On the use of variograms for the prediction of time series

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Abstract: We consider the prediction of stationary stochastic processes with non-zero mean. When the covariance of the process is known, but the mean is not, the classical approach is to first estimate the mean from the past data, and then apply an optimal predictor to the zero-mean residuals. Bastin and Henriet [1] showed that an alternative was to use a predictor based on 'variograms' rather than covariance information, thus avoiding the estimation of the mean. We show here that the two predictors are identical when the unknown mean is replaced by its minimum variance estimate. We also examine, through simulation, how the two predictors compare when the statistics are unknown.

Keywords: Time series analysis, Prediction, Variogram, Minimum variance prediction.

1. Introduction

We consider a discrete scalar stochastic process \( \{ y_0, y_1, \ldots, y_t, \ldots \} \) with constant but not necessarily zero mean:

\[
E \{ y_t \} = m. \tag{1}
\]

We define the 'variogram' of the process as the semi-variance of the increments

\[
\gamma(t, t-\tau) = \frac{1}{2} E \{ (y_t - y_{t-\tau})^2 \}. \tag{2}
\]

We shall assume throughout that the variogram is stationary, i.e.

\[
\gamma(t, t-\tau) = \gamma(\tau) = \frac{1}{2} E \{ (y_t - y_{t-\tau})^2 \}. \tag{3}
\]

A process with the properties (1) and (3) is called intrinsic (see e.g. [2]). If the process is wide-sense stationary, then the (auto)covariance can be defined as

\[
R(\tau) = E \{ (y_t - m)(y_{t-\tau} - m) \}. \tag{4}
\]

For a wide-sense stationary process, the covariance function and the variogram are related by

\[
\gamma(\tau) = \sigma^2 - R(\tau), \quad \text{with } \sigma^2 = R(0). \tag{5}
\]

Note that an intrinsic random process is always wide-sense stationary, but the converse is not true. The class of intrinsic processes is larger and includes Wiener processes as a special case. Except when specifically stated, we shall from now on assume that the process \( \{ y_t \} \) is wide-sense stationary.

In this paper we shall derive different minimum variance unbiased (MVU) expressions for \((d+1)\)-step ahead predictions of the \( \{ y_t \} \) process under a variety of assumptions. In Sections 2 to 4 we shall assume known second-order statistics and consider Levinson predictors with growing memory: the predicted value at time \( t = N \) uses all available past data. In Section 2 we shall briefly recall the expressions of the classical Levinson predictor (CLP) for \( y_{N+1} \), given \( \{ y_0, y_1, \ldots, y_{N-1} \} \), under the assumptions that the constant mean \( m \) and the covariance (or the variogram) are known. In Section 3 we consider the case where the mean is unknown. Two different MVU predictors can be used in this case:

1. one can compute an unbiased estimate \( \hat{m} \), and then replace the mean by its estimate \( \hat{m} \) in the expressions of the CLP of Section 2. This predictor will be called Approximate Levinson Predictor (ALP);

2. alternatively, one can use a MVU predictor of the form \( \sum_{i=1}^{N} b_i y_{N-i} \), in which the \( b_i \) are computed from the variogram function. This predictor, derived by Bastin and Henriet [1], who called it the modified Levinson predictor, does not involve the mean or its estimate in any way.
2. Processes with known mean and covariance function

When the mean is known, the classical \((d+1)\)-step-ahead Levinson predictor (CLP) for \(Y_{N+d}\) given \(y_0, \ldots, y_{N-1}\) has the form (see e.g. [3])

\[
\hat{y}_{N+d} = m + \sum_{i=1}^{N} a_i (y_{N-i} - m) = m + a^T (Y - mU)
\]  

(6)

where

\[
a^T = (a_1, \ldots, a_N), \quad U^T = (1, 1, \ldots, 1),
\]

\[Y^T = (y_{N-1}, \ldots, y_0).
\]

The prediction error \(\hat{y}_{N+d} - y_{N+d}\) is unbiased. The minimization of the prediction error variance \(E((\hat{y}_{N+d})^2)\) with respect to \(a\), leads to the following system of \(N\) linear equations:

\[
Ra = R_0
\]

(7)

where

\[
R = E\{(Y - mU)(Y - mU)^T\}, \quad R_0 = E\{(Y - mU)(y_{N+d} - m)\}.
\]

Using (5), we can also write

\[
R = \sigma^2 UU^T - I, \quad R_0 = \sigma^2 U - I_0,
\]

(9)

\[
\Gamma = \begin{bmatrix} \gamma(0) & \gamma(1) & \ldots & \gamma(N-1) \\ \gamma(1) & \gamma(0) & \ldots & \gamma(N-2) \\ \vdots & \ddots & \ddots & \vdots \\ \gamma(N-1) & \gamma(N-2) & \ldots & \gamma(0) \end{bmatrix},
\]

(10a)

\[
\Gamma_0 = \begin{bmatrix} \gamma(d+1) \\ \gamma(d+2) \\ \vdots \\ \gamma(d+n) \end{bmatrix}.
\]

(10b)

Note that \(\gamma(0) = 0\). Substituting (9) in (7) yields an alternative system of equations for \(a\) in terms of the variogram:

\[
\begin{bmatrix} \Gamma \\ U^T \sigma^{-2} \end{bmatrix} \begin{bmatrix} a \\ a \sigma^2 \end{bmatrix} = \begin{bmatrix} \Gamma_0 \\ 1 \end{bmatrix},
\]

(11)

where

\[
a \triangleq 1 - a^T U = 1 - \sum_{i=1}^{N} a_i.
\]

(12)

Using matrix and vector notations, (11) can be rewritten as \(A_1 \lambda_1 = c\), with obvious definitions for \(A_1, \lambda_1\) and \(c\). The optimal prediction error variance, \(V_e \triangleq E((\hat{y}_{N+d})^2)\), can be written in a number of ways:

\[
V_e = \sigma^2 - a^T R_0 = a \sigma^2 + a^T \Gamma_0
\]

\[= \sigma^2 - R_0^T R^{-1} R_0 = c A_1^{-1} c.
\]

(13)

3. Processes with unknown mean and known second-order statistics

We now consider the case where the constant mean \(m\) is unknown, but where the covariance function \(R(\tau)\) or the variogram \(\gamma(\tau)\) are assumed known. Recall that they are related by (5).

3.1. The approximate Levinson predictor

The most obvious strategy is to replace the mean in (6) by a linear unbiased estimate based on the past data:

\[
\hat{m} = \sum_{i=1}^{N} \xi_i y_{N-i} = \xi^T Y
\]

(14)
with the unbiasedness condition
\[ \xi^T U = 1. \] (15)

The CLP of (6) is then replaced by the approximate Levinson predictor (ALP):
\[ y_{N+d}^* = \hat{m} + a^T(Y - \hat{m}U) \] (16)

where \( a \) is the solution of (7), as before. This estimator was called approximate classical Levinson predictor (ACLP) in [1]. The prediction error can be written
\[ \bar{y}_{N+d} = y_{N+d}^* - y_{N+d} \]
\[ = m + a^T(Y - mU) - y_{N+d} + \alpha(\hat{m} - m). \] (17)

The sum of the first two terms in (17) is the optimal CLP, so that the sum of the first three terms is the CLP prediction error. Therefore, the prediction error variance
\[ V_a = E \left\{ (y_{N+d}^* - y_{N+d})^2 \right\} \]
is
\[ V_a = V_c + \alpha^2 \sigma_{\hat{m}}^2 \]
\[ + 2\alpha E \left\{ \left[ m + a^T(Y - mU) - y_{N+d} \right] [\hat{m} - m] \right\} \]
\[ = V_c + \alpha^2 \sigma_{\hat{m}}^2 \]
\[ + 2\alpha E \left\{ a^T(Y - mU) - y_{N+d} \right\} \left[ (Y - mU)^T \xi \right] \]
since \( \hat{m} \) is unbiased. \( \sigma_{\hat{m}}^2 \) denotes the variance of \( \hat{m} \). The third term in the above expression is zero by (7). Therefore
\[ V_a = V_c + \alpha^2 \sigma_{\hat{m}}^2. \] (18)

It follows from (18) that \( V_a \) will be minimum if \( \sigma_{\hat{m}}^2 \) is minimum, i.e. if \( \hat{m} \) is chosen as the MVU estimate of \( m \). The corresponding estimator will be called MVALP, for Minimum Variance Approximate Levinson Predictor. The MVU estimate for \( \hat{m} \) is obtained as follows:
\[ \sigma_{\hat{m}}^2 = E \left\{ (\hat{m} - m)^2 \right\} = E \left\{ [\xi^T(Y - mU)]^2 \right\} \]
\[ = \xi^T \Sigma \xi = \alpha^2 - \xi^T \Sigma \xi. \] (19)

Minimizing \( \xi^T \Sigma \xi \) w.r.t. \( \xi \) subject to (15) yields
\[ \xi = (U^T R^{-1} U)^{-1} R^{-1} U. \] (20)

After lengthy manipulations, using (5), \( \xi \) can also be expressed in terms of the variogram function \( \gamma(\tau) \):
\[ \xi = \left( U^T R^{-1} U \right)^{-1} R^{-1} U. \] (21)

The corresponding minimum error variance for the mean estimate will be denoted \( \sigma_{\hat{m}}^2 \):
\[ \sigma_{\hat{m}}^2 = \left( U^T R^{-1} U \right)^{-1} = \sigma^2 - \left( U^T R^{-1} U \right)^{-1}. \] (22)

Expression (18) shows that the ALP yields a larger error variance than the CLP, and that the two error variances coincide when \( \sigma_{\hat{m}}^2 \rightarrow 0 \), as should be expected. We shall denote by \( \bar{V}_a \) the prediction error variance of the MVALP. Using (12), (7), (22) and (13), we can write
\[ \bar{V}_a = V_c + \alpha^2 \left( U^T R^{-1} U \right)^{-1} \]
\[ = V_c + \left( 1 - R_0^{-1} R_0 \right) \left( U^T R^{-1} U \right)^{-1} \]
\[ = \sigma^2 - R_0^{-1} R_0 \]
\[ + \left( 1 - R_0^{-1} R_0 \right) \left( U^T R^{-1} U \right)^{-1}. \] (24)

Note that this last expression is entirely in terms of the covariance function of \( \{ y_i \} \).

### 3.2. The modified Levinson predictor (MLP)

When the mean \( m \) is unknown, an alternative strategy is to seek the MVU predictor of the following form:
\[ \tilde{y}_{N+d} = \sum_{i=1}^{N} b_i y_{N-i} = b^T Y \] (25)

together with the constraint, imposed by unbiasedness, that
\[ \sum_{i=1}^{N} b_i = 1, \text{ i.e. } b^T U = 1. \] (26)

Minimization of \( E \{(\tilde{y}_{N+d})^2\} \) w.r.t. \( b \) subject to (26) yields the following linear system of \( (N+1) \) equations:
\[
\begin{bmatrix}
R & -U \\
U^T & 0
\end{bmatrix}
\begin{bmatrix}
b \\
\mu
\end{bmatrix} =
\begin{bmatrix}
R_0 \\
1
\end{bmatrix},
\]
where \( \mu \) is a Lagrange coefficient. Alternatively, using (5), we get
\[ U^T \begin{bmatrix} \xi \\ 0 \end{bmatrix} = T_0. \] (28a)
or, with obvious matrix and vector notations,
\[ A_2 \lambda_2 = c. \]  
\( (28b) \)

The prediction error variance can be written in a number of ways:
\[ V_m = \sigma^2 + b^T R_b - 2 b^T R_0 = 2 b^T \Gamma_0 + b^T \Gamma b \]  
\( (29a) \)
\[ = \mu + \sigma^2 - b^T R_0 = \mu + b^T \Gamma_0 = c^T A_2^{-1} c. \]  
\( (29b) \)

The predictor MLP was proposed by Bastin and Henriet [1], who showed that
\[ V_m = V_c + \alpha^2 (U^T R^{-1} U)^{-1} \]  
\( (30) \)

with \( \alpha \) defined by (12). This, together with (23), shows that
\[ V_m = \tilde{V}_u \leq V_u. \]  
\( (31) \)

The inequality in (31) follows from the fact that \( \tilde{V}_u = \min_{\gamma} V_u \). We show in the next section that the MV books and the MLP are identical, which of course explains the equality in (31).

4. The MV books and the MLP are identical

**Proof.** If follows from (16) and (14) that the MV books can be written
\[ y_{N+t}^* = (1 - a^T U) \hat{m} + a^T Y \]
\[ = (a \xi^T + a^T) Y. \]  
\( (32) \)

Therefore, we need to prove that
\[ a + a \xi = b \]  
\( (33) \)
where \( a, \xi, b \) are solutions of (7), (20) and (27) respectively, and with \( a \) given by (12).

The solution of (27) is unique, because it is the vector \( b \) that minimizes
\[ E\{ (y_{N+t})^2 \} = b^T R_b + \sigma^2 - 2 b^T R_0 \]
subject to (26). It is also trivial to see that \( a + a \xi \) satisfies the last equation of (27). Therefore, to prove (33), it remains to be shown that there exists a \( \mu \) such that
\[ R (a + a \xi) - \mu U = R_0. \]  
\( (34) \)

It follows immediately from (7), (20) and (22) that this is so for
\[ \mu = \alpha \sigma^2. \]  
\( (35) \)

This concludes the proof.

In the process of proving our main result, we have shown that the solution \( \mu \) of (27) and (28) is \( \alpha \sigma^2 \). This yields some closed form expressions for \( b \) and some new expressions for \( \mu \) in terms of either \( \Gamma (\tau) \) or \( \gamma (\tau) \). From (35), (27) and (28) we get
\[ \mu = \frac{1 - U^T R^{-1} R_0}{U^T R^{-1} U} = \frac{U^T \Gamma^{-1} R_0 - 1}{U^T \Gamma^{-1} U}. \]  
\( (36) \)

Using (35), (12) and (22), we have
\[ \mu = \frac{1 - U^T R^{-1} R_0}{U^T R^{-1} U} = \frac{U^T \Gamma^{-1} R_0 - 1}{U^T \Gamma^{-1} U}. \]  
\( (37) \)

The second equality in (37) is obtained by multiplying (36) to the left by \( U^T \), and using (26), (12) and (22). This then allows us to write two expressions for \( b \) in terms of \( \Gamma (\tau) \) or \( \gamma (\tau) \) only:
\[ b = R^{-1} R_0 + \frac{1 - U^T R^{-1} R_0}{U^T R^{-1} U} R^{-1} U \]
\[ = \frac{U^T \Gamma^{-1} R_0 - 1}{U^T \Gamma^{-1} U} \Gamma^{-1} U. \]  
\( (38a) \)

The formulas (38a) and (38b) are remarkable because the expressions in terms of \( \Gamma (\tau), \Gamma_0 \) are identical. Note that the first term of (38a) is \( a \), while the second term is \( \alpha \xi \). (Recall (33)) This is not so, however, for (38b), because \( R^{-1} R_0 \neq \Gamma^{-1} \Gamma_0 \). Finally, note that the expressions (37) and (38) can also be obtained from (27) using a matrix inversion lemma.

In Bastin and Henriet [1], it was claimed that \( \hat{V}_n - V_m = \alpha^2 \sigma^2 \geq 0 \), and that therefore the MLP was better than the MV books. This was based on the fact that \( \hat{V}_n \) had been erroneously computed as \( \hat{V}_n = \hat{V}_c + \alpha^2 (\hat{a}_n^2 + \sigma^2) \) rather than the correct expression (18). Note, however, that the equality \( \hat{V}_n = \hat{V}_u \) holds only if the unbiased estimator \( \hat{m} \) is chosen to be the minimum variance estimator. If the sample mean estimator
\[ \hat{m} = \frac{1}{N} \sum_{i=1}^{N} y_{N-i} \]  
\( (39) \)
is used in (16), then \( V_m \leq V_u \).

5. The case of unknown statistics: Heuristic comparison

In this section we want to compare the ALP and the MLP in the case where \( m, \Gamma (\tau) \) and \( \gamma (\tau) \)
are unknown and must be estimated from the data. In such cases it is impossible to use the growing memory Levinson filters described above, because it does not make sense to estimate $N$ predictor coefficients from $N$ data. We shall therefore compare finite-order predictors (of order $N$) whose coefficients $a_i$, $b_i$ are computed as before, but with $m$, $R(\tau)$ and $\gamma(\tau)$ replaced by their sample estimates $\hat{m}$, $\hat{R}(\tau)$ and $\hat{\gamma}(\tau)$. The ALP (16) and the MLP (25) are now replaced, respectively, by

$$y_{t+1}^* = \hat{m} + \sum_{i=1}^{N} a_i (y_{t-i} - \hat{m})$$  \hspace{1cm} (40)$$

and

$$\hat{y}_{t+1} = \sum_{i=1}^{N} b_i y_{t-i}$$ \hspace{1cm} (41)$$

with the $a_i$ and $b_i$ computed as indicated. The sample estimates are obtained using all $t$ data, assuming $t \gg N$:

$$\hat{m} = \frac{1}{t} \sum_{k=1}^{t} y_{t-k},$$  \hspace{1cm} (42a)$$

$$\hat{R}(\tau) = \frac{1}{t - \tau} \sum_{k=1}^{t-\tau} (y_{t-k} - \hat{m})(y_{t-k-\tau} - \hat{m}),$$ \hspace{1cm} (42b)$$

$$\hat{\gamma}(\tau) = \frac{1}{2(t - \tau)} \sum_{k=1}^{t-\tau} (y_{t-k} - y_{t-k-\tau})^2.$$  \hspace{1cm} (42c)$$

Note that in the growing memory predictors of Section 3 and 4, the predictor length coincides with the number of data upon which the mean estimate is based. This is not so in the fixed length predictor (40). Therefore the result (33) of Section 4 no longer holds.

However, if we redefine $Y$ as

$$Y^T = (y_{t-1}, \ldots, y_{t-N})$$

and $R$ and $R_0$ accordingly, and if we denote by $V_c$, $V_a$ and $V_m$ the prediction error variances, respectively, of the finite length predictors CLP, ALP and MLP using exact covariances for the computation of the $a_i$ and $b_i$ and (42a) for the estimation of $\hat{m}$, then the expression (30) for $V_m$ is still valid, and therefore

for $t = N$: \hspace{1cm} $V_a \geq V_m$, \hspace{1cm} (43a)$$

for $t \to \infty$:\hspace{1cm} $\sigma_{a_m}^2 \to 0$ and hence $V_a \to V_c \leq V_m$. \hspace{1cm} (43b)$$

On the basis of this observation, we would like to compare the finite length ALP (40) and the MLP (41) in the practical case where the unknown $m$, $R(\tau)$ and $\gamma(\tau)$ are estimated from increasing data using (42) \footnote{Of course, in such case other predictors might be used such as maximum likelihood or least squares predictors derived directly from the data, but our aim in this discussion is to compare the ALP and MLP predictors.}. We would also like to know whether the predictor coefficients should be estimated using $\hat{R}(\tau)$ or $\hat{\gamma}(\tau)$. (Recall that all predictors can be computed using either covariance or variogram formulas.)

An exact comparison of predictor error variances is extremely complicated, but the following heuristic arguments can be made.

(1) Clearly, for $t \to \infty$, the estimators $\hat{m}$, $\hat{R}(\tau)$ and $\hat{\gamma}(\tau)$ converge to their true values, and therefore the ALP will converge to the CLP. Hence, asymptotically the ALP is better than the MLP: see (43b).

(2) However, for small sample sizes ($t$ small), there is a good reason to think that the MLP, with its coefficients computed from the variogram formulas (38b), should be preferred over the ALP with $\hat{m}$ replaced by its sample mean. One argument is that the MLP does not require a preliminary estimate of the mean, and that the $\hat{\gamma}(\tau)$ are unbiased estimates that are independent of the mean. The other reason is that, for $t = N$, $V_a \geq V_m$ when second-order statistics are known. One would think that this result would still hold for small sample sizes when exact covariances or variograms are replaced by estimated ones, although this would be extremely hard to prove.

(3) The computation of the MLP using the variogram formulas (38b) requires $N + d$ statistics, \{\$\hat{\gamma}(\tau), \tau = 1, \ldots, N + d\},$ while the computation of the MLP using the covariance formulas (38a), as well as the computation of the ALP, require $N + d + 2$ statistics.

(4) For intrinsic (but not necessarily wide-sense stationary) processes with known variograms, the MLP estimator (38b) is the optimal linear predictor: it can be derived directly without going through (5). In such case $R(\tau)$ and $\sigma^2$ may not exist. Therefore the MLP (38b) covers a wider class of random processes, and should be preferred in case of doubt on the wide-sense stationarity of the process. As it turns out, stationarity is very difficult to validate in practice. If covariance
estimates are used under the false belief that the process is stationary, this may lead to completely erroneous results, as the following example, due to Matheron [5], shows. Consider a Wiener process with variogram $\gamma(\tau) = |\tau|$, and suppose we have observed $(y_0, y_1, \ldots, y_t)$. If the user believes the process is stationary and computes $\hat{m}$ and $\hat{R}(\tau)$ by (42), then it can be shown that, for $\tau \geq 0$,

$$E\{\hat{R}(\tau)\} = \frac{\tau^2 - 1}{3\tau} - \frac{4}{3} \tau + \frac{2}{3} \frac{\tau^2}{\tau}.$$  \hspace{1cm} (44)

It is a parabola; an apparent variance of $\hat{R}(0) = (\tau^2 - 1)/3\tau$ will be found, whereas the true variance is infinite. The sample variogram (42c), on the other hand, is unbiased.

6. Simulations

The ALP (with the sample mean used for $\hat{m}$ and the coefficients $a_i$ computed from the sample covariances) and the MLP (with the coefficients computed from the sample variograms) have been compared on simulated data generated from a large number of ARMA($p, q$) models, using short time series. For each run, the ND available data have been split up into ND = NE + NP data. The first NE data were used to estimate the predictor coefficients; the remaining NP data were then used for validation: the mean square prediction error obtained on these NP data was computed. For each model, different combinations were chosen for the order of the predictor $N$, the prediction horizon $d$, the number of data used for estimation NE, and the number of data used for prediction NP. For each one of those, the mean square prediction errors $V_a$ (for the ALP) and $V_m$ (for the MLP) were computed as the average over NR independent runs. The conclusions drawn from these simulations are as follows.

(1) The simulations do not confirm the heuristic arguments (2) of Section 5: even though the MLP was almost always better than the ALP, particularly for short time series (NE small), there were cases the opposite was true.

(2) For processes with exponentially decaying covariances, the MLP turned out to be consistently better. For processes with damped oscillatory covariances, the ALP was sometimes better.

(3) As the process gets closer to white noise (i.e. with a covariance decaying rapidly to zero) the superiority of one predictor over the other (see point 2) decreases. Typical results are shown in Table 1: they are a good illustration of conclusions 2 and 3 above. Simulations with higher-order models have also been performed: they confirm these conclusions.

<table>
<thead>
<tr>
<th>Table 1</th>
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<tbody>
<tr>
<td>Model used to generate data</td>
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<tr>
<td>$(y_k - 5) - 0.95(y_{k-1} - 5) = e_k$</td>
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<tr>
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<tr>
<td>$(y_k - 3) - 0.7(y_{k-1} - 3) = e_k$</td>
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<td>$(y_k - 5) - 0.5(y_{k-1} - 5) = e_k$</td>
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<tr>
<td>$(y_k - 5) + 0.95(y_{k-1} - 5) = e_k$</td>
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<td>$(y_k - 3) + 0.7(y_{k-1} - 3) = e_k$</td>
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Test 1: $N = 5$, $d = 3$, NE = 30, NP = 20, NR = 10.
Test 2: $N = 3$, $d = 1$, NE = 15, NP = 10, NR = 20.

$e_k$ = zero mean white Gaussian noise with unit variance.
$V_a$ = average over NR runs of the mean square prediction error using the ALP and covariance estimates.
$V_m$ = average over NR runs of the mean square prediction error using the MLP and variogram estimates.

7. Concluding remarks

We have shown that, with known second-order moments but unknown mean, the MLP, introduced in [1], is identical to the classical Levinson predictor in which the unknown mean is replaced by its minimum variance unbiased estimate. It is therefore better than any approximate Levinson predictor using any other mean estimate. One might have expected this property to carry over to the case of fixed-length predictors used on short time series with unknown (and hence estimated) second-order statistics. Simulations show that this is true in most cases, but not all. This result indicates that, even though the variogram based predictor is not consistently better than the covariance based one, in the case of estimated statistics it deserves to be considered and perhaps further
studied by the control community. It should also be recalled that, when the process is not wide-sense stationary but has independent increments, the variogram based predictor is optimal, while the covariance based predictor is not.

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References
