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Supplement of

Evaluation of simulated responses to climate forcings: a flexible statistical framework using confirmatory factor analysis and structural equation modelling – Part 1: Theory

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Contents

S1 Assessing the overall forcing effect by using the Confirmatory Factor Analysis (CFA) model specification

This section complements Sect. 3 and 4 in the article devoted to presenting

- the ME model used in D&A studies for assessing the individual contribution of the forcings studied (Sect. 3),
- the corresponding basic CFA model suggested within our framework (Sect. 4).

Here, we present the ME model used in D&A studies for assessing the overall effect of several forcings, and the corresponding CFA model developed within our framework.

S1.1 The Measurement Error (ME) model used in D&A studies and its link to the CFA model specification

Combining the notations and definitions of our framework with those used in D&A studies, a ME model used in D&A studies for assessing the overall response to the combination of the forcings of interest, is given by:

$$\begin{cases} x_{\mathrm{comb}\,t} = & \xi^{S}_{\mathrm{comb}\,t} + \quad \nu_t. \\ y_t = & \beta \cdot \xi^{S}_{\mathrm{comb}\,t} + \quad \nu_{0\,t}, \end{cases} \tag{S1}$$

The model above corresponds to the ME model with a vector of explanatory variables given in Eq. (2) in the article. The distributional assumptions of its variables are similar to those associated with the model in Eq. (2) in the article. The decomposition of the overall temperature response to all forcings $\xi^{T}_{\mathrm{ALL}\,t}$ is also similar to that performed in the article (see Eq. 3), that is, the extraction of $\xi^{S}_{\mathrm{comb}\,t}$ from $\xi^{T}_{\mathrm{ALL}\,t}$ does not give rise to an error in the equation for y_t over and above the random internal temperature variability $\nu_{0\,t}$:

$$\xi^{T}_{\mathrm{ALL}\,t} = \beta \cdot \xi^{S}_{\mathrm{comb}\,t}, \tag{S2}$$

of which, in addition, follows that the combination of the reconstructed forcings is supposed to represent the correponding true combination of real-world forcings generating $\xi^{T}_{\mathrm{ALL}\,t}$.

Both detection and consistency tests are analogous to those performed under the ME model defined in Eq. (2) in the article, that is, H_0: $\beta = 0$ and H_0: $\beta = 1$, respectively.

To see why the consistency between the simulated and true temperature responses is a necessary condition for performing the attribution, note that the hypothesis of consistency implies the equality between $\xi^{T}_{\mathrm{ALL}\,t}$ and $\xi^{S}_{\mathrm{comb}\,t}$ in Eq. (S2). Thus, model (S1) under the hypothesis of consistency takes the following form:

$$\begin{cases} x_{\mathrm{comb}\,t} = & \xi^{T}_{\mathrm{ALL}\,t} + \quad \nu_t, \\ y_t = & \xi^{T}_{\mathrm{ALL}\,t} + \quad \nu_{0\,t}. \end{cases} \tag{S3}$$

As follows from (S3), the observational data y_t (and x_t as well due to consistency) is a function of the true overall temperature response, which makes it reasonable to attribute this detected temperature response to the real-world forcings under consideration. Hence, model (S3) supports the idea of modelling $\xi^{T}_{\mathtt{f}}$, where $\mathtt{f}$ may represent either an individual forcing or a combination of forcings, as a common latent factor for both observed and simulated temperatures. In addition, the model provides an alternative interpretation of consistency, namely that the combination of the specified forcing(-s) exhibits an equal influence on both observed and simulated climate changes. We use this alternative interpretation within our CFA (and SEM).

In the matrix form given in Eq. (S1), the ME model is represented as an unstandardised CFA model with one common latent factor and two observable indicators for this latent common factor. The standardisation of $\xi^S_{\text{comb}\,g}$ leads to a 2-indicator 1-factor CFA model, abbr. ME-CFA(2,1) model:

$$\begin{cases} x_t = & \alpha \cdot \tilde{\xi}^S_{\text{comb}\,t} + & \nu_t. \\ y_t = & \kappa \cdot \tilde{\xi}^S_{\text{comb}\,t} + & \nu_{0\,t}, \end{cases} \tag{S4}$$

where $\tilde{\xi}^S_{\text{comb}\,t} = \xi^S_{\text{comb}\,t} \Big/ \sqrt{\sigma^2_{\text{comb}}}$, $\alpha = \sqrt{\sigma^2_{\text{comb}}}$, and $\kappa = \beta \cdot \sqrt{\sigma^2_{\text{comb}}}$.

As indicated by its name, the ME-CFA(2,1) model is a ME model rewritten as a CFA model, and the model corresponds to the ME-CFA(6,5) model in Eq. (6) in the article.

As follows from (S4), the ratio κ/α gives us back β in Eq. (S1). Thus, the hypotheses tested under the ME model specification can also be tested under the CFA model specification. More precisely, the hypothesis H_0: $\beta = 0$ corresponds to testing H_0: $\kappa = 0$, while the hypothesis of consistency H_0: $\beta = 1$ is equivalent to testing H_0: $\kappa/\alpha = 1$, or equivalently H_0: $\kappa = \alpha$.

S1.2 The CFA(2,1) model

To formulate the corresponding CFA model, the first step is to express $\xi^S_{\text{comb}\,t}$, embedded in x_{comb}, and $\xi^T_{\text{ALL}\,t}$, embedded in y_t, as a linear function of the true temperature response $\xi^T_{\text{comb}\,t}$ in a similar way as it was done in Eq. (8) and (9) in the article. We get:

$$x_{\text{comb}\,t} = \xi^S_{\text{comb}\,t} + \tilde{\delta}_{\text{comb}\,t} = \gamma_1 \cdot \xi^T_{\text{comb}\,t} + \underbrace{\zeta^S_{\text{comb}\,t} + \tilde{\delta}_{\text{comb}\,t}}_{=\delta_{\text{comb}\,t}}, \tag{S5}$$

$$y_t = \xi^T_{\text{ALL}\,t} + \tilde{\nu}_t = \gamma_2 \cdot \xi^T_{\text{comb}\,t} + \underbrace{\zeta^T_{\text{ALL}\,t} + \tilde{\nu}_t}_{=\nu_t}, \tag{S6}$$

Eq. (S5) and (S6) together constitute an 2-indicator 1-factor CFA model, abbr. CFA(2,1) model, with $\xi^T_{\text{comb}\,t}$ as a common latent factor:

$$\begin{cases} x_{\text{comb}\,t} & = & \gamma_1 \cdot \xi^T_{\text{comb}\,t} & + & \delta_{\text{comb}\,t} \\ y_t & = & \gamma_2 \cdot \xi^T_{\text{comb}\,t} & + & \nu_t \end{cases} \tag{S7}$$

where the specific factors $\delta_{\text{comb}\,t}$ and ν_t are assumed to be both mutually independent and independent of $\xi^T_{\text{comb}\,t}$. This model corresponds to the CFA(7,6) model given in Table 2 in the article. Importantly, in both CFA models, the overall temperature response $\xi^T_{\text{comb}\,t}$ (and $\xi^S_{\text{comb}\,t}$ as well) is treated as a repeatable outcome of a random variable, assumed to have a zero-mean and the variance $\sigma^2_{\xi^T_{\text{comb}}}$ (and $\sigma^2_{\xi^S_{\text{comb}}}$, respectively).

Due to the simplicity of the CFA(2,1) model, we can exemplify the process of determining the model identifiability algebraically. To begin with, the covariance structure equations, $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}(\boldsymbol{\theta})$, under the CFA(2,1) model are given by the following three unique (nonduplicated) equations:

$$
\begin{aligned}
\sigma^2_{x_\text{comb}} &= \gamma_1^2 \cdot \sigma^2_{\xi^T_\text{comb}} + \sigma^2_{\delta_\text{commb}} \\
\sigma_{x_\text{comb}\, y} &= \gamma_1 \cdot \gamma_2 \cdot \sigma^2_{\xi^T_\text{comb}} \\
\sigma^2_y &= \gamma_2^2 \cdot \sigma^2_{\xi^T_\text{comb}} + \sigma^2_\nu .
\end{aligned}
\tag{S8}
$$

It is clear that none of the five model parameters, γ_1, γ_2, $\sigma^2_{\xi^T_\text{comb}}$, $\sigma^2_{\delta_\text{comb}}$ and σ^2_ν, can be determined (identified) from the three equations. However, by introducing the restriction $\sigma^2_{\xi^T_\text{comb}} = 1$ and treating $\sigma^2_{\delta_\text{comb}}$ as known a priori, the remaining model parameters, i.e. γ_1, γ_2, and σ^2_ν, become identified.

Standardising latent factors to have unit variance is a typical restriction in CFA used to assign a scale to latent factors to fully interpret the factor loadings. As we see, it aids the identification as well. Another way of establishing a scale for a latent factor is to fix a factor loading to unity with respect to one of its indicators.

Under the above-specified restrictions, each parameter is not only identified but is just-identified. This means that there is only one distinct subset of equations in Eq. (S8) that is uniquely solvable for γ_1, γ_2, and σ^2_ν, respectively. The resulting solutions are:

$$
\begin{aligned}
\gamma_1 &= \sqrt{\sigma^2_{x_\text{comb}} - \sigma^2_{\delta_\text{comb}}} \\
\gamma_2 &= \sigma_{x_\text{comb}\, y} \Big/ \sqrt{\sigma^2_{x_\text{comb}} - \sigma^2_{\delta_\text{comb}}} \\
\sigma^2_\nu &= \sigma^2_y - (\sigma_{x_\text{comb}\, y})^2 / (\sigma^2_{x_\text{comb}} - \sigma^2_{\delta_\text{comb}}),
\end{aligned}
\tag{S9}
$$

provided $\sigma^2_{x_\text{comb}} \geq \sigma^2_{\delta_\text{comb}}$ and $\sigma^2_y \geq (\sigma_{x_\text{comb}\, y})^2 / (\sigma^2_{x_\text{comb}} - \sigma^2_{\delta_\text{comb}})$. The solution is unique, apart from a possible change of sign of the factor loadings γ_1 and γ_2, which merely corresponds to changing the sign of the latent factor. If $\sigma_{x_\text{comb}\, y} > 0$, the sign for both factor loadings should be the same.

Replacing the population variances and covariance of the indicators in Eq. (S9) by their unbiased estimates, $s^2_{x_\text{comb}}$, $s_{x_\text{comb}\, y}$ and s^2_y, the exact ML solution of the model parameters is obtained:

$$
\begin{aligned}
\widehat{\gamma}_1 &= \sqrt{s^2_{x_\text{comb}} - \sigma^2_{\delta_\text{comb}}} \\
\widehat{\gamma}_2 &= s_{x_\text{comb}\, y} \Big/ \sqrt{s^2_{x_\text{comb}} - \sigma^2_{\delta_\text{comb}}} \\
\widehat{\sigma}^2_\nu &= s^2_y - \widehat{\gamma}_2{}^2,
\end{aligned}
\tag{S10}
$$

provided the conditions for admissible estimates analogous to those in Eq. (S9) are met.

Applying the principles of CFA and the previously mentioned alternative interpretation of the consistency (see Sect. 1.1), the hypothesis of consistency is tested by investigating whether γ_1 equals γ_2. In practice, it means that the model parameters are estimated under the restriction $\gamma_1 = \gamma_2$. Imposing this equality-constraint makes the model overidentified with 1 degree of freedom because the two remaining free parameters, i.e. γ_2 and σ^2_ν, become overidentified.

Overidentifiability means that one can find more than one subset of the equations in $\mathbf{\Sigma} = \mathbf{\Sigma}(\boldsymbol{\theta})$ by which one can solve uniquely for free model parameters. In our CFA(2,1) model, when $\sigma^2_{\xi^T_{\text{comb}}} = 1$ and $\sigma^2_{\delta_{\text{comb}}}$ is treated as known a priori, constraining γ_1 to γ_2 leads to two distinct solutions for γ_2 and to two distinct solutions for σ^2_{ν}:

$$\begin{aligned}
\gamma_2 &= \sqrt{\sigma^2_{x_{\text{comb}}} - \sigma^2_{\delta_{\text{comb}}}} \quad \text{or} \quad \gamma_2 = \sqrt{\sigma_{x_{\text{comb}}\,y}}, \\
\sigma^2_{\nu} &= \sigma^2_y - (\sigma^2_{x_{\text{comb}}} - \sigma^2_{\delta_{\text{comb}}}) \quad \text{or} \quad \sigma^2_{\nu} = \sigma^2_y - \sigma_{x_{\text{comb}}\,y}.
\end{aligned} \tag{S11}$$

provided $\sigma^2_{x_{\text{comb}}} \geq \sigma^2_{\delta_{\text{comb}}}$, $\sigma_{x_{\text{comb}}\,y} \geq 0$, $\sigma^2_y \geq (\sigma^2_{x_{\text{comb}}} - \sigma^2_{\delta_{\text{comb}}})$ and $\sigma^2_y \geq \sigma_{x_{\text{comb}}\,y}$.

Given that the model is correct, the multiple solutions for each overidentified parameter in the population are equal so each of the parameters has a unique solution. For a given sample, however, the two estimates of each parameter will not be exactly the same. Therefore, the ML-method seeks the optimal values for the parameters by minimising numerically the discrepancy function defined in Eq. (A2) in the Appendix in the article.

Under overidentifiability, $\mathbf{\Sigma}(\widehat{\boldsymbol{\theta}})$ does not fit the data, i.e. the sample variance-covariance matrix $\boldsymbol{S}$, perfectly. This permits us to assess the overall model fit. Provided that the solution obtained is admissible, which here means that $\widehat{\sigma}^2_{\nu} > 0$ [1], the model fit can be assessed statistically by means of the χ^2 test statistic, given in Eq. (A5) in the Appendix, and heuristically by various goodness-of-fit indexes, e.g. those defined in Eqs. (A6) - (A8) in the Appendix. If the model fits adequately, we may say that there is not enough evidence to reject the hypothesis of consistency.

Note that even if the hypothesis of consistency turns out to be rejected, it is still possible to draw conclusions about the effect of the real-world forcing `f` on the temperature by using the estimate of γ_2 obtained by fitting the CFA(2,1) model without hypothesising $\gamma_1 = \gamma_2$.

Other hypotheses, under which the CFA(2,1) model remains identified, are:

- $H_0 : \gamma_1 = \gamma_2 = 0$. The resulting factor model has zero latent factors and one free parameter, σ^2_{ν}, which gives us two degrees of freedom;
- $H_0 : \gamma_2 = 0$. Under this restriction, one needs to estimate two free parameters, γ_1 and σ^2_{ν}, which give us 1 degree of freedom. The resulting factor model hypothesises that the overall effect of the true forcing `f` is not detected in observational data. Although the model does not hypothesise consistency, it nevertheless has implications for consistency, provided the model is not rejected. If the estimate of γ_1 turns out to be insignificant, we may say that consistency is compatible with the data, while it is suspect if the estimate of γ_1 differs significantly from zero.

At this point, it is important to clarify that the rejection of any overidentified CFA model does not unambiguosly point to any particular constraint as at fault (Mulaik, 2010).

The CFA(2,1) model becomes *underidentified* under the hypothesis H_0: $\gamma_1 = 0$. This is because both free parameters, γ_2 and σ^2_{ν}, are to be determined from one and the same equation for σ^2_y in Eq. (S8).

The question remains whether it is possible to get a priori knowledge about $\sigma^2_{\delta_{\text{comb}}}$. As follows from Eq. (S5), $\sigma^2_{\delta_{\text{comb}}}$ is a sum of two variances: the variance of ζ^S_{comb} and the variance of $\tilde{\delta}_{\text{comb}}$. Knowledge about the latter is possible to derive from x_{comb} ensemble, containing simulations forced by an identical reconstruction of forcing `f` under different initial conditions.

[1] In statistical literature, a negative solution for a specific-factor variance is termed Heywood case.

The variance of ζ^S_{comb}, on the other hand, cannot be a priori estimated due to the absence of appropriate sources. Ensemble simulations cannot be used because time series $\{\zeta^S_{\text{comb}\,t}\}$ is the same for each of them due to treating $\xi^S_{\text{comb}\,t}$s as repeatable.

Given this limitation, the identifiability of the CFA(2,1)- model can be achieved only by setting the variance of δ_{comb} to the variance of $\tilde{\delta}_{\text{comb}}$. Consequently, the variance of ζ^S_{comb} has to be assumed to be negligible. Importantly, this assumption does not make the model disadvantageous, rather the other way round. This is because setting $\sigma^2_{\zeta^S_{\text{comb}}}$ to zero corresponds to hypothesising that the (large-scale) shape of the simulated temperature response to forcing $\mathtt{f}$ is correctly represented in the climate model under consideration. So, if model (S7) estimated under the restriction $\gamma_1 = \gamma_2$ is not rejected then we have no reasons to reject the hypotheses that both magnitude and shape of the simulated temperature response are correctly simulated by the climate model under consideration.

One way to estimate $\sigma^2_{\tilde{\delta}_{\text{comb}}}$ is to use one of the estimators definied in Eqs. (14) and (15), accompanied by the CFA($k_{\text{comb}}, 1$) model given in Eq. (18) and its modified version the CFA($k_{\text{comb}}, 0$) model, respectively.

S2 Theoretical definition of Structural Equation Model (SEM)

S2.1 A standard representation of SEM

A structural equation model consists of two submodels: a *latent variable model*, linking latent variables to each other, and a *measurement model*, linking latent variables to their indicators.

Submodel 1: Latent Variable Model

A structural equation for the latent variable model is as follows (Bollen, 1989; Jöreskog and Sörbom, 1988):

$$\boldsymbol{\eta} = \boldsymbol{B}\boldsymbol{\eta} + \boldsymbol{\Gamma}\boldsymbol{\xi} + \boldsymbol{\zeta}, \tag{S12}$$

where

- $\boldsymbol{\eta}$ an $m \times 1$ vector of latent endogenous (dependent) variables, i.e. the variables that are determined within the model;
- $\boldsymbol{\xi}$ an $n \times 1$ vector of latent exogenous (independent) variables, i.e. the variables whose causes lie outside the model;
- $\boldsymbol{\zeta}$ an $m \times 1$ vector of latent errors in equations (random disturbance terms). Each ζ_i represents influences on η_i that are not included the structural equation for η_i;
- $\boldsymbol{B}$ an $m \times m$ matrix of coefficients, representing direct effects of η-variables on other η-variables. $\boldsymbol{B}$ always has zeros on the diagonal, which ensures that a variable is not an immediate cause of itself;
- $\boldsymbol{\Gamma}$ an $m \times n$ matrix of coefficients, representing direct effects of ξ-variables on η-variables.

Further, model (S12) assumes that

- $\mathrm{E}(\boldsymbol{\eta}) = 0,\ \mathrm{E}(\boldsymbol{\xi}) = 0,\ \mathrm{E}(\boldsymbol{\zeta}) = 0,$
- $\boldsymbol{\zeta}$ is uncorrelated with $\boldsymbol{\xi}$ (otherwise, inconsistent coefficient estimators are likely),

- $\boldsymbol{I} - \boldsymbol{B}$ is nonsingular,
- ζ_{it}, $i = 1, 2, \ldots, m$, is homoscedastic, meaning that the associated covariance matrix of $\boldsymbol{\zeta}$, $\boldsymbol{\Psi}$, is the same for all time points t. It is also assumed no autocorrelation among the observations on ζ_i.

Importantly, the structure of $\boldsymbol{\Psi}$ depends on whether a model is *recursive* or *nonrecursive*. Recursive models are systems of equations that contain no reciprocal causation, implying that the $\boldsymbol{B}$ matrix can be written as a lower triangular matrix. In this case, the errors in equations are assumed to be uncorrelated, entailing that $\boldsymbol{\Psi}$ is diagonal.

Unlike recursive models, nonrecursive models contain reciprocal causation and/or feedback loops, entailing that $\boldsymbol{B}$ is not lower triangular. Under such models, ζ-disturbances can be assumed either correlated or not.

The variance-covariance matrix of $\boldsymbol{\xi}$ is a $n \times n$ symmetrical matrix denoted $\boldsymbol{\Phi}$. That is, exogenous latent variables can be correlated, implying that $\boldsymbol{\Phi}$ in that case is not diagonal. Notice that the covariance matrix of $\boldsymbol{\eta}$ is not a free parameter matrix in the model. However, one can calculate this matrix afterwards (if required) according to the following formula:

$$\mathbf{Cov}(\boldsymbol{\eta}) = (\boldsymbol{I} - \boldsymbol{B})^{-1} \left(\boldsymbol{\Gamma}\,\boldsymbol{\Phi}\,\boldsymbol{\Gamma}' + \boldsymbol{\Psi}\right) \left[(\boldsymbol{I} - \boldsymbol{B})^{-1}\right]'. \tag{S13}$$

Submodel 2: Measurement model

As a matter of fact, vectors $\boldsymbol{\eta}$ and $\boldsymbol{\xi}$ are not observed. Instead, vectors $\boldsymbol{y}' = (y_1, y_2, \ldots, y_p)$ and $\boldsymbol{x}' = (x_1, x_2, \ldots, x_q)$ are observed, such that

$$\boldsymbol{y} = \boldsymbol{\Lambda}_y \boldsymbol{\eta} + \boldsymbol{\epsilon}, \tag{S14}$$

$$\boldsymbol{x} = \boldsymbol{\Lambda}_x \boldsymbol{\xi} + \boldsymbol{\delta}, \tag{S15}$$

where

$\boldsymbol{y}$ a $p \times 1$ vector of observed indicators of $\boldsymbol{\eta}$;

$\boldsymbol{x}$ a $q \times 1$ vector of observed indicators of $\boldsymbol{\xi}$;

$\boldsymbol{\epsilon}$ a $p \times 1$ vector of measurement errors for $\boldsymbol{y}$ with the associated covariance matrix $\boldsymbol{\Theta}_\epsilon(p \times p)$;

$\boldsymbol{\delta}$ a $q \times 1$ vector of measurement errors for $\boldsymbol{x}$ with the associated covariance matrix $\boldsymbol{\Theta}_\delta(q \times q)$;

$\boldsymbol{\Lambda}_y$ a $p \times m$ matrix of coefficients relating $\boldsymbol{y}$ to $\boldsymbol{\eta}$;

$\boldsymbol{\Lambda}_x$ a $q \times n$ matrix of coefficients relating $\boldsymbol{x}$ to $\boldsymbol{\xi}$.

The model assumptions are:

- $\mathrm{E}(\boldsymbol{\eta}) = 0$, $\mathrm{E}(\boldsymbol{\xi}) = 0$, $\mathrm{E}(\boldsymbol{\epsilon}) = 0$, and $\mathrm{E}(\boldsymbol{\delta}) = 0$,
- $\boldsymbol{\epsilon}$ is uncorrelated with $\boldsymbol{\eta}$, $\boldsymbol{\xi}$, and $\boldsymbol{\delta}$, and
- $\boldsymbol{\delta}$ is uncorrelated with $\boldsymbol{\xi}$, $\boldsymbol{\eta}$, and $\boldsymbol{\epsilon}$.

To summarise, the full SEM is defined by three equations:

$$\begin{aligned} \text{Latent variable model:} \quad & \boldsymbol{\eta} = \boldsymbol{B}\boldsymbol{\eta} + \boldsymbol{\Gamma}\boldsymbol{\xi} + \boldsymbol{\zeta} \\ \text{Measurement model for } \boldsymbol{y}: \quad & \boldsymbol{y} = \boldsymbol{\Lambda}_y\boldsymbol{\eta} + \boldsymbol{\epsilon} \\ \text{Measurement model for } \boldsymbol{x}: \quad & \boldsymbol{x} = \boldsymbol{\Lambda}_x\boldsymbol{\xi} + \boldsymbol{\delta} \end{aligned} \tag{S16}$$

Rewriting $\boldsymbol{\eta}$ in the reduced form, that is,

$$\boldsymbol{\eta} = (\boldsymbol{I} - \boldsymbol{B})^{-1}(\boldsymbol{\Gamma}\boldsymbol{\xi} + \boldsymbol{\zeta}). \tag{S17}$$

and substituting (S17) for $\boldsymbol{\eta}$ in Eq. (S16) permits us to derive the expression for the covariance matrix of the observed variables as a function of the model parameters, $\boldsymbol{\Sigma}(\boldsymbol{\theta})$ (Bollen, 1989, p. 325):

$$\boldsymbol{\Sigma}(\boldsymbol{\theta}) = \begin{bmatrix} \boldsymbol{\Sigma}_{yy}(\boldsymbol{\theta}) & \\ \boldsymbol{\Sigma}_{xy}(\boldsymbol{\theta}) & \boldsymbol{\Sigma}_{xx}(\boldsymbol{\theta}) \end{bmatrix}, \tag{S18}$$

where

$$\boldsymbol{\Sigma}_{yy}(\boldsymbol{\theta}) = \boldsymbol{\Lambda}_y\,\boldsymbol{A}\left(\boldsymbol{\Gamma}\,\boldsymbol{\Phi}\,\boldsymbol{\Gamma}' + \boldsymbol{\Psi}\right)\boldsymbol{A}'\boldsymbol{\Lambda}_y' + \boldsymbol{\Theta}_\epsilon$$

$$\boldsymbol{\Sigma}_{xy}(\boldsymbol{\theta}) = \boldsymbol{\Lambda}_x\,\boldsymbol{\Phi}\,\boldsymbol{\Gamma}'\,\boldsymbol{A}'\,\boldsymbol{\Lambda}_y'$$

$$\boldsymbol{\Sigma}_{xx}(\boldsymbol{\theta}) = \boldsymbol{\Lambda}_x\,\boldsymbol{\Phi}\,\boldsymbol{\Lambda}_x' + \boldsymbol{\Theta}_\delta,$$

where $\boldsymbol{A} = (\boldsymbol{I} - \boldsymbol{B})^{-1}$.

The full SEM model reduces to a general CFA model if one sets all elements in $\boldsymbol{B}$, $\boldsymbol{\Gamma}$, $\boldsymbol{\Theta}_\epsilon$, $\boldsymbol{\Lambda}_y$ and $\boldsymbol{\Psi}$ to $\boldsymbol{0}$. Note that in practice setting all those matrices to zero does not necessarily mean that all η-variables are literally eliminated from the model. They can instead be regarded as ξ-variables.

This straightforward connection between SEM and CFA immediately implies that the issues of estimation, hypothesis testing, identifiability, and model evaluation for SEM parallel those associated with CFA, discussed in the Appendix in the article.

However, due to the higher complexity of SEM, the determination of its identifiability status algebraically can be much more tedious and thus more error-prone. In case the model of interest is very complex, researchers may resort to several rules that aid in the identification of the model, or, as advised by Jöreskog and Sörbom (1988), confine themselves to determining which of the parameters can be solved for and which cannot without solving the equations explicitly.

Another feature associated with SEM only is the notions of indirect and total effects. In CFA, it is relevant to talk only about direct effects, more precisely, direct effects of ξ-variables on their indicators, x-variables. In SEM models, ξ-variables may, in addition, have direct effects on η-variables, meaning that they indirectly affect the indicators of η-variables. Direct and indirect effects together constitute the total effect. In this work, we do not proceed with discussing this topic in greater depth because *(i)* the hypothesis of primary interest, i.e. the hypothesis of consistency between the latent simulated and true temperature responses to forcings, concerns only direct effects of latent variables, and *(ii)* without knowing the ability of the suggested

SEM model to address the question of interest in practice, it is quite unmotivated to discuss what additional questions can be addressed by means of this model.

S2.2 An alternative representation of SEM

The representation of a general structural equation model given above is known as a standard representation. Being sufficient for capturing the relation between variables within some analyses, the standard representation might be insufficient within other analyses due to its restrictions. For example, it is not allowed that observed variables influence latent variables, in particular the endogenous ones, which in the context of the present work would prevent climatologically defensible causal links from observable temperatures (simulated and/or observed) to the latent temperature responses due to the Land and GHG forcings. To overcome those restrictions, a two-equation model has been suggested (see Bollen, 1989, Ch.9):

$$\boldsymbol{\eta}^+ = \boldsymbol{B}^+ \boldsymbol{\eta}^+ + \boldsymbol{\zeta}^+ \tag{S19}$$

$$\boldsymbol{y}^+ = \boldsymbol{\Lambda}_y^+ \boldsymbol{\eta}^+, \tag{S20}$$

where $\boldsymbol{\eta}^+$, $\boldsymbol{B}^+$, $\boldsymbol{\zeta}^+$, and $\boldsymbol{y}^+$ are related to the variables from the standard representation in the following way:

$$\boldsymbol{\eta}^+ = \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{x} \\ \boldsymbol{\eta} \\ \boldsymbol{\xi} \end{bmatrix}, \quad \boldsymbol{\zeta}^+ = \begin{bmatrix} \boldsymbol{\epsilon} \\ \boldsymbol{\delta} \\ \boldsymbol{\zeta} \\ \boldsymbol{\xi} \end{bmatrix}, \quad \boldsymbol{y}^+ = \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{x} \end{bmatrix} \tag{S21}$$

$$\boldsymbol{B}^+ = \begin{bmatrix} \mathbf{0} & \mathbf{0} & \boldsymbol{\Lambda}_y & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{\Lambda}_x \\ \mathbf{0} & \mathbf{0} & \boldsymbol{B} & \boldsymbol{\Gamma} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \end{bmatrix}, \qquad \boldsymbol{\Lambda}_y^+ = \begin{bmatrix} \boldsymbol{I}_{p+q} & \mathbf{0} \end{bmatrix}$$

where $\boldsymbol{I}_{p+q}$ is an order-$(p+q)$ identity matrix picking out the observed variables from $\boldsymbol{\eta}^+$. The $\boldsymbol{\Lambda}_y^+$ is consequently $(p+q) \times (p+q+m+n)$. Further,

- $\boldsymbol{\eta}^+$ and $\boldsymbol{\zeta}^+$ are $(p+q+m+n) \times 1$,
- $\boldsymbol{y}^+$ is $(p+q) \times 1$, and
- $\boldsymbol{B}^+$ is $(p+q+m+n) \times (p+q+m+n)$.

The final matrix for this alternative representation is the covariance matrix for $\boldsymbol{\zeta}^+$ denoted $\boldsymbol{\Psi}^+$. Its relation to the standard parameters is

$$\boldsymbol{\Psi}^+ = \begin{bmatrix} \boldsymbol{\Theta}_\epsilon & & & \\ \mathbf{0} & \boldsymbol{\Theta}_\delta & & \\ \mathbf{0} & \mathbf{0} & \boldsymbol{\Psi} & \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \boldsymbol{\Phi} \end{bmatrix}. \tag{S22}$$

Substituting the reduced form of $\boldsymbol{\eta}^{+}$, given by

$$\boldsymbol{\eta}^{+} = \left(\boldsymbol{I} - \boldsymbol{B}^{+}\right)^{-1} \boldsymbol{\zeta}^{+}, \tag{S23}$$

into (S19), the reproduced covariance matrix of $\boldsymbol{\eta}^{+}$ is derived:

$$\boldsymbol{\Sigma}_{\boldsymbol{\eta}^{+}}(\boldsymbol{\theta}) = \left(\boldsymbol{I} - \boldsymbol{B}^{+}\right)^{-1} \boldsymbol{\Psi}^{+} \left((\boldsymbol{I} - \boldsymbol{B}^{+})^{-1}\right)'. \tag{S24}$$

Inserting (S23) into (S20) gives the reproduced covariance matrix of the observed variables only:

$$\boldsymbol{\Sigma}_{\boldsymbol{y}^{+}}(\boldsymbol{\theta}) = \left(\boldsymbol{\Lambda}_{y}^{+} \left(\boldsymbol{I} - \boldsymbol{B}^{+}\right)^{-1}\right) \boldsymbol{\Psi}^{+} \left(\boldsymbol{\Lambda}_{y}^{+} \left(\boldsymbol{I} - \boldsymbol{B}^{+}\right)^{-1}\right)' \tag{S25}$$

The matrices $\boldsymbol{B}^{+}$ from Eq. (S21) and $\boldsymbol{\Psi}^{+}$ from Eq. (S22) make explicit the implicit constraints of the standard representation. However, by changing the fixed zero elements in these matrices we can relax many of those constraints. An important point to keep in mind, when relaxing the assumptions of the standard representation, is that the resulting model should be identified.

S3 Equations for the basic nonrecursive SEM model, presented in the article, using the standard representation

For the sake of convenience, we reproduce here the path diagram of the SEM model presented in Fig. 2 in the article.

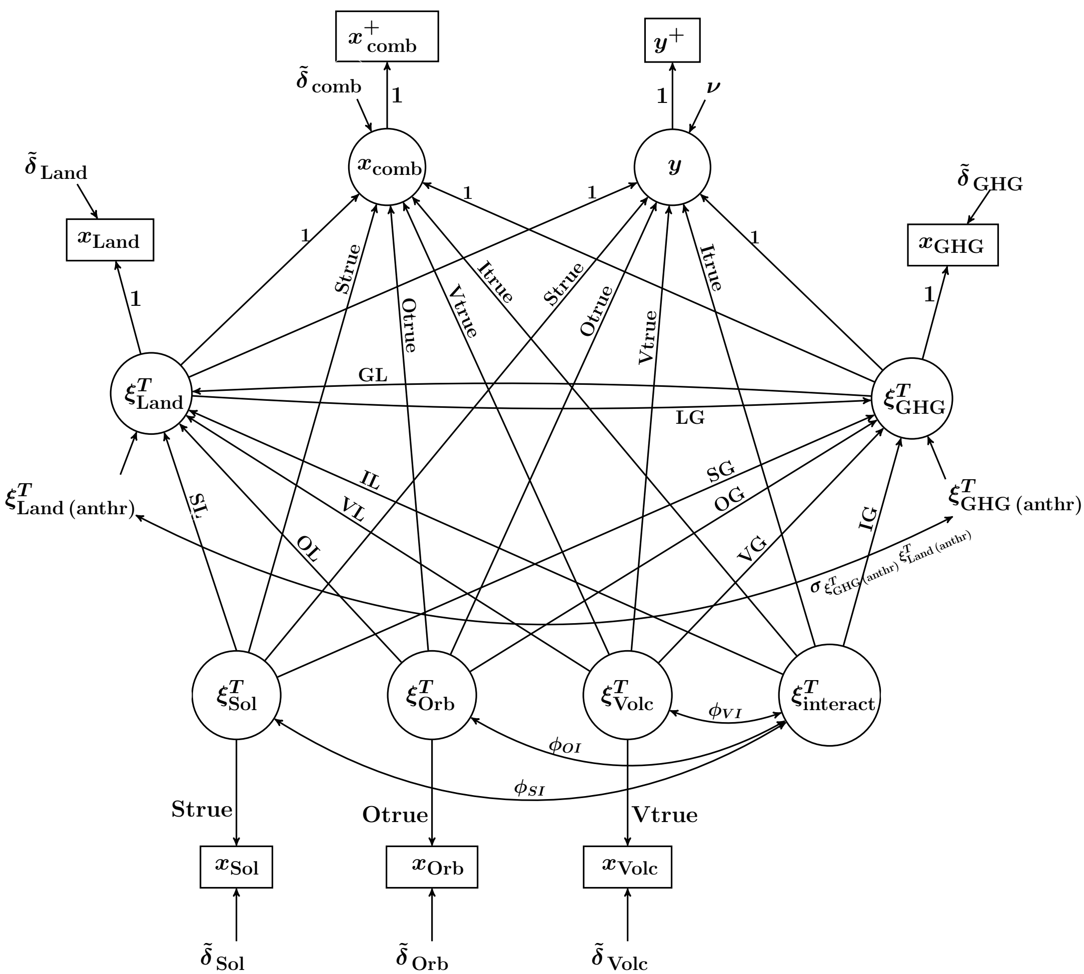

Figure S1. Path diagram of a nonrecursive (i.e. containing reciprocal relationships) SEM model under the hypothesis of consistency. The variance of each specific factor $\tilde{\delta}_{\mathrm{f}}$ is assumed to be known a priori.

Combining our notations used in Fig. S1 and the notations associated with the standard general representation of a structural equation model, the structural equation model depicted in Fig. S1 can be represented by the following equations:

1. The latent variable model:

$$\underbrace{\begin{bmatrix} \xi^T_{\text{Land}} \\ \xi^T_{\text{GHG}} \\ x_{\text{comb}} \\ y \end{bmatrix}}_{=\boldsymbol{\eta}} = \underbrace{\begin{bmatrix} 0 & \text{GL} & 0 & 0 \\ \text{LG} & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix}}_{=\boldsymbol{B}} \cdot \underbrace{\begin{bmatrix} \xi^T_{\text{Land}} \\ \xi^T_{\text{GHG}} \\ x_{\text{comb}} \\ y \end{bmatrix}}_{=\boldsymbol{\eta}} + \underbrace{\begin{bmatrix} \text{SL} & \text{OL} & \text{VL} & \text{IL} \\ \text{SG} & \text{OG} & \text{VG} & \text{IG} \\ \text{Strue} & \text{Otrue} & \text{Vtrue} & \text{Itrue} \\ \text{Strue} & \text{Otrue} & \text{Vtrue} & \text{Itrue} \end{bmatrix}}_{=\boldsymbol{\Gamma}} \cdot \underbrace{\begin{bmatrix} \xi^T_{\text{Sol}} \\ \xi^T_{\text{Orb}} \\ \xi^T_{\text{Volc}} \\ \xi^T_{\text{interact}} \end{bmatrix}}_{=\boldsymbol{\xi}} + \underbrace{\begin{bmatrix} \xi^T_{\text{Land (anthr)}} \\ \xi^T_{\text{GHG (anthr)}} \\ \tilde{\delta}_{\text{comb}} \\ \nu \end{bmatrix}}_{=\boldsymbol{\zeta}},$$

where the variance-covariance matrices of $\boldsymbol{\xi}$ and $\boldsymbol{\zeta}$ are given by

$$\Phi_{\boldsymbol{\xi}} = \begin{pmatrix} 1 & 0 & 0 & \phi_{SI} \\ & 1 & 0 & \phi_{OI} \\ & & 1 & \phi_{VI} \\ & & & 1 \end{pmatrix} \quad \text{and} \quad \Psi_{\boldsymbol{\zeta}} = \begin{pmatrix} \sigma^2_{\xi^T_{\text{Land (anthr)}}} & \sigma_{\xi^T_{\text{Land (anthr)}}\xi^T_{\text{Land (anthr)}}} & 0 & 0 \\ & \sigma^2_{\xi^T_{\text{GHG (anthr)}}} & 0 & 0 \\ & & \sigma^{2\,*}_{\tilde{\delta}_{\text{comb}}} & 0 \\ & & & \sigma^2_{\nu} \end{pmatrix}, \text{ respectively,}$$

and where $\sigma^{2\,*}_{\tilde{\delta}_{\text{comb}}}$ is assumed to be known a priori.

2. The measurement model for $\boldsymbol{x}$-variables, i.e. the indicators of the latent exogenous variables $\boldsymbol{\xi}$:

$$\underbrace{\begin{bmatrix} x_{\text{Sol}} \\ x_{\text{Orb}} \\ x_{\text{Volc}} \end{bmatrix}}_{=\boldsymbol{x}} = \underbrace{\begin{bmatrix} \text{Ssim} & 0 & 0 & 0 \\ 0 & \text{Osim} & 0 & 0 \\ 0 & 0 & \text{Vsim} & 0 \end{bmatrix}}_{=\boldsymbol{\Lambda}_x} \cdot \underbrace{\begin{bmatrix} \xi^T_{\text{Sol}} \\ \xi^T_{\text{Orb}} \\ \xi^T_{\text{Volc}} \\ \xi^T_{\text{interact}} \end{bmatrix}}_{=\boldsymbol{\xi}} + \underbrace{\begin{bmatrix} \tilde{\delta}_{\text{Sol}} \\ \tilde{\delta}_{\text{Orb}} \\ \tilde{\delta}_{\text{Volc}} \end{bmatrix}}_{=\tilde{\boldsymbol{\delta}}},$$

where the variance-covariance matrix of $\tilde{\boldsymbol{\delta}}$ is given by $\boldsymbol{\Theta}_{\tilde{\boldsymbol{\delta}}} = \text{diag}\left(\sigma^{2\,*}_{\tilde{\delta}_{\text{Sol}}},\, \sigma^{2\,*}_{\tilde{\delta}_{\text{Orb}}},\, \sigma^{2\,*}_{\tilde{\delta}_{\text{Volc}}}\right)$. Each of the three variances is assumed to be known a priori.

3. The measurement model for $\boldsymbol{y}$-variables, i.e. the indicators of the latent endogenous variables $\boldsymbol{\eta}$:

$$\underbrace{\begin{bmatrix} x_{\text{Land}} \\ x_{\text{GHG}} \\ x^{+}_{\text{comb}} \\ v^{+} \end{bmatrix}}_{=\boldsymbol{y}} = \underbrace{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}}_{=\boldsymbol{\Lambda}_y} \cdot \underbrace{\begin{bmatrix} \xi^T_{\text{Land}} \\ \xi^T_{\text{GHG}} \\ x_{\text{comb}} \\ v \end{bmatrix}}_{=\boldsymbol{\eta}} + \underbrace{\begin{bmatrix} \tilde{\delta}_{\text{Land}} \\ \tilde{\delta}_{\text{GHG}} \\ 0 \\ 0 \end{bmatrix}}_{=\boldsymbol{\epsilon}},$$

where the variance-covariance matrix of $\boldsymbol{\epsilon}$ is given by $\boldsymbol{\Theta}_{\boldsymbol{\epsilon}} = \text{diag}(\sigma^{2\,*}_{\tilde{\delta}_{\text{Land}}}, \sigma^{2\,*}_{\tilde{\delta}_{\text{GHG}}}, 0, 0)$, where $\sigma^{2\,*}_{\tilde{\delta}_{\text{Land}}}$ and $\sigma^{2\,*}_{\tilde{\delta}_{\text{GHG}}}$ are regarded as known a priori.

Having elucidated the correspondence between our notations and the notations associated with the general SEM given in Sect. S2.1 and S2.2, it is not difficult to rewrite the equations above in accordance with the alternative representation summarised in Eqs. (S19) - (S21). However, we omit here the alternative representation of the SEM model in Fig. S1 due to the considerable size of the resulting matrices.

S4 Fitting the CFA($k_{\mathtt{f}}, 1$) model, defined in Eq. (18) in the article, to an ensemble with five replicates in the *R* package **sem**

Let us repeat the definition of the CFA($k_{\mathtt{f}}, 1$) model, given in Eq. (18) in the article. Given an $x_{\mathtt{f}}$ ensemble containing $k_{\mathtt{f}}$ members, the CFA($k_{\mathtt{f}}, 1$) model is given by:

$$
\begin{array}{ccccc}
x_{\mathtt{f}\,\mathrm{repl.1}\,t} & = & \alpha_{\mathtt{f}} \cdot \tilde{\xi}^{S}_{\mathtt{f}\,t} & + & \tilde{\delta}_{\mathtt{f}\,\mathrm{repl.1}\,t} \\
x_{\mathtt{f}\,\mathrm{repl.2}\,t} & = & \alpha_{\mathtt{f}} \cdot \tilde{\xi}^{S}_{\mathtt{f}\,t} & + & \tilde{\delta}_{\mathtt{f}\,\mathrm{repl.2}\,t} \\
\vdots & & \vdots & & \vdots \\
x_{\mathtt{f}\,\mathrm{repl.}k_{\mathtt{f}}\,t} & = & \alpha_{\mathtt{f}} \cdot \tilde{\xi}^{S}_{\mathtt{f}\,t} & + & \tilde{\delta}_{\mathtt{f}\,\mathrm{repl.}k_{\mathtt{f}}\,t},
\end{array}
\tag{S26}
$$

where $\tilde{\xi}^{S}_{\mathtt{f}\,t} = \xi^{S}_{\mathtt{f}\,t}/\sqrt{\sigma^2_{\xi^S_{\mathtt{f}}}}$, $\alpha_{\mathtt{f}} = \sqrt{\sigma^2_{\xi^S_{\mathtt{f}}}}$, and $\tilde{\xi}^{S}_{\mathtt{f}\,t}$ is assumed to be uncorrelated with all $\tilde{\delta}_{\mathtt{f}\,\mathrm{repl.}i}$. The CFA($k_{\mathtt{f}}, 1$) model is formulated under the following assumptions:

(i) the variances of $\tilde{\delta}_{\mathtt{f}\,\mathrm{repl.}i}$:s are equal,

(ii) the $\tilde{\delta}_{\mathtt{f}\,\mathrm{repl.}i\,t}$ sequences are mutually uncorrelated across all $k_{\mathtt{f}}$ replicates, and

(iii) the magnitude of the forcing effect is the same for each ensemble member.

Below the main steps of fitting the CFA($k_{\mathtt{f}}, 1$) model, where $k_{\mathtt{f}} = 5$, are provided.

Step 1. Specify the model of interest in an *R*-file:

Define the latent factors with the corresponding factor loadings

```
xi_f -> x_repl1,  alpha, NA
xi_f -> x_repl2,  alpha, NA
xi_f -> x_repl3,  alpha, NA
xi_f -> x_repl4,  alpha, NA
xi_f -> x_repl5,  alpha, NA
```

 # where NA denotes an arbitrary starting value for the parameter α. But one can also specify a starting value instead of NA.

Define the variance of the latent factor

```
xi_f <-> xi_f,    NA, 1
```

Define the specific factors with the corresponding variances, i.e. $\sigma^2_{\tilde{\delta}_{\mathtt{f}}}$ for each replicate

```
x_repl1 <-> x_repl1,   sigma2_delta,  NA
x_repl2 <-> x_repl2,   sigma2_delta,  NA
x_repl3 <-> x_repl3,   sigma2_delta,  NA
x_repl4 <-> x_repl4,   sigma2_delta,  NA
x_repl5 <-> x_repl5,   sigma2_delta,  NA
```

 # Note that specific factors are not represented explicitly.

Step 2. Save the file above, e.g. $Model\_1.R$

Step 3. Construct the data set for the analysis

```
MYDATA<-cbind(x_1, x_2, x_3, x_4, x_5)
```

Name the observed variables in the same way as in Step 1.

```
colnames(MYDATA)<-c("x_repl1","x_repl2", "x_repl3","x_repl4","x_repl5")
```

Compute the variance-covariance matrix of the observed variables

```
S2<-cov(MYDATA);
```

Step 4. Estimation

Load the sem package

```
library(sem)
```

Define the heuristic indices of interest

```
opt <- options(fit.indices = c("GFI", "AGFI","SRMR"))
```

Read in the model of interest

```
model_1<-specifyModel("Model_1.R")
```

Fit the model and save the results to a model fit object

```
result_model_1<- sem(model_1, S2, N=100, fit.indices=TRUE)
```

 # where N is a number of observations

To see the result of the estimation

```
summary(result_model_1)
```

S5 Figures

330 Here the plots of data analysed in Sect. 6 in the article are provided.

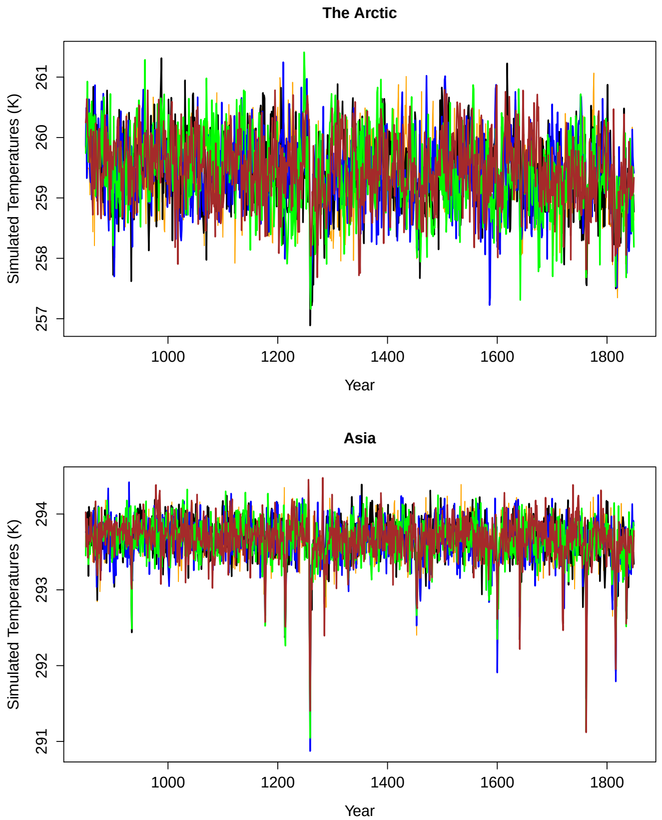

Figure S2. Original time series of the five replicates within the x_{Volc} ensemble for two regions. All time series have the time unit of 1 year and cover the period $850 - 1849$ AD.

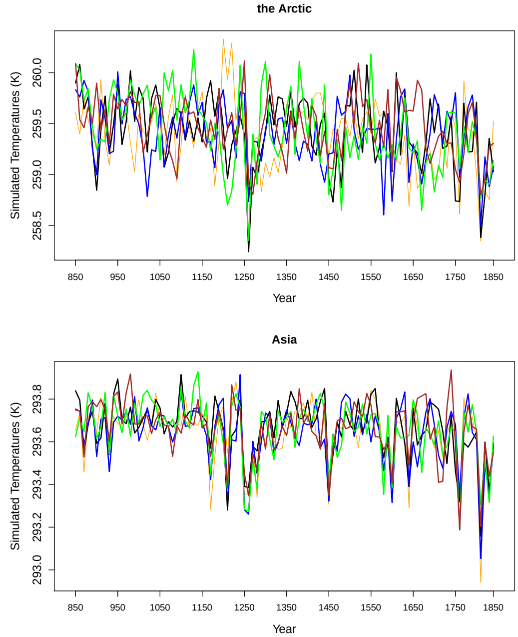

Figure S3. Decadally resolved residual series, defined in Eq. (6.2.1) in the article and associated with two x_{Volc} ensembles for two regions. All time series have the time unit of 10 year and cover the period $850 - 1849$ AD.

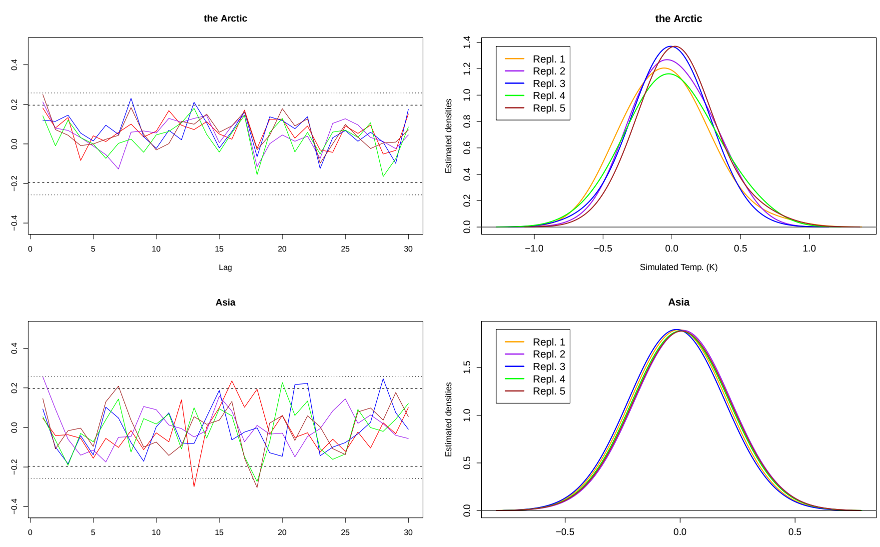

Figure S4. Autocorrelation functions (the left column) and density functions (the right column) of decadally resolved residual series, defined in Eq. (19) in the article and associated with two x_{Volc} ensembles for two regions. The residual time series have the time unit of 10 year and cover the period $850 - 1849$ AD. The two-sided 95% and 99% bounds in the left column, denoted by dashed lines, are equal to $\pm 1.96/\sqrt{100}$ and $\pm 2.58/\sqrt{100}$, respectively.

References

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Jöreskog, K.G. and Sörbom, D.: LISREL 7: a guide to the program and applications, SPSS INC, 1988.

Mulaik, S. A.: Foundations of Factor Analysis, 2nd edition, Chapman&Hall/CRC, ISBN 9781420099614, 2010.