

Multi-pattern fingerprint method for detection and attribution of climate change

K. Hasselmann

Max-Planck-Institut für Meteorologie, Bundesstrasse 55, D-20146 Hamburg, Germany

Received: 19 April 1996 / Accepted: 21 April 1997

Abstract. The multi-variate optimal fingerprint method for the detection of an externally forced climate change signal in the presence of natural internal variability is extended to the attribution problem. To determine whether a climate change signal which has been detected in observed climate data can be attributed to a particular climate forcing mechanism, or combination of mechanisms, the predicted space–time dependent climate change signal patterns for the candidate climate forcings must be specified. In addition to the signal patterns, the method requires input information on the space–time dependent covariance matrices of the natural climate variability and of the errors of the predicted signal patterns. The detection and attribution problem is treated as a sequence of individual consistency tests applied to all candidate forcing mechanisms, as well as to the null hypothesis that no climate change has taken place, within the phase space spanned by the predicted climate change patterns. As output the method yields a significance level for the detection of a climate change signal in the observed data and individual confidence levels for the consistency of the retrieved climate change signal with each of the forcing mechanisms. A statistically significant climate change signal is regarded as consistent with a given forcing mechanism if the statistical confidence level exceeds a given critical value, but is attributed to that forcing only if all other candidate climate change mechanisms (from a finite set of proposed mechanisms) are rejected at that confidence level. Although all relations can be readily expressed in standard matrix notation, the analysis is carried out using tensor notation, with a metric given by the natural-variability covariance matrix. This simplifies the derivations and clarifies the invariant relation between the covariant signal patterns and their contravariant fingerprint counterparts. The signal patterns define the reduced vector space in which the climate trajectories are analyzed, while the fingerprints are needed to project the climate trajectories onto this reduced space.

1 Introduction

There is mounting evidence that the global warming due to increasing atmospheric greenhouse gas concentrations predicted by state-of-the-art coupled ocean-atmosphere global circulation models (CGCMs) is beginning to emerge from the background noise of natural climate variability (see summary in IPCC Second Assessment Report, Santer et al. 1996a). However, much of the evidence is still qualitative or circumstantial. There have been relatively few attempts to assign a quantitative measure to the probability that a climate change signal distinct from natural climate variability can be detected in observed climate data.

A basic obstacle for quantitative signal-to-noise analyses is that they require information on the space–time structure of both the predicted climate signal and the climate variability. While the predicted signal properties can be inferred from model computations, the estimation of the required space–time covariance structure of natural climate variability from model simulations and observations is more difficult. Thus, although general multi-variate theories for the optimal detection of a space–time dependent climate change signal in the presence of natural climate variability noise have now been developed (Hasselmann 1979; Bell 1982, 1986; Hasselmann 1993, referred to in the following as H; North et al. 1995; North and Kim 1995; Hegerl and North 1997), there have been relatively few quantitative applications of these methods (Santer et al. 1995a; Hasselmann et al. 1995; Hegerl et al. 1996, 1997). The latter authors conclude (with various caveats regarding the uncertain estimation of the natural climate variability) that a climate change signal distinct from internal natural climate variability can be detected today with a statistical significance exceeding 95%. We refer to Santer et al. (1996a) for a more complete summary of recent detection studies.

The theoretical formulation of the attribution problem appears to have received less attention than the theory of detection. The problem of attributing a detected climate change signal to a given forcing mechanism has been variously discussed in the literature, but the investigations have been largely qualitative. With the exception of the

recent investigation of Hegerl et al. (1997), the estimation of a quantitative ‘attribution confidence level’, in analogy with the signal-to-noise ‘detection significance level’, has not been attempted.

In contrast to the detection problem, for which it is sufficient to establish that a climate change has occurred which cannot be ascribed, within some given statistical significance limit, to natural (internal) climate variability, attribution requires in addition the demonstration that the detected climate change signal is indeed most likely (in the statistical sense of scientific confirmation theory, see Earman 1992) due to the assumed cause, e.g. an increase in greenhouse gas concentrations, rather than some other external forcing mechanism, like a change in the solar constant or modified land-use practices (see Pennell et al. 1993). As the first step, it must be demonstrated that the retrieved climate change signal is consistent, within given error bounds, with the signal predicted by the assumed forcing mechanism. In the next step, it must then be demonstrated that the signal cannot be explained by other candidate mechanisms. The outcome of such a multiple-forcing test may well be that the signal is consistent with several different forcing mechanisms, or combinations of forcing mechanisms, or that the detected climate change is not consistent with any of the proposed mechanisms or combinations of mechanisms.

A discrimination between competing forcing mechanisms can clearly be meaningfully attempted only if all candidate mechanisms and their associated climate change signals are specified. This implies that the multi-variate fingerprint method must be applied in its general multi-pattern form, rather than in the reduced single-signal pattern version used in most previous detection studies.

Attribution analyses are necessarily limited to tests of consistency. Even if it has been shown that a detected climate change signal is consistent with only one forcing mechanism, or combination of forcing mechanisms, within a finite set of candidate mechanisms, it can never be ruled out that there exist other, overlooked forcing mechanisms, that could also produce the observed climate change signal. Both single- and multi-pattern attribution tests must be regarded as truncated approximations of an ideally infinite sequence of consistency tests applied to all conceivable climate forcing mechanisms. Unequivocal attribution is achieved only in the hypothetical infinite-sequence limit. But it is questionable whether such a limit can be meaningfully defined, quite apart from its practicality (Earman 1992). We must, therefore, restrict ourselves in principal to a statistical definition of attribution that applies only in the limited sense of establishing a ranking within a given finite set of candidate forcing mechanisms.

The attribution method applied in this study represents an extension of the general multi-pattern fingerprint approach developed by H for the problem of climate change detection. After reviewing briefly the multi-variate fingerprint detection method in Sect. 2, the extension to the attribution problem is developed in Sect. 3. The final Sect. 4 gives a summary of the results and presents some conclusions.

2 The detection problem

Here we review briefly the multi-fingerprint method of multi-variate climate change detection, following the approach of H for the general space–time dependent problem. We return, for better illustration of the interrelationship between fingerprint and signal patterns, to the co- and contra-variant tensor notation of Hasselmann’s (1979) earlier analysis of the spatial signal-to-noise problem (see also the Appendix and Thacker 1995).

2.1 Terminology

We shall use the term climate change in the following to denote the response of the climate system to external forcing, as opposed to natural internal climate variability generated by interactions within the climate system. According to this terminology, climate variations due to volcanic activity or variations in the solar constant are classed as (natural) climate change, rather than as climate variability. An alternative terminology refers to these variations also as natural variability, climate variability being regarded as a superposition of externally forced and internally generated components, the term climate change being reserved for anthropogenic climate modifications only. However, for the detection and attribution problem our definitions will be found to be more convenient. Thus, climate change in our terminology can be of either natural or of anthropogenic origin, while climate variability is always natural. The definition loses precision if interactions between climate change and internal natural climate variability are considered, but in our applications we shall regard the climate state to first order simply as a linear superposition of climate change and climate variability.

The present definitions are more consistent than alternative earlier attempts to distinguish between climate change and climate variability on the basis of time scales, or in terms of climate change ‘events’ as opposed to ‘continuous’ climate fluctuations. In practice, the time scales of internal climate variability and externally forced climate change overlap, so that for a given finite time scale it is not possible to distinguish between ‘events’ and ‘continuous fluctuations’. Indeed, the impossibility of distinguishing between externally generated climate change and internal climate variability on the basis of time scale considerations alone is the essence of the detection and attribution problem.

We consider a vector time series $\phi_a(t)$ of climate data, which we assume can be represented as a superposition

$$\phi_a = \phi_a^s + \tilde{\phi}_a \quad (1)$$

of a climate change signal ϕ_a^s and a natural-variability component $\tilde{\phi}_a$. The index a refers to different types of climate data, e.g. temperature or precipitation, and to the location or averaging region of the data. The data set can represent either observed data or synthetic data from a model simulation. The climate vector ϕ_a need not represent a dynamically complete description of the climate state. In fact, in detection and attribution applications, ϕ_a will normally consist of only a small subset of the

components of the complete climate state vector needed, for example, for a dynamical model integration. We require only that the time-lagged second moments $R_{ab}(t, \tau) = \langle \tilde{\phi}_a(t + \tau) \tilde{\phi}_a(t) \rangle$ can be estimated from observations or model simulations with sufficient accuracy for a meaningful signal-to-noise analysis. Here and in the following, cornered parentheses $\langle \dots \rangle$ denote ensemble means, the climate variability is assumed to have zero mean, $\langle \tilde{\phi}_a(t) \rangle = 0$ (the ensemble mean having been subtracted in the definition of the climate state) and the statistics are assumed to be stationary, so that R_{ab} depends only on the time lag τ , or cyclostationary, so that R_{ab} is periodic with respect to the variable t .

For a general space–time dependent analysis, it will be convenient to use a compressed notation in which the trajectory of the observed climate vector is denoted as a vector $\psi = (\psi_i) \equiv (\phi_a(t_b))$ with a composite index $i \equiv (a, b)$ composed of the climate state index a and the index b of the discretized time variable $(t_b) = (t_1, t_2, \dots)$. The time-lagged second moments $R_{ab}(\tau)$ or $R_{ab}(t, \tau)$ are represented in this compressed notation by the covariance matrix

$$C_{ij} = \langle \psi_i \psi_j \rangle. \quad (2)$$

We point out, however, that although we shall refer to the vector ψ as the climate state trajectory, all relations derived in the following apply formally also to the case that ψ represents some time dependent derived product of $\phi_a(t)$ (for example, running climate trends defined over finite time intervals, see Santer et al. 1995a; Hegerl et al. 1996, 1997), so that $\psi = \psi(t)$. All following relations apply then for a given time. The inclusion of the time variable together with the space variables in a fully space–time dependent detection and attribution analysis has the advantage of formally maximizing the significance levels for both detection and attribution; it is also more consistent from a general signal analysis viewpoint. However, the separate treatment of the time dependence, as in Santer et al. (1995a) and Hegerl et al. (1996, 1997), yields more insight into the time evolution of the climate change signal.

To decide whether an observed trajectory ψ contains a climate change signal that can be distinguished from noise, we need to estimate the probability that ψ represents a realization of the natural variability ensemble $\tilde{\psi}$. For this we need to know the multi-variate probability distribution $p(\tilde{\psi})$ of $\tilde{\psi}$. We make the usual assumption that the distribution is Gaussian,

$$p(\tilde{\psi}) = (2\pi)^{-n/2} |C|^{-1/2} \exp[-\tilde{\rho}^2/2], \quad (3)$$

where

$$\tilde{\rho}^2 = C^{ij} \tilde{\psi}_i \tilde{\psi}_j \quad (4)$$

and n is the dimension of the vector ψ_i , $|C|$ the determinant of C_{ij} and C^{ij} denotes the inverse of the covariance matrix,

$$C^{ij} C_{jk} = \delta_k^i. \quad (5)$$

Repeated tensor indices are summed in accordance with the tensor summation convention.

We distinguish here and in the following between lower-index covariant tensor forms (including vectors) and upper-index contravariant tensors. Co- and contravariant tensor components are related through the metric, which we identify with the covariance matrix C_{ij} . Thus the operations of index raising and lowering are defined by

$$\begin{aligned} X^{\dots i \dots} &= C^{ij} X^{\dots j \dots} \\ X^{\dots i \dots} &= C_{ij} X^{\dots j \dots} \end{aligned} \quad (6)$$

The definition of the climate trajectory vector as a covariant vector is arbitrary in the present context. The role of co- and contravariant variables can be interchanged. We adopt here the original assignments of Hasselmann (1979).

We note that the results presented later can all be readily expressed, as in H, in standard matrix notation, without distinguishing between co- and contravariant tensors. However, in this case insight into the invariant nature of the theory with respect to arbitrary linear transformations is lost, including, in particular, the dual relation between the fingerprint and signal patterns (Eq. (20) below). Furthermore, one can no longer appeal to the trivial case of a unit covariance matrix in the derivation of the basic relations (20), (21). However, an alternative matrix notation which similarly expresses the invariant structure of the theory is presented in the Appendix.

For each trajectory ψ there exists a constant probability surface $\rho^2(\tilde{\psi}) = C^{ij} \tilde{\psi}_i \tilde{\psi}_j = \text{const} = C^{ij} \psi_i \psi_j$ which contains the vector ψ . We consider then the integral

$$\bar{P}_\rho = \int_{\tilde{\rho}^2 > \rho^2} p(\tilde{\psi}) d\tilde{\psi}_1 \dots d\tilde{\psi}_n \quad (7)$$

of the n -dimensional probability density over the region $\tilde{\rho}^2(\tilde{\psi}) > \rho^2(\psi)$ outside the surface $\rho^2(\tilde{\psi}) = \rho^2(\psi) = \text{const}$. If \bar{P}_ρ is small, 5%, say, the null hypothesis that ψ represents a realization of the natural variability ensemble is said to be rejected with a risk \bar{P}_ρ . Conversely, a climate change signal is said to have been detected in the data at a significance level $P_\rho = (1 - \bar{P}_\rho)$ (95%).

We note that our definition of climate change detection refers only to the probability of the null hypothesis, based on the relation between the observed climate trajectory and the natural climate variability. We make no reference to the probability of the alternative hypothesis of the existence of an external forcing mechanism that produces the climate change. This is not feasible within the framework of conventional statistics, since there exists no data ensemble for the definition of such a probability. However, it is possible to extend the present detection and attribution analysis within a Bayesian framework by introducing subjective prior probabilities (“degrees of belief”) for the various candidate forcing mechanisms. Observations condition the prior probabilities, yielding modified posterior probabilities (see Earman 1992). Although the Bayesian approach is attractive in capturing some of the uncertainties related to the “degree of belief” in external forcings and model predictions which are central issues in much of the controversy associated with the detection and attribution problem, we shall remain here within the framework of conventional statistics based on existing ensembles of realizations.

2.2 Reduction of the detection space

In practice, this straightforward statistical detection test can be applied successfully only if the vector dimension n of the climate state trajectory is small. Unfortunately, the situation is normally just the reverse: the discretization of a set of time series of gridded climate data will normally yield a vector ψ of very high dimension. The problem of many dimensions is that even a relatively large climate change signal ψ^s relative to the noise component in some given but unknown direction in phase space cannot be detected in the presence of noise distributed over a large number of other components. For successful detection and attribution, the dimension of the detection space must be strongly reduced, ideally to a single dimension by specifying the direction of the anticipated climate change signal, or to a small number of climate change patterns if more than one candidate forcing mechanism is considered.

The impact of the number of dimensions on the detection power can best be demonstrated by transforming to ortho-normal variables

$$\psi'_i = T_j^i \psi_j \quad (8)$$

$$\psi'^i = \hat{T}_j^i \psi^j, \quad (9)$$

where \hat{T}_j^i denotes the transposed inverse of the transformation matrix T_j^i ,

$$T_j^i \hat{T}_k^i = \delta_k^j. \quad (10)$$

In the ortho-normal system, the covariance matrix and its inverse are transformed to the unit co- and contra-variant matrices I_{ij} and I^{ij} , respectively,

$$C'_{ij} = \langle \tilde{\psi}'_i \tilde{\psi}'_j \rangle = T_i^k T_j^l C_{kl} = I_{ij} \quad (11)$$

$$C'^{ij} = \langle \tilde{\psi}'^i \tilde{\psi}'^j \rangle = \hat{T}_k^i \hat{T}_l^j C^{kl} = I^{ij}. \quad (12)$$

The transformation T_j^i can be obtained by first diagonalizing C_{ij} by a rotation to EOF (empirical orthogonal function) variables and then rescaling all EOFs to unit variance. In the space-time dependent problem, the EOFs consist of the set of all frequency-dependent complex EOFs of the discrete covariance spectrum of the time series $\phi_a(t_b)$. The estimation of C_{ij} and the associated transformation T_j^i from finite data sets is not straightforward; it is discussed in some detail in H and Hegerl et al. (1996) for the case of stationary statistics. One needs generally to perform an initial reduction of the dimension of the observed climate space ψ , for example by projection on to a small number of EOFs (typically 10) with adequately defined statistics. This follows already from the consideration that the rank of the estimated covariance matrix cannot be larger than the effective number of statistically independent data samples used to estimate the covariances. The reduction problem is basically the same but becomes more critical in the cyclostationary case. For the present theoretical discussion, however, these problems are irrelevant and we shall simply regard C_{ij} and the transformation T_j^i as given.

In the ortho-normal system the quadratic form (4) is transformed to the Euclidean form

$$\rho'^2 = \sum_i (\tilde{\psi}'_i)^2 \quad (13)$$

and the probability distribution (3) is reduced to the product expression

$$p(\tilde{\psi}') = \prod_i (2\pi)^{-1/2} \exp[-\tilde{\psi}'_i^2/2]. \quad (14)$$

Assume now that the direction of the anticipated climate change signal in the ortho-normal system is known, and that the system has been rotated such that this is the direction ψ_1 . If the magnitude of the signal is a , the detection significance level of the signal in the case of a uni-variate test in the ψ_1 -direction is given by

$$P_a^{(1)} = (2\pi)^{-1/2} \int_{-a}^a \exp[-\tilde{\psi}'_1^2/2] d\tilde{\psi}'_1 \quad (15)$$

This may be compared with the probability

$$P_a^{(n)} = \int_{\hat{\rho}^2 \leq a^2} \prod_i (2\pi)^{-1/2} \exp[-\tilde{\psi}'_i^2/2] d\tilde{\psi}'_1 \cdots d\tilde{\psi}'_n. \quad (16)$$

of detecting the climate change signal in the full n -dimensional space. The integral (16) can be expressed in terms of the incomplete Γ -function. However, an upper bound $\hat{P}_a^{(n)}$ on $P_a^{(n)}$, which illustrates more clearly the origin of the detection degradation as the number of dimensions is increased, can be obtained more simply by replacing the spherical integration domain $\hat{\rho}^2 \leq a^2$ in (16) by the larger cubical domain encompassing the n -sphere, $|\psi_1| < a$, $|\psi_2| < a$, \dots , $|\psi_n| < a$. One obtains in this case

$$P_a^{(n)} < \hat{P}_a^{(n)} = (P_a^{(1)})^n \quad (17)$$

Thus the significance level for the detection of a climate change signal of amplitude $|\psi_1| = a = 2$, say, in the ortho-normal coordinate system, corresponding to a univariate value $P_2^{(1)} \approx 95\%$, is reduced to less than $0.95^{10} \approx 0.6$ in a 10-dimensional detection exercise, and to less than $0.95^{100} \approx 0.006$ for 100 dimensions! A reduction of the detection space to a small number of 1–3 signal patterns is therefore essential for effective climate change detection.

2.3 The optimal fingerprint

In the ortho-normal coordinate system, it is self-evident from the isotropic symmetry of the problem that if the signal lies in the direction of the first coordinate, the univariate detection test should also be carried out with respect to the first coordinate. How does this result transform to a signal ψ_i^s oriented in some given guess-pattern direction g_i in an arbitrary coordinate system? To estimate the amplitude of the signal from the observed data ψ in the general case we write

$$\psi_i = dg_i + \psi_i^r \quad (18)$$

where the coefficient d (the *detection variable*) is determined by the scalar multiplication of the observed data with a suitably defined fingerprint f^i ,

$$d = f^i \psi_i, \quad (19)$$

and ψ_i^r is a residual which we wish to minimize.

It is common practice in many applications to determine the coefficient d by minimizing the mean square error $\sum_i \langle (\psi_i^r)^2 \rangle$. However, in the present case this is not

appropriate. Firstly, the mean square error is not invariant with respect to linear transformations to other variables. Secondly, our goal for the purpose of detection is to not to maximize the explained variance in a particular reference system, but rather to maximize the squared signal-to-noise ratio $d^2/\langle \tilde{d}^2 \rangle$ for an arbitrary reference system, where $\tilde{d} = f^i \tilde{\psi}_i$ is the detection variable determined by the natural climate variability in the absence of a climate change signal. Since the signal-to-noise ratio is independent of the scaling of d , for detection applications we need to determine only the direction of the fingerprint. It was shown in H, and is shown again trivially below (see also Hasselmann 1979), that the maximization of the signal-to-noise ratio yields the fingerprint

$$f^i = C^{ij} g_j \equiv g^i, \quad (20)$$

where the signal pattern and fingerprint can be normalized, without loss of generality, such that

$$C^{ij} g_i g_j = f^i g_i = C_{ij} f^i f^j = 1. \quad (21)$$

Thus, the optimal fingerprint represents the contravariant counterpart of the covariant guess pattern. (We nevertheless use different symbols for the fingerprint and signal rather than distinguishing the two only by the position of the index to emphasize the basic difference in the role of the two patterns. In the detection literature this distinction is sometimes overlooked.)

In the present co- and contravariant notation the result (20), (21) follows immediately from the argument indicated above that in the special case of an ortho-normal reference system, $C^{ij} = I^{ij} =$ unit matrix, the fingerprint and signal pattern must have the same directions for reasons of isotropic symmetry:

$$f'^i = I^{ij} g'_j = C'^{ij} g'_j, \quad (22)$$

where we may define g'_i, f'^i as unit vectors,

$$I^{ij} g'_i g'_j = C'^{ij} g'_i g'_j = 1, \quad (23)$$

$$I_{ij} f'^i f'^j = C'_{ij} f'^i f'^j = 1. \quad (24)$$

Since Eqs. (22)–(24) are tensor relations, they must hold not only in the ortho-normal reference system, but in any reference system, as expressed by Eqs. (20), (21).

If we progress now from the question of detection to the problem of attribution, the scaling of the fingerprint pattern and detection variable is no longer irrelevant. In this case we need to estimate the amplitude of the retrieved climate change signal in order to compare it with the predicted amplitude. The amplitude scaling defined by the normalization condition (21) has the reasonable property that it minimizes the statistical mean square residual $\rho^{r2} = C^{ij} \psi'_i \psi'_j$ defined with respect to the metric C_{ij} . This can again be immediately seen in the ortho-normal reference system and must then be valid, since ρ^{r2} is an invariant scalar, in any reference system.

The invariant least square solution can be derived from maximum likelihood arguments. If it is assumed that the probability distribution of climate trajectories $\tilde{\psi}$ can be represented as a normal distribution with covariance matrix C_{ij} and an unknown non-zero mean $\langle \tilde{\psi}_i \rangle = d' g_i$ in

the direction of the signal pattern, the value of d' which yields a maximum probability density for the given realization ψ is given by $d' = d$. We shall return to this later in the attribution problem, when we derive an alternative maximum likelihood estimate of the climate change signal allowing not only for the natural variability of the observed data but also for the uncertainty of the predicted climate change signal.

Geometrically, the relation between the fingerprint and signal guess patterns can be best understood by rotating to the EOF representation, for which $C_{ij} = \sigma_{(i)}^2 I_{ij}$, $C^{ij} = \sigma_{(i)}^{-2} I^{ij}$, where $\sigma_{(i)}$ denotes the variance of the i 'th EOF (the summation convention is not applied to indices in parentheses). Writing

$$g_i = \sum_m c_{(m)} e_i^{(m)}, \quad (25)$$

where $c_{(m)}$ denotes the coefficient of the m 'th EOF $e_i^{(m)}$, the fingerprint pattern is given, according to (20), by

$$f^i = \sum_m c_{(m)} \sigma_{(m)}^{-2} I^{ij} e_j^{(m)} \quad (26)$$

The factor $\sigma_{(m)}^{-2}$ in (26) attenuates the high-noise EOF components in the fingerprint pattern relative to the low-noise components. Thus, the optimal fingerprint is obtained by turning the original signal vector away from directions of high noise towards low noise directions (see Hasselmann 1979, Fig. 1).

2.4 The multi-pattern case

These results can be readily generalized to the case of p signal patterns g_v , $v = 1, \dots, p$ (see H). If the climate trajectory is represented as an optimal linear combination

$$\psi_i = d^v g_{vi} + \psi'_i \quad (27)$$

of the guess patterns (applying the summation convention also to the indices v of the p guess patterns), the condition that the quadratic form $\rho^{r2} = \rho^2(\psi')$, see Eq. (4), for the residual is minimized (maximizing also the multi-variate signal-to-noise ratio for the coefficient vector $\mathbf{d} = (d^v)$) yields, as determining equations for the coefficients d^v of the retrieved climate change signal the set of p linear equations

$$D_{\nu\mu} d^\mu = f^i_\nu \psi_i \quad (v = 1, \dots, p), \quad (28)$$

where

$$f^i_\nu = C^{ij} g_{\nu j} (= g^i_\nu) \quad (29)$$

denotes the fingerprint of the ν 'th guess pattern, in analogy with the definition (20) in the single pattern case, and

$$D_{\nu\mu} = f^i_\nu g_{\mu i} = C^{ij} g_{\nu i} g_{\mu j}. \quad (30)$$

The solution can be expressed in a concise form by introducing the operations of index raising and lowering also for Greek guess-pattern indices, using as the metric the matrix $D_{\nu\mu}$ defined by the scalar products of the signal

patterns. Introducing the covariant multi-pattern detection coefficients, given, in analogy with the definition for the scalar single-pattern detection coefficient d , Eq. (19), by

$$d_v = f_v^i \psi_i, \quad (31)$$

the contravariant detection coefficients may be expressed as

$$d^v = D^{\nu\mu} f_\mu^i \psi_i = f^{vi} \psi_i, \quad (32)$$

where $D^{\nu\mu}$ denotes the inverse of $D_{\nu\mu}$,

$$D^{\nu\mu} D_{\mu\lambda} = \delta_\lambda^\nu. \quad (33)$$

It follows from Eq. (32) that $D^{\nu\mu}$ represents the covariance matrix of the natural variability components \tilde{d}^v of the contravariant detection coefficients,

$$D^{\nu\mu} = \langle \tilde{d}^\nu \tilde{d}^\mu \rangle = f^{vi} f^{\mu j} \langle \tilde{\psi}_i \tilde{\psi}_j \rangle = f^{vi} g_{ji}, \quad (34)$$

while

$$D_{\nu\mu} = \langle \tilde{d}_\nu \tilde{d}_\mu \rangle = f_\nu^i f_\mu^j \langle \tilde{\psi}_i \tilde{\psi}_j \rangle = f_\nu^i g_{\mu i} \quad (35)$$

represents the corresponding covariance matrix of the natural variability contribution of the covariant detection coefficients.

Depending on the context, the multi-pattern detection problem is seen to lead to a detection vector that can appear either in a co- or a contravariant form with respect to the metric $D_{\nu\mu}$. We shall refer to the contravariant detection coefficients d^v , which appear in the original representation (27) of the climate trajectory in terms of the signal patterns, as *pattern amplitudes*. The covariant detection coefficients d_ν , defined by the straightforward generalization, Eq. (31), of the expression (19) for the scalar detection variable, will be termed simply the *detection variables*. The detection variables arise naturally in the multivariate detection test (see H), while the pattern amplitudes are the appropriate coefficients occurring in the representation of the climate change signal in terms of the predicted signal patterns.

For a multi-variate detection test we need to consider the p -dimensional Gaussian probability distribution of the natural-variability pattern amplitudes \tilde{d}^v or detection variables \tilde{d}_ν , in the absence of a climate change signal,

$$p_d(\tilde{\mathbf{d}}) = (2\pi)^{-p/2} |D|^{-1/2} \exp[-\tilde{\rho}_d^2/2], \quad (36)$$

where

$$\tilde{\rho}_d^2 = D_{\nu\mu} \tilde{d}^\nu \tilde{d}^\mu = D^{\nu\mu} \tilde{d}_\nu \tilde{d}_\mu, \quad (37)$$

and

$$|D| = |D^{\nu\mu}| \quad (38)$$

if Eq. (36) refers to the pattern amplitudes, or

$$|D| = |D_{\nu\mu}| \quad (39)$$

if the equation refers to the detection variables. The significance level for the detection of a given estimated detection vector \mathbf{d} in the p -dimensional guess-pattern detection space (expressed, say, in terms of the detection variables) is then given by

$$P_{\rho_d} = \int_{\tilde{\rho}_d^2 < \rho_{\tilde{d}(d)}^2} p_d(\tilde{\mathbf{d}}) d\tilde{d}_1 \cdots d\tilde{d}_p. \quad (40)$$

As pointed out already, the detection of a multi-pattern climate change signal becomes successively more difficult as the number of patterns increases, so that the multi-pattern detection approach is feasible only for a relatively small number of candidate patterns of order two or three.

An application of the complete space–time dependent, multi-pattern optimal fingerprint approach to climate change detection as summarized above has not yet been attempted. Santer et al. (1995a) and Hegerl et al. (1996) applied a single-pattern analysis in which the time dependence of the signal was represented as a linear trend. An optimization of the fingerprint pattern in the time domain through the application of an appropriate spectral filter (see H), was not attempted, the optimization being limited to a rotation in the time-independent pattern space. Hegerl et al. (1997) have recently applied a two-pattern analysis to distinguish between the effects of greenhouse gas emissions, anthropogenic aerosols and variations in solar insolation in a detection study based on new CGCM global warming simulations including different combinations of forcings. The time dependence of the signal was represented as a running linear trend, the optimization of the fingerprint pattern being limited again to the spatial domain. However, a novelty of the analysis was that the authors considered not only the detection question, but also the attribution problem, which we now consider.

3 The attribution problem

In the detection problem only a single hypothesis is tested, the null hypothesis that the observed climate evolution ψ in some pre-determined direction \mathbf{g} can be attributed to internal natural climate variability. For the attribution problem we need to consider now further hypotheses regarding the cause of a detected climate change. We assume there exist generally several candidate mechanisms $\nu = 1, \dots, p$, each of which is characterized by a predicted climate change signal. In contrast to the detection problem, where we needed to know only the normalized directions \mathbf{g}_ν of the signal patterns, we specify now also the predicted amplitudes a^ν of the signals.

To decide whether the climate change signal $\psi_{(v)}^o$ inferred from observations is consistent with a given signal $\psi_{(v)}^m$ predicted from a model simulation, we must assign to each predicted climate change signal an error covariance matrix, in analogy with the natural variability covariance matrix required for the detection test. We assume again that the error distributions are Gaussian. The consistency of the retrieved climate change signal with the predicted signal is then tested by comparing the difference between the two signals with the differences which could be expected from the estimated signal errors. We shall be concerned only with the distinction between different signals in the space spanned by the p predicted signal patterns. Thus, we need consider only the projection of the signal pattern errors in this signal pattern space.

We assume that the p predicted signal patterns are linearly independent and therefore do indeed span a p -dimensional space. However, we can allow also additional forcing mechanisms which generate climate change

signals lying in this space (for example, by explicitly considering linear combinations of the p basic forcing mechanisms, such as a combined greenhouse gas and aerosol forcing, see Hegerl et al. 1997). If the pattern amplitudes of such linearly combined climate change signals are prescribed, the attribution (or consistency) tests can be applied in the same way to these signals as to the p base signals. Formally, one of the original base signals needs only to be replaced by the linear combination selected for the consistency test (note that the signal patterns \mathbf{g}_ν are assumed to be normalized by Eq. (21), but are not necessarily orthogonal).

The consistency test described in the following is carried out for each forcing mechanism separately. The outcome can be that one, none, or some sub-set of the forcings is consistent with the inferred climate change. If the observations are found to be consistent with exactly one forcing mechanism, and the null hypothesis that the retrieved climate change signal is consistent with natural climate variability is rejected, the retrieved climate change is attributed to that mechanism.

3.1 Consistency and attribution tests

Having retrieved the observed climate change signal

$$\psi^o = d^\mu \mathbf{g}_\mu, \quad (41)$$

with pattern amplitudes d^μ given by the solutions of Eq. (28), we investigate now for each proposed forcing mechanism ν whether the retrieved signal is consistent with the predicted climate change signal

$$\psi^m = a^{(\nu)} \mathbf{g}_{(\nu)} \quad (42)$$

inferred from a model simulation (the summation convention does not apply to the index (ν) , which appears here and in the following in parentheses as a fixed parameter).

To this end we compare the difference

$$\delta\psi_{(\nu)} = \psi_{(\nu)}^m - \psi^o = (\delta_{(\nu)}^\mu a^{(\nu)} - d^\mu) \mathbf{g}_\mu \quad (43)$$

between the predicted and retrieved climate change signals with the differences which can be expected from the errors incurred in the model computation of $\psi_{(\nu)}^m$ and in the estimation of ψ^o from observations. Thus for a given process ν we compare the difference

$$\varepsilon_{(\nu)}^\mu = \delta_{(\nu)}^\mu a^{(\nu)} - d^\mu \quad (44)$$

between the predicted and retrieved pattern amplitudes with the p -dimensional probability distribution of the net errors $\tilde{\varepsilon}_{(\nu)}^\mu$ of the amplitude differences arising from statistical and model errors (the fact that this is more convenient than considering the error ellipsoids of the predicted and retrieved climate signals separately was pointed out by J. Waszkewitz, personal communication).

The natural variability sampling errors \tilde{d}^μ incurred in the determination of the retrieved pattern amplitudes were considered in the previous section. They can be characterized by a covariance matrix $D^{\mu\lambda} = \langle \tilde{d}^\mu \tilde{d}^\lambda \rangle = C^{ij} g_{\mu i} g_{\lambda j}$ Eq. (34).

The errors incurred in computing the predicted climate change signals from models consist of two parts: sampling errors due to the natural variability of the model, and systematic errors of the model itself. The sampling errors can be estimated from long control simulations (see Hegerl et al. 1996, 1997) or Monte Carlo experiments (Cubasch et al. 1994). They can be reduced by computing the mean of two or more climate change simulations (Cubasch et al. 1994; Hegerl et al. 1997). The errors due to systematic model errors are more difficult to determine, but can be estimated by intercomparing climate change simulations of different models. We assume that the net errors from both sources can be characterized by a model amplitude error covariance matrix $M_{(\nu)}^{\mu\lambda}$.

Since the modelled and retrieved signal errors are statistically independent, the covariance matrix $E_{(\nu)}^{\mu\lambda}$ characterizing the errors of the differences $\varepsilon_{(\nu)}^\mu$ between the modelled and retrieved pattern amplitudes is given by the sum

$$E_{(\nu)}^{\mu\lambda} = M_{(\nu)}^{\mu\lambda} + D^{\mu\lambda} \quad (45)$$

of the covariance matrices of the predicted and retrieved pattern amplitude errors.

The probability distribution of the amplitude differences $\tilde{\varepsilon}_{(\nu)}^\mu$ due to statistical sampling and model errors is accordingly given by the Gaussian distribution

$$p_\varepsilon(\tilde{\varepsilon}_{(\nu)}) = (2\pi)^{-p/2} |E_{(\nu)}|^{-1/2} \exp[-\tilde{\rho}_\varepsilon^2/2], \quad (46)$$

where $|E_{(\nu)}| = |E_{(\nu)}^{\mu\lambda}|$,

$$\tilde{\rho}_\varepsilon^2 = \hat{E}_{\mu\lambda}^{(\nu)} \tilde{\varepsilon}_{(\nu)}^\mu \tilde{\varepsilon}_{(\nu)}^\lambda, \quad (47)$$

and $\hat{E}_{\mu\lambda}^{(\nu)}$ is the inverse of $E_{(\nu)}^{\mu\lambda}$,

$$E_{(\nu)}^{\mu\sigma} \hat{E}_{\sigma\lambda}^{(\nu)} = \delta_{\lambda}^\mu. \quad (48)$$

For the consistency test we apply the same approach as in the detection test. The null hypothesis is replaced now by the consistency hypothesis, and the retrieved pattern amplitude vector by the difference amplitude vector. Apart from this change in terminology, the concepts are identical to those introduced for the detection test. For any given amplitude difference vector $\varepsilon_{(\nu)}$ there exists a surface $\rho_\varepsilon^2 = \text{const}$ which contains the vector. We consider then the integral

$$\bar{P}_{\rho_\varepsilon} = \int_{\tilde{\rho}_\varepsilon^2 > \rho_\varepsilon^2} p_\varepsilon(\tilde{\varepsilon}_{(\nu)}) d\tilde{\varepsilon}_{(\nu)}^1 \cdots d\tilde{\varepsilon}_{(\nu)}^p \quad (49)$$

of the p -dimensional probability density p_ε over the region $\tilde{\rho}_\varepsilon^2(\tilde{\varepsilon}_{(\nu)}) > \rho_\varepsilon^2(\varepsilon_{(\nu)})$ outside the surface $\tilde{\rho}_\varepsilon^2(\tilde{\varepsilon}_{(\nu)}) = \rho_\varepsilon^2(\varepsilon_{(\nu)}) = \text{const}$.

If $\bar{P}_{\rho_\varepsilon}$ is small, 5%, say, the hypothesis that the retrieved climate change signal is consistent with the forcing mechanism ν is said to be rejected with a risk of $\bar{P}_{\rho_\varepsilon}$, or at a significance level of $P_{\rho_\varepsilon} = (1 - \bar{P}_{\rho_\varepsilon})$ (95%).

We note that a positive outcome of the statistical detection test (i.e. the rejection of the null hypothesis) is formally analogous to a negative outcome of the consistency test (i.e. the rejection of the consistency hypothesis). A positive outcome of the consistency test should therefore be expressed formally in the double negative form that the retrieved climate change signal is not inconsistent with the proposed forcing mechanism at a given significance level P . However, if the chosen significance level P is high, 95%, say, this statement is rather weak (a high significance

level is normally chosen to yield a strong statement for the converse case that the attribution test is rejected). To avoid the cumbersome double negative wording, while at the same time conveying more accurately the statistical significance of a positive outcome of a consistency test, we shall replace the statement that 'a retrieved climate change signal is *not inconsistent* with a given forcing mechanism at a *significance level of P (95%)*' by the simpler positive statement that 'a climate change signal is *consistent* with the forcing mechanism within the P (95%)- *confidence region*' (in analogy with the terminology of power spectral analysis) or 'at a *confidence level of \bar{P} (5%)*'. Note that the stringency of the consistency test increases with decreasing P or increasing \bar{P} . For $P \rightarrow 0$, the confidence region contracts to zero, requiring zero error between the retrieved and predicted pattern amplitudes for a positive outcome of the consistency test, while the confidence level \bar{P} for a consistent signal increases to 100%. For the acceptance of a consistency test as positive, it will generally be advisable to select a consistency confidence level somewhat higher than 5%, of the order of 10%–20%. Still higher confidence levels, however, incur the risk of erroneously rejecting valid attributions.

As outcome of the combined multi-pattern detection/attribution exercise we can then assign a statistical *significance level*, defined by Eq. (40), for the detection of a climate change signal within the space spanned by the p predicted signal patterns; and a *consistency confidence level* for each proposed climate change mechanism v , defined, in analogy with the risk associated with the null hypothesis, by Eq. (49).

The result of the test will consist generally of one of the following combinations (see Fig. 1):

1. A statistically significant climate change signal a consisting of a superposition of predicted climate change signals is detected in the observed data at a given significance level. The retrieved climate change signal is consistent with only one of the predicted signals at a prescribed consistency confidence level. Thus the observed climate change signal can be attributed to the single forcing mechanism that passed the consistency test.

2. A statistically significant climate change signal b is detected which is consistent with several or all of the predicted climate change signals.

3. A statistically significant climate change signal c is detected which is statistically consistent with none of the predicted signals.

4. The retrieved climate change signal d is not statistically significant, but the signal is statistically consistent with at least one of the predicted signals. In this case the positive consistency tests are nullified by the negative outcome of the detection test: the retrieved signal cannot be distinguished from the internal natural-variability noise, even though it is consistent with some of the predicted externally forced signals.

5. The retrieved climate change signal e is not statistically significant and the retrieved climate change signal is not consistent with any of the predicted signals.

We note that the attribution of a detected climate change signal to a particular forcing mechanism is successful only in the first of these possible outcomes.

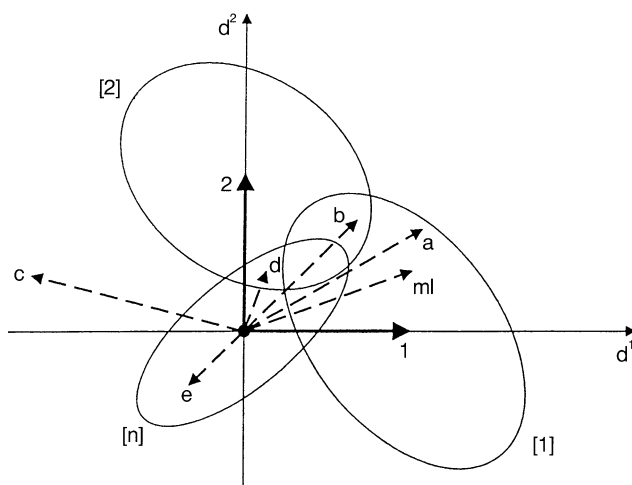


Fig. 1. Predicted (1, 2) and retrieved ($a - e$) climate change signals in the (d^1, d^2) plane for two candidate forcing mechanisms (1) and (2). Ellipse [n] indicates the significance region for detection, ellipses [1] and [2] the consistency confidence regions for the two forcing mechanisms. Retrieved signal a : successful detection, consistency only with forcing (1); climate change is attributed to mechanism (1); the vector ml indicates the estimated maximum likelihood signal. Retrieved signal b : successful detection, signal consistent with both forcing mechanisms; no attribution possible. Retrieved signal c : successful detection, signal consistent with neither prediction; Retrieved signal d : signal consistent with forcing 2, detection insignificant (nullifying consistency); Retrieved signal e : detection insignificant, signal consistent with neither prediction

One can consider various modifications of the test procedure. Rather than determining the retrieved climate change signal in the p -dimensional space of all proposed signal patterns, the detection and attribution test can be carried out as a single-pattern analysis separately for each individual mechanism (yielding the same set of possible test outcomes). This has the advantage of enhancing the probability of detection of any given forcing signal. However, it provides less discrimination between competing mechanisms when the signal patterns are not orthogonal. The signal pattern a of Fig. 1, for example, fails the consistency test for the forcing mechanism 2 in the full signal pattern space, but would pass an individual pattern consistency test for this process (as is apparent from a visual projection of the retrieved signal vector onto the direction of the signal pattern 2). Thus in contrast to the two-pattern analysis, a unique attribution is no longer achieved (see also the similar example discussed in Hegerl et al. 1997).

Another modification is suggested if one of the predicted signals is consistent with a zero amplitude with acceptable probability, and the detection/attribution test also returns a small amplitude for that signal. One can then repeat the test leaving out that forcing mechanism, in the expectation that the significance and confidence levels for the detection and attribution of the other signals are thereby enhanced.

We note, however, that in our formulation of the attribution problem we have not considered the possibility

that a proposed forcing mechanism, once introduced, simply does not exist. A proposed mechanism can only be rejected as not consistent statistically with the observations, or the retrieved signal, although consistent statistically with the predicted signal, can be so small that it is nevertheless not distinguishable statistically from zero.

To establish an optimal trade-off between a high detection significance level (requiring a small number of patterns) and the ability to discriminate between different competing climate forcing mechanisms (requiring a larger number of patterns), a series of detection/attribution tests at different levels may be applied, each successive level involving an increase in the number of patterns. A similar optimal trade-off between statistical significance and the number of predictors has been applied in the construction of a hierarchy of statistical linear prediction models from a finite data set, see Barnett and Hasselmann (1979).

3.2 Maximum likelihood estimate of the climate change signal

If a detected climate change signal has been successfully attributed to a particular forcing mechanism v , one may ask whether the climate change signal retrieved from the observations is necessarily the best estimate of the climate change signal. The retrieved signal is determined by projection of the observed climate trajectory onto the p -dimensional space spanned by the signal patterns of all candidate forcing mechanisms, without regard to the predicted amplitude of the signal pattern to which the retrieved climate change is subsequently attributed. An improved estimate may be expected by an approach which takes account of the information contained not only in the observations but also in the predicted amplitudes, allowing for the errors in both.

This consideration forms the basis of the maximum likelihood method. Both information sources are included together in a single optimization procedure. In contrast to the detection problem, the pattern amplitudes $d_{(v)}^{\mu}$ in the representation (41) are no longer determined solely by the condition that the statistical mean square residual error should be minimized, but also by the requirement that the detected climate change should be compatible, as far as possible, with the climate change mechanism v (in anticipation of this requirement we have included now the parameter index (v) in the pattern amplitudes $d_{(v)}^{\mu}$).

To satisfy optimally both of these requirements, we replace the previous statistical least square condition, which yielded the solution (32) for the coefficients $d_{(v)}^{\mu}$, by a maximum-likelihood condition which takes into account the probability distribution not only of the natural-variability noise (which is equivalent to the statistical least square condition) but also of the signal amplitudes. The coefficients $d_{(v)}^{\mu}$ are chosen such that the joint probability distribution $\hat{p} = \hat{p}(\psi^r, \varepsilon_{(v)}) = p(\psi^r)p_{\varepsilon}(\varepsilon_{(v)})$ of the residual noise ψ^r and the coefficient difference vector $\varepsilon_{(v)}$ is maximized for the given predicted climate change signal and observed climate change realization. According to Eqs.

(3), (27), (46), we have

$$\begin{aligned} \ln \hat{p} &= \ln p(\psi^r) + \ln p_{\varepsilon}(\varepsilon_{(v)}) \\ &= \text{const} - \frac{C^{ij}}{2} (\psi_i - d_{(v)}^{\mu} g_{\mu i}) (\psi_j - d_{(v)}^{\lambda} g_{\lambda j}) \\ &\quad - \frac{\hat{E}_{\mu\lambda}^{(v)}}{2} (\delta_{(v)}^{\mu} a^{(v)} - d_{(v)}^{\mu}) (\delta_{(v)}^{\lambda} a^{(v)} - d_{(v)}^{\lambda}) \end{aligned} \quad (50)$$

Variation of (50) with respect to $d_{(v)}^{\mu}$ yields then the maximum-likelihood set of equations $\partial \ln \hat{p} / \partial d_{(v)}^{\mu} = 0$ for the determination of the pattern amplitudes $d_{(v)}^{\mu}$:

$$(D_{\mu\lambda} + \hat{E}_{\mu\lambda}^{(v)}) d_{(v)}^{\lambda} = d_{\mu} + \hat{E}_{\mu(v)}^{(v)} a^{(v)} \quad (51)$$

Equation (51) differs from the previous determining equation (28) for the pattern amplitudes in the multi-pattern optimal-detection case through the terms proportional to the inverse $\hat{E}_{\mu\lambda}^{(v)}$ of the pattern amplitude error covariance matrix $E_{(v)}^{\mu\lambda}$.

If $\hat{E}_{\mu\lambda}^{(v)}$ is small compared with $D_{\mu\lambda}$, i.e. if the errors in the predicted signal pattern amplitudes are large compared with the pattern amplitudes and amplitude errors derived from the observations, one recovers the previous optimal detection solution. Since nothing is known in effect *a priori* about the magnitudes of the signals, no restriction is placed on the optimal-detection solution. The pattern coefficients d^{μ} are given in this case by the contravariant counterparts of the covariant detection variables d_{μ} with respect to the metric $D_{\mu\lambda}$ (the covariance matrix characterizing the natural variability of the detection variables, Eq. (34)). A detected climate change signal is always trivially consistent in this limit with the proposed forcing mechanism, since the retrieved climate change signal will always lie within the very large error bounds of the prediction.

The opposite limit of large $\hat{E}_{\mu\lambda}^{(v)}$ compared with $D_{\mu\lambda}$, i.e. very accurately determined differences between the predicted and retrieved pattern coefficients relative to the statistical errors in the retrieved optimal-detection pattern coefficients, formally yields the solution

$$d_{(v)}^{\mu} = \delta_{(v)}^{\mu} a^{(v)}, \quad (52)$$

i.e. the maximum likelihood signal is identical to the predicted signal. However, this limit is unaccessible, since the errors in the differences between the predicted and retrieved pattern amplitudes are always larger, according to Eq. (45), than the statistical errors in the retrieved optimal-detection pattern coefficients. The largest values of $\hat{E}_{\mu\lambda}^{(v)}$ are obtained when the model errors $M_{(v)}^{\mu\lambda}$ vanish, so that Eq. (45) yields $E_{(v)}^{\mu\lambda} = D^{\mu\lambda}$. In this case Eq. (51) reduces to

$$2D_{\mu\lambda} d_{(v)}^{\lambda} = d_{\mu} + \hat{D}_{\mu(v)} a^{(v)} \quad (53)$$

Multiplication from the left with $D^{\sigma\mu}$ yields the solution

$$d_{(v)}^{\sigma} = \frac{1}{2} (d^{\sigma} + \delta_{(v)}^{\sigma} a^{(v)}), \quad (54)$$

i.e. the maximum likelihood solution is given by the mean of the predicted and original retrieved solution.

In practice, neither limiting case will apply, and the maximum likelihood solution will lie somewhere between the original retrieved climate change signal and the limiting, maximally modified solution (54) (Fig. 1, signal vector ml).

4 Summary and conclusions

The general multi-pattern optimal fingerprint method for the detection of a space–time dependent climate change signal in the presence of natural climate variability can be readily extended to the problem of attribution. A co- and contra-variant tensor notation, based on a metric given by the space–time dependent covariance matrix C_{ij} of the natural climate variability, simplifies the analysis and clarifies the invariant structure of the theory. The optimal fingerprint patterns f_v^i for detection are identified as the contravariant counterparts of the covariant signal patterns, $f_v^i = C^{ij}g_{vj} = g_v^i$. For the multi-pattern problem it is useful to introduce a second metric $D_{\nu\mu}$, defined by the scalar products $D_{\nu\mu} = g_{\nu i}g_{\mu j}C^{ij}$, in the p -dimensional space of signal patterns $g_{\nu i}$. The covariant detection variables $d_\nu = f_v^i\psi_i$ represent then the simplest set of coefficients for establishing the detection significance level, while the contravariant coefficients $d^\nu = D^{\nu\mu}d_\mu$, which require the inversion of the metric $D_{\nu\mu}$, define the amplitudes of the signal patterns g_ν estimated from the observed data. The matrices $D_{\nu\mu}$ and $D^{\nu\mu}$ represent the covariance matrices of the natural variability of the co- and contravariant detection coefficients, respectively.

In contrast to the detection of a climate change signal, for which only the directions of the predicted signal patterns need to be specified, attribution requires also a specification of the predicted signal amplitudes and their error statistics. The multi-pattern attribution analysis involves three steps: (1) an estimate of the observed climate change signal in the p -dimensional signal pattern space, (2) a test of the null hypothesis that the retrieved climate change signal can be explained by natural climate variability, and (3) tests of the statistical consistency of the retrieved climate change signal with each of the proposed forcing mechanisms.

The outcome of the analysis is an estimated overall statistical *significance level* for the detection of a net climate change signal and a set of *consistency confidence levels* characterizing the statistical consistency of the retrieved climate change signal with each of the proposed climate forcing mechanisms. Positive and negative outcomes of the different tests can occur in all combinations. Attribution is achieved only if the detection test is positive and the retrieved signal is consistent with only one of the proposed forcing mechanisms. However, even in this case the term attribution can still be interpreted only in the limited sense of consistency, since the possibility cannot be excluded that the retrieved signal can be explained by other forcing mechanisms not considered in the analysis.

The highest significance levels for detection and confidence levels in consistency tests can be achieved if only a single forcing mechanism is considered. If several forcing mechanisms are proposed, one could therefore consider carrying out a detection/consistency analysis for each

individual mechanism separately. However, this approach lacks discrimination: more mechanisms pass the consistency test in a series of separate single-pattern analyses than when the retrieved climate change signal is represented in a multi-pattern phase space. In general, the detection power decreases while the discrimination power increases with the number of patterns used in a multi-pattern detection/attribution analysis.

An effective strategy for arriving at an optimal trade-off between detection and attribution could therefore be to carry out a sequence of tests in which the number of patterns is successively increased. The sequence is terminated when the detection significance level falls below a prescribed level. In practice, however, the exponential dependence of the detection significance level on the number of signal patterns will limit multi-pattern tests to two or three patterns.

The main difficulty in the practical application of these theoretically rather straightforward concepts is the estimation of the space–time dependent covariance matrix of natural climate variability, and also the errors of the predicted climate change signals. Unfortunately, these difficulties cannot be circumvented and must therefore be faced if one wishes to arrive at quantitative estimates of statistical significance and consistency levels for climate change detection and attribution. A first application of the concepts presented in this study to real data is given in Hegerl et al. (1997), who attempt a combined quantitative assessment of our present ability to detect climate change signals in observed data and to attribute the retrieved signals to greenhouse gas warming with or without aerosol forcing.

Acknowledgements. The author is grateful for constructive comments by Gabriele Hegerl, Myles Allen and Gerald North. The work was partially supported by NOAA's Office of Global Programs' Climate Change Data and Detection Program Element, and DOE's Office of Health and Environmental Research.

Appendix

Alternative matrix notation

All tensor relations derived in this paper can be expressed in standard matrix notation. In most cases this simply requires suppression of the indices, in some cases the transpose of a matrix must be used and the order of factors must be changed. The notational changes are elementary and are left to the reader who is more comfortable with matrix notation. In the present multi-pattern analysis, in which vectors and matrices are needed for climate trajectory space (Latin indices), pattern space (Greek indices), and the product of both spaces, the explicit tensor index notation was found to be easier to work with than matrix notation, in which these distinctions are lost.

The main advantage of the tensor notation, however, is that it expresses the invariance of the problem with respect to the choice of climate variables and patterns. Although we considered here only linear transformations and no derivatives, so that the full power of tensor calculus developed for differential geometry was not invoked, an

invariant notation for linear transformations requires already a distinction between co- and contravariant tensors, and the restriction of matrix multiplications to contractions over pairwise co- and contravariant indices. Once the problem has been expressed in invariant form, all derivations can be carried out in some convenient coordinate system, for example in a system with unit covariance matrix, for which the basic results are self-evident.

It is also possible to express the invariance of the theory using a generalized matrix notation in which the product $A \odot B$ between two matrices A, B is defined with respect to the metric $C^{-1} =$ inverse covariance matrix as

$$A \odot B \equiv AC^{-1}B, \quad (55)$$

All matrix operations in the vector space of climate trajectories space (Latin indices) can then be expressed in terms of this generalized matrix product. Standard matrix multiplications arise only in pattern space (Greek indices). Contravariant tensors no longer appear, the only contravariant tensor C^{-1} being absorbed in the definition (55). There is then also no need to introduce contravariant fingerprint patterns separately from the covariant signal patterns, since the dual relation between the patterns is absorbed in the application of the generalized matrix product (55) in the projection of the climate trajectory into the reduced pattern space.

Using this notation, the general multi-pattern representation (27) (retaining still the distinction between upper and lower Greek indices and the summation convention for the pattern space),

$$\psi = d^v \mathbf{g}_v + \psi^r, \quad (56)$$

yields, on application of the statistical least square condition $\psi^{rT} \odot \psi^r = \min$, as determining Eq. (28) for the pattern amplitudes:

$$D_{v\mu} d^\mu = \mathbf{g}_v^T \odot \psi \quad (v = 1, \dots, p), \quad (57)$$

where (Eq. 30)

$$D_{v\mu} = \mathbf{g}_v^T \odot \mathbf{g}_\mu. \quad (58)$$

The remaining relations may be similarly rewritten in this generalized matrix notation.

References

Barnett TP, Hasselmann K (1979) Techniques of linear prediction, with application to oceanic and atmospheric fields in the tropical Pacific. *Rev Geophys* 17: 949–968
 Bell TL (1982) Optimal weighting of data to detect climate change: application to the carbon dioxide problem. *J Geophys Res* 87: 11161–11170

Bell TP (1986) Theory of optimal weighting of data to detect climate change, *J Atmos Sci* 43: 1694–1710
 Cubasch U, Santer BD, Hellbach A, Hegerl G, Höck H, Maier-Reimer E, Mikolajewicz U, Stössel A, Voss R (1994) Monte Carlo climate change forecasts with a global coupled ocean-atmosphere model. *Clim Dyn* 10: 1–19
 Earman J (1992) Bayes or bust? A critical examination of bayesian confirmation theory. MIT Press, Cambridge, Mass, 272 pp
 Hasselmann K (1979) On the signal-to-noise problem in atmospheric response studies. In Shaw DB (ed) *Meteorology of tropical oceans*. pp 251–259, Royal Meteorological Society, London
 Hasselmann K (1993) Optimal fingerprints for the detection of time-dependent climate change. *J Clim* 6: 1957–1969
 Hasselmann K, Bengtsson L, Cubasch U, Hegerl GC, Rodhe H, Roeckner E, v.Storch H, Voss R, Waszkewitz J (1995) Detection of anthropogenic climate change using a fingerprint method, *Modern dynamical meteorology, Proc Wiin-Nielsson Symposium, ECMWF Rep* pp 203–221
 Hegerl GC, North GR (1997) Statistically optimal methods for detecting anthropogenic climate change. *J Clim* 10: 1125–1133
 Hegerl GC, v.Storch H, Hasselmann K, Santer BD, Cubasch U, Jones PD (1996) Detecting greenhouse gas induced climate change with an optimal fingerprint method. *J Clim* 9: 2281–2306
 Hegerl GC, Hasselmann K, Cubasch U, Mitchell JFB, Roeckner E, Voss R, Waszkewitz J (1997) Multi-fingerprint detection and attribution of greenhouse gas, greenhouse gas-plus-aerosol and solar forced climate change, *Clim Dyn* 13: 613–634
 North GR, Kim KY (1995) Detection of forced climate signals, part II: simulation results. *J Clim* 8: 409–417
 North GR, Kim KY, Shen SP, Hardin JW (1995) Detection of forced climate signals, part I: filter theory. *J Clim* 8: 401–408
 Pennell WT, Barnett TP, Hasselmann K, Holland WR, Karl TR, North GR, MacCracken MC, Moss ME, Pearman G, Rasmusson EM, Santer BD, Smith WK, v.Storch H, Switzer P, Zwiers F (1993) The detection of anthropogenic climate change, *Proc 4th Symp Global Change Studies, Anaheim (Cal) Jan. 17–19, 1993, Am. Meteorol. Soc.* 21–28
 Santer BD, Mikolajewicz U, Brüggemann W, Cubasch U, Hasselmann K, Höck H, Maier-Reimer E, Wigley TM (1995a) Ocean variability and its influence on the detectability of greenhouse warming signals. *J Geophys Res* 100: 10 693–10 725
 Santer BD, Taylor KE, Penner JE, Wigley TML, Cubasch U, Jones PD (1995b) Towards the detection and attribution of an anthropogenic effect on climate. *Clim Dyn* 12: 77–100
 Santer BD, Wigley TML, Barnett TP, Anyamba E (1996a) Detection of climate change and attribution of causes, IPCC Second Scientific Assessment, Houghton JT et al. (ed) 407–444, Cambridge University Press, UK
 Santer BD, Taylor DE, Wigley TM, Jones PD, Karoly DJ, Mitchell JFB, Oort AH, Penner JE, Ramasvamy V, Schwarzkopf MD, Stouffer RS, Tett SFB (1996b) A search for human influences on the thermal structure of the atmosphere. *Nature* 382: 39–46
 Thacker WC (1995) Indices characterizing patterns of climate change (preprint)