Available online at www.sciencedirect.com
SCIENCE DIRECT®
Journal of Sound and Vibration 290 (2006) 676–689
JOURNAL OF SOUND AND VIBRATION
www.elsevier.com/locate/jsvi

Analysis of the maximum likelihood, total least squares and principal component approaches for frequency response function estimation

P.R. White*, M.H. Tan, J.K. Hammond

Institute of Sound and Vibration Research, University of Southampton, Highfield, Southampton SO17 1BJ, UK

Received 1 August 2003; received in revised form 19 November 2004; accepted 15 April 2005
Available online 24 August 2005

Abstract

This paper considers the problem of estimation frequency response functions (FRFs) for a single-input single-output (SISO) system in the presence of additive noise on both input and output measurements. It demonstrates that principle component analysis (PCA) can be employed to solve such problems and demonstrates that this is equivalent to the methods based on total least squares (TLS). FRF estimation is also cast as a problem in statistical inference and the use of the principle of maximum likelihood (ML) leads to a novel development of a generalised TLS scheme. This analysis also provides a framework within which one can compute asymptotic expressions for the variance of such estimators.

1. Introduction

The problem of estimating the dynamic characteristics of a linear time-invariant system (e.g. its transfer function or impulse response) from measurements of its input and output is of long-standing interest in many areas of engineering. In many areas of engineering the solution to this problem is realised in the frequency domain, leading to the estimation of the system's frequency

*Corresponding author. Tel.: +44 23 8059 2274; fax: +44 23 8059 3190.
E-mail address: prw@isvr.soton.ac.uk (P.R. White).

0022-460X/$ - see front matter © 2005 Elsevier Ltd. All rights reserved.
doi:10.1016/j.jsv.2005.04.029

response function (FRF). This paper reconsiders the problem of FRF estimation for a single-input single-output (SISO) system.

Traditional experimental response testing procedures are subject to several potential confounding factors. In particular, the measurements can often be undermined by various factors including nonlinear system behaviour, change of system characteristics with time, instability and, most commonly, the contamination of the data by additive measurement noise. It is the general problem of FRF estimation in the presence of uncorrelated additive measurement noise that forms the focus for this paper. Fig. 1 depicts the generic problem we consider in block diagram form. Note in this figure Fourier transform (FT) pairs are indicated by the symbol $\leftrightarrow$.

It is crucial to the problem of FRF estimation that the most appropriate statistical estimation procedure is followed in order to obtain an accurate estimate for the identification of the system under investigation. There are two classical transfer function estimators commonly in use; these estimators are based on least-squares optimisation methods and are commonly referred to as $H_1(f)$ and $H_2(f)$. Both these methods are commonly regarded within the framework of least-squares estimation, which assumes that any noise is present on only one of the measured signals. An alternative technique, in which noise is assumed on both signals, is based on the concept of total least squares (TLS) and is commonly referred to as $H_s(f)$. All three methods have been widely applied are integral to a great many analysis tasks.

The goal of this paper is to provide an alternative framework in which all three methods can be derived. Specifically, we show that all three methods can be legitimately regarded as maximum-likelihood (ML) methods. This observation not only intimately links the three techniques but also allows one to infer that the estimators share the rich and well-known benefits of ML schemes; as opposed to the relative porosity of general properties of least-squares techniques. In particular, we shall use the observation that the schemes are ML techniques in order to derive expressions for the variance of the TLS FRF estimator.

The remainder of this paper is organised as follows: Section 2 recaps the properties of the three well-established techniques. Section 3 discusses the interpretation of the FRF estimation as a problem in linear regression and explains how principle component analysis (PCA) can be used as a tool to solve this problem. Section 4 is dedicated to the use of the method of ML to the problem of FRF estimation. Besides developing the optimal (in a ML sense) estimator performance metrics are also derived. Simulation studies presented in Section 5 serve as a verification of the theoretical results established herein, with a summary and conclusions being given in Section 6.

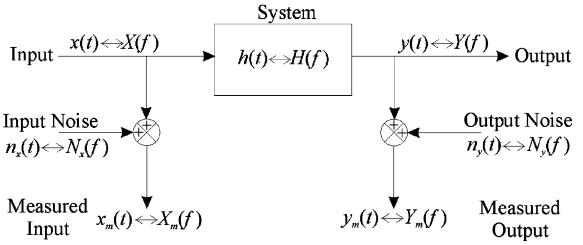

Fig. 1. Measurement configuration.

2. Least-squares FRF estimation

The two most familiar FRF estimation methods are $H_1(f)$ and $H_2(f)$. With reference to Fig. 1, these can be defined as [1]

$$H_1(f) = \frac{\hat{S}_{x_m y_m}(f)}{\hat{S}_{x_m x_m}(f)} \tag{1}$$

and

$$H_2(f) = \frac{\hat{S}_{y_m y_m}(f)}{\hat{S}_{y_m x_m}(f)}, \tag{2}$$

where $\hat{S}_{ab}(f)$ is an estimator for the cross-spectral density between $a(t)$ and $b(t)$ and if $a(t) = b(t)$ then this spectrum is referred to as an auto-spectral density or a power spectrum. Assuming the system under investigation is truly linear and the two additive measurement noises $n_x(t)$ and $n_y(t)$ are mutually uncorrelated and uncorrelated with the input signal, then the statistical behaviour of these two FRF estimators in the presence of additive measurement noise is well established. The important results can be summarised as: for the case of measurements with only output noise, estimator $H_1(f)$ is unbiased; whereas for the case of measurements with only input noise, estimator $H_2(f)$ is unbiased; and when noise is present on both the input and output both $H_1(f)$ and $H_2(f)$ are biased. In the latter case one can further show that [1]

$$E[H_1(f)] \leqslant H(f) \leqslant E[H_2(f)], \tag{3}$$

where $E[\,]$ denotes the expectation operator. This result allows one to approximately bracket the correct result by computing both transfer function estimators. It should be noted that Eq. (3) is developed using the mean values for $H_1(f)$ and $H_2(f)$ and there is no guarantee that for finite data lengths it will hold true. A more correct fashion by which to bound estimates of the transfer function is to use the concept of a confidence interval. For example, it can be shown [1,2] that the confidence interval for the magnitude of a transfer function estimated via $H_1(f)$ is given by [1,2]

$$|H_1(f)|^2 \cdot \left\{ 1 \pm \frac{4}{N-2} \cdot \left(\frac{1}{\gamma^2_{x_m y_m}(f)} - 1 \right) f_{2,N-2}(1-\beta) \right\}, \tag{4}$$

where $f_{2,N-2}(\beta)$ is the inverse cumulative distribution of the F-distribution with "2, $N-2$" dof (for large N $f_{2,N-2}(\beta) \approx -\log(1-\beta)$) and $\gamma^2_{x_m y_m}(f)$ is the coherence function between the measured variables which is given by

$$\gamma^2_{x_m y_m}(f) = \frac{|S_{x_m y_m}(f)|^2}{S_{x_m x_m}(f) S_{y_m y_m}(f)}. \tag{5}$$

Besides the above most commonly used transfer function estimators, $H_1(f)$ and $H_2(f)$, there exists an alternative estimator $H_s(f)$ [3] based upon the concept of TLS [4]. The estimator

$H_s(f)$ is defined as

$$H_s(f) = \frac{\hat{S}_{y_m y_m}(f) - s\hat{S}_{x_m x_m}(f) + \sqrt{\{s\hat{S}_{x_m x_m}(f) - \hat{S}_{y_m y_m}(f)\}^2 + 4s|\hat{S}_{x_m y_m}(f)|^2}}{2\hat{S}_{y_m x_m}(f)} \tag{6}$$

and s is a scale factor that allows one to manipulate the FRF estimates. By letting $s = 0$ one obtains $H_2(f)$ and the case where $s \to \infty$ one can show that $H_s(f) \to H_1(f)$. Hence, if one varies s over the range $[0, \infty]$ the estimator $H_s(f)$ takes values in the range $[H_1(f), H_2(f)]$. The case of $s = 1$ defines an additional FRF estimator, namely $H_v(f)$ [5–8]. This paper concentrates on the interpretation and analysis of the estimator $H_s(f)$, along with the special case $H_v(f)$.

3. PCA and FRF estimation

PCA is one of the most effective multivariate data analysis techniques. It takes the form of an eigenvalue decomposition (EVD) of the covariance matrix. The direction of the resulting eigenvectors represent the direction of principal components and these components are weighted according to value of the corresponding eigenvalues. The sum of the eigenvalues is equal to the total variance (power) of the original variables. The principle components represent a linearly transformed version of the input data, with the benefit that the transformed variables are uncorrelated. This approach also allows one to identify components of low power that may be removed from the data set without significantly affecting the data, thus producing a dimensionally reduced form of the original data. The aim of the method is to introduce parsimony to the analysis.

This section aims to discuss how PCA can be used to estimate FRFs. However, to illuminate this presentation we shall regard the problem of FRF estimation as an example of linear regression.

3.1. FRF estimation as a problem in linear regression

In order to compute the FRF estimators given by Eqs. (1), (2), and (6) one first needs to estimate the spectra involved. One can employ a variety of spectral estimation techniques, but for the purposes of this analysis we shall assume the use of a direct (segment averaging) technique. In direct spectral estimation algorithms the measured signals $x_m(t)$ and $y_m(t)$ are first partitioned into overlapping segments of equal length, a window is then applied and the estimate of, say the cross-spectrum, is defined as

$$\hat{S}_{x_m y_m}(f) = \frac{1}{N}\sum_{n=1}^{N} X^*_{m_n}(f) Y_{m_n}(f) \tag{7}$$

in which $X_{m_n}(f)$ and $Y_{m_n}(f)$ are the FTs of the nth (windowed) segment of $x_m(t)$ and $y_m(t)$, respectively, N is the total number of segments. From hereon, it is tacitly assumed that the length of each window is sufficiently large so that the biasing effects of the window can be neglected.

Within such a framework the standard transfer function estimators can be derived by regression analysis [2] based on the observation that in the absence of noise the input–output relationship of

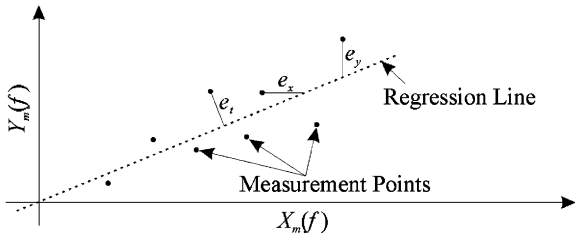

Fig. 2. Different forms of errors in linear regression.

a linear time-invariant system is given by

$$Y(f) = H(f)X(f). \tag{8}$$

The problem is to estimate the function $H(f)$ based on N observations corresponding to the FTs of each segment, i.e. $X_{m_n}(f)$ and $Y_{m_n}(f)$ for $n = 1, \ldots, N$. In order to visualise these estimators we shall temporarily consider that $X_{m_n}(f)$ and $Y_{m_n}(f)$ are real valued. Fig. 2 shows a set of measured points and various error measures that can be adopted.

If one minimises the sum of the squared vertical errors (e_y) between the fitted line and the data points then the estimator $H_1(f)$ is obtained, whereas if the sum of the squared horizontal errors (e_x) is the quantity to be minimised then the estimator $H_2(f)$ results. Whereas if it is the sum of the perpendicular errors (e_t) that is minimised then the TLS estimator $H_v(f)$ is realised. These interpretations are powerful intuitive tools allowing one to readily identify the merits of the algorithms. The drawback of such an interpretation is that it adds little to the mathematic underpinning.

3.2. Principal component approach for estimating transfer characteristics

It has already been shown in the previous section that the above FRF estimators can be derived from a geometric standpoint, relying upon the fact that in the frequency domain the problem of estimating a transfer function is a linear regression problem [2]. In this section we seek to demonstrate how PCA can be employed to obtain a FRF estimate.

The derivation of principal components for such processes can be derived as follows: from a measurement vector $\boldsymbol{\theta}_n(f)$ containing the input and output data

$$\boldsymbol{\theta}_n(f) = \begin{bmatrix} X_{m_n}(f) \\ Y_{m_n}(f) \end{bmatrix}_{n=1,\ldots,N}. \tag{9}$$

The covariance matrix $\mathbf{R}(f)$ is defined as

$$\mathbf{R}(f) = E[\boldsymbol{\theta}_n(f)\boldsymbol{\theta}_n(f)^{\mathrm{H}}] = \mathbf{Q}^{\mathrm{H}}\boldsymbol{\Lambda}\mathbf{Q}, \tag{10}$$

where $\boldsymbol{\Lambda}$ is a diagonal matrix containing the ranked eigenvalues of $\mathbf{R}(f)$ and the orthonormal transformation matrix $\mathbf{Q}$ is the matrix containing the corresponding eigenvectors as its columns and $^{\mathrm{H}}$ denotes the conjugate transpose (Hermition). The principle components $\mathbf{z}_n$ of the data $\boldsymbol{\theta}_n(f)$ are defined through a transformation matrix $\mathbf{T}$ as

$$\mathbf{z}_n = \mathbf{T}\boldsymbol{\theta}_n(f) = \mathbf{Q}^{\mathrm{H}}\boldsymbol{\theta}_n(f). \tag{11}$$

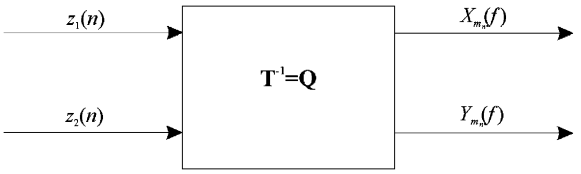

Fig. 3. Virtual two-input-two-output system representing the inverse transformation from principal components to the measured variables.

If PCA is carried out on noise-free input output data then in addition to the actual SISO process involving $X_{m_n}(f)$ and $Y_{m_n}(f)$ (as shown in Fig. 1) one can also consider representing the system by a virtual two-input-two-output (TITO) process, depicted in Fig. 3. In this virtual system, the principal components $z_1(n)$ and $z_2(n)$ are inputs and the original signals $X_{m_n}(f)$ and $Y_{m_n}(f)$ are the outputs. PCA solves the inverse problem by finding the transformation that maps the two correlated variables into two uncorrelated variables.

If the system is linear, so that $Y_{m_n}(f) = \beta X_{m_n}(f)$, then only one distinct eigenvalue exists whose value is equal to the sum of the powers of the inputs. The ratio of the two values in the associated eigenvector determines the scale factor β.

To estimate a transfer function, this procedure is applied frequency bin by frequency bin. The spectral correlation matrix is estimated using

$$\hat{\mathbf{R}}(f) = \begin{bmatrix} \hat{S}_{x_m x_m}(f) & \hat{S}_{y_m x_m}(f) \\ \hat{S}_{x_m y_m}(f) & \hat{S}_{y_m y_m}(f) \end{bmatrix}. \tag{12}$$

The eigenvalues and the eigenvectors of the above given matrix can be computed leading to

$$\lambda_{1,2} = \frac{\hat{S}_{x_m x_m}(f) + \hat{S}_{y_m y_m}(f) \pm \sqrt{(\hat{S}_{x_m x_m}(f) - \hat{S}_{y_m y_m}(f))^2 + 4|\hat{S}_{x_m y_m}(f)|^2}}{2}, \tag{13}$$

$$\left\{\frac{t_{1,k}}{t_{2,k}}\right\}_{k=1,2} = \frac{\hat{S}_{y_m y_m}(f) - \hat{S}_{x_m x_m}(f) \pm \sqrt{(\hat{S}_{x_m x_m}(f) - \hat{S}_{y_m y_m}(f))^2 + 4|\hat{S}_{x_m y_m}(f)|^2}}{2\hat{S}_{y_m x_m}(f)}, \tag{14}$$

where $\{t_{i,j}\}$ are the elements of the transformation matrix $\mathbf{T}$. The eigenvector associated with the largest eigenvalues corresponds to the addition case in Eq. (14) and it is this ratio that represents an estimate of the transfer function, $H_{\mathrm{PCA}}(f)$.

$$H_{\mathrm{PCA}}(f) = \frac{\hat{S}_{y_m y_m}(f) - \hat{S}_{x_m x_m}(f) + \sqrt{(\hat{S}_{x_m x_m}(f) - \hat{S}_{y_m y_m}(f))^2 + 4|\hat{S}_{x_m y_m}(f)|^2}}{2\hat{S}_{y_m x_m}(f)}. \tag{15}$$

Evidently this estimator is exactly that associated with the TLS solution, namely $H_v(f)$, see Eq. (6) with $s = 1$. This is not a surprising result since the TLS solution can be obtained from an eigen-decomposition of the spectral correlation matrix [4], which is exactly the same mechanism used to compute the PCA estimate. The interesting observation is the novel viewpoint that this result provides.

4. Statistical interpretation of transfer function estimation

In this section we shall approach the problem depicted in Fig. 1 from another perspective, namely as a problem of statistical inference. For the purposes of the initial discussion we shall assume that the spectra of the noise processes $S_{n_x n_x}(f)$ and $S_{n_y n_y}(f)$ are known. In which case the problem of estimating the transfer function from input–output data involves only two unknown variables: the FRF $H(f)$ and the input spectrum $S_{xx}(f)$ (note the output spectrum $S_{yy}(f)$ can be inferred from the knowledge of $H(f)$ and $S_{xx}(f)$). It is assumed that all the signals are Gaussian and that $X(f)$, $N_x(f)$ and $N_y(f)$ are mutually uncorrelated. The assumption of Gaussianity is not very restrictive, since even if the time series $x(t)$ is non-Gaussian, then the act of taking a Fourier transform involves linear combinations of the data, which, by virtue of the Central Limit Theorem, tends to make the Fourier coefficients close to Gaussian [9].

The methodology adopted is that of an ML estimator; the primary reason for this is that ML estimators are guaranteed to be unbiased and asymptotically efficient [10,11]. Therefore, for large data sets one can be confident that the ML estimator approximately satisfies the Cramer–Rao lower bound (CRLB) ensuring that, asymptotically, no unbiased estimator will achieve a better performance than an ML estimator.

In our probabilistic framework the data vector is represented as a bivariate complex Gaussian whose probability density function is

$$\Pr\{\boldsymbol{\theta}_n(f)\} = \frac{1}{\pi|\mathbf{R}(f)|} \cdot \mathrm{e}^{-\boldsymbol{\theta}_n(f)^{\mathrm{H}}\mathbf{R}(f)^{-1}\boldsymbol{\theta}_n(f)}. \tag{16}$$

The spectral correlation matrix can be expressed in terms of the two unknowns as

$$\mathbf{R}(f) = \begin{bmatrix} S_{xx}(f) + S_{n_x n_x}(f) & H(f)^* S_{xx}(f) \\ H(f) S_{xx}(f) & |H(f)|^2 S_{xx}(f) + S_{n_y n_y}(f) \end{bmatrix}. \tag{17}$$

If one has a set of N measurement vectors, denoted by $\boldsymbol{\Theta}_n(f)$, and assuming the individual measurement vectors to be uncorrelated then the pdf of $\boldsymbol{\Theta}_n(f)$ is given by

$$\Pr\{\boldsymbol{\Theta}_n(f)\} = \frac{1}{\pi^N|\mathbf{R}(f)|^N} \cdot \mathrm{e}^{-\sum_{n=1}^{N} \boldsymbol{\theta}_n(f)^{\mathrm{H}}\mathbf{R}(f)^{-1}\boldsymbol{\theta}_n(f)}. \tag{18}$$

The ML of the probability density function $\Pr\{\boldsymbol{\Theta}_n(f)\}$ is regarded as a function of the unknown parameters and is maximised with respect to those unknowns. Since the logarithmic function is monotonic then one can equivalently maximise $L = \log\{\Pr\{\boldsymbol{\Theta}_n(f)\}\}$. Therefore the problem is to solve the following equations to obtain the two unknown parameters:

$$\frac{\partial L}{\partial H(f)} = 0 \quad \text{and} \quad \frac{\partial L}{\partial S_{xx}(f)} = 0. \tag{19}$$

Taking logarithms of Eq. (18) leads to the log likelihood function L being written as

$$L = -N\,\log(\pi) - N\,\log(|\mathbf{R}(f)|) - \frac{1}{|\mathbf{R}(f)|} \cdot \sum_{n=1}^{N} \boldsymbol{\theta}_n(f)^{\mathrm{H}}\tilde{\mathbf{R}}\boldsymbol{\theta}_n(f), \tag{20}$$

where $\tilde{\mathbf{R}}$ is the adjoint of $\mathbf{R}(f)$. The derivative of this function with respect to an arbitrary parameter, denoted here as α, can be written as

$$\frac{\partial L}{\partial \alpha} = \frac{1}{|\mathbf{R}(f)|^2} \frac{\partial |\mathbf{R}(f)|}{\partial \alpha} \left\{ \sum_{n=1}^{N} \boldsymbol{\theta}_n(f)^{\mathrm{H}} \tilde{\mathbf{R}} \boldsymbol{\theta}_n(f) - N|\mathbf{R}(f)| \right\} - \frac{1}{|\mathbf{R}(f)|} \sum_{n=1}^{N} \boldsymbol{\theta}_n(f)^{\mathrm{H}} \frac{\partial \tilde{\mathbf{R}}}{\partial \alpha} \boldsymbol{\theta}_n(f). \quad (21)$$

The ML estimate of α is given by the value that renders this derivative zero, implying that

$$\left(\frac{\partial |\mathbf{R}(f)|}{\partial \alpha} \right)^{-1} \sum_{n=1}^{N} \boldsymbol{\theta}_n(f)^{\mathrm{H}} \frac{\partial \tilde{\mathbf{R}}}{\partial \alpha} \boldsymbol{\theta}_n(f) = \sum_{n=1}^{N} \boldsymbol{\theta}_n(f)^{\mathrm{H}} \mathbf{R}(f)^{-1} \boldsymbol{\theta}_n(f) - N. \quad (22)$$

In this problem where there are a pair of unknown parameters one needs to solve a pair of equations of the form (22). These two equations have identical right-hand sides so the following equation must be satisfied:

$$\frac{\partial |\mathbf{R}(f)|}{\partial S_{xx}(f)} \sum_{n=1}^{N} \boldsymbol{\theta}_n(f)^{\mathrm{H}} \frac{\partial \tilde{\mathbf{R}}}{\partial H(f)} \boldsymbol{\theta}_n(f) = \frac{\partial |\mathbf{R}(f)|}{\partial H(f)} \sum_{n=1}^{N} \boldsymbol{\theta}_n(f)^{\mathrm{H}} \frac{\partial \tilde{\mathbf{R}}}{\partial S_{xx}(f)} \boldsymbol{\theta}_n(f). \quad (23)$$

After some algebra this equation reduces to

$$H(f)^2 \hat{S}_{y_m x_m}(f) + H(f)\{\hat{S}_{x_m x_m}(f)\kappa(f) - \hat{S}_{y_m y_m}(f)\} - \hat{S}_{x_m y_m}(f)\kappa(f) = 0 \quad (24)$$

in which $\kappa(f)$ represents the ratio $S_{n_y n_y}(f)/S_{n_x n_x}(f)$. The solutions of this quadratic equation are

$$H(f) = \frac{\hat{S}_{y_m y_m}(f) - \kappa(f)\hat{S}_{x_m x_m}(f) \pm \sqrt{\{\hat{S}_{x_m x_m}(f)\kappa(f) - \hat{S}_{y_m y_m}(f)\}^2 + 4|\hat{S}_{x_m y_m}(f)|^2 \kappa(f)}}{2\hat{S}_{y_m x_m}(f)}. \quad (25)$$

In order to address the question of which sign to take in Eq. (25) one need only consider the limiting cases for $\kappa(f)$. The choice of the positive sign corresponds to the TLS solution and represents the solution where L is maximised whereas the negative sign indicates a worst case solution, i.e. minimum likelihood solution. This indicates that the ML estimator is equivalent to the $H_s(f)$ estimator with the parameter s equal to $\kappa(f)$.

Note that whilst the problem was originally defined obtaining estimates for two unknowns, $H(f)$ and $S_{xx}(f)$, in fact these two elements decouple, so that the problem of estimating the true FRF does not require one to estimate the true input spectrum. Such a decoupling is extremely useful but could not be readily justified prior to the above analysis. The noise spectra, knowledge of which has been assumed throughout this derivation, only enter the solution through the parameter $\kappa(f)$. Thus it is necessary to know the ratio of the noise spectra in order to select appropriate value of the parameter s, but it is not necessary to estimate the absolute levels of the noises.

4.1. Asymptotic performance

The observation that the FRF estimators based on TLS and PCA are equivalent to ML solutions of appropriate problems is not only of academic interest. The wealth of available knowledge pertaining to ML estimators also applies to the TLS and PCA estimators in this case.

More specifically, it is well known that ML estimators are [10]

(i) Unbiased.
(ii) Asymptotically efficient, that is to say that for large N the ML estimators achieve the CRLB.
(iii) Are distributed according to Gaussian statistics.

Combining these properties one can conclude that the error associated with the ML estimators are approximately distributed as $N(0,\sigma^2)$, where σ^2 is the CRLB. This observation will be exploited to allow one to define the confidence intervals for the ML estimator.

There remains the issue of computing the CRLB. Since estimation of $H(f)$ and $S_{xx}(f)$ decouple then one is essentially dealing with a single (complex valued) parameter estimation problem. Furthermore, rather than treating the problem as one of estimating a single complex parameter, $H(f)$, we can consider it as a problem in two real valued parameters, namely $H_R(f) = \mathrm{Re}\{H(f)\}$ and $H_I(f) = \mathrm{Im}\{H(f)\}$.

It is well known that the CRLBs for multi-parameter problems are given by the diagonal elements of the $\mathbf{J}^{-1}$, where $\mathbf{J}$ is the Fisher information matrix defined by

$$J_{p,q} = E\left[-\frac{\partial^2 L}{\partial\alpha_p\partial\alpha_q}\right] = E\left[\frac{\partial L}{\partial\alpha_p}\frac{\partial L}{\partial\alpha_q}\right], \tag{26}$$

where α_p and α_q are the parameters being estimated. For Gaussian problems, like the one we consider, it can be shown that [12]

$$J_{p,q} = E\left[\frac{\partial L}{\partial\alpha_p}\frac{\partial L}{\partial\alpha_q}\right] = N\,\mathrm{Tr}\left\{\mathbf{R}(f)^{-1}\frac{\partial\mathbf{R}(f)}{\partial\alpha_p}\mathbf{R}(f)^{-1}\frac{\partial\mathbf{R}(f)}{\partial\alpha_q}\right\} \quad (p,q)\in(1,2), \tag{27}$$

where $\alpha_1 = H_R(f)$ and $\alpha_2 = H_I(f)$. From the definition spectral correlation matrix it is simple to show that

$$\frac{\partial\mathbf{R}(f)}{\partial H_R(f)} = S_{xx}(f)\begin{bmatrix}0 & 1\\ 1 & 2H_R(f)\end{bmatrix}, \tag{28a}$$

$$\frac{\partial\mathbf{R}(f)}{\partial H_I(f)} = S_{xx}(f)\begin{bmatrix}0 & -i\\ i & 2H_I(f)\end{bmatrix}. \tag{28b}$$

Substituting these expressions into Eq. (27) and after some algebra one can show that

$$\mathbf{J} = \frac{2NS_{xx}(f)^2}{|\mathbf{R}(f)|^2}\{|\mathbf{R}(f)|I + 2S_{n_xn_x}(f)^2\,\underline{H}\,\underline{H}^t\}, \tag{29}$$

$$|\mathbf{R}(f)| = S_{xx}(f)S_{n_yn_y}(f) + S_{n_xn_x}(f)S_{n_yn_y}(f) + S_{n_xn_x}S_{yy}(f) \tag{30}$$

in which $\underline{H} = [H_R(f)H_I(f)]^t$ and CRLBs can be evaluated, with the aid of the matrix inversion lemma (Woodbury's Identity) [13], one can show that

$$\mathrm{CRLB}\{H_R(f)\} = \frac{|\mathbf{R}(f)|}{NS_{xx}(f)^2}\left(1 - \frac{S_{n_xn_x}(f)^2H_R(f)^2}{2S_{n_xn_x}(f)^2|H(f)|^2 + |\mathbf{R}(f)|}\right), \tag{31a}$$

$$\mathrm{CRLB}\{H_I(f)\} = \frac{|\mathbf{R}(f)|}{NS_{xx}(f)^2}\left(1 - \frac{S_{n_xn_x}(f)^2 H_I(f)^2}{2S_{n_xn_x}(f)^2|H(f)|^2 + |\mathbf{R}(f)|}\right). \tag{31b}$$

For large signal-to-noise ratios (SNRs), i.e. $S_{xx}(f), S_{yy}(f) \gg S_{n_xn_x}(f), S_{n_yn_y}(f)$; Eqs. (31a,b) can be significantly simplified by neglecting quadratic terms in the noise spectra, so that

$$|\mathbf{R}(f)| \approx S_{xx}(f)S_{n_yn_y}(f) + S_{yy}(f)S_{n_xn_x}(f) \gg 2S_{n_xn_x}(f)^2|H(f)|^2 \tag{32}$$

in which case the CRLBs become

$$\mathrm{CRLB}\{H_R(f)\} = \mathrm{CRLB}\{H_I(f)\} \approx \frac{|H(f)|^2}{N}\left\{\frac{S_{n_yn_y}(f)}{S_{yy}(f)} + \frac{S_{n_xn_x}(f)}{S_{xx}(f)}\right\}. \tag{33}$$

Therefore, the approximate CRLBs are proportional to the sum of the inverse SNRs on the input and the output. It should also be noted that the $1/N$ factor in Eq. (33) indicates that the ML estimator is consistent. The assumption invoked in approximating Eq. (32) by Eq. (33) also imposes the independence of $H_R(f)$ and $H_I(f)$. By virtue of property (iii) of the ML estimators then the random variable

$$\frac{N|H_s(f)|^2}{|H(f)|^2\{(S_{n_yn_y}(f)/S_{yy}(f)) + (S_{n_xn_x}(f)/S_{xx}(f))\}} = \frac{N\{H_R(f)^2 + H_I(f)^2\}}{|H(f)|^2\{(S_{n_yn_y}(f)/S_{yy}(f)) + (S_{n_xn_x}(f)/S_{xx}(f))\}} \tag{34}$$

is a Chi-squared random variable with 2 dof and hence

$$\mathrm{Var}\{|H_s(f)|^2\} = \frac{4|H(f)|^4}{N}\left\{\frac{S_{n_yn_y}(f)}{S_{yy}(f)} + \frac{S_{n_xn_x}(f)}{S_{xx}(f)}\right\}^2. \tag{35}$$

This allows one to write the confidence interval for the squared magnitude of $H_s(f)$ as

$$|H_s(f)|^2\left[1 \pm \log(\beta)\frac{4}{N}\left\{\frac{S_{n_yn_y}(f)}{S_{yy}(f)} + \frac{S_{n_xn_x}(f)}{S_{xx}(f)}\right\}^2\right], \tag{36}$$

where the fact that the 100β percentile of a Chi-squared distribution, with 2 dof, is given by $\log(\beta)$ has been exploited. The equivalence between Eqs. (36) and (4) can be shown by assuming large N (so that $N - 2 \approx N$) and noting that for the case of output noise only then $S_{n_xn_x}(f) = 1 - \gamma^2_{x_my_m}(f)$.

In order that Eq. (36) can be used in practice one needs to first estimate the input power spectrum $S_{xx}(f)$, from which $S_{yy}(f)$ can simply be obtained. This could be approached in various ad hoc fashions, herein we retain the philosophy of ML and solve Eq. (21), with $\alpha = S_{xx}(f)$, and replacing $H(f)$ by its ML estimate (25). Again after some algebra one can obtain the optimal estimator of $S_{xx}(f)$ as

$$S_{xx}(f) = \frac{S_{x_mx_m}(f)\kappa(f) + S_{y_my_m}(f)}{\kappa(f) + |H_s(f)|^2}. \tag{37}$$

This estimate of the input spectrum only depends upon the ratio $\kappa(f)$ and not on the absolute levels of the noise spectra.

By using Eqs. (36) and (37) in conjunction one can obtain confidence intervals for the squared magnitude of the transfer function estimator $H_s(f)$. Notice how, whilst the estimators of $H(f)$ and $S_{xx}(f)$, Eqs. (25) and (37), respectively, only require the knowledge of the ratio of the noise spectra, in order to compute the confidence intervals one requires the absolute levels of the noise spectra, i.e. values for $S_{n_x n_x}(f)$ and $S_{n_y n_y}(f)$.

5. Results

A series of simulation studies has been undertaken to validate the results of the theoretical analyses presented. These simulations have all been based on estimating the FRF of a simple digital system containing two pole and two zeros. In particular the poles and zeros were all located at a radius of 0.95, with the poles being located at angle of $\pm\pi/4$ and zeros at $\pm 3\pi/4$. The system was excited by Gaussian white noise (with unit variance) and the simulated input and output measurements were corrupted using independent, additive Gaussian noise. In each trial 1000 realisations of the processes were constructed, with the FRFs being estimated using various methods and the means and variances being computed across these realisations. Each realisation consisted of 1 million samples and the spectra were estimated using segment averaging based on FFTs of 256 samples and employing a Hanning window. This regime allowed us to compute the mean and variances of the FRF estimators with a high degree of confidence.

Fig. 4 illustrates the mean of the three FRF estimators: $H_1(f)$, $H_2(f)$ and $H_v(f)$. The measurement noises were unit variance, white and Gaussian. The estimator $H_1(f)$ yields a biased estimator of the true FRF. Since the input SNR is constant the bias in $H_1(f)$ is a constant multiplicative factor, which appears as a constant offset on a decibel scale. The behaviour of the $H_2(f)$ estimator is more complex because the SNR of the output measurement varies as a function of frequency, due to shaping effects of the system. Consequently when the output signal level is low, e.g. at frequencies near the zeros (like the anti-resonance in the high-frequency region of our example FRF), the SNR is correspondingly low and the bias is large. Conversely where the output signal's amplitude is large, e.g. at frequencies near the poles (like the resonance in the low-frequency region of the example FRF), the SNR is large and the bias is small. In this case the estimator $H_v(f)$ yields an (almost) unbiased estimate of the FRF. Note $H_v(f)$ corresponds $H_s(f)$

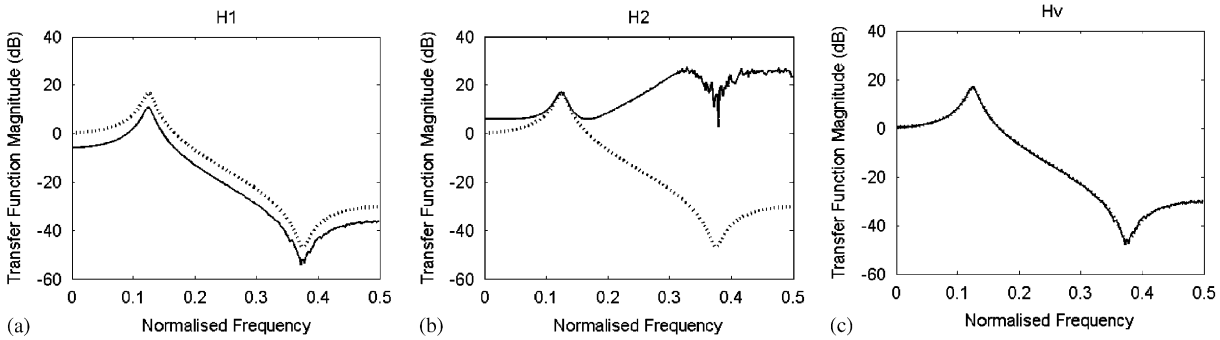

Fig. 4. Mean of the FRF estimators: computed using white measurement noise. (a) Estimator $H_1(f)$, (b) estimator $H_2(f)$ and (c) estimator $H_v(f)$—theoretical FRF shown as a dotted line, estimator shown as the solid line.

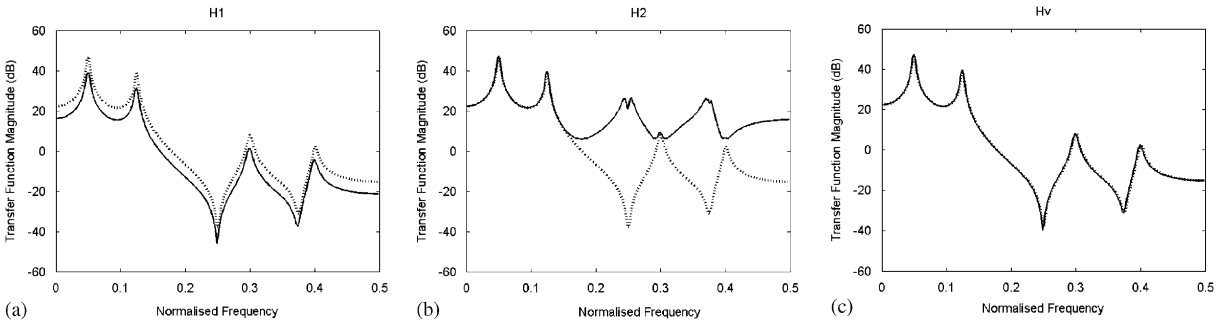

Fig. 5. Mean of the FRF estimators for a system with multiple poles and zeros: computed using white measurement noise. (a) Estimator $H_1(f)$, (b) estimator $H_2(f)$ and (c) estimator $H_v(f)$—theoretical FRF shown as a dotted line, estimator shown as the solid line.

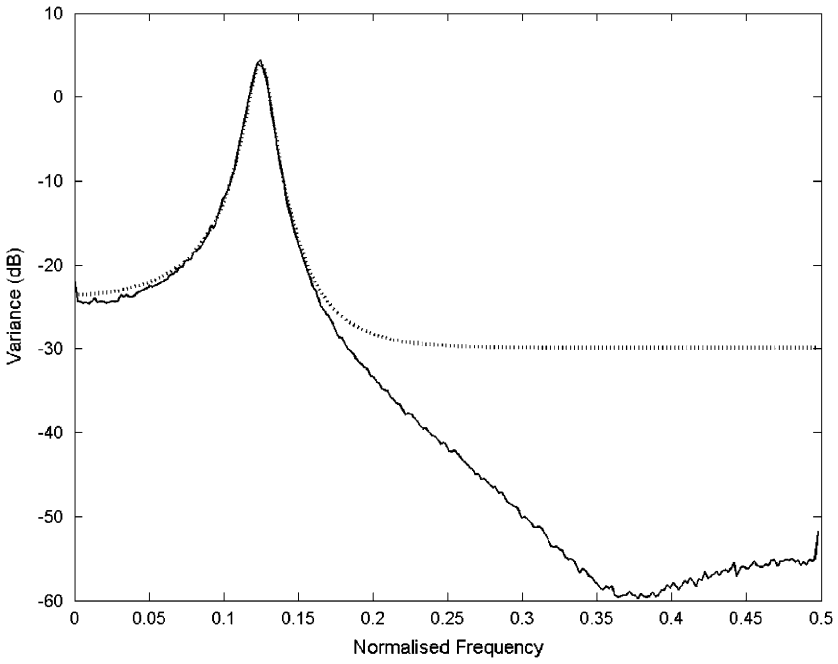

Fig. 6. Variance of ML spectral estimator (solid line—measured variance, dotted line—theoretical prediction of the variance, see Eq. (35)).

with $\kappa(f)$ set to unity, which is the appropriate value for this simulation. The small disparities between the theoretical FRF and mean of the estimator $H_v(f)$ are due to the effect of the window.

Fig. 5 shows a similar set of results this time using a system model that more closely matches systems encountered in realistic measurement scenarios. This model contains of four resonances and two anti-resonances. The observations made with regards to Fig. 4 continue to remain valid in this case.

Fig. 6 depicts the variance of the estimator $H_v(f)$ computed across the 1000 realisations of the processes and as predicted by Eq. (35). The theoretical prediction can be seen to be good in the

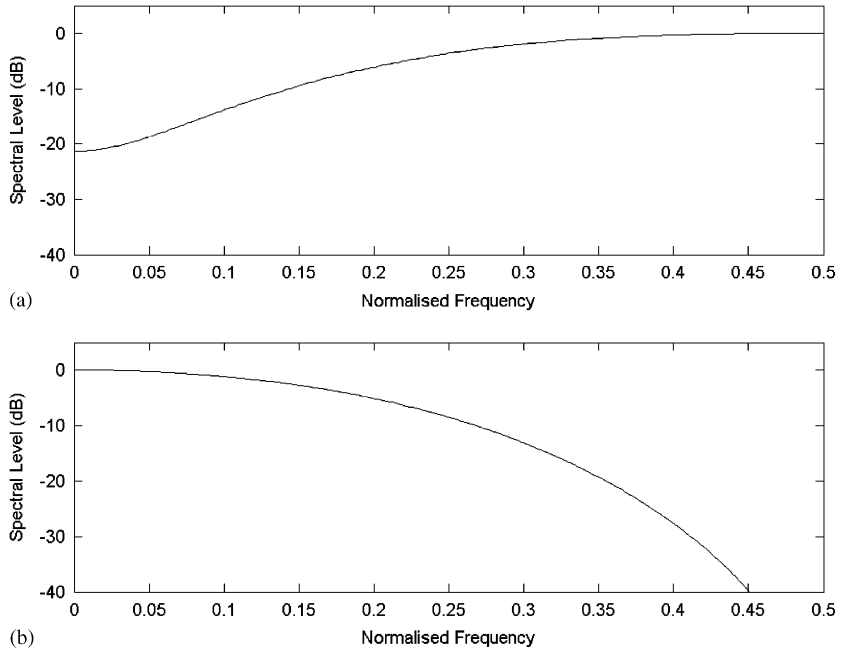

Fig. 7. Measurement noise spectra. (a) Input noise and (b) output noise.

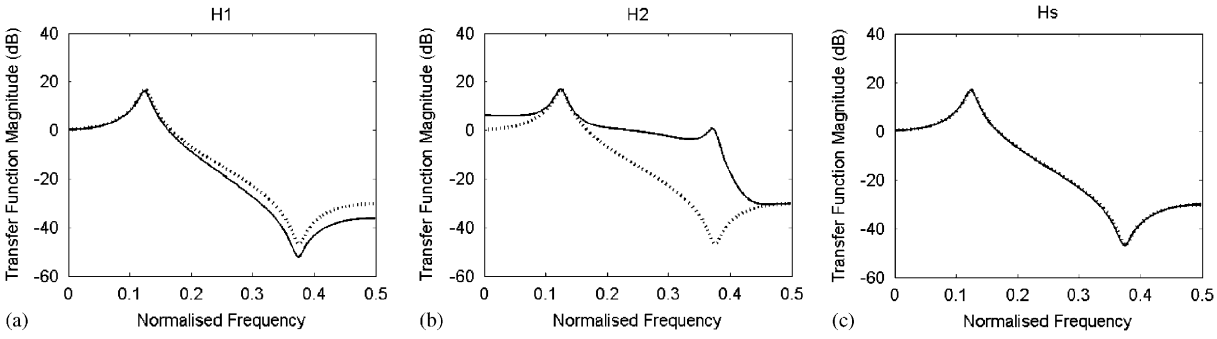

Fig. 8. Means of FRF estimators: computed using coloured measurement noise. (a) Estimator $H_1(f)$, (b) estimator $H_2(f)$ and (c) estimator $H_s(f)$—theoretical FRF shown as a dotted line, estimator shown as the solid line.

region where the SNR is large, but the variance is poorly predicted in the high-frequency region, where the SNR is low. This is a consequence of the approximation (33) used in deriving Eq. (35) becoming invalid. This allows confirms that the variance expression (35) provides a suitable basis for the quality measures, such as confidence intervals (36).

The final simulation study used coloured measurement noises, the colouration being realised by filter with low-order FIR filters. The spectra of the two noise processes are shown in Fig. 7. Fig. 8 illustrates the behaviour of the three FRF estimators $H_1(f)$, $H_2(f)$ and $H_s(f)$. In this case it is necessary to use the estimator $H_s(f)$ since $\kappa(f) \neq 1$. The general behaviour of $H_1(f)$ and $H_2(f)$

remains consistent, so that $H_1(f)$ has a large bias when the input SNR is low and $H_2(f)$ has a large bias when the output SNR is low. Clearly the estimator $H_s(f)$ remains very nearly unbiased. Once again small deviations from the theoretical predictions are due to the finite window size.

6. Summary

This paper has considered the problem of FRF estimation from two different standpoints. It has shown the principle of PCA can be applied to the problem of FRF estimation and the resulting algorithm corresponds to the TLS FRF estimator $H_v(f)$. The second approach to FRF estimation that has been considered is that of statistical inference. The principle of ML has been applied to derive optimal estimators for the FRF. The resulting algorithm corresponds to the established $H_s(f)$ FRF estimator, with the parameter s equated to the ratio of the measurement noise spectra. This estimator is unbiased in the presences of both input and output noise. In addition by exploiting the general properties of ML estimators an expression for the variance of the $H_s(f)$ estimator has been derived. The assertions made in this paper have been validated via a series of simulation studies.

References

[1] J.S. Bendat, A.G. Persol, *Random Data Analysis and Measurement Procedures*, Wiley, New York, 1986.
[2] G.M. Jenkins, D.G. Watts, *Spectral Analysis and its Applications*, Holden-Day, San Francisco, CA, 1968.
[3] A.L. Wicks, H. Vold, The H_s frequency response function estimator, *Proceedings of the Fourth International Modal Analysis Conference (IMAC)*, 1986, pp. 897–899.
[4] G.H. Golub, C.F. Van Loan, An analysis of the total least squares problem, *SIAM Journal of Numerical Analysis* 17 (6) (1980) 883–893.
[5] H. Vold, J.R. Crowley, G.T. Rocklin, New ways of estimating frequency response functions, *Sound and Vibration* 18 (11) (1984) 34–38.
[6] R.J. Allemang, D.L. Brown, Experimental modal analysis, in: C.M. Harris (Ed.), *Shock and Vibration Handbook*, fourth ed., McGraw-Hill, New York, 1996.
[7] J. Leuridan, D. De Vis, A comparison of some frequency response function measurement techniques, *Proceedings of the Fourth International Modal Analysis Conference (IMAC)*, 1986, pp. 908–918.
[8] G.T. Rocklin, J.R. Crowley, H. Vold, Comparison of H_1, H_2 and H_v frequency response functions, *Proceedings of the Third International Modal Analysis Conference (IMAC)*, 1985, pp. 272–278.
[9] D. Brillinger, M. Rossenblatt, Asymptotic theory of kth-order spectra, in: B. Harris (Ed.), *Spectral Analysis of Time Series*, Wiley, New York, 1967, pp. 153–188.
[10] H.L. Van Trees, *Detection, Estimation, and Modulation Theory: Part 1*, Wiley, New York, NY, 1968.
[11] S.M. Kay, *Modern Spectral Estimation: Theory and Application*, Prentice-Hall, Englewood Cliffs, NJ, 1988.
[12] R.O. Schmidt, *A Signal Subspace Approach to Multiple Emitter Location and Spectral Estimation*, PhD Thesis, Stanford University, 1992.
[13] S. Haykin, *Adaptive Filter Theory*, third ed., Prentice-Hall, Englewood Cliffs, NJ, 1996.