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Explicit expressions for the variogram of first-order intrinsic autoregressions

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Abstract: Exact and explicit expressions for the variogram of first-order intrinsic autoregressions have not been known. Various asymptotic expansions and approximations have been used to compute the variogram. In this note, an exact and explicit expression applicable for all parameter values is derived. The expression involves Appell's hypergeometric function of the fourth kind. Various particular cases of the expression are also derived.

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1. Introduction

Let $\{X_{u,v} : u, v \in \mathbb{Z}\}$ be a homogeneous first-order intrinsic autoregression on the two-dimensional rectangular lattice \mathbb{Z}^2 [12, 3] with generalized spectral density function

$$f(w,\eta) = \kappa \left(1 - 2a\cos w - 2b\cos\eta\right)^{-1}$$

for $w \in (-\pi, \pi], \eta \in (-\pi, \pi]$ and the conditional expectation structure

$$\mathsf{E}(X_{u,v} \mid \cdots) = a \left(x_{u-1,v} + x_{u+1,v} \right) + b \left(x_{u,v-1} + x_{u,v+1} \right), \tag{1}$$

where $a > 0, b > 0, a + b = \frac{1}{2}$ and $\operatorname{Var}(X_{u,v} | \cdots) = \kappa$. We can assume without loss of generality that $\kappa = 1$ and that $\{X_{u,v}\}$ is Gaussian, see [4]. It follows that the difference $X_{u,v} - X_{u+s,v+t}$ has a well defined distribution with zero mean and lag (s, t) variogram

$$\nu_{st}(a,b) := \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \frac{1 - \cos(sx)\cos(ty)}{1 - 2a\cos x - 2b\cos y} \,\mathrm{d}x\mathrm{d}y\,. \tag{2}$$

The computation of (2), both analytically and numerically, has been a subject of considerable interest. The symmetric case a = b = 1/4 was considered by McCrea and Whipple [14], Spitzer [20] and Besag and Kooperberg [3]. Besag and Mondal [4] derived explicit expressions for $\nu_{s,s}$ and $\nu_{s,0}$ for the asymmetric case with the latter expressed as a finite sum of incomplete beta functions. Duffin and Shaffer [9, Theorem 4] and Besag and Mondal [4, Theorem 2] provided asymptotic expansions for $\nu_{s,t}$ in terms of $r = \sqrt{4bs^2 + 4at^2}$ for the symmetric and asymmetric cases. Their approach was to exploit a recurrence equation with respect to integer time variables s and t [4, Eq. (4)]. See also [2] and [12].

The aim of this note is to derive an explicit expression for (2) for general s, t, a and b. Our approach to find the explicit formula for $\nu_{st}(a, b)$ is quite different.

The expression given in Section 2 involves Appell's hypergeometric function of the fourth kind [10, page 1008] defined by

$$F_4[\alpha,\beta;\gamma,\gamma';x,y] = \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{(\alpha)_{j+k}(\beta)_{j+k}}{(\gamma)_j (\gamma')_k} \frac{x^j}{j!} \frac{x^k}{k!}$$
(3)

for $\sqrt{|x|} + \sqrt{|y|} < 1$, where $(w)_{\ell} := w(w+1)\cdots(w+\ell-1)$ denotes Pochhammer symbol with $(w)_0 \equiv 1$. Various particular cases of the general expression, involving simpler functions, are derived in Section 3.

A transformation formula between F_4 and Appell's hypergeometric function, F_2 , defined by

$$F_2[\alpha, \beta, \beta'; \gamma, \gamma'; x, y] := \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} \frac{(\alpha)_{j+k}(\beta)_j(\beta')_k}{(\gamma)_j (\gamma')_k} \frac{x^j}{j!} \frac{x^k}{k!} \qquad |x| + |y| < 1$$

is $[19, \S5.4]$

$$F_4\left[\alpha, (\alpha+1)/2; \gamma+\frac{1}{2}, \gamma'+\frac{1}{2}; x^2, y^2\right] = (1+x+y)^{-\alpha} F_2\left[\alpha, \gamma, \gamma'; 2\gamma, 2\gamma'; \frac{2x}{x+y+1}, \frac{2y}{x+y+1}\right].$$

This formula has been proved earlier (in equivalent form) in [1, p. 11, Eq. (3.1)], see [22, Eq. (175), §9.4.] too. In-built numerical routines for the computation of F_2 are available, see [8, §3.1.3] and especially [7, §2]. Reduction procedures for F_4 to lower order analytical expressions have been developed by Niukkanen [15], Paramonova and Niukkanen [16] and references therein.

2. Main result

Theorem 1 expresses (2) in terms of Appell's hypergeometric function of the fourth kind defined in (3). It applies for $|a| + |b| < \frac{1}{2}$. The case $|a| + |b| = \frac{1}{2}$ is considered by Theorem 2.

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Theorem 1. For all $s, t \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}, |a| + |b| < \frac{1}{2}$ we have

$$\nu_{st}(a,b) = F_4\left[\frac{1}{2}, 1; 1, 1; 4a^2, 4b^2\right] - \binom{s+t}{s}a^s b^t \\ \times F_4\left[\frac{1}{2}(s+t+1), \frac{1}{2}(s+t) + 1; s+1, t+1; 4a^2, 4b^2\right].$$
(4)

Proof. By equation 3.915(2) in [10], we can write

$$\nu_{st}(a,b) = \frac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} \int_0^{\infty} \left(1 - \cos(sx)\cos(ty)\right) e^{-(1-2a\cos x - 2b\cos y)z} dxdydz$$
$$= \int_0^{\infty} e^{-x} \left(J_0(-2axi)J_0(-2bxi) - i^{s+t}J_s(-2axi)J_t(-2bxi)\right) dx, \quad (5)$$

where $i = \sqrt{-1}$ and $J_s(x)$ denotes the Bessel function of the first kind of order s. Setting

$$\mathcal{I}_{st}(a,b) := \mathbf{i}^{s+t} \int_0^\infty e^{-x} J_s(-2ax\mathbf{i}) J_t(-2bx\mathbf{i}) \,\mathrm{d}x,$$

we can rewrite (5) as

$$\nu_{st}(a,b) = \mathcal{I}_{00}(a,b) - \mathcal{I}_{st}(a,b).$$
(6)

Consider now, for instance, the Laplace-transform formula 3.12.15(20) in [17], viz

$$\int_{0}^{\infty} e^{-pt} t^{\lambda} J_{\mu}(At) J_{\nu}(Bt) dt = \frac{A^{\mu} B^{\nu}}{2^{\mu+\nu} p^{\lambda+\mu+\nu+1}} \frac{\Gamma(\lambda+\mu+\nu+1)}{\Gamma(\mu+1)\Gamma(\nu+1)} \times F_{4} \left[\frac{1}{2} (\lambda+\mu+\nu+1), \frac{1}{2} (\lambda+\mu+\nu+2); \mu+1, \nu+1; -\frac{A^{2}}{p^{2}}, -\frac{B^{2}}{p^{2}} \right]$$
(7)

for $\Re\{\lambda+\mu+\nu\} > -1$, $\Re\{p\} > |\Im\{A\}|+|\Im\{B\}|$. Setting p = 1, $\lambda = 0$, A = -2ai, B = -2bi in (7), one deduces

$$\mathcal{I}_{st}(a,b) = \binom{s+t}{s} a^s b^t F_4\left[\frac{1}{2}(s+t+1), \frac{1}{2}(s+t)+1; s+1, t+1; 4a^2, 4b^2\right].$$
(8)

The result of the theorem follows from (6) and (8).

Remark 1. The explicit expression in (4) has some applicability. Although one assumes that $|a| + |b| = \frac{1}{2}$ in (1) the case $|a| + |b| < \frac{1}{2}$ has been of interest. For instance, consider Example 3.3 in [3]. This example is based on the data provided by Table 2 in [11]. The data are the yields from a 28×7 uniformity trial on spring barley, carried out in 1979 at the Plant Breeding Institute, Cambridge, England. [11] fitted the model given by (1) to the data and found that the maximum likelihood estimates are $\hat{a} = 0.4848$ and $\hat{b} = 0.0132$. So, for this example, we have $\hat{a} + \hat{b} = 0.4980 < \frac{1}{2}$.

Theorem 2. For all $a \in (0, \frac{1}{2})$ we have

$$\nu_{st}\left(a, \frac{1}{2} - a\right) = \lim_{\theta \to 0+} \nu_{st}\left(a\sqrt{1-\theta}, \left(\frac{1}{2} - a\right)\sqrt{1-\theta}\right). \tag{9}$$

Proof. Consider the Laplace transform (7) for $p = (1 - \theta)^{-1/2}$ and $\lambda = 0$. The resulting Appell's function F_4 obviously converges on the edge $a + b = \frac{1}{2}$ of the convergence region. Noting that ν_{st} is a difference of two F_4 terms, the result follows by Abel's summation method.

Remark 2. The limit in (9) gives an approximation formula, viz

$$\nu_{st}(a, \frac{1}{2} - a) \approx F_4\left[\frac{1}{2}, 1; 1, 1; 4a^2(1 - \theta), 4\left(\frac{1}{2} - a\right)^2(1 - \theta)\right] \\ - \binom{s+t}{s} \frac{a^s\left(\frac{1}{2} - a\right)^t}{(1 - \theta)^{-(s+t)/2}} F_4\left[\frac{1}{2}(s + t + 1), \frac{1}{2}(s + t) + 1; s + 1, t + 1; 4a^2(1 - \theta), 4\left(\frac{1}{2} - a\right)^2(1 - \theta)\right],$$
(10)

where the quality of approximation is controlled by suitably chosen small $\theta > 0$.

Remark 3. To show the usefulness of (9) we compared it with the corresponding formula given in Besag and Mondal [4]. We computed both these formulas for a = 0.1 and s, t = 6, 7, ..., 10. Table 1 shows the exact and approximate values of ν_{st} .

TABLE 1 Exact and approximate values of $\nu_{st}(0.1, 0.4)$ for $s, t = 6, 7, \dots, 10$

s	t	Exact	Approx in [4]	Using (9)
6	6	2.9893	2.9883	2.9887
6	7	3.0170	3.0161	3.0169
6	8	3.0468	3.0459	3.0462
6	9	3.0780	3.0771	3.0778
6	10	3.1102	3.1094	3.1095
7	6	3.0899	3.0893	3.0895
7	7	3.1117	3.1110	3.1111
7	8	3.1354	3.1347	3.1348
7	9	3.1605	3.1599	3.1599
7	10	3.1869	3.1863	3.1864
8	6	3.1813	3.1808	3.1810
8	7	3.1987	3.1982	3.1983
8	8	3.2178	3.2173	3.2176
8	9	3.2384	3.2379	3.2380
8	10	3.2602	3.2597	3.2598
9	6	3.2645	3.2641	3.2643
9	7	3.2786	3.2783	3.2785
9	8	3.2943	3.2939	3.2940
9	9	3.3114	3.3110	3.3112
9	10	3.3297	3.3292	3.3293
10	6	3.3406	3.3404	3.3406
10	7	3.3523	3.3520	3.3520
10	8	3.3654	3.3651	3.3653
10	9	3.3798	3.3794	3.3795
10	10	3.3952	3.3949	3.3952

It is evident from Table 1 that our formula performs consistently better than that due to [4]. Note that the exact values and the approximate values due to [4] were taken from Table 1 in [4]. The expression in (9) was computed using the in-built routines mentioned in Section 1.

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3. The symmetric case a = b = 1/4

Here, we present technical details to calculate $\nu_{s,t}(\frac{1}{4}, \frac{1}{4})$. Using Burchnall-formula [22, §9.4, Eq. (149)], we can transform

$$F_4[\alpha,\beta;\gamma,\gamma';x,x] = {}_4F_3\left[\begin{array}{cc}\alpha,\ \beta,\ \frac{1}{2}(\gamma+\gamma'),\ \frac{1}{2}(\gamma+\gamma'-1) & ;\\ \gamma,\ \gamma',\ \gamma+\gamma'-1 & ;\end{array}\right]$$

The asymptotics of the generalized hypergeometric series $_{p+1}F_p$, $p \geq 3$ have been studied by Bühring and Srivastava [6], Saigo and Srivastava [18] and by A.K. Srivastava [21]. Since we are faced with

$${}_{4}F_{3}\left[\begin{array}{ccc}\frac{1}{2}(s+t+1), \ \frac{1}{2}(s+t)+1, \ \frac{1}{2}(s+t)+1, \ \frac{1}{2}(s+t+1) \\ s+1, \ t+1, \ s+t+1 \end{array}; 1\right],$$
(11)

we have a hypergeometric term

$${}_{4}F_{3}\left[\begin{array}{ccc}\alpha_{1}, \ \alpha_{2}, \ \alpha_{3}, \ \alpha_{4} & ; \\ \beta_{1}, \ \beta_{2}, \ \beta_{3} & ; \end{array}\right]$$

that is zero-balanced, i.e. we have $\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4 = \beta_1 + \beta_2 + \beta_3$. To account for the asymptotics of this ${}_4F_3[\cdots; 1-\theta]$ as $\theta \to 0+$, consider equation (4.2) in [6] for p = 3:

$${}_{4}F_{3}\begin{bmatrix}\alpha_{1}, \alpha_{2}, \alpha_{3}, \alpha_{4} & ;\\ \beta_{1}, \beta_{2}, \beta_{3} & ;\\ \end{bmatrix} = \frac{1}{\Gamma}\left\{L + B - \ln\theta\right\} + O(\theta) + O(\theta\ln\theta) \quad (12)$$

valid for $\theta \to 0+$. Here

$$\Gamma = \frac{\Gamma(\alpha_1)\Gamma(\alpha_2)\Gamma(\alpha_3)\Gamma(\alpha_4)}{\Gamma(\beta_1)\Gamma(\beta_2)\Gamma(\beta_3)}$$
(13)

and

$$L = -2\gamma - \Psi(\alpha_1) - \Psi(\alpha_2),$$

where $\gamma = -\Psi(1)$ denotes the Euler-Mascheroni constant and $\Psi(x) = \frac{d}{dx} \ln \Gamma(x)$ denotes the digamma function. The *B* in (12) can be represented by various forms, see (4.6), (4.7), and (4.12) in [6]. An example is [6, Eq. (4.7)]:

$$B = \sum_{k=1}^{\infty} \frac{(\beta_3 + \beta_1 - \alpha_4 - \alpha_3)_k (\beta_3 + \beta_2 - \alpha_4 - \alpha_3)_k}{k(\alpha_1)_k (\alpha_2)_k} \times {}_{3}F_2 \begin{bmatrix} \beta_3 - \alpha_3, & \beta_3 - \alpha_4, & -k & ;\\ \beta_3 + \beta_1 - \alpha_4 - \alpha_3, & \beta_3 + \beta_2 - \alpha_4 - \alpha_3 & ; \end{bmatrix} .$$
(14)

An advantage of this formula is that it is a single infinite series of hypergeometric terms and the series for each hypergeometric term is finite because of the -k in the numerator. Combining (11), (13) and (14), we can write $L_{st} := L$, $B_{st} := B$ and $\Gamma_{st} := \Gamma$ as

$$B_{st} = \sum_{k=1}^{\infty} \frac{4^k \left(s + \frac{1}{2}\right)_k \left(t + \frac{1}{2}\right)_k}{k(s+t+1)_{2k}} {}_3F_2 \begin{bmatrix} \frac{1}{2}(s+t), & \frac{1}{2}(s+t+1), & -k \\ s + \frac{1}{2}, & t + \frac{1}{2} \end{bmatrix} (15)$$

and

$$\Gamma_{st} = \Gamma = \binom{s+t}{s} \frac{\pi}{4^{s+t}},$$

respectively. Note, for instance, that

$$B_{ss} = \Psi(s+1) - \Psi\left(s + \frac{1}{2}\right) \qquad s \in \mathbb{N}_0,$$
(16)

see the Appendix. Finally, routine calculations show that:

$$\nu_{st}\left(\frac{\sqrt{1-\theta}}{4}, \frac{\sqrt{1-\theta}}{4}\right) = \frac{\ln 4 + B_{00} - \ln \theta}{\pi} - \binom{s+t}{s} \frac{(1-\theta)^{(s+t)/2}}{4^{s+t}\Gamma_{st}} \left\{ L_{st} + B_{st} - \ln \theta \right\} + O(\theta) + O(\theta \ln \theta) = \frac{1}{\pi} \left\{ \ln 16 + B_{00} + 2\gamma + \Psi(\frac{1}{2}(s+t+1)) + \Psi(\frac{1}{2}(s+t)+1) - B_{st} \right\} + O(\theta) + O(\theta \ln \theta) \qquad \theta \to 0_+$$
(17)

for all $(s, t) \in \mathbb{N}_0^2$.

Theorem 3. For all $s, t \in \mathbb{N}_0$ we have

$$\nu_{st}\left(\frac{1}{4}, \frac{1}{4}\right) = \frac{1}{\pi} \left\{ \ln 4 + 2 \sum_{k=1}^{s+t} \frac{1}{k} - B_{st} \right\}.$$
 (18)

Proof. In (17) assume that s+t is even. So, applying properties of the digamma function, Ψ , to expression (17), we conclude

$$\Psi\left(\frac{1}{2}(s+t+1)\right) + \Psi\left(\frac{1}{2}(s+t)+1\right) = -2\gamma - \ln 4 + \sum_{k=0}^{\frac{1}{2}(s+t)-1} \frac{1}{k+\frac{1}{2}} + \sum_{k=1}^{\frac{1}{2}(s+t)} \frac{1}{k}.$$

For odd s + t repeat this procedure.

Corollary 3.1. For all $s \in \mathbb{N}_0$,

$$\nu_{ss}\left(\frac{1}{4}, \frac{1}{4}\right) = \frac{4}{\pi} \sum_{k=0}^{s-1} \frac{1}{2k+1}.$$
(19)

Proof. Consider (18) for s = t. By (16) it follows

$$\nu_{s,s}\left(\frac{1}{4},\frac{1}{4}\right) = \frac{2}{\pi} \left\{ \ln 4 + \gamma + \Psi\left(s + \frac{1}{2}\right) \right\} = \frac{2}{\pi} \left\{ \ln 4 + \gamma + \Psi\left(\frac{1}{2}\right) + \sum_{k=0}^{s-1} \frac{1}{k + \frac{1}{2}} \right\},$$

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Remark 4. The equation (19) is well-known in the literature, see [3, Example 3.2], where the authors refer back to [20, p. 148].

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Appendix

Here we prove (16). Using the transformation given by Bühring [5, Eq. (4.1)], one can express B_{st} in (15) as

$$B_{st} = \sum_{k=1}^{\infty} \frac{4^k \left(s + \frac{1}{2}\right)_k \left(\frac{1}{2}(t - s + 1)\right)_k}{k \left(\frac{1}{2}(s + t + 1)\right)_k \left(\frac{1}{2}(s + t) + 1\right)_k} {}_3F_2 \begin{bmatrix} \frac{1}{2}(s + t), & \frac{1}{2}(s - t), & -k & ; \\ s + \frac{1}{2}, & \frac{1}{2}(s - t + 1) - k & ; \end{bmatrix}.$$

If s = t then the hypergeometric term reduces to 1, so

$$B_{ss} = \sum_{k=1}^{\infty} \frac{\left(\frac{1}{2}\right)_k}{k \left(s+1\right)_k} = \int_0^1 \sum_{k=1}^{\infty} \frac{\left(\frac{1}{2}\right)_k x^{k-1}}{(s+1)_k} dx$$

$$= \frac{1}{2(s+1)} \int_0^1 \sum_{k=1}^{\infty} \frac{\left(\frac{3}{2}\right)_{k-1}(1)_{k-1}}{(s+2)_k} \frac{x^{k-1}}{(k-1)!} dx$$

$$= \frac{1}{2(s+1)} \int_0^1 {}_2F_1 \left[\begin{array}{c} \frac{3}{2}, 1 & \vdots \\ s+2 & \vdots \\ s+2 & \vdots \\ s+2 & \vdots \\ s+2 & z \\ s+2 \\ s+2 & z \\ s+2 \\ s+2 & z \\ s+2 \\$$

where the last two steps follow by equation 1.512(5) in [10] and equation 3.13(42) in [13], respectively. The proof is complete.

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