

2

Empirical model reduction and the modelling hierarchy in climate dynamics and the geosciences

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Modern climate dynamics uses a two-fisted approach in attacking and solving the problems of atmospheric and oceanic flows. The two fists are: (i) observational analyses; and (ii) simulations of the geofluids, including the coupled atmosphere–ocean system, using a hierarchy of dynamical models. These models represent interactions between many processes that act on a broad range of spatial and time scales, from a few to tens of thousands of kilometers, and from diurnal to multidecadal, respectively. The evolution of virtual climates simulated by the most detailed and realistic models in the hierarchy is typically as difficult to interpret as that of the actual climate system, based on the available observations thereof. Highly simplified models of weather and climate, though, help gain a deeper understanding of a few isolated processes, as well as giving clues on how the interaction between these processes and the rest of the climate system may participate in shaping climate variability. Finally, models of intermediate complexity, which resolve well a subset of the climate system and parameterise the remainder of the processes or scales of motion, serve as a conduit between the models at the two ends of the hierarchy.

We present here a methodology for constructing intermediate models based almost entirely on the observed evolution of selected climate fields, without reference to dynamical equations that may govern this evolution; these models parameterise unresolved processes as multivariate stochastic forcing. This methodology may be applied with equal success to actual observational data sets, as well as to data sets resulting from a high-end model simulation. We illustrate this methodology by its applications to: (i) observed and simulated low-frequency variability of atmospheric flows in the Northern Hemisphere; (ii) observed evolution of tropical sea-surface temperatures; and (iii) observed air–sea

interaction in the Southern Ocean. Similar results have been obtained for (iv) radial-diffusion model simulations of Earth's radiation belts, but are not included here because of space restrictions. In each case, the reduced stochastic model represents surprisingly well a variety of linear and nonlinear statistical properties of the resolved fields. Our methodology thus provides an efficient means of constructing reduced, numerically inexpensive climate models. These models can be thought of as stochastic–dynamic prototypes of more complex deterministic models, as in examples (i) and (iv), but work just as well in the situation when the actual governing equations are poorly known, as in (ii) and (iii). These models can serve as competitive prediction tools, as in (ii), or be included as stochastic parameterisations of certain processes within more complex climate models, as in (iii). Finally, the methodology can be applied, with some modifications, to geophysical problems outside climate dynamics, as illustrated by (iv).

2.1 Introduction

Comprehensive general circulation models (GCMs) are governed by a nonlinear set of partial differential equations that, given the climate's state at an initial time t_0 , predict the climatic fields at future times $t_0 + k\Delta t$. These climatic fields – such as atmospheric winds, temperature and humidity, oceanic currents, temperatures and salinities, sea-ice areas and concentrations, among others – are discretised on a spatial grid spanning the entire volume of the Earth's fluid envelope. The governing equations so discretised are but approximations to the original partial differential equations, and are complemented by a large number of semi-empirical relations that connect locally the large-scale fields with subgrid-scale processes, like clouds and radiation. In the absence of the small-scale processes, these approximations could become progressively more accurate as the grid size Δx and time step Δt tend to zero in a judicious manner. Limited computer power poses restrictions on the minimal grid size and, therefore, on the maximal dimension D of the grand climate-state vector, $\mathbf{X} \equiv (X_1, X_2, \dots, X_D)$; there are also restrictions on the appropriate treatment of the small-scale processes as the grid size is progressively reduced.

While D is finite, it is still very large. To facilitate analyses of climatic variability, it is reasonable to use data compression techniques, such as empirical orthogonal function (EOF) analysis, also known as principal component (PC) analysis; see Preisendorfer (1988). Suppose that we have archived a long simulation of a climate model, $\{\mathbf{X}^{(n)}\}$, $n = 1, 2, \dots, N$, as an $N \times D$ array, whose d -th column represents N consecutive values of a climate variable, X_d : $(X_d^{(1)}, X_d^{(2)}, \dots, X_d^{(N)})$. Assuming that the climate is stationary, we first subtract from each of our D variables their

time-mean values, thus redefining the climate state in terms of anomalies $X_d^{(n)} \rightarrow X_d^{(n)} - N^{-1} \sum_{n=1}^N X_d^{(n)}$. The climate-state anomaly vector $\mathbf{X}$ will thus have zero time mean.

Let us now define a new time series, $\mathbf{x}_1 \equiv (x_1^{(1)}, x_1^{(2)}, \dots, x_1^{(N)})$, as a weighted average of D original time series: $x_1^{(n)} = e_1^{(1)} X_1^{(n)} + e_2^{(1)} X_2^{(n)} + \dots + e_D^{(1)} X_D^{(n)}$, where the weights $e_d^{(1)}$ are chosen to maximise the variance of the $\mathbf{x}_1$ time series, subject to the normalisation constraint $\mathbf{e}^{(1)} \cdot \mathbf{e}^{(1)} \equiv e_1^{(1)} e_1^{(1)} + e_2^{(1)} e_2^{(1)} + \dots + e_D^{(1)} e_D^{(1)} = 1$, where $\mathbf{a} \cdot \mathbf{b}$ denotes the inner product of the vectors $\mathbf{a}$ and $\mathbf{b}$. The time series $\mathbf{x}_1$ so obtained is called the leading PC, while the set of weights $\mathbf{e}^{(1)}$ represents a spatial pattern referred to as the leading EOF of our multivariate climate field. One can compute the second PC–EOF pair, $\mathbf{x}_2, \mathbf{e}^{(2)}$, by maximising the variance of $\mathbf{x}_2$ subject to the normalisation constraint $\mathbf{e}^{(2)} \cdot \mathbf{e}^{(2)} = 1$ and the additional orthogonality constraint $\mathbf{e}^{(1)} \cdot \mathbf{e}^{(2)} = 0$. Higher-order PCs and EOFs, up to D , can be found in a similar way, with $\mathbf{e}^{(d)}$ computed to satisfy d orthonormality constraints. In other areas of fluid dynamics, in particular in turbulence theory, this statistical approach goes by the name of proper orthogonal decomposition (Tennekes & Lumley 1972). Thus, the multivariate climate field can be decomposed into the sum of orthonormal spatial patterns $\mathbf{e}^{(d)}$, or EOFs, whose corresponding time series $\mathbf{x}_d$, or PCs, turn out to be orthogonal, while their variances decrease monotonically with d .

The latter property has important consequences, since typically a limited number M of leading EOFs, $M \ll D$, accounts for a major fraction of climate variance. It thus appears reasonable to think of climate evolution in terms of variability associated with leading EOF modes. A few leading EOF modes are sometimes referred to as *teleconnection* patterns (Wallace & Gutzler 1981), since they reflect correlations between variables at spatial locations separated by distances much larger than the typical decorrelation radius of atmospheric fields. Our description of the EOF analysis above is intentionally oversimplified. Even if it were computationally feasible to apply this statistical method directly to the full climate-state vector of a comprehensive GCM, many technical challenges would have to be addressed: treatment of physically and thus dimensionally distinct variables, for example, wind and temperature; choice of optimal inner product in computing covariances while respecting quadratic invariants, like energy or enstrophy and several others. A more comprehensive coverage of these issues is beyond the scope of the present discussion.

Let us consider multivariate dynamical equations with quadratic nonlinearity as a prototype of the discretised equations describing climate evolution (Lorenz 1963; Ghil & Childress 1987, ch. 5):

$$\dot{\mathbf{X}} = \hat{\mathbf{F}} + \hat{\mathbf{L}}\mathbf{X} + \hat{\mathbf{N}}(\mathbf{X}, \mathbf{X}); \quad (2.1)$$

here $\mathbf{X}$ is a D -dimensional state vector and the dot denotes the time derivative. Denoting the matrix transpose by superscript T and substituting the EOF decomposition

$$\mathbf{X} = \mathbf{x} \cdot \mathbf{e}^T \quad (2.2)$$

into (2.1), multiplying these equations on the right by $\mathbf{e}$ and using the orthonormality of the EOFs, we rewrite the governing equations in the EOF basis (Schubert 1985; Selten 1995, 1997; Kwasniok 1996, 2004; Branstator & Haupt 1998; Achatz & Branstator 1999; D’Andrea & Vautard 2001; Achatz & Opsteegh 2003a,b; Franzke *et al.* 2007):

$$\dot{\mathbf{x}} = \tilde{\mathbf{F}} + \tilde{\mathbf{L}}\mathbf{x} + \tilde{\mathbf{N}}(\mathbf{x}, \mathbf{x}) \quad (2.3a)$$

or, componentwise,

$$\dot{x}_i = \tilde{F}_i + \tilde{L}_{ij}x_j + \tilde{N}_{ijk}x_jx_k; \quad (2.3b)$$

the repeated indices, throughout the chapter, imply summation, and i, j, k vary from 1 to D .

Since a moderate number, M , of leading EOFs account for a major fraction of climate-state vector variance, it is natural to consider only the first M of (2.3b), while neglecting in them all the terms that involve higher-order PCs, x_i , $i > M$. This is the simplest approach to obtaining a reduced climate model and it is called the bare-truncation model. It turns out, however, that while the trailing EOF modes may not account for a large fraction of variance, their interaction with the resolved modes over time is important for the dynamics of the resolved modes, as the bare-truncation models typically experience systematic biases. These biases can be partially corrected for empirically by introducing ad hoc linear damping terms of the form $-r_{ij}x_j$ to parameterise the neglected interactions between the resolved and unresolved modes (Selten 1995; Achatz & Branstator 1999). Strounine *et al.* (2008) advance this idea one step further by combining it with data assimilation methods (Dee *et al.* 1985; Kondrashov *et al.* 2008) and estimating, in addition to the linear damping coefficients, the parameters of additive ‘random-noise’ error associated with the statistical linear fit; this random term is subsequently introduced into the reduced model as stochastic forcing. The parameterisation of interactions between the resolved and unresolved modes here involves a stochastic component and increased linear damping, as in Farrell & Ioannou (1993, 1995) but, unlike in these authors’ work, retains the quadratic nonlinearity of the bare-truncation equations.

A systematic theoretical approach to model reduction is due to Majda *et al.* (1999, 2001, 2002, 2003, 2006; hereafter MTV). In the limit of significant time scale separation between the fastest resolved and slowest unresolved EOF modes,

the MTV procedure derives the functional form of the reduced equations, based on standard projection methods from the theory of stochastic differential equations (Khasminsky 1963; Kurtz 1973; Gardiner 1985). The self-interaction of the fast, unresolved modes is modelled by a stochastic process, and the reduced equations include modified forcing, linear terms, quadratic and cubic nonlinearities, as well as additive and multiplicative noise terms; the latter terms consist of products of stochastic and resolved variables. The reduced-model coefficients are formally predicted by the MTV approach, provided the lag-covariance structure of all unresolved modes is given. Franzke *et al.* (2005) and Franzke & Majda (2006) applied this approach to the analysis of intermediate complexity models describing variability of midlatitude atmospheric flow, but managed to achieve only modest agreement between the statistical characteristics of the full and reduced models. The reason behind this partial success may lie in the nature of climatic EOF spectra: overall, higher-order modes do have shorter time scales, and somewhat smaller spatial scales, than the leading modes, but there is no pronounced time-scale separation between the resolved and unresolved modes, as required by the stochastic-process theory on which the MTV approach to model reduction is based. While Majda and colleagues have shown that the MTV formulation may still be approximately valid for some idealised systems without such a spectral gap (e.g. Majda *et al.* 2008), this is apparently not the case for the prototype models of atmospheric variability considered by Franzke *et al.* (2005) and Franzke & Majda (2006).

The problem of constructing a reduced model that describes key features of the climate system can be addressed in a data-driven, rather than model-driven approach, by using inverse stochastic modelling. This data-driven approach lacks the dynamical appeal inherent in model-based reduction methods; it offers, though, greater practical flexibility by allowing one to work directly with appropriate subsets of climatic fields. The inverse modelling approach does not require either the equations that govern the fields of interest, nor the laws that couple a given climate subsystem to the rest of the system. By the same token, empirical methodologies are in no way restricted by the necessity to explicitly separate between slow and fast dynamics within a climate subsystem of interest.

The simplest type of inverse stochastic model is the so-called linear inverse model (LIM; Penland 1989, 1996; Penland & Ghil 1993), which has the form

$$dx_i = L_{ij}x_j dt + d\xi_i(t), \quad (2.4)$$

where $d\xi_i(t)$, $i = 1, 2, \dots, M$ is a vector-valued white-noise process characterised by the $M \times M$ noise covariance matrix $\mathbf{Q}$, and $\mathbf{L}$ is the $M \times M$ dynamics matrix, which is assumed to be constant and stable. The LIM procedure aims at finding $\mathbf{Q}$ and $\mathbf{L}$ given observations of a vector-valued time series $\mathbf{x}(t) \equiv [x_1(t), x_2(t), \dots, x_M(t)]$ that represents, for example, M leading PCs of the field(s) of interest. The

matrices $\mathbf{Q}$ and $\mathbf{L}$ in (2.4) satisfy a fluctuation–dissipation relation, which involves $\mathbf{C}(\tau)$, the lag-covariance matrix of the process $\mathbf{x}$ at lag τ (Gardiner 1985):

$$\mathbf{L}\mathbf{C}(0) + \mathbf{C}(0)\mathbf{L}^T + \mathbf{Q} = 0. \quad (2.5)$$

The Green’s function for (2.4), $\mathbf{G}(\tau) = \exp(\mathbf{L}\tau)$, can be expressed in terms of $\mathbf{C}(\tau)$ as

$$\mathbf{G}(\tau) = \mathbf{C}(\tau)\mathbf{C}^{-1}(0), \quad (2.6)$$

while the optimal forecast of $\mathbf{x}_f(\tau)$ given the initial state $\mathbf{x}(0)$ is

$$\mathbf{x}_f(\tau) = \mathbf{G}(\tau)\mathbf{x}(0). \quad (2.7)$$

Equations (2.5, 2.6) are valid exactly for the stochastic differential equation (2.4). In linear inverse modelling, the true lag-covariance matrix $\mathbf{C}$ is replaced by the sample covariance matrix using the actual available data, while (2.6) can be exploited to estimate $\mathbf{L}$ using different lags τ and thus check whether the linear form of (2.4) is supported by the data (Penland & Ghil 1993; DelSole 2000). Note that the dynamics operator $\mathbf{L}$ in (2.4) is in general different from $\tilde{\mathbf{L}}$ in (2.3), since it represents not only the linear part of the bare-truncation operator, but also parameterises, in a linear fashion and along with the white-noise forcing term, the nonlinear interactions between the resolved modes, as well as linear and nonlinear effects associated with the unresolved modes. Linear inverse models have shown some success in predicting seasonal-to-interannual variability associated with the El Niño/Southern Oscillation (ENSO: Penland & Sardeshmukh 1995), variability of sea-surface temperatures in the tropical Atlantic (Penland & Matrosova 1998), and even the much more nonlinear and chaotic extra-tropical atmospheric variability in the Northern Hemisphere (Penland & Ghil 1993; Winkler *et al.* 2001).

In most geophysical situations, however, the assumptions of linear, stable dynamics and white-noise forcing used to construct LIMs are only valid to a certain degree of approximation. In particular, when nonlinearity is strong enough, the matrices $\mathbf{L}$ and $\mathbf{Q}$ obtained from data can exhibit substantial dependence on the time scales considered (Penland & Ghil 1993): in this case, estimates of the matrices $\mathbf{L}$ and $\mathbf{Q}$ via (2.5, 2.6) using lag-covariance information for different lags, τ , produce different results. Another problem has to do with serial correlations in the model’s estimated stochastic forcing.

Let us consider N observations of a vector time series

$$\mathbf{x}^{(n)} = (x_1^{(n)}, x_2^{(n)}, \dots, x_M^{(n)}), \quad n = 1, 2, \dots, N, \quad (2.8)$$

sampled at time intervals of Δt . If we denote the time increments in x as

$$\Delta x_i^{(n)} \equiv x_i^{(n+1)} - x_i^{(n)}, \quad (2.9)$$

the discrete representation of (2.4) has the same symbolic form as the original stochastic differential equations, with Δ replacing d . The i -th row of the dynamics matrix $\mathbf{L}$ can be estimated by multiple linear regression (MLR; Wetherill 1986) of the response time series, Δx_i , using the vector-valued time series of $\mathbf{x}$ as predictors, while the residual time series, $r_i^{(n)}$, can be defined according to

$$r_i^{(n)} \Delta t \equiv \Delta x_i^{(n)} - L_{ij} x_j^{(n)} \Delta t. \quad (2.10)$$

The serial correlation problem arises if the lag-correlation function of $\mathbf{r}$ has long tails, thus contradicting the LIM assumption of white-noise forcing. The standard way of dealing with serial correlations is to use higher-order autoregressive models, referred to in the literature as autoregressive–moving average (ARMA) models (Wetherill 1986; Box *et al.* 1994). DelSole (1996, 2000) considered ARMA models in his study of stochastic parameterisations of quasi-geostrophic turbulence.

Recently, Kravtsov *et al.* (2005b) proposed an empirical model formulation that addresses both of the above weaknesses of LIMs by introducing nonlinear, multilevel extensions of (2.4). An important application of this methodology is to diagnose simulations of complex dynamical models by studying their stochastic–dynamic prototypes, derived empirically using the output from the full model (Kondrashov *et al.* 2006); hence this methodology has been called Empirical Model Reduction (EMR). The EMR approach has also been applied to observational data sets, including Northern Hemisphere geopotential heights (Kravtsov *et al.* 2005b), tropical sea-surface temperatures (SSTs) (Kondrashov *et al.* 2005) and a combined SST–sea-level wind data set over the Southern Ocean (Kravtsov *et al.* 2008).

The purpose of the present chapter is to overview the EMR methodology and applications, compare it with other available model reduction and data modelling approaches, and evaluate its role in the climate modeling hierarchy (Ghil & Robertson 2000; Ghil 2001; Held 2005; McWilliams 2007). We describe the general EMR formulation in Section 2.2, while referring interested readers to Appendices A and B for technical details. Section 2.3 discusses EMR models of simulated and observed atmospheric low-frequency variability in the Northern Hemisphere (Kravtsov *et al.* 2005b; Kondrashov *et al.* 2006), with emphasis on the application of this approach to the analysis of a detailed dynamical model. This section also provides comparisons with the results of MTV model reduction (Franzke & Majda 2006; Strounine *et al.* 2008).

The predictive capabilities of EMR models are illustrated in Section 2.4 using the example of tropical SST modelling. In Section 2.5, we outline yet another potential application of EMR models to stochastic parameterisation of a subset of processes within a more complex climate model; we deal in this case with air–sea interaction over the Southern Ocean (Kravtsov *et al.* 2008). Empirical model prediction applications are not restricted to climate dynamics, and an example of such

an application to a space-physics problem (Shprits 2009, personal communication) is quite instructive, but beyond the space allotted to this chapter. Section 2.6 contains a summary of the paper's results and the authors' outlook on the problems of model reduction in the geosciences.

2.2 Empirical Model Reduction (EMR)

We consider N observations of the M -valued vector $\mathbf{x}$, as in (2.8), sampled at intervals Δt , and define the increments $\Delta \mathbf{x}$ as the differences between consecutive observations according to (2.9). In most of the following examples, the vector time series $\mathbf{x}$ will be represented by M leading PCs of the field(s) of interest. The first step of EMR uses multiple linear regression to find a set of coefficients N_{ijk} , L_{ij} and F_i ($i, j, k = 1, 2, \dots, M$) that minimise, for each i separately, the root-mean-square (rms) distance, χ_i , between the discrete time series of $\Delta x_i^{(n)}$, $n = 1, 2, \dots, N$, and the test function $(N_{ijk} x_j x_k + L_{ij} x_j + F_i)\Delta t$:

$$\chi_i^2 \equiv \sum_{n=1}^N (r_i^{(n)})^2; \quad r_i^{(n)} \Delta t \equiv \Delta x_i^{(n)} - (N_{ijk} x_j^{(n)} x_k^{(n)} + L_{ij} x_j^{(n)} + F_i) \Delta t, \quad (2.11)$$

where $i = 1, 2, \dots, M$, $n = 1, 2, \dots, N$, and $r_i^{(n)}$ is the discrete N -valued time series of the i -th regression residual.

For large enough M , the distribution of the residuals will typically tend to Gaussian, with all non-Gaussian features of $\mathbf{x}$ accounted for by the nonlinear terms in (2.11). At the same time, inspection of the lag-covariance structure of $\mathbf{r}$ often identifies long-tailed autocorrelations, which indicates that modelling of the residual as white-noise forcing is not justified in such cases. In order to address this issue, we introduce an extended state vector $[\mathbf{x}; \mathbf{r}]$ of dimension $2M$, and fit a multiple linear regression model $\Delta r_i \rightarrow L_{ij}^{(1)}[\mathbf{x}; \mathbf{r}]_j \Delta t$, where the summation over j now runs from 1 to $2M$. This model defines the first-level residual $r_{1,i}^{(n)}$, with $i = 1, 2, \dots, M$, and $n = 1, 2, \dots, N$, as

$$r_{1,i}^{(n)} \Delta t \equiv \Delta r_i^{(n)} - L_{ij}^{(1)}[\mathbf{x}; \mathbf{r}]_j \Delta t. \quad (2.12)$$

The discrete vector time series, $\mathbf{r}_1$, is in turn tested for whiteness; if the test fails, additional model levels are introduced as necessary, to model the evolution of the previous-level residuals as a linear function of the extended state vector that involves the variables of all preceding levels, until the L -th level residuals $\mathbf{r}_L$ become white. In subsequent inverse modelling, this residual is substituted by the vector-valued, discrete-time white-noise process $\Delta \xi_i(t)$, $i = 1, 2, \dots, M$, with lag-0 covariance matrix $\mathbf{Q}$ computed from the sample covariance of $\mathbf{r}_L$.

The EMR, discrete-time model with L levels in addition to the main level has thus the following form:

$$\begin{aligned}
 \Delta x_i^{(n)} &= (N_{ijk} x_j^{(n)} x_k^{(n)} + L_{ij} x_j^{(n)} + F_i) \Delta t + r_i^{(n)} \Delta t, \\
 \Delta r_i^{(n)} &= L_{ij}^{(1)} [\mathbf{x}; \mathbf{r}]_j \Delta t + r_{1,i}^{(n)} \Delta t, \\
 \Delta r_{1,i}^{(n)} &= L_{ij}^{(2)} [\mathbf{x}; \mathbf{r}; \mathbf{r}_1]_j \Delta t + r_{2,i}^{(n)} \Delta t, \\
 &\dots \\
 \Delta r_{L-1,i}^{(n)} &= L_{ij}^{(L)} [\mathbf{x}; \mathbf{r}; \mathbf{r}_1; \mathbf{r}_2; \dots; \mathbf{r}_{L-1}]_j \Delta t + \Delta \xi_i(t).
 \end{aligned} \tag{2.13}$$

In all applications discussed herein, we use a time step of $\Delta t = 1$, thus rescaling our time by the sampling interval. When linearised and rewritten as a single equation, the system (2.13) is formally equivalent to an ARMA model (Box *et al.* 1994; DelSole 1996, 2000), but the multilevel form offers greater algorithmic simplicity and is easier to interpret dynamically as well as statistically. In particular, the dependence of the ‘hidden variables’ $\mathbf{r}_l$ on the observable state vector $\mathbf{x}$ may account for two-way feedbacks between the resolved and unresolved variables. Berloff & McWilliams (2002) used similar multilevel strategy to account for stochastic ocean-eddy effects in statistical simulations of tracer trajectories produced by a model of the wind-driven ocean gyres.

The major technical difficulty in applying (2.13) to geophysical problems lies in the large number of regression coefficients that need to be estimated at the main level of the EMR model: the total number of coefficients for each of the M main-level equations is $M(M + 1)/2 + M + 1$. This number makes the dimension of matrices used in the multiple linear regression inversion uncomfortably large even for moderate values of M ; more importantly, it may result in overfitting due to lack of linear independence among the predictors. As a result, the estimated regression coefficients will not be statistically robust; that is, they may change substantially if a different data subsample is used to estimate them. This is called the collinearity or multicollinearity problem (Wetherill 1986; Press *et al.* 1994). The numerical procedures that choose an optimal subset of predictors to avoid multicollinearity and overfitting are referred to as *regularisation* techniques.

A key regularisation tool is cross-validation, in which one chooses randomly a subset of the vector time series (typically 80% of original data points), applies a given regression technique, and then uses the regression model to reconstruct the segments of the time series that were omitted in the model identification step. The performance of the regression technique may then be assessed according, for example, to the smallness of the differences between the regression-based prediction and the actual values of the time series. One can use cross-validation in

a number of different ways when constructing an EMR model; see Appendices A and B.

Appendix A introduces the methods of principle component regression (PCR; Wetherill 1986) and partial least-squares (PLS; Abdi 2003) regression, which linearly transform original predictor variables into a much smaller set of optimal predictors. This transformation means that the actual number of regression coefficients determined is much less than the number of original predictor variables; thus the $M(M + 1)/2 + M + 1$ regression coefficients in each of the main-level equations (2.13) are in fact linear combinations of a much smaller number of independent coefficients. Appendix B describes a fine-tuning procedure for model selection developed by Kravtsov *et al.* (2008), which combines the usage of PCR and PLS with iterative identification of trivial regression coefficients in the original predictor space. Removing the latter coefficients may help study the interactions that give rise to the nonlinear dynamical features simulated by the EMR models (see Section 2.3).

2.3 Application to extra-tropical atmospheric variability

We analyse the output of a global, three-level quasi-geostrophic (QG3) atmospheric model with topography (Marshall and Molteni 1993; D’Andrea & Vautard 2001; Kondrashov *et al.* 2004). The model equations describe the evolution of winds at each of three pressure-coordinate levels, representing the lower, middle and upper troposphere; the troposphere contains about 80% of atmospheric mass and has an average thickness of about 10 km. The equations that govern the QG3 model have the form

$$\dot{q} = -J(\psi, q) - D\psi + S, \quad q = \Lambda\psi, \quad (2.14)$$

where ψ is the streamfunction, and q is the potential vorticity; q is related to ψ via the linear Laplace–Beltrami operator Λ , while the linear operator D parameterises frictional and radiative damping effects, and S is the constant forcing. The equations also include a quadratic advective nonlinearity written in terms of the Jacobian operator J .

Despite its simple form, the QG3 model has a fairly realistic climatology and complex variability, which also compares favourably with the observed atmospheric behaviour; it has been used therefore extensively in theoretical studies of extra-tropical flows. In addition to synoptic variability associated with baroclinic eddies and a time scale of a few days, the model is characterised on longer time scales by the existence of a few persistent and recurrent flow patterns, or regimes (Reinhold & Pierrehumbert 1982; Legras & Ghil 1985; Molteni 2002), as well as by intraseasonal oscillations (Kondrashov *et al.* 2004). Selten & Branstator (2004)

identified signatures of nonlinearity in the model's phase-space mean tendencies (see also Franzke *et al.* 2007); they argued that the dimension of the subspace in which these nonlinear effects are apparent is as low as three.

Such a low-dimensionality of the model's low-frequency variability prompts the development of reduced models, which have considerably fewer degrees of freedom compared to the full QG3 model (Selten 1997; D'Andrea & Vautard 2001; D'Andrea 2002; Kravtsov *et al.* 2005b; Franzke & Majda 2006; Kondrashov *et al.* 2006; Strounine *et al.* 2008). The performance of these models should be judged according to their ability to represent accurately both linear and nonlinear aspects of the full model's behaviour, in particular intraseasonal oscillations and multiple regimes. The reduced models can be studied further to track down dynamical causes of each type of behaviour. The various reduced models differ in part by the way they parameterise the effect of higher-frequency synoptic transients on lower-frequency modes. This effect is referred to in the literature as the synoptic-eddy feedback (Robinson 1996, 2000; Lorenz & Hartmann 2001, 2003; Kravtsov *et al.* 2003, 2005a).

The original QG3 model is global and projected onto spherical harmonics with a total wavenumber not exceeding 21; this so-called T21 version has $D = 3 \times 483 = 1449$ scalar variables (Marshall & Molteni 1993; D'Andrea & Vautard 2001; D'Andrea 2002; Kondrashov *et al.* 2004, 2006; Kravtsov *et al.* 2005b; Strounine *et al.* 2008). A hemispheric version has also been investigated (Selten 1997; Selten & Branstator 2004; Franzke & Majda 2006; Franzke *et al.* 2007). The two model versions produce somewhat different Northern Hemisphere variability; both exhibit, however, similar teleconnection patterns and are also characterised by intraseasonal oscillations. The goal of model reduction methodologies is to construct a model that captures as well as possible the evolution of $M \propto O(10)$ leading EOFs of the full model, and thus reproduces the key features of the full model's variability.

Before even choosing the dynamics coupling a set of the leading EOFs, one may want to optimise the choice of the EOFs, which depends on the inner product used in defining the covariances. The standard choice in the above-mentioned studies of the QG3 model's global version was the use of an inner product consistent with the energy norm. A reduced model constructed in the subspace of the leading EOFs so obtained, though, does not conserve any quadratic invariants of the flow, unless additional approximations are made to project model fields into the subspace of truncated EOFs (Rinne & Karhila 1975; Schubert 1985; Selten 1995); the latter approximations, however, have a detrimental effect on the performance of such a reduced model. Franzke & Majda (2006) proposed to use the energy norm (Ehrendorfer 2000) instead of the streamfunction norm. This choice ensures that the projected equations will conserve the total energy at any truncation, in the

absence of forcing and dissipation. Strounine *et al.* (2008) have also considered an inner product consistent with the potential-*enstrophy* norm; the equations written in this basis conserve the potential *enstrophy* at any truncation.

We now present and discuss results produced by the EMR and MTV methods in reducing the QG3 model. To make the comparison as fair as possible, both reduced models have 10 resolved components ($M = 10$) that represent the leading energy-norm EOFs of the global QG3 version. For the EMR, we use a three-level ($L = 2$) model (2.13), constructed based on a 30 000-day archive of the QG3 simulation documented by Kondrashov *et al.* (2004, 2006). In deriving this EMR model, PCR-and-PLS regularisation (see Appendix A) resulted in reducing the number of independent regression coefficients from $M[M(M + 1)/2 + M + 1 + 2M + 3M] = 1160$ to $O(100)$.

To deal with the lack of scale separation in the QG3 model, Franzke & Majda (2006) had introduced a few free parameters in front of the various groups of terms predicted by the MTV theory and then applied a trial-and-error procedure to ‘tune’ these parameters in order to achieve better approximations of the statistics of the original, full model’s behavior. Following Strounine *et al.* (2008), we replaced this tuning by sequential estimation of the parameters (Dee *et al.* 1985; Ghil 1997; Kondrashov *et al.* 2008).

Franzke and Majda’s (2006) empirical fitting also addresses another practical issue in applying the MTV approach to climate problems. While the mathematical expressions for MTV model coefficients are predicted by the theory, these coefficients are given in terms of integrals that involve lagged autocovariances of unresolved modes, over all lags. Accurate numerical computation of these integrals requires very long and frequently sampled libraries of the full model’s evolution: Franzke & Majda (2006) used in fact a 1 000 000-day model simulation sampled at half-day intervals. Strounine *et al.*’s (2008) sequential parameter estimation can use QG3 model simulations that are as short as 30 000 days, a number comparable with actual atmospheric data sets, and achieve better statistical fits than those of Franzke & Majda’s (2006).

Figures 2.1 and 2.2 compare the QG3 and EMR models in terms of one-dimensional probability density functions (PDFs) and autocorrelation functions (ACFs), respectively, for each of the nine leading PCs. Analogous comparisons between the QG3 and MTV models are given in Figs. 2.3 and 2.4. The EMR model generates time series with PDFs that are almost indistinguishable from those of the QG3 model (Fig. 2.1), including a strongly skewed PDF for EOF-1 and slightly skewed PDF for EOF-4. The fit for the ACFs is not quite as good (Fig. 2.2), but still fairly tight for short lags, up to five days. At longer lags, the EMR model underestimates the time scale of the QG3 model’s first PC, and exhibits smaller, slightly oscillatory deviations for the other leading PCs.

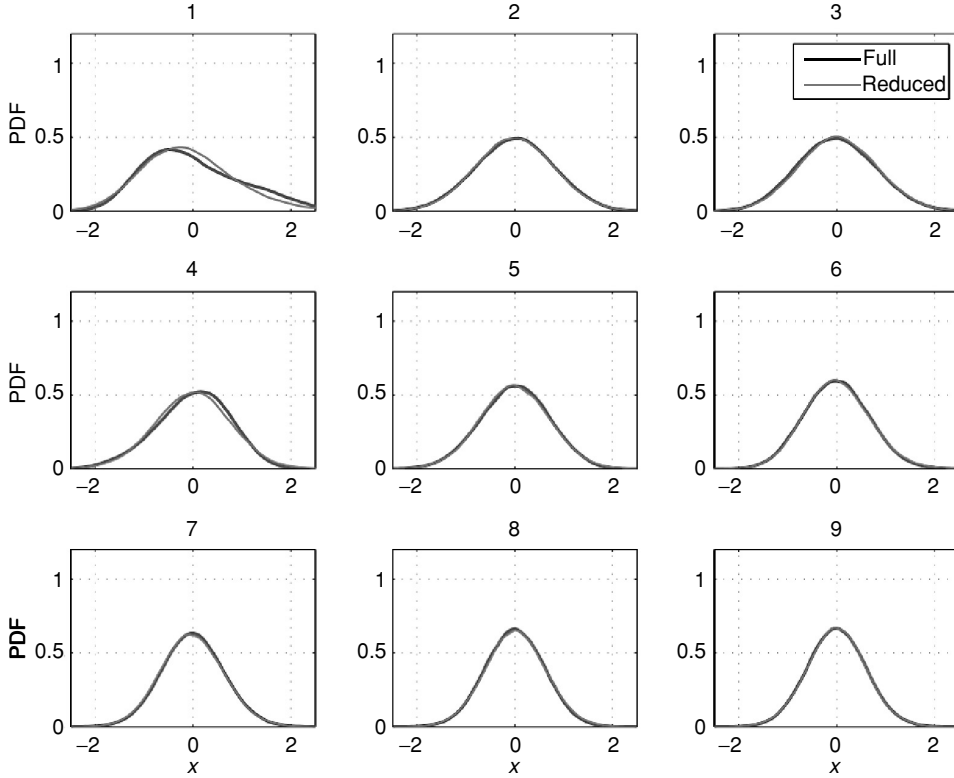


Figure 2.1 Individual probability density functions (PDFs) of the nine leading PCs for the EMR model constructed in the phase space of energy-norm EOFs based on the QG3 model simulation; EOF indices are given in the caption of each panel.

The results for the MTV model are uniformly worse relative to the EMR model for all PCs, with respect to both the PDF (Fig. 2.3) and ACF (Fig. 2.4) comparisons. The MTV model without the sequential parameter estimation of its semi-empirical coefficients (not shown) exhibits even more substantial biases in its PDFs, while its ACFs are fairly similar to those in Fig. 2.4. The quantitative correspondence between the ACFs of the QG3 and MTV models is similar to that reported by Franzke & Majda (2006) for their hemispheric version of the QG3 model (their Fig. 13). On the other hand, their results for PDFs (their Fig. 14) show greater deviations from those of the QG3 model than those in Fig. 2.3 here; the improvement reported herein is presumably due to our use of sequential parameter estimation, rather than trial-and-error tuning.

The performance of our EMR model in capturing nonlinear features of the QG3 model's behaviour is better illustrated by comparing multidimensional PDFs of the full and reduced model solutions. Figure 2.5 shows the PDFs of the data sets

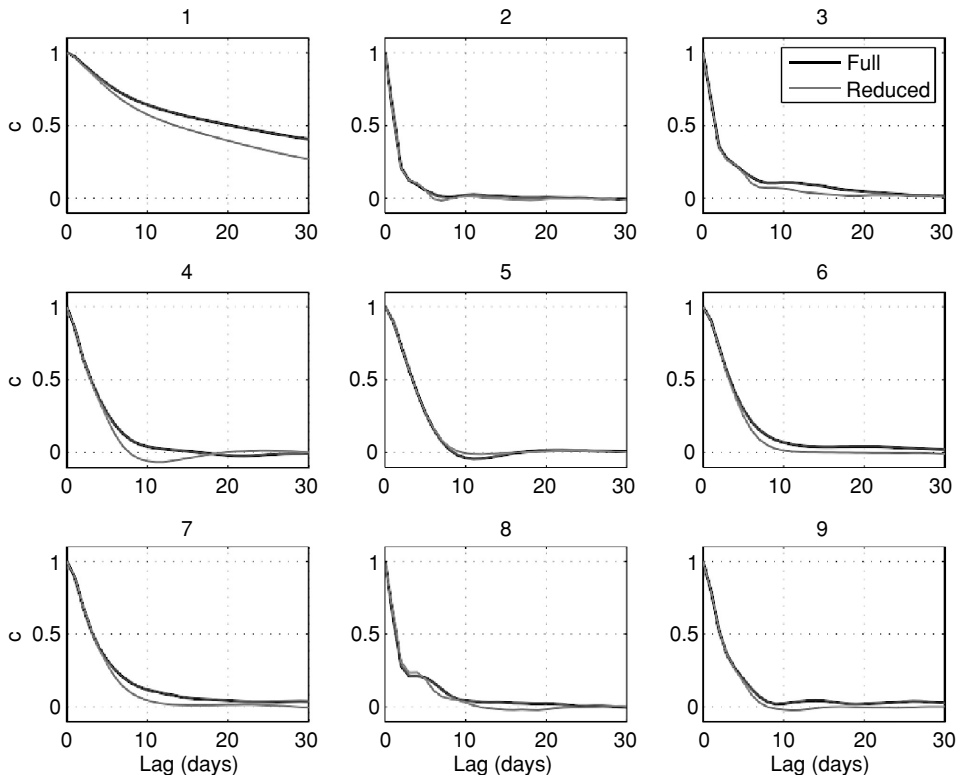


Figure 2.2 The same as Fig. 2.1, but for the autocorrelation functions (ACFs) of the the nine leading PCs for EMR model.

produced by the QG3 and the EMR model, constructed in the phase space of 15 leading streamfunction-norm EOFs (Kondrashov *et al.* 2004; Kravtsov *et al.* 2005b; Kondrashov *et al.* 2006). The clusters were found by mixture modelling of the PDFs (Smyth *et al.* 1999; Hannachi & O’Neill 2001) using an optimal mix of $k = 4$ Gaussian components in a phase subspace of the four leading EOFs. The locations, shapes and sizes of clusters, and hence the general shape of the PDF, are reproduced quite well by the EMR model in Fig. 2.5.

The composites over the data points that belong to each of the clusters in Fig. 2.5 represent, in physical space, the patterns of four planetary flow regimes (Legras & Ghil 1985; Ghil & Childress 1987, ch. 6; Mo & Ghil 1987; Cheng & Wallace 1993; Kimoto & Ghil 1993a,b; Hannachi 1997; Smyth *et al.* 1999; Hannachi & O’Neill 2001; Molteni 2002). In Fig. 2.5a, cluster AO^- (labelled 2 in the figure) occupies a distinctive region on the PDF ridge that stretches along PC-1. It corresponds to the low-index phase of the well-known Arctic Oscillation (AO), which may be related to a more regional North Atlantic Oscillation (NAO) (Deser 2000; Wallace 2000).

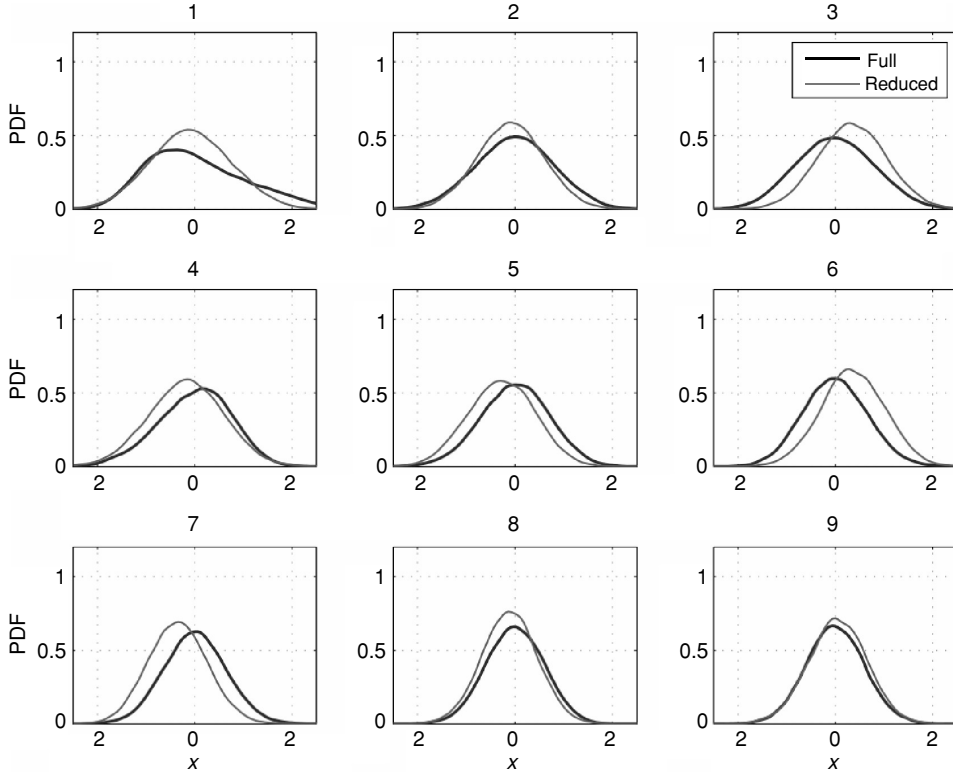


Figure 2.3 Same as Fig. 2.1, but for the MTV model.

The clusters AO^+ , NAO^- and NAO^+ are located around the global PDF maximum, with the centroid of AO^+ to the left and below, NAO^+ above, and NAO^- slightly to the right of this maximum, respectively. These four regimes are not identical to but in fairly good agreement with the observational results of Cheng & Wallace (1993) and Smyth *et al.* (1999); see also Ghil & Robertson (2002) and Kondrashov *et al.* (2004, 2006).

The streamfunction anomalies associated with each regime centroid of the QG3 model are plotted in Fig. 2.6. The spatial correlations between these anomaly patterns and those obtained from the EMR model (not shown) all exceed 0.9. They are thus much higher than the correlations obtained by D’Andrea & Vautard (2001) and D’Andrea (2002), who used a reduced deterministic model obtained by a statistical–dynamical approach to reproduce the behaviour of the largest scales in the QG3 model. We have also computed Gaussian-mixture PDFs of the MTV model simulations (not shown), which however failed to reproduce the PDFs of the full QG3 model (see Fig. 16 of Strounine *et al.* 2008).

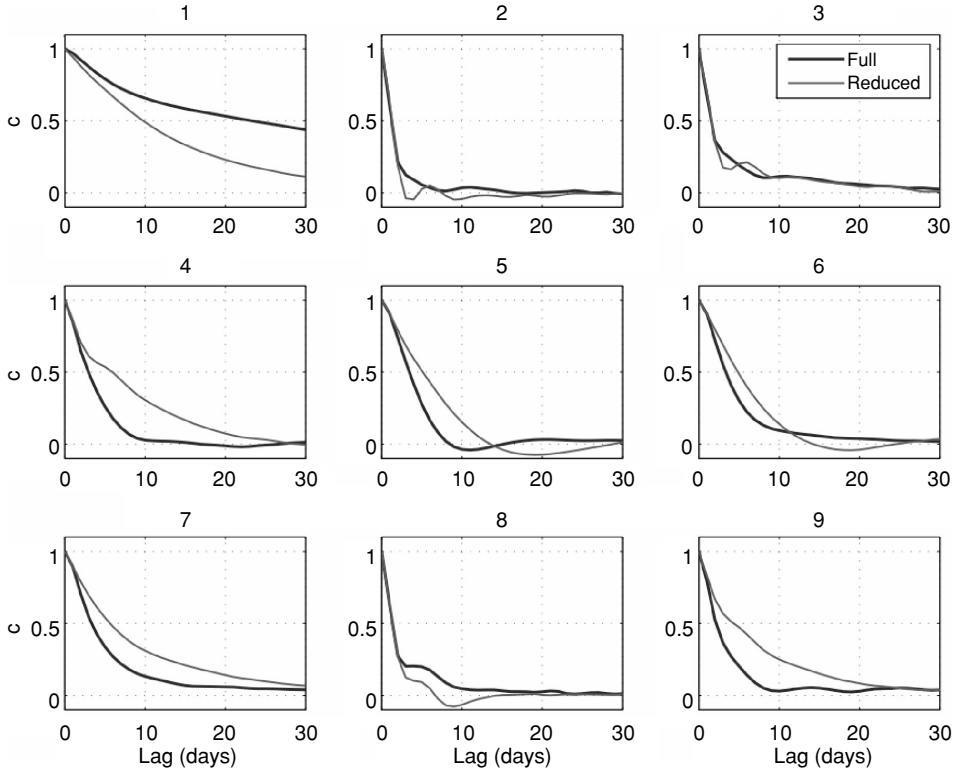


Figure 2.4 Same as Fig. 2.2, but for the MTV model.

The results above indicate a fair degree of success of the EMR models in capturing key characteristics of the QG3 model. Kondrashov *et al.* (2006) built upon this success and conducted a detailed study of the origin of the QG3 model's multiple regimes and low-frequency oscillations, and of possible connections between them. They showed how to use the EMR models' much greater flexibility in studying the dynamic and stochastic contributions to these episodic and oscillatory features present in the QG3 model, as well as in atmospheric observations of low-frequency variability (LFV); see also Ghil and Robertson (2002) and Ghil *et al.* (2003). Kondrashov *et al.* (2006) applied standard tools from numerical bifurcation theory for deterministic dynamical systems to the quadratically nonlinear deterministic operator of their optimal EMR model, and used a continuation method on the variance of the multilevel noise process. This somewhat ad hoc combination of continuation methods allowed them to move all the way from fixed points of the deterministic operator to the multiple regimes of the complete EMR model, with its optimal parameter values.

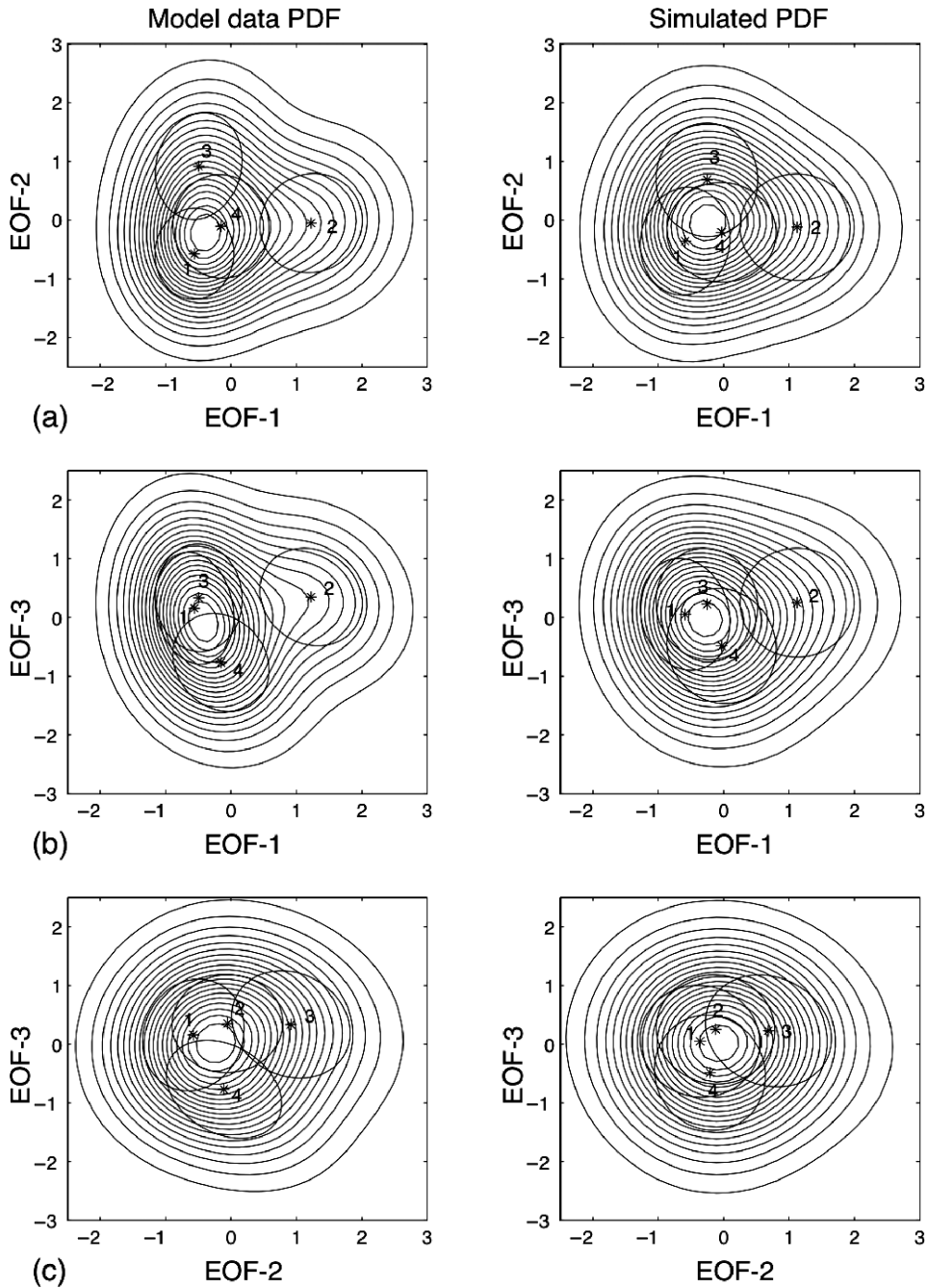


Figure 2.5 PDFs of the QG3 model (left panels) and EMR model (right panels), projected onto the planes of the three leading EOFs: (a) EOF-1–EOF-2; (b) EOF-1–EOF-3; and (c) EOF-2–EOF-3. The ellipses superimposed on the PDFs are obtained by Gaussian-mixture modelling. Cluster centroids are plotted as asterisks, while projections of cluster boundaries are shown as ellipses, the semi-axes of which equal one standard deviation of the cluster, in each direction. Shown are projections onto EOF planes: the cluster centroid indices correspond to AO^+ , AO^- , NAO^+ and NAO^- , in this order (see text and Fig. 2.6). Reproduced from Kravtsov *et al.* (2005b), with the permission of the American Meteorological Society.

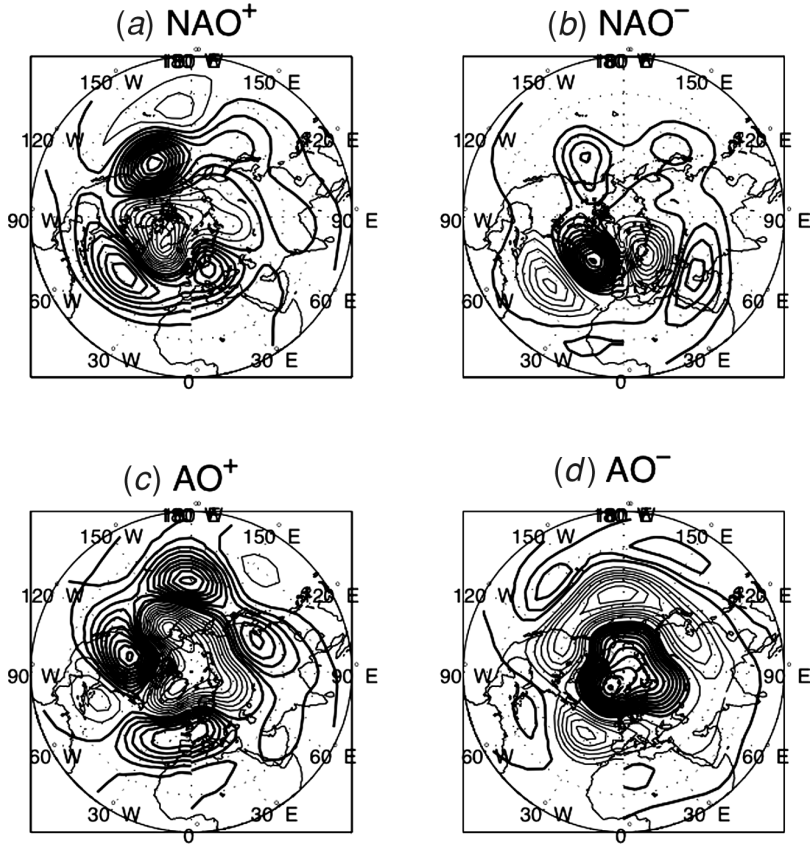


Figure 2.6 Mixture-model centroids, showing streamfunction anomaly maps at the middle level of the QG3 model: (a) NAO^+ ; (b) NAO^- ; (c) AO^+ ; (d) AO^- . Contour interval (CI) is $10^6 \text{ m}^2 \text{ s}^{-1}$; heavy contours: positive anomalies, light contours: negative anomalies.

An attractive feature of EMR methodology is its flexibility with respect to the basis functions in which the model is constructed; for example, in fitting the behaviour of the above QG3 model, the EMR models work equally well in the streamfunction or energy-norm bases. Much like the linear operator of LIM models (2.4) differs from that of the truncated linear part of the full governing equations (2.3b), the EMR's nonlinear operator is also different from its bare-truncation counterpart. Therefore, irrespective of the basis used and in spite of other useful features of the EMR models, a cautionary note is in order: the stability of the EMR model is not guaranteed, since the empirical fit does not conserve quadratic invariants of the QG3 model, but rather parameterises all the important interactions within a given functional form of the EMR model. In contrast, an MTV model constructed in a basis that conserves quadratic invariant(s) is stable, as long as this

stability is not affected by the additional, semi-empirical coefficients. We will return to a point-by-point comparison of EMR with other mode reduction methodologies in Section 2.6.

Since the EMR procedure is entirely data based, it can be applied directly to the observational data sets, for which the full model does not have to be known. For example, Kravtsov *et al.* (2005b) studied low-frequency variability in the observed Northern Hemisphere's geopotential heights by constructing a nine-variable, two-level EMR model thereof; they were able to reproduce the multidimensional PDF and power spectra of the observed fields, with a quantitative success that is quite similar to the QG3 model fit discussed here. It turned out, however, that the EMR model's dynamical operator in this case does possess unstable directions, which led to occasional run-away model realisations with unphysically large values of the model variables, consistent with the lack of quadratic invariants mentioned above. These authors developed a simple strategy to avoid such rare situations altogether, by tracking the instantaneous norm of the EMR model's state vector. If the values of this norm exceeded a certain threshold, the time series being modelled were 'rewound' by a few time steps and restarted with a different realisation of the random forcing.

In summary, the EMR methodology provides a means to construct skillful nonlinear reduced models with stochastic forcing that need not be white in time. Empirical model reduction models are based solely on the data output from a full dynamical model, or directly on observational data. Regularisation techniques ensure that the number of independent regression coefficients to be estimated in an EMR model is much smaller than the number of variables in the full model or the number of coefficients in the absence of regularisation. While the stability of a nonlinear EMR model is not guaranteed a priori, simple engineering fixes are available to avoid unstable directions in the empirical model's dynamical operator. The EMR model based on QG3 output reproduces key features of the full model better than the models based on alternative methodologies, such as that of Selten (1995), D'Andrea (2002) or MTV, and can thus be used for a detailed dynamical and stochastic diagnosis of the full QG3 model (Kondrashov *et al.* 2006).

2.4 Modelling of tropical sea-surface temperatures (SSTs)

The EMR methodology can be used to simulate and predict phenomena whose dynamical modelling requires fairly complex and computationally expensive models. Among such phenomena is the ENSO, which dominates interannual climate signals centered in the tropical Pacific Ocean (Philander 1990), and has a substantial effect on the atmospheric circulation and air-sea interaction through many parts of the globe, via atmospheric or oceanic teleconnections (Alexander *et al.* 2002).

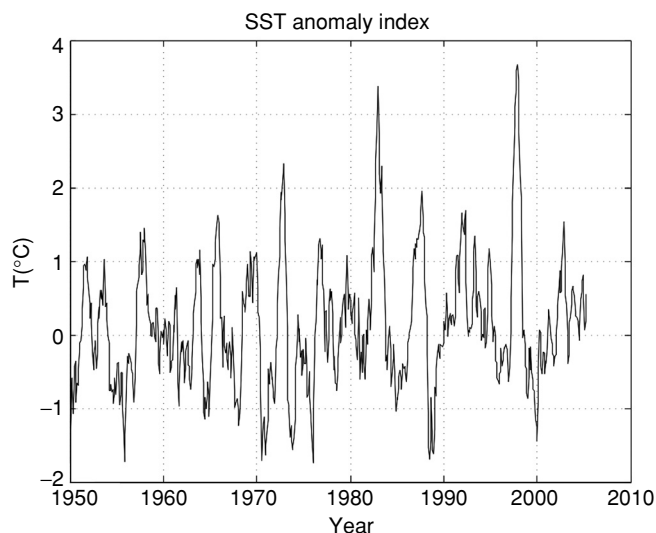


Figure 2.7 Time series of Niño-3 index, defined as the sea-surface temperature (Kaplan *et al.* 1998) averaged over the rectangular box (5° S– 5° N, 150° – 90° W); this box is also outlined in light solid black in Fig. 2.8a,b.

Figure 2.7 shows a widely used index of ENSO activity, the so-called Niño-3 index, computed as the average of SST over a rectangular box located in the tropical Pacific, with coordinates (5° S– 5° N, 150° – 90° W). The pronounced positive-anomaly events in this time series are associated with warm, El Niño episodes in the eastern tropical Pacific, while the negative events point to La Niña conditions. A striking property of ENSO is that El Niño events are in general stronger than La Niñas, thus suggesting that the dynamics of ENSO involves nonlinear processes (Neelin *et al.* 1994, 1998; Ghil & Robertson 2000). At the same time, most detailed numerical models used for operational ENSO predictions significantly underestimate this nonlinearity (Hannachi *et al.* 2003), and the quality of their forecasts is still far from satisfactory (Barnston *et al.* 1994, 1999; Ghil & Jiang 1998; Landsea & Knaff 2000).

Kondrashov *et al.* (2005) constructed a 20-variable, single-level (1-L) and two-level (2-L) EMR models of ENSO based on a 645-month-long monthly time series of SST anomalies given on a $5^{\circ} \times 5^{\circ}$ grid over the 30° S– 60° N latitude belt (Kaplan *et al.* 1998). Despite the seasonal cycle having been removed from the observed time series, the EMR models were extended to include seasonal dependence by making the main-level linear operator's coefficients 12-month periodic and estimating additional regression parameters in the usual way.

Figure 2.8 displays the cross-validated hindcast skill of the 1-L and 2-L EMR models; the skill was defined in terms of anomaly correlation between

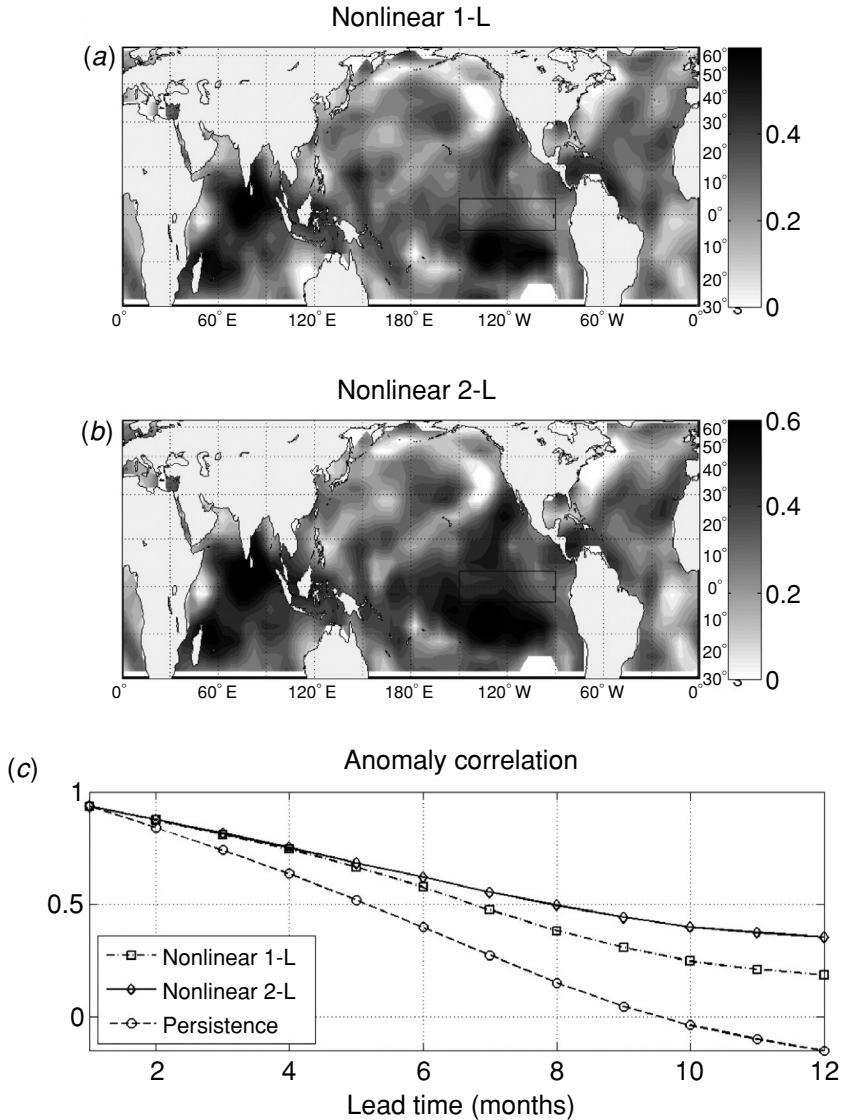


Figure 2.8 Comparison of predictive skill for one-level (1-L) and two-level (2-L) EMR models. Anomaly correlation map for nine-month-lead cross-validated hindcasts using (a) the 1-L model and (b) the 2-L model. (c) Niño-3 hindcast skill in terms of anomaly correlation for the 1-L model (dash-dotted line with squares) and the 2-L model (solid line with diamond symbols), with damped persistence forecast (dashed line with circles) being used as a reference skill. The Niño-3 SST anomaly is defined as the area average over the rectangular box shown in panels (a) and (b). Adapted from Kondrashov *et al.* (2005), with the permission of the American Meteorological Society.

the actual and forecasted time series of SST anomalies. The geographical distribution of the 9-month-lead skill is shown in panels (a) and (b) for the 1-L and 2-L models, respectively. Note that while the skill patterns for both models are fairly similar, the 2-L EMR model is significantly more skillful compared to its 1-L counterpart. This is the case for other lead times, as shown for the Niño-3 index forecast (Fig. 2.8c); note that the anomaly correlation of 0.5–0.6 is considered fairly useful for planning purposes. The skill of the 2-L quadratic EMR model with seasonal dependence is fairly competitive with that of fully coupled atmosphere–ocean GCMs; see also the results of a multimodel prediction scheme implemented by the International Research Institute (IRI) for climate and society: http://iri.columbia.edu/climate/ENSO/currentinfo/SST_table.html.

The ability of EMR models to capture nonlinearity and seasonal dependence of ENSO is best illustrated using box-plot statistics (e.g. Hannachi *et al.* 2003), which show the spread around the mean and skewness of a given time series, as well as its outliers.

Figure 2.9 shows the box plots of the observed Niño-3 index (Fig. 2.9a), along with those of ensemble simulations of the 2-L linear and quadratic EMR models (Figs. 2.9b,c). The linear model was obtained using full EMR methodology of Section 2.2, augmented by the seasonal dependence of regression coefficients at the main level, except that nonlinear predictors in the main level of (2.13) were neglected throughout the procedure. The linear EMR model is successful in describing the seasonal dependence of the Niño-3 variance, with maximal variability in boreal winter; compare panels (a) and (b). It does not, however, capture the positive skewness of the observed Niño-3 time series, while the quadratic EMR model does; compare panels (a) and (c).

Kondrashov *et al.*'s (2005) most comprehensive and skilful quadratic EMR model with seasonal dependence had 20 state variables at the main level, and one additional level. These authors showed that this model's forecast capabilities were due to its ability to capture ENSO's leading quasi-quadrennial (Jiang *et al.* 1995) and quasi-biennial oscillatory modes. As pointed out by Ghil & Jiang (1998) and Ghil & Robertson (2000), capturing these two modes is of the essence for successful ENSO prediction beyond six months. Kondrashov *et al.* (2005) demonstrated that these modes are present as inherent periodicities within the dynamical operator of their EMR model, by carrying out month-by-month linear stability analyses, as well as Floquet analysis of the model's seasonal cycle (Strong *et al.* 1995; Jin *et al.* 1996).

To summarise, EMR methodology allows one to come up with a skillful predictive model and then use it to study the dynamical causes of the observed variability in situations in which comprehensive dynamical models based on first principles are either unavailable or else very complex and difficult to interpret.

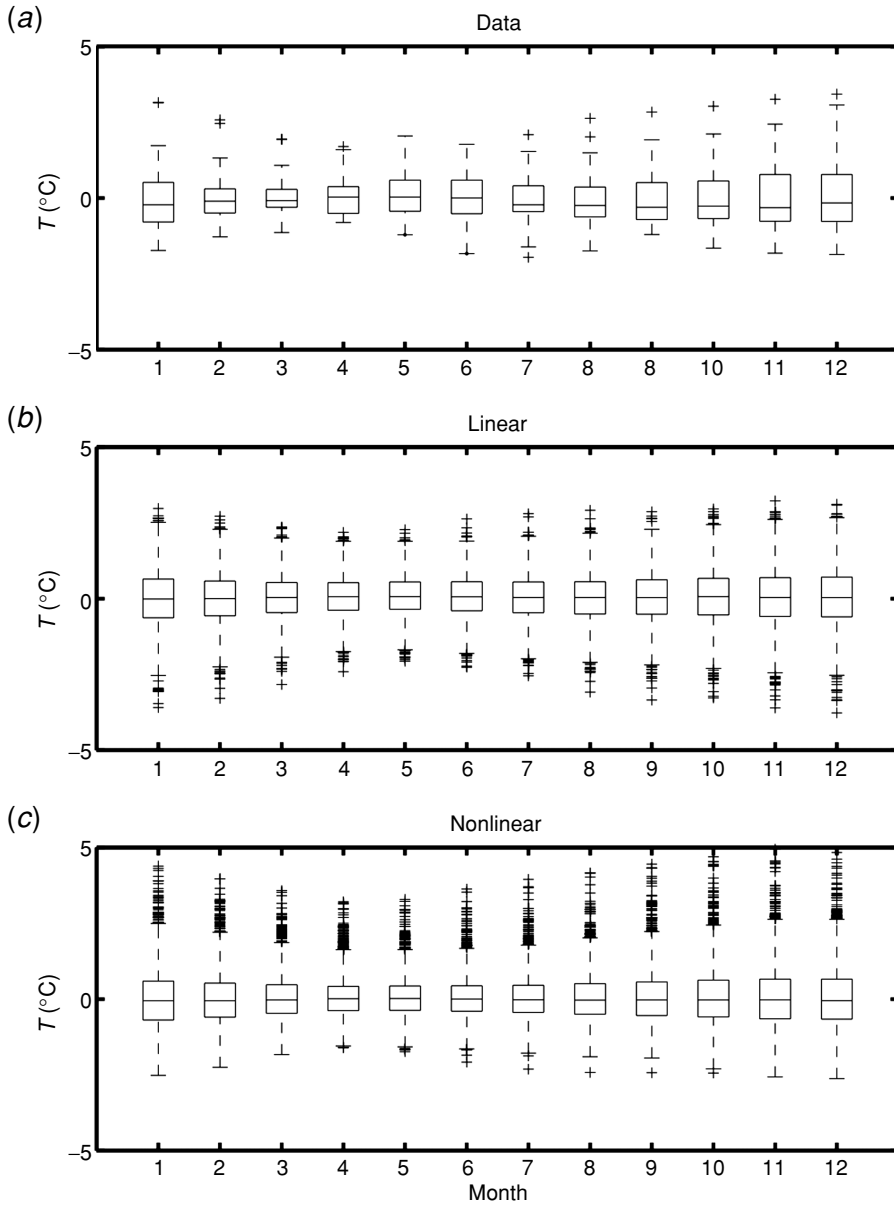


Figure 2.9 Seasonal dependence of EMR model fit to ENSO statistics, visualised as box-plot statistics for each month of the year, for (a) the observed Niño-3 index (1950–2003); (b) a 100-member ensemble of 645-month-long runs of the 2-L linear EMR model; and (c) same as in (b), but for the quadratic EMR model. The horizontal line within each box marks the median, while the height of the box represents the interquartile range (IQR), which is defined as the distance between the first and the third quartiles and is a robust measure of spread. The whiskers represent the most extreme data values within $1.5 \times \text{IQR}$, while points beyond the last of the whiskers represent outliers and are indicated by individual tick marks. Reproduced from Kondrashov *et al.* (2005), with the permission of the American Meteorological Society.

2.5 Stochastic parameterisation of air–sea interaction over the Southern Ocean

Another possible application of the EMR models we discuss here is to parameterise certain processes within a more complex dynamical model. The processes considered in this section pertain to air–sea interaction over the Southern Ocean. To this end, Kravtsov *et al.* (2008) have analysed five years of remotely sensed data sets of SSTs and sea-level wind (SLW; Liu 2002) over the Southern Ocean. The microwave sensors installed on recently launched NASA satellites provide an unprecedented quantity and quality of observations in this otherwise poorly known but important part of the world ocean (Kawanishi *et al.* 2003).

The EMR model of SLW over the Southern Ocean developed by Kravtsov and colleagues describes the evolution of winds in the phase subspace of 100 leading vector-wind EOFs, and also accounts for ocean–atmosphere coupling via dependence of the SLW equations on the SST anomalies; the latter anomalies are represented in the subspace of the 75 leading EOFs of the SST field. The larger number of EOFs required, in both SST and SLW, is due to the need to span a considerable range of spatial scales. The best EMR model has three levels, including the bilinear main level, in which the products of SST and SLW variables are also included as predictors, in addition to linear terms; the main level includes seasonal forcing, too, as described in Section 2.4.

This model captures detailed features of SLW variability on a wide range of time scales, from daily to interannual, and spatial scales spanning the range from hundreds of kilometres to the basin scale. Note that capturing details of non-local aspects of the SLW variability, i.e. teleconnections – along with the local aspects – is essential for the intended coupling of the EMR model to a more comprehensive climate model.

Kravtsov *et al.* (2008) also showed evidence for the coupled dynamics at work behind certain aspects of SLW variability. In order to do so, they computed ensemble-averaged evolution of the SLW anomalies for a 100-member ensemble using the EMR model forced by the history of the observed SST anomalies; the ensemble members differed by the realisation of the third-level white-noise process. This SST-driven evolution was compared with the evolution for the SLW-only stochastic model, in which SST anomalies were artificially set to zero. The authors then computed the standard deviation, in time, of the ensemble-averaged wind speed for both cases, at each grid point: the results of this computation for the SST-forced model are shown in Fig. 2.10.

The standard deviation in the SST-dependent case is much larger, at all grid points, than that in the SLW-only case (not shown). Its distinctive large-scale spatial pattern suggests that this SLW variability is forced by long-term, ocean-induced

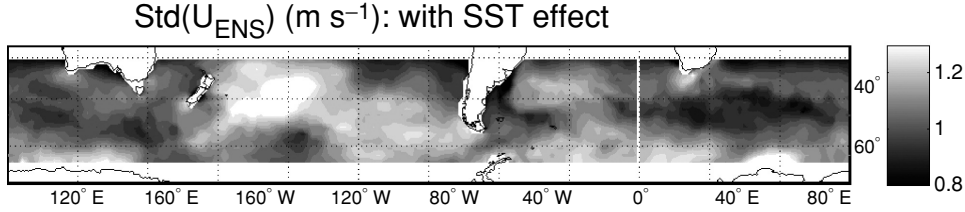


Figure 2.10 Sea-surface temperature effect on the sea-level wind as modelled by the EMR model of air–sea interaction over the Southern Ocean (65° – 30° S). Shown is the standard deviation of the wind speed time series near sea level. These time series, at each spatial grid point, were computed as the ensemble average of 100 simulations of the EMR model constructed in the phase space of 100 leading EOFs of sea-level wind and forced by the observed history of SST anomalies.

SST anomalies. Bretherton & Battisti (2000) proposed alternative explanations to such findings in the atmospheric GCMs forced by North Atlantic SSTs. On the other hand, Goodman & Marshall (1999) formulated a theory of interannual-to-decadal coupled variability that is potentially applicable to the Southern Ocean. Their theory predicts the existence of coupled modes, given a certain spatial phase relationship between SST patterns and SST-induced SLW anomalies; this phase relationship gives rise to Ekman pumping anomalies that force and modify the oceanic circulation and the associated SST field. One possible use of the EMR model would be to check whether it supports such a phase relationship between SLP and SLW on interannual time scales.

Another very promising way to apply the EMR model of SLW is, however, to couple it to an oceanic general circulation model. This can be achieved by blending the SST-dependent SLW model with the atmospheric boundary layer model of Seager *et al.* (1995). The latter model needs the specification of boundary-layer winds to compute ocean–atmosphere heat fluxes. These winds can be supplied by the EMR model, and would then be used to compute the atmosphere–ocean momentum flux. The ocean model forced by heat, moisture and momentum fluxes will, in turn, predict the evolution of the SST field, which will affect the future SLW anomalies. Experiments with such a hybrid coupled GCM of the Southern Ocean regions are currently underway; they may provide valuable insights into the dynamics of climate variability there.

2.6 Concluding remarks

2.6.1 Summary

We developed a systematic, albeit empirical strategy for constructing parsimonious, dynamic–stochastic models that are able to capture key aspects of a given climate

subsystem's evolution. Our approach, called Empirical Model Reduction (EMR) is indeed fully empirical, being based entirely on utilising the information embedded in the observed or simulated time series, via parametric regression fitting (see Section 2.2); in other words, our methodology doesn't use, or require at all, the knowledge of the true, and presumably much more complex, dynamical model that governs the evolution of the climate subsystem under consideration.

The EMR models are extensions of the linear inverse models (LIMs) of Penland and associates (Penland 1989, 1996; Penland & Ghil 1993) that may include quadratic – and higher-order polynomial, if necessary – combinations of predicted variables in the dynamical operator of the main model level; additional model levels are also included to capture the lagged autocorrelations possibly present in the main-level stochastic forcing. The number of model levels is chosen to ensure that the forcing at the last level can be well approximated by a vector-valued white-noise process. The stochastically forced simulations of an EMR model can then be exploited to analyse various aspects of the actual, observed evolution of the system or one that is generated by a high-end model thereof. The actual regression fitting of an EMR model's coefficients is carried out by regularisation methods, such as principal component regression (PCR; Press *et al.* 1994) and partial least-squares (PLS; Abdi 2003); these methods substantially reduce – by as much as two orders of magnitude, depending on the particular problem at hand – the number of independent coefficients to be estimated (see Appendices A and B).

Section 2.3 documents a remarkable success of EMR methodology in reducing a fairly sophisticated, nonlinear model of the extra-tropical atmosphere, with more than a thousand degrees of freedom (the QG3 model: Marshall & Molteni 1993) to a dynamic–stochastic model with ten main-level variables and $O(100)$ independent coefficients. The original QG3 model is well known for having a fairly realistic climatology and complex variability, which also compares favourably with the observed atmospheric behaviour. The coefficients here were estimated based on a 30 000-day-long simulation of the full QG3 model.

The EMR model accurately reproduces non-Gaussian features of the PDF of the full model, computed in the phase subspace of the ten resolved variables (see Figs. 2.1, 2.2, 2.5 and 2.6 here). It also reproduces surprisingly well the intraseasonal oscillations (Ghil *et al.* 2003) that characterise the full QG3 model's low-frequency variability (Kravtsov *et al.* 2005b; Kondrashov *et al.* 2006). Kondrashov *et al.* (2006) studied the deterministic operator of the EMR model, as well as its stochastic forcing, to analyse the dynamical causes behind the persistent and recurrent states associated with the non-Gaussian PDF, the intraseasonal oscillations, as well as the connections between the two (see also Ghil & Robertson 2002). Kondrashov and colleagues applied standard tools from numerical bifurcation theory for deterministic dynamical systems to the quadratically nonlinear deterministic

operator of their optimal EMR model, and used a continuation method on the variance of the multilevel noise process. This somewhat ad hoc combination of continuation methods allowed them to move all the way from fixed points of the deterministic operator to the multiple regimes of the complete EMR model.

In situations when the full dynamical model is not available, or otherwise is very complex and difficult to implement efficiently or to interpret, the EMR methodology can be used to set up a competitive analysis and prediction scheme for the phenomena of interest. Section 2.4 illustrates the predictive capabilities of an EMR-based model using the example of tropical sea-surface temperature (SST) evolution (Kondrashov *et al.* 2006; see Fig. 2.7 here). Their 20-variable, three-level EMR model with quadratic main-level and seasonally-dependent coefficients in its linear part has a forecast skill in predicting El Niño–Southern Oscillation (ENSO) events that is comparable with that of state-of-the-art dynamical and statistical models (see Fig. 2.8). The EMR prediction scheme of these authors is currently a member of the multimodel forecast ensemble developed by the International Research Institute (IRI) for Climate and Society.

The successful EMR forecasts are rooted in the EMR model’s ability to capture major oscillatory signals associated with ENSO behaviour; namely, the quasi-quadrennial and quasi-biennial oscillations (Jiang *et al.* 1995). These signals can be explained in terms of eigenmodes of the EMR model’s dynamical operator (Kondrashov *et al.* 2006). In addition, the nonlinear EMR model successfully reproduces the observed asymmetry between larger positive (El Niño) and smaller negative (La Niña) anomalies of the ENSO cycle (see Fig. 2.9), as well as the seasonal dependence of ENSO predictability, including the well-known ‘spring barrier’ to interannual forecast skill.

The EMR models can also serve to parameterise stochastically a subset of processes within a more complex dynamical model. As an example, Section 2.5 outlines a strategy for coupling an EMR model of air–sea interaction over the Southern Ocean with a comprehensive ocean model. In this case, the EMR modelling bypasses dynamical consideration of a fairly complex chain of SST effects on the sea-level winds (SLWs) to construct a statistical model of SST-dependent SLW evolution (Kravtsov *et al.* 2008). The subsequent coupling uses SST fields produced by the ocean model to force the EMR and predict SLW distribution. This distribution affects in turn the atmospheric boundary layer and atmosphere–ocean heat, moisture and momentum fluxes, and, therefore, the oceanic variables.

The EMR model used here has 100 SLW variables and 75 SST variables, and features a bilinear SST–SLW main-level structure. This fairly large model dimension is necessary since coupling to the ocean model requires a wide range of spatial scales in the simulated SLW field. Note that, despite a fairly short five-year training interval and large number of predictors, the regularisation techniques described

in Appendices A and B are successful in obtaining robust model coefficients: the model's dynamical operator is stable and simulates well both local and non-local statistical properties of the observed SLW. These results (see Fig. 2.10) demonstrate the applicability of the EMR methodology to problems of intermediate size.

Finally, the EMR methodology is in no way restricted to the problems of climate dynamics; EMR modelling has also been applied to describe the variability of the Earth's radiation belts (Shprits 2009, personal communication).

2.6.2 Discussion

The EMR models belong to a class of multivariate parametric stochastic models forced by additive, state-independent noise. Alternative statistical formulations used in climate dynamics involve empirical fitting to the Fokker–Planck equation (Gardiner 1985). Such fits result in non-parametric, univariate or bivariate models that include state-dependent or multiplicative noise (Sura 2003; Sura & Gille 2003; Sura *et al.* 2006; Sura & Newman 2008; Sura & Sardeshmukh 2008). The extreme truncation of these models to one or two dimensions only is due to the limited amount of data, which is typically insufficient to obtain reliable estimates of higher-dimensional analogues of drift and diffusion coefficients.

This approach is therefore applied either to scalar teleconnection indices (Feldstein 2000; Stephenson *et al.* 2000) or to the time series of a climatic field at a single location. In the latter case, in order to get reliable estimates of model parameters given relatively sparse observations, one may also concatenate data sets from multiple locations, which are situated far enough from each other so that their respective time series may be assumed to be uncorrelated (Sura 2003). The scalar stochastic differential equations so obtained describe local features of interactions between processes evolving on different time scales. They are successful in interpreting certain non-Gaussian aspects of SLW (Sura 2003; Monahan 2004, 2006a,b), as well as of SST (Sura *et al.* 2006; Sura & Newman 2008; Sura & Sardeshmukh 2008) variability. These stochastic models are not suitable, however, for modelling non-local aspects of climatic variability (compare the results of Deloncle *et al.* 2007, with those of Sura *et al.* 2005); the ability to capture non-local effects is a considerable advantage of the EMR-based models.

Sura *et al.* (2005) applied the above methodology to explain non-Gaussian features in the phase subspace of the observed atmospheric winds in terms of dynamics involving multiplicative noise. Berner (2005) and Branstator & Berner (2005) independently used similar ideas to analyse long output from an atmospheric GCM. Kravtsov & Branstator (2006, personal communication) performed EMR modelling of the same GCM simulation and produced surrogate time series, whose

statistical properties were subsequently analysed by estimating the drift and diffusion matrices of planar subspaces of the EMR-simulated data. The drift and diffusion coefficient structure, as well as the mean phase-space tendencies computed for the EMR-based surrogate were very similar to those based on the GCM-generated data set.

These results demonstrate that the multiplicative-noise explanations of non-Gaussian atmospheric behaviour depend on how the climate ‘signal’ and ‘noise’ are defined; in the EMR approach, the signal and the noise are equivalent to the unresolved and resolved variables. For example, for the EMR model of Kravtsov and Branstator, with its nine resolved variables, the non-Gaussianity is clearly due to quadratic nonlinearity in the model’s deterministic propagator. On the other hand, if only the two leading EMR variables are interpreted as signal, and the others as ‘noise,’ the same quadratic combinations of the first two variables with the rest become manifestations of multiplicative noise. The same comments apply to attribution of various features in the phase-subspace mean tendencies to either interaction between the resolved modes or that between the resolved and unresolved modes (Franzke *et al.* 2007; Majda *et al.* 2008).

Purely empirical models, such as the EMR models, are very flexible in their choice of predictor fields, including bases other than EOFs, such as those proposed by Kwasniok (1996, 2004) and DelSole (2001); see also Crommelin & Majda (2004). These models are in general not limited by various restrictions and constraints inherent to reduction methods that are based entirely or to a large extent on properties of the full governing equations. This flexibility of empiricism comes, however, at the expense of the lack of an easy, immediate interpretation of results in terms of formal model properties, such as that offered, at least at first sight, by the latter methods. The simplest approach of incorporating dynamical information into simplified models of geophysical flows is to linearise the full governing equations with respect to their long-term time-mean state and introduce a combination of linear damping and stochastic forcing terms to achieve time-variable climates that resemble those of the full nonlinear model (Branstator 1992, 1995; Farrell & Ioannou 1993, 1995; Zhang & Held 1999; DelSole 2004).

Another possibility is to follow an empirical–dynamical approach and write the governing equations in a truncated EOF basis, while parameterising the interaction between the resolved and unresolved modes empirically (Selten 1993, 1995; Achatz & Branstator 1999; D’Andrea & Vautard 2001; D’Andrea 2002; Achatz & Opsteegh 2003a,b). Finally, Majda *et al.* (1999, 2001, 2002, 2003, 2006; abbreviated as MTV) presented a model reduction methodology based on standard projection methods for stochastic differential equations (Khasminsky 1963; Kurtz 1973; Gardiner 1985), which is rigorously correct for systems with

substantial time-scale separation between the resolved and unresolved modes; in some cases, these results carry over to the situations without such a spectral gap (Majda *et al.* 2002, 2003; Majda & Timofeyev 2004). However, when applied to prototype barotropic (Franzke *et al.* 2005) and baroclinic (Franzke and Majda 2006) atmospheric models, the results are less striking (see our Section 2.3 here and Strounine *et al.* 2008), presumably due to the fairly continuous atmospheric power spectra violating the main assumption of the MTV methodology.

In general, Strounine *et al.* (2008) found that reduced models with an equal number of resolved variables perform better when a larger amount of statistical information is used in model construction. Thus, the EMR models with quadratic nonlinearity and additive noise reproduce very well spectral properties of the full model's variability, such as autocorrelations and spectra, as well as the model's, and the extra-tropical atmosphere's, multiple flow regimes that induce non-Gaussian features in the model's PDF. The empirical-dynamical models capture some of the basic statistical properties of the full model's variability, such as the variance and integral correlation time scales of the leading PCs, as well as some of the regime-behaviour features; but they fail to reproduce the detailed structure of autocorrelations and distort the statistics of the regimes. The MTV-type models that use sequential estimation of additional parameters (see also Section 2.3 here) do capture the univariate statistics of the leading PCs to a degree comparable with that of empirical-dynamical models, but do much less well on the full model's nonlinear dynamics, in particular on its multivariate PDF.

The EMR methodology thus occupies by now an important position at the lower and intermediate rungs of the full climate modelling hierarchy (Schneider & Dickinson 1974; Ghil & Robertson 2000; Held 2005). Further improvements in reduced models of various types can only benefit from, and to, a more complete and systematic exploration of this hierarchy.

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Appendix A. PCR and PLS regression

The multicollinearity problem can be avoided by finding linear combinations of original predictors whose time series are uncorrelated, while each linear combination accounts for the maximum possible fraction of the total variance. A natural way to determine this modified set of predictors is to apply PC analysis to the original vector of predictors, and then use cross-validation for finding the optimal number of PCs to retain in the regression; this procedure is called principal component regression (PCR; Wetherill 1986). Note that for the LIM model constructed in the phase space of the data set's EOFs (Penland 1989, 1996), the predictor variables are already uncorrelated. On the other hand, the predictors in the main level of (2.13) are the original set of PCs augmented by their quadratic combinations. Therefore, applying PC analysis to this new multivariate data set generally produces a different set of predictors.

Principal component regression does a fairly good job in picking the smallest set of uncorrelated predictors that capture most of the variance. However, the choice of the PCR predictors does not involve at all the information about how well these predictors are correlated with the response variable. The procedure that does take into account this additional information is called partial least-squares (PLS) regression; see Abdi (2003) for a brief, but comprehensive review. It is reasonable and advisable to apply PLS to the set of optimal predictors determined via PCR cross-validation, rather than to the original, much larger set of predictors.

Similarly to the PCR procedure, the leading PLS predictor is defined as a linear combination of the original predictor time series, but in this case the quantity being maximised is the correlation between this time series and the predictor time series. We found that applying PLS to each response variable, i.e. to each model tendency in (2.13), individually produces better results than the matrix formulation of the PLS algorithm; in the latter, one also considers linear combinations of all response variables and finds two sets of coefficients that define the mode of response and the mode of predictor variables that are maximally correlated (Abdi 2003). In the general multivariate case, the weights of the leading PLS mode are found using singular value decomposition (SVD; Press *et al.* 1994) as the first right singular vector of the matrix $\mathbf{X}^T\mathbf{Y}$, where $\mathbf{X}$ and $\mathbf{Y}$ are the matrices whose columns are the time series of the predictor and response variables, respectively. The right singular vectors of $\mathbf{X}^T\mathbf{Y}$ define the weights for the response variables; in the univariate case, the single such weight is naturally equal to 1.

The time series of the leading PLS mode is obtained by summing the original time series of the predictor variables with the weights obtained as above. The signal associated with the leading PLS mode is then regressed out of the response-variable time series, as well as out of all the predictor time series; once again, we only retain

the residual of the linear regression of each of these time series onto the time series associated with the leading PLS mode. The procedure just described is then applied to the ‘reduced’ response and predictor time series to obtain the next PLS mode, and so on. The optimal number of modes to retain in this PLS procedure is also determined by cross-validation.

Appendix B. Selection of predictor variables

A few regression coefficients found by the application of PCR and PLS regularisation, as described in Appendix A, can be translated by trivial matrix manipulation into the coefficients of the EMR model in the original predictor-variable basis. Many of these coefficients are fairly small and do not contribute much to the predictive capability of the EMR model. The following procedure iteratively fine-tunes the selection of the predictor variables by throwing out original predictors whose corresponding regression coefficients are not significantly different from zero (Kravtsov *et al.* 2008).

This selection procedure is also based on subsampling of the original predictor and response variables. We first obtain 100 sets of regression coefficients by applying PCR-and-PLS regularisation to 100 randomly sampled subsets of the full original time series, each of which includes 80% of the original data points. The regression coefficients so obtained are then translated into the original predictor-variable space.

Now if the interval between the 2nd and 97th percentile of a given regression coefficient obtained as described above contains zero, we exclude the corresponding predictor variable from consideration, thus forming a new, smaller subset of predictor variables. This subset is in turn subsampled 100 times and subjected to PCR and PLS regression to identify coefficients not significantly different from zero, and so on, until all coefficients of the final set of predictors are found to be significant. The final regression coefficients are then found by applying the PCR-and-PLS regularisation to the fully sampled set of optimal predictors.

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