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PIPs and POPs: The Reduction of Complex Dynamical Systems Using Principal Interaction and Oscillation Patterns

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A general method is described for constructing simple dynamical models to approximate complex dynamical systems with many degrees of freedom. The technique can be applied to interpret sets of observed time series or numerical simulations with high-resolution models, or to relate observation and simulations. The method is based on a projection of the complete system on to a smaller number of "principal interaction patterns" (PIPs). The coefficients of the PIP expansion are assumed to be governed by a dynamic model containing a small number of adjustable parameters. The optimization of the dynamical model, which in the general case can be both nonlinear and time-dependent, is carried out simultaneously with the construction of the optimal set of interaction patterns. In the linear case the PIPs reduce to the eigenoscilations of a first-order linear vector process with stochastic forcing (principal oscillation patterns, or POPs). POPs are linearly related to the "principal prediction patterns" used in linear forecasting applications. The POP analysis can also be applied as a diagnostic tool to compress the extensive information contained in the high-dimensional cross-spectral covariance matrix representing the complete second-moment structure of the system.

1. INTRODUCTION

To gain insight into the behavior of complex dynamical systems with many degrees of freedom, a standard strategy is to devise simpler analog systems which contain only a few degrees of freedom but nevertheless succeed in capturing the principal dynamical properties of the full system. In the case of climate modeling, some form of system reduction is essential if one wishes to model the many interactions between the different climate subsystems which span many orders of magnitude of different time scales. A high-resolution model, such as a general circulation model (GCM), cannot be integrated long enough to cover more than a small fraction of the time scales occurring in natural climate variability, so that a trade-off must be found between the number of degrees of freedom of the model and the spectral bandwidth of the simulation. Apart from the need to remain within finite computational restraints, system reduction is also the standard approach to "understanding" the system. Various reduced systems have been proposed, for example, to deduce the overall response characteristics of the global climate system or to explain particular phenomena, such as the El Niño/Southern Oscillation or atmospheric blocking.

The simplest and most commonly used method of system reduction is scale truncation. The nonresolved components of the system beyond the cutoff scale are normally parameterized in the form of mean interaction terms and a residual stochastic forcing contribution. The latter can often be the dominant term responsible for the time variability of the reduced system [cf. *Hasselmann*, 1976].

In this paper an alternative method of system reduction is considered, based on the observation that the dynamical behavior of complex systems often appears to be dominated by interactions between only a few characteristic "patterns". A number of hypotheses which have been proposed to explain climate fluctuations in terms of internal feedback processes rather than short time scale stochastic forcing have been formulated implicitly in terms of such interaction patterns. However, the identification of the basic interaction structures in observed data or in the simulation data of high-resolution model runs has often proved elusive.

In the following discussion a general method for constructing reduced dynamical models is introduced which addresses this problem. The models combine internal linear or nonlinear interactions within the reduced system with residual stochastic forcing, both of which can contribute to the natural variability of the system. The basic technique is straightforward: the reduced dynamical model is constructed by finding the optimal model, within a given model class, which best fits the data in a generalized least squares sense. In defining the model class for the fitting procedure, the interaction patterns, parameter values of the dynamical model, and statistical structure of the stochastic forcing are not specified. The optimal model fit then yields the set of "principal interaction patterns" (PIPs), the model parameter values, and the (cross) spectra of the stochastic forcing. In the linear case the PIPs reduce to (damped) normal modes (principal oscillation patterns, or POPs).

The approach may be regarded as a combination and extension of standard methods of expanding statistical fields with many degrees of freedom in terms of empirical orthogonal functions (EOFs) or "principal prediction patterns" (PPPs) and the autoregressive moving average (ARMA) technique of constructing dynamical models for systems with a few degrees of freedom.

EOFs yield an optimal representation of the covariance structure of fields at a given time, but they are not designed to reveal the structure of the time evolution or the internal dynamics of the system. Principal prediction patterns provide an optimal representation of the linear prediction of one field in terms of another field [cf. *Davis*, 1976; *Barnett and Preisendorfer*, 1987]. If the two fields represent the same physical field taken at different times, the prediction represents a forecast, and the principal prediction patterns therefore contain some time evolution information. However, this cannot normally be translated into an explicit dynamical model without further assumptions. Although EOFs and PPPs can be used, and occasionally have been used, to construct reduced dynamical models, they are not optimized for this purpose.

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ARMA methods, on the other hand, have been developed specifically to construct dynamical models. In its standard form [cf. *Box and Jenkins*, 1976; *Kashyap and Rao*, 1976], the technique is basically linear and applies for systems with relatively few degrees of freedom. The method can be readily generalized to nonlinear systems and to systems with time-dependent model parameters. For many climate modeling applications, the nonlinearity and annual modulation of the system are indeed essential characteristics which need to be included at the outset in the formulation of the reduced dynamical model. The main restriction of such a generalized ARMA approach, however, is still the limitation to a few degrees of freedom. The ARMA technique as such contains no provision for projecting the full system onto a smaller set of dominant patterns. This aspect is addressed in the present study.

Although the primary motivation for the paper is to construct reduced dynamical models, the POPs technique for the linear case may also be applied simply as a diagnostic tool (just as the ARMA technique can be applied to estimate spectra using maximum entropy methods). A complete description of the space-time dependent covariance structure of a statistically stationary field requires the specification of the complete cross-spectral covariance matrix for each frequency band of the spectrum or, equivalently, the complete sets of complex EOFs for each frequency. The POPs essentially identify those regions of the spectrum which can be described by the same patterns for an extended frequency interval. They therefore provide a simultaneous optimization of the representation of the second moments of the field with respect to both the spatial and frequency dependence.

Alternative techniques for combining spatial structure information with reduced time-dependence information have been proposed in which an extended EOF analysis is carried out for an enlarged set of time series, consisting of the original time series argumented by a finite number of time-lagged time series [cf. *Weare and Nasstrom*, 1982] or by the Hilbert transforms of the original time series [cf. *Wallace and Dickinson*, 1972; *Horel*, 1984]. The main difference in the POP technique, compared with these methods, is that it ties the different patterns more closely into the structure of the spectrum (see also section 4).

Another diagnostic application of the POP method is the determination of the perturbation eigenmodes of complex model systems, e.g., an ocean circulation model (E. Maier-Reimer et al., paper in preparation, 1988). If the model is driven by white noise stochastic forcing, a POP analysis of the response automatically extracts the system's normal modes.

The general nonlinear PIP formalism is developed in section 2, while the simplifications resulting for POPs in the linear case are discussed in section 3. The relation between the complete cross-spectral matrix representation of the second moments of the field and the POPs expansion is considered in section 4. The conclusions are summarized in section 5.

2. Principal Interaction Patterns: The General Case

Consider a system represented by the state vector $\Phi = (\Phi_1, \Phi_2, \cdots, \Phi_n)$, whose evolution is governed by a set of first-order equations

$$\frac{d\Phi}{dt} = \mathbf{F}(\Phi) \tag{1}$$

where $\mathbf{F}$ is some nonlinear, time-dependent function of Φ (the time dependence is suppressed in the notation). The dimension n of the system is assumed to be high: for numerical high-resolution models, n is typically of order 10^4–10^6, while for observational data, n may be of order 10^2.

attempt now to construct a simplified dynamical model approximating (1) which involves a significantly smaller number of degrees of freedom m, where m is perhaps of order 2–10. The reduction is carried out in two steps.

First, the dimension of the state vector is reduced by approximating Φ as a superposition $\hat{\Phi}$ of m time-independent principal interaction patterns, $\mathbf{p}_v$,

$$\Phi = \hat{\Phi} + \rho \tag{2}$$

where

$$\hat{\Phi} = \sum_v z_v(t)\mathbf{p}_v \tag{3}$$

and ρ is the residual error.

For this section and section 3, it is convenient to introduce a matrix notation in which, in an extension of Dirac's bra-ket notation, the structure of a matrix is depicted by left and right delimiters, indicating the dimensions of the left and right indices of the matrix, respectively. A transposed matrix is represented by a mirror image delimiter pair; a matrix multiplication contains two adjacent mirror image delimiters. Thus the state vector Φ is represented as the one column matrix $\Phi_{i1} = |\Phi\rangle$, the set of patterns $\mathbf{p}_v$ as the rectangular matrix $p_{iv} \equiv |p)$, the set of coefficients z_v as the one-column vector $z_{v1} \equiv (z\rangle$ (or as the transposed row vector $\langle z)$), and the symmetrical $n \times n$ matrix in (4) as $M_{ij} \equiv |M|$ (see Table 1). Following standard practice, we shall replace the delimiter pair represented by double verticals in matrix multiplications by a single vertical delimiter.

The matrix form of (3) is then given by

$$|\hat{\Phi}\rangle = |p)(z\rangle \tag{3'}$$

The coefficients $z_v(t)$ for a given set of patterns $\mathbf{p}_v$ are determined, in the standard manner, by requiring that the square modulus $\langle \rho | M | \rho \rangle$ of the error ρ with respect to some suitably defined metric M is minimized. One obtains

$$(z\rangle = (d|M|\Phi\rangle \tag{4}$$

where $|d)$ is the set of adjoint patterns to $|p)$, defined as the set of vectors within the space spanned by $|p)$, which are orthonormal (with respect to the matrix M) to the set $|\mathrm{p})$,

$$(d|M|p) = (I) \qquad (\equiv \delta_{v\mu}) \tag{5}$$

or explicitly,

$$|d) = |p)(N^{-1}) \tag{6}$$

where

$$(N) = (p|M|p) \tag{7}$$

In statistical applications, in which Φ is regarded as a particular realization taken from a statistical ensemble of states, the metric M is usually chosen as the inverse of the covariance matrix of Φ. If Φ is Gaussian and is defined such that its expectation value vanishes, surfaces of constant $\langle \Phi | M | \Phi \rangle$ in Φ phase space then correspond to surfaces of constant probability density. This choice of M has the property that it maximizes the statistical significance of patterns extracted from Φ

TABLE 1. Notation

(Right) Delimiter	Associated Dimension⟩
|	1
|	n, equal to the dimension of state vector Φ
)	m, equal to the number of patterns $\mathbf{p}_v$, $v = 1, \ldots m$
|	dimension of predictand field Ψ

		Column Vectors		
Vector	Vector Index Notation	Matrix Index Notation	Bra-ket Notation	Definition
$\boldsymbol{\Phi}$	Φ_i	Φ_{i1}	$\|\Phi\rangle$	state vector
$\hat{\boldsymbol{\Phi}}$	$\hat{\Phi}_i$	$\hat{\Phi}_{i1}$	$\|\hat{\Phi}\rangle$	modeled state vector
$\boldsymbol{\rho}$	ρ_i	ρ_{i1}	$\|\rho\rangle$	error of modeled state vector
$\mathbf{z}$	z_v	z_{v1}	$(z\|$	pattern expansion coefficients
$\mathbf{c}$	c_v	c_{v1}	$(c\|$	pattern coefficients
$\boldsymbol{\Psi}$	Ψ_a	Ψ_{a1}	$\|\Psi\rangle$	predictand field
$\mathbf{p}$	p_i	p_{i1}	$\|p\rangle$	single expansion pattern
$\mathbf{q}$	q_i	q_{i1}	$\|q\rangle$	single projection pattern
$\bar{\mathbf{q}}$	$\bar{q}_i$	$\bar{q}_{i1}$	$\|\bar{q}\rangle$	$\|\bar{q}\rangle = \|M\|q\rangle$

Matrix	Index Notation	Bra-ket Notation	Definition
M	M_{ij}	$\|M\|$	metric used for pattern expansion
$\bar{M}$	$\bar{M}_{ij}$	$\|\bar{M}\|$	metric used for PIP model error minimization
M'	$M_{\alpha\beta}{}'$	$\|M\|$	metric used for PPP model error minimization
$\mathbf{p}_v$	p_{iv}	$\|p)$	set of expansion patterns
$\mathbf{d}_v$	d_{iv}	$\|d)$	set of adjoint patterns: $(d/M/p) = (I)$
N	$N_{v\mu}$	(N)	$(p/M/p)$
D	$D_{v\mu}$	(D)	linear model matrix
$\mathbf{q}_v$	q_{iv}	$\|q)$	set of projection patterns: $\|q) = \|d)\ (D^T)$
K	K_{ai}	$\|K\|$	predictand-predictor covariance matrix
C	C_{ij}	$\|C\|$	predictor covariance matrix
$\bar{K}$	K_{ia}	$\|\bar{K}\|$	$\|C^{-1}\|K^T\|M'\|$

which are associated with specific externally generated "signals", as opposed to the internal background noise of the statistical ensemble of states $\boldsymbol{\Phi}$ [cf. *Hasselmann*, 1979].

In the second step of the reduction procedure, a set of m (in general nonlinear, time-dependent) evolution equations

$$\frac{dz_v}{dt} = G_v(z;\, \alpha_1, \alpha_2, \cdots \alpha_p) + n_v \tag{8}$$

is postulated for the coefficients $z_v(t)$ of the expansion (4). The reduced model (8) is specified a priori only as a member of a model class: the evolution equations contain a number of free parameters $\alpha_1, \alpha_2, \cdots \alpha_p$, which still need to be determined. In addition to the deterministic evolution functions G_v, the evolution equations contain an (unknown stochastic) forcing term n_v, representing the residual errors of the reduced dynamical system. The class of model G_v must be specified a priori in accordance with some preconceived notion or hypothesis regarding the type of dynamical process governing the evolution of the system.

The unknown model parameters α_j and PIPs $\mathbf{p}_v$ are now determined simultaneously by minimizing the error

$$\varepsilon = \{\langle \dot{\hat{\Phi}} - \dot{\Phi} \,|\, \bar{M} \,|\, \dot{\hat{\Phi}} - \dot{\Phi} \rangle\} \tag{9}$$

between the rate of change $\dot{\boldsymbol{\Phi}} \equiv d\boldsymbol{\Phi}/dt$ of the true system and the rate of change $\dot{\hat{\boldsymbol{\Phi}}} \equiv d\hat{\boldsymbol{\Phi}}/dt$ of the approximate system, as determined from (3), (4), (6), and (8), but without inclusion of the unknown noise term n_v. The braces in (9) denote expectation values (or, if the system cannot be regarded as a stochastic process, as the time integral over the period for which the reduced model is applied).

The metric $\bar{M}$ of the scalar product in (9) may be defined differently from the scalar product (4). For example, it may be appropriate to choose the matrix $\bar{M}$ as the inverse of the covariance matrix of $\hat{\boldsymbol{\Phi}}$, rather than $\boldsymbol{\Phi}$.

Substituting (8) into (3), we obtain

$$\varepsilon = \{\langle G)(p \,|\, \bar{M} \,|\, p)(G\rangle - 2\langle \hat{\Phi} \,|\, M \,|\, p)(G\rangle + \langle \hat{\Phi} \,|\, M \,|\, \hat{\Phi}\rangle\} \tag{10}$$

Variation of ε with respect to α_j and $\mathbf{p}_v$, respectively, then yields as the determining equations for our model

$$\frac{1}{2}\frac{\partial \varepsilon}{\partial \alpha_j} = 0 = \left\{\langle G)(p \,|\, \bar{M} \,|\, p)\left\langle \frac{\partial G}{\partial \alpha_j}\right\rangle - \langle \hat{\Phi} \,|\, \bar{M} \,|\, p)\left\langle \frac{\partial G}{\partial \alpha_j}\right\rangle\right\} \tag{11}$$

$$\frac{1}{2}\frac{\partial \varepsilon}{\partial \,|\, p)}\,\delta \,|\, p) = 0 = \{[\langle G)(p| - \langle \hat{\Phi}|]\,|\,\bar{M}\,|\,\delta p)(G\rangle\} + \left\{[\langle G)(p \,|\, \bar{M} \,|\, p) - \langle \hat{\Phi} \,|\, \bar{M} \,|\, p)]\,\frac{\partial (G\rangle}{\partial (z\rangle}\,\delta(z\rangle\right\} \tag{12}$$

where, according to (4), (6)

$$\delta(z\rangle = (N^{-1})(\delta p \,|\, M \,|\, |\Phi\rangle - (N^{-1}) \cdot [(\delta p \,|\, M \,|\, p) + (p \,|\, M \,|\, \delta p)](N^{-1})(p \,|\, M \,|\, \Phi\rangle \tag{13}$$

Equations (11) and (12) are in general nonlinear and can be solved only by iterative techniques. In practice, the determination of the optimal solution will be less forbidding than the structure of the equations appears to imply. For a prescribed set of patterns, the minimization with respect to α_j can be carried out using minimization routines available in standard libraries (the dimension of the parameter vector α_j is assumed to be small). Conversely, for given α_j the matrix equation (12)

for the determination of the optimal patterns can also be solved iteratively, for example, by considering small perturbations about a reference set of patterns and then applying linear techniques. For a linear model, (12) reduces to a straightforward matrix eigenvalue problem (compare section 3). The full minimization problem can thus be solved by minimizing iteratively with respect to $\mathbf{p}_v$ and α_j. Alternatively, the full parameter set $\mathbf{p}_v$, α_j can be determined simultaneously, using recently developed adjoint gradient techniques designed for optimizing systems with many degrees of freedom [cf. *Navon and Legler*, 1987].

It has been assumed that the class of models is formulated such that the optimal solution which minimizes ε is uniquely determined. This will generally require some restriction in the form of the dynamical model. For example, an alternative representation equivalent to (3) can be obtained by any linear transformation of the set of patterns within the space spanned by the patterns. If the resulting linear transformation of the coefficient vector z_v yields a model which still belongs to the class of models defined by (8), the optimal model is clearly defined only to within an arbitrary linear transformation. In this particular case the solution can be made unique by requiring, for example, that the linear terms in the Taylor expansion of the dynamical equations are diagonal. For the case of a linear system, the principal interaction patterns reduce then to principal oscillation patterns, which are defined as the normal modes of the system. Alternatively, the representation can be made unique by introducing the patterns successively, keeping the previously defined patterns fixed when the next pattern is determined.

The general technique outlined in this section can clearly be modified in various respects. The set of adjoint vectors $|d)$ need not be defined through (4) and (5), but can be determined simultaneously with the PIPs as part of the minimization condition on ε. Furthermore, the model can be required to satisfy additional side conditions, either rigorously or approximately, which can be included with appropriate weighting in the definition of the error function ε. In most applications the model will be constructed for a particular time scale range. This can be taken into consideration by passing the original data $\mathbf{\Phi}(t)$ through an appropriate filter. Alternatively, the minimizing function itself can be defined as a weighted integral over the frequency domain (this procedure lends itself most readily to linear models).

3. Principal Oscillation Patterns: The Linear Case

The evolution equations (8) for the reduced dynamical system are given in the linear case by

$$\frac{d\langle z|}{dt} = (D)\langle z| + \langle n| \tag{14}$$

or, invoking (4),

$$\frac{d|\hat{\Phi}\rangle}{dt} = |p)(D)(d|M|\Phi\rangle + \text{residual forcing} \tag{15}$$

where $(D) \equiv D_{v\mu}$ represents a constant matrix. The elements of (D) correspond to the parameters α_j in the general formulation of section 2. Since the square matrix (D) will normally be nonsymmetrical, the transpose matrix $(D^T) \equiv D_{\mu v}$ is indicated explicitly by an superscript T in the following discussion to avoid ambiguity in the delimiter notation.

Through a (complex) linear transformation, the form (14) can normally be diagonalized (we shall ignore degenerate cases where this is not possible). We denote the linear patterns, $\mathbf{p}_v$, of the optimal model after diagonalization, which represent the eigenmodes of the linear system (14), as principal oscillation patterns. The POPs occur as complex conjugate pairs, if the eigenvalues are complex (damped oscillations), or as single real patterns for real eigenvalues (exponentially damped modes).

Before considering the POPs further, it is helpful to relate the present approach to the alternative, but essentially equivalent, expansion in terms of principal prediction patterns (PPPs). For this purpose, we introduce a set of "projection patterns" $|q) \equiv q_{iv}$, defined by

$$|q) = |d)(D^T) \tag{16}$$

where $|d)$ is the set of adjoint patterns given by (6).

Equation (15) then takes the form

$$\frac{d}{dt}|\hat{\Phi}\rangle = |p)(q|M|\hat{\Phi}\rangle \tag{17}$$

Since, for a given set of patterns $|p)$ (and nonsingular (D)), the patterns $|q)$ are uniquely determined through (16) if (D) is given and vice versa, the model can be optimized with respect to the set of parameters $|p)$, (D), as in the original formulation of the model or, alternatively, with respect to the pattern sets $|p)$, $|q)$. The latter approach corresponds to an expansion in terms of PPPs.

PPPs are normally introduced in the more general context of deriving an optimal linear prediction of a predictand field $\mathbf{\Psi} \equiv \Psi_\alpha$ from a predictor field $\boldsymbol{\phi} \equiv \phi_i$, using an expansion of only a finite number of predictand and predictor (projection) patterns [cf. *Davis*, 1976; *Barnett and Preisendorfer*, 1987]. The dimensions of Ψ_α and ϕ_i can be different. We denote the field $\mathbf{\Psi}$ in matrix notation as $|\Psi\rangle$. In our particular case, however, $\mathbf{\Psi} \equiv \dot{\mathbf{\Phi}}$, so that the predictor and predictand fields have identical dimension.

In the general problem one seeks an optimal prediction

$$|\Psi(t)\rangle = |p)\langle c(t)| \tag{18}$$

for the predictand field $\mathbf{\Psi}$ in terms of m constant patterns $\mathbf{p}_v \equiv p_{\alpha v} \equiv |p)$, $v = 1, \cdots m$, where the coefficients $c_v(t) \equiv \langle c|$ of the expansion are derived from the predictor field $\mathbf{\Phi}$ by a projection

$$\langle c| = (q|M|\Phi\rangle \tag{19}$$

using m projection patterns $\mathbf{q}_v \equiv q_{iv} \equiv |q)$, $v = 1, \cdots m$

Thus

$$|\hat{\Psi}\rangle = |p)(q|M|\Phi\rangle \tag{20}$$

The pattern sets $|p)$ and $|q)$ are determined by minimizing the mean square error

$$\varepsilon = \{\langle \Psi - \hat{\Psi}|M'|\Psi - \hat{\Psi}\rangle\} = \min \tag{21}$$

defined with respect to some metric $|M'| \equiv M_{\alpha\beta}'$. (This will generally differ from the metric $|\bar{M}| \equiv \bar{M}_{ij}$ in (9), introduced in section 2, since Ψ_α and ϕ_i have different dimensions. However, in our application we may set $M' = \bar{M}$).

The condition (21) alone clearly does not specify the pattern sets $|p)$, $|q)$ uniquely, since (20) and (21) are invariant with respect to an arbitrary linear transformation $|p') = |p)(L)$, $|q') = |q)(L^{-1T})$. However, we may make the solution unique

by requiring that the pattern pairs $\mathbf{p}_v$, $\mathbf{q}_v$ are introduced in sequence (and, say, by suitably normalizing the patterns p_v). In this case, we need consider only one pattern pair, $\mathbf{p}_v$, $\mathbf{q}_v \equiv \mathbf{p}$, $\mathbf{q}$, at a time and can thus drop the index v (i.e., we may replace $|\, p)$ by $|\, p\rangle$. The predictand field $\mathbf{\Psi}$ is redefined at each step as the original field minus the field already predicted from the patterns introduced previously.

The (local) minimization of ε yields the relations

$$\frac{1}{2}\frac{\partial \varepsilon}{\partial \langle p|} = \langle q|M|[-|K^T| + |C|M|q\rangle\langle p|]|M'| = 0 \quad (22)$$

$$\frac{1}{2}\frac{\partial \varepsilon}{\partial |q\rangle} = \langle p|M'|[-|K| + |p\rangle\langle q|M|C|]|M| = 0 \quad (23)$$

where

$$|K| \equiv K_{\alpha i} = \{\Psi_\alpha \phi_i\} \quad (24)$$

and

$$|C| \equiv C_{ij} = \{\phi_i \phi_j\} \quad (25)$$

Multiplying (22) and (23) from the right with $|M'|^{-1}$, and $(|C|M|)^{-1}$, respectively, one obtains two coupled eigenvalue equations for $|p\rangle$ and

$$|\bar{q}\rangle = |M|q\rangle \quad (26)$$

namely,

$$|K|\bar{q}\rangle - \lambda'|p\rangle = 0 \quad (27)$$

$$|\bar{K}|p\rangle - \lambda''|\bar{q}\rangle = 0 \quad (28)$$

where

$$\lambda' = \langle \bar{q}|C|\bar{q}\rangle \quad (29)$$

$$\lambda'' = \langle p|M'|p\rangle \quad (30)$$

and

$$|\bar{K}| = |C^{-1}|K^T|M'| \quad (31)$$

Separation of $|p\rangle$ and $|\bar{q}\rangle$ then yields the pair of eigenvalue equations

$$|K|\bar{K}|p\rangle - \lambda|p\rangle = 0 \quad (32)$$

$$|\bar{K}|K|\bar{q}\rangle - \lambda|\bar{q}\rangle = 0 \quad (33)$$

with the same eigenvalues

$$\lambda = \lambda'\lambda'' \quad (34)$$

for $|p\rangle$ and $|\bar{q}\rangle$. The values λ', λ'' follow from λ after introduction of a suitable normalization for $|p\rangle$, say, for example, $\lambda'' = 1$ (equation (30)).

The matrices $|K|\bar{K}| = [|K|C^{-1}|K^T|]\,[|M|]$ and $|\bar{K}|K| = [|C^{-1}|]\,[|K^T|M'|K|]$ in the eigenvalue equations (32) and (33) consist of quadratic products of symmetrical, positive definite matrices, indicated here by the square parentheses. It follows that the eigenvalues are real and positive and that the eigenvectors are also real. The eigenvectors themselves are in general not orthogonal but are related to an equivalent orthogonal set by a linear transformation.

The absolute minimum of ε is given by the eigenvector pair with the largest eigenvalue λ, and the sequence of predictor patterns is accordingly given by the ordered sequence of eigensolutions of (32) and (33).

To derive the POPs for a linear model, the most straightforward procedure is accordingly the following: (1) determine the sequence of PPPs by solving (32) and (33); (2) evaluate the linear model coefficient matrix D by inverting (16); and (3) diagonalize (14) by transforming to the (complex) eigenoscillations of the linear system (14).

The inversion of (16) in the second step is readily carried out by making use of the orthogonality of the vector sets $|p)$ and $|d)$. One obtains, applying (5)–(7),

$$(D) = (q|M|p) \quad (35)$$

Although this approach is presumably the simplest when dealing with purely linear systems, it may be more convenient to resort to the general nonlinear formalism when the linear model is to be investigated within a hierarchy of nonlinear models in which the linear model occurs as a limiting case. The dynamical model would then be formulated at the outset in terms of a model which is diagonalized in the first-order, linear approximation.

In the diagonalized reference frame the POP expansion of the field Φ is given by

$$\Phi = \sum_v A_v(t)\mathbf{p}_v(t) + \text{complex conjugate} \quad (36)$$

where the complex amplitudes A_v satisfy the standard damped harmonic oscillator equation

$$\frac{dA_v}{dt} - i\Omega_v A_v = N_v(t) \quad (37)$$

$$\Omega_v = \omega_v + i\mu_v$$

The residual forcing term $N_v(t)$, frequencies Ω_v, and patterns

$$\mathbf{p}_v = \mathbf{p}_v^{(1)} + i\mathbf{p}_v^{(2)} \quad (38)$$

are generally complex. For eigenmodes with zero frequency ω_v, however, the complex conjugate pattern pair $\mathbf{p}_v$, $\mathbf{p}_v^*$ reduces to a single, real pattern $\mathbf{p}_v^{(1)}$ representing an exponentially decaying mode $\sim \exp(-\mu_v t)$.

In general, both real and imaginary patterns $\mathbf{p}_v^{(1)}$, $\mathbf{p}_v^{(2)}$ will be continually excited by the residual complex stochastic forcing $N_v(t)$. Each excitation pulse gives rise to a damped oscillation, in which the originally excited pattern $\mathbf{p}_v^{(1)}$, say, is transformed into the pattern $\mathbf{p}_v^{(2)}$ after a quarter period $\pi/2\omega_v$, returning back to the original pattern with opposite sign after another quarter period, and so on. Depending on the form of the patterns $\mathbf{p}_v^{(1)}$ $\mathbf{p}_v^{(2)}$, the oscillation can appear as a standing wave, a traveling wave, a local pulsation, or as various combinations of these. The general oscillation represents a damped amphodromic wave of the form considered extensively in the harmonic analysis of tides or in the eigenoscillation theory for ocean basins.

In contrast to the nondynamical expansion in terms of EOFs, the amplitudes of different POPs are generally correlated. This applies also for the amplitudes of a PPP expansion, and it must be expected to hold generally for any expansion procedure based on dynamical models. Even when the different system components are dynamically decoupled by transforming to normal-mode coordinates, as in the POP representation, correlations between the different modes are introduced by the residual forcing $N_v(t)$ in (38), which cannot be assumed to be uncorrelated.

A more detailed discussion of POPs, in the context of a meteorological application, is given by *von Storch et al.* [this issue].

4. Relation Between POPs and Cross-Spectral EOF Analysis

In applications to a multivariate, stationary, stochastic process $\Phi_i(t)$, the POPs analysis is not only useful as method of constructing optimal linear dynamical models, but also provides a simple diagnostic tool for compressing the extensive information required for a complete characterization of the second-moment statistics of the process into a manageable set of numbers and patterns.

The second moments of a statistically stationary process $\Phi_i(t)$ can be characterized by the covariance function

$$R(t) \equiv R_{ij}(t) = \{\Phi_i(t+\tau)\Phi_j(t)\}$$

or equivalently, by its Fourier transform, the complex cross spectrum $F_{ij}(\omega)$.

The cross spectrum may also be formed directly from the Fourier representation of the process itself,

$$\Phi_i(t) = \int \phi_i(\omega) \exp(i\omega t)\, d\omega \tag{39}$$

through the relation

$$\{\phi_i^*(\omega)\phi_j(\omega')\} = F_{ij}(\omega)\delta(\omega - \omega') \tag{40}$$

where $\phi_j^*(\omega)$ denotes the complex conjugate, and the reality of Φ_i requires

$$\phi_j^*(\omega) = \phi_j(-\omega) \tag{41}$$

$$F_{ij}(\omega) = F_{ji}(-\omega) = F_{ij}^*(-\omega) \tag{42}$$

At each frequency ω, the cross spectrum F_{ij} may be diagonalized by transforming from $\phi_i(\omega)$ to the coefficients $c_\alpha(\omega)$ of the expansion with respect to the complex EOFs, $e_{i\alpha}(\omega)$ [cf. *Brillinger*, 1981]:

$$\phi_i(\omega) = \sum_\alpha e_{i\alpha} c_\alpha(\omega) \tag{43}$$

where the EOFs satisfy the eigenvalue equation

$$\sum_j F_{ij} e_{j\alpha} = \lambda_\alpha e_{i\alpha} \tag{44}$$

The set of variables $c_\alpha(\omega)$ provides a completely orthogonalized representation of $\Phi_i(t)$,

$$\{c_\alpha^*(\omega)c_\beta(\omega')\} = \delta_{\alpha\beta}\delta(\omega - \omega')\lambda_\alpha(\omega) \tag{45}$$

Thus the spectrum $\lambda_\alpha(\omega)$, together with the set of EOFs $e_{i\alpha}(\omega)$, may be regarded as the most compact complete representation of the second-momentum structure of $\Phi_{it}(t)$. However, the information content is still formidable, as a different set of EOFs and eigenvalues is required for each frequency band.

The POP analysis may be regarded as an attempt to interpolate both the EOF pattern structure and the EOF energy levels across the frequency spectrum. Translating (37) into the frequency domain and again using lower-case symbols for the Fourier transforms, the POP amplitude cross spectrum for a given noise cross spectrum is given by

$$\{a_\nu(-\omega)a_\mu(\omega)\} = \frac{\{n_\nu(-\omega)n_\mu(\omega)\}}{(\Omega_\nu + \omega)(\Omega_\mu - \omega)} \tag{46}$$

(the quadratic products must be formed here using the negative frequency amplitudes rather than complex conjugate amplitudes, since (41) and the second part of (42) do not hold for the complex processes $A_\nu(t)$ and $N(t)$).

Up to this point the second moments of the POP amplitudes have simply been expressed in terms of the second moments of the forcing. If we require the same number of POPs to describe the process as spectral EOFs, and if the forcing cross spectrum is as complex as the response, clearly nothing has been gained. However, it is the basic premise of the present dynamic model expansion, as in the general ARMA approach, that the dominant structures in the spectrum may be attributed to a relatively small number of dynamical processes represented explicitly in the model, rather than to the external stochastic forcing which is left as a residual after one has identified the dominant internal processes. Thus it is assumed that the residual forcing is white in the frequency domain, or is at least smoothly varying, exhibiting no marked resonances of the type represented by the denominator in (46). In this case, the structure of the cross spectrum can be characterized by the (relatively few) POP patterns, the positions of the quasi-resonance POP frequencies Ω_ν in the complex frequency plane, and the strengths and cross correlations of the effective forcing at these frequencies.

The advantage of the POP technique as a method of compressing the detailed information contained in the complete cross-spectral matrix clearly comes to bear only for relatively broad spectra containing many frequency bands. In the limit of a single-frequency, very narrow band spectrum, the set of POPs reduces to the set of complex EOFs at that frequency.

An alternative technique for compressing the information content of a broadband cross spectrum is to apply a complex EOF analysis in the time domain to a set of time series consisting of the original time series and their Hilbert transforms [*Brillinger*, 1981; *Horel*, 1984]. This is equivalent to treating the entire cross spectrum formally as a single-frequency band, i.e., to averaging over the (one-sided) cross spectrum. Both techniques yield similar sets of reduced patterns, but the POP analysis, in addition, provides information on the frequency structure of the spectrum by identifying the spectral peaks (the POP eigenfrequencies) and peak widths (the inverse damping time scales) associated with different patterns. In the limit of the single-frequency, narrow-band spectrum, the Hilbert transform method again becomes equivalent to the POP and the spectral EOF analysis techniques.

5. Conclusions

A general method has been described for constructing optimal reduced dynamical models for systems with many degrees of freedom. The technique combines the approach used in empirical orthogonal function or principal prediction pattern analyses, in which systems with a large number of degrees of freedom are reduced to a few dominant patterns, with ARMA methods for constructing simple dynamical models from data. Both methods have been generalized to nonlinear and time-dependent systems.

The simultaneous determination of the optimal set of principal interaction patterns and the optimal dynamical model describing the evolution of the PIP amplitudes yields a coupled nonlinear eigenvalue problem for the PIPs and a standard minimization problem for the dynamical model parameters. The full nonlinear problem can generally be solved numerically by a Newton method, i.e., by iterating a local linear minimization problem.

In the linear case the PIPs reduce to principal oscillation patterns, which represent the eigenoscillations of the reduced linear dynamical system.

As a diagnostic tool, the POPs provide a smoothed repre-

sentation of the cross-spectral covariance matrix of the full system in the frequency domain. The extensive information contained in the complete cross spectrum is reduced to a finite set of patterns characterized by a finite set of complex resonant frequencies.

Examples and applications are given in the papers of *von Storch et al.* [this issue] and E. Maier-Reimer et al. (manuscript in preparation, 1988).

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