Nonlinear Model Selection for PARMA Processes Using RJMCMC

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Abstract-Many prediction studies using real life measurements such as wind speed, power, electricity load and rainfall utilize linear autoregressive moving average (ARMA) based models due to their simplicity and general character. However, most of the real life applications exhibit nonlinear character and modelling them with linear time series may become problematic. Among nonlinear ARMA models, polynomial ARMA (PARMA) models belong to the class of linear-in-the-parameters. In this paper, we propose a reversible jump Markov chain Monte Carlo (RJMCMC) based complete model estimation method which estimates PARMA models with all their parameters including the nonlinearity degree. The proposed method is unique in the manner of estimating the nonlinearity degree and all other model orders and model coefficients at the same time. Moreover, in this paper, RJMCMC has been examined in an anomalous way by performing transitions between linear and nonlinear model spaces.

I. INTRODUCTION

Autoregressive moving average (ARMA) models have been utilized often especially in time series prediction studies due to the ease of estimation by methods such as that of Box-Jenkins [1] and their generality encompassing both *autoregressive* (AR) and *moving average* (MA) models. ARMA models have been used in diverse areas of applications such as speech [2], [3], seismology [4], video [5], image [6], etc. Particularly, they have been applied in energy and meteorological prediction studies of solar radiation [7], [8], electricity demand [9], [10] and wind speed [11], [12].

However, many real life problems exhibit nonlinear characters. *Nonlinear ARMA* (NARMA) or specifically, *polynomial ARMA* (PARMA) models appear as alternatives in modelling problems including nonlinearity and have been used in prediction studies in many different areas such as in energy prediction studies for electricity load [13], wind speed [14], modelling a nonlinear networked control system [15] and forecasting of financial returns [16].

Reversible jump Markov chain Monte Carlo (RJMCMC) is a Bayesian model identification method which was firstly introduced in [17]. RJMCMC has been defined as an extended and generalized version of the MCMC algorithm and offers transitions between parameter spaces of different dimensions. In the literature, RJMCMC has been generally used in linear model estimation studies such as AR models [18], [19],

autoregressive integrated moving average (ARIMA) models [20] and *fractional* ARIMA models [21].

Contrary to the general practice which employs RJMCMC on problems which include exploring spaces of varying dimensions of the same classes of models, RJMCMC offers much wider interpretation than just exploring spaces of different dimensions. In previous studies [22], [23], we have shown that RJMCMC can be used as a model determination method which performs transitions between linear and nonlinear model spaces for *polynomial AR* (PAR) and *polynomial MA* (PMA) models.

In this paper, the formulation in previous studies [22], [23] has been reconstructed into a general framework which estimates the nonlinearity degree of PARMA models. In addition to the nonlinearity degree, AR and MA orders and all the model coefficients have been estimated at the same time. Results have been depicted in figures and tables for synthetically generated PARMA models.

The rest of the paper is organized as follows: PARMA models and general RJMCMC definition are examined in Sections II and III, respectively. In Section IV, RJMCMC construction for PARMA model estimation is studied in detail. Numerical results about the study are presented with figures and a table in Section V. Section VI concludes the paper with a brief summary.

II. PARMA MODELS

The Volterra based *linear-in-the-parameters* PARMA models can be defined as:

$$x_{l} = \mu + \sum_{d=1}^{p} \sum_{\tau_{1}=1}^{k} \dots \sum_{\tau_{d}=\tau_{d-1}}^{k} a_{\tau_{1},\dots,\tau_{d}}^{(d)} \prod_{j=1}^{d} x_{l-\tau_{j}} + e_{l} + \sum_{d=1}^{p} \sum_{\tau_{1}=1}^{q} \dots \sum_{\tau_{d}=\tau_{d-1}}^{q} b_{\tau_{1},\dots,\tau_{d}}^{(d)} \prod_{j=1}^{d} e_{l-\tau_{j}}, \quad (1)$$

where l = 1, ..., n and p, k and q refer to the nonlinearity degree, the AR order and the MA memory of the model, respectively. In addition, vector $\mathbf{e} = [e_1, e_2, ..., e_n]$ represents the *iid* excitation sequence with distribution $\mathcal{N}(\mathbf{0}, \sigma_e^2 \mathbf{I}_n)$, $a_{\tau_1,...,\tau_d}^{(d)}$ and $b_{\tau_1,...,\tau_d}^{(d)}$ are the d^{th} ordered coefficients of AR and MA parts, respectively. A PARMA model can be represented with the notation: $P^{(p)}ARMA(k,q)$.

The system of equations in (1) can be easily represented in matrix vector form for a $P^{(p)}ARMA(k,q)$ model by using the linear-in-the-parameters property:

$$\mathbf{x} = \mu + \mathbf{X}\mathbf{a}^{(p,k)} + \mathbf{E}\mathbf{b}^{(p,q)} + \mathbf{e}, \qquad (2)$$

where $n \times \eta$ matrix **X**, η -vector $\mathbf{a}^{(p,k)}$, $n \times \gamma$ matrix **E** and γ -vector $\mathbf{b}^{(p,q)}$ are given as:

$$\mathbf{X} = \begin{bmatrix} x_0 & \dots & x_{1-k} & x_0^2 & x_0x_{-1} & \dots & x_{1-k}^p \\ x_1 & \dots & x_{2-k} & x_1^2 & x_1x_0 & \dots & x_{2-k}^p \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{n-1} & \dots & x_{n-k} & x_{n-1}^2 & x_{n-1}x_{n-2} & \dots & x_{n-k}^p \end{bmatrix},$$
(3)

$$\mathbf{a}^{(p,k)} = \begin{bmatrix} a_1^{(1)}, \dots, a_k^{(1)}, a_{1,1}^{(2)}, a_{1,2}^{(2)}, \dots, a_{k,k}^{(2)}, \dots, \underbrace{a_{k,k,\dots,k}^{(p)}}_{\mathbf{p}^{\text{th order}}} \end{bmatrix}^T, \quad (4)$$

$$\mathbf{E} = \begin{bmatrix} e_0 & \dots & e_{1-q} & e_0^2 & e_0e_{-1} & \dots & e_{1-q}^p \\ e_1 & \dots & e_{2-q} & e_1^2 & e_1e_0 & \dots & e_{2-q}^p \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ e_{n-1} & \dots & e_{n-q} & e_{n-1}^2 & e_{n-1}e_{n-2} & \dots & e_{n-q}^p \end{bmatrix},$$
(5)

$$\mathbf{b}^{(p,q)} = \begin{bmatrix} b_1^{(1)}, \dots, b_q^{(1)}, b_{1,1}^{(2)}, b_{1,2}^{(2)}, \dots, b_{q,q}^{(2)}, \dots, \underbrace{b_{q,q,\dots,q}^{(p)}}_{\mathbf{p}^{\text{th order}}} \end{bmatrix}^T, \tag{6}$$

where η and γ are the lengths of parameter vectors $\mathbf{a}^{(p,k)}$ and $\mathbf{b}^{(p,q)}$, respectively.

III. REVERSIBLE JUMP MCMC

Following [17], assume that we propose a move m with probability p_m from a Markov chain state κ to κ' . These states have parameter vectors θ and θ^* , respectively with different dimensions. Given the observed data \mathbf{x} , the general expression for the acceptance ratio, $\alpha(\kappa \to \kappa')$, is;

$$\min\left\{1, \frac{f(\boldsymbol{\theta}^*|\mathbf{x})p_m^{\mathrm{R}}}{f(\boldsymbol{\theta}|\mathbf{x})p_m\chi(\mathbf{u})} \left|\frac{\partial\boldsymbol{\theta}^*}{\partial(\boldsymbol{\theta},\mathbf{u})}\right|\right\},\tag{7}$$

where p_m^{R} represents the probability for the reverse move of $m, \chi(\mathbf{u})$ is the proposal distribution for the auxiliary variable vector \mathbf{u} which is required to provide dimension matching for the move m and $\left|\frac{\partial \theta^*}{\partial(\theta,\mathbf{u})}\right|$ is the magnitude of the Jacobian.

In each RJMCMC run, the standard Metropolis-Hastings algorithm is applied for within-model moves, which we call as *life* move. For between-model moves, namely *birth* and *death* moves, reversible jump mechanism is applied.

IV. RJMCMC CONSTRUCTION FOR PARMA MODEL ESTIMATION

PARMA model estimation via RJMCMC includes 3 stages at each iteration. At each stage, one of the model parameters (p, k or q) has been proposed while the others remain at their recent values. Model order in question is increased and decreased with probabilities P_{birth} and P_{death} , respectively and remains at the same order with probability P_{life} . If the proposed model order is accepted, RJMCMC performs a training procedure by applying 10 consecutive life moves to update the newly estimated model coefficients. All these steps have been repeated at each stage for each model order (p, k or q).

In the case of a birth move corresponding to a model change from k = 2 to k' = 3 when q = 0 and p = 2, in order to satisfy the dimension matching, it's required to propose $\lambda = 9 - 5 = 4$ candidate model coefficients from a proposal distribution, $\chi(\mathbf{u})$, which is:

$$\chi(\mathbf{u}) = \prod_{i=1}^{\lambda} \mathcal{U}(-\delta, \delta), \quad \text{and} \quad \delta = \frac{0.02}{E[|\mathbf{x}|]}, \tag{8}$$

where $E[|\mathbf{x}|]$ is the expectation of the absolute value of the observed data vector \mathbf{x} .

The upper and lower bounds of the joint distribution are chosen to depend on the given data. By doing so, distinct limits can be arisen due to the fact that the magnitudes of different data sets may vary in different ranges. Consequently, this *adhoc* choice adds variety for the candidates. Moreover, after some trial-error process, we see that keeping the interval narrower (smaller δ values) increases the number of acceptable moves. That's why we have chosen a value of 0.02 for the nominator part in equation (8).

Furthermore, each of the newly proposed model coefficients have been chosen to be independent from the recent coefficients which causes a unity Jacobian.

RJMCMC construction for PARMA model estimation is presented in detail in the sequel.

A. Bayesian Hierarchy

The target distribution of RJMCMC is a joint posterior density and can be expressed as $f(\theta|\mathbf{x})$ with parameter vector $\boldsymbol{\theta} = \{p, k, q, \mathbf{a}^{(p,k)}, \mathbf{b}^{(p,q)}, \sigma_e^2, \sigma_a^2, \sigma_b^2\}$. This density can be decomposed via Bayes Theorem:

$$f(\boldsymbol{\theta}|\mathbf{x}) \propto f(\mathbf{x}|p,k,q,\mathbf{a}^{(p,k)},\mathbf{b}^{(p,q)},\sigma_e^2)f(\mathbf{a}^{(p,k)}|p,k,\sigma_a^2) \times f(\mathbf{b}^{(p,q)}|p,q,\sigma_b^2)f(\sigma_a^2)f(\sigma_b^2)f(\sigma_e^2)f(p)f(k)f(q).$$
(9)

B. Likelihood Definition

In a previous study [24], it has been stated that for white inputs and narrowband Volterra based models output follows Gaussian characteristics. We have experimentally verified this by testing the output process of a PARMA model.

Furthermore, in [25] a Gaussian approximate likelihood has been used in restoration of nonlinearly distorted AR signals when the whole system follows a nonlinear AR model characteristics. Consequently, choosing a Gaussian likelihood for PARMA models appears as a good practical approximation.

Moreover, in [1], an approximation of the likelihood function of ARMA models has been provided by performing a recursive estimation procedure in the model itself for the unobserved excitation values. This approach has been used in model estimation studies for Bayesian analysis of ARMA based time series models [19]–[21]. Thus, an approximate likelihood function for a $P^{(p)}ARMA(k,q)$ has been examined in this study as,

$$f(\mathbf{x}|\boldsymbol{\theta}) = \frac{1}{\sqrt{(2\pi\sigma_e^2)^{(n-q_{\max})}}} \exp\left(\frac{-1}{2\sigma_e^2} \sum_{t=q_{\max}+1}^n e_t^2\right) \quad (10)$$
$$\approx \mathcal{N}(\mathbf{x} - \mathbf{X}\mathbf{a}^{(p,k)} - \mathbf{E}\mathbf{b}^{(p,q)}|\mathbf{0}, \sigma_e^2 \mathbf{I}_{n-q_{\max}}). \quad (11)$$

Please see Section IV-F for the details of the estimation process of the unobserved excitation sequence.

C. Priors

In the previous studies, general practice is to use uniform priors for model order parameters [19]–[23]. Correspondingly, in this study, we assume that each model is equally likely and we choose uniform priors for model orders p, k, and q with upper bounds $p_{\text{max}}, k_{\text{max}}$ and q_{max} , respectively.

$$f(p) = \mathcal{U}(1, p_{\max}), \quad f(k) = \mathcal{U}(1, k_{\max}), \quad f(q) = \mathcal{U}(1, q_{\max}).$$
(12)

We choose priors for model coefficients and variances as shown below so as to provide conditional conjugacy:

$$f(\mathbf{a}^{(p,k)}|p,k,\sigma_a^2) = \mathcal{N}(\mathbf{a}^{(p,k)}|\mathbf{0},\sigma_a^2 \mathbf{I}_{\mathbf{w}}),$$
(13)

$$f(\mathbf{b}^{(p,q)}|p,q,\sigma_b^2) = \mathcal{N}(\mathbf{b}^{(p,q)}|\mathbf{0},\sigma_b^2\mathbf{I_z}),$$
(14)

$$f(\sigma_a^2) = \mathcal{IG}(\sigma_a^2 | \alpha_a, \beta_a), \tag{15}$$

$$f(\sigma_b^2) = \mathcal{IG}(\sigma_b^2 | \alpha_b, \beta_b), \tag{16}$$

$$f(\sigma_e^2) = \mathcal{IG}(\sigma_e^2 | \alpha_e, \beta_e). \tag{17}$$

where w and z are the length of coefficients vectors $\mathbf{a}^{(p,k)}$ and $\mathbf{b}^{(p,q)}$, respectively, $\mathcal{IG}(\cdot)$ refers to an inverse Gamma distribution and $\alpha_a, \beta_a, \alpha_b, \beta_b, \alpha_e, \beta_e$, are hyperparameters for variances.

D. Between Model Moves

Between model moves require to change dimension of parameter space. If proposed move requires an increase in dimension, RJMCMC performs a **birth** move. In the contrary case, **death** move has been performed.

Assume a **birth** move has been proposed from AR order k to k' when p and q are fixed. Then, resulting acceptance ratio is $\alpha_{\text{birth}} = \min\{1, r_{\text{birth}}\}$ where r_{birth} can be given as:

$$r_{\text{birth}} = \frac{f(\mathbf{x}|p,k',q,\mathbf{a}^{(p,k')},\mathbf{b}^{(p,q)},\sigma_e^2)}{f(\mathbf{x}|p,k,q,\mathbf{a}^{(p,k)},\mathbf{b}^{(p,q)},\sigma_e^2)} \times \frac{f(\mathbf{a}^{(p,k')}|p,k',\sigma_a^2)}{f(\mathbf{a}^{(p,k)}|p,k,\sigma_a^2)} \times \frac{P_{\text{death}}}{P_{\text{birth}}\chi(\mathbf{u})} \times \left|\frac{\partial \mathbf{a}^{(p,k')}}{\partial (\mathbf{a}^{(p,k)},\mathbf{u})}\right|.$$
(18)

When a **death** move has been proposed from k to k', no new parameters are being proposed. Since birth and death moves are reversible move pairs, $\alpha_{\text{death}}(k \rightarrow k')$ can be written in terms of $\alpha_{\text{birth}}(k' \rightarrow k)$. By definition, if

$$\alpha_{\text{birth}}(k' \to k) = \min\{1, r'_{\text{birth}}\},\tag{19}$$

then we can directly write

$$\alpha_{\text{death}}(k \to k') = \min\{1, 1/r'_{\text{birth}}\}.$$
 (20)

E. Within Model Moves

When k' = k, a **life** move will be proposed with acceptance ratio, $\alpha_{\text{life}} = \min \{1, r_{\text{life}}\}$ with

$$r_{\text{life}} = \frac{f(\mathbf{x}|p,k',q,\mathbf{a}^{(p,k')},\mathbf{b}^{(p,q)},\sigma_e^2)}{f(\mathbf{x}|p,k,q,\mathbf{a}^{(p,q)},\mathbf{b}^{(p,q)},\sigma_e^2)} \times \frac{f(\mathbf{a}^{(p,k')}|p,k',\sigma_a^2)}{f(\mathbf{a}^{(p,k)}|p,k,\sigma_a^2)} \times \frac{\psi(\mathbf{a}^{(p,k)}|p,k',\mathbf{a}^{(p,k')})}{\psi(\mathbf{a}^{(p,k')}|p,k,\mathbf{a}^{(p,k)})}$$
(21)

where the proposal distribution $\psi(\cdot)$ is:

$$\psi(\mathbf{a}^{(p,k)}|p,k',\mathbf{a}^{(p,k')}) = \mathcal{N}(\mathbf{a}^{(p,k')}|\mu_n,\Sigma_n^{-1}), \quad (22)$$

with $\mu_n = \sigma_e^{-2} \Sigma_n^{-1} \mathbf{X}^{\mathsf{T}} (\mathbf{x} - \mathbf{B} \boldsymbol{\epsilon}^{(p,q)})$ and $\Sigma_n = \sigma_e^{-2} \mathbf{X}^T \mathbf{X} + \sigma_a^{-2} \mathbf{I}_{\mathbf{w}}$.

F. Update Moves

After the 3 stage mechanism for model order estimation has been executed, at each iteration several update moves are performed to update variance parameters and initial unobserved excitation vector $\mathbf{e}^{(0)} = [e_1, e_2, \dots, e_q]$ via Gibbs sampling.

The full conditional distribution for σ_e^2 is [19]:

$$f(\sigma_e^2 | \mathbf{x}, p, q, \mathbf{b}^{(\mathbf{p}, \mathbf{q})}) = \mathcal{IG}(\sigma_e^2 | \alpha_{en}, \beta_{en}), \qquad (23)$$

where $\alpha_{en} = \alpha_e + \frac{1}{2}n$, $\beta_{en} = \beta_e + \frac{1}{2}\mathbf{e}^T\mathbf{e}$. Similarly, the full conditionals for coefficient vector variances appear as:

$$f(\sigma_a^2 | \mathbf{x}, p, k, \mathbf{a}^{(p,k)}) = \mathcal{IG}(\sigma_a^2 | \alpha_{an}, \beta_{an}), \qquad (24)$$

$$f(\sigma_b^2 | \mathbf{x}, p, q, \mathbf{b}^{(p,q)}) = \mathcal{IG}(\sigma_b^2 | \alpha_{bn}, \beta_{bn}),$$
(25)

where parameters for these inverse Gamma functions are $\alpha_{an} = \alpha_a + \frac{1}{2}w$, $\beta_{an} = \beta_a + \frac{1}{2}(\mathbf{a}^{(p,k)})^T \mathbf{a}^{(p,k)}$, $\alpha_{bn} = \alpha_b + \frac{1}{2}z$ and $\beta_{bn} = \beta_b + \frac{1}{2}(\mathbf{b}^{(p,q)})^T \mathbf{b}^{(p,q)}$.

Initial excitation vector, $e^{(0)}$ can be sampled from the distribution:

$$\mathbf{e}^{(0)} \sim \mathcal{N}(\mathbf{0}, \sigma_e^2 \mathbf{I}_q) \tag{26}$$

where σ_e^2 is the sampled value from (23). Complete excitation vector **e** has been estimated at each iteration via (1) starting from e_{q+1} up to e_n by using $\mathbf{e}^{(0)}$.

V. NUMERICAL RESULTS

In this study, 10 PARMA models have been generated for simulations. Each model generates 20 different data sets with zero mean ($\mu = 0$) where each has a length of 750 samples. Each data set is driven with a Gaussian excitation sequence with variance of σ_e^2 .

In all the MCMC methods, selection of the initial values of the parameters does not have a direct affect on the final result. It only changes the convergence time to be long or short according to the selection [26], [27]. We have chosen the initial values by taking these issues into consideration. Hyperparameters $\alpha_a, \alpha_b, \alpha_e, \beta_a, \beta_b$ and β_e are selected as 1. Each of the initial values p_0, k_0 and q_0 is also set to 1. Upper bounds, $p_{\text{max}}, k_{\text{max}}$ and q_{max} , for model orders have been selected as 5, 6 and 6, respectively. Model orders change with probability of 0.15 to up (birth) and down (death) and remain

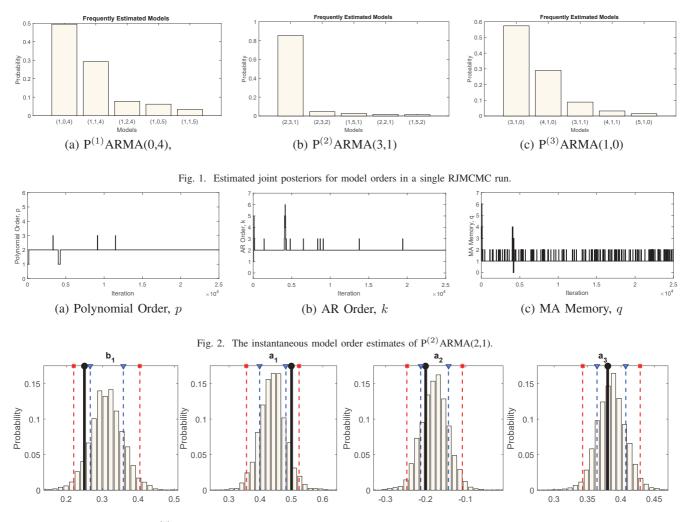


Fig. 3. Estimated posteriors for $P^{(1)}ARMA(3,1)$ Coefficients (b* = [0.25, 0.5, -0.2, 0.38]). Black vertical line with "o" marker is the correct coefficient value, vertical dashed lines with " ∇ " and "*" markers refer to $\pm \sigma$ and $\pm 2\sigma$ CIs, respectively.

at the same (life) with a probability of 0.7. Each RJMCMC run performs 25000 iterations including a burn-in period of 10000 iterations.

In order to measure model coefficient estimation performance of the proposed method, the *normalized mean* square error (NMSE) which is defined as NMSE = $\frac{1}{w+z} \sum_{i=1}^{w+z} \frac{(h_i - \hat{h}_i)^2}{\|\mathbf{h}\|_2^2}$ has been used. Here, vector **h** includes both AR and MA model coefficients vectors $\mathbf{a}^{(p,k)}$ and $\mathbf{b}^{(p,q)}$ and $\hat{\mathbf{h}}$ is its estimate.

Table I demonstrates results after 20 RJMCMC runs. These results reveal that for all 10 PARMA models, RJMCMC estimates correct model orders with the highest percentages. In addition, RJMCMC exhibits great performance on model coefficients estimation with NMSE values between 6×10^{-4} and 1×10^{-2} for all the models.

Figure 1 depicts the estimated joint posteriors of model order for 3 example PARMA models in a single RJMCMC run. Each sub-figure shows 5 frequently estimated models and their probabilities after burn-in period. Examining the figure, we can

TABLE I MODEL ESTIMATION RESULTS

| | (1,3,0) | (1,0,4) | (1,3,1) | (1,2,2) | (2,1,1) |
|--|-------------------|---------------------|-------------------|-------------------|-------------------|
| % Perf. Of Detection Avg. NMSE # of Coeff. | 85 0.0015 3 | 65 0.0022 4 | 80 0.0081 4 | 80 0.0145 4 | 95 0.0079 4 |
| | (2,2,1) | (2,3,1) | (3,1,0) | (3,0,1) | (3,1,1) |
| % Perf. Of Detection Avg. NMSE # of Coeff. | 90 0.0050 7 | 100 0.0056 11 | 70 0.0006 3 | 80 0.0011 3 | 80 0.0030 6 |

clearly state that models which have highest probabilities are the correct models and these posteriors depict that RJMCMC estimates the correct models.

In Figure 2, instantaneous estimates for each model order p, k and q for a P⁽²⁾ARMA(2,1) model, have been shown for a single RJMCMC run with 25000 iterations. Burn-in period is also shown in Figure 2 in order to see the transient character of the algorithm.

Figure 3 shows the posterior probabilities for models coefficients of $P^{(1)}ARMA(3,1)$ in a single RJMCMC run. Vertical black line corresponds to the correct model coefficient value for each sub-figure. Coefficient estimates for only correctly estimated model orders after burn-in period have been used to obtain the distributions in this figure. Resulting posteriors show that RJMCMC estimates model coefficients with a remarkable performance and the correct model coefficient values stand in 95% *confidence interval* (CI) ($\pm 2\sigma$) for b_1 and a_1 and 68% CI ($\pm \sigma$) for a_2 and a_3 of the estimated posteriors.

VI. CONCLUSIONS

In this study we present a general framework for Volterra based linear-in-the-parameters nonlinear model estimation problems by extending our previous works on PAR and PMA models to PARMA models. We have utilized RJMCMC algorithm which has been generally used for linear model estimation problems, in the manner of performing transitions between linear and nonlinear model spaces.

We propose a method which can estimate all parameters of PARMA or its special cases PAR, PMA, linear AR, MA, ARMA processes. In addition, RJMCMC has been used to estimate the nonlinearity degree of the models which is generally assumed to be known in the literature.

Numerical results demonstrate promising performance of the proposed method in estimating model orders and corresponding model coefficients concurrently.

ACKNOWLEDGEMENT

Oktay Karakuş is funded as a visiting scholar at ISTI-CNR, Pisa, Italy by The Scientific and Technological Research Council of Turkey (TUBITAK) under grant program 2214/A.

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