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Effects of Hidden Unit Sizes and Autoregressive Features in Mental Task Classification

Ramaswamy Palaniappan, and Nai-Jen Huan

Abstract—Classification of electroencephalogram (EEG) signals extracted during mental tasks is a technique that is actively pursued for Brain Computer Interfaces (BCI) designs. In this paper, we compared the classification performances of univariate-autoregressive (AR) and multivariate autoregressive (MAR) models for representing EEG signals that were extracted during different mental tasks. Multilayer Perceptron (MLP) neural network (NN) trained by the backpropagation (BP) algorithm was used to classify these features into the different categories representing the mental tasks. Classification performances were also compared across different mental task combinations and 2 sets of hidden units (HU): 2 to 10 HU in steps of 2 and 20 to 100 HU in steps of 20. Five different mental tasks from 4 subjects were used in the experimental study and combinations of 2 different mental tasks were studied for each subject. Three different feature extraction methods with 6th order were used to extract features from these EEG signals: AR coefficients computed with Burg's algorithm (ARBG), AR coefficients computed with stepwise least square algorithm (ARLS) and MAR coefficients computed with stepwise least square algorithm. The best results were obtained with 20 to 100 HU using ARBG. It is concluded that i) it is important to choose the suitable mental tasks for different individuals for a successful BCI design, ii) higher HU are more suitable and iii) ARBG is the most suitable feature extraction method.

Keywords—Autoregressive, Brain-Computer Interface, Electroencephalogram, Neural Network.

I. INTRODUCTION

OVER the last ten years, the volume and pace of Brain Computer Interface (BCI) research have grown tremendously [1, 2]. In 1995 there were no more than six active BCI research groups, and in the year 2000, there were more than 20 [2]. BCI designs are very useful for completely paralysed individuals to communicate with their external surroundings using their brain thoughts. These individuals could have become completely paralysed after being involved in an accident or due to some diseases. BCI designs are also suitable for use in simple hands off menu selection on the screen.

There are a few non-invasive methods for obtaining these brain signals to be utilised in a BCI design.

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Electroencephalogram (EEG) signals recorded at the scalp during particular mental tasks have been used by some of the research groups [3-8]. Some others have utilised single-trial visual evoked potential signals where the subjects gaze at a screen full of alphabets or menus. Synchronisation and desynchronisation of μ -rhythm extracted during sensory motor tasks is another method for BCI design [9-11]. Reviews of some of these technologies and developments in this area are given by Vaughan *et al* [1], Wolpaw *et al* [2] and Mason and Birch [6].

In this paper, we adopted classification of EEG signals extracted during mental tasks for our BCI design. The advantage of this method over the other existing BCIs is that it does not require any in-between interface but the choice of mental tasks, feature extraction methods and classifiers could affect the performance greatly. Therefore, our objective in this paper is to study the performance of a bi-state BCI design across different mental task combinations, 3 different AR feature extraction methods and 2 sets of hidden units (HU); one higher and one lower.

The EEG signals were recorded during 5 different mental tasks from 4 healthy subjects. These mental tasks were: geometrical figure rotation, mathematical multiplication, mental letter composing, visual counting and a baseline-resting task. The 3 different feature extraction methods were

- 6th order autoregressive (AR) coefficients computed with Burg's algorithm (ARBG)
- 6th order autoregressive (AR) coefficients computed with stepwise Least Squares algorithm (ARLS)
- 6th order multivariate autoregressive (MAR) coefficients computed with stepwise Least Squares algorithm

These features were then used by a MLP-BP NN with single hidden layer which consisted of

- 2 to 10 HU in steps of 2, or
- 20 to 100 HU in steps of 20

to classify different combinations of 2 mental tasks. Two mental tasks were chosen because the output of the studied BCI design is bi-state. The output of this BCI design could be used with some translation schemes like Morse Code [7] or to control the movement of a cursor to select a target on a computer screen, which would provide a communication channel for paralysed individuals to communicate with others.

II. METHODOLOGY

A. Data

The EEG data used in this study were collected by Keirn and Aunon [5]. The subjects were seated in an Industrial Acoustics Company sound controlled booth with dim lighting and noise-less fan (for ventilation). An Electro-Cap elastic electrode cap was used to record EEG signals from positions C3, C4, P3, P4, O1 and O2 (shown in Figure 1), defined by the 10-20 system [12] of electrode placement. The impedances of all electrodes were kept below 5 K Ω . Measurements were made with reference to electrically linked mastoids, A1 and A2. The electrodes were connected through a bank of amplifiers (Grass7P511), whose band-pass analog filters were set at 0.1 to 100 Hz. The data were sampled at 250 Hz with a Lab Master 12-bit A/D converter mounted on a computer. Before each recording session, the system was calibrated with a known voltage. Signals were recorded for 10s during each task and each task was repeated for 10 sessions where the sessions were held on different weeks. The EEG signal for each mental task was segmented into 20 segments with length 0.5 s, so each EEG segment was 125 samples in length.

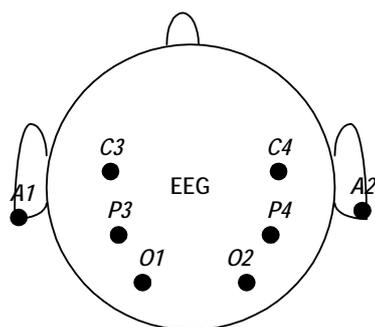


Fig. 1 Electrode placement

In this paper, EEG signals from 4 subjects performing 5 different mental tasks were used¹. In the original dataset, there were 7 subjects participating in the study but we chose only 4 subjects here as the other 3 had fewer than 10 sessions or some errors in the recording. These mental tasks were:

- a) Baseline task. The subjects were asked to relax and think of nothing in particular. This task was used as a control and as a baseline measure of the EEG signals.
- b) Math task. The subjects were given nontrivial multiplication problems, such as 42 times 18 and were asked to solve them without vocalising or making any other physical movements. The tasks were non-repeating and designed so that an immediate answer was not apparent. The subjects verified at the end of the task whether or not he/she arrived at the solution and no subject completed the task before the end of the 10 s recording session.
- c) Geometric figure rotation task. The subjects were given 30 s to study a particular three-dimensional block object, after

which the drawing was removed and the subjects were asked to visualise the object being rotated about an axis. The EEG signals were recorded during the mental rotation period.

- d) Mental letter composing task. The subjects were asked to mentally compose a letter to a friend or a relative without vocalising. Since the task was repeated several times the subjects were told to continue with the letter from where they left off.
- e) Visual counting task. The subjects were asked to imagine a blackboard and to visualise numbers being written on the board sequentially, with the previous number being erased before the next number was written. The subjects were instructed not to verbalise the numbers but to visualise them. They were also told to resume counting from the previous task rather than starting over each time.

Keirn and Aunon [5] specifically chose these tasks since they involve hemispheric brainwave asymmetry (except for the baseline task). For example, it was shown by Osaka [13] that arithmetic tasks exhibit a higher power spectrum in the right hemisphere whereas visual tasks do so in the left hemisphere. As such, Keirn and Aunon [5] and later Anderson *et al* [3] proposed that these tasks are suitable for brain-computer interfacing.

B. Feature Extraction

In this paper, we have used 3 different AR feature extraction methods to extract features from the EEG signals and then classifying the features using 2 sets of different number of HU in the MLP-BP NN architecture. In the first method, AR coefficients were computed using Burg's method [14-16]. In the second method, AR parameters were estimated by using stepwise Least Square algorithm with data from a single channel used at a time and in the third method, the multivariate AR coefficients were estimated using stepwise Least Square algorithm with data from 6 channels used all at once. The following discussion details the 3 different feature extraction processes.

1) 6th order AR coefficients with Burg's algorithm

A real valued, zero mean, stationary, nondeterministic, autoregressive process of order p is given by

$$x(n) = -\sum_{k=1}^p a_k x(n-k) + e(n), \quad (1)$$

where p is the model order, $x(n)$ is the signal at the sampled point n , a_k are the real valued AR coefficients and $e(n)$ represents the error term independent of past samples. The term autoregressive implies that the process $x(n)$ is seen to be regressed upon previous samples of itself. The error term is assumed to be a zero mean noise with finite variance, σ_p^2 . In applications, the values of a_k and σ_p^2 have to be estimated from finite samples of data $x(1), x(2), x(3), \dots, x(N)$.

In this paper, we used Burg's method [14-16] to estimate the AR coefficients. The method is more accurate as compared to other methods like Levinson-Durbin as it uses the data point directly. Furthermore, Burg algorithm uses

¹ The data is available online at <http://www.cs.colostate.edu/eeg/index.html#Data>.

more data points by minimising both forward error and backward error. Order 6 was used for the AR process because other researchers [3, 5] have suggested the use of order 6 for AR process for mental task classification. Therefore, we had 6 AR coefficients for each channel, giving a total of 36 features for each EEG segment from a mental task.

2) 6th order AR coefficients with stepwise least square algorithm

An m -variate AR(p) model for a stationary time series of state vectors $v_v \in \mathfrak{R}^m$, observed at equally spaced instants v , is defined by

$$v_v = w + \sum_{i=1}^p A_i v_{v-i} + \varepsilon_v, \quad \varepsilon_v = \text{noise}(C), \quad (2)$$

where the m -dimensional vectors $\varepsilon_v = \text{noise}(C)$ are uncorrelated random vectors with mean zero and covariance matrix $C \in \mathfrak{R}^{m \times m}$, and the matrices $A_1, A_2, \dots, A_p \in \mathfrak{R}^{m \times m}$ are the coefficient matrices of the AR model [19]. The parameter vector $w \in \mathfrak{R}^m$ is a vector of intercept terms that is included to allow for a nonzero mean of the time series,

$$\langle v_v \rangle = (I - A_1 - \dots - A_p)^{-1} w, \quad (3)$$

where $\langle \bullet \rangle$ denoted an expected value.

If the coefficient matrices A_1, A_2, \dots, A_p and the intercept vector w of an AR model are estimated with the method of least squares, the residual covariance matrix \hat{C} of the estimated model is a fairly reliable estimator of the noise covariance matrix C . The least squares estimates of AR parameters are obtained by casting an AR model in the form of an ordinary regression model and estimating the parameters of regression model with the method of least squares. The least squares modeling criterion is widely used in connection with the AR model because it is particularly suitable for solving the related optimization problem [17]. Numerically, the least squares problem for the ordinary regression model can be solved with standard methods that involve the factorization of a data matrix. However, in this study, stepwise least squares algorithm by Neumaier and Schneider [18] was used to estimate the parameter due to its computational efficiency and stability. Mathematical details of this method are given in Appendix B.

Although the m -variate AR(p) model is generally used with multi-channels, in this paper, we have used only a single channel at a time in the computation of parameters instead of multi-channel and unexpectedly obtained good results. The model order was fixed at 6 to ensure a fair comparison with the above-mentioned method. Therefore, we had a total of 6 AR coefficients for each channel, giving a total of 36 features for each EEG segment from a mental task.

C. MLP-BP NN

In this paper, MLP NN with single hidden layer trained by the BP algorithm [19] was used to classify different combinations of 2 mental tasks represented by the different EEG features. Figure 2 shows the architecture of the MLP-BP NN used in

this study. Both the hidden and output layer used hyperbolic tangent function as activation function. The inputs were normalised from -1 to 1 using the minimum and maximum value of each feature as this would improve the NN training. As mentioned earlier, for experiments involving ARBG and ARLS, the number of inputs was 36 while for MAR, it was 216. Weights and biases were initialised according to the Nguyen-Widrow algorithm. This algorithm chooses values in order to distribute the active region of each neuron in the unit evenly across the unit's input space. Advantages of this initialisation over purely random weights and biases are faster training and the use of more or all the available hidden units.

BP algorithm with adaptive learning rate and momentum stabilisation was used to train the MLP NN. This training algorithm was chosen after some preliminary experiments. The output units were set at 2 so that the NN could classify into either of the 2 categories representing the mental task. There were 2 experiments conducted with different number of HU:

- 2 to 10 in steps of 2, and
- 20 to 100 in steps of 20

In other words, one experiment was conducted with 2, 4, 6, 8, 10 HU and the other with 20, 40, 60, 80, 100 HU.

A total of 200 EEG patterns (20 segments for EEG each signal x 10 sessions) were used for each subject for each mental task in all the experiments. Therefore, for each experiment, there were 400 EEG patterns from 2 mental tasks, where half of the patterns were used in training and the remaining half in testing.

A modified 10 fold cross validation technique was used to increase the reliability of the results. In this method, the entire data for an experiment (i.e. 400 EEG patterns) were split into 10 parts. Training and testing were conducted for 5 times where for each time, we used 5 randomly selected parts for training and the rest 5 different parts for testing. So for each HU size, the MLP-BP training and testing were repeated for 5 times. Overall, the training and testing were repeated for 6000 times (10 HU sizes x 10 mental task combinations x 3 features extraction methods x 5 cross-validation repetitions x 4 subjects). Training was conducted until the mean square error (between desired and target) fell below 0.0001 or reached a maximum iteration limit of 1000. The mean square error denotes the error limit to stop NN training. The desired target output was set to 1.0 for the particular category representing the mental task of the EEG pattern being trained, while for the other category, it was set to 0.

Figure 3 shows the overall flow of the methodology.

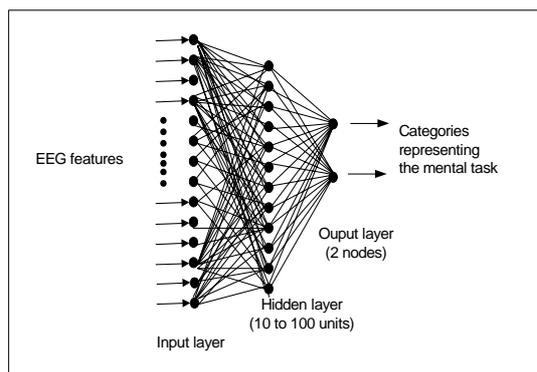


Fig. 2 MLP-BP NN architecture

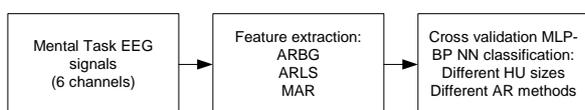


Fig. 3 Flow of Methodology

III. RESULTS

Table I shows the MLP-BP NN classification results using ARBG, ARLS and MAR methods with 2 to 10 HU in steps of 2 and 20 to 100 HU in steps of 20 for subject 1. Tables 2, 3 and 4 show similar results for subjects 2, 3 and 4, respectively. The classification performances are shown in terms of percentage. Only the averaged classification percentages using the modified 10 fold cross validation techniques from either 2 to 10 HU in steps of 2 and 20 to 100 HU in steps of 20 are shown instead of their individual classification percentages. This is to save space. The additional row, 'average' shows the average of these averages over the 10 different mental task combinations. The term coefficient variation (CV) represents standard deviation divided by the mean.

TABLE I
MLP-BP NN CLASSIFICATION RESULTS FOR SUBJECT 1

Mental task combination	Feature extraction method						Best feature extraction method and HU number
	ARBG		ARLS		MAR		
	20-100	2-10	20-100	2-10	20-100	2-10	
	No. of HU						
	Averaged classification (%)						
Baseline, Count	81.72	80.58	80.96	79.82	74.16	74.38	ARBG HU 20-100
Baseline, Letter	82.02	79.66	79.84	77.02	73.22	72.66	ARBG HU 20-100
Baseline, Maths	82.80	81.40	81.38	79.60	74.46	72.14	ARBG HU 20-100
Baseline, Rotation	83.08	81.84	83.04	79.62	77.48	76.18	ARBG HU 20-100
Letter, Count	82.88	80.46	82.86	80.52	74.08	72.78	ARBG HU 20-100
Letter, Rotation	80.22	76.82	78.62	76.16	73.54	72.80	ARBG HU 20-100
Maths, Count	80.26	77.82	78.70	76.80	72.34	70.16	ARBG HU 20-100
Maths, Letter	81.08	78.64	79.28	76.70	73.76	72.86	ARBG HU 20-100
Maths, Rotation	79.98	79.04	78.48	77.26	74.98	73.48	ARBG HU 20-100
Rotation, Count	78.32	77.38	77.80	76.40	73.96	73.08	ARBG HU 20-100
Average	81.24	79.36	80.10	77.99	74.20	73.05	ARBG HU 20-100
Coefficient variation	0.02	0.02	0.02	0.02	0.02	0.02	
Maximum	83.08	81.84	83.04	80.52	77.48	76.18	ARBG HU 20-100
Best mental task combination	Baseline	Baseline	Baseline	Letter	Baseline	Baseline	
	Rotation	Rotation	Rotation	Count	Rotation	Rotation	

TABLE II
MLP-BP NN CLASSIFICATION RESULTS FOR SUBJECT 2

Mental task combination	Feature extraction method						Best feature extraction method and HU number
	ARBG		ARLS		MAR		
	20-100	2-10	20-100	2-10	20-100	2-10	
	No. of HU						
	Averaged classification (%)						
Baseline, Count	71.28	69.40	71.66	69.26	68.18	66.04	ARLS HU 20-100
Baseline, Letter	73.00	70.70	73.70	72.00	69.08	66.54	ARLS HU 20-100
Baseline, Maths	73.80	72.16	74.40	71.90	68.26	67.48	ARLS HU 20-100
Baseline, Rotation	71.18	69.46	71.10	70.08	67.64	65.74	ARBG HU 20-100
Letter, Count	75.24	73.30	75.04	72.58	68.64	67.22	ARBG HU 20-100
Letter, Rotation	71.48	68.88	70.90	67.78	70.74	69.04	ARBG HU 20-100
Maths, Count	71.50	69.72	72.42	69.02	71.96	70.74	ARLS HU 20-100
Maths, Letter	73.70	70.48	72.74	70.78	71.30	69.28	ARBG HU 20-100
Maths, Rotation	72.08	70.14	71.96	71.12	70.88	70.14	ARBG HU 20-100
Rotation, Count	74.96	71.82	73.66	71.78	72.84	70.92	ARBG HU 20-100
Average	72.82	70.61	72.76	70.63	69.97	68.31	ARBG HU 20-100
Coefficient variation	0.02	0.02	0.02	0.02	0.03	0.03	
Maximum	75.24	73.30	75.04	72.58	72.84	70.92	ARBG HU 20-100
Best mental task combination	Letter, Count	Letter, Count	Letter, Count	Letter, Rotation	Rotation	Rotation	

TABLE III
MLP-BP NN CLASSIFICATION RESULTS FOR SUBJECT 3

Mental task combination	Feature extraction method						Best feature extraction method and HU number
	ARBG		ARLS		MAR		
	20-100	2-10	20-100	2-10	20-100	2-10	
	No. of HU						
	Averaged classification (%)						
Baseline, Count	70.46	68.64	69.14	68.24	63.08	63.26	ARBG HU 20-100
Baseline, Letter	68.30	65.92	68.36	66.70	61.34	60.24	ARLS HU 20-100
Baseline, Maths	71.24	69.64	69.60	67.38	62.40	62.08	ARBG HU 20-100
Baseline, Rotation	71.72	67.86	70.74	68.20	62.82	59.94	ARBG HU 20-100
Letter, Count	71.08	68.98	70.60	67.82	64.04	61.56	ARBG HU 20-100
Letter, Rotation	79.66	76.90	77.86	74.98	72.24	70.38	ARBG HU 20-100
Maths, Count	76.38	76.46	76.98	75.00	69.36	67.18	ARLS HU 20-100
Maths, Letter	78.26	75.36	76.22	75.14	70.60	69.82	ARBG HU 20-100
Maths, Rotation	77.84	75.80	76.54	74.84	71.04	71.00	ARBG HU 20-100
Rotation, Count	80.28	78.38	77.94	76.02	72.58	71.06	ARBG HU 20-100
Average	74.54	72.39	73.42	71.43	66.95	65.66	ARBG HU 20-100
Coefficient variation	0.06	0.06	0.05	0.06	0.07	0.07	
Maximum	80.28	78.38	77.94	76.02	72.58	71.06	ARBG HU 20-100
Best mental task combination	Rotation	Rotation	Rotation	Rotation	Rotation	Rotation	

TABLE IV
MLP-BP NN CLASSIFICATION RESULTS FOR SUBJECT 4

Mental task combination	Feature extraction method						Best feature extraction method and HU number
	ARBG		ARLS		MAR		
	20-100	2-10	20-100	2-10	20-100	2-10	
	No. of HU						
	Averaged classification (%)						
Baseline, Count	84.18	82.50	84.32	81.52	72.26	70.68	ARLS HU 20-100
Baseline, Letter	83.72	81.92	82.14	78.90	72.40	71.66	ARBG HU 20-100
Baseline, Maths	84.66	83.74	83.88	83.10	71.60	69.92	ARBG HU 20-100
Baseline, Rotation	84.22	82.70	83.00	81.88	73.92	72.54	ARBG HU 20-100
Letter, Count	83.80	82.98	82.68	81.04	70.56	70.44	ARBG HU 20-100
Letter, Rotation	78.82	77.44	78.98	77.62	74.80	71.52	ARLS HU 20-100
Maths, Count	78.60	76.52	77.54	75.28	73.02	71.34	ARBG HU 20-100
Maths, Letter	79.58	79.08	79.66	78.10	73.72	70.36	ARLS HU 20-100
Maths, Rotation	78.38	77.54	78.82	76.62	73.42	72.18	ARLS HU 20-100
Rotation, Count	78.44	77.26	79.66	77.28	72.84	72.78	ARLS HU 20-100
Average	81.44	80.17	81.07	79.13	72.85	71.34	ARBG HU 20-100
Coefficient variation	0.04	0.04	0.03	0.03	0.02	0.01	
Maximum	84.66	83.74	84.32	83.10	74.80	72.78	ARBG HU 20-100
Best mental task combination	Maths	Maths	Count	Maths	Rotation	Count	

IV. DISCUSSION

Overall, it could be seen from Tables 1-4 that 20-100 HU gave significantly better results as compared to 2-10 HU for all the feature extraction methods using Student t-test ($p < 0.00001$) from all 4 subjects for all 3 feature extraction methods. This is also the case when comparing the averaged and best classification performances. When comparing best classification performance for each mental task combination, MAR method never gave the best performance for any of the subjects. In this regard, ARBG method gave the best classification performance more number of times as compared to ARLS for all the subjects. For subject 1, only ARBG method gave the best classification performance for all the mental task combinations. However, the classification performances between ARBG and ARLS were closer to each other as compared to MAR, which are most likely due to the similarity of the uni-variate AR modeling for ARBG and ARLS. Classification performances using MAR method also varied hugely between different mental task combinations as compared to ARBG and ARLS, which is shown by the CV values in the tables.

As far as the best mental task combinations are concerned, it varied for different subjects. For subject 1, the mental task that gave the best performance was baseline-rotation (83.08%), while it was letter-count (75.24%), rotation-count (80.28%) and baseline-maths (84.66%) for subjects 2, 3 and 4. It is also interesting to note that for subject 3, the best mental task combination was rotation-count for all the feature extraction methods.

V. CONCLUSION

In this paper, we have studied the effects of AR features and number of MLP-BP hidden units on the classification performance for designing BCIs. Classification results indicated 20-100 HU gave better performance for all the subjects with the ARBG method as the best method to extract features from EEG signals. This conclusion is based on the average and best classification performance over all the mental task combinations as it is difficult to conclude based on classification performance of single mental task pairs. Though more HU might increase the training and testing time for MLP-BP NN, it is advantageous as it generally results in higher classification performances compared to lower HU. Finally, we showed that it is appropriate to design individual BCIs, i.e. those that are suitable for use by a particular individual. Our experimental results showed that we cannot expect to build universal BCIs for use by all. This is because the thought patterns from different individuals are not the same and therefore different mental tasks result in varying classification performance. The results showed that in most cases, the suitable mental task pairs for each subject (i.e. the mental task pair that gave the best classification performances) are invariant to the feature extraction method. Therefore, it is more important to choose suitable mental task pairs for each individual as compared to the feature extraction method for a successful BCI design.

APPENDIX

Suppose an m -dimensional time series of $N+p$ state vector v_v ($v=1-p, \dots, N$) is available, the time series consisting of p pre-sample state vector v_{1-p}, \dots, v_0 and N state vectors v_1, v_2, \dots, v_N that form what we call the effective sample. The parameters A_1, A_2, \dots, A_p, w and C of an AR(p) model of fixed order are to be estimated.

The following description of multivariate AR is extracted from [18]. An AR(p) model can be cast in the form of a regression model

$$v_v = B u_v + \varepsilon_v, \quad \varepsilon_v = \text{noise}(C), \quad v=1, 2, \dots, N \quad (\text{A.1})$$

with parameter matrix

$$B = (w \ A_1 \ A_2 \ \dots \ A_p) \quad (\text{A.2})$$

and with predictors

$$u_v = \begin{pmatrix} 1 \\ v_{v-1} \\ \vdots \\ v_{v-p} \end{pmatrix}, \quad (\text{A.3})$$

of dimension $n_p = mp + 1$. Casting an AR model in the form of a regression model is an approximation in that in a regression model, the predictors u_v are assumed to be constant, whereas the state vectors v_v of an AR process are a realization of a stochastic process. The approximation of casting an AR model into the form of a regression model amounts to treating the first predictor

$$u_1 = \begin{pmatrix} 1 \\ v_0 \\ \vdots \\ v_{1-p} \end{pmatrix}. \quad (\text{A.4})$$

In terms of the moment matrices

$$U = \sum_{v=1}^N u_v u_v^T, \quad V = \sum_{v=1}^N v_v v_v^T, \quad W = \sum_{v=1}^N v_v u_v^T, \quad (\text{A.5})$$

where the least squares estimate of the parameter matrix B can be written as

$$\hat{B} = W U^{-1}. \quad (\text{A.6})$$

The residual covariance matrix

$$\hat{C} = \frac{1}{N - n_p} \sum_{v=1}^N \hat{\varepsilon}_v \hat{\varepsilon}_v^T \quad \text{with} \quad \hat{\varepsilon}_v = v_v - \hat{B} u_v. \quad (\text{A.7})$$

is an estimate of the noise covariance matrix C and can be expressed as

$$\hat{C} = \frac{1}{N - n_p} (V - W U^{-1} W^T). \quad (\text{A.8})$$

The residual covariance matrix \hat{C} is proportional to a Schur complement of the matrix

$$\Gamma = \begin{pmatrix} U & W^T \\ W & V \end{pmatrix} = \sum_{v=1}^N \begin{pmatrix} u_v \\ v_v \end{pmatrix} \begin{pmatrix} u_v^T & v_v^T \end{pmatrix}, \quad (\text{A.9})$$

which is the moment matrix $\Gamma = K^T K$ belonging to the data matrix

$$K = \begin{pmatrix} u_1^T & v_1^T \\ \vdots & \vdots \\ u_N^T & v_N^T \end{pmatrix}, \quad (\text{A.10})$$

The least squares estimates can be computed from a QR factorization of the data matrix

$$K = QR, \quad (\text{A.11})$$

with an orthogonal matrix Q and an upper triangular matrix

$$R = \begin{pmatrix} R_{11} & R_{12} \\ 0 & R_{22} \end{pmatrix}. \quad (\text{A.12})$$

The QR factorization of the data matrix K leads to the Cholesky factorization $\Gamma = K^T K = R^T R$ of the moment matrix.

$$\begin{pmatrix} U & W^T \\ W & V \end{pmatrix} = R^T R = \begin{pmatrix} R_{11}^T R_{11} & R_{11}^T R_{12} \\ R_{12}^T R_{11} & R_{12}^T R_{12} + R_{22}^T R_{22} \end{pmatrix}, \quad (\text{A.13})$$

and from this Cholesky factorization, one finds the representation

$$\hat{B} = (R_{11}^{-1} R_{12})^T \text{ and } \hat{C} = \frac{1}{N - n_p} R_{22}^T R_{22}, \quad (\text{A.14})$$

for the least squares estimates of the parameter matrix B and of the noise covariance matrix C . The estimated parameter matrix \hat{B} is obtained as the solution of a triangular system of equations, and the residual covariance matrix \hat{C} is given in a factored form that shows explicitly that the residual covariance matrix is positive semi-definite.

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