d\xi d\eta}{\sqrt{\eta^2 - 1}} dr$$

which can be easily integrated over ξ , getting

$$\frac{(n-2)(1-r^2)^{(n-4)/2}}{\pi(1-\rho^2)^{(n-1)/2}} \cdot \left(\frac{1-\rho^2}{\eta-\rho r}\right)^{n-1} \frac{d\eta}{\sqrt{\eta^2-1}} dr$$

And the last substitution is

$$\eta = \frac{1-\rho r z}{1-z}$$

(z going from 0 to 1) replaces $\eta - \rho r$ by

$$\frac{1-\rho r}{1-z}$$

$d\eta$ by

$$\frac{1-\rho r}{(1-z)^2} dz$$

and $\sqrt{\eta^2-1}$ by

$$\frac{\sqrt{2z(1-\rho r)} \cdot \sqrt{1-\frac{1+\rho r}{2}z}}{1-z}$$

getting

$$\frac{(n-2)(1-r^2)^{(n-4)/2} z^{-1/2} \left(1-\frac{1+\rho r}{2}z\right)^{-1/2}}{\sqrt{2}\pi} \cdot \frac{(1-\rho^2)^{(n-1)/2} (1-z)^{n-2}}{(1-\rho r)^{n-3/2}} dz dr$$

Maple tells us that

$$\int_0^1 z^k (1-z)^m (1-az)^\ell dz = \frac{\Gamma(k+1)\Gamma(m+1)}{\Gamma(k+m+2)} F(-\ell, k+1; m+k+2; a)$$

which in our case means

$$\frac{\Gamma(\frac{1}{2})\Gamma(n-1)}{\Gamma(n-\frac{1}{2})} F(\frac{1}{2}, \frac{1}{2}; n-\frac{1}{2}; \frac{1+\rho r}{2})$$

The final answer is thus

$$\frac{(n-2)(n-2)!(1-\rho^2)^{(n-1)/2}}{\sqrt{2}\pi\Gamma(n-\frac{1}{2})} \cdot \frac{(1-r^2)^{(n/2-2)}}{(1-\rho r)^{n-3/2}} F(\frac{1}{2}, \frac{1}{2}; n-\frac{1}{2}; \frac{1+\rho r}{2}) dr$$