

EFFICIENT INPUT SIGNAL DESIGN FOR THIRD-ORDER VOLTERRA MODEL IDENTIFICATION

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Abstract: The present work addresses the identification of third-order Volterra models from input-output process data. Building on previous studies regarding input sequence design for third-order Volterra models (Soni and Parker, 2004), a new reduced-length sequence is designed to identify third-order sub-diagonal kernels. This input sequence leads to a 30% reduction in the data required to accurately estimate the sub-diagonal kernel. Identification of second- and third-order off-diagonal kernels is carried out using a random binary sequence (RBS). These input sequences exploit the third-order Volterra model structure and use the prediction error variance expression as a measure of model fidelity. The utility of the proposed approach is demonstrated on an isothermal polymerization reactor case study. The reduced length sequence shows excellent performance and results in an 47% improvement in the sum-squared error (SSE) value of the third-order sub-diagonal kernel. *Copyright ©2005 IFAC*

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1. INTRODUCTION

One of the main impediments to the widespread implementation of nonlinear model based control schemes in industry is the availability of suitable nonlinear models (Lee, 1999). A number of researchers have focused on fundamental nonlinear model development (Zamamiri *et al.*, 2002; Crowley *et al.*, 2000). While these models provide physical insight and have model parameters with physical correspondence, these models are time-consuming to develop and often have a high state dimension. This complexity in the system model manifests directly in the controller design and implementation which may be computationally intensive. Since theoretically achievable controller performance in a model based control scheme is directly related to model quality (Morari and Zafriou, 1989), control-relevant nonlinear models are essential. An alternative to the use of fundamental models is to em-

ploy an empirical, or black-box, model. In empirical modeling, a mathematical model structure is chosen and model parameters are calculated to best fit the process input-output behavior. Since these models are based only on input-output data, they are comparably easier to develop. However the model parameters often do not have any physical correspondence. In spite of this limitation, a vast majority of industrial model predictive control (MPC) algorithms employ empirical dynamic models (Qin and Badgwell, 1999). Hence, nonlinear empirical dynamic model identification is an academically as well as an industrially relevant problem.

The choice of the input signal is one of the primary design elements in a system identification scheme. The chosen input sequence should be persistently exciting to elicit sufficient output response in order to allow identification of the parameters in the model structure. It is also desired to be plant-friendly, such that it provides enough excitation to identify the model parameters without causing excessive actuator movement,

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and without causing the plant to deviate significantly from its nominal operating point. The input sequence must also be as short as possible so as not to interfere with the nominal plant operation. The metric used to analyze plant-friendliness in this work is the friendliness factor f , as reported in (Parker *et al.*, 2001). An alternative approach is to use multisine signals with a goal of minimizing the crest-factor (ratio of the ℓ_∞ norm of the input to its ℓ_2 norm). The multisine signals can be designed to emphasize the frequency region of interest, and minimization of the crest factor improves the signal to noise ratio of the output thereby making the sequence plant friendly (Braun *et al.*, 2002). In the context of this work input signals are designed with a goal of minimizing actuator wear due to frequent transitions in the input sequence.

2. THIRD-ORDER VOLTERRA MODELS

The general form of the Volterra model is given as:

$$y(k) = h_0 + \sum_{i=1}^N \sum_{j_1=1}^M \cdots \sum_{j_N=1}^M h_i(j_1, \dots, j_N) u(k-j_1) \cdots u(k-j_N) \quad (1)$$

In this equation, N is the model order and M is the model memory, the duration over which the past inputs have a significant effect on the current output, $y(k)$. The Volterra model kernels are given by $h_i(j_1, \dots, j_N)$ and this model is capable of capturing a variety of nonlinear systems behavior (Doyle III *et al.*, 1995; Seretis and Zafiriou, 1997). An example is the ability to capture asymmetric output responses to symmetric changes in the input; this behavior is shown by many chemical engineering systems including reactors and distillation columns. The identification problem involves designing input sequences that excite the Volterra model kernels and identifying the same from the resultant input-output data. One approach used to estimate the Volterra kernels is the cross-correlation method (Doyle III *et al.*, 1995; Pearson *et al.*, 1995). Cross-correlation is essentially a statistical technique which uses the interaction between the input and output of a system to identify the Volterra kernels. An $n+1$ -level input sequence (at a minimum) is required to identify a Volterra model of order n by cross-correlation (Nowak and Veen, 1994). For a detailed description of this technique the interested reader is referred to (Wiener, 1958; Schetzen, 1980). In the present sequence tailoring approach, the third-order Volterra model is first decomposed in the following manner (Parker *et al.*, 2001):

$$\hat{y}(k) = h_0 + L(k) + D(k) + S(k) + O(k) \quad (2)$$

$$L(k) = \sum_{i=1}^M h_1(i) u(k-i)$$

$$D(k) = \sum_{i=1}^M h_2(i, i) u^2(k-i) + \sum_{i=1}^M h_3(i, i, i) u^3(k-i)$$

$$S(k) = 3 \sum_{i=1}^M \sum_{j \neq i}^M h_3(i, i, j) u^2(k-i) u(k-j)$$

$$O(k) = \sum_{i=1}^M \sum_{j \neq i}^M h_2(i, j) u(k-i) u(k-j) + \sum_{i=1}^M \sum_{j \neq i}^M \sum_{\ell \neq j \neq i}^M h_3(i, j, \ell) u(k-i) u(k-j) u(k-\ell)$$

Here, L , D , S , and O represent the linear, nonlinear diagonal, third-order sub-diagonal, and nonlinear off-diagonal terms, respectively. The Volterra model can be assumed symmetric without loss of generality (Rugh, 1981).

2.1 Third-order Volterra model Identification

The identification of the Volterra model coefficients is carried out based on the decomposition (2). As a metric to analyze model fitness, consider the third-order Prediction Error Variance (PEV) expression:

$$\begin{aligned} \sigma_p^2 = & \sigma_0^2 + \sigma_u^2 \sum_{i=1}^M \delta_1^2(i) + (\kappa + 2) \sigma_u^4 \sum_{i=1}^M \delta_2^2(i, i) \\ & + 2 \sigma_u^4 \sum_{i=1}^M \sum_{j=1}^{i-1} \delta_2^2(i, j) + (m_6 - \frac{m_4^2}{\sigma_u^2}) \sum_{i=1}^M \delta_3^2(i, i, i) \\ & + 9(\kappa + 2) \sigma_u^6 \sum_{i=1}^M \sum_{j \neq i}^M \delta_3^2(i, i, j) \\ & + 6 \sigma_u^6 \sum_{i=1}^M \sum_{j \neq i}^M \sum_{\ell \neq j \neq i}^M \delta_3^2(i, j, \ell) \end{aligned} \quad (3)$$

The first term represents the bias term whereas the second, third, and fourth terms describe the contributions due to coefficient errors in the linear, second-order diagonal, and the second-order off-diagonal terms. The last three terms represent the third-order diagonal, third-order sub-diagonal and the third-order off-diagonal contributions to the PEV, respectively. In this work, input sequences are designed based on the structure and coefficients of the terms in (2) and (3). Thus, an input-sequence with a high variance, a high kurtosis, and a high value of the coefficient $(m_6 - \frac{m_4^2}{\sigma_u^2})$, would be a candidate to identify the linear and nonlinear diagonal kernels. For the third-order sub-diagonal terms, if an input sequence is designed such that no more than two points have non-zero values within the model memory M then the third-order off-diagonal contribution to $\hat{y}(k)$ would be zero identically (according to (2)). Furthermore, the ratio of the coefficient of the third-order sub-diagonal term to that of the second-order off-diagonal term in (3) is:

$$\frac{C_{3SD}}{C_{2OD}} = 4.5(\kappa + 2) \sigma_u^2 \quad (4)$$

Thus, a sequence with a high kurtosis (κ) and a high variance would ensure that the third-order sub-diagonal terms dominate. Finally, an RBS is employed to estimate the off-diagonal kernels. The theoretical kurtosis of an RBS is -2 so the off-diagonal term contributions dominate the PEV expression if an RBS of high input variance is designed.

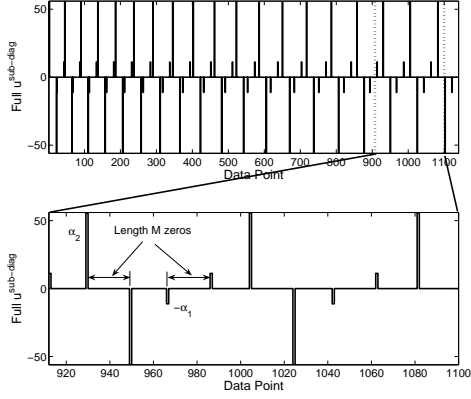


Fig. 1. Full length input sequence used for sub-diagonal identification. Bottom: zoom of the plot to show pulses α_1 and α_2 and M length zeros.

2.2 Estimation of bias, linear, and nonlinear diagonal parameters

Since the bias, linear, and nonlinear diagonal kernels are involved in calculating the sub- and off-diagonal kernels, their identification is carried out first to improve subsequent kernel estimates. Akin to the results of (Florian Jr. and Parker, 2002), a $4M + 4$ length deterministic input sequence is used to estimate the bias, linear, and diagonal parameters, and is given as:

$$u(k) = \begin{cases} \beta_1 & k = 0 \\ 0 & 1 \leq k \leq M \\ -\beta_1 & k = M + 1 \\ 0 & M + 2 \leq k \leq 2M + 1 \\ \beta_2 & k = 2M + 2 \\ 0 & 2M + 3 \leq k \leq 3M + 2 \\ -\beta_2 & k = 3M + 3 \\ 0 & 3M + 4 \leq k \leq 4M + 3 \end{cases} \quad (5)$$

This sequence ensures that the contributions due to the nonlinear sub-diagonal and off-diagonal terms are zero identically, $(u(k-i)u(k-j) = 0 \quad \forall i \neq j \quad (i, j \leq M))$. The parameters β_1 and β_2 represent the pulse heights of the input-sequence and are selected such that $\beta_2 = 56 > \beta_1 = 11.2$. The smaller pulse precedes the larger pulse to ensure that any residual error from the large pulse response does not corrupt the small pulse output data. Based on the definition of a friendliness factor in (Parker *et al.*, 2001), this sequence has a friendliness factor $f = 93\%$.

2.3 Estimation of sub-diagonal parameters

The estimation of the sub-diagonal parameters is carried out as in (Soni and Parker, 2004). The input, shown in Figure 1, is a plant-friendly ($f = 94\%$) CSRS sequence with a value of 13,102 for the ratio given by (4). This ensures that the third-order sub-diagonal kernel contributions dominate. Furthermore, for this sequence the contribution due to the third-order off-diagonal terms is zero identically *i.e.* $u(k-i)u(k-j)u(k-l) = 0 \quad \forall i \neq j \neq l$ and $(i, j, l \leq M)$. The total length of the sequence is $3M(M-1)$ and the pulse heights α_1 and α_2 are 11.2 and 56 respectively.

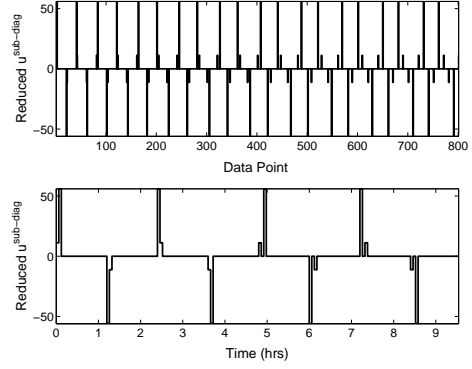


Fig. 2. Reduced length input sequence used for sub-diagonal identification. Bottom: zoom of the plot over the first two sub-units to show increasing pulse separation

2.4 Identification of off-diagonal parameters

The identification of the off-diagonal kernels uses residualization and a cross-correlation technique, as in (Parker *et al.*, 2001).

3. REDUCED SEQUENCE FOR SUB-DIAGONAL IDENTIFICATION

The input sequence used for the sub-diagonal identification in Section 2.3 is of length 1140 for a value of $M = 20$. In many cases, the value of M may be high so that a substantial amount of data is required to estimate the third-order sub-diagonal kernel. On the contrary, short input sequences are plant-friendly as they lead to a reduction in the duration for which the plant operates in identification mode, thereby reducing off-specification product. This motivates the design of a reduced length input-sequence for third-order sub-diagonal kernels. The main reason for the large number of data-points in the sub-diagonal sequence in Section 2.3 was the presence of M zeros after every other pulse, as shown in Figure 1 (bottom). While this effectively eliminated interactions between all but the intended pulses, it added significantly to sequence length without adding input excitation.

The structural basis of the reduced-length sequence (Figure 2) is similar to the one in Section 2.3; the reduced-length sequence also involves two pulses, and the gap between them successively increases. A key difference can be observed by considering the first sub-unit of the reduced-length input sequence:

$$u(k) = \begin{cases} \gamma_1 & k = 1 \\ \gamma_2 & k = 2 \\ 0 & 3 \leq k \leq M \\ -\gamma_2 & k = M + 1 \\ -\gamma_1 & k = M + 2 \\ 0 & M + 3 \leq k \leq 2M \\ \gamma_2 & k = 2M + 1 \\ \gamma_1 & k = 2M + 2 \\ 0 & 2M + 3 \leq k \leq 3M \\ -\gamma_1 & k = 3M + 1 \\ -\gamma_2 & k = 3M + 2 \\ 0 & 3M + 3 \leq k \leq 4M \end{cases} \quad (6)$$

For this input sequence, the input data from points $2M + 1$ to $4M$ is the same as that from $M + 1$ to $2M$, with the exception that the order of the pulses is interchanged; *i.e.* γ_2 forms the first, and γ_1 the second pulse. This was done for two main reasons. First, to avoid singularities in the solution of the estimator equations. Second, when only the first $2M$ points were used as a sub-unit, the resulting sub-diagonal kernels were poorly estimated owing to the interchanging order of pulses for each sub-unit. The addition of the second $2M$ points averages out the contribution of both pulse orders, *i.e.* (γ_1, γ_2) and (γ_2, γ_1) , resulting in smooth estimates for the sub-diagonal kernel. For the next sub-unit there is a gap of one point between the two pulses. This gap length successively increases by one, until the gap length is of $(\frac{M}{2} - 1)$ points. This results in $\frac{M}{2}$ sub-units, each of length $4M$ so that the total length of this sequence is $2M^2$. An important benefit of the four pulse-pair sequence sub-unit is that each coefficient is estimated from four points instead of two for the sequence in Section 2.3. This makes the estimator algorithm more robust to noise.

To calculate the estimator equations for the reduced-length sequence, consider Figure 3. From the figure, two distinct regions a and b can be identified. The region a (length $M - q$) corresponds to the output data-set used to estimate the $h_3(p, p + q, p + q)$ and $h_3(p, p, p + q)$ kernel coefficients for $q = 1, 2, \dots, \frac{M}{2}$ and $p = 1, 2, \dots, M - q$. The region b (length $M - i$) data are used to estimate the $h_3(i, i + j, i + j)$ and $h_3(i, i, i + j)$ kernel coefficients for $i = M - 1, M - 2, \dots, \frac{M}{2} + 1$ and $j = 1, 2, \dots, M - i$. Note that the first two points of the next sub-unit, $4M + 1$ and $4M + 2$, are also required for estimation of the kernels. For each of the next sub-units, the length of region a decreases by 1, whereas that of region b increases by 1, until the $\frac{M}{2}$ sub-unit where they have the same length. This can be visualized in terms of a right triangle. For the first sub-unit, region a is the hypotenuse and region b is the opposite vertex. For each successive sub-unit, the regions move towards the center, until they finally converge for the $\frac{M}{2}$ sub-unit and are of the same length.

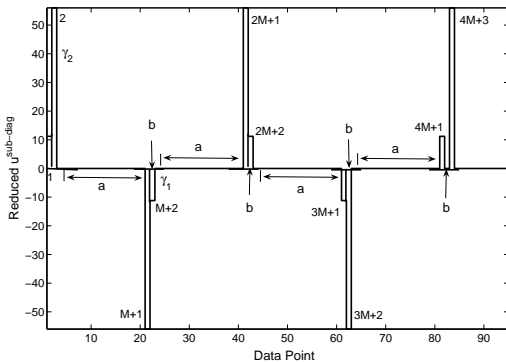


Fig. 3. A schematic of the first sub-unit of the reduced sequence.

For simplicity consider estimating only the $h_3(1, 2, 2)$, and the $h_3(1, 1, 2)$ kernels:

$$\begin{bmatrix} y(3) \\ y(M+3) \\ y(2M+3) \\ y(3M+3) \end{bmatrix} = \begin{bmatrix} \gamma_1^2 \gamma_2 & \gamma_2^2 \gamma_1 \\ -\gamma_2^2 \gamma_1 & -\gamma_1^2 \gamma_2 \\ \gamma_2^2 \gamma_1 & \gamma_1^2 \gamma_2 \\ -\gamma_1^2 \gamma_2 & -\gamma_2^2 \gamma_1 \end{bmatrix} \begin{bmatrix} h_3(1, 2, 2) \\ h_3(1, 1, 2) \end{bmatrix}$$

$$Y = \mathcal{A} \begin{bmatrix} h_3(1, 2, 2) \\ h_3(1, 1, 2) \end{bmatrix} \quad (7)$$

The solution to these kernel contributions is given as:

$$\begin{bmatrix} h_3(1, 2, 2) \\ h_3(1, 1, 2) \end{bmatrix} = (\mathcal{A}^T \mathcal{A})^{-1} \mathcal{A}^T Y$$

This can now be generalized for the a regions of the entire sequence so that the solution is:

$$\mathcal{H} = (u^T u)^{-1} u^T \mathcal{Y} \quad (8)$$

In this equation, \mathcal{Y} is a column vector of output data points. u is a non-square block-diagonal matrix, with \mathcal{A} in (7) along the main diagonal. The column vector \mathcal{H} represents the sub-diagonal coefficients. The calculation for the kernel contributions corresponding to the b regions for the entire sequence proceed in a similar manner, with the exception that the matrix along the block diagonal of u is given by:

$$\begin{bmatrix} -\gamma_2^3 & \gamma_2^3 \\ \gamma_1^2 \gamma_2 & -\gamma_2^2 \gamma_1 \\ -\gamma_1^3 & \gamma_1^3 \\ \gamma_2^2 \gamma_1 & -\gamma_1^2 \gamma_2 \end{bmatrix}$$

The equations thus derived are equivalent to those obtained by starting from the PEV expression and minimizing the sum-squared prediction error (as in (Soni and Parker, 2004)) given by:

$$J_{sd} = \sum_{k=1}^{2M^2+1} \{z(k) - \hat{z}(k)\}^2 \quad (9)$$

In this equation, $\hat{z}(k)$ is the model output prediction in response to the reduced-length input sequence.

4. IDENTIFICATION ALGORITHMS

The following algorithms for third-order Volterra model identification are considered:

Algorithm 1

- (1) The bias, linear, and nonlinear diagonal parameters are estimated using a four-pulse, five-level, $4M + 4$ length (84 point) sequence.
- (2) The second-order off-diagonal kernel is estimated using a cross-correlation technique as in (Parker *et al.*, 2001). A 12,000 point RBS is used as the input sequence. Pre-whitening is used to eliminate the contributions of the bias, the linear, and the nonlinear diagonal kernels.

- (3) A tailored sequence with length $3M(M - 1)$ (1140 points) is used to excite the system and residuals are calculated by subtracting off the bias, linear, and nonlinear diagonal contributions. Third-order sub-diagonal coefficients are estimated from these residuals.
- (4) The third-order off-diagonal terms are estimated similar to the second-order off-diagonal kernels. Pre-whitening is used to eliminate the contributions of the bias, linear, second-order, third-order diagonal, and the third-order sub-diagonal kernels.

Algorithm 2

- (1) The estimation of bias, linear, and nonlinear diagonal kernels is carried out as in Algorithm 1.
- (2) The sequence described in Section 3 (801 points) is used to calculate the third-order sub-diagonal kernels. Pre-whitening is first carried out to eliminate the contributions of the bias, the linear, and the nonlinear diagonal kernels.
- (3) The second- and third-order off-diagonal terms are estimated as in Algorithm 1.

Algorithm 3 (Cross-correlation)

- (1) The estimation of bias, linear, and nonlinear diagonal kernels is carried out using a 600 point random quaternary sequence (RQS).
- (2) The second-order off-diagonal kernel is estimated as in Algorithm 1. Pre-whitening is used to eliminate the contributions of the bias and the linear kernel.
- (3) For the 380 unique third-order sub-diagonal kernels a 3800 point RQS is employed. Pre-whitening is used to eliminate the contributions of the bias, linear, and second-order kernels.
- (4) The third-order off-diagonal terms are estimated as in Algorithm 1. Pre-whitening is used to eliminate the contributions of the bias, linear, and second-order kernels.

5. CASE STUDY AND RESULTS

5.1 Polymerization Reactor Model

In order to test identification algorithm performance, the isothermal free-radical polymerization of methyl-methacrylate using azo-bis-isobutyronitrile as an initiator and toluene as a solvent (Congalidis *et al.*, 1989) was treated as the “real” system. The system equations are given as:

$$\begin{aligned}
 \dot{x}_1 &= 60 - 10x_1 - 2.45684x_1\sqrt{x_2} \\
 \dot{x}_2 &= 80u - 10.1022x_2 \\
 \dot{x}_3 &= 0.0024121x_1\sqrt{x_2} + 0.112184x_2 - 10x_3 \quad (10) \\
 \dot{x}_4 &= 245.979x_1\sqrt{x_2} - 10x_4 \\
 y &= \frac{x_4}{x_3}
 \end{aligned}$$

In this system the output y is the number average molecular weight (NAMW) of the polymer whereas

Table 1. SSE values for the nominal study

Kernel	Algorithm 1	Algorithm 2	Algorithm 3
Linear	3.45×10^{-6}	3.45×10^{-6}	6.67×10^{-3}
2 nd Diag.	9.20×10^{-8}	9.20×10^{-8}	7.74×10^{-6}
2 nd Off-diag.	9.14×10^{-8}	9.14×10^{-8}	1.55×10^{-7}
3 rd Diag.	1.27×10^{-10}	1.27×10^{-10}	1.02×10^{-7}
3 rd Sub-diag.	1.01×10^{-9}	6.89×10^{-10}	3.89×10^{-8}
3 rd Off-diag.	7.93×10^{-11}	7.90×10^{-11}	3.47×10^{-10}

Table 2. Data Reduction and Kernel Estimate % Improvement versus Algorithm 3

Kernel	Algorithm 1	Algorithm 2	Data Redn.
Linear	99	99	7×
2 nd Diag.	98	98	7×
2 nd Off-diag.	41	41	–
3 rd Diag.	99	99	7×
3 rd Sub-diag.	97	98	3.3(4.75)×
3 rd Off-diag.	77	77	–

the input u is the initiator flow-rate. The nominal operating point was selected as the mid-point of the operation range of the reactor and is the same as used in (Soni and Parker, 2004). The system was converted to deviation form, and the input and output were scaled according to (Parker *et al.*, 2001). Carlemann linearization of the nonlinear system was performed (Rugh, 1981), and truncation to third-order terms yielded a bilinear system in state-space form. Finally, the bilinear state-space system was discretized using the fourth-order Runge-Kutta algorithm. A sampling time (Δt) of 0.06 hr and model-memory M of 20, were selected to allow comparison with (Parker *et al.*, 2001). From the discretized equations, the Volterra kernels for the system were calculated analytically (Rugh, 1981). A third-order Volterra model was thus obtained which allows for a comparison with the Algorithms presented in the previous section.

5.2 Volterra Identification Results

5.2.1. Nominal (noise-free) results Table 1 shows the sum squared errors (SSE) between the kernel estimates, identified from the Algorithms in Section 4, and the analytically derived kernels. It is observed in Table 2 that both Algorithm 1 and Algorithm 2 outperform Algorithm 3, while requiring markedly less data. The key advance of the current work versus that accomplished previously (Soni and Parker, 2004) is the improved estimates for the third-order sub-diagonal kernel. These estimates yield more accurate off-diagonal kernels for Algorithm 2 due to a reduction in error propagation during pre-whitening.

5.2.2. Results in the presence of noise In order to test the performance of the identification algorithm in the presence of noise, additive, uncorrelated, white noise with a variance equal to 5% of the output variance, for a signal-to-noise ratio of 5 decibels, was added to the output. Akin to the nominal study, the results are reported as SSE values in Table 3. Once again, it is observed that the tailored identification algorithms outperform the cross-correlation approach.

Table 3. SSE values in the presence of noise

Kernel	Algorithm 1	Algorithm 2	Algorithm 3
Linear	1.76×10^{-4}	1.76×10^{-4}	7.18×10^{-3}
2 nd Diag.	9.24×10^{-8}	9.24×10^{-8}	6.12×10^{-6}
2 nd Off-diag.	9.25×10^{-8}	9.25×10^{-8}	1.89×10^{-7}
3 rd Diag.	1.84×10^{-10}	1.84×10^{-10}	1.14×10^{-7}
3 rd Sub-diag.	2.59×10^{-9}	2.33×10^{-9}	4.31×10^{-8}
3 rd Off-diag.	8.27×10^{-11}	8.22×10^{-11}	3.68×10^{-10}

Five repeat-units of the linear and nonlinear diagonal identification sequence were used to improve the noise sensitivity of the coefficient estimates. An improvement of 77, 16, and 20% was observed for linear, second- and third-order diagonal kernels, respectively, compared to the case when just one unit of this sequence was used for identification. Even with five repeat-units, the resulting sequence was still 30% shorter than the cross-correlation sequence used in Algorithm 3.

6. SUMMARY

In this work, a tailored reduced-length input sequence design was presented to identify the third-order sub-diagonal kernel of a third-order Volterra model. This design was based on the PEV expression and also exploited the Volterra model structure. Random binary signals were used to estimate the off-diagonal kernels using a cross-correlation technique. The identification of the linear, nonlinear diagonal, and third-order sub-diagonal kernels was carried out using 80% less data than the cross-correlation approach. For the third-order sub-diagonal kernel, the reduced-length sequence was 30% shorter than the full sequence and showed a 47% improvement in the SSE value. Finally, improvement in other kernels improved the quality of the off-diagonal kernels. It is interesting to note that tailored algorithms 1 and 2 provide both superior coefficient estimates and a substantial reduction in data requirements. This work thus presents an efficient and plant-friendly algorithm for the estimation of third-order Volterra models.

7. ACKNOWLEDGMENTS

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