

## APPENDIX TO PART I

This Appendix, designated as **A2**, contains additional analytical results for Part II of the NOTEBOOK, and follows the notational conventions in Appendix A1.

### A2.1. Covariograms for Sums of Independent Spatial Processes

First recall that the covariance of any random variables,  $Z_1$  and  $Z_2$ , with respective means,  $\mu_1$  and  $\mu_2$ , is given by

$$\begin{aligned}
 \text{(A2.1.1)} \quad \text{cov}(Z_1, Z_2) &= E[(Z_1 - \mu_1)(Z_2 - \mu_2)] = E(Z_1 Z_2 - Z_1 \mu_2 - \mu_1 Z_2 + \mu_1 \mu_2) \\
 &= E(Z_1 Z_2) - E(Z_1) \mu_2 - \mu_1 E(Z_2) + \mu_1 \mu_2 \\
 &= E(Z_1 Z_2) - \mu_1 \mu_2 - \mu_1 \mu_2 + \mu_1 \mu_2 \\
 &= E(Z_1 Z_2) - \mu_1 \mu_2
 \end{aligned}$$

so that if  $Z_1$  and  $Z_2$  are *independent* then

$$\text{(A2.1.2)} \quad E(Z_1 Z_2) = E(Z_1)E(Z_2) = \mu_1 \mu_2 \Rightarrow \text{cov}(Z_1, Z_2) = 0$$

Hence if a given covariance stationary stochastic process,  $\{Y(s) : s \in R\}$ , with mean,  $\mu$ , is the sum of two *independent* covariance stationary components

$$\text{(A2.1.3)} \quad Y(s) = Y_1(s) + Y_2(s), \quad s \in R,$$

with respective means,  $\mu_1$  and  $\mu_2$ , then it follows by definition that  $\mu = \mu_1 + \mu_2$ , and that  $Y_1(s)$  and  $Y_2(v)$  are independent for all  $s, v \in R$ . Hence for any  $h \geq 0$  and  $s, v \in R$  with  $\|s - v\| = h$ , we see that the *covariogram*,  $C$ , of the  $Y$ -process must satisfy,

$$\begin{aligned}
 \text{(A2.1.1)} \quad C(h) &= \text{cov}[Y(s), Y(v)] \\
 &= E[Y(s) \cdot Y(v)] - E[Y(s)] \cdot E[Y(v)] = E[Y(s) \cdot Y(v)] - \mu^2 \\
 &= E\left[\left(Y_1(s) + Y_2(s)\right)\left(Y_1(v) + Y_2(v)\right)\right] - (\mu_1 + \mu_2)^2 \\
 &= E\left[Y_1(s)Y_1(v) + Y_1(s)Y_2(v) + Y_2(s)Y_1(v) + Y_2(s)Y_2(v)\right] \\
 &\quad - (\mu_1^2 + 2\mu_1\mu_2 + \mu_2^2)
 \end{aligned}$$

$$\begin{aligned}
&= E[Y_1(s)Y_1(v)] + E[Y_1(s)]E[Y_2(v)] + E[Y_2(s)]E[Y_1(v)] + E[Y_2(s)Y_2(v)] \\
&\quad - (\mu_1^2 - \mu_1\mu_2 - \mu_2\mu_1 + \mu_2^2) \\
&= E[Y_1(s)Y_1(v)] + \mu_1\mu_2 + \mu_2\mu_1 + E[Y_2(s)Y_2(v)] - (\mu_1^2 - \mu_1\mu_2 - \mu_2\mu_1 + \mu_2^2) \\
&= (E[Y_1(s)Y_1(v)] - \mu_1^2) + (E[Y_2(s)Y_2(v)] - \mu_2^2) \\
&= \text{cov}[Y_1(s), Y_1(v)] + \text{cov}[Y_2(s), Y_2(v)] \\
&= C_1(h) + C_2(h)
\end{aligned}$$

where  $C_1$  and  $C_2$  are the respective covariograms for the  $Y_1$  and  $Y_2$  components of  $Y$ .

## A2.2. Expectation of the Sample Covariance Estimator under Spatial Dependence

Given any collection of  $2n$  jointly distributed random variables,  $\{(Y_{1i}, Y_{2i}), i = 1, \dots, n\}$  where the pairs  $(Y_{1i}, Y_{2i})$  have common means  $E(Y_{1i}) = \mu_1$ ,  $E(Y_{2i}) = \mu_2$  and covariance  $\text{cov}(Y_{1i}, Y_{2i}) = \sigma_{12}$  for all  $i = 1, \dots, n$ , consider the following estimator of  $\sigma_{12}$ ,

$$(A2.2.1) \quad \hat{\sigma}_{12} = \frac{1}{n-1} \sum_{i=1}^n (Y_{1i} - \bar{Y}_1)(Y_{2i} - \bar{Y}_2)$$

where  $\bar{Y}_j = \frac{1}{n} \sum_{i=1}^n Y_{ji}$ ,  $j = 1, 2$ . Here  $\hat{\sigma}_{12}$  and  $\sigma_{12}$  are taken to correspond to the estimator  $\hat{C}(h)$  of the covariance  $C(h)$  in expressions (4.10.2) and (4.10.1), respectively. To analyze this estimator, it is convenient to begin with the rescaled version

$$(A2.2.2) \quad \tilde{\sigma}_{12} = \frac{n}{n-1} \hat{\sigma}_{12} = \frac{1}{n} \sum_{i=1}^n (Y_{1i} - \bar{Y}_1)(Y_{2i} - \bar{Y}_2)$$

and recall the following standard decomposition of sums of squares:

$$\begin{aligned}
(A2.2.3) \quad \tilde{\sigma}_{12} &= \frac{1}{n} \sum_{i=1}^n (Y_{1i}Y_{2i} - Y_{1i}\bar{Y}_2 - \bar{Y}_1Y_{2i} + \bar{Y}_1\bar{Y}_2) \\
&= \frac{1}{n} \sum_{i=1}^n Y_{1i}Y_{2i} - \left(\frac{1}{n} \sum_{i=1}^n Y_{1i}\right)\bar{Y}_2 - \bar{Y}_1\left(\frac{1}{n} \sum_{i=1}^n Y_{2i}\right) + n\left(\frac{1}{n}\bar{Y}_1\bar{Y}_2\right) \\
&= \frac{1}{n} \sum_{i=1}^n Y_{1i}Y_{2i} - \bar{Y}_1\bar{Y}_2 - \bar{Y}_1\bar{Y}_2 + \bar{Y}_1\bar{Y}_2 \\
&= \frac{1}{n} \sum_{i=1}^n Y_{1i}Y_{2i} - \bar{Y}_1\bar{Y}_2
\end{aligned}$$

But since

$$(A2.2.4) \quad \bar{Y}_1 \bar{Y}_2 = \left( \frac{1}{n} \sum_{i=1}^n Y_{1i} \right) \left( \frac{1}{n} \sum_{i=1}^n Y_{2i} \right) = \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n Y_{1i} Y_{2j}$$

it follows from (A2.2.2) through (A2.2.4) that

$$(A2.2.5) \quad \begin{aligned} E(\hat{\sigma}_{12}) &= \frac{n}{n-1} E(\tilde{\sigma}_{12}) = \frac{n}{n-1} \left[ \frac{1}{n} \sum_{i=1}^n E(Y_{1i} Y_{2i}) - E(\bar{Y}_1 \bar{Y}_2) \right] \\ &= \frac{n}{n-1} \left[ \frac{1}{n} \sum_{i=1}^n E(Y_{1i} Y_{2i}) - \frac{1}{n^2} \sum_{i=1}^n \sum_{j=1}^n E(Y_{1i} Y_{2j}) \right] \\ &= \frac{n}{n-1} \left[ \frac{1}{n} \sum_{i=1}^n E(Y_{1i} Y_{2i}) - \frac{1}{n^2} \sum_{i=1}^n E(Y_{1i} Y_{2i}) - \frac{1}{n^2} \sum_{i=1}^n \sum_{j \neq i} E(Y_{1i} Y_{2j}) \right] \\ &= \frac{n}{n-1} \left[ \frac{n-1}{n^2} \sum_{i=1}^n E(Y_{1i} Y_{2i}) - \frac{1}{n^2} \sum_{i=1}^n \sum_{j \neq i} E(Y_{1i} Y_{2j}) \right] \\ &= \frac{1}{n} \sum_{i=1}^n E(Y_{1i} Y_{2i}) - \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} E(Y_{1i} Y_{2j}) \end{aligned}$$

Finally, if we let  $\mu_j \equiv E(Y_{ji})$ ,  $j=1,2$ , then since by definition,  $E(Y_{1i} Y_{2i}) = \sigma_{12} + \mu_1 \mu_2$  and  $E(Y_{1i} Y_{2j}) = \text{cov}(Y_{1i}, Y_{2j}) + \mu_1 \mu_2$  both hold for all  $i=1, \dots, n$  and  $j \neq i$ , it follows from (A2.2.5) that

$$(A2.2.6) \quad \begin{aligned} E(\hat{\sigma}_{12}) &= \frac{n}{n-1} (\sigma_{12} + \mu_1 \mu_2) - \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j=1}^n (\text{cov}(Y_{1i}, Y_{2j}) + \mu_1 \mu_2) \\ &= \sigma_{12} + \mu_1 \mu_2 - \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} \text{cov}(Y_{1i}, Y_{2j}) - \frac{n(n-1)}{n(n-1)} \mu_1 \mu_2 \\ &= \sigma_{12} - \frac{1}{n(n-1)} \sum_{i=1}^n \sum_{j \neq i} \text{cov}(Y_{1i}, Y_{2j}) \end{aligned}$$

### A2.3. A Bound on the Binning Bias of Empirical Variogram Estimates

Here it suffices to consider the variogram,  $\gamma(h)$ , on the interval of distance values,  $d_{k-1} \leq h < d_k$ , for a typical bin  $k$ . Recall from (4.7.1) that for a given sample of values  $(Y(s_i) : i=1, \dots, n)$ , if  $N_k$  denotes the set of *distance pairs*,  $(s_i, s_j)$ , in bin  $k$ , and if the distance between each such pair is denoted by  $h_{ij} = \|s_i - s_j\|$ , then the *lag distance*,  $h_k$ , for bin  $k$  is defined to be

$$(A2.3.1) \quad h_k = \frac{1}{|N_k|} \sum_{(s_i, s_j) \in N_k} h_{ij}$$

Recall also that if the  $\varepsilon_k$ -linear approximation to  $\gamma(h)$  on this interval is denoted by

$$(A2.3.2) \quad l_k(h) = a_k \cdot h + b_k$$

then by definition,

$$(A2.3.3) \quad h \in [d_{k-1}, d_k) \Rightarrow |\gamma_k(h) - l_k(h)| \leq \varepsilon_k$$

In this context we have the following bound on the bias of the empirical variogram estimates,

$$(A2.3.4) \quad \hat{\gamma}(h_k) = \frac{1}{2|N_k|} \sum_{(s_i, s_j) \in N_k} (Y(s_i) - Y(s_j))^2$$

at lag distance,  $h_k$  :

**Proposition A2.1.** *If for any bin,  $k = 1, \dots, \bar{k}$ , the true variogram,  $\gamma(h)$ , has an  $\varepsilon_k$ -linear approximation, then at lag distance,  $h_k$ , it must be true that*

$$(A2.3.5) \quad |E[\hat{\gamma}(h_k)] - \gamma(h_k)| \leq 2\varepsilon_k$$

**Proof:** If for each  $(s_i, s_j) \in N_k$  we let

$$(A2.3.6) \quad \gamma_{ij} = \gamma(h_{ij}) = \frac{1}{2} E \left[ (Y(s_i) - Y(s_j))^2 \right]$$

with  $h_{ij} = \|s_i - s_j\|$ , then by (A2.3.4),

$$(A2.3.7) \quad \begin{aligned} E[\hat{\gamma}(h_k)] &= E \left[ \frac{1}{2|N_k|} \sum_{(s_i, s_j) \in N_k} (Y(s_i) - Y(s_j))^2 \right] \\ &= \frac{1}{|N_k|} \sum_{(s_i, s_j) \in N_k} \left\{ \frac{1}{2} E \left[ (Y(s_i) - Y(s_j))^2 \right] \right\} \\ &= \frac{1}{|N_k|} \sum_{(s_i, s_j) \in N_k} \gamma_{ij} \end{aligned}$$

But since  $h_{ij} \in [d_{k-1}, d_k)$  for all  $(s_i, s_j) \in N_k$ , we see from (A2.3.2) that  $|\gamma_{ij} - l_k(h_{ij})| \leq \varepsilon_k$ , and thus that

$$(A2.3.8) \quad -\varepsilon_k \leq \gamma_{ij} - l_k(h_{ij}) \leq \varepsilon_k \text{ for all } (s_i, s_j) \in N_k$$

Hence by summing this set of inequalities and taking averages [with the observation that  $(1/|N_k|) \sum_{(s_i, s_j) \in N_k} \varepsilon_k = (|N_k| / |N_k|) \varepsilon_k = \varepsilon_k$ ], we have

$$(A2.3.9) \quad -\varepsilon_k \leq \frac{1}{|N_k|} \sum_{(s_i, s_j) \in N_k} [\gamma_{ij} - l_k(h_{ij})] \leq \varepsilon_k$$

Next, by using (A2.3.1), (A2.3.2) and (A2.3.7), the middle expression of (A2.3.9) can be rewritten as,

$$(A2.3.10) \quad \begin{aligned} \frac{1}{|N_k|} \sum_{(s_i, s_j) \in N_k} [\gamma_{ij} - l_k(h_{ij})] &= \frac{1}{|N_k|} \sum_{(s_i, s_j) \in N_k} \gamma_{ij} - \frac{1}{|N_k|} \sum_{(s_i, s_j) \in N_k} l_k(h_{ij}) \\ &= E[\hat{\gamma}(h_k)] - \frac{1}{|N_k|} \sum_{(s_i, s_j) \in N_k} [a_k h_{ij} + b_k] \\ &= E[\hat{\gamma}(h_k)] - a_k \left( \frac{1}{|N_k|} \sum_{(s_i, s_j) \in N_k} h_{ij} \right) - b_k \\ &= E[\hat{\gamma}(h_k)] - a_k h_k - b_k \\ &= E[\hat{\gamma}(h_k)] - l_k(h_k) \end{aligned}$$

so that (A2.3.9) is seen to imply that

$$(A2.3.11) \quad -\varepsilon_k \leq E[\hat{\gamma}(h_k)] - l_k(h_k) \leq \varepsilon_k$$

But since  $h_k \in [d_{k-1}, d_k)$  it also follows from (A2.3.3) that  $|l_k(h_k) - \gamma(h_k)| \leq \varepsilon_k$  and hence that

$$(A2.3.12) \quad -\varepsilon_k \leq l_k(h_k) - \gamma(h_k) \leq \varepsilon_k$$

Finally, by adding (A2.3.11) and (A2.3.12) we may conclude that

$$(A2.3.13) \quad \begin{aligned} -2\varepsilon_k &\leq (E[\hat{\gamma}(h_k)] - l_k(h_k)) + (l_k(h_k) - \gamma(h_k)) \leq 2\varepsilon_k \\ &\Rightarrow -2\varepsilon_k \leq E[\hat{\gamma}(h_k)] - \gamma(h_k) \leq 2\varepsilon_k \\ &\Rightarrow |E[\hat{\gamma}(h_k)] - \gamma(h_k)| \leq 2\varepsilon_k \end{aligned}$$

and thus that (A2.3.5) must hold. ■