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Holonomic properties and recurrence formula for the distribution of sample correlation coefficient

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Abstract.
This paper presents the holonomic properties and recurrence formula for the distribution of the sample correlation coefficient. The probability density function (pdf) is holonomic. Therefore, it is computed exactly based on the holonomic gradient method (HGM). The initial values for computation are expressed in terms of Gaussian hypergeometric functions with specific parameters that can be transformed to a rational equation of gamma functions. Using the integral algorithm in the D-module theory, the cumulative distribution function (cdf) is also holonomic. It can be computed using HGM. Next, we derive the recurrence formula for the Gaussian hypergeometric function related to the degrees of freedom and apply it to exact computation of the pdf under a fixed population correlation coefficient and increasing degrees of freedom. We conclude with discussion of the quantile function of the sample correlation coefficient which satisfies a nonlinear differential equation of second order.

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§1. Introduction

First, we let $(X_1, Y_1), \ldots, (X_N, Y_N)$ be random vectors that are distributed identically and independently as a bivariate normal distribution with population correlation coefficient $\rho = \rho(X, Y)$. For the distribution of the sample correlation coefficient, we assume means $\mu_X = \mu_Y = 0$ and variances

$\sigma_X^2 = \sigma_Y^2 = 1$ without loss of generality. Then the sample correlation coefficient r is defined as $r = s_{XY}/(s_X s_Y)$, where $s_{XY} = \frac{1}{N}\sum_{i=1}^{N}(X_i - \bar{X})(Y_i - \bar{Y})$, $s_X = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(X_i - \bar{X})^2}$, $s_Y = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(Y_i - \bar{Y})^2}$, $\bar{X}$ and $\bar{Y}$ respectively denote the sample means of X and Y. The probability density function (pdf) $f(r)$ (written here as $f(r,\rho)$) is given by [8] as

(1.1)
$$f(r,\rho) = \frac{n-1}{\sqrt{2\pi}} \frac{\Gamma(n)}{\Gamma(n+\frac{1}{2})} \frac{(1-\rho^2)^{\frac{n}{2}}(1-r^2)^{\frac{n-3}{2}}}{(1-\rho r)^{n-\frac{1}{2}}} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; n+\frac{1}{2}; \frac{1+\rho r}{2}\right),$$

where $n = N-1$ and ${}_2F_1(a,b;c;x)$ is the Gaussian hypergeometric function defined as

$${}_2F_1(a,b;c;x) = \sum_{k=0}^{\infty} \frac{(a)_k(b)_k}{(c)_k}\frac{x^k}{k!}, \quad (a)_k = \prod_{i=0}^{k-1}(a+i), \quad \text{and} \quad (a)_0 = 1.$$

Here a, b, c lie in $\mathbb{C}$, the set of complex numbers. Full details of this function are given by [2]. In fact, $f(r,\rho)$ is a regular function for $-1 < r < 1$ and $-1 < \rho < 1$. The function ${}_2F_1(a,b;c;x)$ satisfies the following differential equation:

$$\left[x(1-x)\partial_x^2 - (c + (a+b+1)x)\partial_x - ab\right] {}_2F_1(a,b;c;x) = 0.$$

Letting $\partial_1 = \frac{\partial}{\partial r}$ and $\partial_2 = \frac{\partial}{\partial \rho}$, then we take the differential operators annihilating $f(r,\rho)$ as

$$h_1 := h_1(r,\rho,\partial_1) = c_{12}\partial_1^2 + c_{11}\partial_1 + c_{10}, \tag{1.2}$$

$$h_2 := h_2(r,\rho,\partial_2) = c_{22}\partial_2^2 + c_{21}\partial_2 + c_{20}, \tag{1.3}$$

$$h_3 := h_3(r,\rho,\partial_1,\partial_2) = c_{32}\partial_2 + c_{31}\partial_1 + c_{30}. \tag{1.4}$$

It follows that $h_i f(r,\rho) = 0$ $(i = 1,2,3)$, where c_{ij} are

$$\begin{aligned} c_{12} &= (1-\rho^2 r^2)(1-r^2)^2, \\ c_{11} &= r(1-r^2)\{2n(1-\rho^2) - 6 - \rho^2 + 7\rho^2 r^2\} \\ c_{10} &= n^2(r^2-\rho^2) + n(1-5r^2+4\rho^2 r^2) - 3(1-2r^2-2\rho^2 r^2+3\rho^2 r^4) \\ c_{22} &= (1-\rho^2)^2(1-r^2\rho^2),\ c_{21} = \rho(1-\rho^2)\{2n(1-r^2) - r^2(1-\rho^2)\} \\ c_{20} &= n\{1+(1-2r^2)\rho^2 + n(-r^2+\rho^2)\},\ c_{32} = -(1-r^2)(1-\rho^2)\rho \\ c_{31} &= r(1-r^2)(1-\rho^2),\ c_{30} = -n(1-r^2)\rho^2 + (n-3)r^2(1-\rho^2). \end{aligned} \tag{1.5}$$

Hotelling [8] gave h_1 and h_3, and implied the existence of h_2 without specifying it. In that report, Hotelling [8] presented a typographical error as $r(1-5r^2+4\rho^2r^2)$ instead of $n(1-5r^2+4\rho^2r^2)$ in the coefficient c_{10}. These h_1, h_2 and h_3 can also be obtained from the package `HolonomicFunctions.m` in Mathematica 11 developed by Koutschan [9, 10].

In the framework of algebraic statistics for the holonomic gradient method (HGM), we use r and ρ as indeterminate variables. The holonomic gradient descent method (HGD) was proposed in an earlier report of a study by [12]. That report describes an attempt to find the optimal parameters of the likelihood function for the Fisher–Bingham distribution in directional analysis. Koyama et al. [11] presented the accelerated algorithm of [12]. Hashiguchi et al. [5] proposed HGM for use in the numerical computation for the distribution on the largest eigenvalue of the Wishart matrix. Siriteanu et al. [15, 16] applied HGM for MIMO Zero-Forcing performance evaluation. Hashiguchi et al. [6] performed numerical computation for the distribution of the ratio of two Wishart matrices.

This paper presents discussion of the holonomic properties and HGM for use on the distribution of the sample correlation coefficient under a normal population. Fisher [3] obtained the pdf of the sample correlation coefficient. Hotelling [8] provided a useful representation using the Gaussian hypergeometric function. From the perspective of asymptotic property, Fisher [3] also proposed Fisher's z-transformation, which has asymptotic normality with great rapidity. Asymptotic expansion with higher order for the transformation was explained by [14]. Nakagawa et al. [13] clarified the role of computer algebra to obtain the asymptotic expansion based on the module of symmetric polynomials. Greco [4] obtained the explicit expression for any sample size through a relation that enables us to calculate exact values of pdf and the cumulative distribution function (cdf). In addition, Barabesi and Greco [1] used the relation to obtain Student's t and Snedecor F distribution functions. The distribution of the sample correlation coefficient is calculable numerically using several methods. However, we specifically examine holonomic properties and numerical computations using HGM.

§2. Holonomic property of the pdf of r

We examine the pdf of the sample correlation coefficient at the perspective of D-module theory, of which detailed discussion is presented in Chapter 6 of [7]. We restrict the case to two parameters and define the ring of differential operators with rational function coefficients as $R_2 = \mathbb{C}(r, \rho)\,\langle \partial_1, \partial_2 \rangle$. We also define $I_f = \langle h_1, h_2, h_3 \rangle$ as a left ideal of R_2 generated by annihilators h_1, h_2, h_3 of the pdf $f(r, \rho)$, respectively, in (1.2),(1.3) and (1.4). Function $g(r, \rho)$ is a holonomic function if there exists a left ideal I_g of R_2 annihilating g and R_2/I_g has a finite dimension as a vector space. The left ideal I_g and the number of its dimension are called, respectively, the zero-dimensional ideal and holonomic rank if R_2/I_g has a finite dimension. Actually, the following theorem ensures that the pdf $f(r, \rho)$ is a holonomic function as well as $h_2 \in \langle h_1, h_3 \rangle$.

Theorem 2.1. *The term order is defined by the graded lexicographic order with $\partial_1 < \partial_2$. Then the following statements hold.*

1. *Set $G = \{h_1, h_3\}$ as a Gröebner basis of I_f.*
2. *The left ideal I_f is a zero-dimensional ideal. The quotient ring R_2/I_f has a basis $\{1, \partial_1\}$ as a vector space. The holonomic rank of I_f is 2.*

Proof. From direct calculation, the S-polynomial of h_1 and h_3 is reduced to 0, i.e., we have $\mathrm{sp}(h_1, h_3) \longrightarrow^* 0$. This result demonstrates that G is a Groebner basis of I_f from Theorem 6.1.8 in [7]. Because the initial terms of G are $\mathrm{in}_<(h_1) = \partial_1^2, \mathrm{in}_<(h_3) = \partial_2$, the standard monomials are $\{1, \partial_1\}$. From Theorem 6.1.10 in [7], the standard monomials form a vector space basis of R_2/I_f. Therefore, I_f is a zero-dimensional ideal with holonomic rank of 2. $\square$

§3. Numerical computation of the pdf of r using HGM

We establish HGM of the pdf $f(r, \rho)$ for any $r \in (-1, 1)$ and a fixed $\rho \in (-1, 1)$. From Theorem 2.1, we take the vector

$$\overrightarrow{G}(r, \rho) = [f(r, \rho), \partial_1 f(r, \rho)]^\top$$

corresponding to the standard monomials $\{1, \partial_1\}$, where $\top$ is a transposition of a vector or matrix. The Pfaffian system of $\overrightarrow{G}(r, \rho)$ has matrices $A_1(r, \rho)$

and $A_2(r,\rho)$ associated with $\partial_i \overrightarrow{G}(r,\rho) = A_i(r,\rho)\overrightarrow{G}(r,\rho)$ for $i = 1,2$, where $A_1(r,\rho)$ and $A_2(r,\rho)$ are given, respectively, as

$$A_1(r,\rho) = \begin{bmatrix} 0 & 1 \\ -\frac{c_{10}}{c_{12}} & -\frac{c_{11}}{c_{12}} \end{bmatrix}, \quad A_2(r,\rho) = \begin{bmatrix} -\frac{c_{30}}{c_{32}} & -\frac{c_{31}}{c_{32}} \\ d_{21} & d_{22} \end{bmatrix},$$

using $c_{10},\dots,c_{32}$ in (1.5) and

$$d_{21} = \frac{2(n-3)r}{(1-r^2)^2\rho} + \frac{c_{31}}{c_{32}}\frac{c_{10}}{c_{12}}, \quad d_{22} = -\frac{c_{30}}{c_{32}} + \frac{1}{\rho} + \frac{c_{31}}{c_{32}}\frac{c_{11}}{c_{12}}.$$

In the domain $\{(r,\rho) : -1 < r < 1, -1 < \rho < 1\}$, the singularity is $\rho = 0$ for A_2. In this case, we are fortunately able to transform r into $t = r\sqrt{n-1}/\sqrt{1-r^2}$ that distributes the Student t-distribution with $n-1$ degrees of freedom.

For a fixed ρ, we calculate $\overrightarrow{G}(0,\rho)$ as an initial value and move from $\overrightarrow{G}(r,\rho)$ to $\overrightarrow{G}(r+\Delta r,\rho)$. For example, we consider the linear equation as

$$\begin{aligned} \overrightarrow{G}(r+\Delta r,\rho) &\approx \overrightarrow{G}(r,\rho) + \Delta r\, \partial_1 \overrightarrow{G}(r,\rho) \\ &= [I_1 + \Delta r A_1(r,\rho)]\overrightarrow{G}(r,\rho) \end{aligned}$$

with the initial value $\overrightarrow{G}(0,\rho) = [f(0,\rho), \partial_1 f(0,\rho)]^\top$, where

$$f(0,\rho) = C(1-\rho^2)^{\frac{n}{2}}\,{}_2F_1\left(\frac{1}{2},\frac{1}{2};n+\frac{1}{2};\frac{1}{2}\right), \tag{3.1}$$

$$\partial_1 f(0,\rho) = (n-\frac{1}{2})\rho f(0,\rho) + \frac{C\rho(1-\rho^2)^{\frac{n}{2}}}{4(2n+1)}\,{}_2F_1\left(\frac{3}{2},\frac{3}{2};n+\frac{3}{2};\frac{1}{2}\right), \tag{3.2}$$

and

$$C = \frac{n-1}{\sqrt{2\pi}}\frac{\Gamma(n)}{\Gamma(n+\frac{1}{2})}.$$

We take the above initial value $\overrightarrow{G}(0,\rho)$ so that the hypergeometric function ${}_2F_1$ are independent of the value of ρ. We must respectively evaluate ${}_2F_1(\frac{1}{2},\frac{1}{2};n+\frac{1}{2};\frac{1}{2})$ and ${}_2F_1(\frac{3}{2},\frac{3}{2};n+\frac{3}{2};\frac{1}{2})$ in (3.1) and (3.2). However, before evaluating them, we provide the following lemma.

Lemma 3.1. *For $a,b>0$ and $c>1$, we have*

$$\frac{ab}{c}\,{}_2F_1(a+1,b+1;c+1;x) = \frac{c-1}{x}[{}_2F_1(a,b;c-1;x) - {}_2F_1(a,b;c;x)].$$

Proof.

$$\begin{aligned}
\frac{ab}{c}\,{}_2F_1(a+1,b+1;c+1;x) &= \partial_x\,{}_2F_1(a,b;c;x)\\
&= \frac{c-1}{x}\sum_{k=1}^{\infty}\frac{(a)_k(b)_k\,x^k}{k!}\frac{k}{(c-1)(c)_k}\\
&= \frac{c-1}{x}\sum_{k=0}^{\infty}\frac{(a)_k(b)_k\,x^k}{k!}\left\{\frac{1}{(c-1)_k}-\frac{1}{(c)_k}\right\}\\
&= \frac{c-1}{x}[{}_2F_1(a,b;c-1;x)-{}_2F_1(a,b;c;x)]
\end{aligned}$$

□

The following theorem is a direct consequence of Lemma 3.1.

Theorem 3.1.

1. $${}_2F_1\left(\frac{1}{2},\frac{1}{2};n+\frac{1}{2};\frac{1}{2}\right)=\frac{2^{\frac{1}{2}-n}\Gamma(n+\frac{1}{2})\sqrt{\pi}}{\Gamma(\frac{n+1}{2})^2}$$
2. $${}_2F_1\left(\frac{3}{2},\frac{3}{2};n+\frac{3}{2};\frac{1}{2}\right)=2^{\frac{5}{2}-n}\,\Gamma(n+\frac{3}{2})\sqrt{\pi}\left\{\frac{4}{\Gamma(\frac{n}{2})^2}-\frac{2n-1}{\Gamma(\frac{n+1}{2})^2}\right\}$$

Proof. From formula (51) in Section 2.8, p.104 of [2], we have

$$(3.3)\qquad {}_2F_1\left(a,1-a;b;\frac{1}{2}\right)=\frac{2^{1-b}\sqrt{\pi}\,\Gamma(b)}{\Gamma(\frac{a+b}{2})\,\Gamma(\frac{1+b-a}{2})},$$

where b is neither a negative integer nor 0. Substituting $a=\frac{1}{2}$ and $b=n+\frac{1}{2}$ into (3.3), we have statement 1. Next, we set $a=\frac{1}{2}$, $b=\frac{1}{2}$, and $c=n+\frac{1}{2}$ to Lemma 3.1 and use (3.3) again to obtain statement 2. □

Substituting (3.1) and (3.2) with statements 1 and 2 of Theorem 3.1, the initial values $f(0,\rho)$ and $\partial_1 f(0,\rho)$ can be rewritten as

$$(3.4)\qquad f(0,\rho)=\frac{(n-1)(1-\rho^2)^{\frac{n}{2}}\Gamma(n)}{2^n(\Gamma(\frac{n+1}{2}))^2},$$

$$\begin{aligned}
(3.5)\quad \partial_1 f(0,\rho) &= (n-\frac{1}{2})\rho f(0,\rho)\\
&\quad+\frac{(n-1)\rho(1-\rho^2)^{\frac{n}{2}}\Gamma(n)\,\Gamma(n+\frac{3}{2})}{2^n(2n+1)\Gamma(n+\frac{1}{2})}\times\left\{\frac{4}{\Gamma(\frac{n}{2})^2}-\frac{2n-1}{\Gamma(\frac{n+1}{2})^2}\right\}.
\end{aligned}$$

We use the Runge–Kutta method for the numerical computation of $\overrightarrow{G}(r,\rho)$ as shown below.

1. Give the values of ρ, n, r_0 and Δr; set $r \leftarrow 0$.
2. Calculate $\overrightarrow{G}(0, \rho)$ using (3.4) and (3.5).
3. Compute l_1, l_2, l_3 and l_4 as

$$\begin{aligned}
l_1 &\leftarrow \Delta r\, A_1(r, \rho)\overrightarrow{G}(r, \rho),\\
l_2 &\leftarrow \Delta r\, A_1\left(r + \frac{\Delta r}{2}, \rho\right)\left\{\overrightarrow{G}(r, \rho) + \frac{l_1}{2}\right\},\\
l_3 &\leftarrow \Delta r\, A_1\left(r + \frac{\Delta r}{2}, \rho\right)\left\{\overrightarrow{G}(r, \rho) + \frac{l_2}{2}\right\},\\
l_4 &\leftarrow \Delta r\, A_1(r + \Delta r, \rho)\left\{\overrightarrow{G}(r, \rho) + l_3\right\}.
\end{aligned}$$

4. Increment from $\overrightarrow{G}(r, \rho)$ to $\overrightarrow{G}(r + \Delta r, \rho)$ as

$$\overrightarrow{G}(r + \Delta r, \rho) \leftarrow \overrightarrow{G}(r, \rho) + \frac{1}{6}(l_1 + 2l_2 + 2l_3 + l_4).$$

5. Let $r \leftarrow r + \Delta r$.
6. If $r = r_0$, then return $\overrightarrow{G}(r_0, \rho)$ as a result, else go back to the step 3.

Our numerical computation based on the algorithm above is conducted using software (Mathematica 11; Wolfram Research Inc.). Figure 1 portrays the pdf of r with $\rho = 0.5$ and $n = 50$. The black line represents the pdf evaluated by HGM. Open circles represent values computed using a built-in function, `Hypergeometric2F1`, in the software.

3.1. Recurrence relation of the pdf

The pdf of r can also be calculated by application of the recurrence relation of hypergeometric function ${}_2F_1$ with respect to the degrees of freedom n. Letting $f_n = {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; n + \frac{1}{2}; x\right)$ for convenience, then from formula (30) on p. 103 of a report by [2], we obtain

$$f_n = \frac{1}{4x(n-1)^2}(2n-1)(2n-3)[(2x-1)f_{n-1} - (x-1)f_{n-2}], \tag{3.6}$$

where $n \geq 2$. The respective initial terms f_0 and f_1 are

$$f_0 = \frac{1}{\sqrt{1-x}} \quad \text{and} \quad f_1 = \frac{\arcsin\sqrt{x}}{\sqrt{x}}. \tag{3.7}$$

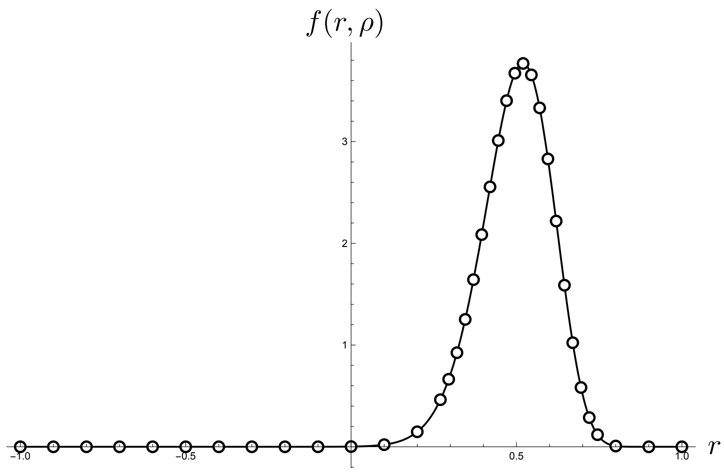

Figure 1: The pdf values were evaluated by HGM, where $\rho = 0.5$ and $n = 50$.

In Figure 2, the open circles are values of the pdf applying (3.7) and (3.6), where $\rho = 0.5$, fixed $r = 0.5$, and the values of n are $1, 25, 50, 100, 150$, and 300. The black curves represent the pdfs of r shown using a built-in function, `Hypergeometric2F1` in the software. It shows how the pdf values are calculated recursively as the number of the degrees of freedom n increases. For $n = 300$, the recurrence formulas (3.7) and (3.6) can compute the values of the pdf for $\rho = 0.5$ and $r = 0.5$, but the function with the built-in function `Hypergeometric2F1` does not work, as shown in Figure 2.

§4. Numerical computation of the cdf of r using HGM

We consider the cdf of r, $F(r, \rho)$, satisfying

$$(c_{12}\partial_1^2 + c_{11}\partial_1 + c_{10})\partial_1 F = (c_{12}\partial_1^3 + c_{11}\partial_1^2 + c_{10}\partial_1)F = 0.$$

The pdf of r, a holonomic function, is also its cdf from Theorem 6.10.14 in [7]. We take the initial value at $r = 0$ as well, such that to calculate $F(r, \rho)$ for any r and a fixed ρ, we need only ascertain the value of

$$F(0, \rho) = \int_{-1}^{0} f(r, \rho)\, dr.$$

By applying the integration algorithm (see Section 6.10 in [7]), the integral

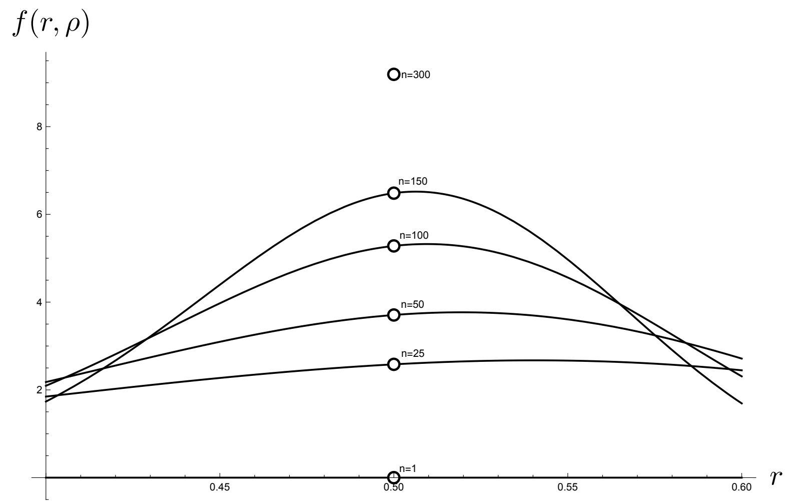

Figure 2: The pdf values were evaluated using the recurrence formulas (3.7) and (3.6) where $\rho = 0.5$. The white circles are at $r = 0.5$.

$F(0, \rho)$ satisfies the following differential equation:

$$\left[(-1+\rho^2)\partial_2^2 + (2\rho - n\rho)\partial_2\right] F(0,\rho) = 0. \tag{4.1}$$

It is obtained using the `HolonomicFunctions.m` package in the software (see Section 1). It is solvable using the initial conditions $F(0, 0) = \frac{1}{2}$ and $F(0, -1) = 1$ (or $F(0, 1) = 0$) as

$$F(0,\rho) = \frac{1}{2} - \frac{\rho(1-\rho^2)^{\frac{n}{2}}\Gamma(\frac{n+1}{2})}{\sqrt{\pi}\,\Gamma(\frac{n}{2})} \times {}_2F_1\left(1, \frac{n+1}{2}; \frac{3}{2}; \rho^2\right), \tag{4.2}$$

which is obtained using the built-in function `DSolve` in the software. In Figure 3, the black line shows the HGM-based cdf evaluation where $\rho = 0.5$ and $n = 50$. White circles represent the empirical frequency of the 10^6 Monte Carlo simulation.

§5. Ordinary differential equation for the quantile of the distribution of r

In this section, we give an ordinary differential equation for the quantiles of the distribution of r. A general method for the ordinary differential equation for a univariate statistic was proposed by Steinbrecher and Shaw [17]. For the distribution function of the sample correlation coefficient $u = F(r, \rho)$, we write its quantile function as $r(u) = F^{-1}(u)$. Then the following theorem holds.

Theorem 5.1. *The quantile function $r(u)$ of the distribution of r has a non-linear differential equation as presented below.*

$$\frac{d^2 r}{du^2} = H(r, \rho) \left(\frac{dr}{du} \right)^2 \tag{5.1}$$

For that equation, $H(r, \rho)$ is given as shown below.

$$H(r, \rho) = \frac{5\rho r^2 + 2(n-3)r + \rho - 2n\rho}{2(r^2 - 1)(\rho r - 1)} - \frac{\rho}{8n+4} \frac{{}_2F_1\left(\frac{3}{2}, \frac{3}{2}; n + \frac{3}{2}; \frac{r\rho+1}{2}\right)}{{}_2F_1\left(\frac{1}{2}, \frac{1}{2}; n + \frac{1}{2}; \frac{r\rho+1}{2}\right)}$$

Proof. From equations (55) and (56) of [17], one can infer that

$$H(r, \rho) = -\frac{d}{dr} \log f(r, \rho),$$

where $f(r, \rho)$ is given as (1.1). □

Taking $r_0 = 0$ and $u_0 = F(0, \rho)$ for a fixed ρ, the equation (5.1) is calculable numerically with the initial values $r(u_0) = 0$ and $r'(u_0) = \frac{dr}{du}\big|_{u=u_0} = \frac{1}{f(0,\rho)}$, where $F(0, \rho)$ and $f(0, \rho)$ are given respectively as (4.2) and (3.4). Figure 4 presents the plot of the quantile function with $\rho = 0.5$ and $n = 50$.

In Figure 4, the black line represents the quantile function of r computed by solving the differential equation (5.1). White circles show the empirical quantile function of 10^6 Monte Carlo simulation. Although the range of the plot is expected to be $-1 < r < 1$, we stop computing when values $|u|$ or $|1 - u|$ become sufficiently small to approximate as $u = 0$ or $u = 1$.

§6. Conclusion

After first explaining the holonomic property of the pdf of the sample correlation coefficient, we constructed methods for HGM-based exact computation of the distribution. Results show that they work very well with pdf and cdf computation. We also discussed numerical computations of the quantile function and derived the recurrence formula for the Gaussian hypergeometric function related to the degrees of freedom. Future work is expected to investigate whether the quantile function is holonomic or not.

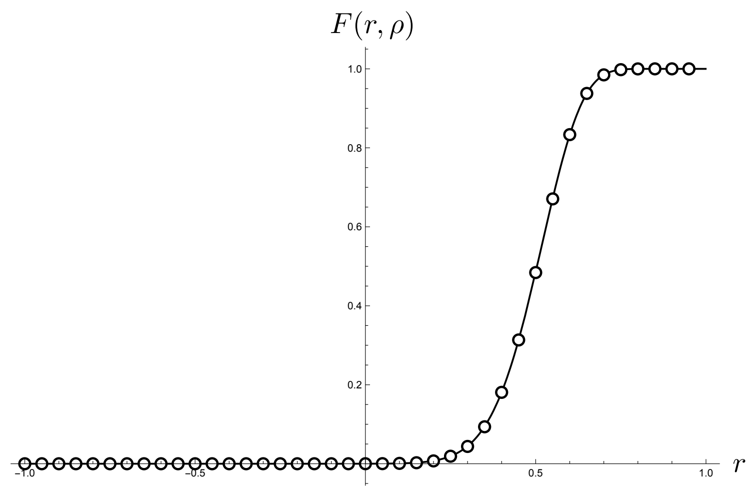

Figure 3: The cdf values evaluated using HGM where $\rho = 0.5$ and $n = 50$.

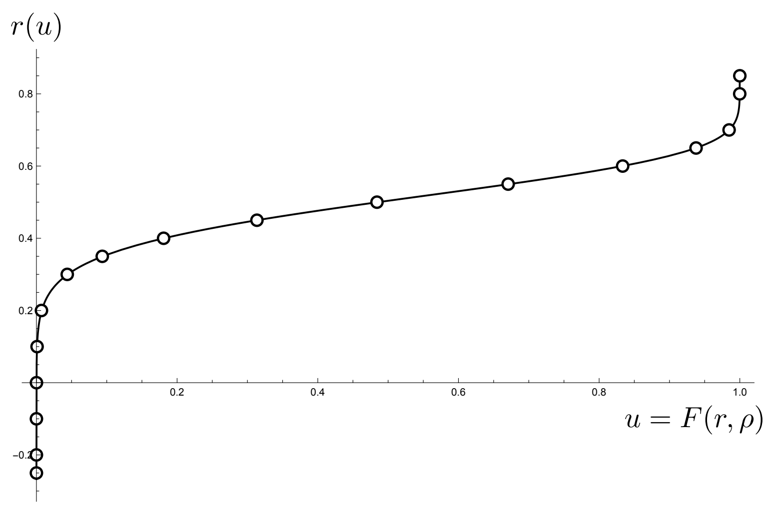

Figure 4: The quantile function of r where $\rho = 0.5$ and $n = 50$.

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