Applying the simple OLS form

Observations $\mathbf{Y}$

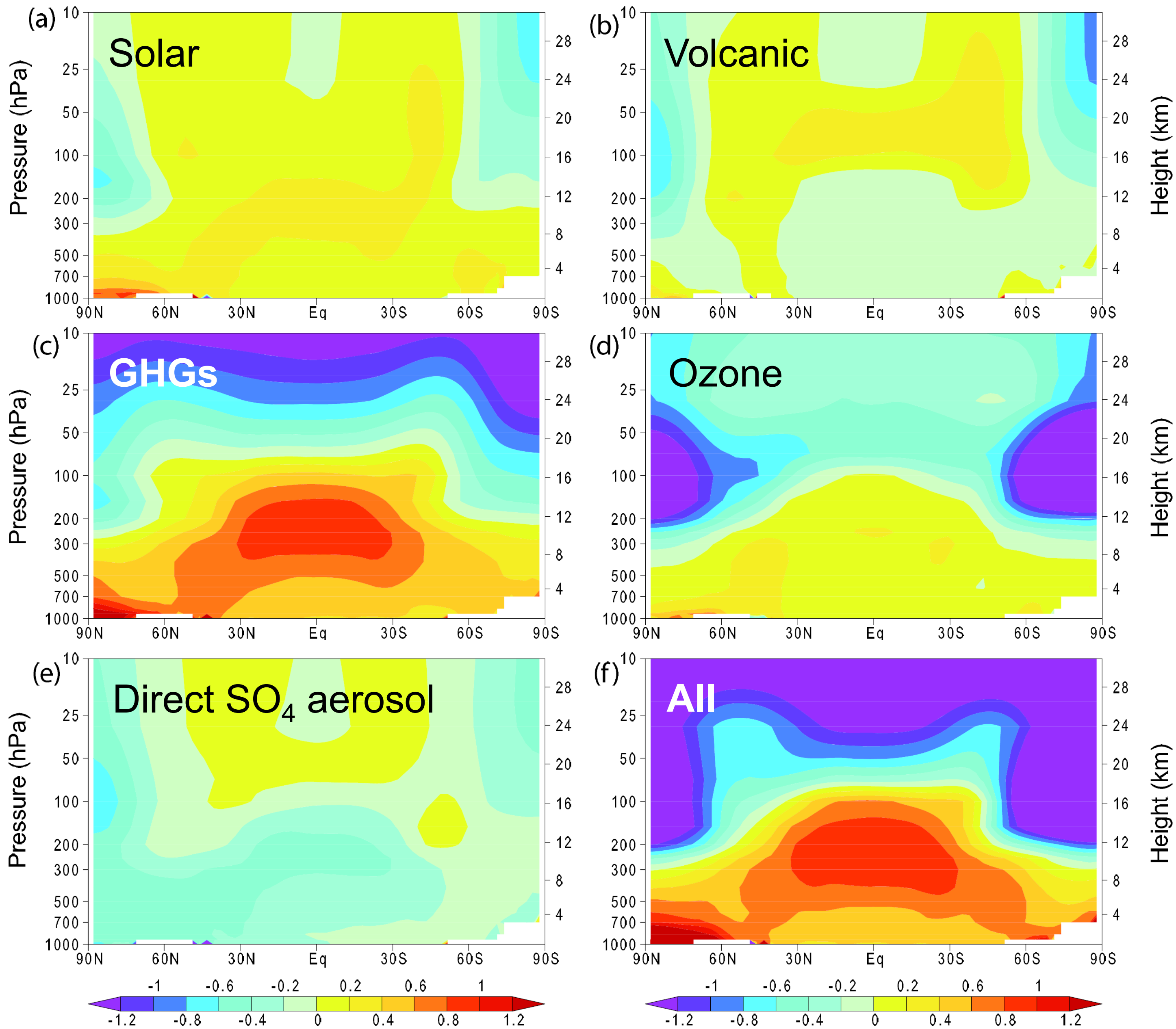
- Most studies of surface air temperature use
  - decadal averages and some kind of spatial averaging
    - To reduce noise from internal variability
    - To reduce the dimension of $\mathbf{Y}$
- Recent studies (e.g., Jones et al, 2013) use
  - Gridded (5°×5°) monthly mean surface temperature anomalies (e.g., HadCRUT4, Morice et al, 2012)
  - Reduced to decadal means for 1901-1920, 1911-1920 … 2001-2010 (11 decades)
  - Often spatially reduced using a “T4” spherical harmonic decomposition ⇒ global array of 5°×5°decadal anomalies reduced to 25 coefficients
  - $\mathbf{Y}_{n\times1}$ therefore has dimension n=11×25=275

Signals $\mathbf{X}_i$, i=1, …, s

- Number of signals s is small
  - s=1 → ALL
  - s=2 → ANT and NAT
  - s=3 → GHG, OANT and NAT
  - s=4 → …
- Can't separate signals that are "co-linear"
- Signals estimated from either
  - single model ensembles (size 3-10 in CMIP5) or
  - multi-model ensembles (~172 ALL runs available in CMIP5 from 49 models, ~67 NAT runs from 21 models , ~54 GHG runs from 20 models)
- Process as we do the observations
  - Transferred to observational grid, "masked", centered, averaged using same criteria, etc.

Examples of forced signals

PCM simulated 20th century temperature response to different kinds of forcing



IPCC WG1 AR4 Fig. 9.1

The generalized regression estimator of $\boldsymbol{\beta}$ is

$$\widehat{\boldsymbol{\beta}} = (\mathbf{X}^t\boldsymbol{\Sigma}^{-1}\mathbf{X})^{-1}\mathbf{X}^t\boldsymbol{\Sigma}^{-1}\mathbf{Y}$$

Need an estimate $\widehat{\boldsymbol{\Sigma}}$ of $\boldsymbol{\Sigma}$

- Usually estimated from control runs
- Even with decadal+T4 filtering, $\boldsymbol{\Sigma}$ is 275x275
  - need >275 110-year “chunks” of control run for a full-rank estimate

➔ Need further dimension reduction

- Constraints on dimensionality
  – Need to be able to invert covariance matrix $\widehat{\boldsymbol{\Sigma}}$
  – Covariance needs to be well estimated
  – Climate model should represent internal variability well
  – Should be able to represent signal vector well

A frequently used dimension reduction approach is projection onto the low order EOFs of $\hat{\boldsymbol{\Sigma}}$

$$\hat{\boldsymbol{\Sigma}} = \mathbf{P}\boldsymbol{\Lambda}\mathbf{P}^{t}$$

$$\mathbf{P}^{t}\mathbf{P} = \mathbf{P}\mathbf{P}^{t} = \mathbf{I}$$

$$\boldsymbol{\Lambda} = \mathbf{diag}(\boldsymbol{\lambda}_1, \dots, \boldsymbol{\lambda}_n)$$

$$\boldsymbol{\lambda}_1 \geq \boldsymbol{\lambda}_2 \geq \cdots \geq \boldsymbol{\lambda}_n \geq \mathbf{0}$$

$$\boldsymbol{\varepsilon} = \sum_{j=1}^{n} \boldsymbol{e}_j \mathbf{P}_j \quad \text{where} \quad \boldsymbol{e}_j = \boldsymbol{\varepsilon}^{t}\mathbf{P}_j$$

$$\mathbf{Var}(\boldsymbol{e}_j) = \boldsymbol{\lambda}_j \ \text{ and } \ \mathbf{Cor}(\boldsymbol{e}_i, \boldsymbol{e}_j) = \mathbf{0} \ \text{ for } \ \boldsymbol{i} \neq \boldsymbol{j}$$

Further constraint on estimating $\boldsymbol{\Sigma}$

– To avoid bias, optimization and uncertainty analysis should be performed separately (Hegerl et al, 1997)

➔ Require ***two*** independent estimates of of the covariance matrix

– An estimate $\widehat{\boldsymbol{\Sigma}}_{\mathbf{1}}$ for the optimization step and to estimate scaling factors $\boldsymbol{\beta}$

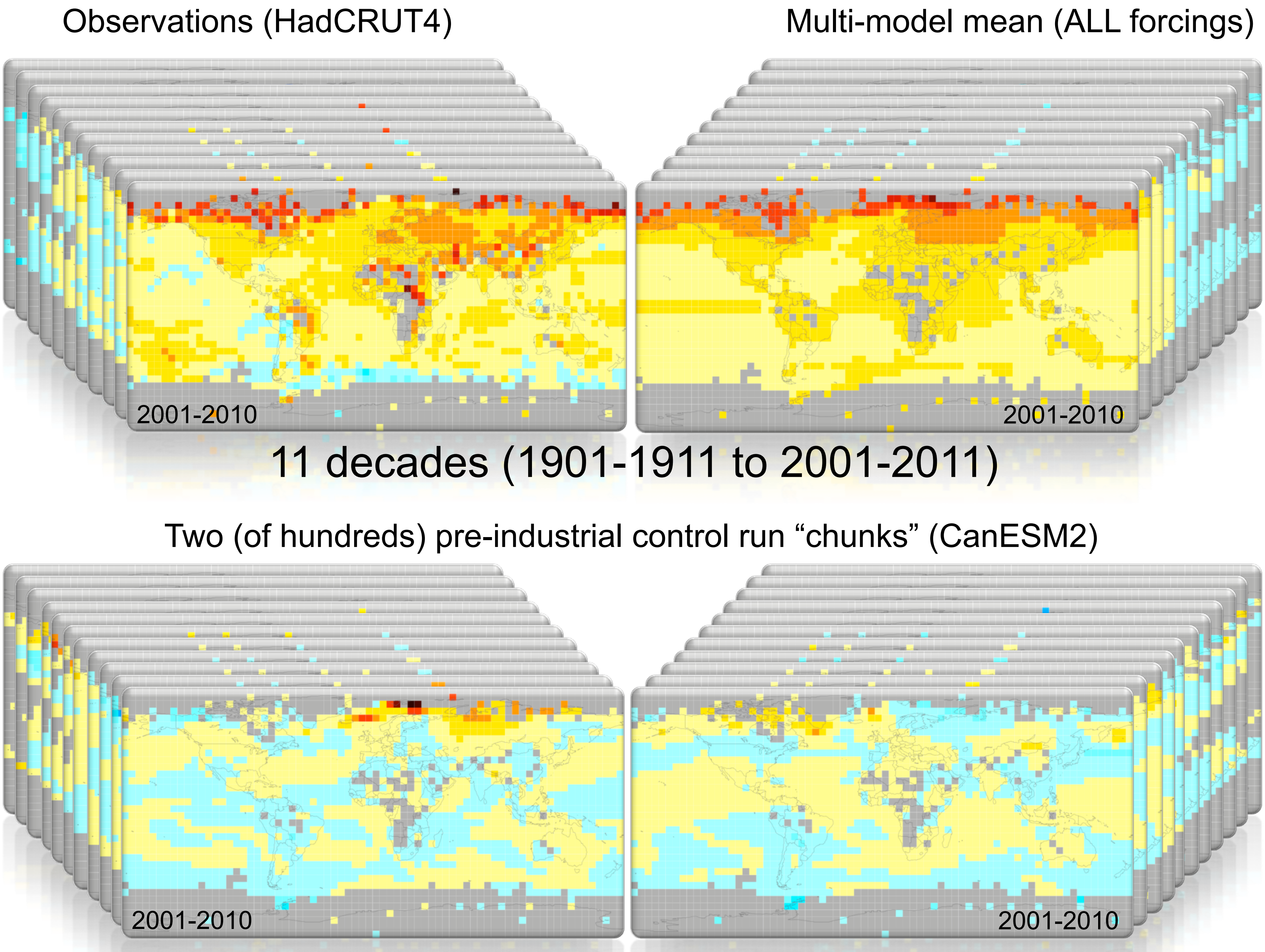
– An estimate $\widehat{\boldsymbol{\Sigma}}_{\mathbf{2}}$ to make estimate uncertainties and make inferences

- Residuals from the regression model, $\hat{\boldsymbol{\varepsilon}} = \mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}}$ are used to assess misfit and evaluate model based estimates of internal variability

Step-by-step procedure

Review of Basic Procedure

1. Determine domain, period of interest, filtering
    - Global, 1901-2010, T4 spatial smoothing, decadal averaging
2. Gather all data
    - Observations
    - Ensembles of historical climate runs
        - ALL and NAT runs (to separate ANT and NAT responses in obs)
    - Control runs (no forcing, needed to estimate internal variability)
3. Process all data
    - Observations
        - homogenize, center, grid, identify where missing
    - Historical climate runs
        - “mask” to duplicate “missingness” of observations,
        - process each run as the observations (no need to homogenize)
        - ensemble average to estimate signals
    - Control runs
        - divide into “chunks”, re-label years
        - process as the historical runs


Observations (HadCRUT4)
Multi-model mean (ALL forcings)
2001-2010
2001-2010
11 decades (1901-1911 to 2001-2011)
Two (of hundreds) pre-industrial control run “chunks” (CanESM2)
2001-2010
2001-2010

Basic procedure …

4. Estimate internal covariance structure for optimization
   - Use 1st sample of ν_1 control run chunks to estimate $\widehat{\mathbf{\Sigma}}_{\mathbf{1}}$

5. Fit the regression model in the reduced space
   - Select an EOF truncation k
   - Obtain an estimate of the scaling factors

$$\widehat{\boldsymbol{\beta}} = (\mathbf{X}^t \widehat{\mathbf{\Sigma}}_{\mathbf{1}}^{-1} \mathbf{X})^{-1} \mathbf{X}^t \widehat{\mathbf{\Sigma}}_{\mathbf{1}}^{-1} \mathbf{Y}$$

   - and an estimate of the residuals $\hat{\boldsymbol{\varepsilon}} = \mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}}$

6. Evaluate goodness of fit …

Basic procedure …

6. Assess whether the residual variance in the observations is consistent with model estimated internal variability

- Allen and Tett (1999)

$$\hat{\boldsymbol{\varepsilon}}^t \widehat{\boldsymbol{\Sigma}}_2^{-1} \hat{\boldsymbol{\varepsilon}} \sim (k-s) F_{k-s, v_2}$$

- Note that this is conditional on $\widehat{\boldsymbol{\Sigma}}_1$ (i.e., it ignores sampling variability in the optimization, Allen and Stott, 2003).

- Ribes et al (2012a) show that

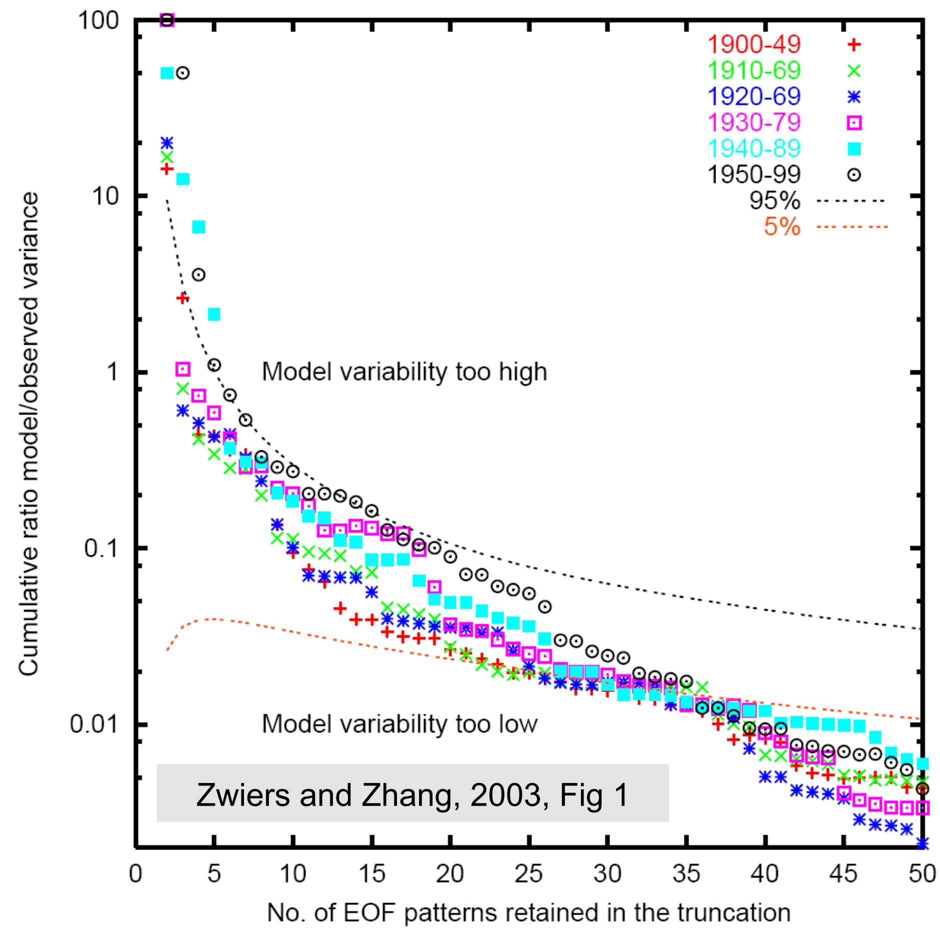
$$\hat{\boldsymbol{\varepsilon}}^t \widehat{\boldsymbol{\Sigma}}_2^{-1} \hat{\boldsymbol{\varepsilon}} \sim \frac{v_2(k-s)}{v_2 - k + 1} F_{k-s, v_2 - k + 1}$$

provides a better approximation for the residual consistency test

Basic procedure …

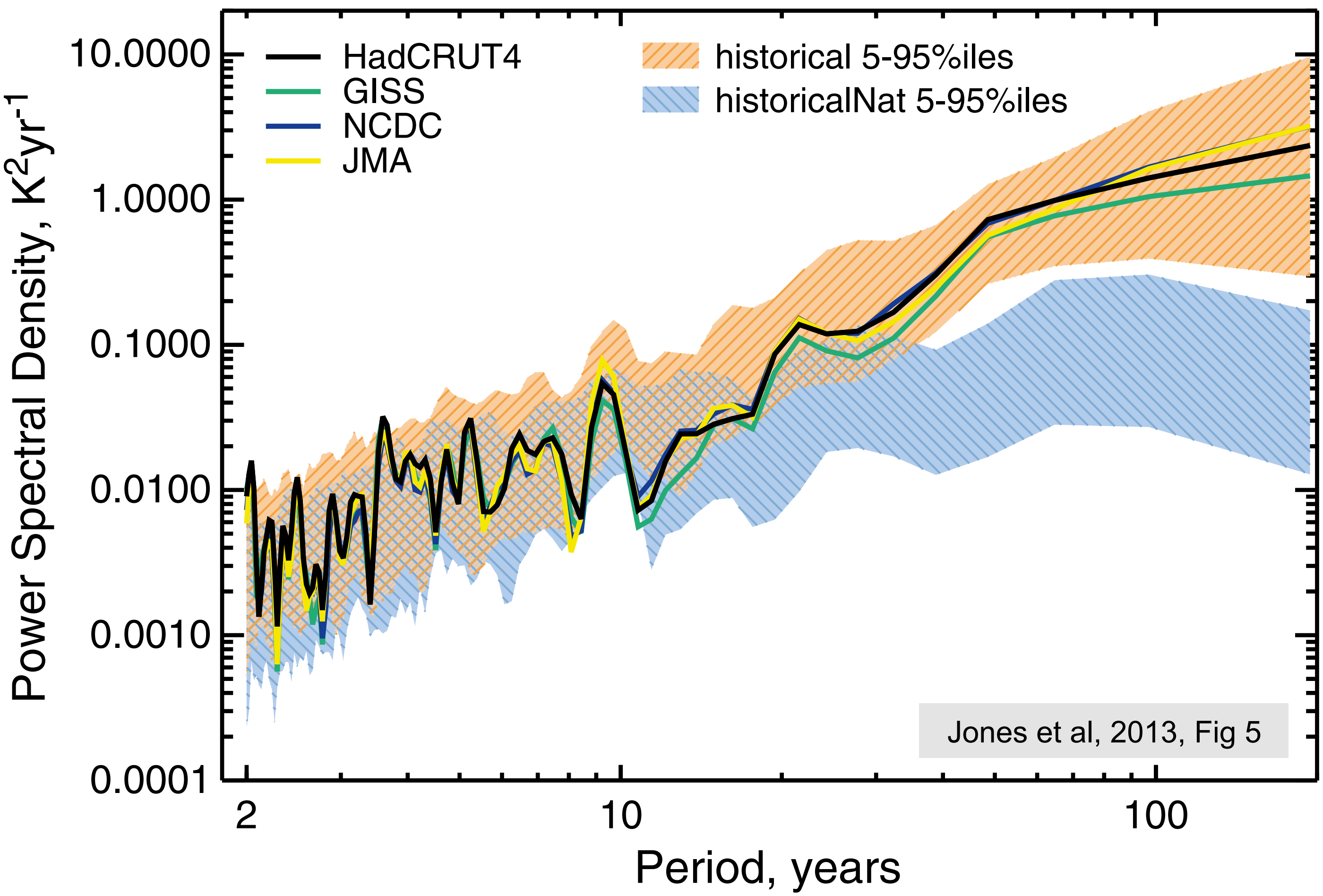
7. Determine EOF truncation point via residual consistency test

   – Global surface air temperature
   – One signal (“GS”)
   – 270 dimensions (5-decades, 30°×40° spatial averages)
   – 1600-yr of control runs (covariance estimated from 10-year overlapping chunks)
   – Residual consistency evaluated with



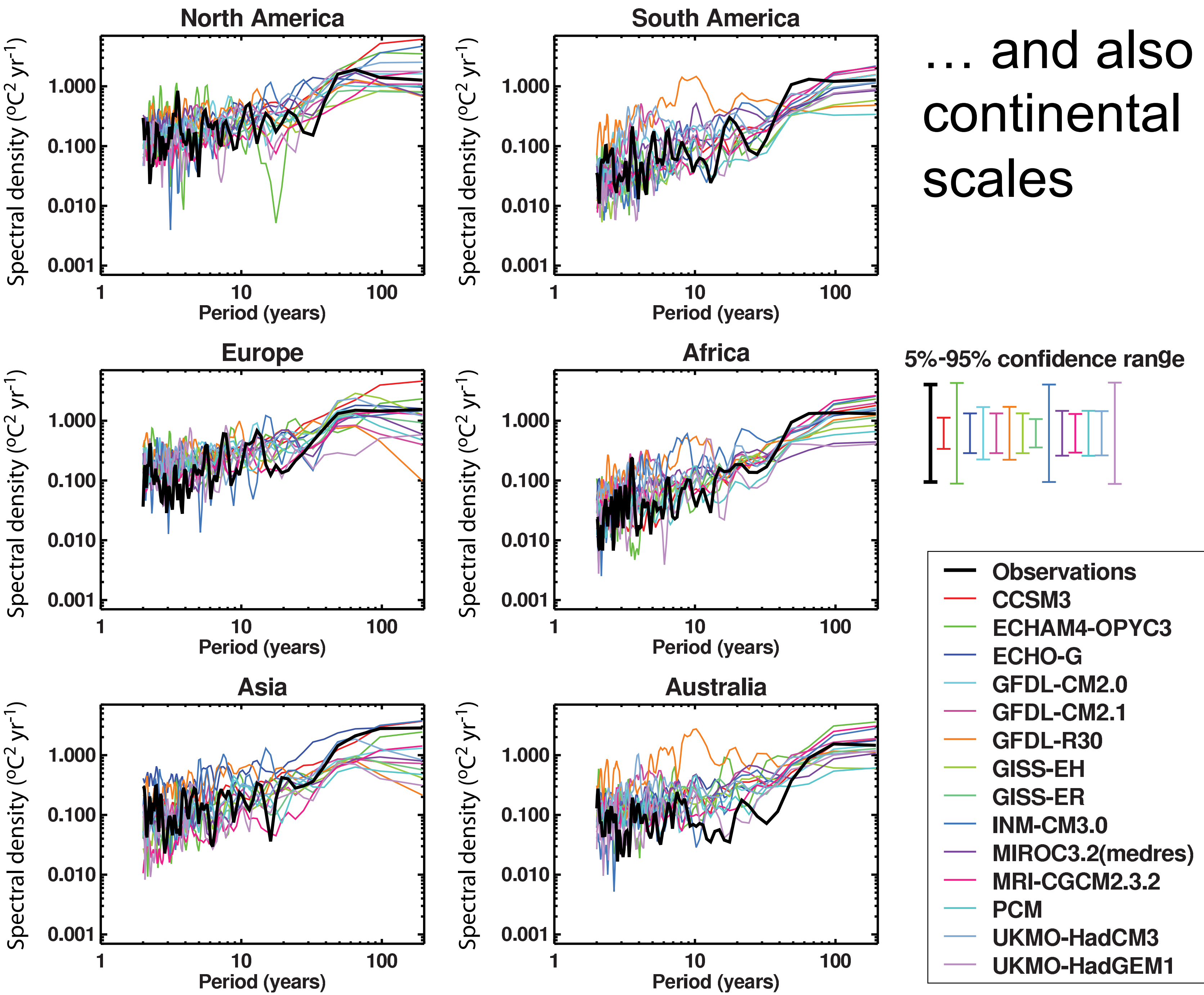
$$\hat{\boldsymbol{\varepsilon}}^t \hat{\boldsymbol{\Sigma}}_2^{-1} \hat{\boldsymbol{\varepsilon}} \sim (k-s) F_{k-s,v_2} \approx \chi^2_{k-s}$$

Models adequately represent surface temperature variability on global scales …



Variability of annual global mean surface temperature (1901-2010) estimated from observations (4 datasets) and ALL and NAT forced models (CMIP3 and CMIP5)

… and also on continental scales



IPCC WG1 AR4 Fig. 9.8

Basic procedure ….

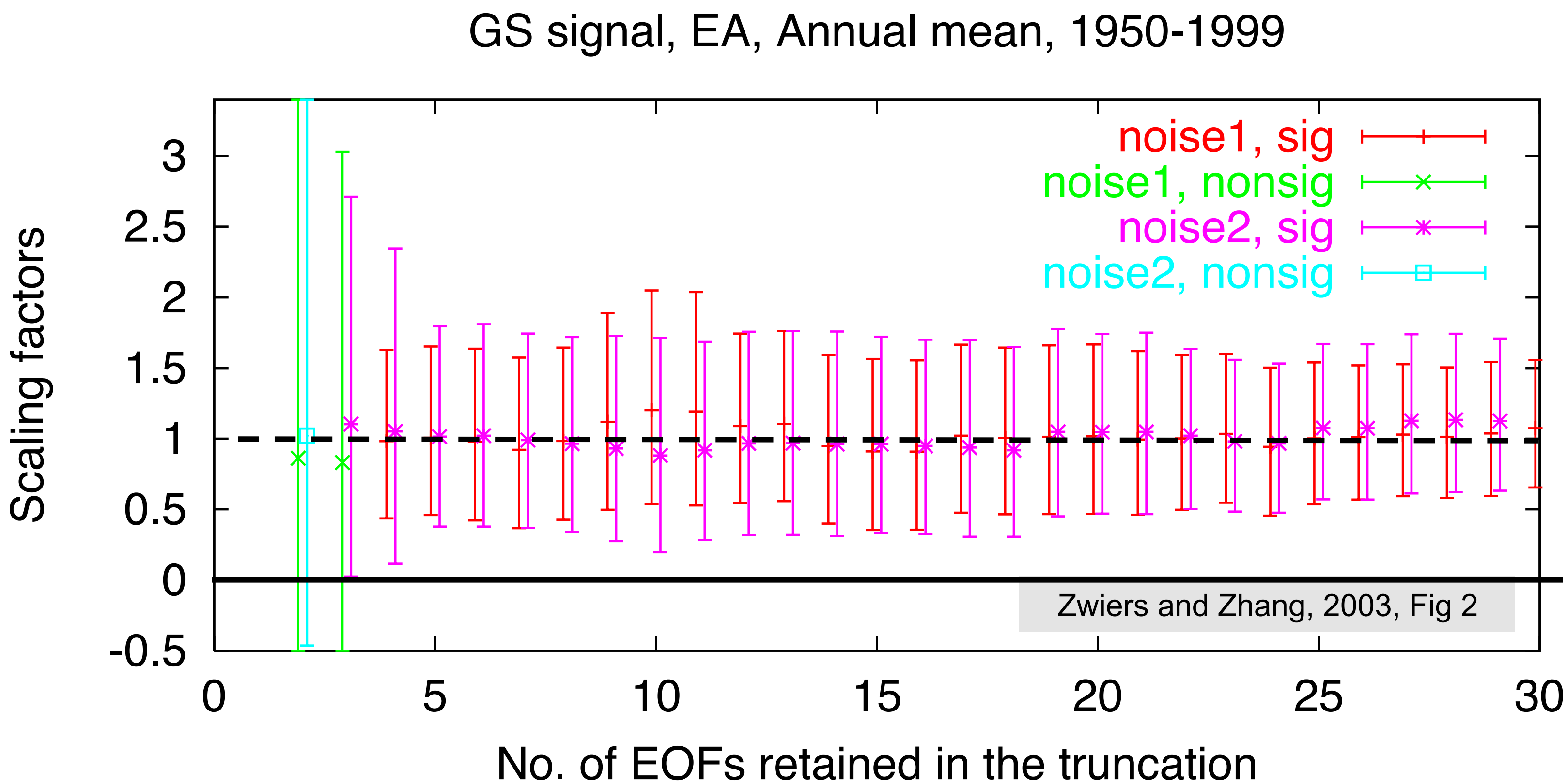
8. Make inferences about scaling factors

   - OLS expression that ignores uncertainty in $\widehat{\boldsymbol{\Sigma}}_{\mathbf{1}}$ looks like…

$$(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})^{t}\widehat{\boldsymbol{\Sigma}}_{\mathbf{2}}^{-\mathbf{1}}(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}) \sim sF_{s,v_2}$$

where $\boldsymbol{\Sigma}_{\boldsymbol{\beta}} = \mathbf{F}_{\mathbf{1}}^{t}\widehat{\boldsymbol{\Sigma}}_{\mathbf{2}}^{-\mathbf{1}}\mathbf{F}_{\mathbf{2}}$ and $\mathbf{F} = \left(\mathbf{X}^{t}\widehat{\boldsymbol{\Sigma}}_{\mathbf{1}}^{-\mathbf{1}}\mathbf{X}\right)^{-\mathbf{1}}\mathbf{X}^{t}\widehat{\boldsymbol{\Sigma}}_{\mathbf{1}}^{-\mathbf{1}}$

A “typical” 1-signal detection result



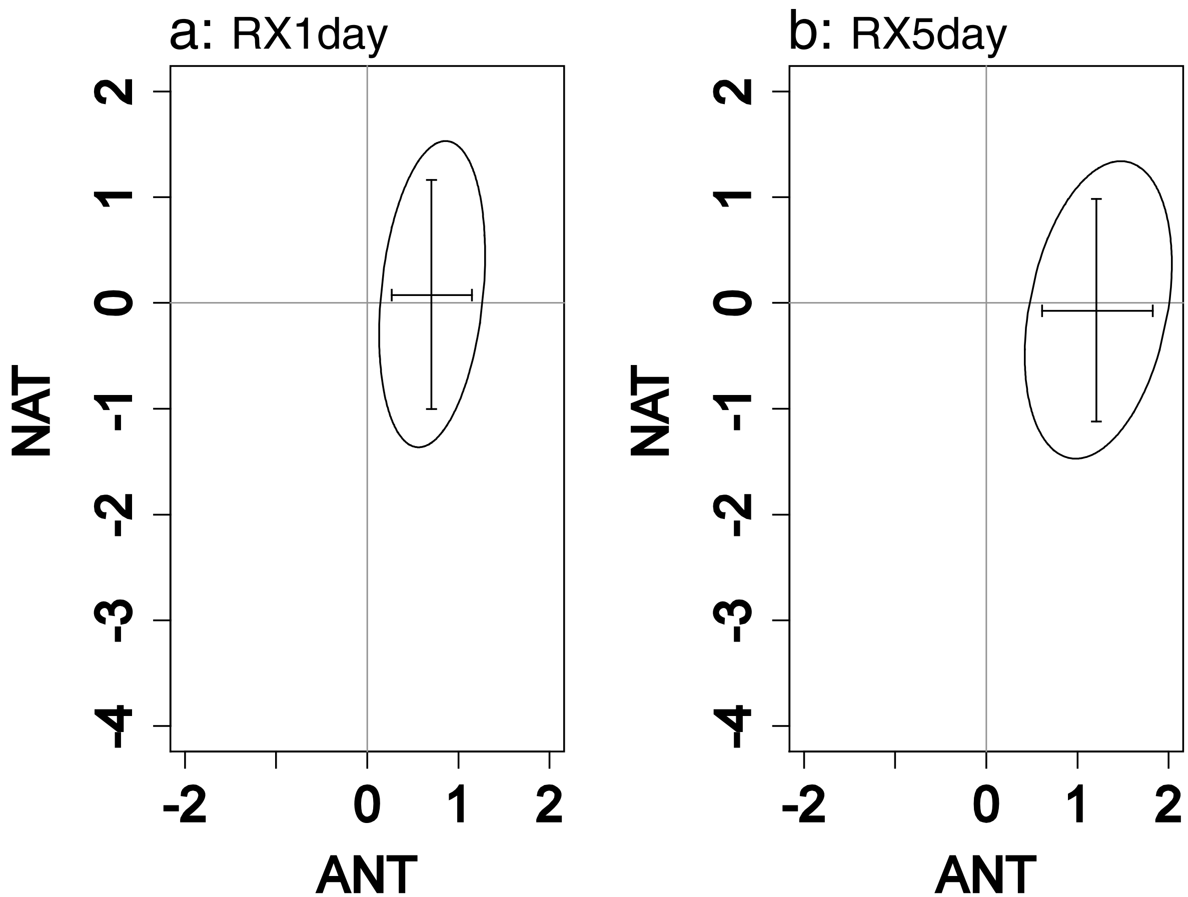
Detection of “GS” signal in Eurasian surface air temperature

A “typical” 2-signal detection result

Northern Hemisphere
1-day and 5-day
extreme precipitation,
1951-2005

Details:

- Two signals (ANT, NAT)
- 33-dimensions (11 5-yr averages, 3 regions)
- 54 ALL runs (14 GCMs)
- 34 NAT runs (9 GCMs)
- >15000-yr of control simulations (31 GCMs)
- total of ~455 “chunks” for estimating covariance matrices



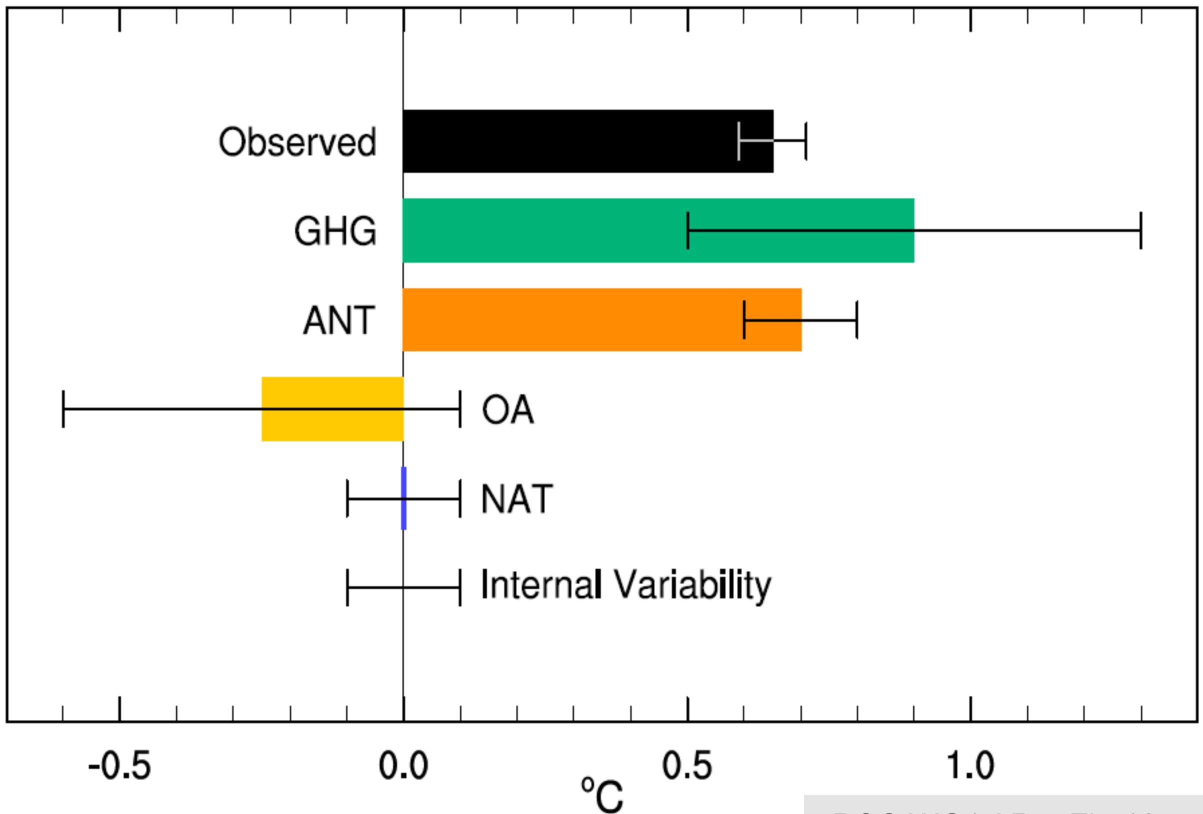
Zhang et al, 2013, Fig. 2

Calculating attributed change

Usual approach is to calculate trend in signal, multiply by scaling factor, and apply scaling factor uncertainty

Observed warming trend and 5-95% uncertainty range based on HadCRUT4 (black).

Attributed warming trends with assessed *likely* ranges (colours).



IPCC WG1 AR5, Fig 10.5

Total least squares

Statistical model for $\mathbf{X}_i$

– a single climate simulation j, j=1,…m_i, for forcing i produces

$$\widetilde{\mathbf{X}}_{i,j} = \mathbf{X}_i + \boldsymbol{\delta}_{i,j}$$

Simulated 110 year change vector	=	Deterministic forced response	+	Internal variability

$$\Rightarrow \quad \widetilde{\mathbf{X}}_{i,\cdot} = \mathbf{X}_i + \boldsymbol{\delta}_{i,\cdot}$$

where $\Sigma_{\delta\delta} = \frac{1}{m_i}\Sigma_{\varepsilon\varepsilon}$

That is, we assume that the $\boldsymbol{\delta}_{i,j}$'s are independent, and that they represent repeated realizations of the internal variability $\boldsymbol{\varepsilon}$ of the observed system.

Leads to a more complicated regression model

$$\mathbf{Y} = \mathbf{Y}^{Forced} + \boldsymbol{\varepsilon}$$
$$\widetilde{\mathbf{X}} = \mathbf{X}^{Forced} + \boldsymbol{\Delta}$$

$$\mathbf{Y}^{Forced} = \mathbf{X}^{Forced}\boldsymbol{\beta}$$

Columns of $\widetilde{\mathbf{X}}$ represent ensemble averages (m_i ensemble members averaged to form column i)

Columns of $\boldsymbol{\Delta}$ are independent of each other, and of $\boldsymbol{\varepsilon}$, with the same covariance structure as $\boldsymbol{\varepsilon}$ except scaled by $1/m_i$

For simplicity, scale $\widetilde{\mathbf{X}}$ by $\mathbf{M} = diag(\sqrt{m_1}, \ldots, \sqrt{m_s})$

→ Columns of $\boldsymbol{\Delta}$ have same covariance matrix as $\boldsymbol{\varepsilon}$
→ Need to remember to undo this later

Fitting the more complicated regression model

$$\mathbf{Y} = \mathbf{Y}^{Forced} + \boldsymbol{\varepsilon}$$
$$\widetilde{\mathbf{X}} = \mathbf{X}^{Forced} + \boldsymbol{\Delta}$$

$$\mathbf{Y}^{Forced} = \mathbf{X}^{Forced}\boldsymbol{\beta}$$

Fitting involves finding the $\mathbf{X}^{Forced}$ and $\boldsymbol{\beta}$ that minimize the “size” of the n×(s+1) matrix of residuals $[\boldsymbol{\Delta}, \boldsymbol{\varepsilon}]$

The assumptions about the covariance structure determine how the “size” of the matrix of residuals is measured

Note that because we scaled $\widetilde{\mathbf{X}}$, the estimate of $\mathbf{X}^{Forced}$ will be too large by a factor of $\mathbf{M}$, which means that we will have to adjust the estimated $\mathbf{X}^{Forced}$ and $\boldsymbol{\beta}$ to compensate

$$\mathbf{Y} = \mathbf{Y}^{Forced} + \boldsymbol{\varepsilon}$$
$$\widetilde{\mathbf{X}} = \mathbf{X}^{Forced} + \boldsymbol{\Delta}$$

$$\mathbf{Y}^{Forced} = \mathbf{X}^{Forced}\boldsymbol{\beta}$$

Find $\mathbf{X}^{Forced}$ and $\boldsymbol{\beta}$ that maximize joint likelihood of $\boldsymbol{\varepsilon}$ and $\boldsymbol{\Delta}$

→ minimize the "size" of the n×(s+1) matrix of residuals

$$[\widetilde{\mathbf{X}} - \widehat{\mathbf{X}}^{Forced}, \mathbf{Y} - \widehat{\mathbf{X}}^{Forced}\widehat{\boldsymbol{\beta}}]$$

n×s n×1

taking into account its covariance structure.

To take care of the covariance structure we "prewhiten" with $\mathbf{P} = \boldsymbol{\Sigma}^{-1/2}$

→ after prewhitening, we minimize

$$\left\|[\widetilde{\mathbf{X}} - \widehat{\mathbf{X}}^{Forced}, \mathbf{Y} - \widehat{\mathbf{X}}^{Forced}\widehat{\boldsymbol{\beta}}]\right\|_f^2$$

where $||\mathbf{A}||_f^2$ is the squared Frobenius norm (sum of eigenvalues of $\mathbf{A}^T\mathbf{A}$)

→ minimize $\left\| \left[\widetilde{\mathbf{X}} - \widehat{\mathbf{X}}^{Forced}, \mathbf{Y} - \widehat{\mathbf{X}}^{Forced}\widehat{\boldsymbol{\beta}} \right] \right\|_f^2$

→ minimize $\left\| \left[\widetilde{\mathbf{X}}, \mathbf{Y} \right] - \left[\widehat{\mathbf{X}}^{Forced}, \widehat{\mathbf{X}}^{Forced}\widehat{\boldsymbol{\beta}} \right] \right\|_f^2$

Note that the matrix on the left is of rank s+1
right is of rank s

Eckart-Young-Mirsky matrix approximation theorem (Huffel and Vandewalle, 1991, pp31) states that:

the minimum loss (measured as the least squared Frobenius norm) between a matrix and its p-lower-rank approximation is the sum of the last p eigenvalues from the singular value decomposition (SVD) of the original matrix.

We require an approximating matrix of only one rank lower

→ minimum loss is given by the last eigenvalue ν_{1+s} in the SVD of the left hand matrix

Let $[\widetilde{\mathbf{X}}, \mathbf{Y}] = \mathbf{Udiag}(\boldsymbol{\nu}_1, \dots, \boldsymbol{\nu}_s, \boldsymbol{\nu}_{s+1})\mathbf{V}^t$

n×(s+1) (s+1)×(s+1) (s+1)x(s+1)

The minimum loss approximation is obtained when

$\widehat{\boldsymbol{\beta}} = \mathbf{V}_{s+1}$ (the last singular vector of $[\widetilde{\mathbf{X}}, \mathbf{Y}]$) and

$$[\widehat{\mathbf{X}}^{Forced}, \widehat{\mathbf{Y}}^{Forced}] = \mathbf{Udiag}(\boldsymbol{\nu}_1, \dots, \boldsymbol{\nu}_s, \mathbf{0})\mathbf{V}^t$$

Don’t forget to rescale $\widehat{\boldsymbol{\beta}}$ and $\widehat{\mathbf{X}}^{Forced}$ with $\mathbf{M}^{-1}$

Aside – the problem of minimizing

$$\left\| [\tilde{\mathbf{X}}, \mathbf{Y}] - [\hat{\mathbf{X}}^{Forced}, \hat{\mathbf{X}}^{Forced}\hat{\boldsymbol{\beta}}] \right\|_f^2$$

is entirely parallel to the generalized linear regression problem.

For OLS we take $\hat{\mathbf{X}}^{Forced} = \tilde{\mathbf{X}}$

$$\left\| [\tilde{\mathbf{X}}, \mathbf{Y}] - [\hat{\mathbf{X}}^{Forced}, \hat{\mathbf{X}}^{Forced}\hat{\boldsymbol{\beta}}] \right\|_f^2 = \left\| [\tilde{\mathbf{X}}, \mathbf{Y}] - [\tilde{\mathbf{X}}, \tilde{\mathbf{X}}\hat{\boldsymbol{\beta}}] \right\|_f^2$$

$$= \left\| \mathbf{Y} - \tilde{\mathbf{X}}\hat{\boldsymbol{\beta}} \right\|_{\boldsymbol{\Sigma}}^2$$

That is, we find an approximation for a vector, rather than a matrix, but measuring distance essentially the same way

Statistical Inferences under TLS

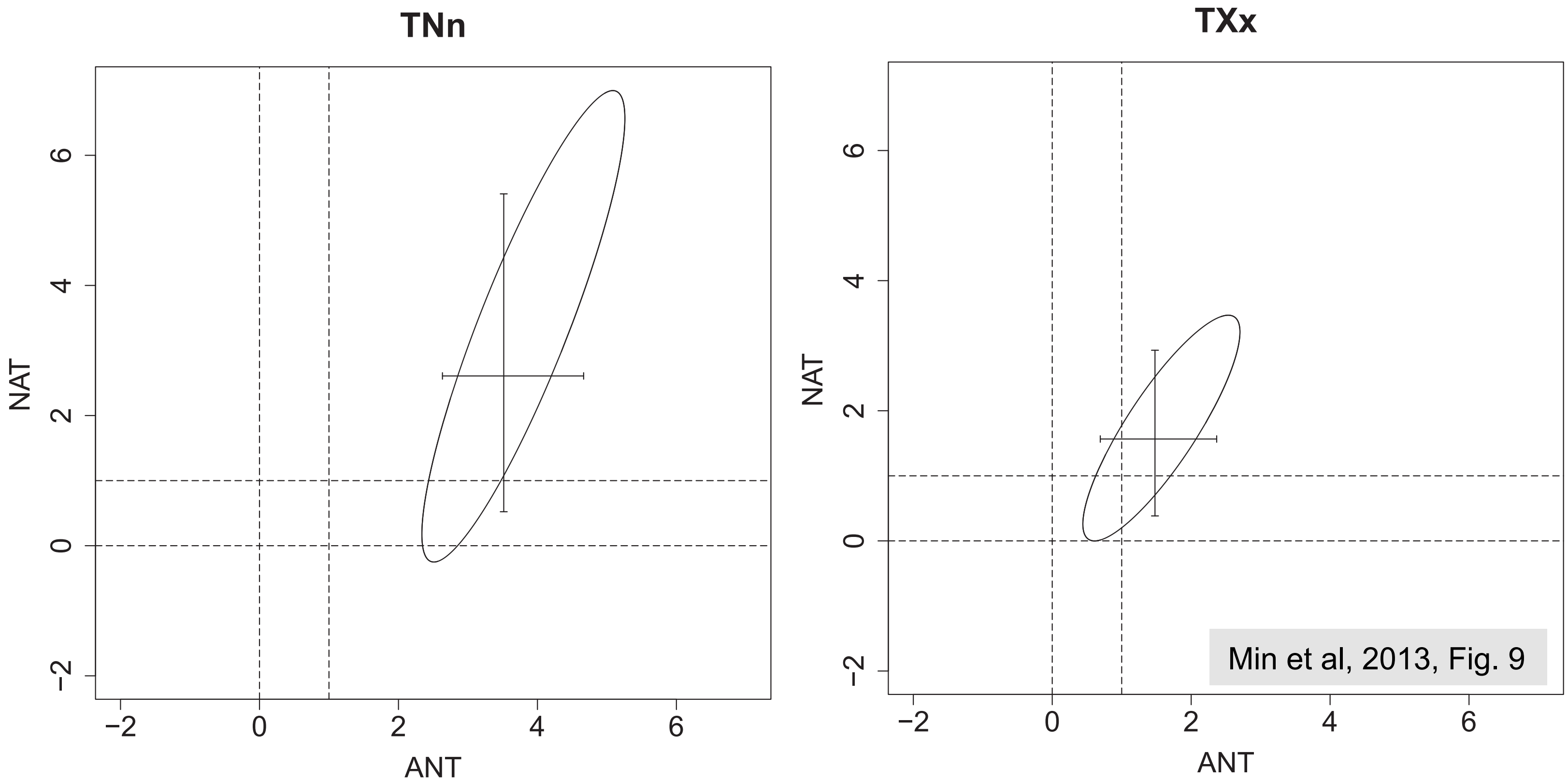
- Residual consistency test
  - Exact distribution not available analytically because the estimation problem is non-linear
  - Approximate distribution suggested by Allen and Stott (2003) is

$$\hat{\boldsymbol{\varepsilon}}^{t}\hat{\boldsymbol{\Sigma}}_{2}^{-1}\hat{\boldsymbol{\varepsilon}} \sim (k-s)F_{k-s,v_2} \approx \chi^2_{k-s} \text{ when } v_2 \gg k$$

  - Ribes et al (2012a) show, using Monte Carlo simulations, that this test operates at actual significance levels well below specified levels for reasonable values of k, v_1, v_2

- Confidence intervals for scaling factors
  - Based on approximation $\psi_{\tilde{\boldsymbol{\beta}}} = \hat{\boldsymbol{\varepsilon}}^{t}_{\tilde{\boldsymbol{\beta}}}\hat{\boldsymbol{\Sigma}}_{2}^{-1}\boldsymbol{\varepsilon}_{\tilde{\boldsymbol{\beta}}} - \hat{\boldsymbol{\varepsilon}}^{t}\hat{\boldsymbol{\Sigma}}_{2}^{-1}\hat{\boldsymbol{\varepsilon}} \sim sF_{s,v_2}$
  - Given a critical value C of F_{s,v_2}, find $\tilde{\boldsymbol{\beta}}'s$ that satisfy $\psi_{\tilde{\boldsymbol{\beta}}} = sC$
  - Nonlinearity makes intervals/regions non-symmetric, particularly when signal is weak relative to noise

Joint 90% confidence region for ANT and NAT detection in TNn and TXx



Details: 1951-2000 TNn and TXx from HadEX (Alexander et al, 2006), decadal time averaging, “global” spatial averaging, CMIP3 models (ANT – 8 models, 27 runs; ALL – 8 models, 26 runs; control – 10 models, 158 chunks)

Covariance matrix estimation

More on covariance matrix estimation

- A key source of uncertainty is the estimate of the covariance matrix
- Even with CMIP5, we often do not have enough information to estimate $\mathbf{\Sigma}$ well
- Several recent studies have attempted to avoid problems with covariance estimation by either
  - not fully optimizing (e.g., Polson et al, 2013; TLS without prewhitening)
  - Keeping dimension small (e.g., Sun et al, 2014; Najafi et al, 2014; Zhang et al, 2013; Min et al, 2013).
- Keeping dimension small
  - Increases signal-to-noise ratio
  - Eliminates the need for EOF truncation
  - Forces explicit space- and time-filtering decisions prior to conducting the D&A analysis
  - Involves a trade off (e.g., we might lose the ability to distinguish between different signals)

More on covariance matrix estimation

- An alternative approach is to use a more sophisticated estimator that the sample covariance matrix
- Ribes (2009, 2012a, 2012b) suggest using the regularized estimator of Ledoit and Wolf (2004), which is given by a weighted average of the sample covariance matrix and the identity matrix

$$\widehat{\boldsymbol{\Sigma}} = \boldsymbol{\lambda}\widehat{\mathbf{C}} + \boldsymbol{\rho}\mathbf{I}$$

- This estimate is always well conditioned, is consistent, and has better accuracy when sample size is small
- Since this estimator is full rank, EOF truncation is not needed
- Its application requires careful predetermination of the level of signal detail we require from the observations
- For example, Ribes et al (2012a) consider the effect of different amounts of spatial filtering of surface temperature

A further challenge

A further challenge - EIV

$$\mathbf{Y} = \mathbf{Y}^{Forced} + \boldsymbol{\varepsilon}$$
$$\widetilde{\mathbf{X}} = \mathbf{X}^{Forced} + \boldsymbol{\Delta}$$

$$\mathbf{Y}^{Forced} = \mathbf{X}^{Forced}\boldsymbol{\beta}$$

- We assumed that columns of $\boldsymbol{\Delta}$ have the same covariance structure as $\boldsymbol{\varepsilon}$
- That is, we assumed that only internal variability makes the signals uncertain
- But model and forcing differences also make the signals uncertain
- Maybe need a more complex representation for $\boldsymbol{\Delta}$**?**
- See Huntingford et al (2006), Hannart et al (2014)

Conclusions

Conclusions

- The method continues to evolve
- Thinking hard about regularization is a good development (but perhaps not most critical)
- Some key questions
  - How do we make objective prefiltering choices?
  - How should we construct the “monte-carlo” sample of realizations that is used to estimate internal variability?
  - Similar question for signal estimates
  - How should we proceed as we push to answer questions about extremes?

Thank you

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