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TUTORIAL ON MULTIVARIATE AUTOREGRESSIVE MODELLING

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ABSTRACT. In the present paper, the theoretical background of multivariate autoregressive modelling (MAR) is explained. The motivation for MAR modelling is the need to study the linear relationships between signals. In biomedical engineering, MAR modelling is used especially in the analysis of cardiovascular dynamics and electroencephalographic signals, because it allows determination of physiologically relevant connections between the measured signals. In a MAR model, the value of each variable at each time instance is predicted from the values of the same series and those of all other time series. The number of past values used is called the model order. Because of the inter-signal connections, a MAR model can describe causality, delays, closed-loop effects and simultaneous phenomena. To provide a better insight into the subject matter, MAR modelling is here illustrated with a model between systolic blood pressure, RR interval and instantaneous lung volume.

KEY WORDS. multivariate autoregressive modelling, cardiovascular dynamics.

INTRODUCTION

The univariate AR model predicts the current values of a time series from the previous values of the same series [1]. A better estimate for a predicted time series may be found if another plausible explanatory variable is included in the model, such as systolic blood pressure (SBP) on RR interval (RRI). A multivariate AR (MAR) model contains not only a model of each time series but also a model of the relationships between the included variables. In biomedical engineering, MAR modelling thus enables one to determine various physiologically relevant connections between the measured signals. To select the correct model structure, we need to know the restrictions implicit in the model and how to apply it. Understanding the physical and/or physiological mechanisms underlying the system is crucial for a correct interpretation of the analysis results, but if this condition is satisfied, MAR modelling can provide valuable information on the operational status of the system under study.

Multivariate AR modelling provides an efficient tool for locating the origins of fluctuations in a variety of processes [2]. It has been applied e.g. to the diagnosis of nuclear reactor status [3] and a paper manufacturing process [4] as well as to the analysis of neurosignals [5] and cardiovascular dynamics [6, 7].

The theoretical background of MAR modelling is scattered in the literature. The aim of this paper is to present a review of the existing literature and to outline a compact

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theoretical basis for MAR modelling. To provide a deeper insight into the presented method, it is here illustrated with a model between SBP, RRI and instantaneous lung volume (ILV).

MODEL IDENTIFICATION

Model identification is based on the assumption that the process to be studied is stationary and stochastic. A stationary time series, by definition, does not change its statistical parameters, i.e., mean value, probability distribution or frequency content, over time [8]. Nonstationarities and dynamic situations in the data result in distorted results.

The MAR model represents each variable as a linear function of both its own previous values and those of all other variables. Thus, the model divides each time series into two additive components, the predictable time series and the prediction error sequence. The latter is also called the noise source of the corresponding time series. The nonlinear interactions between variables are included in the prediction errors.

The MAR model with N variables is defined by the equations

$$\begin{aligned} x_1(n) &= \sum_{i=1}^{M} a'_{11}(i)x_1(n-i) + \cdots \\ &\quad + \sum_{i=1}^{M} a'_{1N}(i)x_N(n-i) + e_1(n) \\ x_2(n) &= \sum_{i=1}^{M} a'_{21}(i)x_1(n-i) + \cdots \\ &\quad + \sum_{i=1}^{M} a'_{2N}(i)x_N(n-i) + e_2(n) \\ x_N(n) &= \sum_{i=1}^{M} a'_{N1}(i)x_1(n-i) + \cdots \\ &\quad + \sum_{i=1}^{M} a'_{NN}(i)x_N(n-i) + e_N(n) \end{aligned} \tag{1}$$

where $x_1(n) \ldots x_N(n)$ is the current value of each time series, $a'_{11}(i) \ldots a'_{NN}(i)$ are predictor coefficients at delay i, M is the model order, indicating the number of previous data points used for modelling, and $e_1(n) \ldots e_N(n)$ are one-step prediction errors (Figure 1). The equations (1)

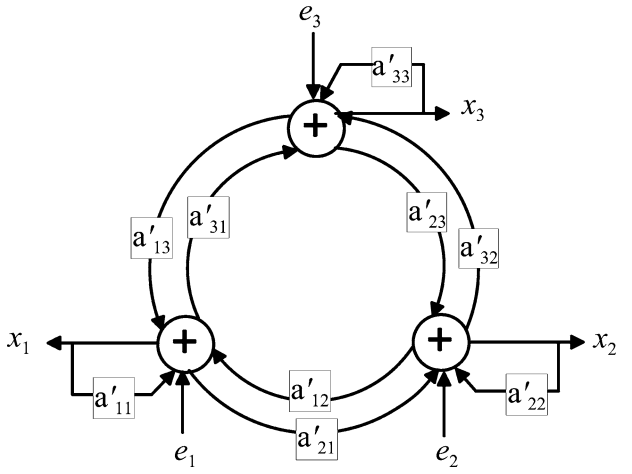

Fig. 1. Structure of a trivariate MAR model.

can be re-written in a matrix form:

$$\begin{aligned} \mathbf{x}(n) &= \sum_{i=1}^{M} \begin{bmatrix} a'_{11}(i) & \cdots & a'_{1N}(i) \\ \vdots & \ddots & \vdots \\ a'_{N1}(i) & \cdots & a'_{NN}(i) \end{bmatrix} \begin{bmatrix} x_1(n-i) \\ \vdots \\ x_N(n-i) \end{bmatrix} \\ &\quad + \begin{bmatrix} e_1(n) \\ \vdots \\ e_N(n) \end{bmatrix} \end{aligned} \tag{2}$$

$\Leftrightarrow$

$$\mathbf{x}(n) = \sum_{i=1}^{M} \mathbf{a}'(i)\mathbf{x}(n-i) + \mathbf{e}(n) \tag{3}$$

where $\mathbf{x}(n)$ is a $(N \times 1)$ column matrix denoting multivariate process at index n, $\mathbf{a}'(i)$ are $(N \times N)$ predictor coefficient matrices, and $\mathbf{e}(n)$ is a $(N \times 1)$ matrix for prediction errors [9]. The multivariate form of the prediction error filter is thus expressed as

$$\mathbf{e}(n) = \sum_{i=0}^{M} \mathbf{a}(i)\mathbf{x}(n-i) \tag{4}$$

where $\mathbf{a}(0) = \mathbf{I}$ and $\mathbf{a}(i) = -\mathbf{a}'(i)$.

The model structure allows the identification of feedback loops, as the transfer functions in both directions between each pair of variables are described by separate off-diagonal elements of the matrices $\mathbf{a}(i)$, i.e. $a_{ij} \neq a_{ji}$ for each $i \neq j$. A MAR model *per se* does not reveal any causal relationships between the variables. Therefore, *a priori* knowledge of the system to be studied is needed.

Usually, the optimum predictor coefficients are estimated by applying the orthogonality principle in the least-squares minimization technique so that the coefficients will produce minimum variance. The predictor coefficients are selected so that $\mathbf{e}(n)$ is orthogonal to $\mathbf{x}(n-k)$, where $k = (1, \ldots, M)$ [9]. This means that the prediction errors for each variable are simultaneously independent of every explanatory vector x_i. This requirement may be stated as

$$E\{\mathbf{e}(n)\mathbf{x}(n-k)^T\} = 0, \quad k = 1, \ldots, M \tag{5}$$

where $(*)^T$ denotes matrix or vector transpose.

By combining (4) and (5) and noting that $E\{\mathbf{x}(n-i)\mathbf{x}(n-k)^T\} = \mathbf{R}_x(k-i)$, we get

$$\sum_{i=0}^{M} \mathbf{a}(i)\mathbf{R}_x(k-i) = 0, \quad k = 1, \ldots, M \tag{6}$$

The optimum set of MAR parameters is found when the mean square prediction error is minimized. This happens when the orthogonality principle applies. Under these conditions, the MAR noise covariance matrix $\mathbf{\Sigma_e}$ is given by [9]

$$\mathbf{\Sigma_e} = \mathbf{e}(n)\mathbf{e}(n)^T = \sum_{i=0}^{M} \mathbf{a}(i)\mathbf{R}_x(-i) \tag{7}$$

Equations (6) and (7) can now be expressed as a single set of equations:

$$\sum_{i=0}^{M} \mathbf{a}(i)\mathbf{R}_x(k-i) = \mathbf{\Sigma_e}\delta(k), \quad k = 0, \ldots, M \tag{8}$$

where $\delta(k)$ is Kronecker delta function ($\delta(k) = 1$ when $k = 0$, otherwise $\delta(k) = 0$) [9, 10].

The values of the correlation matrix are estimated using the sampled data [9, 11]. Usually, a so-called autocorrelation method is used. In the autocorrelation method, the sample correlations are computed assuming that $x(k) = 0$ when $(k < 1)$ or $(k > L)$; L is the number of data samples. In this case, sample correlations $\widehat{\mathbf{R}}_x(k)$ are defined as

$$\hat{\mathbf{R}}_x(i, j) = \frac{1}{L} \sum_{n=-\infty}^{\infty} x(n-i)x(n-j)^T \tag{9}$$

where i, j are sample delay indices.

The presented correlation method is also known as a multichannel Yule-Walker method. In this procedure, the data is actually windowed with a rectangular window, which has a value 1 when $(0 < n \leq L)$ and 0 otherwise. If the amount of data is small, and if there is a high correlation together with long delays, the statistical reliability of the model estimation may be considerably diminished [9].

Using the set of normal equations (8) with $(M + 1)$ matrix equations and $(M + 1)$ unknown matrix parameters, the MAR coefficient matrices $(\mathbf{a}(i), \mathbf{\Sigma_e})$ can be solved by, for instance, using a recursive LWR algorithm [9]. The Levinson-Durbin recursion for univariate model [12, 13] was extended to the multivariate Yule-Walker equations by Whittle [14] and independently by Wiggins and Robinson [15]. This algorithm applies a fast updating procedure to obtain a MAR parameter set $(\mathbf{a}_{M+1}(1), \mathbf{a}_{M+1}(2), \ldots, \mathbf{a}_{M+1}(M+1), \mathbf{\Sigma}_{M+1})$ of order $(M+1)$ by applying the parameter set in the previous order M.

M determines the length of the memory in the model. It must be high enough to describe all relevant delays and fluctuations in the process and low enough to ensure reliable model identification from the measured data. In practise, the model can contain only a few variables without compromising the reliability of model identification from a limited amount of measurement data [9]. There are several objective criteria for the selection of M in the multivariate case, such as the Akaike information criterion (AIC) [16], Akaike's final prediction error and the criterion autoregressive transfer function [17]. These methods find the optimal M for one-step prediction, but this is not necessarily the optimal M for analysing transfer functions in the system. Therefore, none of these criteria is in itself a sufficient method for the selection of M. The autocorrelation function of the residual time series should also be studied, and if M is correct, the residuals should be uncorrelated white noise. In practise, several MAR models are calculated while varying M, and the best model is then chosen.

The multivariate AIC is given by

$$\mathrm{AIC}(M) = L\log(\det\mathbf{\Sigma}_\varepsilon) + 2N^2M \tag{10}$$

where L is the number of data points applied in the estimation.

For reliable parameter identification, the number of parameters must be significantly smaller than the number of data points available, i.e.,

$$N^2M \ll NL \tag{11}$$

PROPERTIES OF NOISE COVARIANCE MATRIX $\mathbf{\Sigma_e}$

Equation (4) gives the prediction errors as a function of variables. By inverting the MAR model, we can calculate the variables as a function of prediction errors (Figure 2a).

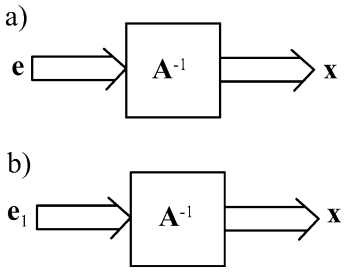

Fig. 2. (a) An inverse model $\mathbf{A}^{-1}$ *can be used to calculate the variables* $\mathbf{x}$ *as a function of prediction errors* $\mathbf{e}$*. (b) Estimation of the contribution of a noise source* $\mathbf{e}_1$ *to the system by setting all the other noise sources to zero.*

The MAR model describes a system where signals explain each other, and dynamic interactions of the system can be analysed. Both MAR coefficients and $\mathbf{\Sigma_e}$ are used to describe the interrelations of the variables. The analysis of interactions is based on an assumption of mutually independent noise sources, which results in diagonal $\mathbf{\Sigma_e}$. In that case, the contribution of a noise source to the system can be studied by setting all the other noise sources to zero (Figure 2b). The noise source contribution function describes the extent of variability originating from the signal's internal noise source in relation to other noise sources. This means that it allows assessment of the strength and direction of the connections between the signals.

When the zero lag MAR coefficient matrix $\mathbf{a}(0) = \mathbf{I}$, all the zero lag effects between the variables have to be included in $\mathbf{\Sigma_e}$. In practise, physical systems are not able to produce responses without some time delay, which may cause a situation where the estimated MAR model contains zero lag relations. Then, the estimated noise sources are not independent of each other and the off-diagonal values of $\mathbf{\Sigma_e}$ tend to differ from zero. Accordingly, it is very important to check the off-diagonal values of $\mathbf{\Sigma_e}$ before starting the analysis. If the off-diagonal values are close to zero, it can be assumed that the identified MAR model can separate each noise source perfectly from the other noise sources, and the non-zero off-diagonal elements of $\mathbf{\Sigma_e}$ can be ignored.

If $\mathbf{\Sigma_e}$ contains significant off-diagonal values, we can try to eliminate the reason by using a higher sampling rate or a different selection of variables in the analysis. Alternatively, we can manipulate the model so that the influences of immediate propagation are removed from $\mathbf{\Sigma_e}$ and transferred into the MAR coefficients.

This is achieved by using the following transformation:

$$\mathbf{\Sigma_e} = \mathbf{b}\Sigma_{\text{diag}}\mathbf{b}^* \tag{12}$$

where $\mathbf{b}$ is a lower triangular matrix calculated by applying Cholesky decomposition to the noise covariance matrix [18].

For MAR coefficients, this means

$$\mathbf{a}_{\text{new}}(k) = \mathbf{b}^{-1}\mathbf{a}(k), \quad k = 0, \ldots, M \tag{13}$$

MODEL ANALYSIS

As in the univariate case, the MAR model analysis (transfer functions, spectra, contributions) is easiest to accomplish in the frequency domain. This also solves the problem of possible instability of the inverse MAR system; in the frequency domain, the concept of spectrally equivalent systems can be applied.

In the MAR system, both the total transfer function from each noise source to each variable in the model and the direct transfer function between the variables x_i and x_j are defined. The total transfer function can be determined by first z-transforming (3):

$$\begin{aligned}\mathbf{X}(z) &= \sum_{i=1}^{M} \mathbf{a}'(i)\mathbf{X}(z)z^{-i} + \mathbf{E}(z) \\ &= (\mathbf{a}'(1)z^{-1} + \cdots + \mathbf{a}'(M)z^{-M})\mathbf{X}(z) + \mathbf{E}(z)\end{aligned} \tag{14}$$

From (14), we get the total transfer function $\mathbf{H}(z)$:

$$\begin{aligned}\mathbf{H}(z) &= \frac{\mathbf{X}(z)}{\mathbf{E}(z)} = \frac{1}{\mathbf{I} - \mathbf{a}'(1)z^{-1} - \cdots - \mathbf{a}'(M)z^{-M}} \\ &= \frac{1}{\mathbf{I} - \mathbf{A}'(z)} = \frac{1}{\mathbf{A}(z)}\end{aligned} \tag{15}$$

In the frequency domain, the total transfer function is then

$$\mathbf{H}(f) = \mathbf{H}(z)|_{z=e^{j2\pi ft}} = \mathbf{A}^{-1}(f) \tag{16}$$

where $\mathbf{A}(f)$is the Fourier transform of $\mathbf{a}(i)$ [9].

The direct transfer function between the variables x_i and x_j in the frequency domain is defined as [19]

$$H_{ij}(f) = -\frac{A_{ij}(f)}{A_{ii}(f)} \tag{17}$$

Reliable identification of a MAR model requires that some unique information is propagated through every transfer path in the model. The signals used for modelling should preferably also have a broad frequency band. Using narrowband signals in the model results in greater transfer function uncertainty at the frequencies where the signals have zero power.

In the univariate case, the spectrum of the modelled time series is obtained by multiplying the prediction error variance with the square of the transfer function. The multivariate spectral matrix contains an autospectrum of each variable and cross-spectra of each variable pair. The prediction error variance is replaced by $\mathbf{\Sigma_e}$, and the univariate transfer function is replaced by a multivariate transfer function. Thus, the spectral matrix for a multivariate AR process can be expressed as

$$\mathbf{P_x}(f) = \mathbf{H}(f)\mathbf{\Sigma_e}\mathbf{H}^*(f) \tag{18}$$

where $(*)^*$ denotes the conjugate transpose of a matrix [19]. If $\mathbf{\Sigma_e}$ is diagonalized, the spectrum is

$$\mathbf{P}_x(f) = \mathbf{A}_{\text{new}}^{-1}(f)\mathbf{b}\Sigma_{\text{diag}}\mathbf{b}^*\left(\mathbf{A}_{\text{new}}^{-1}(f)\right)^* \tag{19}$$

In a three-variable case, the spectral matrix is

$$\mathbf{P_x}(f) = \begin{bmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{bmatrix}_{\mathbf{x}} (f) \tag{20}$$

where $P_{ii}(f)$ is the autospectrum of the ith variable and $P_{ij}(f)$ is the cross-spectrum between the variables x_i and x_j.

Assuming that the noise sources are mutually independent, the multivariate power spectrum can be decomposed into components originating from each noise source:

$$P_{x_{ii}}^{(\text{diag})}(f) = \sum_{j=1}^{N} \left|\mathbf{A}_{ij}^{-1}(f)\right|^2 \mathbf{\Sigma}_{e_{jj}} \tag{21}$$

The superscript $^{(\text{diag})}$ indicates that the off-diagonal elements of $\mathbf{\Sigma_e}$ are ignored. $P_{x_{ii}}^{(\text{diag})}$ indicates the element on the row i and the column i in the matrix $\mathbf{P}_x^{(\text{diag})}$, which is equal to $\mathbf{P}_x$ if $\mathbf{\Sigma_e}$ is diagonal.

An important quantity in multivariate system analysis is the noise source contribution, Γ_{ij}. Noise source contribution analysis decomposes the power of the fluctuation of the variables x_i into components originating from separate noise sources e_j. The effect of each noise source to the system can then be studied separately by setting the other noise sources to zero. Noise source contribution is scaled to a percentage of the power of the fluctuation of x [20]:

$$\Gamma_{ij}^{(\text{diag})}(f) = \frac{\left|\mathbf{A}_{ij}^{-1}(f)\right|^2 \mathbf{\Sigma}_{\mathbf{e}_{jj}}}{\mathbf{P}_{x_{ii}}^{(\text{diag})}(f)} \cdot 100\% \tag{22}$$

If the noise sources are mutually independent, the sum of the contributions from each noise source to the variable x_i is 100%. If the noise sources are correlated, the sum may exceed this value. The noise source contribution is usually examined over a frequency range instead of a single frequency, since the causes of variations are generally broadband.

Another useful parameter for analyzing system dependencies is the squared coherence function. Coherence expresses the frequency domain correlation between the variables x_i and x_j, and it is given by [19]

$$\gamma_{ij}^2(f) = \frac{|P_{ij}(f)|^2}{P_i(f)\,P_j(f)} \tag{23}$$

The value of coherence is between 0 and 1. It is the only reliable measure of correlation at frequencies where both of the variables x_i and x_j have variation (i.e., $P_i(f), P_j(f) \gg 0$). The squared coherence can be considered reliable if it exceeds the value of 0.5 [8]. The value of coherence function at any given frequency can be used as a measure of reliability of any other cross-variable parameter determined at that frequency.

APPLICATION EXAMPLE

A MAR model is here illustrated with a model between SBP, RRI and ILV. The data was measured from a healthy male in a supine position as in [22]. The ILV signal was measured using an impedance pneumograph. Therefore, the utilized method also reflects some cardiovascular activity [21].

Stationary data segments of 5 min were chosen for analysis. The signals were transformed into time series of instantaneous SBP, RRI and ILV and pre-processed as in [22]. A phase lead of RRI to ILV of 2 samples was incorporated into the model, because the onset of RRI change has been shown by neural mechanisms to precede the onset of ILV change [23].

The M of 16 given by AIC results in:

$$\Sigma_{\mathrm{e}} = \begin{bmatrix} 0.2266 & -0.0283 & -0.0181 \\ -0.0283 & 0.1724 & 0.0141 \\ -0.0181 & 0.0141 & 0.0330 \end{bmatrix}$$

Since these signals tend to have immediate transfer paths (i.e. mechanisms that affect within the heartbeat interval) or common noise sources outside this three-variable model, $\mathbf{\Sigma_e}$ is not diagonal. The immediate effects can be taken into account by diagonalising $\mathbf{\Sigma_e}$ and modifying the zero delay coefficient matrix by using (12) and (13). The diagonalised

$\mathbf{\Sigma_e}$ ($\mathbf{\Sigma_{e,\mathrm{diag}}}$) is

$$\mathbf{\Sigma_{e,\mathrm{diag}}} = \begin{bmatrix} 0.2266 & 0 & 0 \\ 0 & 0.1689 & 0 \\ 0 & 0 & 0.0307 \end{bmatrix}$$

and the zero delay coefficient matrix is

$$\mathbf{a}(0) = \begin{bmatrix} 1.0000 & 0 & 0 \\ 0.1248 & 1.0000 & 0 \\ 0.0712 & -0.0703 & 1.0000 \end{bmatrix}$$

The matrix describes the immediate effects of RESP on RRI, of RESP on SBP and of RRI on SBP.

The diagonal model allows estimation of spectra, noise source contributions and transfer functions. In the neural regulation of circulatory function, SBP and RRI exhibit variations at around 0.1 Hz and 0.2 Hz, which are associated with baroreceptor and respiratory activity, respectively (Figure 3) [24]. At these frequencies, the squared coherence between RRI and SBP is greater than 0.6, indicating a tight linear coupling between the time series (Figure 4a). There is a negative phase angle between RRI and SBP, indicating that changes in SBP precede changes in RRI (Figure 4b).

Respiration has a relatively greater effect on RRI variability than on SBP variability (Figure 3). At the respiratory frequency, some 80% of RRI variability originates from respiration (Figure 5). At around 0.1 Hz, 80% originates from RRI's own noise source contribution, while the rest is divided between respiration and SBP.

The transfer function from SBP to RRI describes the clinically important arterial baroreceptor function. Transfer function analysis reveals that SBP variability has the greatest effect on RRI variability at 0.1 Hz (Figure 6). Baroreceptor sensitivity is 12.0 ms/mmHg**,** as assessed by the method of Robbe et al. [25]. The transfer function from respiratory activity to RRI describes respiratory sinus arrhythmia (Figure 7), another measure of clinical importance. Respiration is generally a narrow-band signal and transfer functions calculated from respiration to blood pressure and RR intervals are only reliable within the respiration frequency band. The confidence limits for the magnitude of the transfer function [26] plotted in Figures 6 and 7 also show this.

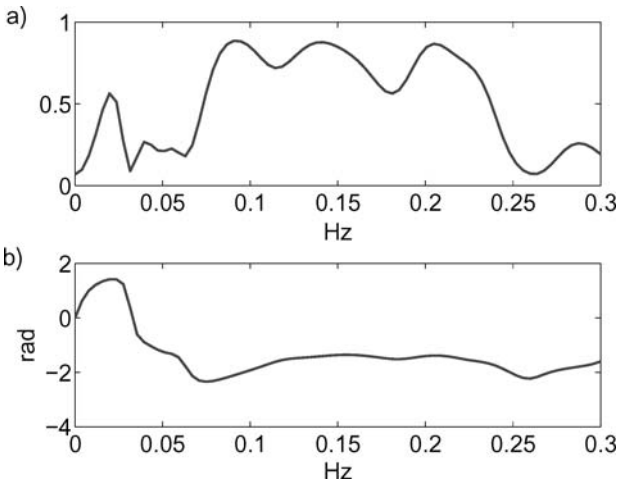

Fig. 4. (a) Squared coherence between RR intervals and systolic blood pressure. (b) Phase angle of the coherence function between RR intervals and systolic blood pressure.

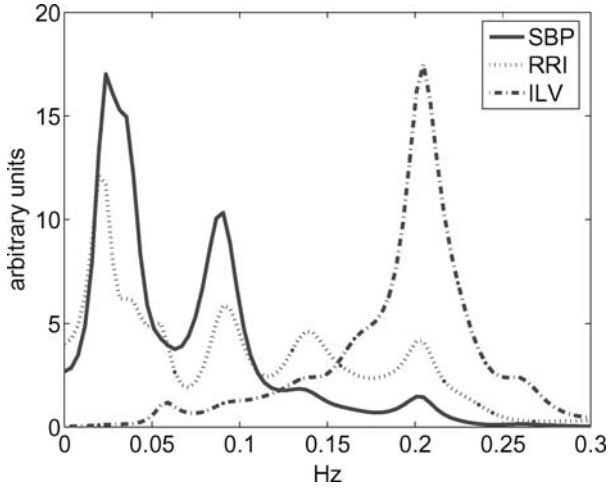

Fig. 3. Autospectra of systolic blood pressure (SBP), RR intervals (RRI) and instantaneous lung volume (ILV).

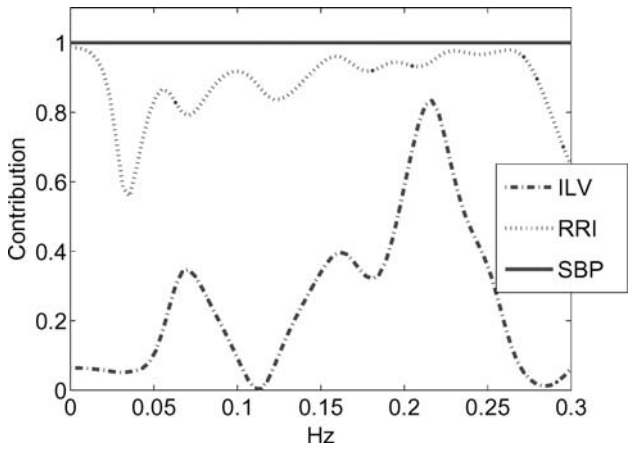

Fig. 5. Noise source contributions from systolic blood pressure (SBP), instantaneous lung volume (ILV) and RR intervals (RRI) to RRI.

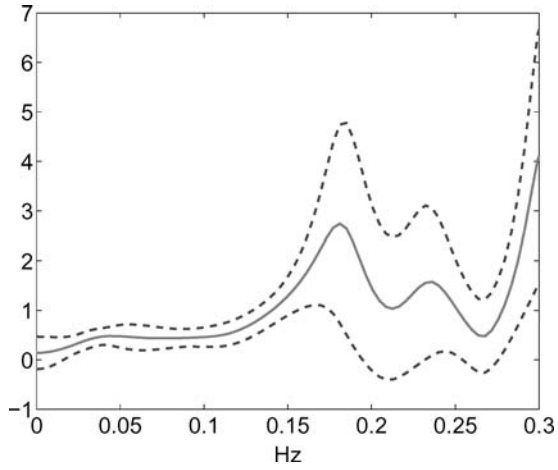

Fig. 6. Transfer function magnitude from systolic blood pressure to RR intervals, mean (solid line) and its 95% confidence limits (broken lines).

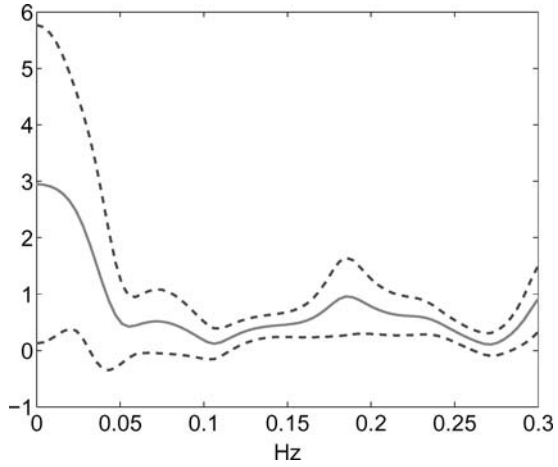

Fig. 7. Transfer function magnitude from instantaneous lung volume to RR intervals, mean (solid line) and its 95% confidence limits (broken lines).

Since SBP and RRI variability above 0.3 Hz is noise, the computed transfer function values above that frequency are also noise.

It is of note, that interactions between SBP and RRI occur physiologically in a closed-loop condition, i.e. in a condition were changes in SBP cause reflex changes in RRI, and, at the same time, changes in RRI affect SBP through changes in cardiac output. Therefore, closed-loop models are physiologically more valid than open-loop models, which account for the effect of SBP on RRI, but do not have link from RRI to SBP. Secondly, in the assessment of arterial baroreflex the effect of respiration is a confounding factor, because it also affects RRI on a beat-to-beat basis. Unless all the three variables are controlled, the calculated arterial baroreflex is likely to be biased, and to have reduced accuracy [27]. All these variables should also be taken into account in the analysis of respiratory sinus arrhythmia. This is possible only if the model is multivariate, closed-loop, and causal, such as our MAR model and the autoregressive techniques that have been previously described [27].

SUMMARY

In the present paper, the theoretical basis of MAR modelling is presented. The process to be studied should be stationary under the modelling period. In the formulation of the model structure, *a priori* knowledge of the system is used. The model is solved by a set of linear equations. In the model identification, correct selection of M, i.e. the length of the model memory, deserves special attention. After the model has been identified, its validity must be checked. It is important to check the off-diagonal values of $\mathbf{\Sigma_e}$ before the analysis. If the off-diagonal values are close to zero, it is possible to assess connections between the variables by examining the effect of each noise separately. Otherwise, the model should be modified. A possibility is to use *a priori* knowledge of the system, and use immediate, pre-defined directions in the transfer paths. The model is analysed by calculating different functions from the model. The presented MAR model is well suited for the analysis of cardiovascular dynamics, because cardiovascular system is inherently a multivariate closed-loop system.

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