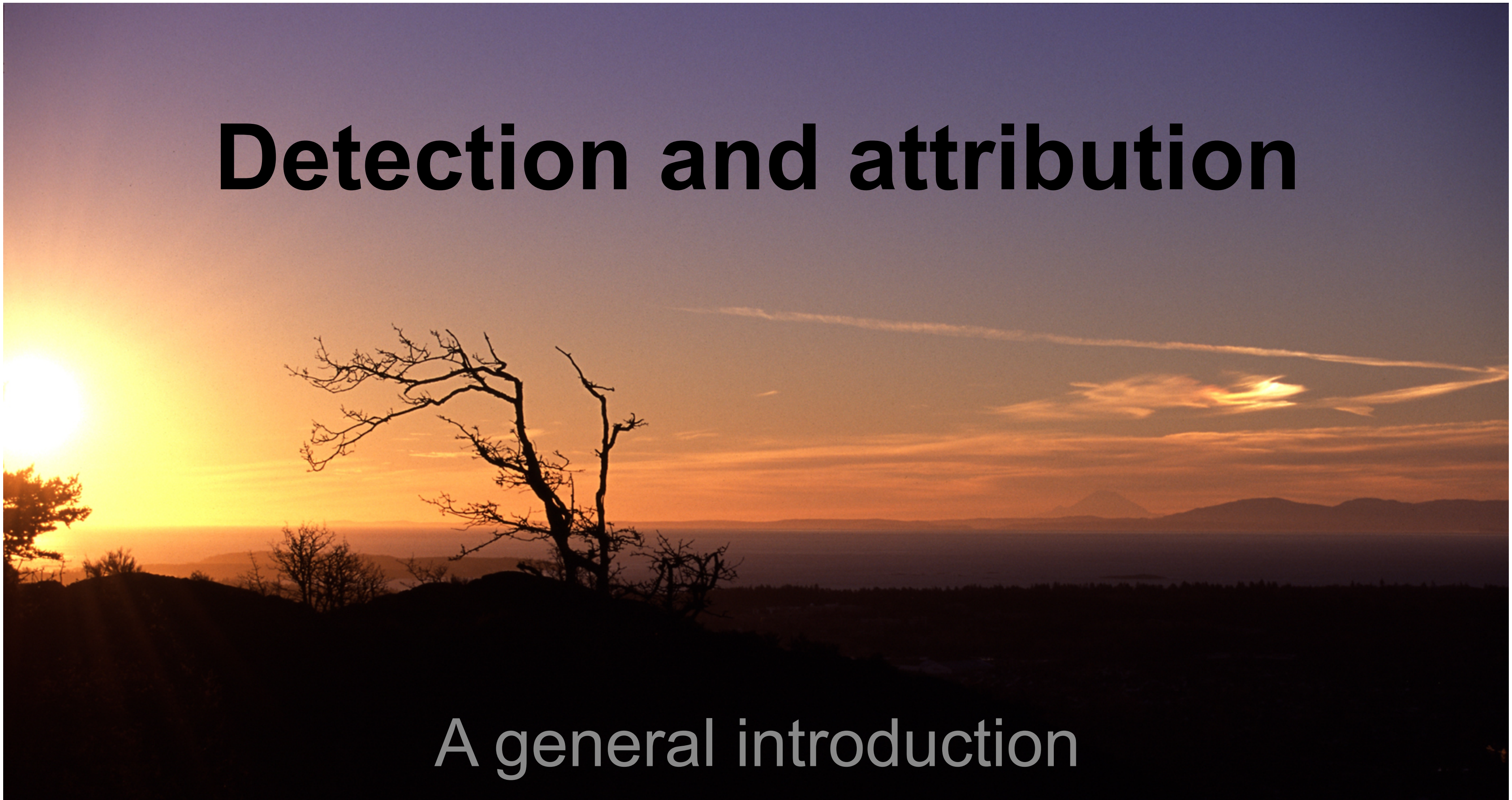


Detection and attribution

A general introduction

Francis Zwiers, Pacific Climate Impacts Consortium, University of Victoria
Qiuzi Wen, Climate Data Analysis Section, Environment Canada

University of Victoria
PACIFIC CLIMATE IMPACTS CONSORTIUM
WCRP World Climate Research Programme WMO IOC ICSU
ICTP The Abdus Salam International Centre for Theoretical Physics IAEA
Environment Canada

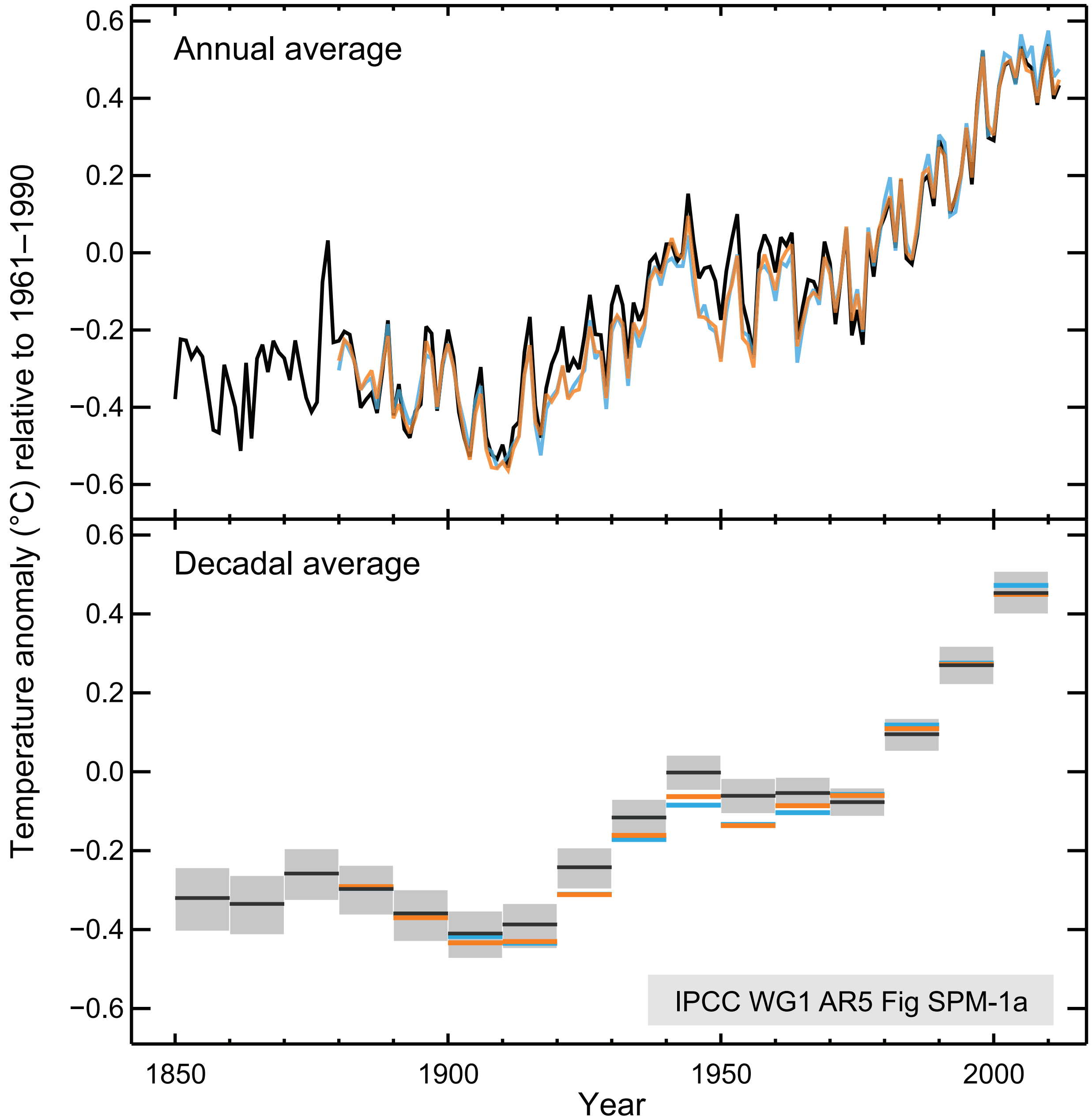

IPCC AR5 Overview

Observed Climate Change

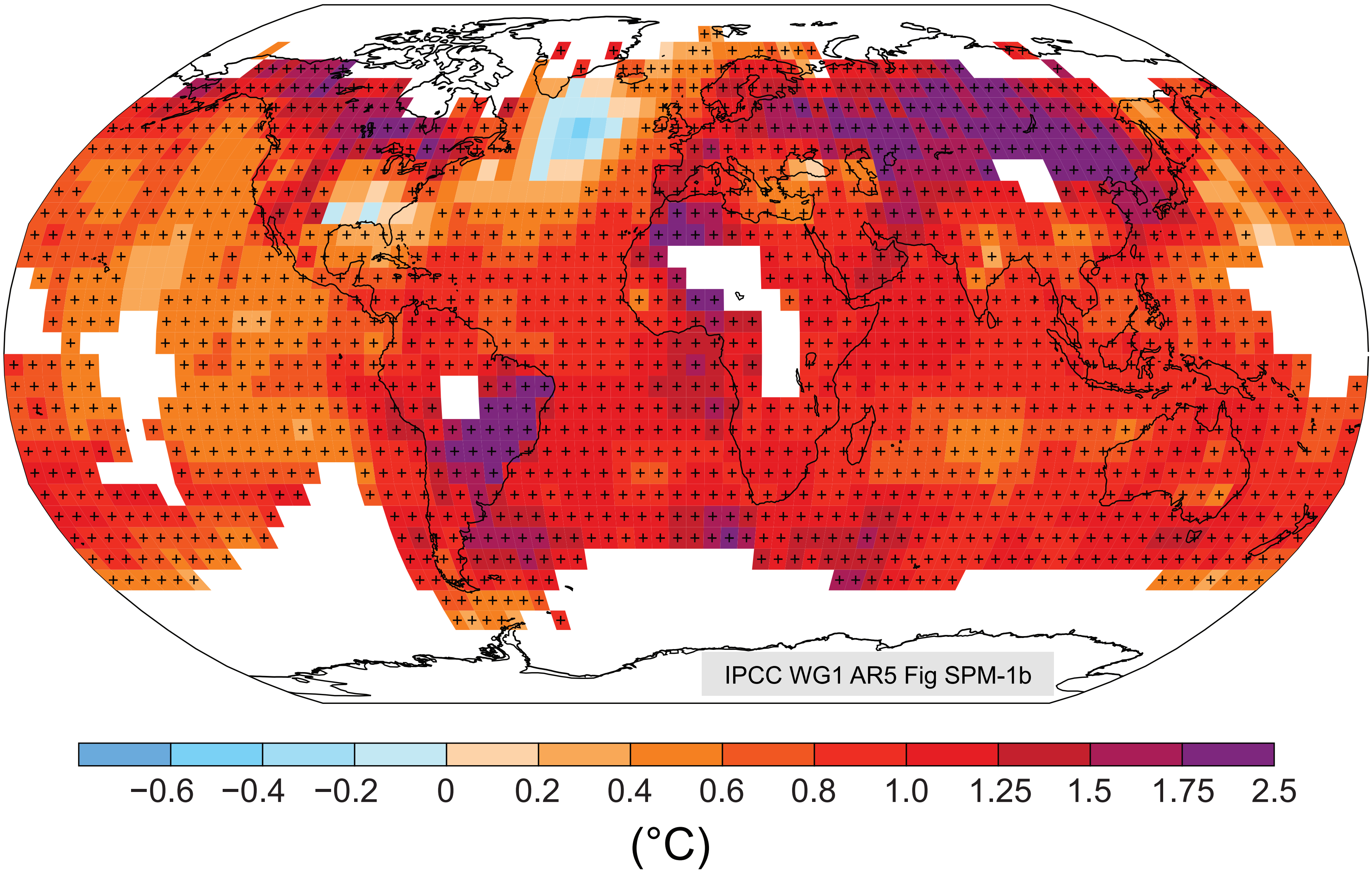
"Warming of the climate system is ***unequivocal***, and since the 1950s, many of the observed changes are unprecedented over decades to millennia. The atmosphere and ocean have warmed, the amounts of snow and ice have diminished, sea level has risen, and the concentrations of greenhouse gases have increased."

IPCC-WG1-AR5 SPM

Observed globally averaged combined land and ocean surface temperature anomaly 1850–2012

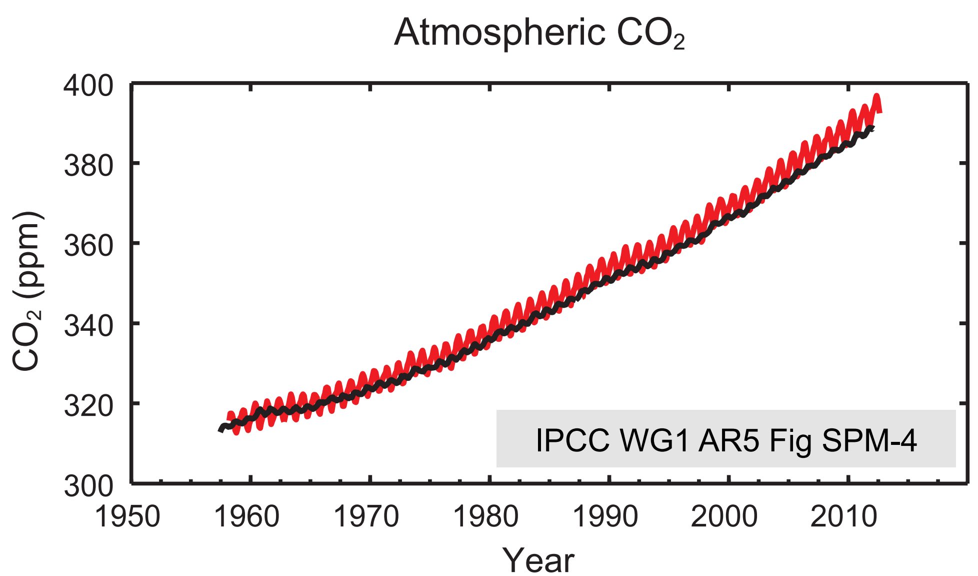


Observed change in surface temperature 1901–2012

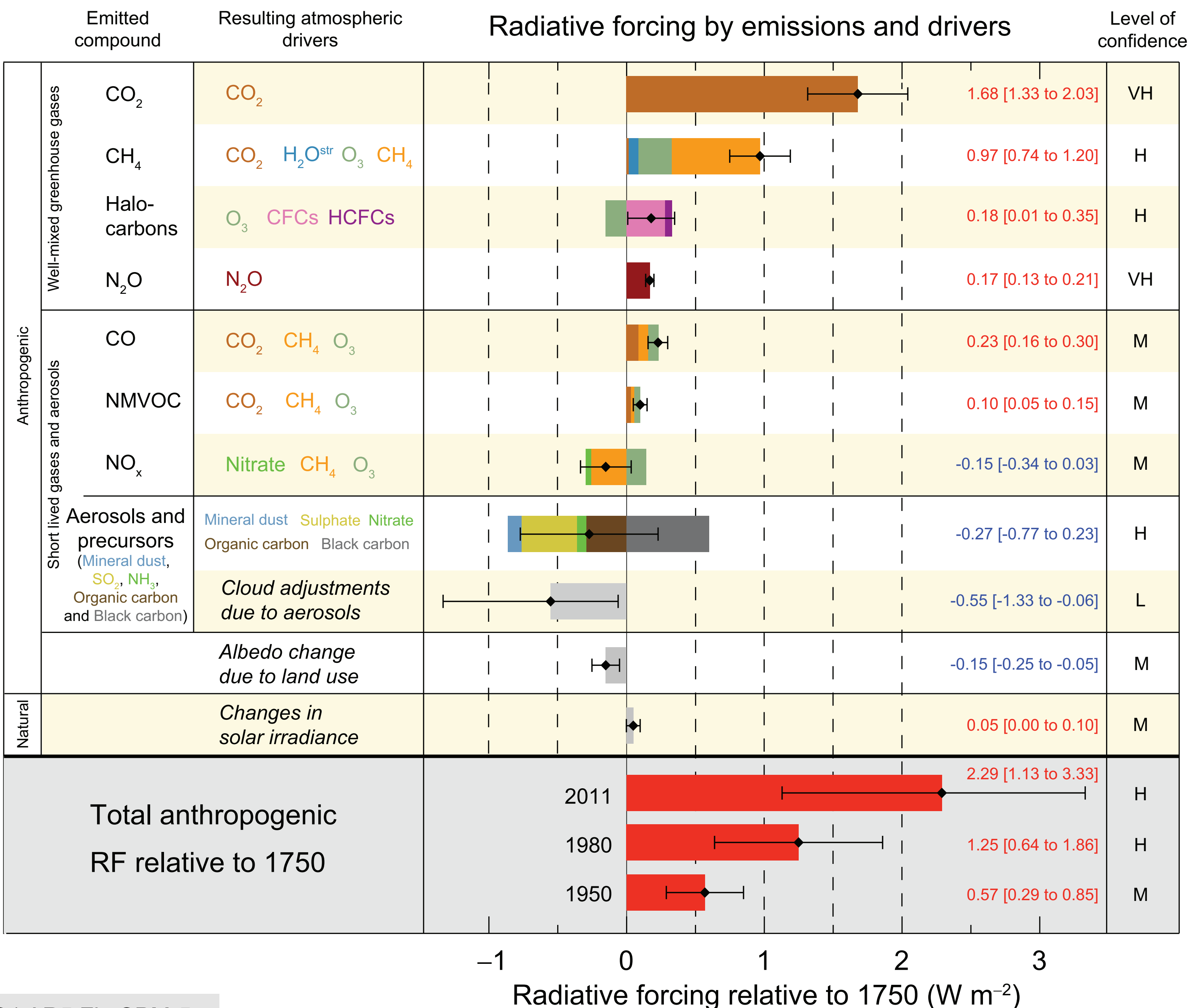


"The atmospheric concentrations of carbon dioxide, methane, and nitrous oxide have increased to levels unprecedented in at least the last 800,000 years.

Carbon dioxide concentrations have increased by 40% since pre-industrial times … " *IPCC WG1 AR5 SPM*



"Total radiative forcing is positive, and has led to an uptake of energy by the climate system." *IPCC WG1 AR5 SPM*



IPCC WG1 AR5 Fig SPM-5

But knowing that the forcing is positive does not mean you have detected the cause of the observed warming ...

Attribution

- are observed changes consistent with

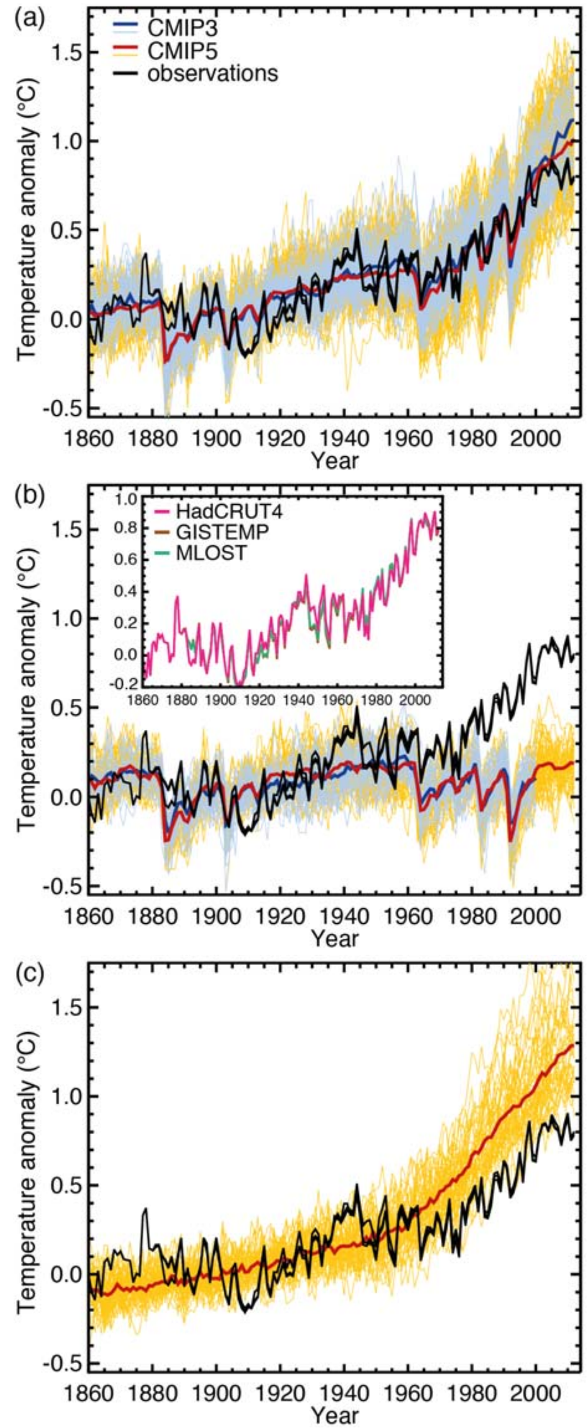
☑expected responses to forcings

☒inconsistent with alternative explanations

All forcing

Solar + volcanic

GHG forcing



IPCC WG1 AR5 Fig TS-9

Attribution results

TAR (2001)

– "most of the observed warming over the last 50 years is **likely** to have been due to the increase in greenhouse gas concentrations"

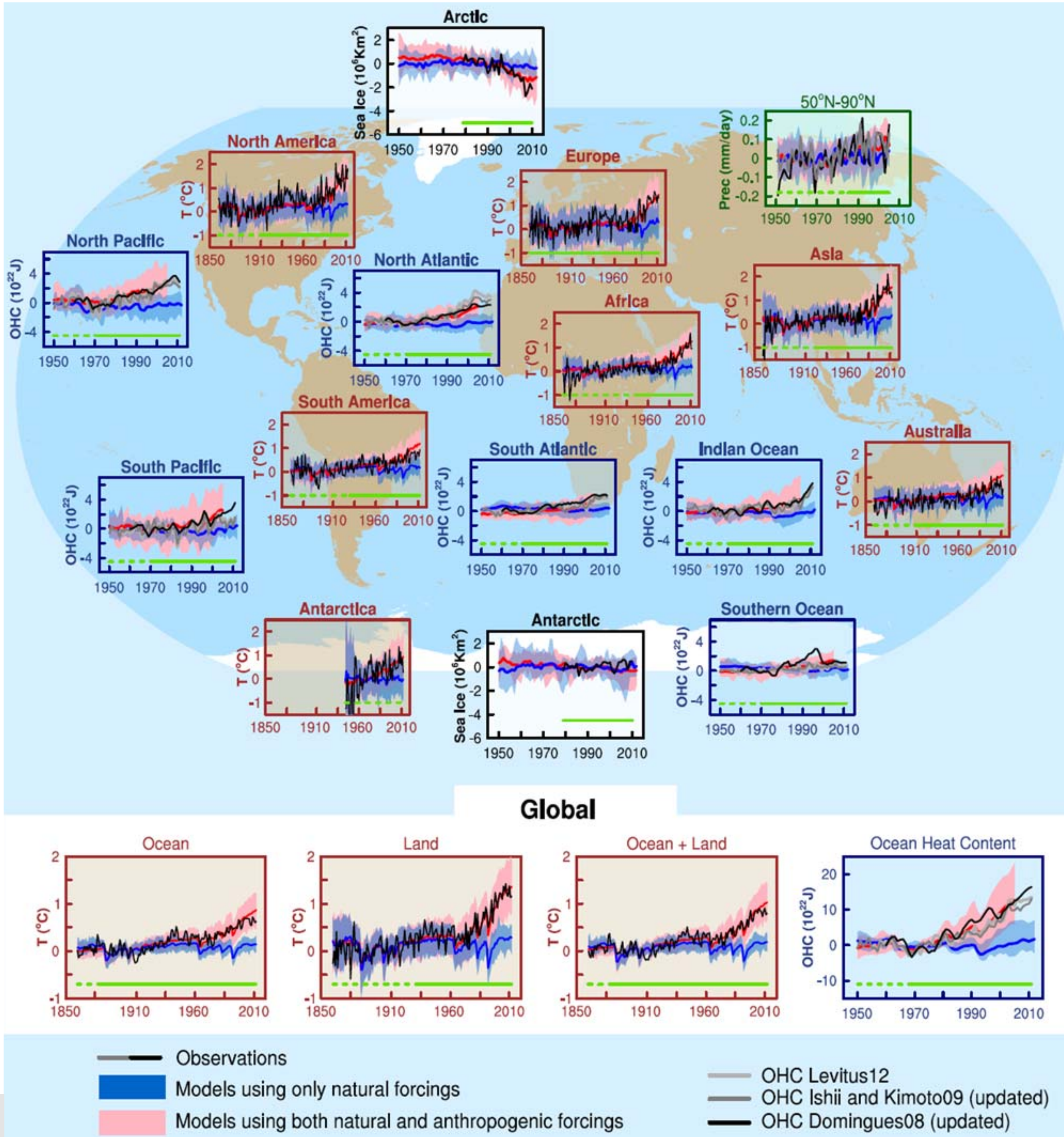
AR4 (2007)

– **likely** replaced with **very likely**
– "GHGs **likely** would have caused more warming than observed"

AR5 (2013)

– "It is **extremely likely** that human influence has been the dominant cause of the observed warming since the mid-20th century."
– "Greenhouse gases contributed a global mean surface warming **likely** to be in the range of 0.5°C to 1.3°C over the period 1951 to 2010 …"

Changes in land surface temperature, sea ice extent, and upper ocean heat content



IPCC WG1 AR5 Fig 10.21

Attribution Summary

- **Warming – human influence has …**
  - caused more than half of the observed increase in global mean surface temperature from 1951-2010 (**extremely likely**).
    - the GHG contribution was between 0.5K and 1.3K (**likely**)
    - internal variability alone cannot account for the observed warming since 1951 (**virtually certain**).
  - caused significant warming on each continent except Antarctica (**likely**)
  - contributed to the warming of the troposphere since 1961 (**likely**) with a dominant influence from GHGs
  - contributed to the cooling of the lower stratosphere since 1979 (**very likely**) with a dominant influence from ozone depleting substances.
  - contributed substantially to global sea level rise since the 1970s (**very likely**).

Attribution Summary (cont'd)

- **Climate extremes – human influence has …**
  - contributed to the observed changes in ***temperature extremes*** since the mid-20th century (**very likely**).
  - substantially increased the probability of occurrence of ***heat waves*** in some locations (**likely**).
  - contributed to intensification of ***heavy precipitation*** on global scales (***medium confidence***).
  - There is ***low confidence*** in attribution of changes in ***tropical cyclone activity*** to human influence.

- **Other aspects – human influence has …**
  - contributed to changes in the **hydrological cycle** (***medium confidence***).
  - contributed to sea ice loss (**very likely**) and snow cover loss (**likely**).

Overview of the methodology

Definition of D & A

- *Detection* of change is defined as the process of demonstrating that climate or a system affected by climate has changed in some defined statistical sense without providing a reason for that change.

- *Attribution* is defined as the process of evaluating the relative contributions of multiple causal factors to a change or event with an assignment of statistical confidence.

- In WG1, casual factors usually refer to *external influences*, which may be *anthropogenic* (GHGs, aerosols, ozone precursors, land use) and/or *natural* (volcanic eruptions, solar cycle modulations).

IPCC Good Practice Guidance Paper on Detection and Attribution, 2010

Four core elements

1. Observations of climate indicators

2. An estimate of external forcing
   – how external drivers of climate change have evolved before and during the period under investigation
   – e.g., GHG and solar radiation

3. A quantitative physically-based understanding of how external forcing might affect these climate indicators.
   – normally encapsulated in a physically-based model

4. An estimate of climate internal variability
   – often, but not always, derived from a physically-based model

General assumptions

- Key forcings have been identified
- Signals are additive
- Noise is additive
- The large-scale patterns of response are correctly simulated by climate models

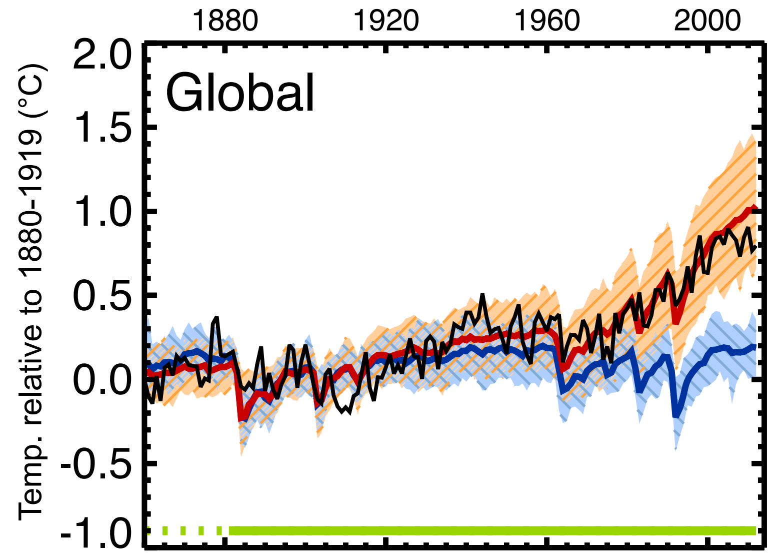
Methodology

- Methods are determined by
  - Assumptions about sources of uncertainty
  - Whether signals are “optimized”
- Invariably D&A relies heavily on climate models
  - D&A is a “small sample” statistical problem
- The objective is always to assess the evidence <u>contained in the observations.</u>
- Methods are simple, yet complex.

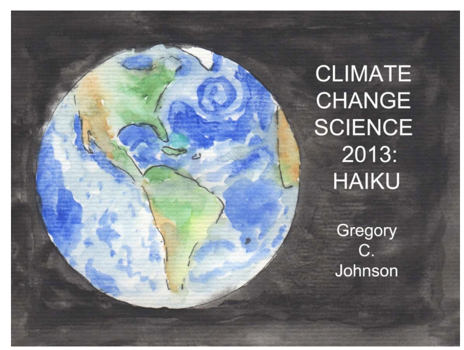
Non-optimal D&A approaches

Non-optimal approach

Qualitatively, we could evaluate the consistency of observed changes with modelled changes



IPCC WG1 AR5 Fig 10.7



Gregory C. Johnson

LA, IPCC WG1 AR5, Chapter 3 (Ocean Observations)

Non-optimal approach

1. Use climate models to estimate "form" of signal
   – Usually the mean F of an ensemble of forced runs

2. Estimate amplitude of signal in the observations
   – A scaled inner-product between a normalized signal and observations

$$S = (F \cdot T)/||F||$$

signal (F) observations (T)

   – Signal could be a pattern of change in space, or in space and time, or across multiple variables

Non-optimal approach

3. Compare S with amplitude of signal in differently forced model runs
4. Compare S with natural variability of signal amplitude in control simulations
   - Calculate amplitude in similar length control run segments
   - Basis for a test of the strength of the signal in the observations

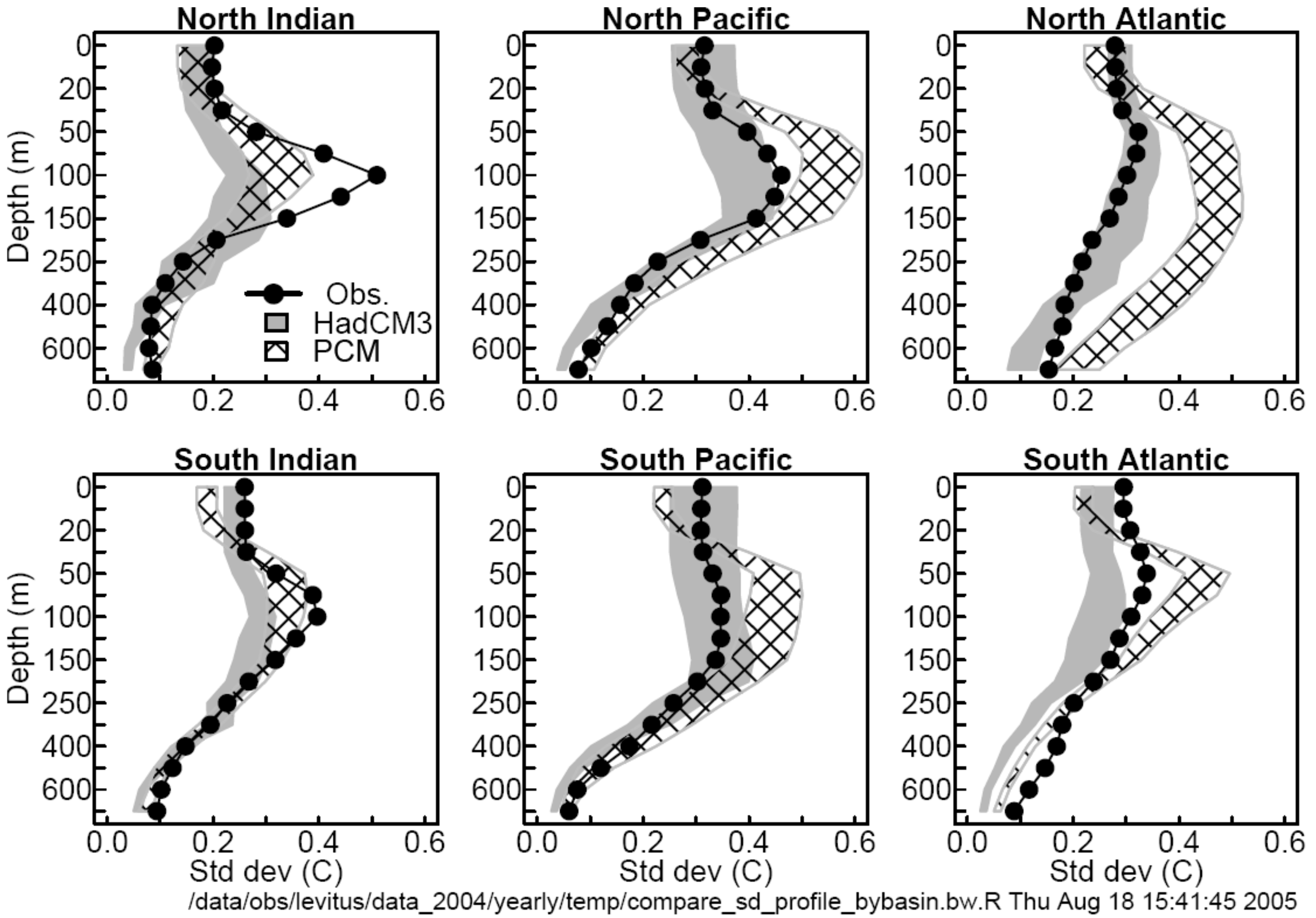
- Note that model output is processed to match observations
   - it is masked to be "missing" where/when observations are missing, etc.
   - the fact that data are missing may have some impact … we want to be sure we are not detecting an "aliased" signal

5. Demonstrate that alternative signals are unlikely to be able to explain observed change

Non-optimal approach

- Some recent studies taking this approach include
  - Barnett et al, 2005; Pierce et al., 2006
    - anthropogenic influence on ocean temperature structure
  - Santer et al, 2007
    - SSTs in tropical cyclone formation regions
  - Barnett et al, 2008
    - western United States surface hydrology
    - temperature, snow pack and stream flow combined
  - Marvel and Bonfils, 2013
    - zonal distribution of global precipitation

Observed and simulated variability

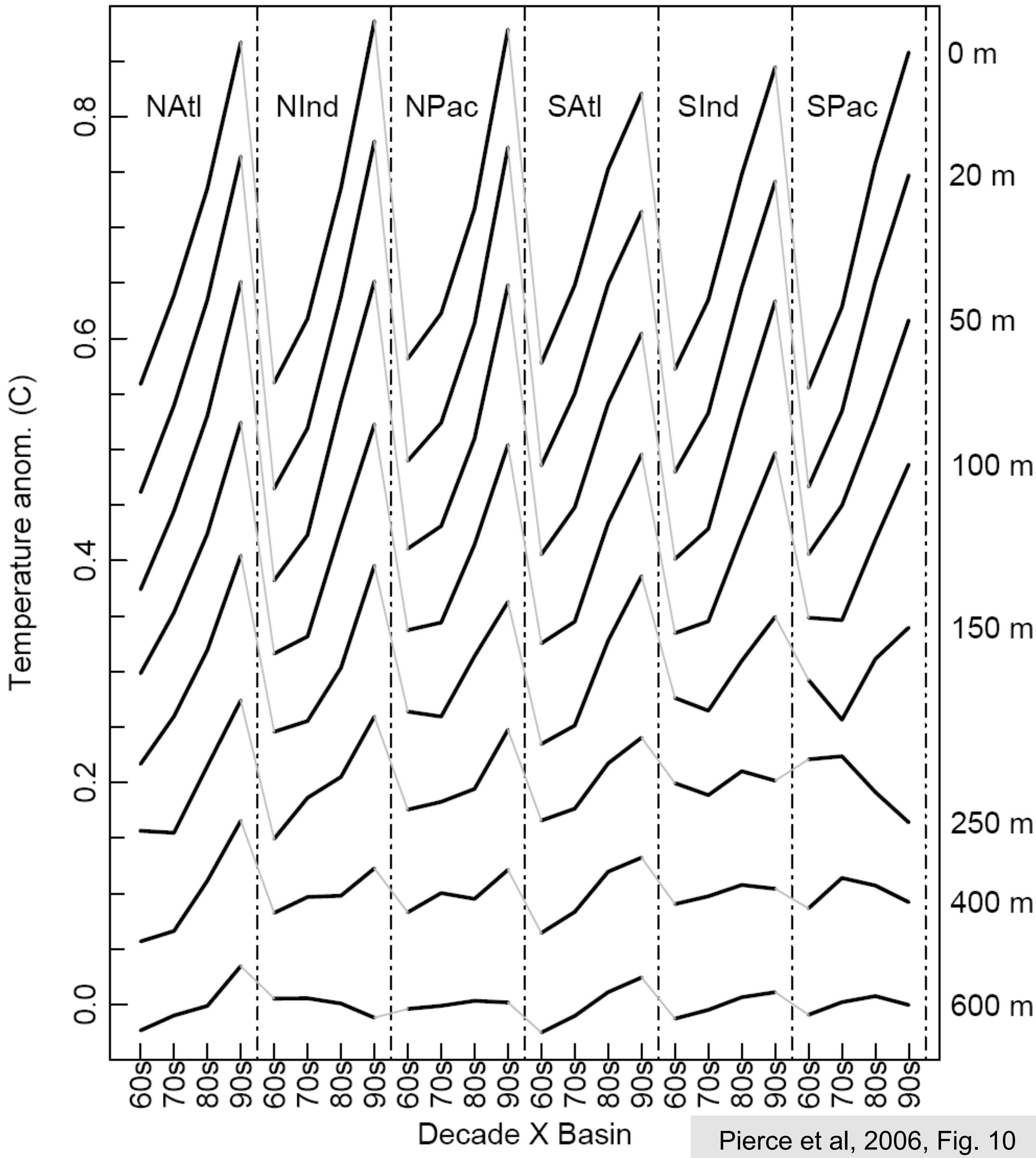


Basin averaged standard-deviation of temperature
(5-year time scale, masked)

Pierce et al, 2006, Fig. 3

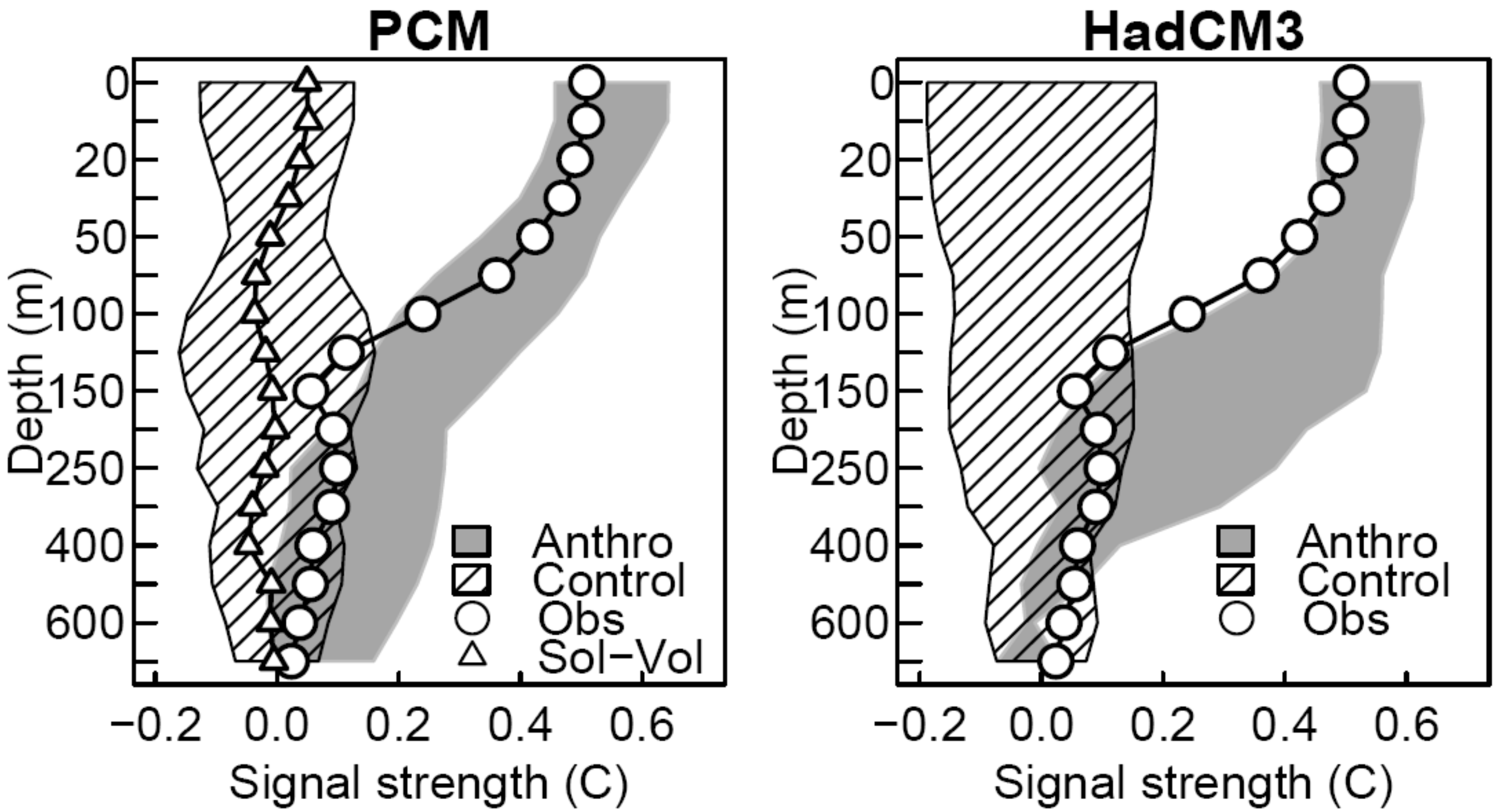
Signal pattern

- Model-simulated temperature changes (by level and ocean basin)
- PCM and HadCM3 combined
- 1960s-1990s
- By basin
- Masked
- Scales offset by 0.1°C



Pierce et al, 2006, Fig. 10

Signal Amplitude



- Using common model fingerprint
- 90% confidence bands are shown

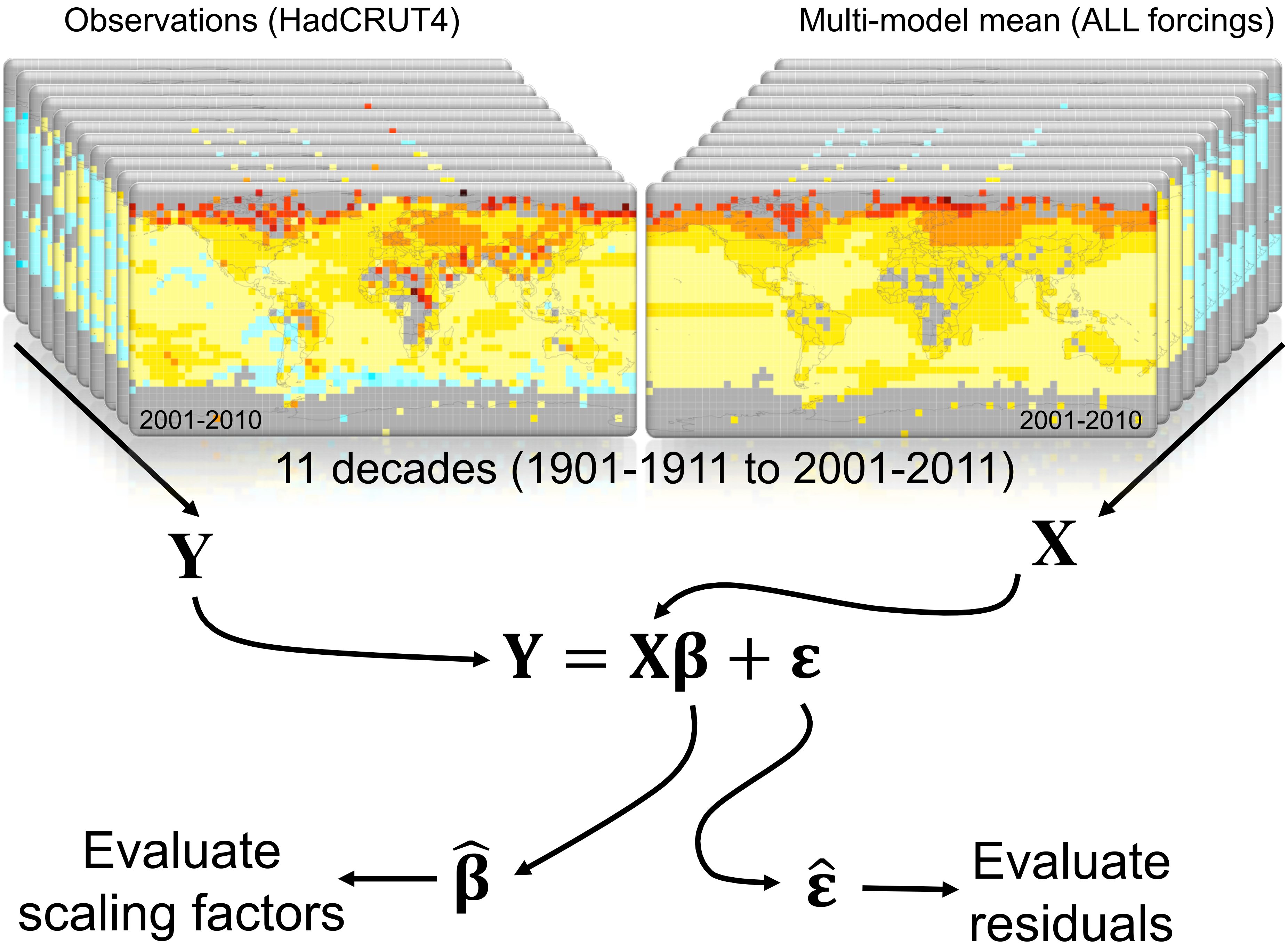
Pierce et al, 2006, Fig. 11

Optimal D&A Approaches

Optimal approach

- Originally developed in a couple of different ways
  - Optimal filtering (North and colleagues, early 1980's)
  - Optimal fingerprinting (Hasselmann,1979; Hegerl et al, 1996; 1997)

- Variants of linear regression
  - Ordinary least squares / Generalized least squares (Allan and Tett, 1999)
  - Total least squares (Allan and Stott, 2003, Ribes et al, 2009, 2012a,b)
  - Errors in variables (Huntingford et al, 2006, Hannart et al, 2014)



Observations (HadCRUT4)
Multi-model mean (ALL forcings)
2001-2010
2001-2010
11 decades (1901-1911 to 2001-2011)
Y
X
Y = Xβ + ε
β̂
ε̂
Evaluate scaling factors
Evaluate residuals

$$\mathbf{Y} = \sum_{i=1}^{s} \beta_i \mathbf{X}_i + \boldsymbol{\varepsilon} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

$\mathbf{Y}$ → Observations

$\mathbf{X}$ → Expected changes – one vector for each "signal"

β → Regression coefficients – aka "scaling factors"

ε → Residuals – internal variability

Idea is to interpret the observations with a regression model, where physics is used to provide representations of expected changes due to external influences, statistics is used to demonstrate a good fit, and physics is used to interpret the fit and rule out other putative explanations

Key statistical questions relate to the β_i's and residuals ε

$$\mathbf{Y} = \sum_{i=1}^{s} \beta_i \mathbf{X}_i + \boldsymbol{\varepsilon} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

Key assumptions

- Responses to forcings are additive
- Expected patterns of response in vectors $\mathbf{X}_i$ are correct
- Residuals ε_j, j=1, …, n are zero-mean
- … some more, discussed later

No assumptions about the "covariance structure" of the residuals

This is a "small sample" statistical inference problem (even if vector $\mathbf{Y}$ is big, covering essentially the globe and the entire instrumental period)

To fit, chose β to minimize $\left\|\mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}}\right\|_{\boldsymbol{\Sigma}}^{2}$

where $\|\mathbf{Z}\|_{\boldsymbol{\Sigma}}^{2} = \mathbf{Z}^{T}\boldsymbol{\Sigma}^{-1}\mathbf{Z}$

That is, we have a choice as to how we measure distance ….

$$\Sigma = \mathrm{I}$$

← Simple least squares, non-optimal

$$\Sigma = diag(\sigma_1^2, \ldots, \sigma_n^2)$$

← Weighted least squares, partially optimized

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \cdots & \sigma_{1,n} \\ \vdots & \ddots & \vdots \\ \sigma_{n,1} & \cdots & \sigma_n^2 \end{pmatrix}$$

← Generalized linear regression, fully optimized

Minimizing $\left\|\mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}}\right\|_{\boldsymbol{\Sigma}}^{2}$ yields

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

Let $\boldsymbol{\Sigma} = \mathbf{P\Lambda P}^t$ where $\boldsymbol{\Lambda} = \boldsymbol{diag}(\boldsymbol{\lambda_1}, \ldots, \boldsymbol{\lambda_n})$

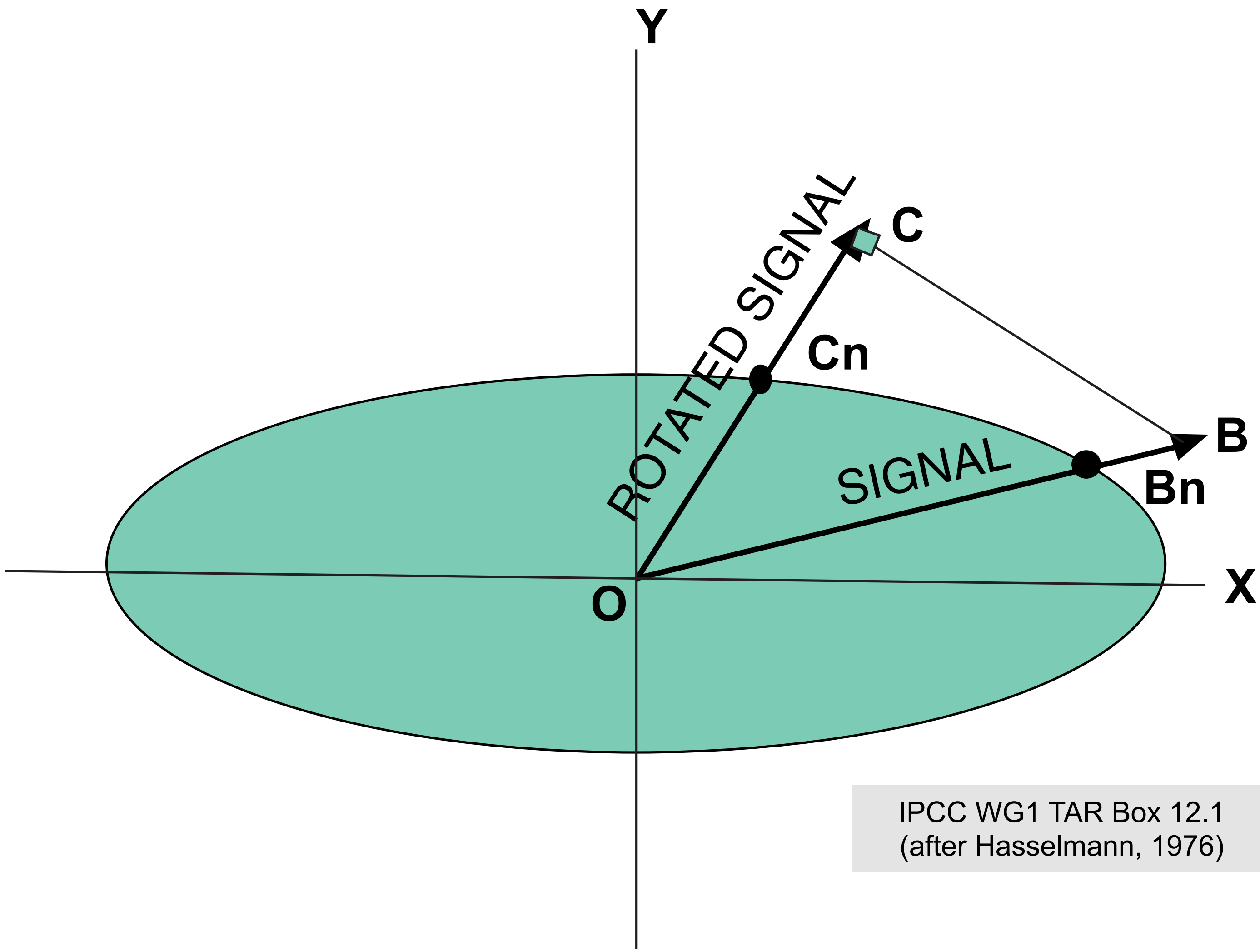
Then $$\widehat{\boldsymbol{\beta}} = (\mathbf{X}^t\mathbf{P}\boldsymbol{\Lambda}^{-1}\mathbf{P}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{P}\boldsymbol{\Lambda}^{-1}\mathbf{P}^t\mathbf{Y}$$
$$= (\acute{\mathbf{X}}^t\acute{\mathbf{X}})^{-1}\acute{\mathbf{X}}^t\acute{\mathbf{Y}}$$

Where $$\acute{\mathbf{X}} = \boldsymbol{\Lambda}^{-1/2}\mathbf{P}^t\mathbf{X}$$
$$\acute{\mathbf{Y}} = \boldsymbol{\Lambda}^{-1/2}\mathbf{P}^t\mathbf{Y}$$

Thus the signals $\mathbf{X}$ and observations $\mathbf{Y}$ are being rotated and scaled

Optimization

- maximize S/N ratio by projecting observations onto the signal component that is least affected by noise



IPCC WG1 TAR Box 12.1
(after Hasselmann, 1976)

Applying the simple OLS form

Observations $\mathbf{Y}$

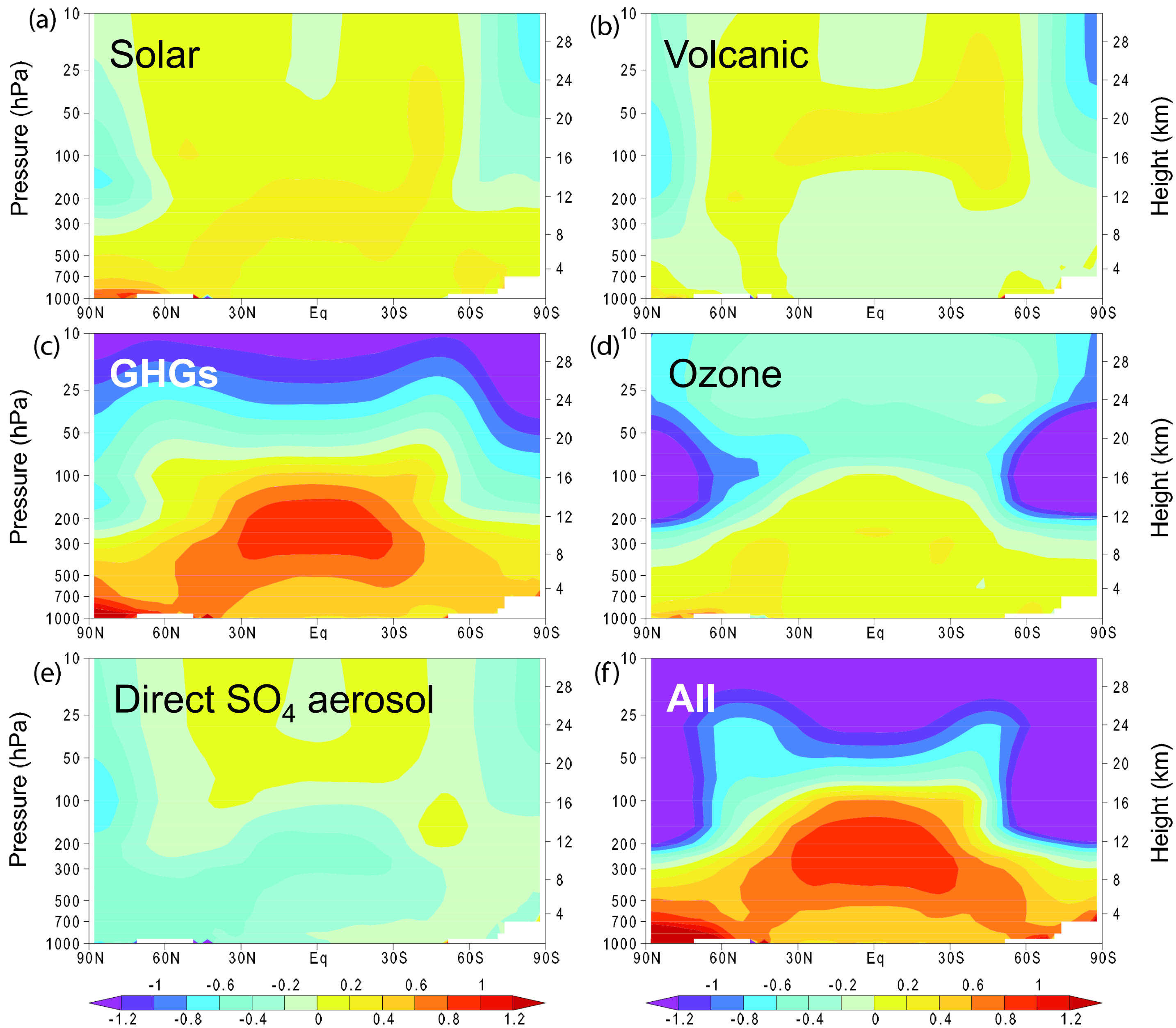
- Most studies of surface air temperature use
  - decadal averages and some kind of spatial averaging
    - To reduce noise from internal variability
    - To reduce the dimension of $\mathbf{Y}$
- Recent studies (e.g., Jones et al, 2013) use
  - Gridded (5°×5°) monthly mean surface temperature anomalies (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
  - $\mathbf{Y}_{n\times 1}$ therefore has dimension n=11×25=275

Signals $\mathbf{X}_i$, $i=1, \ldots, s$

- 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 $\widehat{\boldsymbol{\Sigma}}$

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

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

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

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

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

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

Further constraint on estimating Σ

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

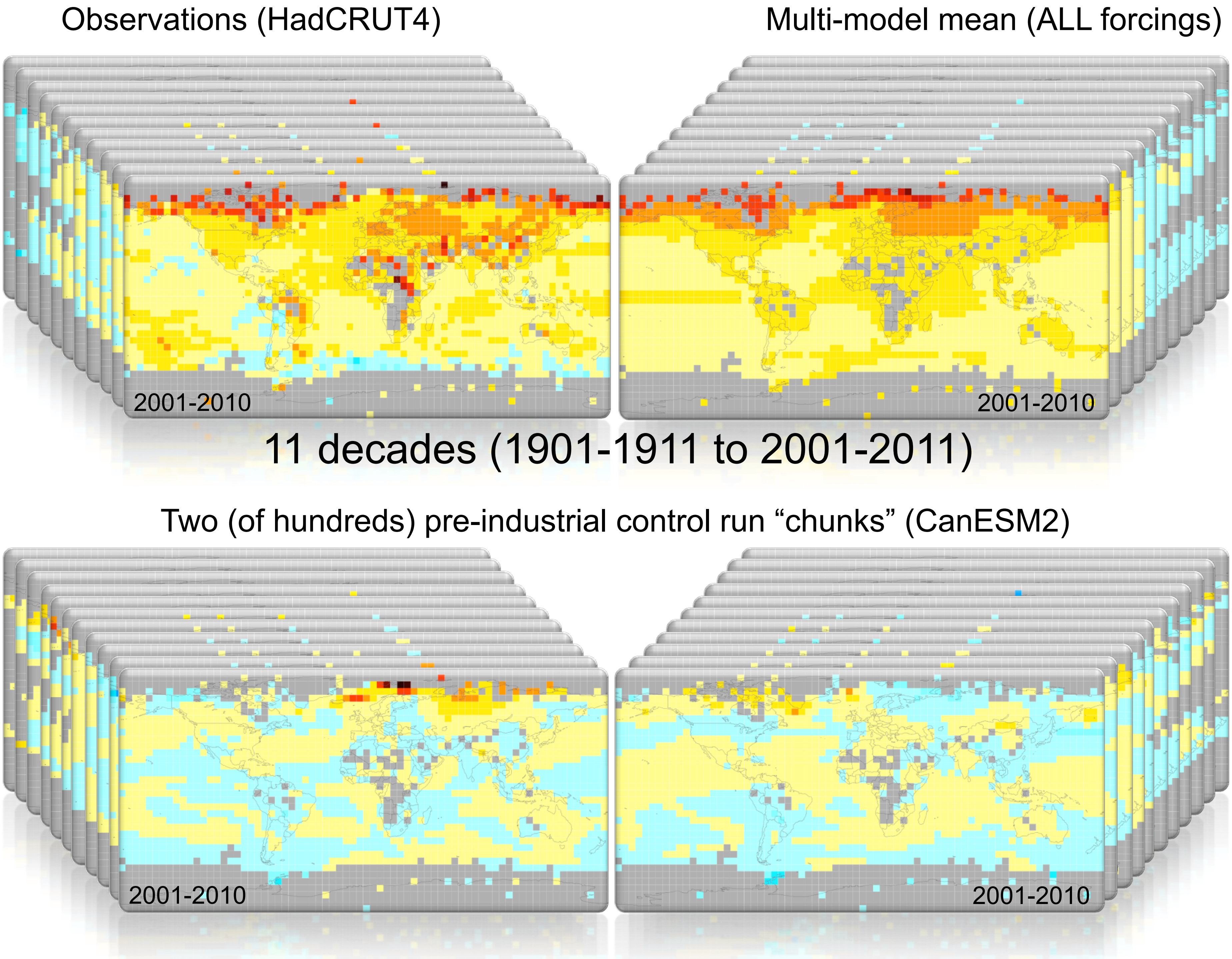
– An estimate $\hat{\boldsymbol{\Sigma}}_{\mathbf{2}}$ to make estimate uncertainties and make inferences

- Residuals from the regression model, $\hat{\boldsymbol{\varepsilon}} = \mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}$ 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 $\widehat{\boldsymbol{\Sigma}}_{\mathbf{1}}$

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

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

   - 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)

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

- Note that this is conditional on $\widehat{\boldsymbol{\Sigma}}_{\mathbf{1}}$ (i.e., it ignores sampling variability in the optimization, Allen and Stott, 2003).

- Ribes et al (2012a) show that

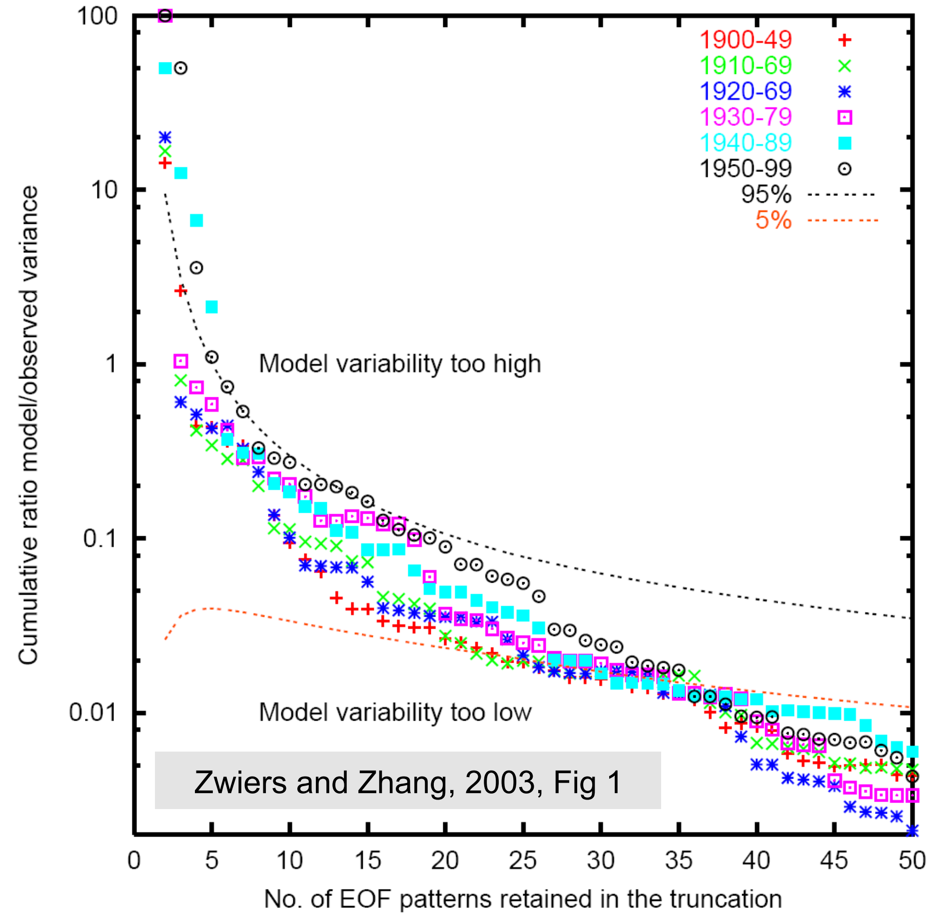
$$\hat{\boldsymbol{\varepsilon}}^t \widehat{\boldsymbol{\Sigma}}_{\mathbf{2}}^{-\mathbf{1}} \hat{\boldsymbol{\varepsilon}} \sim \frac{v_2(k-s)}{v_2-k+1} F_{k-s, v_2-k+1}$$

provides a better approximation for the residual consistency test

Basic procedure …

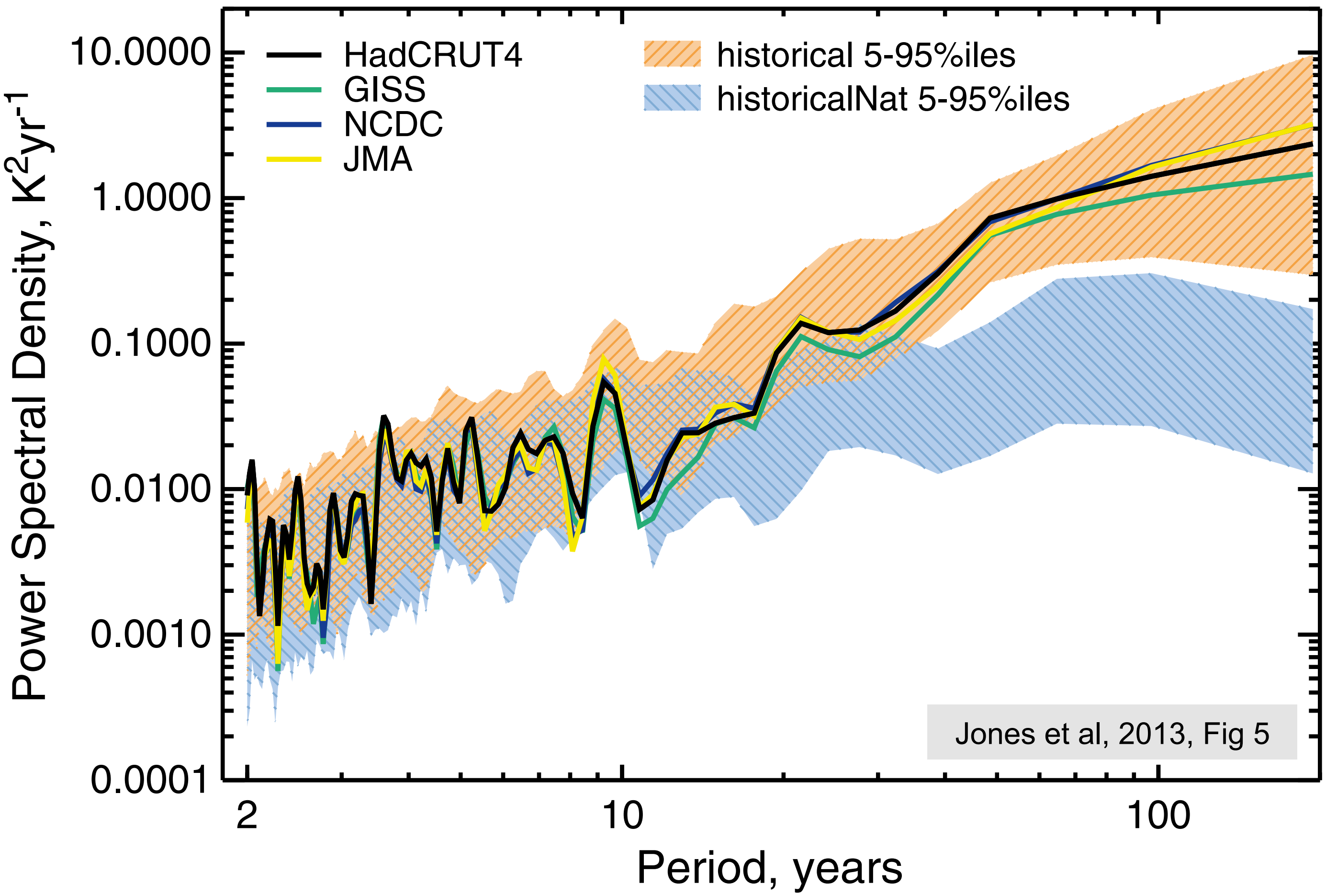
7. Determine EOF truncation point via residual consistency test

   – 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



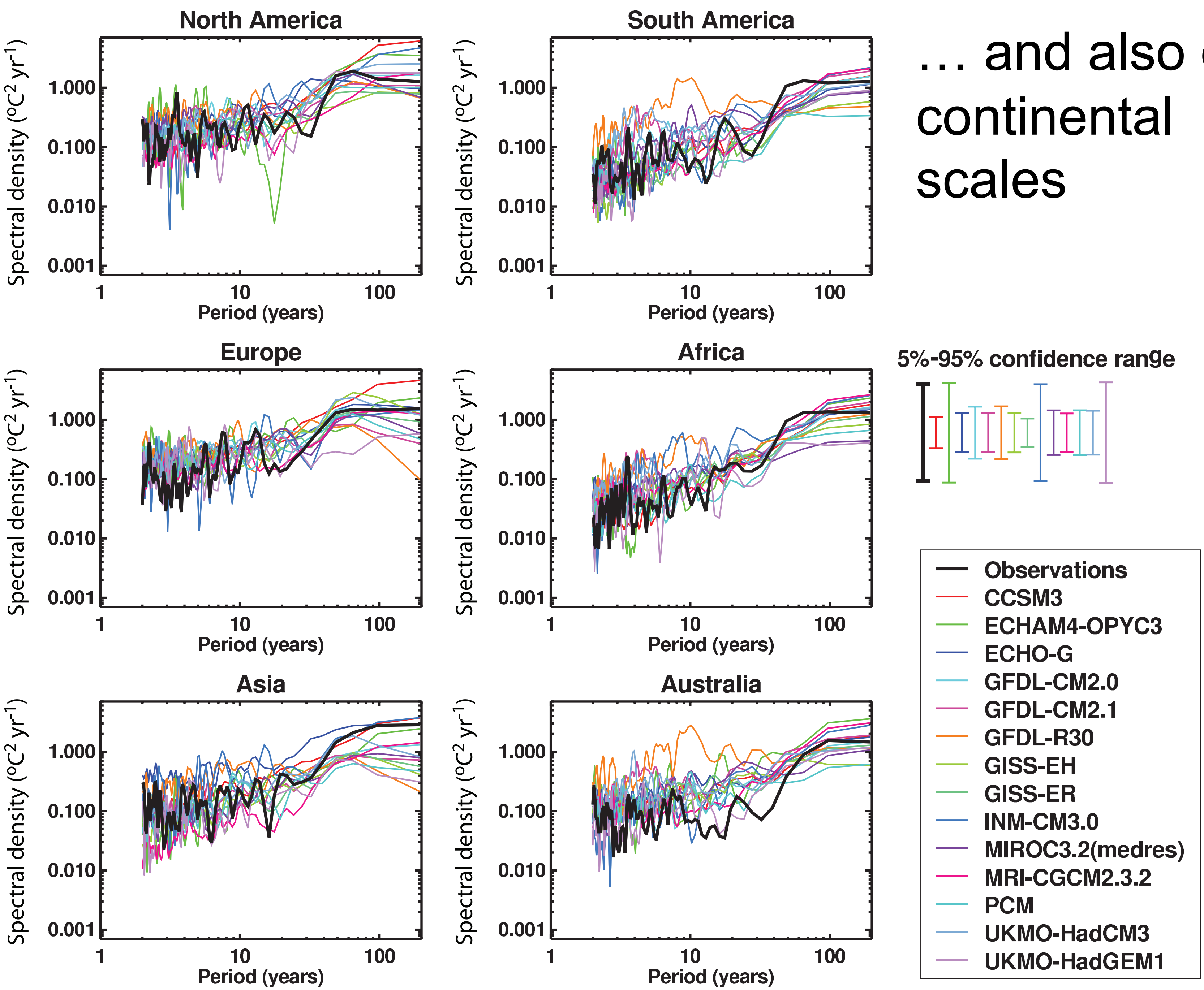
$$\hat{\boldsymbol{\varepsilon}}^t \hat{\boldsymbol{\Sigma}}_2^{-1} \hat{\boldsymbol{\varepsilon}} \sim (k-s) F_{k-s, v_2} \approx \chi^2_{k-s}$$

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 ….

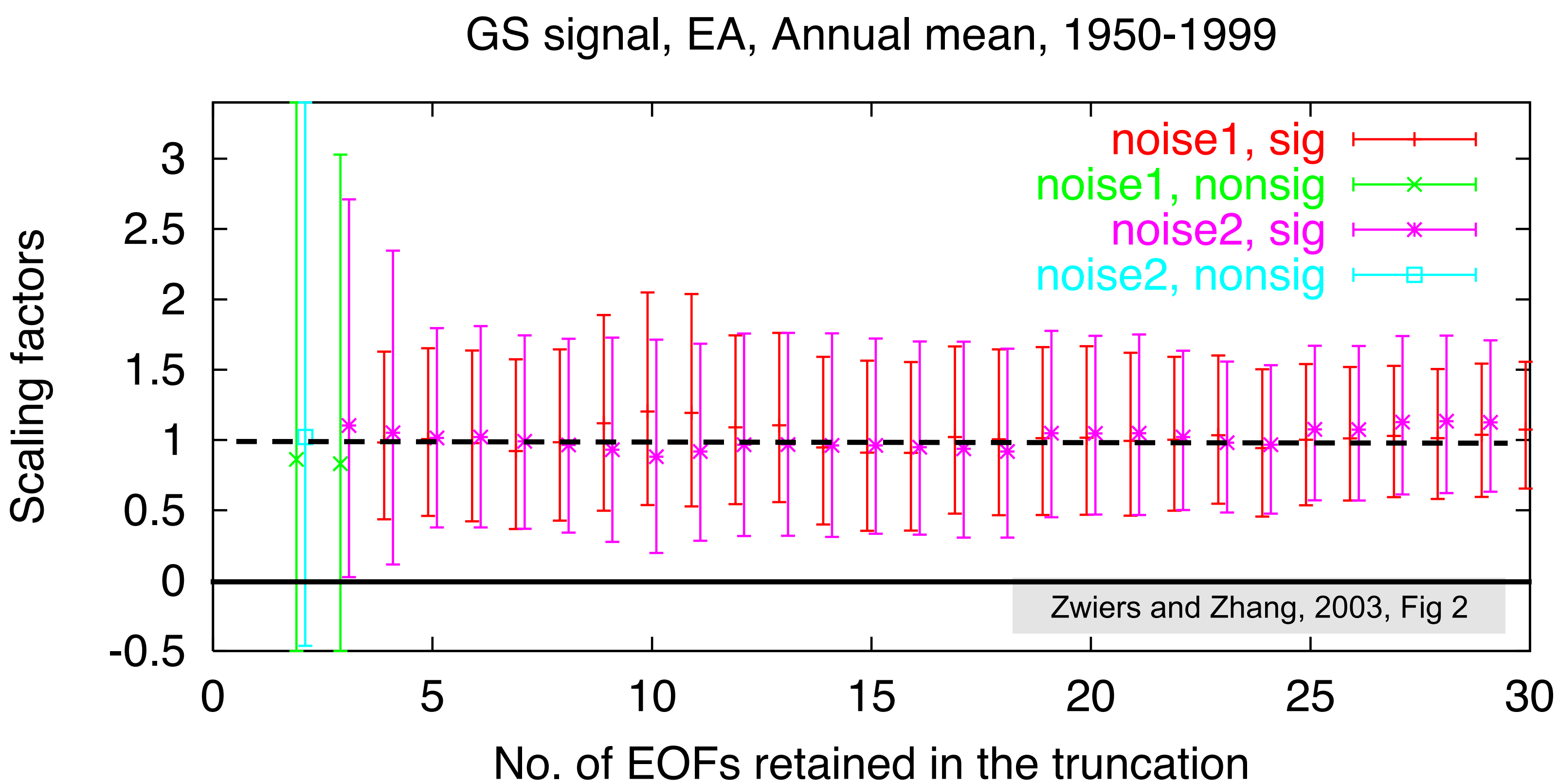
8. Make inferences about scaling factors

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

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

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



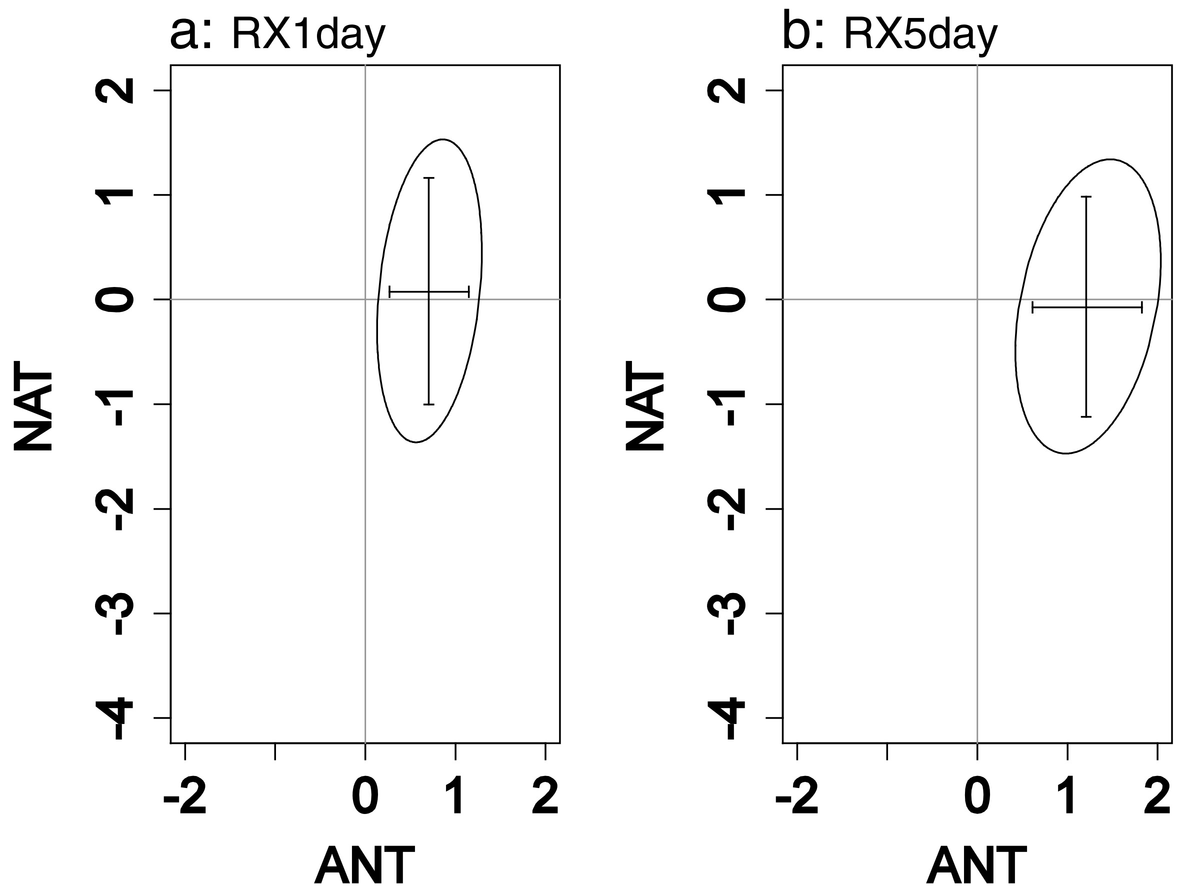
Detection of "GS" signal in Eurasian surface air temperature

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



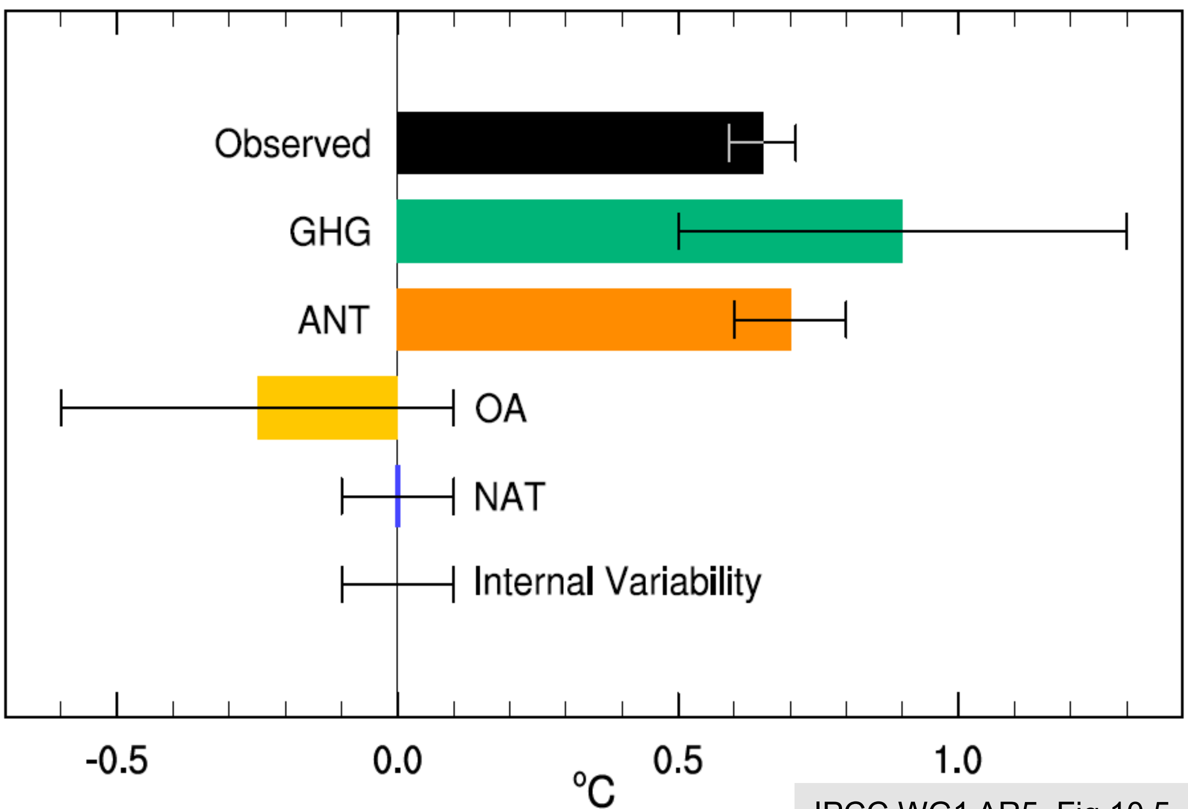
Zhang et al, 2013, Fig. 2

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

Do we really know the signal perfectly, and how do proceed if we don't know it completely?

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 $\Sigma_{\delta\delta} = \dfrac{1}{m_i}\Sigma_{\varepsilon\varepsilon}$

That is, we assume that the $\delta_{i,j}$'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 β that minimize the "size" of the n×(s+1) matrix of residuals $[\Delta, \varepsilon]$

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

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

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

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

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

Aside – the problem of minimizing

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

is entirely parallel to the generalized linear regression problem.

For OLS we take $\widehat{\mathbf{X}}^{Forced} = \widetilde{\mathbf{X}}$

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

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

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

Statistical Inferences under TLS

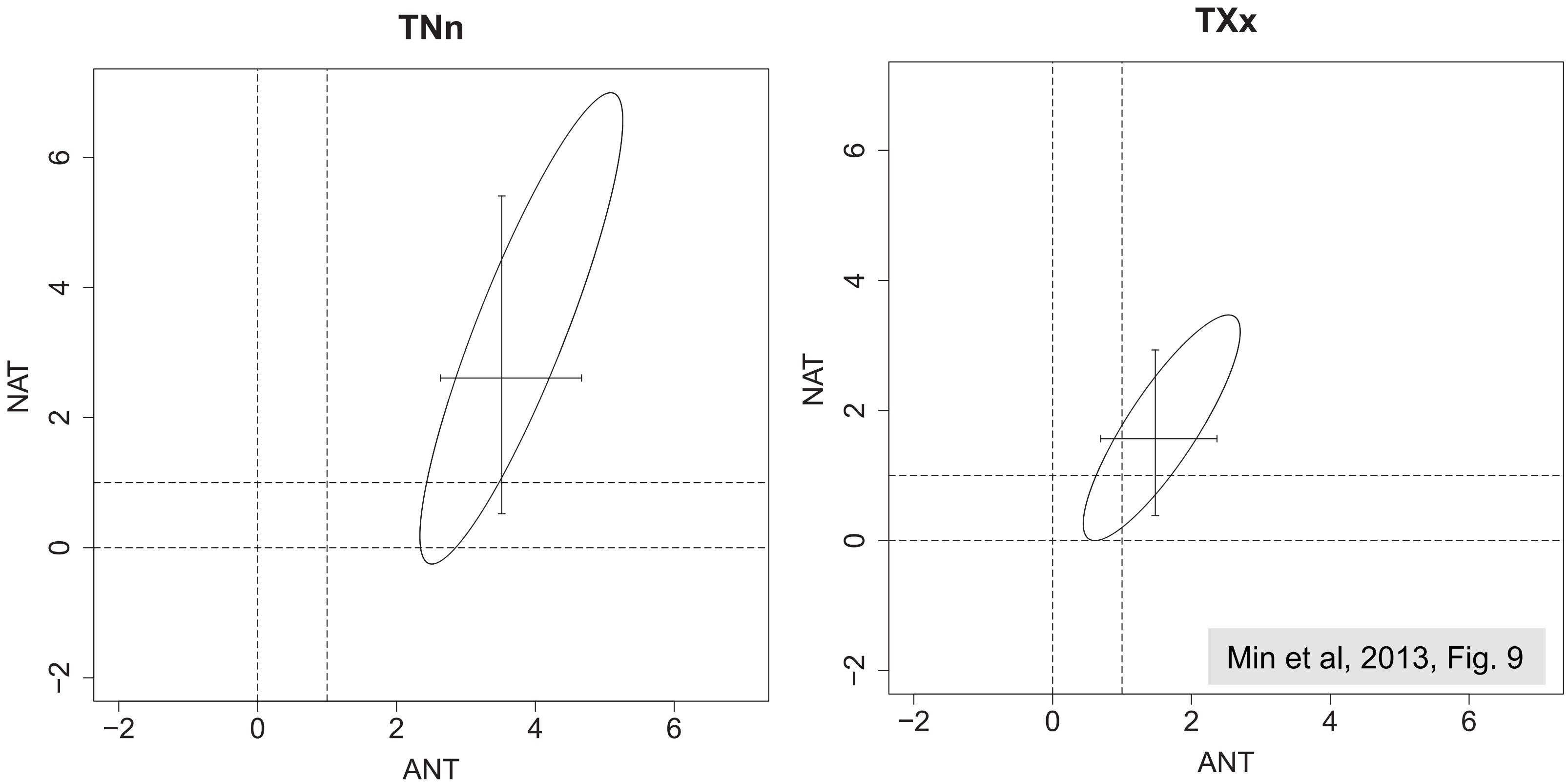
- Residual consistency test
  - Exact distribution not available analytically because the estimation problem is non-linear
  - Approximate distribution suggested by Allen and Stott (2003) is

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

  - 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 $\psi_{\tilde{\boldsymbol{\beta}}} = \hat{\boldsymbol{\varepsilon}}_{\tilde{\boldsymbol{\beta}}}^{t}\widehat{\boldsymbol{\Sigma}}_{\mathbf{2}}^{-\mathbf{1}}\boldsymbol{\varepsilon}_{\tilde{\boldsymbol{\beta}}} - \hat{\boldsymbol{\varepsilon}}^{t}\widehat{\boldsymbol{\Sigma}}_{\mathbf{2}}^{-\mathbf{1}}\hat{\boldsymbol{\varepsilon}} \sim sF_{s,v_2}$
  - 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 Σ 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

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

- 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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