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Application of inverse modelling techniques to palaeoclimatic data

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Abstract

The method of inverse modelling is summarized and illustrated by examples from short-term climate modelling. The application of the technique to palaeoclimatic data is demonstrated by developing a general method for the construction of linear climate response models simulaneously with the time calibration of core records. The approach admits full variability of the time-depth calibration curve under defined integral constraints while determining the optimal linear climate response to astronomical forcing consistent with general dynamical side conditions.

1. Introduction

In the last years the palaeoclimatic data base derived from deep-sea cores and other geological sources has expanded considerably. Continuous profiles of various climatic indices extending over several hundred thousand years or longer now exist for a wide distribution of locations. These data provide not only information on the state of past climates, but also on the dynamics of the climatic system controlling global climatic variations in the time scale range from 10^3 - 10^6 years. However, the relevant dynamic properties cannot be inferred immediately from the data records, but must be extracted from a host of other relations involving the interpretation of climatic indices, the absolute time calibration of core records, and the form of external climatic forcing, as well as the various internal interactions within the climatic system. A useful tool for decomposing such multiple interrelations and establishing the significance of the diagnostic and dynamical conclusions inferred from the data is the method of inverse modelling. The technique has become a standard tool in many areas of geophysics, but has so far found little application in palaeoclimatology (apart from the climatic interpretation of proxy data).

In this paper we summarize briefly the basic concepts of inverse modelling, present a few elementary examples of previous applications in climate dynamics analysis, and outline some potential applications for palaeoclimatology.

2. Inverse modelling methods

The difference between standard "direct modelling" and "inverse modelling" is basically minor. Any model designed to simulate an observed set of n data values $\underset{\sim}{d} = (d_1, \dots d_n)$ will normally contain a number m of adjustable internal parameters $\underset{\sim}{a} = (a_1, \dots a_m)$. The modeller will typically try to "tune" his model through suitable choice of the parameters $\underset{\sim}{a}$ such that the model $\underset{\sim}{\hat{d}}$ approximates the observed data $\underset{\sim}{d}$ as closely as possible (Fig. 1a). The principal difference between the inverse modelling approach and standard direct modelling is that the tuning is not left to the subjective efforts of the modeller, but is automated in the form of a feedback loop (cf. Fig. 1b).

The automization requires the definition of an error function which is minimized in the feedback loop. Normally, some quadratic form

$$\epsilon = \sum_{i,j} M_{ij}(d_i-\hat{d}_i)(d_j-\hat{d}_j) \qquad (1)$$

is chosen where M_{ij} represents a positive definite error metric. The output of the minimization process then defines a set of optimally determined model parameters $\underset{\sim}{a}$ as a function of the observed data $\underset{\sim}{d}$, $\underset{\sim}{a} = \underset{\sim}{a}(\underset{\sim}{d})$. Thus the relation between model parameters and data is inverted relative to the direct modelling approach, in which the simulated data are predicted as output for a given set of input model parameters $\underset{\sim}{a}$, $\underset{\sim}{d} = \underset{\sim}{d}(\underset{\sim}{a})$.

The simple step of automating the model fitting procedure opens up a number of possibilities not amenable to subjective tuning procedures :

(1) The models may contain a fairly large number m of free parameters. The parameters $\underset{\sim}{a}$ may often be related to important physical properties of the system which could not be easily inferred from the data without model inversion techniques (cf. next section).

(2) The errors $\delta\underset{\sim}{a}$ induced in the model parameters by errors $\delta\underset{\sim}{d}$ in the data can be systematically investigated. This enables the assessment of the statistical sugnificance of the model for a given data error covariance matrix.

(3) The ability to carry out a quantitative model error analysis and significance assessment provides further the basis for investigating hierarchies of models involving an increasing number of free parameters. Typically, the effect of introducing additional parameters into a model is to increase the "skill" of the model through the reduction of the error , but at the same time to decrease the "significance" of the model, as expressed in terms of the model error covariance matrix $\langle\delta a_i \delta a_j\rangle$ (cf. Davis, 1977, Barnett and Hasselmann, 1979). The model hierarchy is developed up to a critical order for which the significance falls below some prescribed acceptance level (cf. Fig. 2). By systematically increasing the order of the model until this cut-off point is reached, the maximum content of statistically significant information can be extracted from the data.

(4) The form (1) of the error function can be readily generalized to include further side conditions, such as the requirement that the model should be as smooth as possible, or lie as close as possible to some favoured theoretical model. Without side conditions, the numbers of free paramaters characterizing a model class must be restricted to be smaller than the number of data values. The introduction of continuous integral side conditions is formally equivalent to the introduction of a continuum of artificial data. Thus an infinite dimensional continuum of models may now be considered, without prior limitation of their functional form. The classical inverse modelling papers of Backus and Gilbert (1967) and Gilbert (1971) addressed this general case. The applications to palaeoclimatic data discussed in section 5 also fall in this class.

A basic limitation of the inverse modelling approach is that the models need to be kept relatively simple, since many cycles through the iteration loop (Fig. 1b) are normally required to minimize the error (particularly for more interesting applications involving a large number of model parameters). Some examples from the field of short term climate modelling (one month to a few years) are given in the next section.

. Some examples

Inverse modelling techniques are most useful in situations in which a fairly extensive data set for model construction exists, but the physical concepts proposed to explain the data are still relatively rudimentary and can therefore be cast in rather simple models. A typical case is short term climate variability on time scales of months to years. Extensive time series on global climate variability exist for these periods (sea surface temperatures, atmospheric temperatures and pressures, precipitation, etc.), but relatively little is known of the physics governing the observed climatic fluctuations.

An example of the application of inverse modelling for these time scales is given in Fig. 3, which shows the distribution of near surface currents determining the advection of sea surface temperature (SST) anomalies in the North Pacific (Herterich and Hasselmann, 1983). The currents were inferred alone from SST observations by fitting a simple model of the form

$$\frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i} \left(D_{ij} \frac{\partial T}{\partial x_j}\right) + \lambda T = n \qquad (2)$$

to 25 years of monthly SST anomaly data for 5° (MARSEN) squares in the area shown. In eqn (2), T denotes the SST anomaly, u_i the two-dimensional current vector, D_{ij} a diffusion tensor, λ a feedback parameter and n a (temporal) white noise forcing term representing the short term fluctuations of the heat transfer across the air-sea interface.

The model was optimized by fitting the simulated output to the measured SST auto- and cross spectra. It yielded fields of all coefficients u_i, D_{ij}, λ and the spectral level and spatial correlation scales of the white noise forcing.

Model fitting to the statistical moments (spectra, covariance functions) of the data rather than the data time series themselves is generally appropriate when the input function driving the model is not given explicitly, but is known only in terms of its statistical properties (e.g. Olbers et al., 1976, Long and Hasselmann, 1979). However, the time series can also be used directly in some cases by adjusting the model coefficients such that the unknown residual input n is minimized, cf. Box and Jenkins (1976). In the present example, this technique was not applied, since the model requirement was not that the input should be white, but not necessarily small. A similar analysis has been applied by Lemke et al. (1980) to investigate the variability of sea ice on monthly to interannual time scales and by Lemke (1977) to determine whether the climate variability in the time scale range 10^2 - 10^6 years can be explained as the response to stochastic white noise forcing.

A more detailed analysis of the model dynamics is possible if the input function is known explicitly, so that the input and response functions can be correlated. This approach has been used, for example, in the construction of short-term climate linear regression prediction models (cf. Barnett and Hasselmann, 1979, Hasselmann and Barnett, 1981, Davis, 1978). In palaeoclimatic modelling, the method can be applied to determine the dynamical response characteristics of the climate system to astronomical variations of the solar insolation.

In general, however, the construction of palaeoclimatic models will probably need to be based on a combination of the spectral and time series fitting methods, since the driving terms consist of a superposition of the known Milankovitch input and stochastic forcing terms, which can be described only statistically. An additional complication of palaeoclimatic model construction is that the time calibration of palaeoclimatic records is not known and must be determined as part of the model fitting procedure. We consider this problem in section 5 after a brief discussion of current time calibration approaches in the following section.

4. Continuous dating of palaeoclimatic records

Following the pioneering work of Hays et al. (1976), the use of the insolation forcing in the Milankovitch spectral bands of 19, 23 and 41 ky as time reference is generally regarded as the most effective technique for establishing the time calibration of palaeoclimatic records. The time axis is generally tuned subjectively to maximize the spectral coherence between the input and response at the Milankovitch frequencies (cf. Hays et al., 1976, Morley and Hays, 1981). The method makes no use of the information contained in the system transfer functions at these frequencies. Thus the precise choice of climate response signal and input forcing function is immaterial, provided both signals contain significant energy in the frequency bands in question.

Herterich and Sarnthein (1983) have recently applied this approach in a formal inverse modelling framework. However, the inverse method was applied only in a restricted sense, since the calibration function $z = c(t)$ relating the core depth z to time t was allowed to vary only with respect to 5 adjustable parameters (representing 5 dated levels, as compared with about 30 levels which have been varied in subjective tuning methods). In the general technique discussed in the following section, $c(t)$ can be an arbitrary function of time subject only to certain integral constraints.

Various alternative time calibration techniques have been proposed in which assumptions are introduced, independent of the solar insolation input, to interpolate the sedimentation rates between well dated core levels (Shackleton and Opdyke, 1973, Shackleton and Matthews, 1977, Kominz et al., 1979, Sarnthein et al., 1983). For example, von Grafenstein (1982) and Herterich and Sarnthein (1983), related the sedimentation rate to the (highly variable) carbonate concentration. The method was tested by Herterich and Sarnthein (1983) by subsequently correlating the time calibrated climate signal with the solar insolation. Significant coherences were found in the Milankowitch frequency bands, with coherence levels only slightly lower than the values obtained by direct calibration against the solar input. However, the calibration curve CARPOR obtained in this manner deviated significantly, by time separations of the order 20 - 50 kyrs from calibrations obtained from the solar input. Significantly different calibrations were also obtained by the latter technique depending on whether the Brunhes-Matuyama boundary at 730 ky B.P. was regarded as fixed (STUNE) or variable (TUNE) (cf. Fig. 4). We note that all three calibration curves shown in Fig. 4 exhibit statistically significant coherences in the Milankowitch frequency bands at the 90 - 95 % condifende level, although the differences in time calibration are of the order of one to two Milankowitch periods. The calibration ambiguities are related to the property that the total integrated coherence for the three frequency bands passes through a number of relative maxima of comparable magnitude as the calibration curve in systematically varied. Apparently, it is possible to "swallow a period" in regions in which the signals are low without significantly affecting the coherence.

To resolve the ambiguities, additional considerations are needed. One possibility is to penalize calibration solutions which exhibit rapid changes by including a smoothness requirement in the minimized error function. Another approach is to investigate the complex transfer function representing the response of the calibrated climatic signal to the insolation input and test whether the frequency dependencies of the phase and amplitude are consistent with basic dynamical concepts. Fig. 5 shows the transfer functions associated with the three calibration curves of Fig. 4. Based on simple requirements of continuity and causality, the calibration curve TUNE (variable Brunhes-Matuyama boundary) may be rejected as improbable. The calibration curve STUNE (fixed Brunhes-Matuyama boundary) is more consistent with a simple first-order feedback model (cf. section 5) than the carbonate calibrated solution CARPOR. However, the calibrations CARPOR and STUNE should not be regarded as competitive, but rather as complementary : STUNE models the gradual changes of the sedimentation rate, while CARPOR is determined largely by the short time scale fluctuations of the sedimentation rate which are implied by the observed short term fluctuations of the carbonate concentration.

We note that none of the models yield plausible transfer functions at the eccentricity period of 10^5 years, unless a high Q resonance of the climatic system is assumed at this frequency. This is a well=known consequence of the high energy peak in the climatic record at this period which has motivated a number of model constructions exhibiting quasi self-generated oscillations at this frequency.

Ideally, a flexible, general time calibration and dynamical model fitting procedure should attempt to combine the diverse inputs and constraints determining the time calibration and model dynamics into a single optimization algorithme, in which the bestfit time calibration and optimal dynamical model are generated as joint outputs of the optimization procedure. The outline of such an approach is developed in the following section.

5. Application of inverse modelling to palaeoclimatic data

We begin with the time calibration problem. Let us assume there exists a prior calibrated depth-time relation $z = c^o(t)$ based on a finite number of dated levels and estimates of the sedimentation rates (derived, for example, from the carbonate concentration profile). We attempt now to improve on this calibration by tuning the observed climatic response $\eta(z)$ to the known astronomical forcing function $\xi(t)$.

Since $\xi(t)$ has significant energy only in the three Milankovitch bands centered on the periods 19, 23 and 41 ky, we consider for this purpose only the filtered climatic signal in which all energy is removed except within these bands. To avoid encumbering the notation, we retain the symbol $\eta(t)$ for the filtered climatic signal. For the same reason we consider only a single input and single output function. The extension to the multi-dimensional problem of a number of input functions (cf. discussions in Hays et al., 1976, Berger et al., 1981, Kukla et al., 1981, Bruns, 1981, and Herterich and Sarnthein, 1983) and a number of climatic outputs (representing, for example, different climatic indices at different locations) is of considerable interest for the construction of dynamical models, but is conceptually straight-forward and need not be elaborated here.

In improving the time calibration we wish to stay as close as possible to the original calibration function $z = c^o(t)$ while simultaneously satisfying (again "as well as possible") the following additional constraints : well dated levels $z_i = z_i(t_i)$ should be reproduced; the small scale variability of the deviation $c'(t)$ of the net calibration curve $z = c(t) = c^o(t) + c'(t)$ from the prior calibration $c^o(t)$ should be small; and the transfer functions derived from the time calibrated climatic response should be consistent with general dynamical concepts.

The last condition cannot be formulated without considering the dynamic model fitting problem. We assume here for simplicity that the dynamic response model is linear. Although the basic approach can be extended to nonlinear models, it is no longer possible in this case to restrict the analysis to the Milankovitch forcing frequencies, and the relations become more complex.

For a linear model the (predicted) climatic response $\hat{\eta}(t)$ to the forcing can be represented in the general form

$$\hat{\eta}(t) = \int_{-\infty}^{t} T(t-t')\, \xi(t')dt' \qquad T(\xi) \tag{3}$$

or, in the Fourier domain,

$$\hat{\eta}_\omega = T_\omega \xi_\omega \tag{4}$$

where T, T_ω represent, respectively, the system transfer (Green) function and its Fourier transform

$$T_\omega = \frac{1}{2\pi} \int_{-\infty}^{\infty} T(t) e^{-i\omega t} dt \tag{5}$$

and ξ_ω, $\hat{\eta}_\omega$ are defined as full resolution Fourier transforms over the entire interval $-\tau \leq t \leq 0$ of the given climatic record,

$$(\xi_\omega, \hat{\eta}_\omega) = \frac{1}{\tau} \int_{-\tau}^{0} (\xi, \hat{\eta}) e^{-i\omega t} dt \tag{6}$$

(The statical smoothing required below for the auto- and covariance spectra may be regarded formally as obtained by averaging over neighbouring frequencies).

Without any prior information on the dynamics of the climatic system, the only condition which can be placed on T is the causality relation $T(t) = 0$ for $t < 0$ (already implied in the upper bound t of the integral in eqn (3)) or the equivalent Kronig-Kramers relations between the real and imaginary components of the Fourier transform T_ω. However, elementary preconceptions on the structure of the climate dynamics may suggest a simple form for T. For example, the climatic response to stochastic white noise forcing n(t) has often been successfully modelled by a simple first order Markov process of the form

$$\frac{d\eta}{dt} + \lambda\eta = n(t) \tag{7}$$

with a constant linear feedback factor λ which is represented by a transfer fucntion

$$T(t) = \begin{cases} e^{-\lambda t} & (t > 0) \\ \\ 0 & (t < 0) \end{cases} \tag{8}$$

or

$$T_\omega = \frac{1}{i\omega+\lambda} \tag{9}$$

The next step in complexity would be a second-order system, with which a resonance at some prescribed period could be modelled (10^5 years would be a favoured candidate).

In the following, we assume that the most likely structure of the transfer function T^o, of the form (8), (9), say, has been identified on the basis of some prior physical concepts. In general, the transfer function T^o will depend on a number m of adjustable parameters a_i.

The problem of simultaneously optimizing the time calibration and dynamical model structure under the stated constraints may then be formulated as the problem of minimizing the general error function

$$\epsilon = \epsilon_o + g_1\epsilon_1 + g_2\epsilon_2 + g_3\epsilon_3 + g_4\epsilon_4 \tag{10}$$

with respect to independent variations of the calibration function c, transfer function T_ω and model parameters a_i, where $g_1, \ldots g_4$ represent suitably chosen weighting factors and the individual error functions are defined as follows :

$$\epsilon_o = (\eta(c(t)) - \hat{\eta}(t))^2 dt = (\eta - T(\xi))^2 dt \tag{11a}$$

$$= 2\pi \, \langle|\eta_\omega - T_\omega \xi_\omega|^2\rangle d\omega \tag{11b}$$

describes the basic deviation between the model prediction $\hat{\eta}$, after calibration of the time axis, and the observed climatic time series (c(t)) (within the Milankovitch frequency bands; the cornered parentheses denote smoothing over neighbouring frequency bands, within the bands, which is formally redundant in the integral (11b), but is required later in the variational equations);

$$\epsilon_1 = \sum_i (z_i - c_i(t_i))^2 = \sum_i \int \delta(t-t_i)(c(t)-z_i)^2 dt \qquad (12)$$

represents the sum of the time calibration errors at the levels z_i for which the date t_i are well-known;

$$\epsilon_2 = \int (c-c^o)^2 dt = \int (c'(t))^2 dt \qquad (13)$$

denotesthe mean square deviation of the net calibration function c(t) from the prior calibration $c^o(t)$;

$$\epsilon_3 = \int \left(\frac{d^2c'}{dt^2}\right)^2 dt \qquad (14)$$

expresses the constraint that the deviation c' from the prior calibration function c^o should be as smooth as possible (ϵ_3 could also be replaced by an integral over the square of the slope rather than the curvature of c'), and, finally,

$$\epsilon_4 = \langle|\xi_\omega|^2\rangle |T_\omega - T^o_\omega|^2 d\omega \qquad (15)$$

represents the deviation between the optimal empirical model T and the preferred theoretical model T^o_ω.

We note that the basic error expression ϵ_o depends on both the time calibration and the model, while the errors ϵ_1, ϵ_2, ϵ_3 depend only on the calibration, the error $_4$ only on the model. The usual decoupled methods of time calibration and model construction consider only the basic error function. It can be shown (e.g. by inspection of eqn (16), below) that the optimal time calibration problem is not well posed for an arbitrary calibration function c(t) when formulated solely in terms of ϵ_o (the optimal solution consists of a set of perfect fit segments separated by discontinuities). Thus apart from the inherent attraction of introducing all calibration aspects into a single error function, some form of additional constraint is required to yield a meaningful solution.

The variation of eqn (10) with respect to c' yields as minimum condition for the optimal calibration curve c (or c')

$$\frac{d\eta}{dz}[\eta(c(t))-\bar{\eta}(t)] + g_1 \sum_i (c(t_i)-z_i)\delta(t-t_i) + g_2 c'(t) + g_3 \frac{d^4c'(t)}{dt^4} = 0 \qquad (16)$$

with boundary conditions

$$\frac{d^2c'}{dt^2} = \frac{d^3c'}{dt^3} = 0 \quad \text{at } t = -\tau \text{ and } 0 \qquad (17)$$

The δ-functions in (16) may be removed by integrating across infinitesimal intervals at t_i, yielding the equation

$$g_3 \frac{d^4 c'}{dt^4} + g_2 c' + \frac{d\eta}{dz}(\eta - \hat{\eta}) = 0 \qquad (18)$$

valid for the intervals between the calibration points t_i with matching conditions

$$g_3 \frac{d^3 c'}{dt^3} \Bigg]_{z_i-\varepsilon}^{z_i+\varepsilon} = -g_1(z_i - c(t_i)) \text{ at the calibration points } t_i \qquad (19)$$

The corresponding minimum condition with respect to variations of T_ω yields

$$T_\omega = \frac{\langle \eta_\omega \xi_\omega^* \rangle + g_4 T_\omega^o \langle |\xi_\omega|^2 \rangle}{\langle |\xi_\omega|^2 \rangle (1+g_4)} \qquad (20)$$

(The quadratic mean products may be replaced by the appropriate auto- and cross spectra, from which they differ only by a common normalization factor).

Equation (20) is identical to the usual optimal fit transfer function of linear system theory except for the distorsion towards the favoured model T_ω^o introduced by the terms proportional to g_4. The appropriate value for the weight g_4 can be derived from statistical maximum likelihood considerations based on the statistical uncertainty of the spectral estimates $\langle |\xi_\omega|^2 \rangle$ and $\langle \eta_\omega \xi_\omega^* \rangle$ and the a priori "likelihood" attributed to the validity of the model T_ω^o (cf. Savage, 1962). In practice, g_4 will generally be of order $p^{-\frac{1}{2}}$, where p is the number of degrees of freedom of the spectral estimate.

Finally, the variation with respect to the preferred model parameters, a_i yields the relations

$$(T_\omega - T_\omega^o) \frac{\partial T_\omega^{o*}}{\partial a_i} \xi_\omega \,^2\!\rangle d\omega = 0 \qquad (i=1, \dots m) \qquad (21)$$

The optimal time calibration c, optimal dynamical model T and best fit preferred model T_ω^o are obtained by simultaneous solution of the equations (17) - (21). The solutions can be constructed iteratively : starting from the reference calibration c^o as first guesses for c and a suitable choice of model parameter a_i as first guess for T_ω^o, the associated optimal transfer function T can be determined from (20). This defines a theoretical response $\hat{\eta}$, and the solution of the differential equation (18), with boundary conditions (17) and (19), then yields a first iteration of the calibration function c(t). Similarly, equations (21) determine an iterated set of parameters a_i. The procedure is then repeated, a new T_ω being determined from the new calibration c and new preferred model T_ω^o.

Experience with similar coupled optimal fitting problems in other applications (cf. Herterich and Hasselmann, 1983, Long and Hasselmann, 1979, Olbers et al., 1976) indicates that the convergence of such iterative schemes is normally rather rapid.

As pointed out in section 2, an important aspect of inverse modelling, which we have not been able to consider in this example, is the application of the technique to determine the mapping of data errors or statistical estimation uncertainties into model errors. We have also not discussed possible extensions of the model to include stochastic white noise forcing, an important aspect in trying to model the complete palaeoclimatic record (cf. Kominz et al., 1979).

However, even without these extensions the inverse modelling technique described here determine a general optimal time calibration function and dynamical model, subject only to integral constraints which can be clearly specified, and whose effects can be systematically explored by numerical experimentation. The application of these techniques as a diagnostic tool to investigate climate variability in the time scale range 10^3 - 10^6 years will become indispensible as more palaeoclimatic time series become available for analysis.

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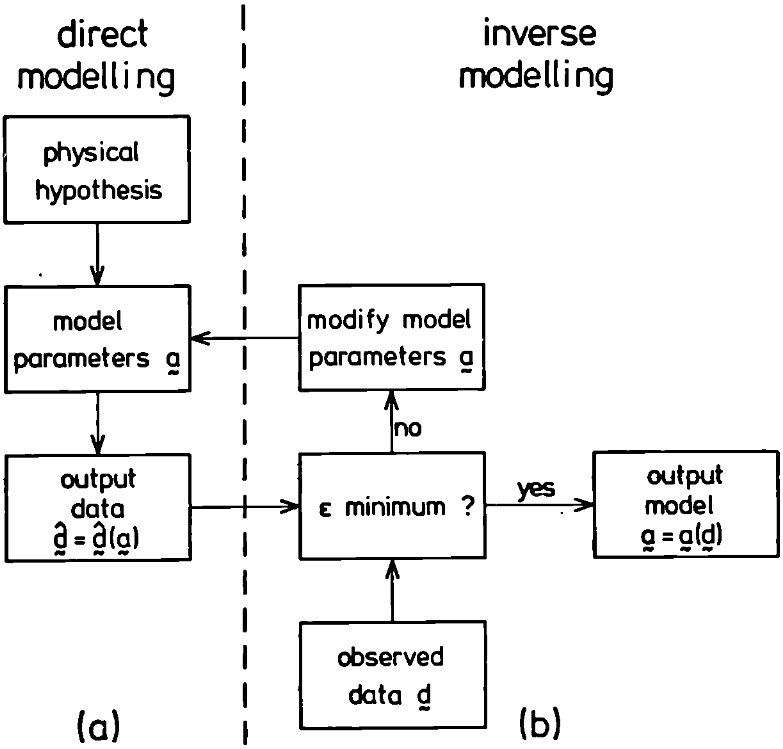

Fig. 1 Relation between direct and inverse modelling methods.
In the inverse modelling approach, the optimally tuned model is found by a closed iteration loop (for very simple, e.g. linear models, the inversion can sometimes be given explicitly).

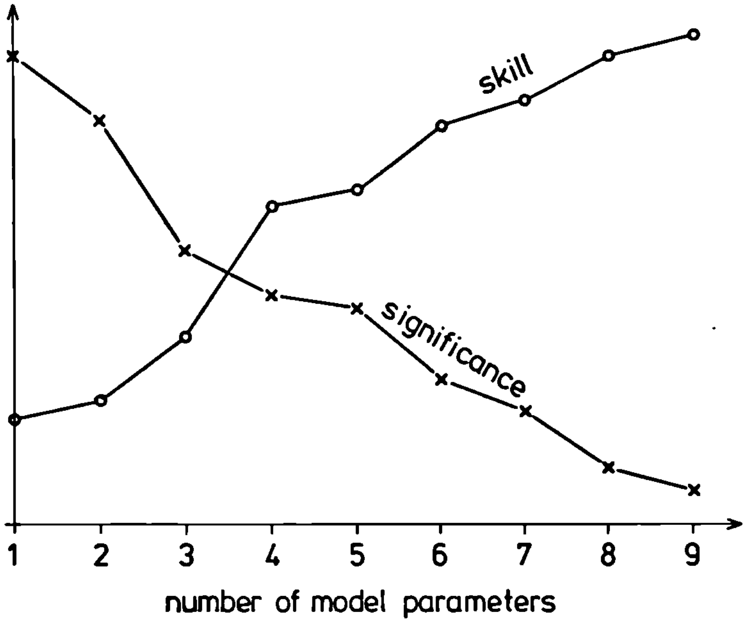

Fig. 2 Contrary dependencies of model skill and significance on number of adjustable model parameters.

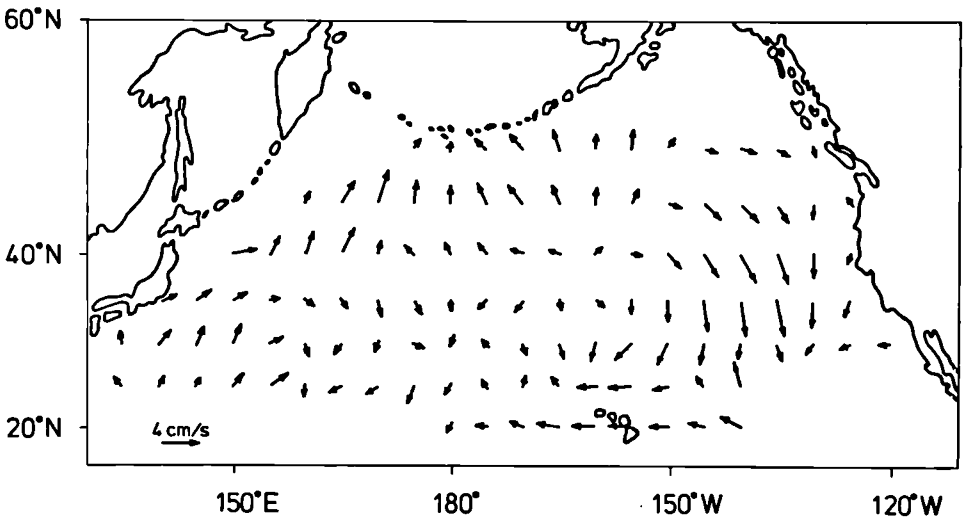

Fig. 3 Field of upper layer ocean currents determining advection of SST as inferred by statistical analysis of SST anomaly time series (from Herterich and Hasselmann, 1983).

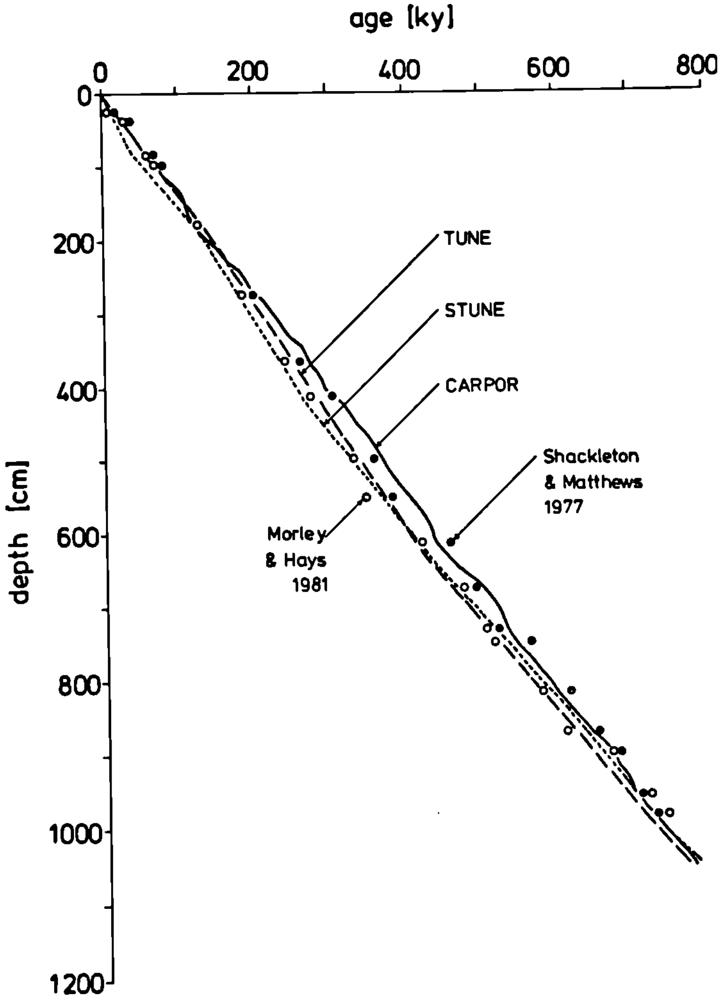

Fig. 4 Time calibration curves for METEOR core 13519 inferred from carbonate concentrations (CARPOR) and cross correlation with July insolation at 65°N with fixed (STUNE) and variable (TUNE) Brunhes-Matuyama boundary (from Herterich and Sarnthein, 1983).

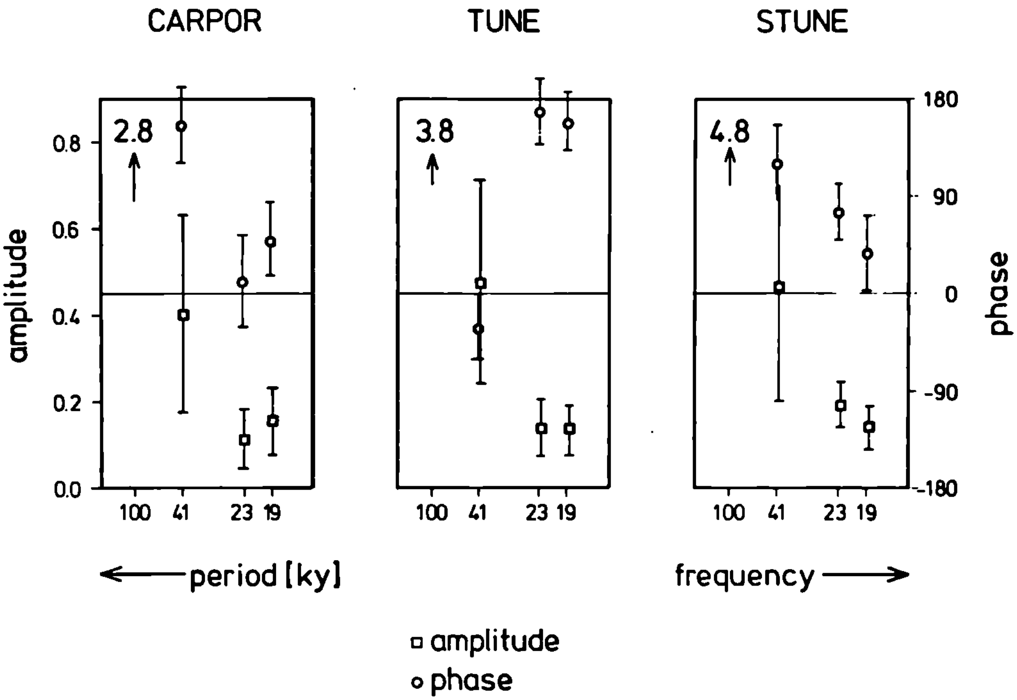

Fig. 5 Transfer functions (amplitude and phase) relating climate response ($\delta^{18}O$) for METEOR core 13519 to July insolation at 65°N for the three time calibrations CARPOR, STUNE and TUNE.