Ocean Engng, Vol. 19, No 6, pp. 511–526, 1992.
Printed in Great Britain.

0029–8018/92 $5.00 + .00
Pergamon Press Ltd

THE EIGENVALUE PROBLEM AS A FORM OF MINIMUM LEAST-SQUARED APPROXIMATION

R. TATAVARTI* and Y. ANDRADE†
Department of Oceanography, Dalhousie University, Halifax, B3H 4J1 Canada

Abstract—Two important tools used in the interpretation of ocean engineering data are the Minimum Least-Squared approximation technique (MLS) and the spectral analysis technique. Often, the inherent assumptions in these analytical techniques are overlooked by users which may, at times, bias the picture of the physics that remains to be understood. The present study focuses on a modified version of the MLS technique and the Empirical Orthogonal Function (EOF) analysis which have many advantages compared to the more commonly used techniques. It is shown that the eigen-decomposition technique of EOF analysis and a variation of the Minimum Least-Squared Approximation, known as the MLS2 technique, are the same, as has been documented in the literature. Unlike the MLS approximation, the MLS2 approximation or the EOF analysis does not depend on which variable is called "independent" or which "dependent", as both the variables are treated symmetrically. Field data collected during the C^2S^2 program from Pointe-Sapin beach, New Brunswick, Canada, were used in a simple example to demonstrate the advantages of employing complex EOF analysis.

INTRODUCTION

THE INCREASING number of satellite observations and the development of more and more sophisticated data acquisition systems are forcing ocean scientists and engineers to develop and apply methods of analysis which can extract maximum information from the observed data without jeopardizing the accuracy. In recent years ocean engineers are extensively using the least-squares approximation and spectral analysis techniques as analytical tools to describe data from the oceanic environment and discuss the relationships between different oceanic parameters.

The method most commonly used when seeking a linear model between two variables is the standard Minimum Least-Squared approximation (MLS), also known as linear regression. This method has an underlying assumption that the variable chosen as independent is assumed to be noiseless. This assumption is frequently overlooked by users. While, in spectral analysis, the time series of one parameter is designated as a base series and the coherence and phase computed between this series and those of other parameters. The underlying assumption that the base series is free of noise obviously produces a bias in favour of the base series. If the coherence between various parameters and the base series is not large the bias can result in considerable distortion in the pattern of amplitudes of the parameters. Moreover, this does not exploit the information contained in the cross-spectra between parameters other than the base

* Present address: Naval Physical and Oceanographic Laboratory, Thrikkakara, Kochi 682 021, India.
† Present address: Instituto de Fomento Pesquero (IFOP), Oceanography Department, Blanco 1067, Valparaiso, Chile.

series. Also, when different waves (modal shapes) are present in the same frequency band, there is considerable difficulty in interpreting the cross-spectrum data as there is no way of determining how many wave structures are present and what is the relative contribution of each wave type to the variance spectra. Thus there is a need for an analysis technique that takes into account the uncertainty in both variables that are being compared. One such technique, which involves the eigen modal decomposition of the covariance matrix, is known as the *Empirical Orthogonal Function* analysis (EOF).

Over the past few decades empirical orthogonal functions have been examined by many scientists from different disciplines, each viewing the concept from his or her own perspective, developing a tool to form a picture of some portion of physical reality. To the mathematician the concept provided a simple way to represent one matrix as another of lower rank. Empirical orthogonal function (EOF) analysis as conventionally applied to oceanographic data is used to decompose spatial and temporally distributed data into modes ranked by their temporal variances. In addition EOF analysis allows the partitioning of huge data sets into signal-like and noise-like parts. The following discussion dwells on the latter properties of the EOF analysis, providing an outline of the rationale for the desired partition and demonstrates with some examples as to how this may be accomplished.

EOF analysis is also known as the Principal Component analysis. This technique originated with Pearson (1901) as a means of fitting planes by orthogonal least-squares, but was later proposed by Hotelling (1933, 1936) for the particular purpose of analysing correlation structures. Since then this technique (and its variations) has (have) been used with success in Archaeology, Biology, Criminology, Dentistry, Economics, Forestry, Geology, etc., and has now become a common procedure in Meteorological and Oceanographic data analysis [for example, see Weare (1979); Aubrey (1980); Weare and Nasstrom (1982); Barnett (1983); Horel (1984); Marsden and Juszko (1987); and more recently Liang and Seymour (1991)]. There are a number of reasons for this popularity. Probably the most important is that this method often enables a description of the variations of a complex geophysical field with a relatively small number of functions and associated time coefficients. This property is especially important in the development of statistical prediction schemes, which rely upon multiple linear regression, where the skill and statistical confidence of prediction depend heavily upon *a priori* methods of reducing the number of available predictors (Davis, 1976; Barnett and Hasselmann, 1979; Marsden and Juszko, 1987). Secondly, the popularity of EOF analysis is due to the fact that the derived empirical functions are often amenable to physical interpretation which may give substantial insight into complex processes such as oceanographic variations (Weare *et al.*, 1976; Aubrey, 1980) or short time climatic changes (Weare, 1979; Servain and Legler, 1986).

The motivation for the present study stems from the need to find an accurate estimator for the spectral gain and phase between two synoptic collocated measurements of wave parameters (wave elevation, η, and current velocity, u), in order to determine the frequency dependent reflection coefficients $R(\omega)$ of natural beaches (Tatavarti *et al.*, 1988). The key to this method of determining $R(\omega)$ was to find an estimator for the spectral gain, which is insensitive to noise in both η and u measurements (Tatavarti, 1989). Hence this study.

The primary objective of this paper is to focus the reader's attention on EOF analysis and its various advantages compared to the more commonly used techniques. Although we do advocate the use of EOF analysis technique as opposed to the least-squared approximation technique, we certainly do not claim that EOF analysis is the panacea for all analytical problems.

EMPIRICAL ORTHOGONAL FUNCTION ANALYSIS

The fundamental theorem of the empirical orthogonal function analysis or the principal component analysis may be stated as follows:

Given a set of variables $u_1, u_2, \ldots, u_p$ with a non-singular variance–covariance matrix $\mathbf{\Sigma}$, it is possible to derive a set of uncorrelated variables $z_1, z_2, \ldots, z_p$ by a set of linear transformations corresponding to the principal axes rotation, that is, the rigid rotation whose transformation matrix $\mathbf{E}$ has as its columns the p eigen vectors of $\mathbf{\Sigma}$. The covariance matrix of this new set of variables is the diagonal matrix $\mathbf{Z} = \mathbf{E}'\mathbf{\Sigma}\ \mathbf{E}$ whose diagonal elements are the p eigenvalues of $\mathbf{\Sigma}$. Note that the prime denotes the transpose of the matrix.

The method of EOF analysis involves an orthogonal transformation wherein each p original variable is described in terms of the p new principal components or modes. An important feature of the new components (modes) is that they account, in turn, for a maximum amount of variance of the variables. More specifically, the first principal component (mode) is that linear combination of the original variables which contributes a maximum to their total variance, the second mode uncorrelated to the first, contributes a maximum to the residual variance, and so on until the total variance is analysed. The sum of all p modes (principal components) is equal to the sum of the variances of the original variables. *In other words, considering only the first EOF we would be looking at the coherent structure of the system.* Therefore, use of the complex empirical orthogonal function analysis appears appropriate since parts of the original coherent signals will tend to occur in the principal mode with the noise splitting into the higher modes.

In what follows, we first review the standard Minimum Least-Squared (MLS) approximation, and then a variation of it named MLS2 and the eigen-decomposition are treated. Finally, a comparison between MLS2 and the eigen problem is made, wherein the EOF decomposition corresponds exactly to a simple variation of the standard MLS approximation, that is, MLS2.

THE METHOD OF MINIMUM LEAST-SQUARED APPROXIMATION (MLS)

Let $\{(u_i, \eta_i)\}$ be a set of n paired measurements where for simplicity the means $(\langle u \rangle, \langle \eta \rangle)$ of the original set have been removed. The criterion function for obtaining estimators is based on fitting the errors or residuals $E_i = \eta_i - \hat{\eta}_i$, where $\hat{\eta}_i = Su_i$ is the value on the fitted line at $u = u_i$. The residuals give the vertical distances between the fitted line and the actual η_i values as illustrated in Fig. 1. In order to determine an optimal straight line slope (S) as model for the data set, the MLS approximation minimizes the function formed by the sum of squared errors (E_i). In this case the error is defined as in Fig. 1

$$E_i(S) = \eta_i - Su_i\,. \tag{1}$$

One method of minimizing (1) is to differentiate Equation (1) with respect to S, set

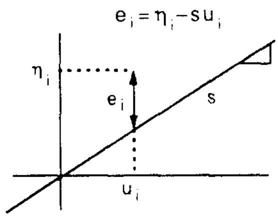

FIG. 1. Error definition for the standard MLS approximation.

the derivative equal to zero, and solve the resulting equation (Weisberg, 1985). That is,

$$\frac{d}{dS}\left\{\sum_{i=1}^{n}[\eta_i - Su_i]^2\right\} = 0 \tag{2}$$

which gives the well-known solution for S

$$S = \frac{\Sigma\, u_i\, \eta_i}{\Sigma\, u_i^2}\,.$$

If we further define a correlation coefficient (ρ) and a variance ratio (σ) as:

$$\rho = \frac{\text{covar}(u, \eta)}{\sigma_u\, \sigma_\eta} \text{ and } \sigma^2 = \frac{\sigma_\eta^2}{\sigma_u^2}$$

where σ_u^2 and σ_η^2 are the variances of u and η, respectively, and covar(u, η) is the covariance between u and η, we can express the slope S of the linear model as:

$$S = \rho\, \sigma\,. \tag{3}$$

A SECOND OPTION FOR THE MLS APPROXIMATION (MLS2)

In the MLS approximation the error is defined as the difference between the η-measurements and its model values. Clearly, one could consider other functions of the data besides vertical errors to derive a criterion for choosing an estimator, but the residuals (the vertical distances between the estimated values and the actual values) are generally believed to be a good choice because they reflect the inherent asymmetry in the roles of the response and the predictor in regression problems. Now we will change the error definition as the minimum distance between the data points (u_i, η_i) to the straight line model. This definition is sketched in Fig. 2.

Following geometrical considerations, the expression for this new error definition (E_i) can be obtained as:

$$E_i = \frac{\eta - Su_i}{\sqrt{1+S^2}}\,. \tag{4}$$

As before, to determine S we resort to the method of minimizing (4). Therefore,

$$\frac{d}{dS}\left\{\sum_{i=1}^{n}\frac{[\eta_i - Su_i]^2}{1+S^2}\right\} = 0\,. \tag{5}$$

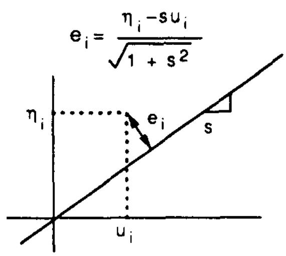

FIG. 2. Error definition for the MLS2 approximation.

Performing the differentiation a quadratic equation on S is obtained which is satisfied by the solutions:

$$S_{1,2} = A \pm \sqrt{1+A^2}, \text{ where } A = \frac{\sigma^2 - 1}{2\rho\sigma}$$

and, ρ and σ are the same as previously defined.

These two solutions are related as $S_1 S_2 = -1$, which in a geometric interpretation means that the two best fitted lines obtained are perpendicular to each other. These two lines are sketched in Fig. 3.

After some algebra, it can be shown that the global minimum depends on the sign of ρ. Therefore the optimal slope of the linear model obtained by the MLS2 approximation is

$$S = A + \frac{\rho}{|\rho|}\sqrt{1+A^2}\,. \tag{6}$$

From Fig. 3, an association between the eigenproblem and the MLS2 appproximation is immediately suspected. In the following it will be proved that the correspondence is indeed exact.

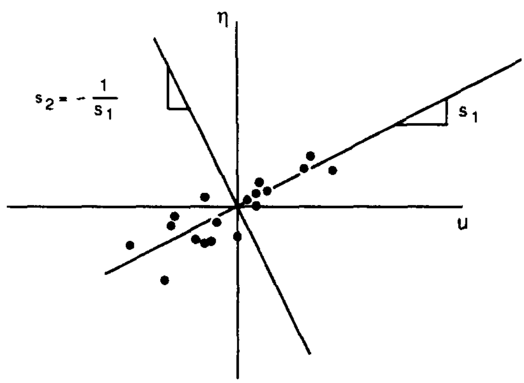

FIG. 3. The two solutions obtained by the MLS2 approximation. S_1 and S_2 correspond exactly to the directions of the eigenvectors obtained by the EOF method.

EMPIRICAL ORTHOGONAL FUNCTIONS OF OBSERVATIONS

Suppose we monitor p variables of interest $\mathbf{u}' = (u_1, u_2, \ldots u_p)$, having a certain multivariate distribution with a mean vector $\mathbf{v}$ and covariance matrix $\mathbf{\Sigma}$.

Expressing a linear combination of the p variables as

$$z_j = \mathbf{e}'\mathbf{u} = \Sigma\, e_{ij} u_i \tag{7}$$

where e_{ij} are the elements of the characteristic vector associated with the characteristic root λ_j of the covariance matrix $\mathbf{\Sigma}$. We ask which $\mathbf{E}$ gives the maximum variance of z. Defining the covariance matrix as

$$\mathbf{\Sigma} = \langle \mathbf{u}\mathbf{u}' \rangle \tag{8}$$

we note from matrix algebra that the variance of z is given by

$$\langle z^2 \rangle = \mathbf{e}'\, \mathbf{\Sigma}\, \mathbf{e}\ . \tag{9}$$

In order to maximize a function of p variables when the variables are connected by an arbitrary number of auxilliary equations, the method of Lagrange Multipliers is well adapted (Anderson, 1984). In general terms this method states that if a function $f(e_{1j}, e_{2j}, \ldots, e_{pj})$ of several variables is to be maximized under the side condition $g\,(e_{1j}, e_{2j}, \ldots, e_{pj}) = 0$, this can be accomplished by constructing a new function

$$F = f(e_{1j}, e_{2j}, \ldots, e_{pj}) - \lambda g\,(e_{1j}, e_{2j}, \ldots, e_{pj}) \tag{10}$$

where λ is a new unknown called the Lagrange Multiplier. Maximizing this new function without any restriction on the variables will produce an index whose scatter would be greater than that of z^2 so we must put some sort of restriction if we are to obtain a sensible answer. Thus we constrain $\mathbf{e}$ by

$$\mathbf{e}'\,\mathbf{e} = 1 \tag{11}$$

now maximizing (9) subject to (11), that is

$$\frac{\partial}{\partial \mathbf{e}}[\mathbf{e}'\,\mathbf{\Sigma}\,\mathbf{e} - \lambda(\mathbf{e}'\mathbf{e} - 1)] = 0 \tag{12}$$

$$\rightarrow 2\,\mathbf{\Sigma}\,\mathbf{e} - 2\lambda\mathbf{e} = 0 \tag{13}$$

that is,

$$\mathbf{\Sigma}\,\mathbf{e} = \lambda\mathbf{e}\ . \tag{14}$$

Thus, the empirical orthogonal functions correspond to the eigenvectors of $\mathbf{\Sigma}$ and the variances of the time series of a given EOF correspond to the eigenvalues. Note that for an eigenvector $\mathbf{e}$

$$\langle z^2 \rangle = \mathbf{e}'\,\mathbf{\Sigma}\,\mathbf{e} = \mathbf{e}'\,(\lambda e) = \lambda\mathbf{e}'\,\mathbf{e} = \lambda \tag{15}$$

that is, λ is the variance of $z_j = \Sigma\, e_{ij} u_j$.

Summarizing, we can say that the first principal component of the complex of the sample values of the responses $u_1, u_2, \ldots, u_p$ is the linear compound

$$z_1 = e_{11}u_1 + \ldots, + e_{p1}u_p \tag{16}$$

whose coefficients e_{i1} are the elements of the characteristic vector associated with the greatest characteristic root λ_1 of the sample covariance matrix of the responses. The e_{i1} are unique up to multiplication by a scale factor, and if they are scaled so that $\mathbf{e}'\mathbf{e} = 1$, the characteristic root is interpretable as the sample variance of $\boldsymbol{\Sigma}$.

But what is the utility of this artificial variate constructed from original responses? In the extreme case, of $\boldsymbol{\Sigma}$ of rank one, the first mode would explain all the variation in the multivariate system. In the more usual case of the data matrix of full rank the importance and the usefulness of the component would be measured by the proportion of the total variance attributable to it. If say 87% of the variation in a system of six responses could be accounted for by a simple weighted average of the response values, it would appear that almost all the variation could be expressed along a single continuum rather than in six-dimensional space. Not only would this appeal to our sense of parsimony but also the coefficients of the six responses would indicate the relative importance of each original variate in the new derived compound.

Having introduced the empirical orthogonal functions analytically as those linear combinations of the responses which explain progressively smaller portions of the total variance, let us now discuss the geometrical interpretation of components as the variates corresponding to the principal axes of the scatter of observations in space. If we can imagine that a sample of p trivariate observations has the scatter plot shown in Fig. 4, where the origin of the response axes has been taken at the sample means, then the swarm of points seems to have a generally ellipsoidal shape, with a major axis z_1 and less well-defined minor axes z_2 and z_3. We can interpret the empirical orthogonal modes of the sample of p trivariate observations as the new variates specified by the axes of a rigid rotation of the original response coordinate system into an orientation corresponding to the directions of maximum variance in the sample scatter configuration. In other words, considering only the first EOF (provided that it explains the largest percentage of the total variance) we would be looking at the improved coherent structure of the system. Hence if the initial responses are a linear superposition of the coherent signal and an incoherent noise then consideration of the first EOF ensures a reduced contribution of the incoherent noise to the new variate. [For a more detailed account on EOF analysis the reader is suggested to refer to Preisendorfer (1988).]

A SIMPLE EXAMPLE

Consider two collocated time series measurements of different physical parameters of a wave system, namely velocity (u) and elevation (η). Suppose the recordings are affected by a large scale coherent signal and an uncorrelated noise (uncorrelated with the signal and the other measurement). Then the measurements $u(t)$ and $\eta(t)$ can be expressed as

$$u(t) = u_s(t) + \varepsilon(t) \tag{17}$$

$$\eta(t) = \eta_s(t) + \zeta(t) \tag{18}$$

where $u_s(t)$ and $\eta_s(t)$ are the true signals and $\varepsilon(t)$ and $\zeta(t)$ are the uncorrelated noises in the two measurements. Then

$$\langle u(t)^2\rangle = \langle u_s(t)^2\rangle + \langle \varepsilon(t)^2\rangle + 2\underbrace{\langle u_s(t)\varepsilon(t)\rangle}_{=0} \tag{19}$$

$$\langle \eta(t)^2\rangle = \langle \eta_s(t)^2\rangle + \langle \zeta(t)^2\rangle \tag{20}$$

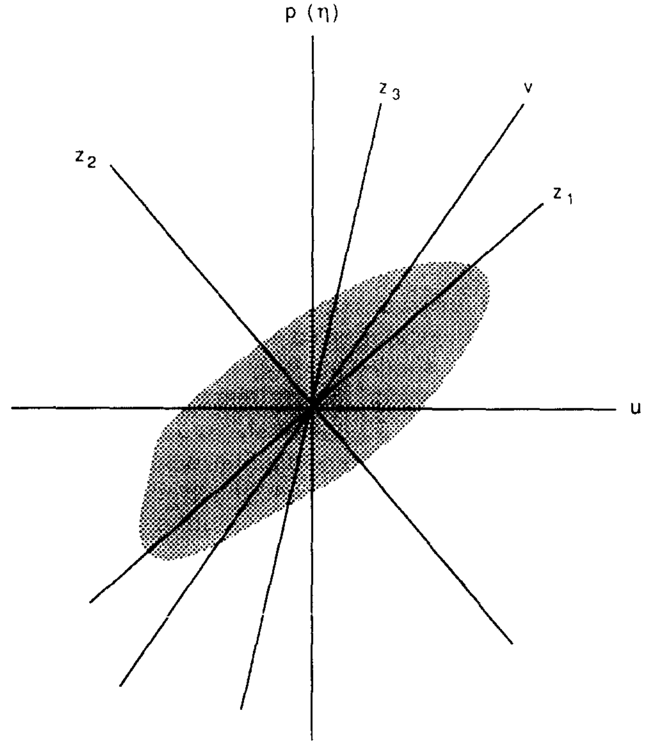

FIG. 4. Principal axes of trivariate observations.

$$\langle u(t)\eta(t)\rangle = \langle u_s(t)\eta_s(t)\rangle \; . \tag{21}$$

Before proceeding further let us transform the units of u using linear wave theory to units of the wave elevation η. Then the covariance matrix $\boldsymbol{\Sigma}$ may be expressed as

$$\boldsymbol{\Sigma} = \begin{bmatrix} \langle u_s^2\rangle + \langle \varepsilon^2\rangle & \langle u_s\eta_s\rangle \\ \langle \eta_s u_s\rangle & \langle \eta_s^2\rangle + \langle \zeta^2\rangle \end{bmatrix} . \tag{22}$$

For convenience, let

$$\langle u_s^2\rangle = \langle \eta_s^2\rangle = \sigma_s^2 \; ; \qquad \langle u_s\eta_s\rangle = \sigma_s\sigma_s\rho \tag{23}$$

$$\langle \varepsilon^2\rangle = \sigma_N^2 \; ; \qquad \langle \zeta^2\rangle = \sigma_N^2 \tag{24}$$

and

$$\sigma_u^2 = \sigma_\eta^2 = \sigma_s^2 + \sigma_N^2 \tag{25}$$

where ρ is the correlation between the two time series measurements. Therefore,

$$\boldsymbol{\Sigma} = \begin{bmatrix} \sigma_u^2 & \sigma_u\sigma_\eta\rho \\ \sigma_u\sigma_\eta\rho & \sigma_\eta^2 \end{bmatrix} \tag{26}$$

rewriting Equation (26) as

$$\Sigma = \sigma_u \sigma_\eta \begin{bmatrix} \sigma & \rho \\ \rho & \sigma^{-1} \end{bmatrix} \tag{27}$$

where $\sigma = \dfrac{\sigma_u}{\sigma_\eta}$.

We compute the eigenvalues by using the relation $\mathbf{\Sigma e} = \lambda \mathbf{e}$ that is,

$$\begin{bmatrix} \sigma & \rho \\ \rho & \sigma^{-1} \end{bmatrix} \begin{bmatrix} e_{1j} \\ e_{2j} \end{bmatrix} = \lambda_j \begin{bmatrix} e_{1j} \\ e_{2j} \end{bmatrix} \tag{28}$$

where e_{1j} and e_{2j} are the elements of the column vector $\mathbf{e_j}$. The above matrix Equation (28) is equivalent to the homogeneous system

$$\sigma e_{1j} + \rho e_{2j} = \lambda_j e_{1j} \tag{29}$$

$$\rho e_{1j} + \sigma^{-1} e_{2j} = \lambda_j e_{2j} \, . \tag{30}$$

But for a non-trivial solution we know that,

$$\begin{vmatrix} \sigma - \lambda & \rho \\ \rho & \sigma^{-1} - \lambda \end{vmatrix} = 0 \, . \tag{31}$$

The function [Equation (31)] is a polynomial in λ of degree 2. Therefore [Equation (29)] has two eigenvalues. Let us now relate the directional tangent (q) of the first eigenvector (associated with the first eigenvalue) with the slope (S) of the linear model obtained by applying the MLS2 approximation. From Equation (28) the two eigenvalues are obtained as:

$$\lambda_{1,2} = \frac{1 + \sigma^2 \pm \sqrt{(1-\sigma^2) + (2\sigma\rho)^2}}{2} \, . \tag{32}$$

From the set of Equations (29) and (30), the directional tangent (q) of the first eigenvector is obtained as:

$$q = \frac{e_{21}}{e_{11}} = \frac{\lambda_1 - 1}{\sigma\rho} \tag{33}$$

and by substituting λ_1 from (32) we obtain:

$$q = A \pm \sqrt{1+A^2}, \text{where } A = \frac{\sigma^2 - 1}{2\rho\sigma} \tag{34}$$

and we choose the positive sign when $\rho > 0$.

By comparing (6) and (34) we find that the slope obtained by the MLS2 approximation is identical to the directional tangent of the first eigenvector.

For convenience let $\sigma = 1$; hence, the eigenvalues are given by

$$\lambda = (1 + \rho), (1 - \rho) \, . \tag{35}$$

As discussed earlier the jth EOF of the p variate observations is the linear compound (16)

$$z_j = e_{1j}u_1 + \ldots, + e_{pj}u_p \tag{36}$$

whose coefficients are the elements of the characteristic vector of the covariance matrix $\mathbf{\Sigma}$ corresponding to the jth largest characteristic root λ_j. If $\lambda_i \neq \lambda_j$, the coefficients of the ith and the jth components are necessarily orthogonal; if $\lambda_i = \lambda_j$, the elements can be chosen to be orthogonal although an infinity of such orthogonal vectors exists. The variance of the jth component is λ_j and the total system variance is thus

$$\lambda_1 + \ldots, + \lambda_p = tr\,\mathbf{\Sigma} \tag{37}$$

where tr denotes the trace of the matrix. The importance of the jth component in a more parsimonious description of the system is measured by

$$\frac{\lambda_j}{tr\,\mathbf{\Sigma}}\,. \tag{38}$$

The algebraic sign and magnitude of e_{ij} indicate the direction and importance of the contribution of the ith response to the jth component.

Incorporating the eigenvalues $(1+\rho,\ 1-\rho)$ in Equations (29) and (30) we can compute the ratios of the elements (e_{1j}, e_{2j}) of the eigenvectors $\mathbf{e}_1$ and $\mathbf{e}_2$. Therefore

$$\mathbf{e}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{39}$$

$$\mathbf{e}_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}. \tag{40}$$

Let us now normalize e_{1j}, e_{2j} such that $e_{1j}^2 + e_{2j}^2 = 1$ and compute the signal to noise ratio (S/N) in the new variable expressed as a linear combination of the initial responses,

$$\frac{\mathbf{S}}{\mathbf{N}} = \frac{e_1^2\langle u_s^2\rangle + e_2^2\langle \eta_s^2\rangle + 2e_1e_2\langle u_s\eta_s\rangle}{e_1^2\langle \varepsilon^2\rangle + e_2^2\langle \zeta^2\rangle} \tag{41}$$

that is,

$$\frac{\mathbf{S}}{\mathbf{N}} = \frac{\sigma_s^2}{\sigma_N^2}\,(1 + 2e_1e_2\rho)\,. \tag{42}$$

Equation (42) shows that the signal to noise ratio of the first empirical orthogonal function is greater than that of the original measurements (σ_s^2/σ_N^2) and is a function of the coherence between the two time series measurements. That is, the higher the coherence between η and u measurements the larger the signal to noise ratio. Therefore, considering only the first mode for further analysis we would be reducing the contribution of uncorrelated noise in the original measurements.

Although the first mode explains most of the total variance the absence of any phase information makes it difficult to physically interpret the results. Hence Wallace and Dickinson's (1972) *complex* EOF analysis technique is considered.

Wallace and Dickinson (1972) demonstrated how one could use the eigenvectors of the cross-spectral matrix instead of the covariance matrix to represent the parameter space structure of a multiple time series. This procedure is similar to the application of EOF analysis of simultaneous multiple time series which have been band pass filtered to eliminate all components outside the band of frequencies being considered. However, the eigenvectors of the cross-spectral matrix are not used to transform the original time series as in the previous case but are applied to an augmented complex time series involving the original time series and its time derivative. It is easy to show that the cross-spectral matrix at the appropriate frequency is simply the covariance matrix of the augmented complex time series of the original time series. Since the cross-spectral matrix is Hermitian, it has a complete set of orthonormal eigenvectors and real eigenvalues, the eigenvectors being *complex*. Therefore one can obtain *complex* modes (that is, shapes with amplitude and phase information). In principle, any set of unit vectors, each representing a particular type of motion, which span the space may be chosen as the basis set for the spectrum representation. A natural set to use is the orthonormal set of eigenvectors $\mathbf{e}_j$ of the spectral density matrix which are obtained from the eigenvalue equation $\Sigma\mathbf{e}_j = \lambda_j\mathbf{e}_j$. These eigenvectors form a complete orthonormal set and can be thought of as the kinematic normal modes for the time series measurements. Moreover, Preisendorfer (1988) clearly showed that in order to solve the travelling wave problem, one needs to resort to complex harmonic analysis first and then perform EOF analysis in the frequency domain.

THE SIMPLE EXAMPLE REVISITED

Let us now form a cross-spectral matrix instead of a covariance matrix for the previous example. Therefore, in this example we would be performing *complex* EOF analysis rather than simple EOF outlined in the previous section. Normally we denote the power and cross-spectra by Γ_{ii} and Γ_{ip}, respectively. Therefore the cross-spectral matrix can be written as

$$\begin{bmatrix} \Gamma_{ii} \;\cdots\; \Gamma_{ip} \\ \Gamma_{pi} \;\cdots\; \Gamma_{pp} \end{bmatrix}. \tag{43}$$

Let us consider real data from collocated measurements of cross-shore velocity, alongshore velocity and pressure (elevation) to form the cross-spectral matrix for a specific frequency band. The alongshore velocity measurement is also considered in order to increase the statistical confidence, since the greater the number of parameters available to form the cross-spectral matrix the greater the statistical confidence, because the EOF analysis fully exploits the interrelationships between all the parameters used in the expansion. To maintain consistency the units of velocity have been transformed to those of elevation using linear wave theory before forming the cross-spectral matrix.

$$\begin{bmatrix} \Gamma_{uu} & \Gamma_{uv} & \Gamma_{u\eta} \\ \Gamma_{vu} & \Gamma_{vv} & \Gamma_{v\eta} \\ \Gamma_{\eta u} & \Gamma_{\eta v} & \Gamma_{\eta\eta} \end{bmatrix}. \tag{44}$$

The data for analysis were collected during Autumn 1983, from Pointe-Sapin beach, New Brunswick, Canada, as part of the Canadian Coastal Sediment Study (C^2S^2) program. Details of the field experiment and a summary of the data collected are reported by Daniel (1985). Measurements of the flow field were made using Model 512 OEM Marsh McBirney electromagnetic current meters and Model 245A-002 Digiquartz pressure transducers. The data set used in this study is from an instrument station located about 60 m offshore from the mean shoreline. The following cross-spectral matrix ($u \times v \times \eta$) is formed from data obtained from Pointe-Sapin beach, New Brunswick, for waves in the frequency band 0.1318–0.1363 Hz.

$$\begin{matrix} 0.002049 & -0.000118-0.000084i & -0.002214-0.000060i \\ -0.000118+0.000084i & 0.000048 & 0.000145-0.000102i \\ -0.002214+0.000060i & 0.000145+0.000102i & 0.002476 \end{matrix} . \qquad (45)$$

Eigenvalues and complex eigenvectors are computed using the IMSL subroutine EIGCH. The normalized eigenvalues are computed to be

$$\lambda = 0.9838, 0.0106, 0.0054 .$$

That is, the principal mode explains 98.4% of the variance. The first EOF can therefore be considered to be that linear combination of the initial responses (u, v, η) which account not only for the maximum variance but also a reduced contribution from the uncorrelated noise. Therefore the components u_1 (0.671,0), v_1 (0.051,144.46) and η_1 (0.739,178.45) may be used for further analysis. The numbers in brackets are, respectively, the amplitudes (in metres) and phases (in degrees).

Figure 5 shows the normalized eigenvalues as a function of the wave frequency. It is clear that the first eigenvalue explains most of the total variance in all frequency bands and hence the appropriate eigenmode for further analysis would be the first mode associated with this eigenvalue. In order to check whether the eigen-modal decomposition really partitions the total variance into different orthonormal modes

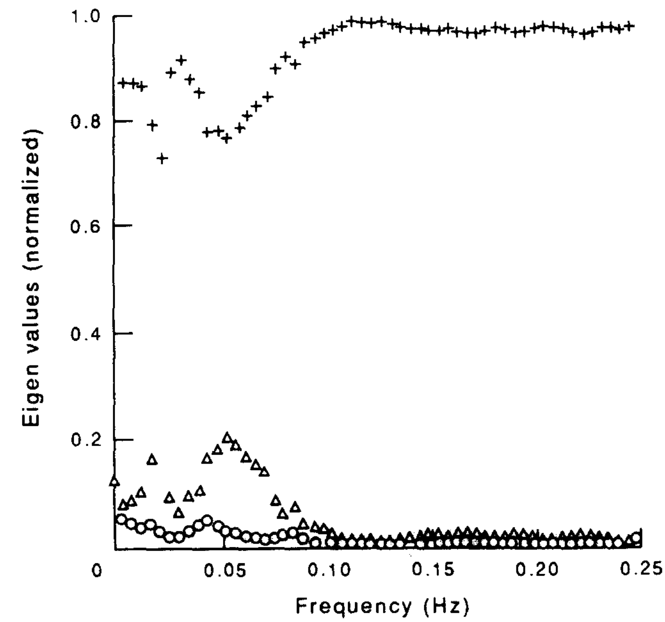

FIG. 5. Normalized eigenvalues as a function of the wave frequency. The eigenvalues indicate the percentage of variance explained by mode 1 (+), mode 2 (△), mode 3 (O).

let us compute the energy flux magnitudes and directions as functions of the wave frequency.

The expression for co-spectrum can be written in terms of the coherent amplitudes and the phase difference between two series as follows

$$C_{\eta u}(\omega) = a_{\eta}(\omega)\, a_u(\omega) \cos \theta_{\eta u}(\omega) \tag{46}$$

$$C_{\eta v}(\omega) = a_{\eta}(\omega)\, a_v(\omega) \cos \theta_{\eta v}(\omega) \tag{47}$$

where $C_{\eta u}(\omega)$ and $C_{\eta v}(\omega)$ are the co-spectra between η and u series, and η and v series, respectively, a_{η}, a_u and a_v are the coherent spectral amplitudes obtained from EOF analysis for each eigenmode, $\theta_{\eta u}$ and $\theta_{\eta v}$ are the corresponding spectral phase differences between η, u and v series obtained from the each eigenmode, and ω is the wave frequency.

We can express the energy flux $\mathbf{F} = |\mathbf{F}|e^{i\alpha}$ (normalized (dimensionless) magnitude and direction) at each frequency as

$$|F|^2 = \frac{C_{\eta u}^2 + C_{\eta v}^2}{a_{\eta}^2(a_u^2 + a_v^2)} \tag{48}$$

$$\alpha = \tan^{-1}\left(\frac{C_{\eta v}}{C_{\eta u}}\right). \tag{49}$$

Figures 6 and 7, respectively, show the direction of the energy flux associated with each mode and the magnitude of the energy flux associated with each mode as a function of the wave frequency for data from Pointe-Sapin beach. It can be seen that the total energy is distributed in three directions, corresponding to the three modes, each orthogonal to the other and that the magnitude of the energy associated with the principal mode is significantly greater at all frequencies when compared to the other modes.

As observed in Equations (39) and (40) it is easy to show that the gain (ratio of the square root of the variances in η and u) of the first eigenmode is equal to the inverse of the negative of the gain of the second eigenmode and that there is a 180° phase shift between the first two eigenmodes. This seems to be an interesting property of the empirical orthogonal function analysis which partitions energy into different orthonormal modes. It is important to recognize that these empirical modes are not a property of any geometry (as in the case of normal modes of a basin), nor do they depend on any dynamical assumptions, but rather they are a property of the time series itself.

CONCLUSIONS

Unlike the standard MLS approximation, the MLS2 approximation or the EOF analysis does not depend on which variable is called "independent" or which "dependent", as both the variables are treated symmetrically. Thus, given the frequency of practical situations in which "independent" variables are recorded with error, methods of MLS2 approximation and EOF are more appropriate for data analysis.

The result stating $S \equiv q$ (where S is the optimal straight line slope and q is the directional tangent of the first eigenvector), is expected if we consider that the total variance in data set is invariant under an orthogonal transformation. If we split the

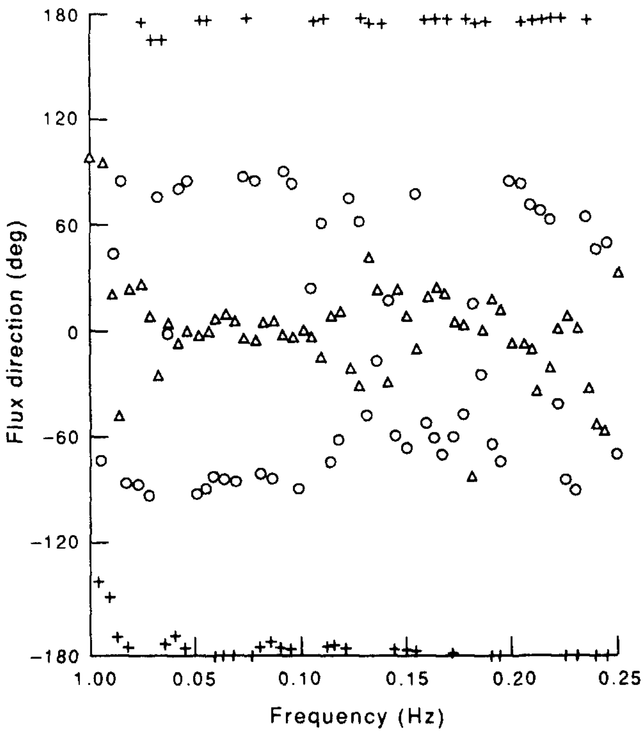

FIG. 6. Direction of energy fluxes (in degrees) as a function of the wave frequency for mode 1 (+), mode 2 (△), mode 3 (○).

total variance (σ_T^2) into orthogonal components ($\sigma_{u'}^2$, $\sigma_{\eta'}^2$) the sum of them will be constant independently of the arbitrary orthogonal reference system selected (u', η'):

$$\sigma_T^2 = \sigma_{u'}^2 + \sigma_{\eta'}^2 \equiv \text{trace}\,\boldsymbol{\Sigma}\ . \tag{50}$$

Referring to the orthogonal splitting of the total variance, the eigenproblem corresponds to finding rotated axes (u', η') such that $\sigma_{u'}^2(\sigma_{\eta'}^2)$ is maximum. In a similar way the MLS2 approximation, with the error defined in Equation (5), corresponds to finding rotated axes (u', η') such that $\sigma_{u'}^2(\sigma_{\eta'}^2)$ is minimum. In other words, this exact equivalence comes from the fact that as total variance is invariant, to maximize one part of it leads to the same result as to minimize the other part.

To summarize the results, we can compare the slope values obtained by using the two different methods: EOF and MLS2. For a certain data set $\{(u_i,\eta_i)\}$ we can always transform the units such that $\sigma^2 \equiv 1$. Therefore under this scaling, expressions (3) and (34) imply that for a linear model $\eta = Su$, the value of S is:

$$S = \begin{cases} \pm 1 & \text{by using EOF} \\ \rho & \text{by using MLS} \end{cases} \qquad \text{if } \sigma^2 \equiv 1\ .$$

Therefore by assuming one of the variables being noiseless (e.g. u), the slope of a linear relation between u and η will be always underestimated.

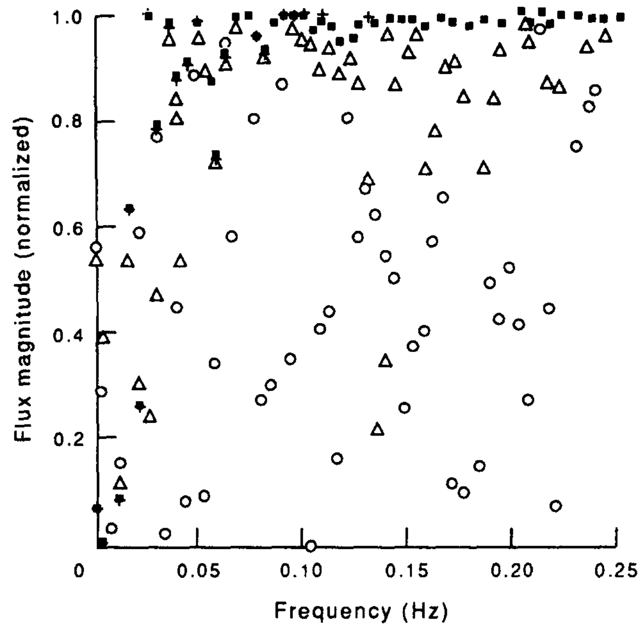

FIG. 7. Normalized (dimensionless) magnitudes of energy fluxes as a function of the wave frequency for mode 1 (■), mode 2 (△), mode 3 (○).

The *complex* empirical modes determined from the eigenvectors of the cross-spectral matrix have the following characteristics:

(i) the empirical modes, which are the properties of the measured time series (not of any geometrical or dynamical assumptions) allow independent orthogonal motions at the same frequency to be separated;

(ii) the relative magnitudes of the first few eigenvalues in the expansion gives an indication of whether one or more wave types are present. If the first eigenvalue explains a significant amount of variance then the remaining eigenvalues may be regarded as due to uncorrelated noise;

(iii) if more than one type of wave structure is present in the same frequency band, the physical interpretation becomes somewhat speculative because the first mode represents a compromise structure which incorporates the correlated (non-orthogonal) features of the waves which are present, while the next mode will be orthogonal to the first mode, which explains the maximum amount of the residual variance and so on.

Acknowledgements—Sincere thanks to Keith Thompson and Tony Bowen of Dalhousie University, Canada, and David Huntley of Polytechnic South West, Plymouth, U.K., for their suggestions and critical remarks on the earlier versions of this manuscript. Suggestions from Dr Seymour, Scripps Institution of Oceanography, U.S.A., and the two anonymous referees are appreciated.

REFERENCES

ANDERSON, T.W. 1984. *An Introduction to Multivariate Statistical Analysis*. John Wiley and Sons, New York.
AUBREY, D.G. 1980. The statistical prediction of beach changes in southern California. *J. geophys. Res.* **85**, 3264–3276.

BARNETT, T.P. 1983. Interaction of the monsoon and Pacific trade wind systems at interannual time scale. Part I: the equatorial zone. *Mon. Weath. Rev.* **111**, 756–773.

BARNETT, T.P. and HASSELMANN, K. 1979. Techniques of linear prediction with application to oceanic and atmospheric fields in the tropical Pacific. *Rev. Geophys. Space Phys.* **17**, 949–968.

DANIEL, P.E. 1985. Data summary index for Canadian Coastal Sediment Study Program at Pointe Sapin, New Brunswick and Stanhope Lane, P.E.I. *NRC Reports*, C^2S^2—15, 16.

DAVIS, R.E. 1976. Predictability of sea surface temperature and sea level pressure anomalies over the North Pacific ocean. *J. phys. Oceanogr.* **6**, 249–266.

HOREL, J.D. 1984. Complex principal analysis: theory and examples. *J. Climate appl. Meteor.* **23**, 1660–1673.

HOTELLING, H. 1933. Analysis of a complex of statistical variables into principal components. *J. Edu. Psych.* **24**, 417–441.

HOTELLING, H. 1936. Relations between two sets of variates. *Biometrica* **28**, 321–377.

LIANG, G. and SEYMOUR, R.J. 1991. Complex principal component analysis of wave-linked sand motions. *Proceedings of the Coastal Sediments '91, ASCE*, pp. 2175–2186.

MARSDEN, R.F. and JUSZKO, B.A. 1987. An eigenvector method for the calculation of directional spectra from heave, pitch and roll buoy data. *J. phys. Oceanogr.* **5**, 750–760.

PEARSON, K. 1901. On lines and planes of closest fit to systems of points in space. *Philosophical Magazine* **6**, 559–572.

PREISENDORFER, R.W. 1988. *Principal Component Analysis in Meteorology and Oceanography*. Elsevier, New York.

SERVAIN, J. and LEGLER, D.M. 1986. Empirical orthogonal function analyses of tropical Atlantic sea surface temperature and wind stress: 1964–1979. *J. geophys. Res.* **91**, 14181–14191.

TATAVARTI, RAO V.S.N. 1989. The reflection of waves on natural beaches. Ph.D. thesis, Dalhousie University, Canada, (175 pp.).

TATAVARTI, RAO V.S.N., HUNTLEY, D.A. and BOWEN, A.J. 1988. Incoming and outgoing wave interactions on beaches. *Proceedings of the 21st Coastal Engineering Conference, Malaga, Spain*, Vol. 1, pp. 136–150.

WALLACE, J.M. and DICKINSON, R.E. 1972. Empirical orthogonal representation of time series in the frequency domain. Part I: theoretical considerations. *J. appl. Meteorology* **1**, 887–892.

WEARE, B.C. 1979. A statistical study of the relationships between ocean surface temperatures and the Indian monsoon. *J. atmos. Sci.* **26**, 2279–2291.

WEARE, B.C. and NASSTROM, J.S. 1982. Examples of extended empirical orthogonal function analyses. *Mon. Weath. Rev.* **110**, 481–485.

WEARE, B.C., NAVATO, A.R. and NEWELL, R.E. 1976. Empirical orthogonal analysis of Pacific sea surface temperatures. *J. phys. Oceanogr.* **6**, 671–678.

WEISBERG, S. 1985. *Applied Linear Regression* (2nd Edn). John Wiley and Sons, New York.