Identification of surface characteristics from large samples

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Surface roughness characteristics have been modelled by autoregressive moving average (ARMA) models. Frequently, extra-large samples from the surface are available. Due to the non-linearity and the computational burden dependence on sample size, the available data can not be sufficiently utilized to fit ARMA models in most cases. In an attempt to sufficiently employ the available data, an innovative ARMA identification approach is presented. The computational burden of this approach is nearly independent of the sample size. The accuracy ratio between the present approach and the non-linear least squares algorithm is determined. Both simulation and application have been conducted to confirm its effectiveness.

1 INTRODUCTION

The characterization of engineering surfaces has been an important issue of research in mechanical engineering (**1–5**). In general, to adequately describe the surface, the sampling interval should be sufficiently small. However, if the sampling interval is too small, the sample size will be too large and a long processing time will be required (**1**). Therefore, a study has been performed to select an optimum sampling in accordance with the error requirement (**1**). This optimum interval is only determined for R_a, the centre-line average roughness. When other descriptions of surface roughness are concerned, alternative optimum intervals must be acquired according to the corresponding accuracy requirements.

The autoregressive moving average (ARMA) model has been acknowledged as an effective description for characterization of various types of engineering surfaces (**6–11**). However, there is a lack of approach to select an optimum interval for ARMA characterization. Furthermore, the accuracy requirement varies from case to case. Hence, more data are expected to be processed for more accurate results. The problem is that the computational burden prevents extensive data from being selected. In fact, since the parameter estimation of ARMA models is non-linear and since the computational burden of the conventional methods [for example the non-linear least squares (NLS) method (**12**) and the maximum likelihood (ML) method (**13**)] are proportional to the sample size, the identification of large samples will be time consuming. Therefore, alternative algorithms for identifying ARMA models are preferred.

If the computational burden is not considered, the NLS and ML associated with some well-known criteria of order selection [for instance Akaike's information criterion (**14**) and the *F-test* (**12**)] could provide adequate tools for ARMA identification. However, since their non-linearities have made the computational burden too extensive, it has been one of the aim's of research to find effective approaches to make the computational burden more manageable in the area of time series analysis during the past two decades. These approaches are usually constructed using a method based on a least squares error criterion and require solutions of linear equations. The autoregressive (AR) and moving average (MA) parameters are estimated separately. Kay and Marple concluded in 1981 (**15**) that ARMA parameter estimation continued to be an active area of research. This conclusion was based on the performance and/or computational complexity associated with the existing approaches. In the 1980s, several approaches have been proposed based on the extended Yule–Walker equations (**16–19**). However, it is known that the performance of the extended Yule–Walker equation estimator is poor (**20**). Recently, Fassois presented a fast ARMA approach to parametric spectral estimation (**21**) which offers a low computational and storage requirement. However, much more overspecified models are obtained that are not suitable for the present case. An LD^2 ARMA identifier (**22**) combined an order selection scheme with a linear, dual, decoupled algorithm to estimate the AR and MA components. In this work, some unavailable quantities (the successively increasing order prediction and innovation filter coefficients) are substituted by their estimates. These quantities are essential to produce the AR and MA parameters. More examples of recent presentations concerning ARMA identification can be found in references (**23**) to (**25**), a number of which have been devoted to linearization primarily to decrease the computational burden.

Although numerous approaches have been proposed to eliminate the non-linearity, the most widely used approaches are still the NLS and ML, especially in mechanical engineering (**6–8**, **10**, **26**). This is caused by the complexity that seems to be a common feature of the aforementioned approaches. Also, the lack of feasible performance evaluation prevents users from understanding the modelling accuracy. Therefore, a novel approach that can decrease the computational burden with less complexity and reliable accuracy evaluation is strongly preferred.

A general solution of this problem is not the objective of the present paper. The concern of this paper is to present a novel identification approach for surface modelling that can decrease the computational burden–accuracy ratio with only a slight additional complexity

The MS was received on 31 March 1992 and was accepted for publication on 14 July 1992.
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0954-4062/92 $3.00 + .05

and a reliable evaluation of the final modelling accuracy. The procedure for the proposed approach in this paper consists of two steps: (a) identifying an AR model from the samples (AR modelling); (b) identifying the ARMA model based upon this AR model (ARMA approximation). It will be shown that the modelling accuracy–computational burden ratio increases with the sample size, although this ratio in conventional methods is nearly constant. However, its computational burden is nearly independent of the sample size. This makes it possible to adequately utilize extra-large samples to improve the modelling accuracy without increasing the computational burden. Also, its additional complexity over the NLS is slight and the final accuracy can be evaluated through a simple equation.

In Section 2, the AR modelling and the ARMA approximation are performed based upon novel algorithms presented in this paper. In Section 3, the properties of the present algorithm and the non-linear least squares estimate are analysed. The minimum size of sample that can confirm that the presented algorithm is superior to the non-linear least squares algorithm in terms of the ratio of the modelling accuracy to the computational burden is determined. In Section 4, simulations are performed to verify the proposed algorithm. In Section 5, the proposed algorithm is employed to identify ARMA models from data of the practical surface profile. In the final section, conclusions are provided.

2 ALGORITHMS

As described in the introduction, the present approach consists of the AR modelling and the ARMA approximation. Parameters of AR models are estimated through the least squares algorithm (**12**) while the order is determined by an innovative order determination criterion, proposed in this section. It will be shown that the order selected by this criterion is optimal, assuming an infinite size of samples. Thus, the resulting AR model must be a sufficiently accurate representation of the samples. By minimizing the distance from an ARMA model to this AR model, parameters of ARMA models can be acquired. From an order determination criterion presented in this paper for ARMA models, the order of an ARMA model can be selected. Since the computational burden for AR models may be ignored and since the computational burden for ARMA approximation is independent of sample size, the computational burden will be dramatically decreased. The block diagram of the approach is presented in Fig. 1. The properties of the presented approach will be discussed in the next section.

2.1 Order determination of AR models

A number of criteria for AR order determination already exists, such as the F-test (**12**), Akaike's final prediction error (FPE) criterion (**27**, **28**), the cross-validatory criterion (**29**), Akaike's information criterion (AIC) (**14**) and the weak parameter criterion (WPC) (**30**), etc. Also, researchers have studied the behaviour or validity of some well-known criteria [for instance the FPE criterion (**31**, **32**) and the AIC (**33**, **34**)]. Although there are extensive methods available, no one method can be regarded as the most appropriate for a wide variety of model applications. When prediction is of primary concern, parameters are frequently estimated by the least squares method. In this case, those methods based upon the *one-step-ahead* prediction error (for example the FPE and the cross-validatory criterion) may be the most suitable of the existing methods due to the relationship between the one-step-ahead prediction error and the squared sum of residuals. Since the least squares algorithm has been selected to estimate AR parameters, these methods are of interest here. However, it has been noted by Gooijer (**29**) that for the FPE and its modifications, the ability of predicting one-step-ahead values of the process is measured over the same data utilized to estimate the parameters of the model. In order to overcome this somewhat unrealistic situation some approaches have been proposed based upon a concept of cross-validity. In cross-validity, a given model specification in the class of AR (p) is estimmated N times, each time deleting one observation from the sample (the number of samples is N). This deleted observation is then predicted using the resulting model estimate. However, it is apparent that this modified approach may not be appropriate for our problem where N is extra large.

Recently, the concept of model distance has been introduced by the present authors to propose a novel order determination criterion for ARMA models. In this sub-section, the model distance is first briefly recalled. Then an order determination criterion for AR models is presented.

2.1.1 Model distance

Suppose the sample of y_t is produced from

$$M:\ \phi(B)y_t = \theta(B)\varepsilon_t \tag{1}$$

where M is a notation for the model (1), B is the backshift operator, $\varepsilon \sim N(0, \sigma_\varepsilon^2)$, and

$$\phi(B) = 1 - \sum_{j=1}^{p} \phi_j B^j = \prod_{j=1}^{p} (1 - \alpha_j B)$$

$$\theta(B) = 1 - \sum_{i=1}^{q} \theta_i B^i = \prod_{i=1}^{q} (1 - \beta_i B)$$

where ϕ_j and θ_i ($j = 1, \ldots, p$; $i = 1, \ldots, q$) are real and $|\alpha_j| < 1, |\beta_i| < 1$ ($j = 1, \ldots, p$; $i = 1, \ldots, q$).

Suppose $\hat{M}$ (ARMA ($\hat{p}$, $\hat{q}$)) is an estimate of M:

$$\hat{M}:\ \hat{\phi}(B)y_t = \hat{\theta}(B)\hat{\varepsilon}_t \tag{2}$$

where $\hat{\varepsilon}_t$ is the residual of $\hat{M}$ and

$$\hat{\phi}(B) = 1 - \sum_{j=1}^{\hat{p}} \hat{\phi}_j B^j, \qquad \hat{\theta}(B) = 1 - \sum_{i=1}^{\hat{q}} \hat{\theta}_i B^i$$

where $\hat{\phi}_j$ and $\hat{\theta}_i$ ($j = 1, \ldots, \hat{p}$; $i = 1, \ldots, \hat{q}$) are real and $|\hat{\alpha}_j| < 1, |\hat{\beta}_i| < 1$ ($j = 1, \ldots, \hat{p}$; $i = 1, \ldots, \hat{q}$).

Let us define

$$D_1(\hat{M} \to M) \equiv \sqrt{\left\{\frac{E_1(\hat{M}) - E_1(M)}{E_1(M)}\right\}}$$

$$\equiv \sqrt{\left\{\frac{\Delta E_1(\hat{M} \to M)}{\sigma_\varepsilon^2}\right\}} \tag{3}$$

as the first-order model distance from $\hat{M}$ to M, where $E_1(M)$ [$E_1(\hat{M})$] is the variance of the one-step-ahead prediction error when the minimum mean squared fore-

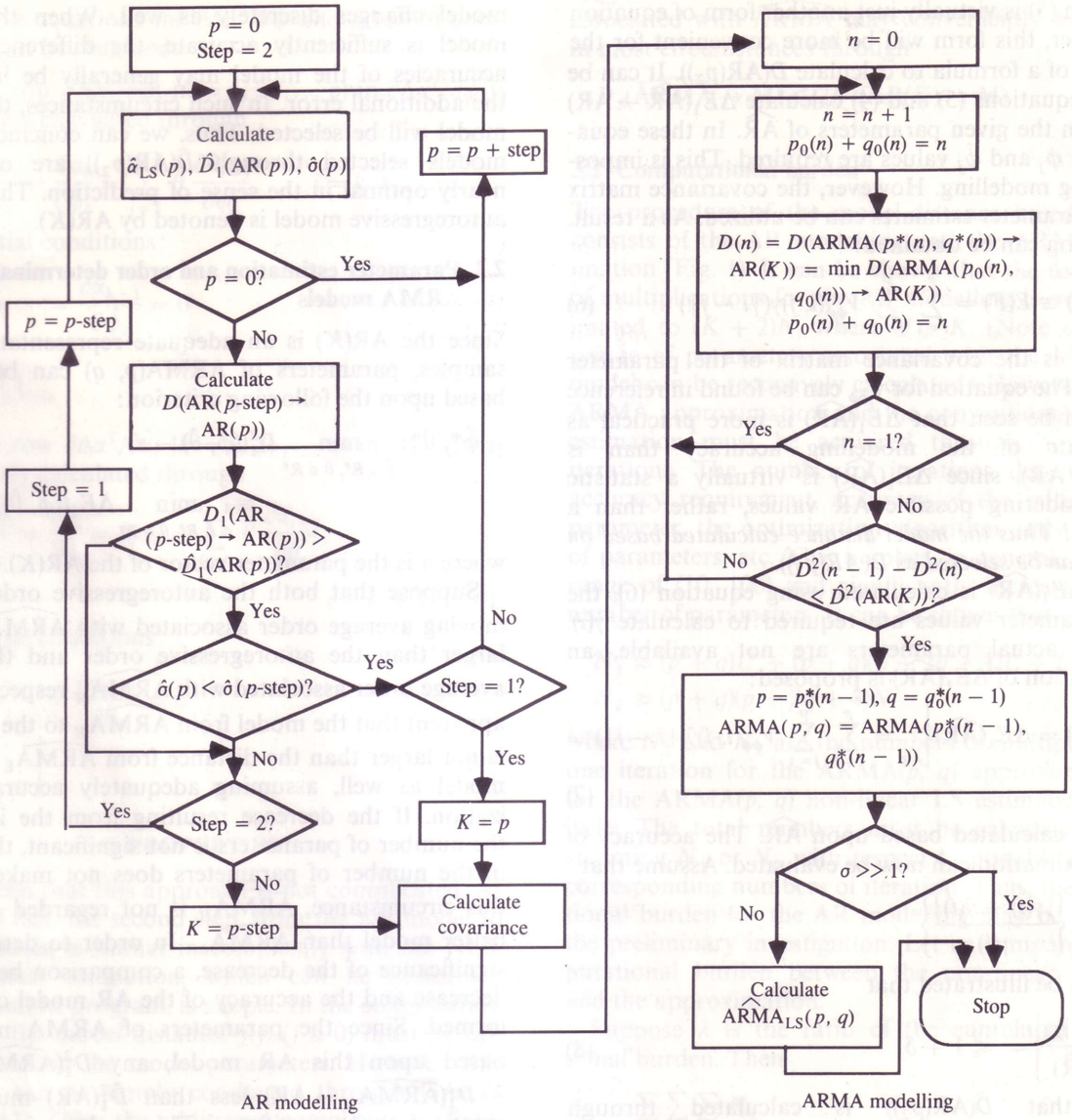


Fig. 1 Identification procedure of ARMA models from large samples

cast is performed using M ($\hat{M}$). Suppose M, $\hat{M}$ assume the following AR model forms:

$$M: y_t = \sum_{j=1}^{\infty} a_j y_{t-j} + \varepsilon_t, \qquad \hat{M}: y_t = \sum_{j=1}^{\infty} \hat{a}_j y_{t-j} + \hat{\varepsilon}_t$$

It can be shown that

$$\Delta E_1(\hat{M} \to M) = \Delta a^T R \Delta a \tag{4}$$

where $\Delta a = (\Delta a_1, \Delta a_2, \ldots, \Delta a_L)^T = (a_1 - \hat{a}_1, a_2 - \hat{a}_2, \ldots, a_L - \hat{a}_L)^T$, $R_{L\times L}(i, j) = \gamma(|j - i|) = E(y_{t-i} y_{t-j})$ and L is a positive infinite integer (which can be taken to be a sufficiently large integer in numerical computations); $\gamma(j)$ can be calculated based upon both ϕ_j, θ_i ($j = 1, \ldots, p$; $i = 1, \ldots, q$) and σ_ε^2 **(12)**.

2.1.2 Order determination

Suppose there is a model AR(p_1) and a model AR(p_2), where AR(p_1) has less parameters than AR(p_2). If the model distance from AR(p_1) to AR(p_2) is large, the difference between these two models is significant. Therefore, if $\hat{\sigma}_{\hat{\varepsilon}}^2$(AR($p_2$)) [the estimate of the residual variance associated with AR(p_2)] is smaller, the increase in the number of parameters from AR(p_1) to AR(p_2) should produce a better model. In this case, the model distance from AR(p_1) to AR(p_2) can be taken as a measure of the improvement in modelling accuracy due to the increase in the number of parameters. However, if the accuracy improvement is not significant so that the model distance [D(AR(p_2))] corresponding to the accuracy estimate of AR(p_2) is larger than the model distance from AR(p_1) and AR(p_2), then AR(p_2) is not a correct selection. The above is simply the principle of the order determination criterion for AR models presented in this section. This criterion can be described as the following: if $D(\text{AR}(p_2)) < D(\text{AR}(p_1) \to \text{AR}(p_2))$ and $\hat{\sigma}_{\hat{\varepsilon}}^2(\text{AR}(p_2)) < \hat{\sigma}_{\hat{\varepsilon}}^2(\text{AR}(p_1))$, select AR($p_2$); otherwise, do not select AR(p_2). Since the model distance is employed, this criterion is of prediction concern corresponding to the least squares estimation.

Let us discuss the computation of D(AR(p_2)). Assume an AR model to be described by ϕ_j ($j = 1, 2, \ldots, p$) and its estimate $\widehat{\text{AR}}$ by $\hat{\phi}_j$ ($j = 1, 2, \ldots, p$). It can be shown that

$$\Delta E_1(\widehat{\text{AR}} \to \text{AR}) \equiv F = \sum_{i=1}^{p} \sum_{j=1}^{p} \Delta\phi_i \Delta\phi_j \gamma(|i - j|) \tag{5}$$

As a result, the corresponding model distance $D(\widehat{\text{AR}} \to \text{AR})$ can be calculated.

Equation (5) is virtually just another form of equation (4). However, this form will be more convenient for the derivation of a formula to calculate $D(\mathrm{AR}(p_2))$. It can be seen that equations (5) and (4) calculate $\Delta E_1(\widehat{\mathrm{AR}} \rightarrow \mathrm{AR})$ based upon the given parameters of $\widehat{\mathrm{AR}}$. In these equations, both ϕ_j and $\hat{\phi}_j$ values are required. This is impossible during modelling. However, the covariance matrix V of the parameter estimates can be utilized. As a result, the following can be obtained:

$$\Delta E_1(\widehat{\mathrm{AR}}) \equiv E(F) = \sum_{i=1}^{p} \sum_{j=1}^{p} V_{\phi\phi}(i, j)\gamma(|i-j|) \tag{6}$$

where $V_{\phi\phi}$ is the covariance matrix of the parameter estimates. The equation for $V_{\phi\phi}$ can be found in reference (**13**). It can be seen that $\Delta E_1(\widehat{\mathrm{AR}})$ is more practical as an estimate of the modelling accuracy than is $\Delta E_1(\widehat{\mathrm{AR}} \rightarrow \mathrm{AR})$, since $\Delta E_1(\widehat{\mathrm{AR}})$ is virtually a statistic when considering possible $\widehat{\mathrm{AR}}$ values, rather than a special $\widehat{\mathrm{AR}}$. *Thus the model distance calculated based on* $\Delta E_1(\widehat{AR})$ *can be selected as* $D(AR(p_2))$.

When $\Delta E_1(\widehat{\mathrm{AR}})$ is calculated using equation (6), the actual parameter values are required to calculate $\gamma(i)$. Since the actual parameters are not available, an approximation of $\Delta E_1(\widehat{\mathrm{AR}})$ is proposed:

$$\Delta \hat{E}_1(\widehat{\mathrm{AR}}) = \Delta E_1(\widehat{\mathrm{AR}})\Big|_{\widehat{\mathrm{AR}}} = \sum_{i=1}^{p} \sum_{j=1}^{p} V_{\phi\phi}(i, j)\hat{\gamma}(|i-j|) \tag{7}$$

where $\hat{\gamma}$ is calculated based upon $\widehat{\mathrm{AR}}$. The accuracy of this approximation can now be evaluated. Assume that

$$\delta = \max\left\{\frac{|\gamma(i) - \hat{\gamma}(i)|}{\gamma(i)}\right\}$$

It can then be illustrated that

$$\left|\frac{\Delta E(\widehat{\mathrm{AR}}|_{\widehat{\mathrm{AR}}})}{\Delta E(\widehat{\mathrm{AR}})}\right| = \leqslant 1 + \delta \tag{8}$$

Assume that $\hat{D}(\mathrm{AR}(p_2))$ is calculated through $\Delta E_1(\mathrm{AR}(p_2))|_{\mathrm{AR}(p2)}$. Thus, the maximum relative error between $\hat{D}^2(\mathrm{AR}(p_2))$ and $D^2(\mathrm{AR}(p_2))$ [which is calculated based upon $\Delta E_1(\mathrm{AR}(p_2))$] will be

$$\max \frac{|\hat{D}^2(\mathrm{AR}(p_2)) - D^2(\mathrm{AR}(p_2))|}{D^2(\mathrm{AR}(p_2))} \approx \delta \tag{9}$$

When $\mathrm{AR}(p_2)$ is a sufficient approximation of AR, δ will be small. In this case, $\hat{D}^2(\mathrm{AR}(p_2))$ is a good estimate of $D^2(\mathrm{AR}(p_2))$.

It is apparent that if $D(\mathrm{AR}(p_2))$ is employed, the selected models are statistically optimal in the sense of minimizing the prediction error. When $\hat{D}(\mathrm{AR}(p_2))$ is utilized, it can be shown that

$$D^2(\mathrm{AR}^*) \leqslant D^2(\mathrm{AR}^{\mathrm{optimal}}) + D^2(\mathrm{AR}^{\mathrm{optimal}})\delta \tag{10}$$

where AR^* is the model selected based upon $\hat{D}(\mathrm{AR}(p_2))$ and $\mathrm{AR}^{\mathrm{optimal}}$ is the selected model based upon $D(\mathrm{AR}(p_2))$ which is optimal. Therefore, the possible incorrect selections will only cause additional errors lying within a range of $D^2(\mathrm{AR}^{\mathrm{optimal}})\delta$. It can be seen that this is an excellent result when the accuracy of the optimal model is sufficient, especially in this case of an extra-large sample size. Also, in most cases the optimal model will be selected when the accuracy of the optimal model is sufficient. As a matter of fact, since the model order varies discretely, the accuracy of the estimated model changes discretely as well. When the optimal model is sufficiently accurate, the difference between accuracies of the model may generally be larger than the additional error. In such circumstances, the optimal model will be selected. Thus, we can conclude that the models selected through $\hat{D}(\mathrm{AR}(p_2))$ are optimal or nearly optimal in the sense of prediction. The resulting autoregressive model is denoted by $\mathrm{AR}(K)$.

2.2 Parameter estimation and order determination of ARMA models

Since the $\mathrm{AR}(K)$ is an adequate representation of the samples, parameters of $\mathrm{ARMA}(p, q)$ can be acquired based upon the following criterion:

$$\hat{\phi}^*, \hat{\theta}^*: \min_{\hat{\phi} \in R^p, \hat{\theta} \in R^q} D_1^2((\hat{\phi}, \hat{\theta}) \rightarrow \alpha) \equiv \min_{\hat{\phi} \in R^p, \hat{\theta} \in R^q} \Delta E_1((\hat{\phi}, \hat{\theta}) \rightarrow \alpha) \tag{11}$$

where α is the parameter vector of the $\mathrm{AR}(K)$.

Suppose that both the autoregressive order and the moving average order associated with $\widehat{\mathrm{ARMA}}_L$ are not larger than the autoregressive order and the moving average order associated with $\widehat{\mathrm{ARMA}}_H$ respectively. It is apparent that the model from $\widehat{\mathrm{ARMA}}_H$ to the AR model is not larger than the distance from $\widehat{\mathrm{ARMA}}_L$ to the AR model as well, assuming adequately accurate optimization. If the decrease resulting from the increase in the number of parameters is not significant, the increase in the number of parameters does not make sense. In this circumstance, $\widehat{\mathrm{ARMA}}_H$ is not regarded as being a better model than $\widehat{\mathrm{ARMA}}_L$. In order to determine the significance of the decrease, a comparison between this decrease and the accuracy of the AR model can be performed. Since the parameters of ARMA models are based upon this AR model, any $D_1^2(\widehat{\mathrm{ARMA}}_L \rightarrow \mathrm{AR}) - D_1^2(\widehat{\mathrm{ARMA}}_H \rightarrow \mathrm{AR})$ less than $\hat{D}_1^2(\mathrm{AR})$ must not be regarded to be significant. This is the principle of the order determination of ARMA models presented in this section.

In order to minimize the model distance from $\mathrm{ARMA}(p, q)$ to $\mathrm{AR}(K)$, the derivative of the distance with respect to $(\hat{\phi}, \hat{\theta})$ is expected. It can be shown [see equation (4)] that

$$\begin{bmatrix} \dfrac{\partial \Delta E_1((\hat{\phi}, \hat{\theta}) \rightarrow \alpha)}{\partial \hat{\phi}} \\ \dfrac{\partial \Delta E_1((\hat{\phi}, \hat{\theta}) \rightarrow \alpha)}{\partial \hat{\theta}} \end{bmatrix} = 2 \begin{bmatrix} \dfrac{\partial \Delta \alpha}{\partial \hat{\phi}} \\ \dfrac{\partial \Delta \alpha}{\partial \hat{\theta}} \end{bmatrix}_{(p+q) \times L} R \Delta \alpha \tag{12}$$

where $\partial \Delta \alpha^{\mathrm{T}} / \partial \hat{\phi}$ and $\partial \Delta \alpha^{\mathrm{T}} / \partial \hat{\theta}$ are $p \times L$ and $q \times L$ matrices respectively. Based upon

$$\left(\frac{\partial \Delta \alpha^{\mathrm{T}}}{\partial \hat{\phi}}\right)_{ki} = \frac{\partial \Delta \alpha^{\mathrm{T}}}{\partial \hat{\phi}_k} = -\frac{\partial \alpha_i}{\partial \hat{\phi}_k},$$

$$\left(\frac{\partial \Delta \alpha^{\mathrm{T}}}{\partial \hat{\theta}}\right)_{ni} = \frac{\partial \Delta \alpha^{\mathrm{T}}}{\partial \hat{\phi}_n} = -\frac{\partial \alpha_i}{\partial \hat{\phi}_n},$$

$$i = 1, 2, \ldots, L; \; k = 1, 2, \ldots, p; \; n = 1, 2, \ldots, q$$

and

$$\hat{\alpha}_i = \hat{\phi}_i - \hat{\theta}_i + \sum_{j=1}^{i-1} \hat{\alpha}_{i-j}\hat{\theta}_j, \quad i = 2, 3, \ldots, L$$

$$\hat{\alpha}_1 = \hat{\phi}_1 - \hat{\theta}_1, \quad \hat{\phi}_j = 0(j > p), \quad \hat{\theta}_j = 0(j > q)$$

the recursive equations for $\partial\Delta\alpha^T/\partial\hat{\phi}$ and $\partial\Delta\alpha^T/\partial\hat{\theta}$ computations can be obtained:

1. The kth row $\partial\Delta\alpha^T/\partial\hat{\phi}_k$ ($k = 1, 2, \ldots, p$) in $\partial\Delta\alpha^T/\partial\hat{\phi}$ is recursively calculated through

$$-\frac{\partial\Delta\alpha_i}{\partial\hat{\phi}_k} = \frac{\partial\hat{\alpha}_i}{\partial\hat{\phi}_k} = \sum_{j=1}^{i-1} \hat{\theta}\,\frac{\partial\hat{\alpha}_{i-j}}{\partial\phi_k}, \qquad i = k+1, \ldots, L$$

with initial conditions:

$$\frac{\partial\hat{\alpha}_1}{\partial\hat{\phi}_k} = \cdots = \frac{\partial\hat{\alpha}_{k-1}}{\partial\hat{\phi}_k} = 0$$

$$\frac{\partial\hat{\alpha}_k}{\partial\hat{\phi}_k} = 1$$

2. The kth row $\partial\Delta\alpha^T/\partial\hat{\theta}_k$ ($k = 1, 2, \ldots, q$) in $\partial\Delta\alpha^T/\partial\hat{\theta}$ is recursively calculated through

$$-\frac{\partial\Delta\alpha_i}{\partial\hat{\theta}_k} = \frac{\partial\hat{\alpha}_i}{\partial\hat{\theta}_k} = \hat{\alpha}_{i-k} - \sum_{j=1}^{i-1} \hat{\theta}\,\frac{\partial\hat{\alpha}_{i-j}}{\partial\theta_k}, \qquad i = k+1, \ldots, L$$

with initial conditions:

$$\frac{\partial\hat{\alpha}_1}{\partial\hat{\theta}_k} = \cdots = \frac{\partial\hat{\alpha}_{k-1}}{\partial\hat{\theta}_k} = 0$$

$$\frac{\partial\hat{\alpha}_k}{\partial\hat{\theta}_k} = -1$$

3 PROPERTIES

It can be seen that this approach is not complicated. As a matter of fact, the second step, from the AR model to ARMA models, is similar in complexity with the NLS. AR parameter estimation, which can be performed using a standard program, is simple. In the computation concerning the model distance, $\gamma(j)$ ($j \geqslant 0$) must be calculated based on the model parameters. However, this calculation can be simply conducted through Green's functions (**12**). Thus, the additional complexity is slight. The discussion now turns to an investigation of the effectiveness of the proposed approach.

In this section, both the computational burden and the modelling accuracy have been related to the size of samples and the number of parameters. In terms of the ratio of modelling accuracy to sample size, the possible benefit can be determined.

3.1 Accuracy

From equation (4) the following inequality can be shown:

$$\Delta E_1(\widehat{\text{ARMA}} \to M) \leqslant [\sqrt{\{\Delta E_1(\widehat{\text{ARMA}} \to \text{AR}(K))\}} + \sqrt{\{\Delta E_1(\text{AR}(K) \to M)\}}]^2$$

Thus, the final modelling accuracy can be estimated from the following inequality:

$$D_1(\widehat{\text{ARMA}} \to M) \leqslant \frac{\sqrt{\{\Delta E_1(\widehat{\text{ARMA}} \to \text{AR}(K))\}} + \sqrt{\{\Delta E_1(\text{AR}(K) \to M)\}}}{\sqrt{\{E_1(M)\}}} \leqslant D_1(\widehat{\text{ARMA}} \to \text{AR}(K)) + D_1(\text{AR}(K) \to M) \tag{13}$$

In most cases, $D_1(\widehat{\text{ARMA}} \to \text{AR}(K)) < \hat{D}_1(\text{AR}(K))$. Also, it will be illustrated in Section 3.3 that $\hat{D}_1(\text{AR}(K)) < D_1(\text{AR}(K) \to M)$. Therefore, the accuracy associated with $\widehat{\text{ARMA}}$ may conveniently be estimated in most circumstances through

$$D_1(\widehat{\text{ARMA}} \to M) \leqslant 2D_1(\text{AR}(K) \to M) \tag{14}$$

3.2 Computational burden

The procedure of the model-distance based approach consists of the AR modelling and the ARMA approximation (Fig. 1). It can be shown that the total number of multiplications for the AR modelling is only approximated to $(K + 2)N$, where $N \gg K$. (Note that the estimate of parameters associated with the higher order model can be recursively calculated.) However, both the ARMA approximation and the conventional parameter estimation must be acquired through a number of iterations. The number of iterations depends on the accuracy requirement, accuracy of the initial iterative parameter, the optimization algorithm and the number of parameters, etc. This number, in general, varies in a range of (10, 100) and significantly increases with the number of parameters. It can be shown that

$$\begin{aligned} N_1 &\approx (p+q)L^2 + (p+q)(p+2q+1)L + L^2/2 \\ N_2 &\approx (p+q)(p+3q+4)N \end{aligned} \tag{15}$$

where N_1 and N_2 are the numbers of multiplications in one iteration for the ARMA(p, q) approximation and for the ARMA(p, q) non-linear LS estimation respectively. The total numbers must be calculated through summing N_1 or N_2 with respect to possible orders and corresponding numbers of iteration. Thus, the computational burden for the AR modelling may be ignored in the preliminary investigation. Let us compare the computational burden between the non-linear estimation and the approximation.

Suppose λ is the ratio of the cumulated computational burden. Then

$$\lambda = \frac{\sum_p \sum_q \sum_{i_1} N_1}{\sum_p \sum_q \sum_{i_2} N_2} \tag{16}$$

where i_1 and i_2 correspond to the number of iterations associated with the ARMA approximation and the non-linear LS estimation respectively. For the sake of convenience, i_1 and i_2 are assumed to be two equivalent constants. Thus, we have

$$\lambda \approx \frac{\sum_p \sum_q N_1}{\sum_p \sum_q N_2} \tag{17}$$

From equations (15) it can be seen that both N_1 and N_2 depend on (p, q). Yet a variety of (p, q) values will be encountered in order to determine order. Suppose the DDS order determination procedure of Pandit and Wu (**12**) is followed. Thus, ARMA(2, 1), ARMA(4, 3) ARMA(6, 5), ARMA(5, 3) and ARMA(4, 4) may be encountered, assuming the final result to be of ARMA(4, 3). Hence, it can be shown that λ can be estimated through

$$\lambda \leqslant \frac{N_1(p^*, q^*)}{N_2(p^*, q^*)} \tag{18}$$

where (p^*, q^*) are the final orders. Thus, from equations

(15), the following can be employed:

$$\lambda = \frac{(p^* + q^*)L^2 + (p^* + q^*)(p^* + 2q^* + 1)L + L^2/2}{(p^* + q^*)(p^* + 3q^* + 4)N} \tag{19}$$

This equation can, in a practical situation where $p^* + 2q^* + 1 < K + 5 = L$, be approximated as

$$\lambda = \frac{2L^2}{(p^* + 3q^* + 4)N} \tag{20}$$

Equation (20) will be employed to determine the benefit of the present algorithm.

In order to demonstrate the decrease in the ratio of computational burden as the sample size increases, some computational results are depicted in Fig. 2 where L is selected to be 45. The computation is performed based upon equations (17) and (15), assuming the DDS order determination procedure of Pandit and Wu is followed. It can be found that the computational burden dramatically decreases as the size of the samples becomes larger.

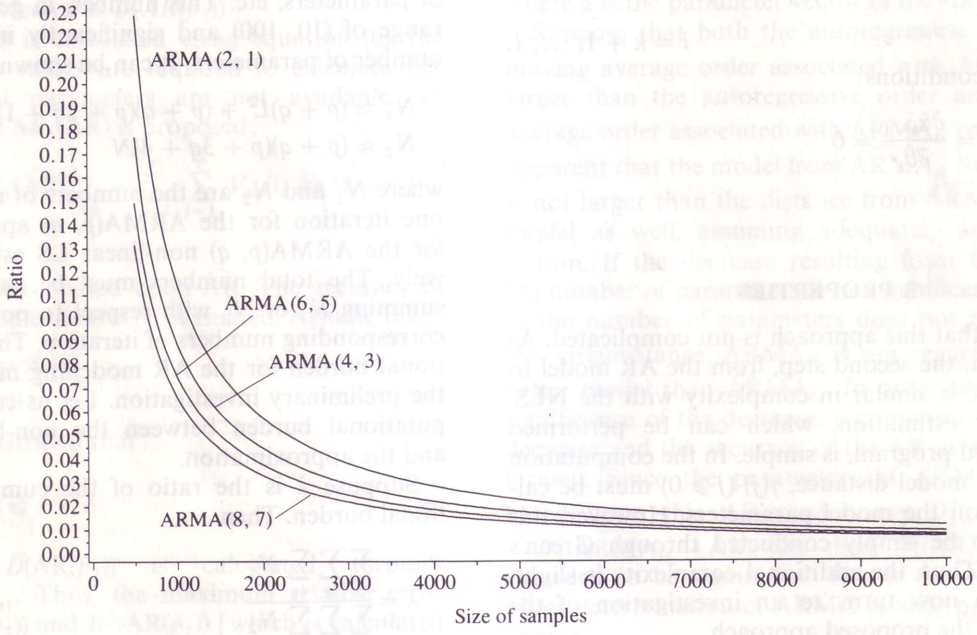
3.3 Estimation accuracy behaviour

Assume that the least squares estimate of AR(K), $\hat{\alpha}_{LS}$, can be denoted by

$$\hat{\alpha}_{LS} = [\Phi^T\Phi]^{-1}\Phi^T Y$$

Thus, the large sample matrix for $\hat{\alpha}_{LS}$ covariance may be obtained utilizing

$$V_{\phi\phi} = [\Phi^T\Phi]^{-1}\sigma_\varepsilon^2 \approx \frac{1}{N} R^{-1}\sigma_\varepsilon^2$$



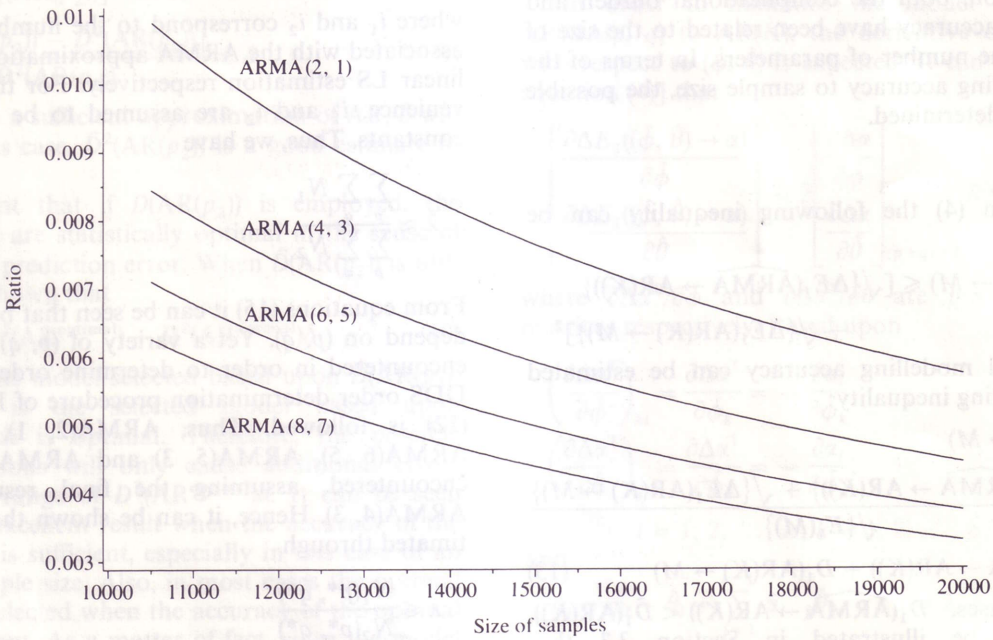


Fig. 2 Ratio of cumulated computational burden versus sample size

Therefore,

$$\Delta E(\mathrm{AR}(K)) = \sum_{j=1}^{K}\sum_{j=1}^{K} V_{\phi\phi}(i,j)\gamma(|i-j|)$$

$$\approx \frac{\sigma_\varepsilon^2}{N}\sum_{i=1}^{K}\sum_{j=1}^{K}(R^{-1})_{ij}R_{ji} = \frac{K}{N}\sigma_\varepsilon^2 \qquad (21)$$

It can be seen that the AR modelling error is proportional to the order and inversely proportional to the sample size in the case where adequately large samples are addressed.

Equation (21) actually provides an accuracy estimate for the case where the actual model is a Kth AR model. In fact, the actual model in this problem will, in general, be an infinite-order AR model. For this infinite AR model, an adequately accurate finite-order AR approximation exists for any given accuracy requirement if the order of the AR approximation can be sufficiently large, if invertibility is assumed. For any given order, a corresponding optimum AR approximation exists. The accuracy estimate provided by equation (21) is simply a correspondence to the error measurement from the estimated AR(K) to the optimum AR(K) approximation. (Note that the estimated AR(K) is the optimal or nearly optimal autoregressive estimate in the case of the given samples. This model is determined through a total consideration of the sample size and the order.) Thus, if it is assumed that all the infinite AR models (all M values) of concern can be sufficiently approximated by AR (K_m), the following can be shown:

$$\Delta E(\mathrm{AR}(K) \to M) \leqslant \frac{K_\mathrm{m}}{N}\sigma_\varepsilon^2 \qquad (22)$$

In most circumstances, K_m can be taken to be 30 (**35**). In this paper, K_m is taken to be 40 for the sake of conclusion validity.

For non-linear least squares estimates of ARMA models, the dependence of modelling accuracy on the sample size and the parameter number can not be as simple as equation (21). The modelling error will, in general, be larger than provided by equation (21). However, for the sake of convenience, it can still be assumed that

$$\Delta E(\widehat{\mathrm{ARMA}}_{\mathrm{LS}}(p,q)) = \frac{p+q}{N}\sigma_\varepsilon^2 \qquad (23)$$

although the actual value will be larger.

3.4 Beneficial sample size

It can be seen that the computational burden for the ARMA approximation is independent of the sample size while the computational burden for the non-linear LS estimation is proportional to the sample size. This implies that the present algorithm may be preferred when the sample size is large enough. It will now be determined which size of sample is sufficiently large.

The concern here is to acquire a more accurate estimate using less computational burden. Thus,

$$\rho = \frac{1/\Delta E}{\text{computational burden}} \qquad (24)$$

is defined as a ratio of modelling accuracy to the computational burden. Hence, the intention is to acquire large ρ. Confirmation of the following inequality can ensure that the present algorithm is superior to the non-linear least squares estimate:

$$\rho_{\widehat{\mathrm{ARMA}}_{\mathrm{present}}} > \rho_{\widehat{\mathrm{ARMA}}_{\mathrm{LS}}} \qquad (25)$$

It can be shown that $\rho_{\widehat{\mathrm{ARMA}}_{\mathrm{LA}}}$ is independent of the sample size because the computational burden is proportional to the sample size. Using equations (20), (21), (23) and (14), the following inequality can be obtained:

$$\frac{N}{8K_\mathrm{m}L^2} > \frac{1}{(p+q)(p+3q+4)}$$

Thus,

$$N > \frac{8K_\mathrm{m}L^2}{(p+q)(p+3q+4)} \qquad (26)$$

The minimum N that satisfies equation (26) can be defined as the beneficial sample size N_b. It is apparent that if the sample size is larger than N_b, the presented algorithm will possess a larger ρ than the non-linear LS algorithm. In this computation, $L = K + 5$. Thus,

$$N_\mathrm{b} = \frac{8K_\mathrm{m}(K+5)^2}{(p+q)(p+3q+4)} \qquad (27)$$

If $D_1(\widehat{\mathrm{ARMA}} \to \mathrm{AR}(K)) > \hat{D}_1(\mathrm{AR}(K))$, N_b should be calculated through the following equation:

$$N_\mathrm{b} = \frac{2K_\mathrm{m}(K+5)^2\left\{1 + \dfrac{D_1(\widehat{\mathrm{ARMA}} \to \mathrm{AR}(K))}{\hat{D}_1(\mathrm{AR}(K))}\right\}^2}{(p+q)(p+3q+4)} \qquad (28)$$

It can be seen that if some β_j (see Section 2.1) is near to the unit circle a large K will be produced. In this circumstance, N_b will tend to increase as K increases. However, in this situation, $\Delta E(\widehat{\mathrm{ARMA}}_{\mathrm{LS}}(p,q))$ may not be estimated by equation (23). A much larger modelling error will be caused as well (**36**). From this point of view, N_b will be much smaller than the value calculated through equation (27).

Some examples showing the beneficial sample sizes may be found in the next section.

3.5 Accuracy ratio

Suppose that the equivalent values of computational burden are costed to identify ARMA models by means of the non-linear least squares algorithm and the present algorithm. The accuracy ratio of the present algorithm to the non-linear least squares algorithm can be obtained. This ratio can be calculated through

$$\sigma = \frac{N/4K_\mathrm{m}}{N'/(p+q)}$$

where N' represents the size of samples for which the non-linear least squares modelling will have the same computational burden cost as that where the present algorithm has a size of samples N. It is evident that σ is a measure of the accuracy improvement due to the utilization of the present algorithm. By equation (20), it can be shown that

$$\sigma = \frac{N}{N_b} \tag{29}$$

It is apparent that the accuracy ratio increases with the sample size utilized to conduct the present algorithm. Some ratios in simulations and in practical cases may be found in the following two sections.

4 SIMULATION

The samples are generated from ARMA models:

$$(1 + 1.45B^2 + 0.518B^4)y_t = (1 - \theta B)\varepsilon_t$$

for $\theta = 0.3$, $\theta = 0.6$, $\theta = 0.7$, $\theta = 0.8$ and $\theta = 0.9$. The number of samples is 10 000. Simulation results are listed in Table 1. The details for order determination can be found in Table 2.

From Table 1, it can be seen that the accuracy ratios are much larger than one. This reveals that more accurate results are produced using the present approach than the conventional non-linear least squares algorithm, assuming equivalent computational burden costs. Also, the correct orders of ARMA models are selected.

In the case of $\theta = 0.9$, $\widehat{D(\text{ARMA} \rightarrow \text{AR})} > \hat{D}(\text{AR}(K) \rightarrow M)$. For this case, equation (28) is employed to calculate N_b rather than equation (27). This ensures that the values of N_b and σ in Table 1 are correct.

5 IDENTIFICATION OF SURFACE PROFILES

Surface profile measurements have been performed on copper plates cut by an abrasive water jet. In the literature, only a few hundred data have been employed to fit the ARMA model. In the present two cases, the sample sizes are 6400 and 30 000 respectively. The measured data are depicted in Figs 3 and 4. The results are listed in Table 3 [for case 2, equation (28) was employed to calculate N_b rather than equation (27) to calculate the accuracy ratio]. It can be seen that the accuracy

Table 1 Modelling results of simulation

	AR modelling			ARMA approximation						
θ	K	α	$\hat{D}^2(\text{AR}(K))$	p	q	ϕ	θ	$D^2(\rightarrow\text{AR}(K))$	N_b	σ
0.3	6	−0.29, −1.52, −0.44, −0.62, −0.17, −0.04	0.0005989	4	1	0.0109, −1.436, 0.0118, −0.4984	0.2991	0.00024127	705	14.2
0.6	10	−0.59, −1.79, −1.06, −1.12, −0.66, −0.38, −0.22, −0.11, −0.05, −0.02	0.0009984	4	1	0.0073, −1.438, 0.0085, −0.5000	0.5932	0.0004299	1310	7.63
0.7	12	−0.69, −1.92, −1.35, −1.44, −1.02, −0.71, −0.50, −0.34, −0.22, −0.13, −0.05, −0.03	0.0012047	4	1	0.0113, −1.438, 0.129, −0.5000	0.7008	0.0007743	1682	5.95
0.8	16	−0.79, −2.07, −1.65, −1.82, −1.46, −1.17, −0.95, −0.76, −0.61, −0.49, −0.38, −0.29, −0.20, −0.13, −0.06, −0.03	0.0016008	4	1	0.0114, −1.437, 0.0122, −0.5000	0.7941	0.0009197	2566	3.90
0.9	22	−0.88, −2.22, −1.98, −2.25, −2.01, −1.78, −1.58, −1.39, −1.23, −1.07, −0.94, −0.81, −0.70, −0.59, −0.49, −0.42, −0.33, −0.29, −0.20, −0.15, −0.06, −0.03	0.0021918	4	1	−0.002, −1.451, −0.000, −0.513	0.8733	0.006869	4242	2.36

Table 2 Order determination

	AR modelling				ARMA approximation			
θ	D^2	$\hat{D}^2(\text{AR}(p))$	$\hat{\sigma}$	Selected	p	q	$D^2(\text{ARMA}(p, q) \rightarrow \text{AR}(K))$	Selected
0.3	2	0.00020	1.2024		2	1	0.26426	
	4	0.39608	0.00040	1.0172		2	2	0.08565	
	6	0.02778	0.00060	1.0033	X	4	1	0.00024	X
	8	0.00006	0.00080	1.0032		4	2	0.00011	
0.6	6	0.13451	0.00060	1.0107		2	1	0.25391	
	8	0.01177	0.00080	1.0045		4	0	0.15351	
	10	0.00203	0.00100	1.0033	X	4	1	0.00043	X
	12	0.00004	0.00120	1.0031		4	2	0.00027	
0.7	8	0.02948	0.00080	1.0083		2	1	0.26647	
	10	0.00921	0.00100	1.0042		2	2	0.19846	
	12	0.00195	0.00120	1.0034	X	4	1	0.00077	X
	14	0.00118	0.00141	1.0032		4	2	0.00071	
0.8	12	0.00716	0.00120	1.0055		2	1	0.28127	
	14	0.00434	0.00140	1.0036		2	2	0.23147	
	16	0.00198	0.00160	1.0028	X	4	1	0.00092	X
	18	0.00004	0.00180	1.0028		5	1	0.00087	
0.9	18	0.00238	0.00180	1.0050		2	1	0.35614	
	20	0.00226	0.00198	1.0039		2	2	0.35230	
	22	0.00229	0.00219	1.0034	X	4	1	0.00687	X
	24	0.00177	0.00241	1.0036		4	2	0.00577	

ratios of the present algorithm to the non-linear least squares algorithm are 6.7 and 4.3 respectively; that is *much more accurate ARMA models have been acquired by the proposed approach than with the non-linear least squares method* with a nearly identical computational burden in both cases.

6 CONCLUSIONS

An innovative approach has been proposed to identify ARMA models from large samples in order to improve modelling accuracy of surface characteristics. The feature of this approach is that its computational burden is independent of the sample size while the computational burden of the conventional algorithm is proportional to the sample size. Thus, extra-large available samples may be utilized sufficiently to improve the modelling accuracy, without a virtual increase in the computational burden. When the sample size is beyond the beneficial sample size, a better accuracy to the computational burden can be produced. It is shown that the

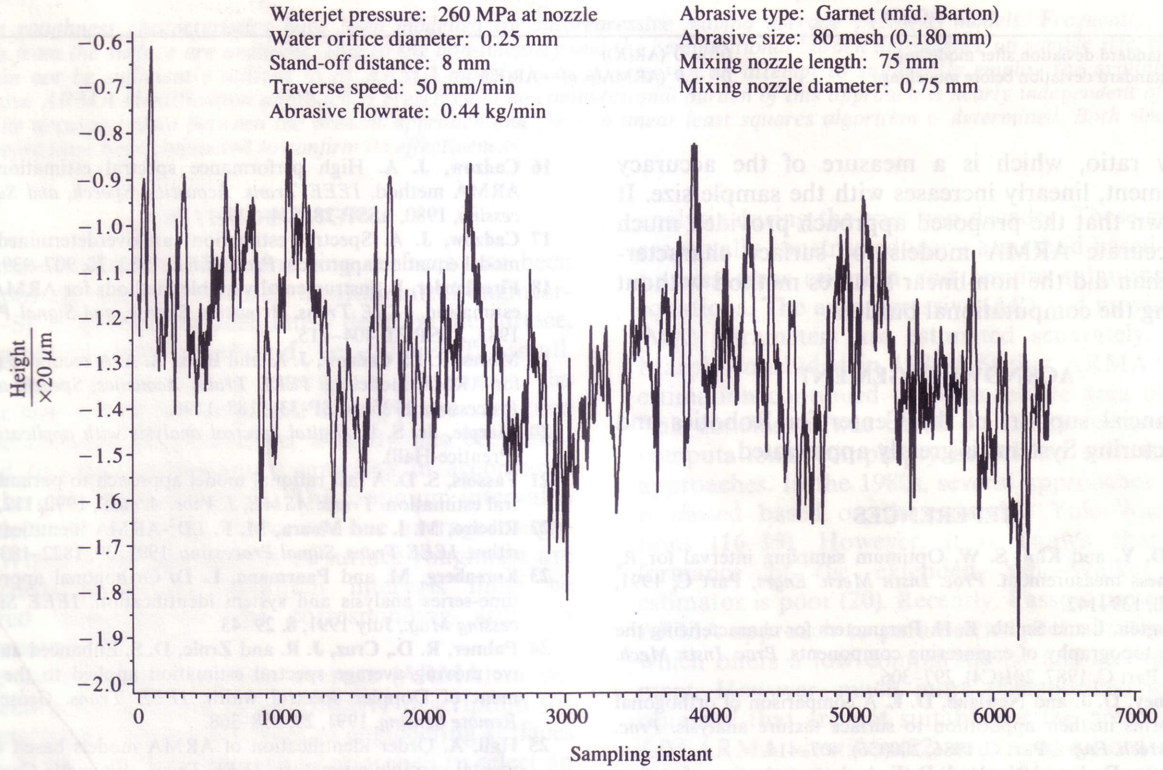


Fig. 3 Surface profile measure: case 1

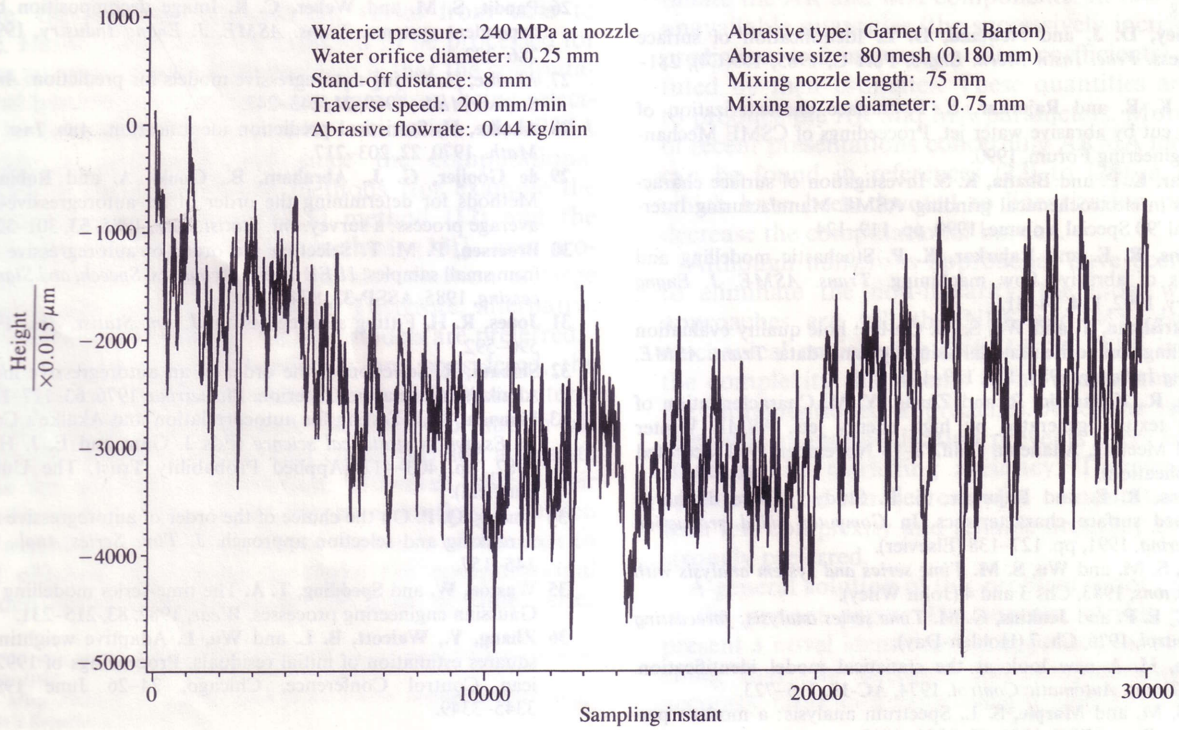


Fig. 4 Surface profile measure: case 2

Table 3 Identification of surface profiles

			AR modelling		ARMA modelling			
Case	N	K	α	$\hat{D}^2$	Model	D^2	σ	$\hat{\sigma}_\varepsilon/\hat{\sigma}_y$
1	6400	4	1.864, −1.098, 0.2776, −0.04968	0.00064	$(1 - 1.60B + 0.608B^2)y_t = (1 + 0.265B)\varepsilon_t$	0.00016	6.7	0.01/0.18
2	30000	22	−0.115, −0.103, −0.113, −0.129, −0.106, −0.113, −0.099, −0.091, −0.098, −0.092, −0.079, −0.061, −0.066, −0.073, −0.075, −0.060, −0.045, −0.040, −0.041, −0.035, −0.038, −0.034	0.00073	$(1 - 1.55B + 0.607B^2 + 0.018B^3) \times (1-B)^2 y_t = (1 - 1.67B - 0.69B^2)\varepsilon_t$	0.003236	4.3	13.2/835

$\hat{\sigma}_\varepsilon$ = standard deviation after modelling
$\hat{\sigma}_y$ = standard deviation before modelling

$\hat{D}^2 = \hat{D}^2(\mathrm{AR}(K))$
$D^2 = D^2(\mathrm{ARMA}(p, q) \rightarrow \mathrm{AR}(K))$

accuracy ratio, which is a measure of the accuracy improvement, linearly increases with the sample size. It was shown that the proposed approach provided much more accurate ARMA models for surface characterization than did the non-linear squares method without increasing the computational burden.

ACKNOWLEDGEMENT

The financial support of the Center for Robotics and Manufacturing Systems is greatly appreciated.

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