Computational Approaches for Parameter Estimation in Climate Models

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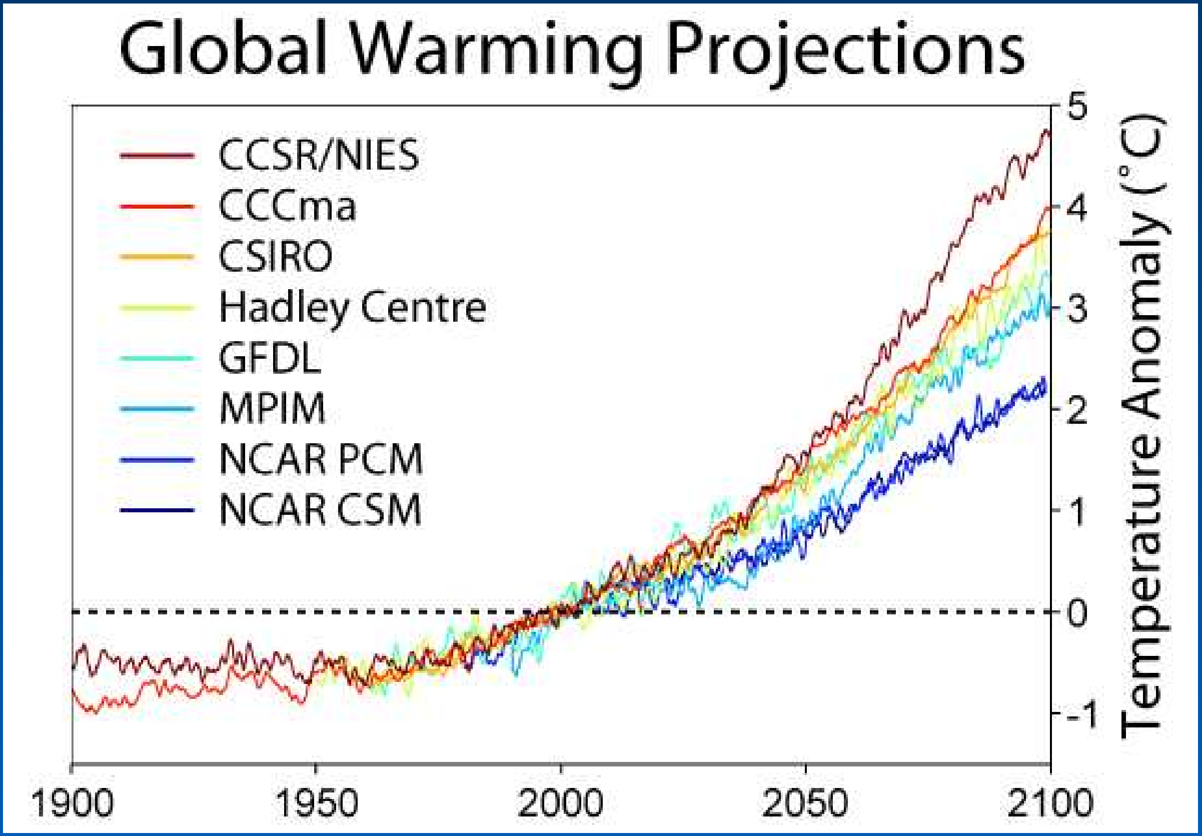
Summary Points

- Parametric uncertainties in climate modeling.
- Estimation of multidimensional probability distributions.
- Climate model, proxy or surrogate to a full ACGM.
- Simulated Annealing based method (MVFSA).
- Adaptive Metropolis as an alternative.
- Comparisons of posterior probability distributions.


Global Warming Projections
CCSR/NIES
CCCma
CSIRO
Hadley Centre
GFDL
MPIM
NCAR PCM
NCAR CSM
Temperature Anomaly (°C)
5
4
3
2
1
0
-1
1900
1950
2000
2050
2100

Comments on Climate Models

- IPCC Third Assessment Report (TAR, 2001): Global temperatures are likely to increase by 1.1 to 6.4°C 1990-2100.
- "more comprehensive and systematic system of model analysis and diagnosis, and a Monte Carlo approach to model uncertainties associated with parameterizations" .
- Recent progress with models of reduced complexity (Forest et al., 2000, 2001, 2002).
- Perturbed physics ensembles with a general circulation model (Allen, 1999; Murphy et al, 2004; Stainforth et al., 2005; Collins et al., 2006).

Range of Model Hierarchies

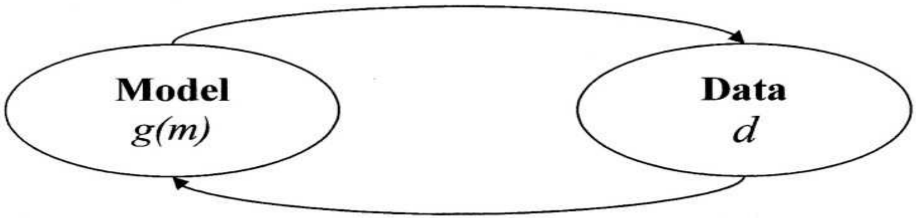
- *General Circulation Models:* Most demanding.
  - 16 processors/24 hours to simulate 10 years of climate.
- *Models of Reduced Complexities:* One or more spatial dimensions are eliminated.
- *Surrogate or Emulator Models:*
  - Mimics equilibrium space-time response of an Atmospheric GCM.
  - To test sampling strategies for parametric uncertainties.

Goals of Present Study

- Estimate probability distributions for parameters in climate models.
- Non-standard methods for state-of-art in the climate literature.
- Improve on the calibration of the climate model.
- "appreciate the ability to detect and attribute the effects of forcings on paleoclimate observations".
- Bayesian approach via posterior distributions.

Forward Problem

g(m)=d



Inverse Problem

m = ?, given d

↕

Bayes Theorem:

$$P(m|d) = \frac{P(d \mid m)P(m)}{\int P(d \mid m)P(m)dm}$$

Surrogate Climate Model

- Jackson and Broccoli (2003): "Changes in Earth's orbital geometry over the past 165kyears".
- Obliquity $\Phi \in (22^\circ, 25^\circ)$, eccentricity, $e \in (0, 0.05)$ and longitude of perihelion, $\lambda \in (0^\circ, 360^\circ)$.
- $d_{obs}(i, j, k)$ is the observed surface temperature at latitude i, longitude j and season k.
- Data simulated using $\Phi = 22.62$, $e = 0.044$, $\lambda = 75.93$.
- $d_{obs}(i, j, k) = g_{ijk}(m) + \eta_{ijk}$, where $m = (\Phi, e, \lambda)$.
- g is the "surface air temperature" to a given change in parameters.

- The surrogate model is

$$g_{ijk}(m) = A_o\Phi' + eA_p cos(\phi_p - \lambda) + R_{ijk}$$

- $\Phi = \Phi_o + A_o\Phi'$, Φ_o is the mean obliquity.
- Φ' is the deviation of obliquity from its 165,000 year mean.
- ϕ_p is the phase of the response to precessional forcing.
- R_{ijk} is a term that is added to represent the effects of internal variability.
- A_o and A_p are the sensitivity of temperature to changes in obliquity and precession respectively.

Cost or Misfit Function

- Measure of the deviation from the observed data and the model.
- For the climate model considered,

$$E(m) = \frac{1}{2N} \sum_{i=1}^{I} \sum_{j=1}^{J} \sum_{k=1}^{K} B_{ijk}^{-1} (d_{obs}(i,j,k) - g_{ijk}(m))^2$$

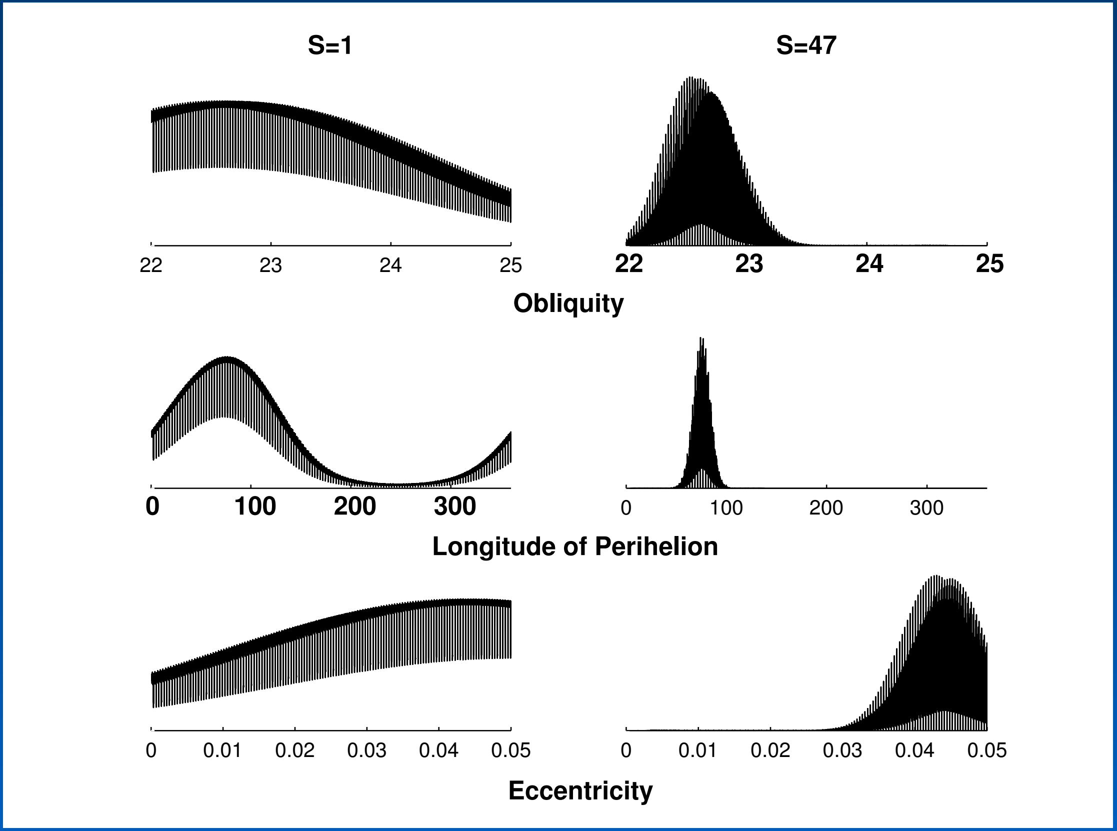
- B_{ijk} is the variance of the observations at each grid point.
- Other functions under study.

- The likelihood function is

$$L(d_{obs}|m, S) \propto exp\{-SE(m)\}$$

- S weights the significance of model-data differences.
- We fixed $S = 1$, $S = 47$ and plot a *profile* likelihood for each parameter.
- Simulation values ($\Phi = 22.625$, $e = 0.043954$, $\lambda = 75.93$).
- 20,000 point grid evaluation.

Likelihood functions for each orbital parameter.

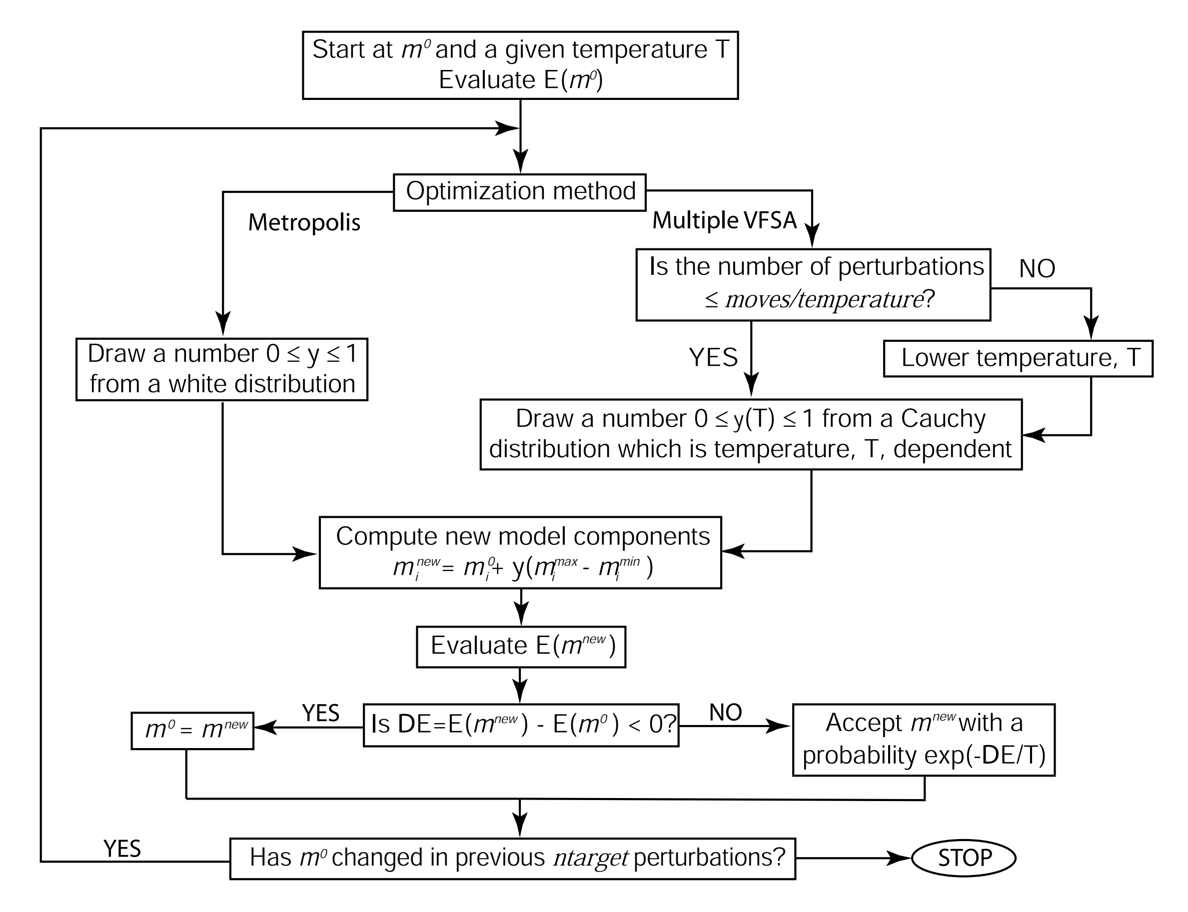


Multiple Very Fast Simulated Annealing

- Ingber (1989). Given a current selection $m_i^{(k)}$,

$$m_i^{(k+1)} = m_i^{(k)} + y_i(m_i^{max} - m_i^{min})$$

- $y_i \sim$ Cauchy distribution.
- Uses a cooling schedule $T_k = T_o exp(-\alpha(k-1)^{1/d})$
- One accepts or rejects $m_i^{(k+1)}$ according to a Metropolis scheme.
- Sen and Stoffa (1996), multiple repetitions.
- Balance between estimating a PPD and finding the global minimum.


Start at m^0 and a given temperature T
Evaluate E(m^0)
Optimization method
Metropolis
Multiple VFSA
Is the number of perturbations ≤ *moves/temperature*?
NO
YES
Lower temperature, T
Draw a number 0 ≤ y ≤ 1 from a white distribution
Draw a number 0 ≤ y(T) ≤ 1 from a Cauchy distribution which is temperature, T, dependent
Compute new model components
$m_i^{new} = m_i^0 + y(m_i^{max} - m_i^{min})$
Evaluate E(m^{new})
Is DE=E(m^{new}) - E(m^0) < 0?
YES
NO
$m^0 = m^{new}$
Accept m^{new} with a probability exp(-DE/T)
YES
Has m^0 changed in previous *ntarget* perturbations?
STOP

Adaptive Methods: Single Component AM

- $m_{i,k-1} = (m_i^{(0)}, ..., m_i^{(k-1)})$ are the sampled values for the *i-th* parameter.

- Variance equation $V_i^{(k)} = s_d V(m_{i,k-1}) + s_d \epsilon$ where

$$V(m_{i,k-1}) = \frac{1}{k-1} \sum_{r=0}^{k-1} (m_i^{(r)} - \overline{m}_i)^2$$

- Updating $m_i^{(k)}$ at iteration k,

  - $z_i \sim N(m_i^{(k-1)}, V_i^{(k)})$

– Accept z_i with probability

$$min\left(1, \frac{\pi(m_1^{(k)}, ..., m_{i-1}^{(k)}, z_i, m_{i+1}^{(k-1)}, ..., m_d^{(k-1)})}{\pi(m_1^{(k)}, ..., m_{i-1}^{(k)}, m_i^{(k-1)}, ..., m_d^{(k-1)})}\right)$$

- We produce samples $\pi(m, S|d_{obs})$.
- "Flat" priors on orbital forcing parameters. $S \sim$ Gamma distribution ($\alpha_0 = 552.25$,$\beta_0 = 11.75$).
- $\pi(m|S, d_{obs})$ is sampled through SC-AM.
- $\pi(S|m, d_{obs})$ is a Gamma $\alpha^* = \alpha_0$ and $\beta^* = \beta_0 + E(m^{(k)})$.

Adaptive Methods: FAM. (Haario et al. 2001)

- All parameters are sampled at once.
- $z \sim q_t(\cdot|m^{(0)}, ..., m^{(t-1)})$,
- z is accepted with probability,

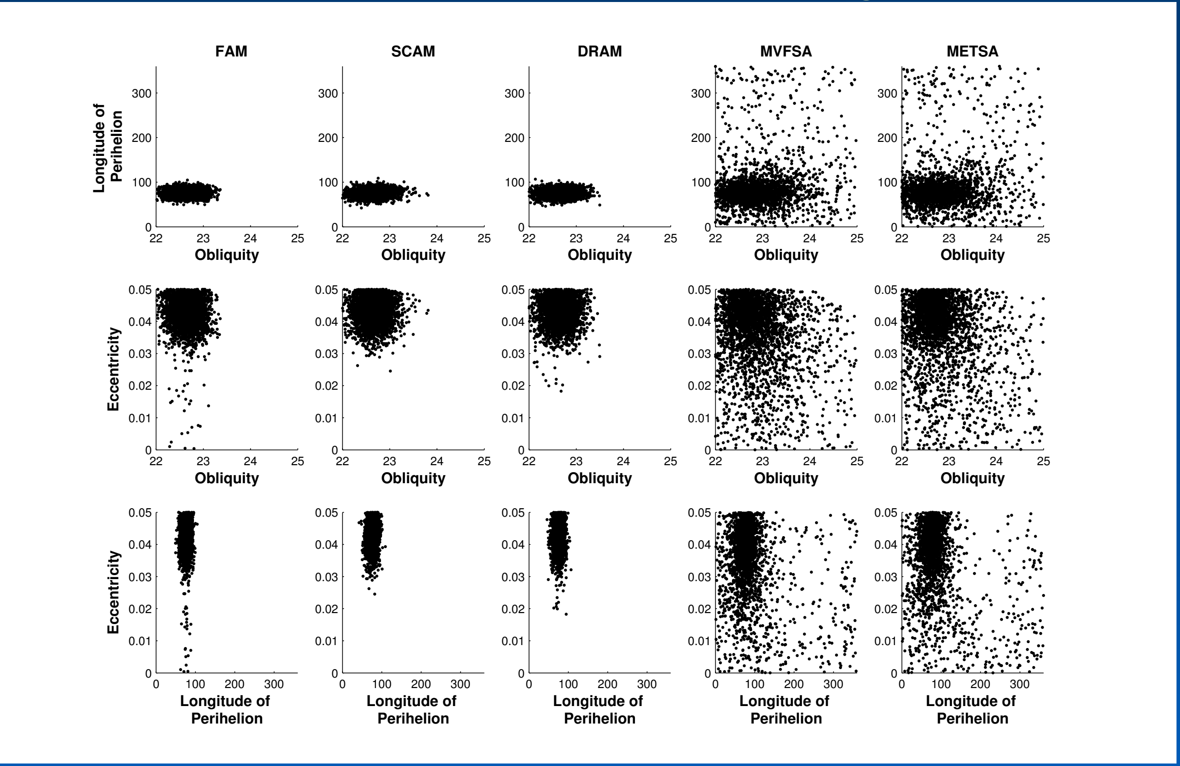
$$\alpha(m^{(t-1)}, z) = min\left(1, \frac{\pi(z)}{\pi(m^{(t-1)})}\right),$$

- $q_t(\cdot)$ is a multivariate Gaussian with mean $m^{(t-1)}$ and covariance matrix C_t.
- Recursively, $C_t = s_d C_{t-1} + s_d \epsilon I_d$, where $s_d > 0$ and $\epsilon > 0$

Adaptive Methods: DRAM (Haario and Mira 2006)

- Combines Delayed Rejection (DR) and Adaptive Metropolis.
- In DR, propose a second state move if first move was rejected.
- The process can be iterated for a fixed or random number.
- DR combines different proposals.
- May use for initial period (burn-in).
- The DR method uses rejected values without losing properties.

Bivariate scatter plots of orbital forcing parameters.



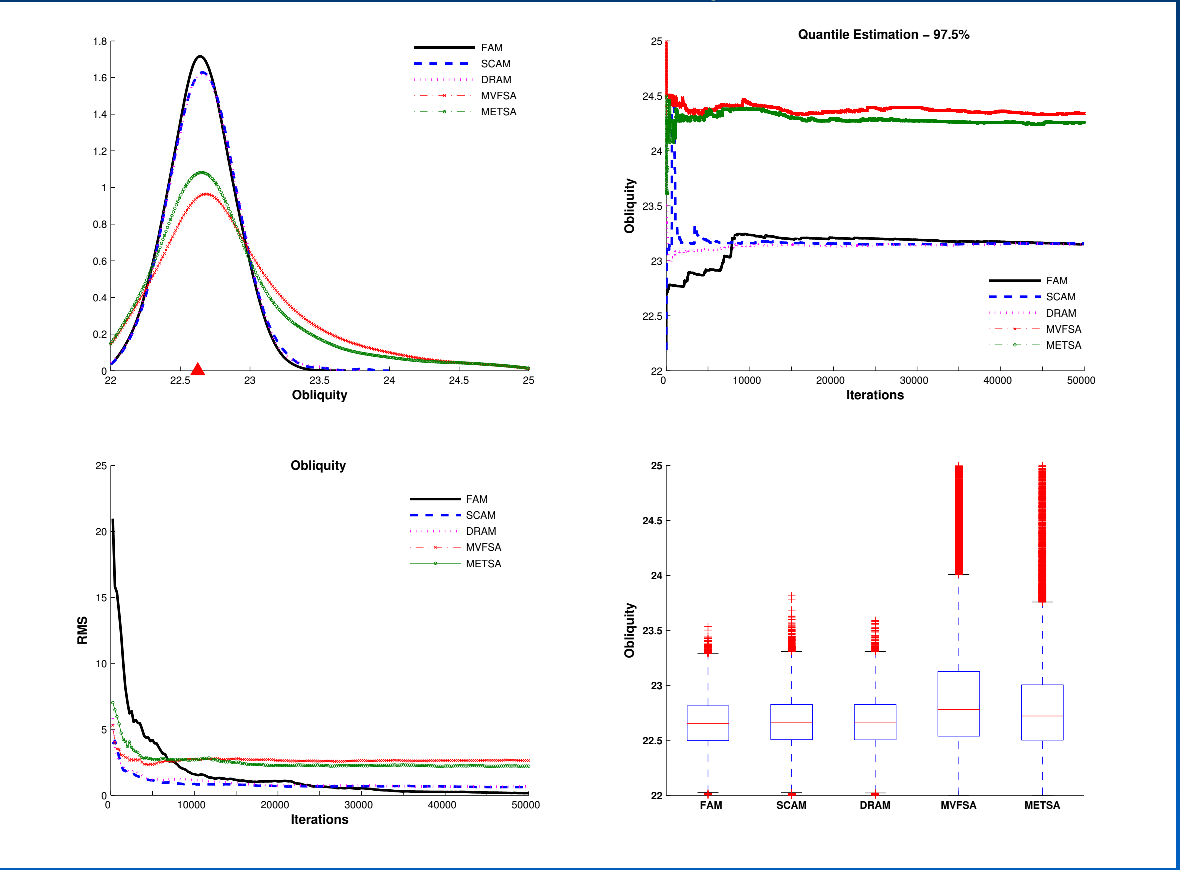
Root Mean Square (RMS) Probability Error

- For every parameter θ, :

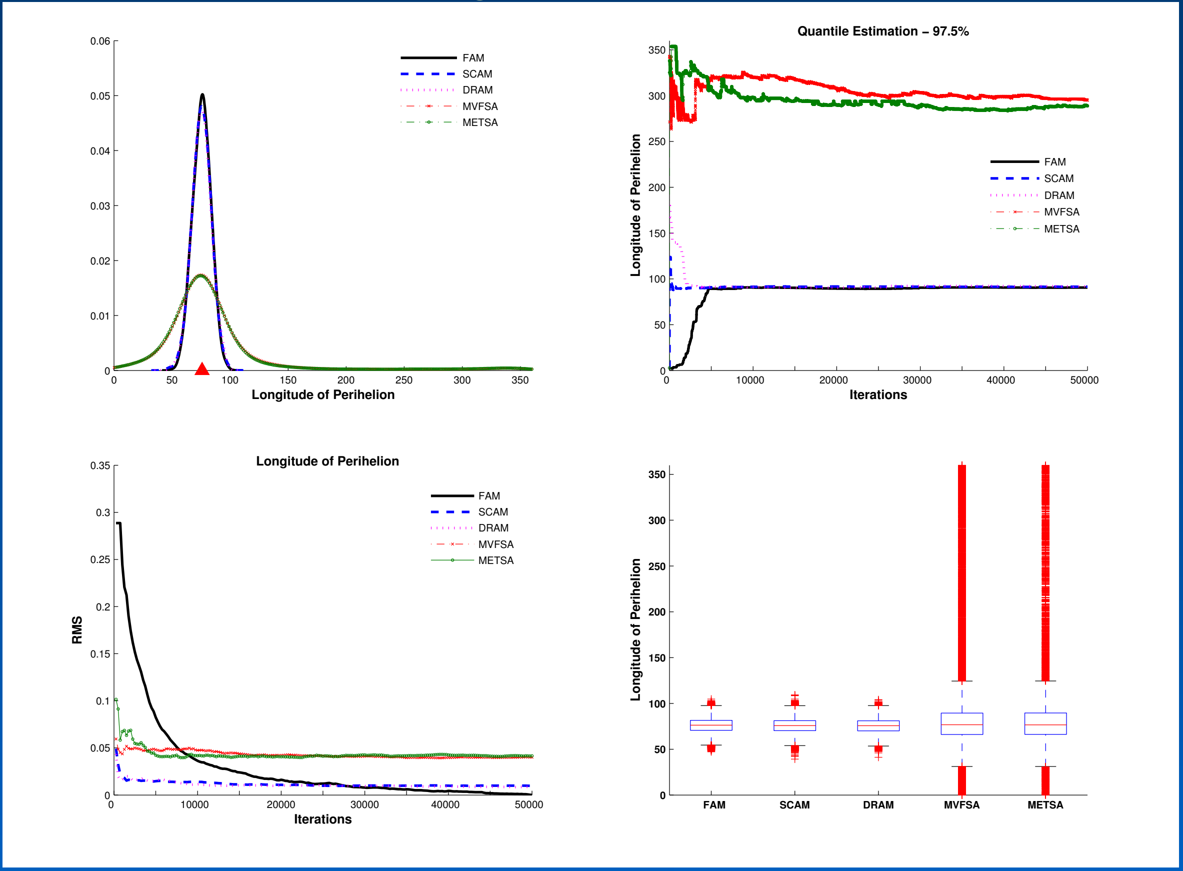
$$RMS_i(\theta) = ||Prob_i^{(\theta)} - Prob_\pi^{(\theta)}||$$

- $Prob_i^{(\theta)}$ is a vector of "bin probabilities" estimated from output at iteration i.
- $Prob_i^{(\theta)}$ probability vector under *target*.
- RMS goes to zero as i goes to infinity.
- $Prob_i^{(\theta)}$ from a *baseline* method.

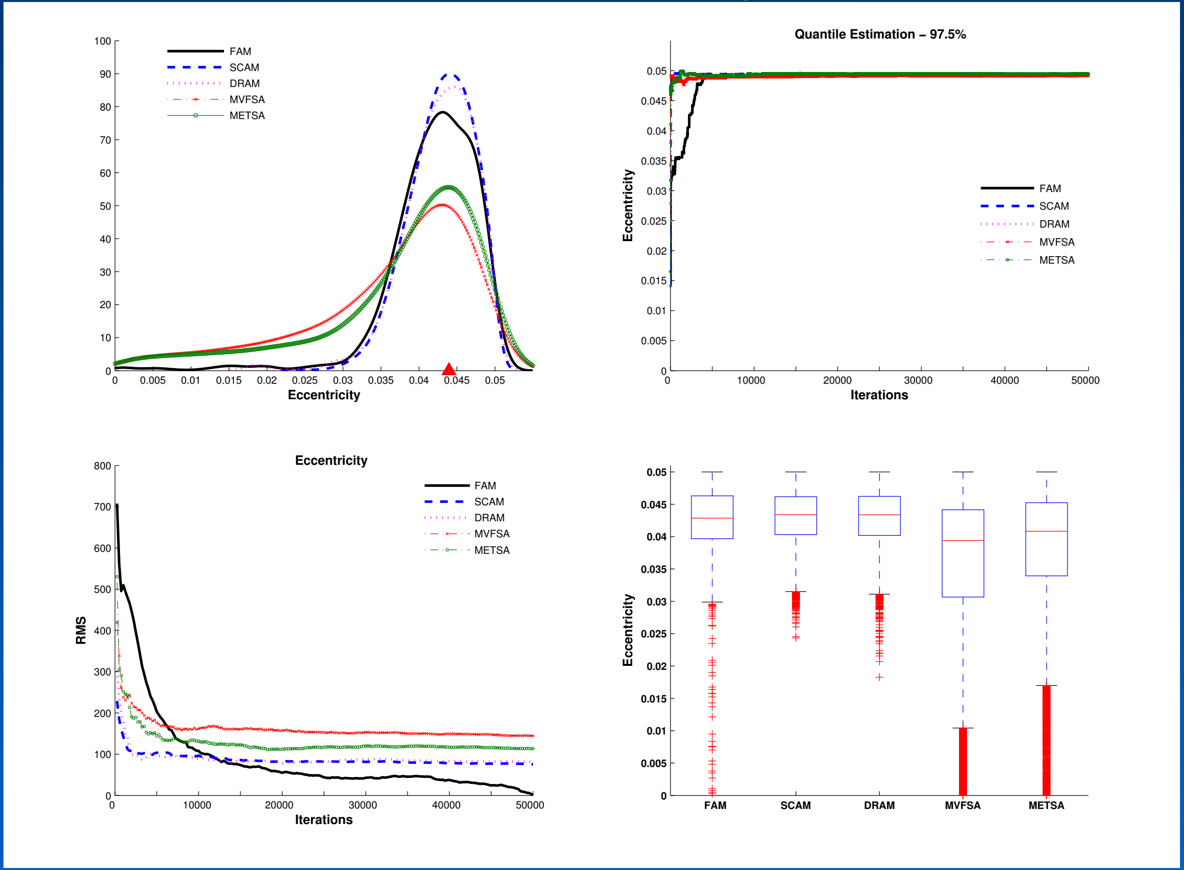
Comparison for Obliquity Parameter.



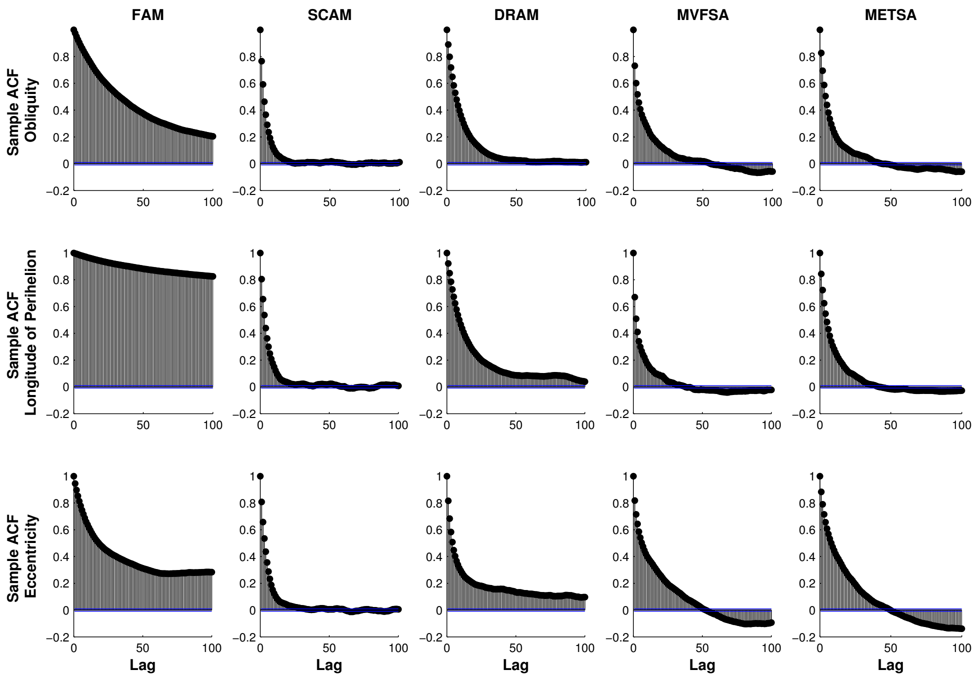
Comparison for Longitude of Perihelion Parameter.



Comparison for Eccentricity Parameter.



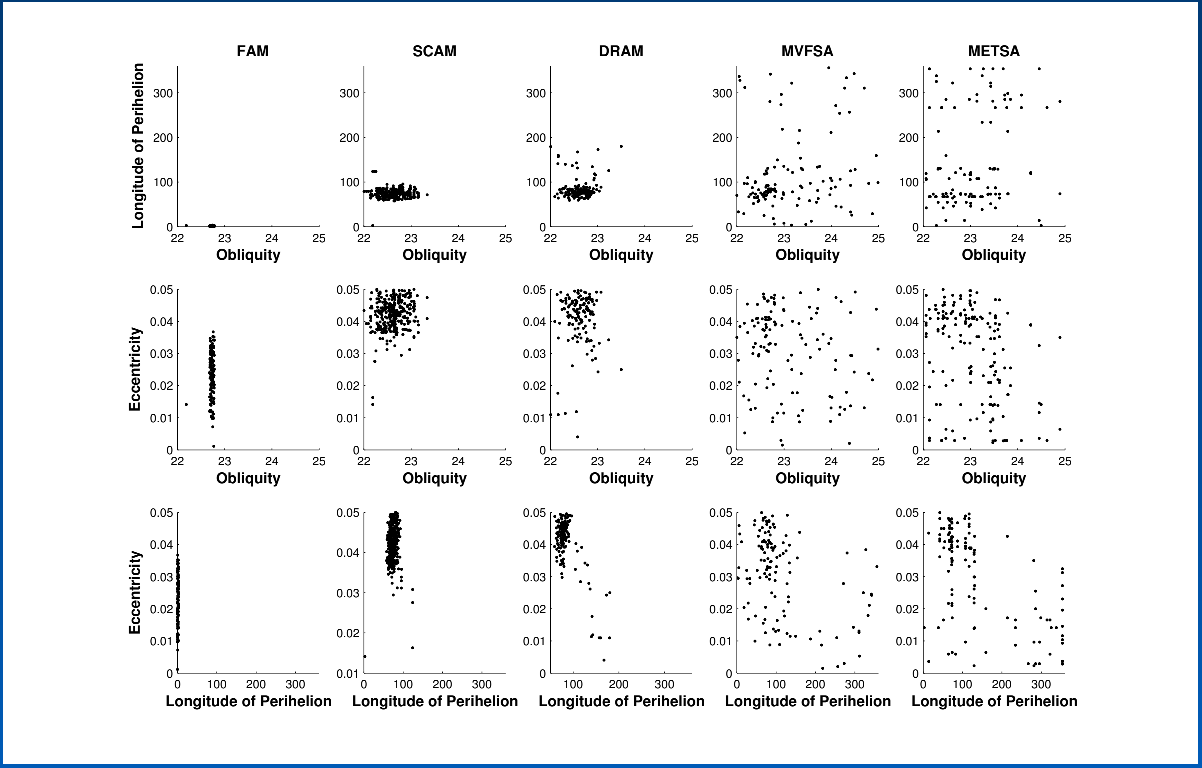
Autocorrelation function of orbital forcing parameters.



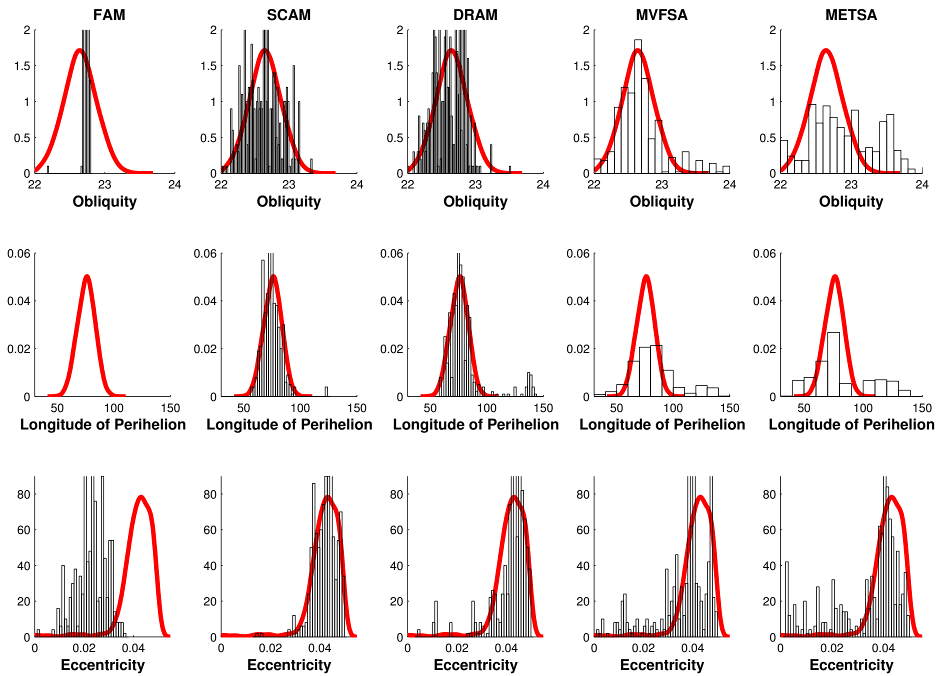
Appraisal of a few forward evaluations

- Impossible to evaluate methods using thousands of iterations.
- We evaluate the methods just with 500 iterations of the climate model.
- 500 is approximately the number of experiments currently performed on the CAM model by the Institute of Geophysics at the University of Texas-Austin.

Bivariate scatter plots with 500 iterations.



Histograms with 500 iterations.

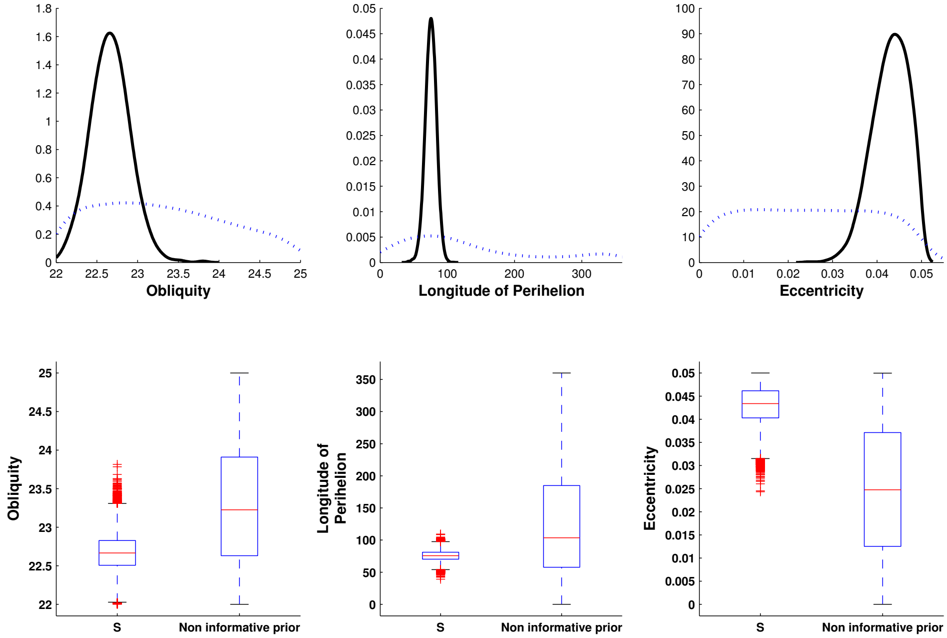


Comparative estimation with 500 evaluations.

Method	$\mathbf{E(m^*)}$	$\Phi_{2.5\%}$	$\Phi_{97.5\%}$	$\lambda_{2.5\%}$	$\lambda_{97.5\%}$	$e_{2.5\%}$	$e_{97.5\%}$
FAM	0.8411	22.6817	22.7813	0.2248	3.4413	0.0101	0.0331
SCAM	0.1912	22.1644	23.1309	60.6625	91.5434	0.0312	0.0495
DRAM	0.1943	22.1665	22.9816	62.7528	141.1550	0.0113	0.0491
MVFSA	0.2019	22.1595	24.5072	18.3329	311.9383	0.0089	0.0482
METSA	0.2029	22.0631	24.2744	38.6806	353.6220	0.0029	0.0481

- Optimal cost function values comparable except for FAM.
- 95 % probability intervals for MVFSA are wide compared to SCAM and DRAM.

Relevance of S parameter.



Final Thoughts

- MVFSA is a fast method to detect optima but has biases.
- DRAM, or SCAM provided nearly identical estimates of the marginal PPD.
- MVFSA has similar modes with broader credible intervals.
- Results mainly apply to unimodal posteriors.
- Model configurations that reflect uncertainties in model development.

* NSF support grant OCE-0415251

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