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A statistical review on the optimal fingerprinting approach in climate change studies

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Abstract

We provide a statistical review of the "optimal fingerprinting" approach presented in Allen and Tett (Clim Dyn 15:419-434, 1999) in light of the severe criticism of McKitrick (Checking for model consistency in optimal fingerprinting: a comment. Clim Dyn 58:405–411, 2022). Our review finds that the "optimal fingerprinting" approach would survive much of McKitrick (2022)'s criticism by enforcing two conditions related to the conduct of the null simulation of the climate model, and the accuracy of the null setting climate model. The conditions we proposed are simpler and easier to verify than those in McKitrick (2022). We provide additional remarks on the residual consistency test in Allen and Tett (1999), showing that it is operational for checking the agreement between the residual covariance matrices of the null simulation and the physical internal variation under certain conditions. We further provide the reason why the Feasible Generalized Least Square method, much advocated by McKitrick (2022), is not regarded as operational by geophysicists.

Keywords Climate change · Feasible generalized least square · Gauss–Markov Theorem · Optimal fingerprinting · Residual consistency test

1 Introduction

The optimal fingerprinting approach with linear regression perspective, proposed in a series of papers starting from Allen and Tett (1999) (hereinafter AT99) followed by Allen and Stott (2003) and Stott et al. (2003), has been the cornerstone in the detection and attribution of climate change due to human activities in the last 20 years, and has been the adopted method by numerous Intergovernmental Panel on Climate Change (IPCC) reports on the climate change. Hasselmann (1979) first proposed to obtain the optimal fingerprints on climate change by maximizing signal-to-noise ratio (SNR). Bell (1982) proposed to compute an optimally weighted average of the discrete data. North et al. (1995) constructed an optimal filter that passes the signals of climate change but suppresses the noise. Hegerl and North (1997) showed that the core of the three approaches were identical and that the standard optimal fingerprints can be expressed as a least square regression problem. AT99 further provided a more practical method using the ordinary least squares(OLS) which provides essentially the same result as maximizing the SNR of Hasselmann (1979).

Recently, McKitrick (2022) (hereinafter M22) offered a very critical assessment on AT99, suggesting there were serious flaws with the approach. The criticism of M22 is well summarized in its abstract "AT99 stated the GM Theorem incorrectly, omitting a critical condition altogether, their GLS method cannot satisfy the GM conditions, and their variance estimator is inconsistent by construction". "Additionally, they did not formally state the null hypothesis of the RCT (residual consistency test) nor identify which of the GM conditions it tests, nor did they prove its distribution and critical values, rendering it uninformative as a specification test."

This paper provides a statistical review of AT99 in light of the critics of M22, makes remarks on the key aspects of the AT99 formulation, and discusses M22's criticism. Along the way, we provide conditions under which the optimal fingerprint approach would stand, which are

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largely based on the quality of the null simulation of the climate models and the accuracy of the covariance matrix offered by the climate models as approximation to the residual covariance of the observations (internal variation). If the null simulation cannot capture the covariance of the internal variation in the physical world, the so called "optimal fingerprints" are only unbiased and consistent, and their variance may not be the smallest as claimed. We further show that the Feasible Generalized Least Square, advocated by M22 is not readily suitable to the context of AT99 before a workable model for the covariance matrix of the residual is available.

Throughout this review, the equation numbers in AT99 and M22 are labeled as (AT.numeric number) and (M.numeric number), respectively, while other equations are labeled separately. Furthermore, the five key assumptions of M22 are marked as M22 (i) etc.

2 Review of AT99's formulation

The main idea of AT99 is to utilize the Gauss–Markov (GM) theorem for homogeneous linear regression to make the detected fingerprints "optimal", which means in statistical terms to obtain unbiased estimates of the regression coefficients with the smallest variation so as to attain the largest signal (regression coefficient estimates) to noise (standard deviation of the estimates) ratio. AT99 tried to utilize the GM theorem's ability to generate the Best Linear Unbiased Estimator (BLUE) for the regression coefficients. The BLUE property would ensure the best signal to noise ratio in the detected human fingerprints on climate change, and thus the "optimal fingerprints".

The road to BLUE is not a direct one, as the homogeneous variance condition in the GM theorem is not readily satisfied. AT99 uses an approach that is uncommon to statisticians and econometricians by estimating the residual covariance matrix from separate simulations of climate models.

M22 criticized that AT99 had left out some conditions for the GM theorem, suggesting that $\tilde{\beta}$ may not have the BLUE property with nonstochastic $\boldsymbol{P}$ and the non-existence of C_N^{-1}, and further questioned the formulation of the RCT. M22 also questioned why not use the seemingly related feasible generalized regression (FGLS) (Wooldridge 2010) and the heteroskedasticity-consistent (HC) method (White 1980) to replace the simulation runs of the climate models to estimate the covariance matrix. We will try to address the criticism of M22 and show in particular that the FGLS is not applicable to the setting of AT99 as the residual covariance is too general to permit a parametric structure required by FGLS.

2.1 Model and key aspects of AT99

The Linear regression model considered in AT99 is

$$(AT.1) \quad \mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \mathbf{u} \tag{1}$$

where $\mathbf{y}$ is a ℓ-dimensional vector of observations on certain climate variables, $\beta = (\beta_1, \dots, \beta_m)^T$ is the regression coefficient vector, $\mathbf{X} = (x_{(1)}, \cdots, x_{(m)})$ is a design matrix of $\ell \times m$ corresponding to m climate system's response-patterns, which are potential fingerprints of climate change and are often obtained from independent runs of certain climate models. In Statistics, the columns vectors of $\mathbf{X}$ are called covariates.

That $\beta_i = 0$ or $\beta_i = 1$ for an $i \in \{1, \dots, m\}$ carries special meaning in the climate change study. If hypothesis $H_0 : \beta_i = 0$ is rejected statistically at a level of significance α, it means a detection of significant climate change factor $x_{(i)}$. Under the detection of $x_{(i)}$, if hypothesis $H_0 : \beta_i = 1$ cannot be rejected statistically at α level, it provides a necessary evidence for attribution of climate change to the factor $x_{(i)}$. Without causing too much confusion, we also call β the fingerprints as $x_{(i)}$ being a fingerprint or not depends on the value of β_i.

The residual $\mathbf{u}$ represents the "climate noise" or "internal variation" which was assumed to be multivariate normally distributed with the covariance matrix

$$(AT.2) \quad \mathbf{C}_N \equiv E\left(\mathbf{u}\mathbf{u}^T\right), \tag{2}$$

where E denotes the mathematical expectation operation.

Remark 1 AT99 did not explicitly present the regression identification condition

$$E(\mathbf{u} \mid \mathbf{X}) = 0, \tag{3}$$

which has drawn heavy criticism in M22 (iii). Our reading is that AT99 assumed that the internal climate variability is independent of the signal and that the climate variability, which implies (3). However, as will be shown in Sect. 2.2 below, (3) is not enough for the validity of AT99's approach.

The major idea of AT99 is to utilize the GM theorem for attaining the best linear unbiased estimator (BLUE) of $\boldsymbol{\beta}$, which can attain the smallest mean square error in the estimated $\boldsymbol{\beta}$-coefficients and hence the highest signal to noise ratio (SNR) in the fingerprint detection.

As $\mathbf{C}_N \neq \sigma^2 \mathbf{I}_\ell$ (here $\mathbf{I}_\ell$ denotes the $\ell \times \ell$ identity matrix) due to the spatial and temporal heterogeneity in the residuals u, to satisfy the homogeneous variance condition required by the GM theorem, AT99 suggested a pre-whitening operator via a $\kappa' \times \ell$ matrix $\mathbf{P}$ of rank $\kappa' \leq \ell$, such that

$$(AT.3) \quad E\left(\mathbf{P}\mathbf{u}\mathbf{u}^T\mathbf{P}^T\right) = \mathbf{P}\mathbf{C}_\mathbf{N}\mathbf{P}^T = \mathbf{I}_{\kappa'}. \tag{4}$$

Remark 2 AT99 was vague about the dimensions of $\mathbf{P}$ and $\mathbf{I}$ in (4), which should be $\mathbf{I}_{\kappa'}$ where κ' is the rank of $\mathbf{P}$ and $\kappa' \le \ell$. In the original GM theorem, $\kappa' = \ell$. There should be another restriction that $\kappa' > m$, the dimension of $\boldsymbol{\beta}$, in order to make $\mathbf{X}^T\mathbf{P}^T\mathbf{P}\mathbf{X}$ used in the generalized least square (GLS) full rank, which was not explicitly assumed in AT99 to ensure a positive degree of freedom in the χ^2-distribution in (AT.18). Our understanding is that if C_N admits the spectral decomposition $C_N = \sum_{i=1}^{\kappa'} \lambda_i^2 v_i v_i^T$ where $\{\lambda_i^2\}_{i=1}^{\kappa'}$ are the non-zero eigenvalues, then $P = (\lambda_1^{-1}v_1, \cdots, \lambda_{\kappa'}^{-1}v_{\kappa'})^T$ and C_N's Moore-Penrose generalized inverse is $C_N^+ = \mathbf{P}^T\mathbf{P}$.

Ignoring the randomness of $\mathbf{P}$ for the moment, the Gauss-Markov theorem would imply that by left multiplying $\mathbf{P}$ on both sides of (1), the ordinary least square (OLS) estimator $\tilde{\boldsymbol{\beta}}$ on the rotated data is

$$(AT.4) \quad \tilde{\boldsymbol{\beta}} = \left(\mathbf{X}^T\mathbf{P}^T\mathbf{P}\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{P}^T\mathbf{P}\,\mathbf{y} = \left(\mathbf{X}^T\mathbf{C}_N^+\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{C}_N^+\mathbf{y} \equiv \mathbf{F}^T\mathbf{y}, \tag{5}$$

where $\mathbf{F}^T = \left(\mathbf{X}^T\mathbf{P}^T\mathbf{P}\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{P}^T\mathbf{P}$, and the covariance of $\tilde{\boldsymbol{\beta}}$ is

$$(AT.6) \quad \mathrm{Var}(\tilde{\boldsymbol{\beta}}) = \left(\mathbf{X}^T\mathbf{C}_N^+\mathbf{X}\right)^{-1}. \tag{6}$$

Remark 3 The $\mathbf{C}_N^+$ is the Moore–Penrose generalized inverse of C_N, in the case of $\kappa' \le \ell$, and $\mathbf{C}_N^+ = C_N^{-1}$ when $\kappa' = \ell$. A more general expression for the variance is

$$\mathrm{Var}(\tilde{\boldsymbol{\beta}}) = \left(\mathbf{X}^T\mathbf{P}^T\mathbf{P}\mathbf{X}\right)^{-1}. \tag{7}$$

A key formulation of AT99 is on the estimation of $\mathbf{C}_N$ via separate simulations of a certain climate model that would be consistent to the null hypothesis of no human forcing on the climate, the so-called null setting in the climate models, representing the internal climate variability. Specifically, $\mathbf{C}_N$ is estimated by

$$(AT.12) \quad \hat{\mathbf{C}}_N = \frac{1}{n}\mathbf{Y}_N\mathbf{Y}_N^T, \tag{8}$$

where the columns of $\mathbf{Y}_N$ ($\ell \times n$ matrix) represent n response vectors of size ℓ from n independent samples of the null setting simulation runs, for instance from the pre-industrial control.

Remark 4a This external way of estimating the covariance matrix $\mathbf{C}_N$ was quite different from the internal way commonly practised in Statistics and Econometrics, which is largely due to the difficulty of modeling C_N parametrically. Indeed, the commonly adopted covariance structures like diagonal or autoregressive structure in FGLS in statistics and econometrics are not useful for climate studies as the climate system has more complex covariance structure.

Remark 4b The n independent samples leading to $\hat{C}_N$ should be mutually independent, and should be independent of the design matrix $\mathbf{X}$. It is noted that the independence alluded above is actually conditional independent upon given the climate models which generate the simulation samples, for instance, the pre-industrial configuration of the models. This independence is explicitly presented in a newly added condition (10) in Sect. 2.2. AT99 was vague about the independence requirements of the samples.

Remark 4c A merit of this external estimation of $\mathbf{C}_N$ is to make the estimation of the error covariance separate from the potential regression model misspecification (for instance omitted variables and non-linearity). Let $\tilde{\mathbf{C}}_N$ be the underlying covariance matrix of the ensembled null simulations to which $\hat{\mathbf{C}}_N$ converges in probability, meaning that

$$\lim_{n\to\infty} P(\|\hat{\mathbf{C}}_N - \tilde{\mathbf{C}}_N\| > \varepsilon) = 0 \text{ for all } \varepsilon > 0,$$

where $\|M\|$ denotes a matrix norm (Frobenius or spectral norm) of matrix M.

A challenge with this external approach is to make $\tilde{\mathbf{C}}_N$ match $\mathbf{C}_N$ of the physical world. This is actually the most important factor that determines the estimated fingerprint $\tilde{\boldsymbol{\beta}}$ being BLUE or not as will be discussed in Sect. 2.3.

Remark 5 A key requirement needed here is that the null simulation experiments should be statistically independent of the observed physical world governing Model (1) in order to ensure the key identification condition (11) in Sect. 2.2. As will be shown later, this independence is a key to ensure $\tilde{\boldsymbol{\beta}}$ being unbiased.

Due to the limitation of the independent samples of the climate models, $\hat{\mathbf{C}}_N$'s rank is only a $\kappa < \ell$, making $\hat{\mathbf{C}}_N$ non-invertible. By resorting to the generalized inverse of $\hat{\mathbf{C}}_N$, $\mathbf{P}$ in (4) can be approximated by a $\mathbf{P}^{(\kappa)}$. Specifically, support $\hat{\mathbf{C}}_N$ admits the spectral decomposition that $\hat{\mathbf{C}}_N = \sum_{i=1}^{\kappa} \hat{\alpha}_i^2\hat{\eta}_i\hat{\eta}_i^T$ where $\{\hat{\alpha}_i^2\}_{i=1}^{\kappa}$ are the positive eigenvalues of $\hat{\mathbf{C}}_N$ ranked in descending order and $\{\hat{\eta}_i\}_{i=1}^{\kappa}$ are the corresponding eigenvectors. One attains the $\kappa \times \ell$ matrix $\mathbf{P}^{(\kappa)}$ as

$$\mathbf{P}^{(\kappa)} = \left(\hat{\alpha}_1^{-1}\hat{\eta}_1, \ldots, \hat{\alpha}_\kappa^{-1}\hat{\eta}_\kappa\right)^T.$$

Then, it can be verified that

$$\mathbf{P}^{(\kappa)}\hat{\mathbf{C}}_N\mathbf{P}^{(\kappa)^T} = \mathbf{I}_\kappa. \tag{9}$$

Remark 6 The reduced rank of $\hat{\mathbf{C}}_N$ implies that $\hat{\mathbf{C}}_N$ may not be a consistent estimator of $\mathbf{C}_N$. This is an aspect that received severe criticism in M22. AT99 seemed to suggest that $\hat{\mathbf{C}}_N$ consistently estimates $\sum_{i=1}^{\kappa} \lambda_i^2 v_i v_i^T$, the first κ-terms in the spectral decomposition of $\mathbf{C}_N$. How to achieve this statistically is a question to us, since, although $\hat{\mathbf{C}}_N$ is consistent to $\tilde{\mathbf{C}}_N$ as implied by the law of large numbers, $\tilde{\mathbf{C}}_N$ may not be C_N.

Remark 7 It is clear that the null independent runs which make up the columns of Y_N should be independent (strictly speaking conditional independence given the null model). Hence, for a fixed ℓ, from the law of large numbers, $\hat{\mathbf{C}}_N$ is a consistent estimator of $\tilde{\mathbf{C}}_N$, as the number of the sample $n \to \infty$. In geophysical terms, ℓ may represent the number of grid locations in the study, namely the number of repeated observations over ℓ locations. For consistent estimation of β, one needs $\tilde{\beta} \to \beta$ in probability, which requires a large ℓ. However, that ℓ is increasing means that $\hat{\mathbf{C}}_N$, $\tilde{C}_N$ and C_N are all high-dimensional covariance matrices. The high dimensionality makes the convergence of $\hat{\mathbf{C}}_N$ to $\tilde{C}_N$ not automatic as demonstrated in Bai and Silverstein (2010). Specifically, $\hat{C}_N$ consistently estimates $\tilde{C}_N$ only when $\ell = o(n)$, the latter means that $\lim_{n\to\infty} \ell/n = 0$. However, the convergence of $\hat{\mathbf{C}}_N$ to $\tilde{C}_N$ is not assured if ℓ/n does not diminish to zero, namely when ℓ is large or the number of independent samples n is small. The high dimensional effects should be taken into consideration since we increasingly encounter global-scale climate change studies with high spatial resolution.

2.2 Unbiasedness and consistency

A key concern of M22 on AT99 is given in M22 (i) and (iv) on the unbiasedness and consistency of the estimated fingerprint $\tilde{\beta}$. We show that even if $\tilde{\mathbf{C}}_N \neq \mathbf{C}_N$ as suspected by M22, $\tilde{\boldsymbol{\beta}}$ is still unbiased and consistent by adding some conditions, addressing the two key concerns of M22.

In order to employ the GM theorem, as commented in Remark 4b, the null climate simulations used to obtain $\hat{\mathbf{C}}_N$ should be independent of the observed physical "experiments" that governs equation (1). Here again the independence should be conditional independence given the null models and the underlying physical model.

Specifically, the following two conditions are needed:

$$\mathbf{P}^{(\kappa)} \text{ is independent of } \{x_i\}_{i=1}^{\ell}, \text{ the row vectors of } \mathbf{X}, \tag{10}$$

and

$$E\big(\mathbf{u} \mid \mathbf{X}, \mathbf{P}^{(\kappa)}\big) = E(\mathbf{u} \mid \mathbf{X}) = 0. \tag{11}$$

The statistical meaning of (11) is conditional independence between $\mathbf{u}$ and $\mathbf{P}^{(\kappa)}$ given $\mathbf{X}$. AT99 did not explicitly present the most primitive regression identification condition $E(\mathbf{u} \mid \mathbf{X}) = 0$, nor mention (10) and (11) above, which had caused criticism in M22 (iii).

It is readily shown that under (11), $E(\mathbf{y} \mid \mathbf{X}, \mathbf{P}^{(\kappa)}) = \mathbf{X}\boldsymbol{\beta}$. Hence,

$$\begin{aligned} E(\tilde{\boldsymbol{\beta}}) &= E\big\{E\big(\tilde{\boldsymbol{\beta}} \mid \mathbf{X}, \mathbf{P}^{(\kappa)}\big)\big\} \\ &= E\left\{ \left(\mathbf{X}^T \mathbf{P}^{(\kappa)^T} \mathbf{P}^{(\kappa)} \mathbf{X}\right)^{-1} \mathbf{X}^T \mathbf{P}^{(\kappa)^T} \mathbf{P}^{(\kappa)} E\big(\mathbf{y} \mid \mathbf{X}, \mathbf{P}^{(\kappa)}\big) \right\} \\ &= \boldsymbol{\beta}. \end{aligned} \tag{12}$$

Then $\tilde{\boldsymbol{\beta}}$ is unbiased, addressing the unbiased issue concerned in M22 (ii).

Recall that $\{\lambda_i^2\}_{i=1}^{\ell}$ and $\{\hat{\alpha}_i^2\}_{i=1}^{\kappa}$ are the eigenvalues of C_N and $\hat{C}_N$ respectively as in Remark 5. And let $\{x_i\}_{i=1}^{\ell}$ be row vectors of X. The consistency of $\tilde{\beta}$, namely, $\tilde{\beta} \xrightarrow{\text{p}} \beta$ as $\ell, n \to \infty$, requires the following conditions.

$$\begin{aligned} &(i)\ \ell^{-1} X^T X \xrightarrow{p} \Sigma_X, \text{ where } \Sigma_X \text{ is non-singular };\\ &(ii)\ \hat{\alpha}_\kappa^{-2} = O_p(1);\ (iii)\ E\big(\lambda_1^2 \hat{\alpha}_\kappa^{-4}\big) = O(1); \end{aligned} \tag{13}$$

where $O_p(1)$ denotes a sequence that is bounded in probability and $O(1)$ denotes a sequence that is bounded (van der Vaart 1998).

From (5),

$$\tilde{\beta} = \big(X^T \hat{C}_N^+ X\big)^{-1} X^T \hat{C}_N^+ Y = \beta + \big(X^T \hat{C}_N^+ X\big)^{-1} X^T \hat{C}_N^+ u. \tag{14}$$

From Condition (13) (i) and (ii),

$$\begin{aligned} \ell^{-1} X^T \hat{C}_N^+ X &= \ell^{-1} X^T \left(\sum_{i=1}^{\kappa} \hat{\alpha}_i^{-2} \hat{\eta}_i \hat{\eta}_i^T \right) X \\ &\leq \hat{\alpha}_\kappa^{-2} \ell^{-1} X^T X = O_p(1). \end{aligned} \tag{15}$$

To show $\ell^{-1} X^T \hat{C}_N^+ u \xrightarrow{p} 0$, we note first that under Condition (11),

$$E(X^T \hat{C}_N^+ u) = E\{X^T \hat{C}_N^+ E(u \mid X, P^{(\kappa)})\} = 0. \tag{16}$$

With (2) and (16), and by Chebyshev's inequality,

$$\begin{aligned} &P\Big(\big\|\ell^{-1} X^T \hat{C}_N^+ u\big\|_F > \delta\Big) \\ &\quad\leq \big(\delta^2 \ell\big)^{-1} \mathrm{tr}\big\{E\big(\ell^{-1} X^T \hat{C}_N^+ u u^T \hat{C}_N^+ X\big)\big\} \\ &\quad= \big(\delta^2 \ell\big)^{-1} \mathrm{tr}\big[E\big\{E\big(\ell^{-1} X^T \hat{C}_N^+ u u^T \hat{C}_N^+ X \mid X, P^{(\kappa)}\big)\big\}\big] \\ &\quad= \big(\delta^2 \ell\big)^{-1} \mathrm{tr}\big\{E\big(\ell^{-1} X^T \hat{C}_N^+ C_N \hat{C}_N^+ X\big)\big\} \end{aligned}$$

for any $\delta > 0$, where tr(M) is the trace of matrix M.

Similar to (15),

$$\ell^{-1}X^T\hat{C}_N^{+}C_N\hat{C}_N^{+}X \le \lambda_{max}^2\left(\hat{C}_N^{+}C_N\hat{C}_N\right)\ell^{-1}X^TX = \lambda_1^2\hat{\alpha}_\kappa^{-4}\ell^{-1}X^TX,$$

where $\lambda_{max}^2(M)$ denotes the largest eigenvalue of matrix M. Thus, under Conditions (13) (i) and (iii) and (10),

$$\begin{aligned}P\left(\left\|\ell^{-1}X^T\hat{C}_N^{+}u\right\|_F > \delta\right) &\le \left(\delta^2\ell\right)^{-1}\mathrm{tr}\left\{E\left(\lambda_1^2\hat{\alpha}_\kappa^{-4}\ell^{-1}X^TX\right)\right\}\\ &= \left(\delta^2\ell\right)^{-1}\mathrm{tr}\left\{E\left(\lambda_1^2\hat{\alpha}_\kappa^{-4}\right)E\left(\ell^{-1}X^TX\right)\right\}\\ &= \left(\delta^2\ell\right)^{-1}O(1) = o(1),\end{aligned}$$

which implies that $\ell^{-1}X^T\hat{C}_N^{+}u = o_p(1)$, where $o_p(1)$ denotes a sequence that converges to zero in probability and $o(1)$ denotes a deterministic sequence that converges to zero (van der Vaart 1998). This together with (14), (15) and the mapping theorem implies that $\tilde{\beta}\xrightarrow{p}\beta$, and hence the consistency of $\tilde{\beta}$.

2.3 BLUE property

We now consider the BLUE property of $\tilde{\beta}$, a key aspect of AT99's approach. It is the focus of other concerns in M22 (ii)-(iv).

We are to show that if Condition (11) and $\tilde{\mathbf{C}}_N = \mathbf{C}_N$ including $\kappa = \kappa'$ are satisfied, then $\tilde{\boldsymbol{\beta}}$ is at least a restricted BLUE and is a full BLUE if κ, the rank of $\tilde{\mathbf{C}}_N$, reaches ℓ, namely $\kappa = \ell$. The restricted BLUE is defined as the minimum variance estimator of $\boldsymbol{\beta}$ among the unbiased estimators having the form $\mathbf{AP}^{(\kappa)}\mathbf{y}$ for the pre-whitening operator $P^{(\kappa)}$ satisfying $P^{(\kappa)}\tilde{C}_NP^{(\kappa)T} = I_\kappa$ and an arbitrary matrix $\mathbf{A}$.

Let us consider an arbitrary linear unbiased estimator $\hat{\boldsymbol{\beta}}$ of $\boldsymbol{\beta}$ such that $\hat{\boldsymbol{\beta}} = \mathbf{AP}^{(\kappa)}\mathbf{y}$ for an arbitrary $m \times \kappa$ constant matrix $\mathbf{A}$, and

$$\mathbf{D} = \mathbf{A} - \left(\mathbf{X}^T\mathbf{P}^{(\kappa)T}\mathbf{P}^{(\kappa)}\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{P}^{(\kappa)T}.$$

The unbiasedness of $\hat{\boldsymbol{\beta}}$ suggests that

$$\begin{aligned}E\left(\hat{\boldsymbol{\beta}} \mid \mathbf{X}, \mathbf{P}^{(\kappa)}\right) &= E\left(\mathbf{AP}^{(\kappa)}y \mid \mathbf{X}, \mathbf{P}^{(\kappa)}\right)\\ &= \boldsymbol{\beta} + \mathbf{DP}^{(\kappa)}\mathbf{X}\boldsymbol{\beta} = \boldsymbol{\beta}.\end{aligned} \tag{17}$$

This means that $\mathbf{DP}^{(\kappa)}\mathbf{X}\boldsymbol{\beta} = 0$ for arbitrary β, and hence $\mathbf{DP}^{(\kappa)}\mathbf{X} = 0$.

It can be shown that

$$\begin{aligned}&\mathrm{Var}\left(\hat{\boldsymbol{\beta}} \mid \mathbf{X}, \mathbf{P}^{(\kappa)}\right)\\ &= E\Big(\left(\mathbf{AP}^{(\kappa)}(\mathbf{X}\beta + u) - \beta\right)\left(\mathbf{AP}^{(\kappa)}(\mathbf{X}\beta + u) - \beta\right)^T \mid \mathbf{X}, \mathbf{P}^{(\kappa)}\Big)\\ &= E\left\{\mathbf{AP}^{(\kappa)}\mathbf{uu}^T\mathbf{P}^{(\kappa)^T}\mathbf{A}^T \mid \mathbf{X}, \mathbf{P}^{(\kappa)}\right\}\\ &= \mathbf{DD}^T + \left(\mathbf{X}^T\mathbf{P}^{(\kappa)^T}\mathbf{P}^{(\kappa)}X\right)^{-1}\mathbf{X}^T\mathbf{P}^{(\kappa)^T}I_k\mathbf{P}^{(\kappa)}X(\mathbf{X}^TP^{(\kappa)^T}\mathbf{P}^{(\kappa)}X)^{-1}\\ &= \mathbf{DD}^T + \mathrm{Var}\left(\tilde{\boldsymbol{\beta}} \mid \mathbf{X}, \mathbf{P}^{(\kappa)}\right),\end{aligned} \tag{18}$$

where the second equation and the third equation utilize $\mathbf{DP}^{(\kappa)}\mathbf{X} = 0$. As $\mathbf{DD}^T \ge 0$, $\mathrm{Var}(\hat{\boldsymbol{\beta}} \mid \mathbf{X}, \mathbf{P}^{(\kappa)}) \ge \mathrm{Var}(\tilde{\boldsymbol{\beta}} \mid \mathbf{X}, \mathbf{P}^{(\kappa)})$.

Remark 8a Note here the class of the linear estimators is restricted by $\mathbf{P}^{(\kappa)}$ when $\kappa < \ell$. The derivation above shows that under Conditions (10) and (11), the estimated coefficient $\tilde{\boldsymbol{\beta}}$ is a restricted BLUE, which would be an unrestricted BLUE if $\kappa = \ell$.

Remark 8b The largest threat to the BLUE property of $\tilde{\boldsymbol{\beta}}$ is $\tilde{\mathbf{C}}_N \ne \mathbf{C}_N$, which would surrender the minimum variance aspect of $\tilde{\boldsymbol{\beta}}$ although $\tilde{\boldsymbol{\beta}}$ is still unbiased and consistent as shown in Sect. 2.2.

2.4 Model inconsistency check

AT99 was aware of the importance of $\tilde{\mathbf{C}}_N$ being a good approximation of $\mathbf{C}_N$. Section 4 of AT99 was devoted to checking for this by examining the potential inconsistency via a χ^2 in (AT.18), which was called the residual consistency test (RCT). The null hypothesis $\mathcal{H}_0$ was worded: "Our null-hypothesis, $\mathcal{H}_0$, is that the control simulation of climate variability is an adequate representation of variability in the real world in the truncated state space which we are using for the analysis, i.e. the subspace defined by the first κ EOFs of the control run does not include patterns which contain unrealistically low (or high) variance in the control simulation of climate variability. Because the effects of errors in observations are not represented in the climate model, $\mathcal{H}_0$ also encompasses the statement that observational error is negligible in the truncated state-space (on the spatio-temporal scales) used for detection. A test of $\mathcal{H}_0$, therefore, is also a test of the validity of this assumption."

M22 complained that "they did not formally state the null hypothesis of the RCT nor identify which of the GM conditions it tests, nor did they prove its distribution and critical values, rendering it uninformative as a specification test" in the abstract and was repeated several times in the paper.

M22's complaint for not stating the null hypothesis formally is understandable as AT99 was not explicit about it, despite using lengthy sentences to illustrate it before (AT.17), as quoted above. M22's assertion that "nor did they prove its distribution and critical values" is an overstatement as they were provided in (AT.18). We provide a derivation on the distribution of the RCT statistics, which shows (AT.18) is only true asymptotically instead of being exactly so as stated.

Remark 9 The null hypothesis $\mathcal{H}_0$ of the RCT is actually $\mathcal{H}_0 : \tilde{\mathbf{C}}_N = \mathbf{C}_N$ where $\tilde{\mathbf{C}}_N$ is the underlying covariance matrix of the null simulation via the climate model representing "the control simulation of climate variability", and $\mathbf{C}_N = \mathrm{Var}(\mathbf{u})$ is "the variability in the real world". It appears that AT99 implicitly assumed ℓ is fixed while $n \to \infty$, which ensures $\hat{\mathbf{C}}_N$ is a consistent estimator of $\tilde{\mathbf{C}}_N$ in light of Remark 7, namely $\hat{\mathbf{C}}_N = \tilde{\mathbf{C}}_N + o_p(1)$. AT99 also assumes the rank of $\tilde{\mathbf{C}}_N$ is the same as that of $\hat{\mathbf{C}}_N$.

In the following, we try to add the technical details leading to the χ^2 distribution in (AT.18). We assume ℓ is fixed, which assures the consistency of $\hat{\mathbf{C}}_N$ to $\tilde{\mathbf{C}}_N$ as indicated above.

Under $\mathcal{H}_0 : \tilde{\mathbf{C}}_N = \mathbf{C}_N$, the rank of $\tilde{\mathbf{C}}_N$, κ, matches the rank of C_N which is κ'. Then, the RCT statistic is

$$
\begin{aligned}
r^2 &= \tilde{\mathbf{u}}^T \hat{\mathbf{C}}_N^+ \tilde{\mathbf{u}} \\
&= \left(\mathbf{Y} - \mathbf{X}\tilde{\boldsymbol{\beta}}\right)^T \hat{C}_N^+ \left(\mathbf{Y} - \mathbf{X}\tilde{\boldsymbol{\beta}}\right) \\
&= \mathbf{Y}^T \left(\mathbf{I}_\ell - \mathbf{F}\mathbf{X}^T\right) \tilde{\mathbf{C}}_N^+ \left(\mathbf{I}_\ell - \mathbf{X}\mathbf{F}^T\right) \mathbf{Y} + o_p(1) \\
&= u^T \left(I_\ell - FX^T\right) \mathbf{C}_N^+ \left(I_\ell - XF^T\right) u + o_p(1) \\
&= \mathbf{u}^{*T} Q \mathbf{u}^* + o_p(1),
\end{aligned} \tag{19}
$$

where $\mathbf{u}^* = Pu \sim N(0, I_{\kappa'})$ according to (4), $Q = C_N^{\frac{1}{2}}(\mathbf{I}_\ell - \mathbf{F}\mathbf{X}^T)C_N^+(\mathbf{I}_\ell - \mathbf{X}\mathbf{F}^T)C_N^{\frac{1}{2}}$ and F is defined in (5). Then, from (4), $PC_N P^T = I_{\kappa'}$. Note that $I_\ell - XF^T$ is idempotent and $(I_\ell - FX^T)C_N^+ = C_N^+(I_\ell - XF^T)$. Thus,

$$
\begin{aligned}
Q^2 &= C_N^{\frac{1}{2}}\left(I_\ell - FX^T\right)C_N^+\left(I_\ell - XF^T\right) \\
&\quad C_N\left(I_\ell - FX^T\right)C_N^+\left(I_\ell - XF^T\right)C_N^{\frac{1}{2}} \\
&= C_N^{\frac{1}{2}}\left(I_\ell - FX^T\right)C_N^+ C_N C_N^+\left(I_\ell - XF^T\right)C_N^{\frac{1}{2}} \\
&= C_N^{\frac{1}{2}}\left(I_\ell - FX^T\right)C_N^+\left(I_\ell - XF^T\right)C_N^{\frac{1}{2}} = Q,
\end{aligned} \tag{20}
$$

implying that Q is idempotent and if $\kappa = \kappa' \leq \ell$,

$$
\begin{aligned}
\mathrm{rank}(Q) &= \mathrm{tr}(Q) \\
&= \mathrm{tr}\left(C_N^{\frac{1}{2}}\left(I_\ell - FX^T\right)C_N^+\left(I_\ell - XF^T\right)C_N^{\frac{1}{2}}\right) \\
&= \mathrm{tr}\left(C_N^{\frac{1}{2}} C_N^+ C_N^{\frac{1}{2}}\right) \\
&\quad - \mathrm{tr}\left(C_N C_N^+ X\left(X^T C_N^+ X\right)^{-1} X^T C_N^+\right) \\
&= \kappa' - m = \kappa - m.
\end{aligned} \tag{21}
$$

Remark 10 AT99 did not provide any details on the χ^2 distribution result in (AT.18), which made M22 suspicious about its validity. From (19), (20) and (21), r^2 is asymptotically $\chi^2_{\kappa-m}$ rather than exactly $\chi^2_{\kappa-m}$ as in (AT.18) even if we assume normally distributed data. The key that leads to Q being idempotent and hence the asymptotic $\chi^2_{\kappa-m}$ distribution is $\tilde{\mathbf{C}}_N = \mathbf{C}_N$ under $\mathcal{H}_0$ while $\ell = \kappa'$ is not needed. As indicated earlier, AT99 was not explicit about κ' but implicitly assumed $\ell = \kappa'$, which was not needed as shown above.

Remark 11 AT99 did not discuss the power of the χ^2-test. A formal power analysis can be conducted as follows. Under the alternative hypothesis $\mathcal{H}_1 : \tilde{\mathbf{C}}_N \neq \mathbf{C}_N$,

$$
r^2 = \mathbf{u}^{*T} \tilde{Q} \mathbf{u}^* + o_p(1), \tag{22}
$$

where $\tilde{Q} = \mathbf{C}_N^{\frac{1}{2}}(\mathbf{I}_\ell - \tilde{\mathbf{F}}\mathbf{X}^T)\tilde{\mathbf{C}}_N^+(\mathbf{I}_\ell - \mathbf{X}\tilde{\mathbf{F}}^T)\mathbf{C}_N^{\frac{1}{2}}$ and $\tilde{\mathbf{F}}$ is similar to F except that it uses $\tilde{\mathbf{P}}$ from the spectral decomposition of $\tilde{C}_N$ rather than $\mathbf{P}$. As $\tilde{Q}$ is no longer idempotent under $\mathcal{H}_1$, r^2 is no longer χ^2 distributed. Let $\{\sigma_j\}_{j=1}^d$ be the eigenvalues of $\tilde{Q}$ and $\{\chi^2_{1j}\}_{j=1}^d$ be the independent χ^2_1 random variables. Then, it can be shown that $r^2 \sim \sum_{j=1}^d \sigma_j \chi^2_{1j}$, which is a weighted independent χ^2_1 distribution and can be used to evaluate the power of the χ^2-test. If $\mathbf{C}_N$ can be consistently estimated, the eigenvalues of $\tilde{Q}$ can be numerically computed and then the power of the RCT can be calculated under (22).

Remark 12 The power of the RCT test in detecting differences between the covariance matrix of the null simulation and that of the residuals in the observed physical world is worth further study. The nonparametric nature of $\tilde{C}_N$ poses challenges for using the likelihood ratio test (Anderson 2003) for the BLUE and the optimal fingerprinting detection approach.

3 Connection to feasible generalized least square

After pointing out the problems of the optimal fingerprints approach of AT99, M22 advocated using the Feasible Generalized Least Square (FGLS) (Carroll 1982; Wooldridge 2010) and the heteroskedasticity-consistent (HC) method (White 1980). However, the FGLS and the HC methods

are not readily suitable for the setting of AT99 without careful modeling and statistical inference.

Remark 13 The key issue rests on the form of C_N, the covariance matrix of the residual u, which takes a nonparametric form in AT99 and is modeled and simulated via a climate model. The rationale is that, as commented by a referee, "climate variability has a fairly complex structure", which is "not easily amenable to representation by a small number of parameters with a simple space-time structure". This is sharply different from the FGLS which assumes a parametric form for C_N, namely C_N has a known pattern via a parameter θ so that $C_N = C_N(\theta)$. The latter means that C_N can be estimated with one replication of ℓ observations $\{x_i, y_i\}_{i=1}^{\ell}$ as commonly practiced in Statistics and Econometrics (Wooldridge 2010). As AT99 does not assume a known pattern for C_N, it cannot be estimated with merely ℓ samples from one replication of observations. AT99 got around the problem by estimating C_N via repeated simulation of a null climate model that they assumed to be close to the underlying null climate system.

Another difficulty with achieving the parametric model $C_N(\theta)$ required by the FGLS is that ℓ, the dimension of C_N, grows as ℓ increases. White (1980)'s HC and the FGLS approaches require C_N having a known parametric form depending on a finite number of parameters, so that as $\ell \to \infty$, the parameters and hence the covariance matrix can be estimated consistently. However, this is not the case for AT99's setting, where C_N's dimension grows with ℓ and yet there is no available parametrization for C_N.

The covariance structure used in the spatial statistics, for instance, the Matérn covariance models (Cressie 1993; Guttorp and Gneiting 2006), may be useful for the FGLS. However, careful modeling and hypothesis testing are needed before it can be used for the climate change studies.

4 Conclusion

Our review finds that the approach outlined in AT99 can survive M22's criticism by assuming three key conditions, which are the independence condition (10), the conditional independence condition (11) and $\tilde{\mathbf{C}}_N = \mathbf{C}_N$. The first two are related to how the null simulation of the climate model is conducted, and can be readily realized. The last one depends on how accurate the null climate model is in approximating the real covariance matrix $\mathbf{C}_N$ of the internal variation in the physical world, which touches on the core issue of climate system modeling. The quality of the climate modeling is improving as shown by the improved accuracy of longer term weather forecasting. However, whether the climate modeling is accurate enough to warrant $\tilde{\mathbf{C}}_N = \mathbf{C}_N$ is an issue one should aware of.

When $\tilde{\mathbf{C}}_N \neq \mathbf{C}_N$, the estimated fingerprints are no longer optimal. We have shown the estimated coefficients to the fingerprints by AT99 are unbiased and consistent to the underlying β under extra Conditions (13) after Conditions (10) and (11). Furthermore, we have shown that the RCT is valid asymptotically.

The above assessment should answer the main criticism of M22 as in "AT99 stated the GM Theorem incorrectly, omitting a critical condition altogether, their GLS method cannot satisfy the GM conditions, and their variance estimator is inconsistent by construction" and "Additionally, they did not formally state the null hypothesis of the RCT (residual consistency test) nor identify which of the GM conditions it tests, nor did they prove its distribution and critical values, rendering it uninformative as a specification test."

The conditions N1-N6 listed in M22 to repair AT99 are too complicated, many of them are unnecessary, and some are harder to justify. In contrast, Condition (10)–(11) and (13) are readily justifiable with simple physical meanings.

For easy reference of readers, we list in the following the main issues of AT99.

(i) AT99 did not present Condition (3), and neglected the independence Condition (10) and Condition (11): $E(u \mid X) = E(u \mid X, P^{(k)}) = 0$. These conditions are the key to the unbiasedness and consistency of the estimated fingerprints $\tilde{\beta}$ as shown in Remark 1 and Sect. 2.2 for details.

(ii) AT99 was vague on the ranks of C_N and the simulated null $\tilde{C}_N$. It should define the rank of C_N as κ', where $\kappa' \leq \ell$, while the rank of $\tilde{C}_N$ is κ. See Remarks 2 and 3 for details.

(iii) The claim that the estimated fingerprints $\tilde{\beta}$ is BLUE needs two more conditions: $C_N = \tilde{C}_N$ and $\kappa = \ell$ in addition to (10) and (11). If $\kappa < \ell$, $\tilde{\beta}$ is only a restricted BLUE among estimators in the form of $\mathbf{A}\mathbf{P}^{(\kappa)}\mathbf{y}$. See Remarks 8a and 8b for details.

(iv) The optimality of the estimated fingerprint critically depends on $C_N = \tilde{C}_N$, which may not be readily attained. Our analysis shows the estimated fingerprints are unbiased and consistent under weaker conditions.

(v) The distribution of the RCT statistic r^2 is not exactly $\chi^2_{\kappa-m}$ as in (AT.18) and (AT.19), but only valid asymptotically, requiring the sample size n being large. See Remark 10 for details.

The framework of AT99 has been extended to more general settings of fingerprint detection and attribution studies. Tett et al. (2002) followed similar approach as AT99 but proposed to estimate the covariance matrix by intraensemble variability of climate models aside from null setting control runs. Allen and Stott (2003) extended AT99's approach by allowing errors in the variables (EIV) $x_{(i)}$. Ribes et al. (2013) considered the EIV setting with a high dimensional aspect and used a high dimensional covariance matrix estimator (Ledoit and Wolf 2004). As these works are very much based on the pre-whitening rotation method advocated in AT99, that tries to use the GM for optimality, our comments on and repairs to AT99 are applicable to these works as well.

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Declarations

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