What drives the glacial-interglacial cycle? A Bayesian approach to a long-standing model selection problem

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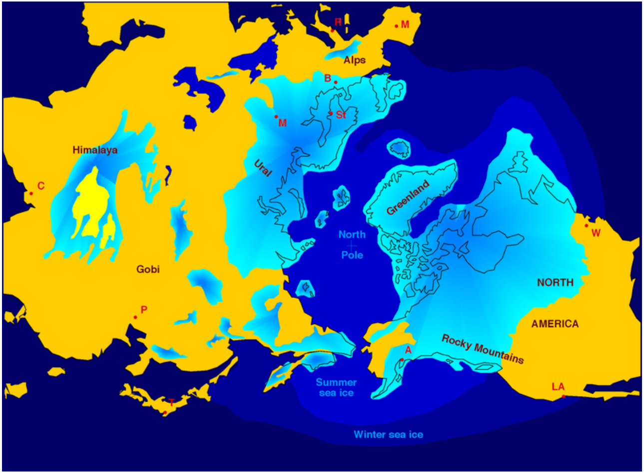
Glacial-Interglacial cycle

We're currently in the quaternary ice age

Last glacial period ended about 10,000 years ago (start of the Holocene)



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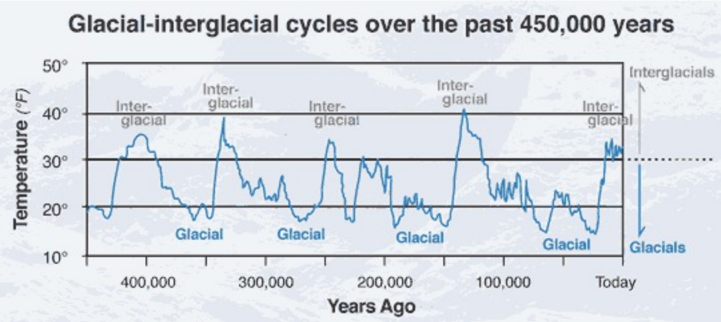
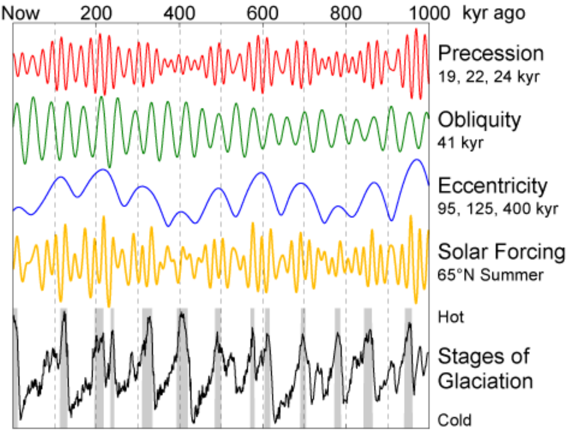


Cycle characterised by saw-toothed behaviour: slow accumulation and rapid terminations.
Approx 100 kyr period between cycles, but previously a 40 kyr period was observed.

Milankovitch theory



Eccentricity: orbital departure from a circle, controls duration of the seasons
Obliquity: axial tilt, controls amplitude of seasonal cycle
Precession: variation in Earth's axis of rotation, affects difference between seasons

Insolation at 65° north: combination of these three terms, considered important.

100kyr problem

Spectral analysis suggest the climate response has a period of $\approx$ 100kyr, but the orbital forcing at this period is small.

Eccentricity has 95 and 125kyr periods, but accounts for only 2% of the variation compared to the shifts caused by obliquity (41kyr period) and precession (21kyr period).

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Explanatory hypotheses

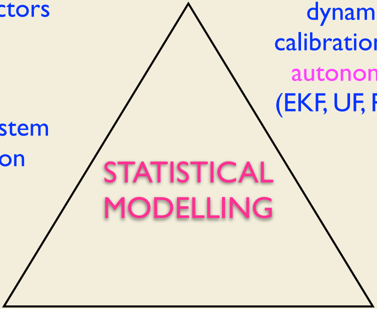
- Earth's climate may have a natural frequency of 100kyr caused by natural feedback processes
- 100kyr eccentricity cycle acts as a "pacemaker" to the system, amplifying the effect of precession and obliquity at key moments, triggering a termination.
- 21kyr precession cycles are solely responsible, with ice building up over several precession cycles, only melting after four or five such cycles.

strange non-chaotic attractors

Dynamical Systems

dynamical system calibration for the non-autonomous system (EKF, UF, Particle Filter)

dynamical system identification



STATISTICAL MODELLING

Bayesian Calibration

Observation analysis

Simulation

experiment design emulation global sensitivity analysis

Current practice

Climate scientists want[1] to use palaeo-data to gather evidence for different hypotheses. They typically want to

- Compare models (and estimate parameters)
- Compare effects of different aspects of the solar forcing (all components have been argued for)
- Produce climate reconstructions (temperature chronologies)
- ...

[1] In my imagination.

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Current approaches tend to be statistically naive

- Models fit by eye,
- Model selection rarely tackled in a statistical manner, and when they do, questionable approaches are taken.

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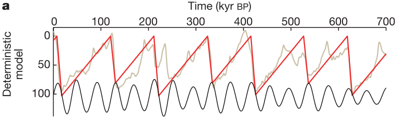
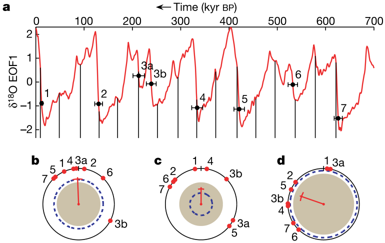
Example

Huybers and Wunsch 2005 argue that obliquity is the primary driver of glacial cycle





- Reduce the dataset to 7 termination times
- Look at the consistency of the phase of each component at terminations
- They propose a random walk model of ice volume with a 100kyr period

$$V_{t+1} = V_t + N(1, 2) \text{ and if } V_t > 90, \text{ terminate}$$

 and estimate the distribution of the test statistic under H_0 (obliquity and termination are independent) by looking at obliquity phase during terminations in the model.

Our aim

Most simple models of the [...] glacial cycles have at least four degrees of freedom [parameters], and some have as many as twelve. Unsurprisingly [...this is] insufficient to distinguish between the skill of the various models (Roe and Allen 1999)

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Can we do any better?

- Aim to demonstrate the power of the Bayesian approach; demonstrate that a full analysis is feasible
- Use all the data, not just the termination times
- Estimate parameters rather than using hand tuned models
- Deal with noisy records and age-model uncertainty

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Essentially a demonstration of recent Monte Carlo methodology (SMC^2, PMCMC), and GPU computation.

Many aspects of the modelling could be improved, and be incorporated within this framework.

$\delta^{18}O$ time-series

^{18}O is heavier than ^{16}O, and so its circulation behaviour varies with temperature

By examining the variation in the ratio $\delta^{18}O$ in marine sediments and ice cores, we can learn about historic ocean temperatures and ice volume

The raw measurements are of $\delta^{18}O$ as a function of depth in a core: age must be inferred. Moreover, the data are noisy, often contain hiatuses, are compacted etc.

Models

A phenomenological approach is taken: idealised simple models based on a few hypothesised relationships that capture some aspect of the climate system.

Let $X_t \in \mathbb{R}^p$ be the state of the climate at time t. Typically $X_{1,t}$ = ice volume, and other components many represent CO_2, ocean temp, etc, or be left undefined.

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- Oscillators synchronised on the solar forcing (Saltzman and Maasch 1991),

$$\begin{aligned}
dX_1 &= -\left(X_1 + X_2 + vX_3 + F(\gamma_P, \gamma_C, \gamma_E)\right) dt + \sigma_1 dW_1 \\
dX_2 &= \left(rX_2 - pX_3 - sX_2^2 - X_2^3\right) dt + \sigma_2 dW_2 \\
dX_3 &= -q\left(X_1 + X_3\right) dt + \sigma_3 dW_3
\end{aligned}$$

- Models with switches in the ice volume (Tziperman 2006)

$$\begin{aligned}
dX_1 &= \left((p_0 - KX_1)(1 - \alpha X_2) - (s + F(\gamma_P, \gamma_C, \gamma_E))\right) dt + \sigma_1 dW_1 \\
X_2 &: \quad \text{switches from 0 to 1 when } X_1 \text{ exceeds some threshold } X_u \\
X_2 &: \quad \text{switches from 1 to 0 when } X_1 \text{ decreases below } X_l
\end{aligned}$$

- Models with switches dependent upon thresholds in the forcing (Parrenin and Paillard 2012)

Statistical model

These models are forced with some aspect of the solar forcing

$$\frac{\mathrm{d}X_t}{\mathrm{d}t} = g(X_t, \theta) + F(t, \gamma)$$

where $\gamma = (\gamma_P, \gamma_C, \gamma_E)$ controls the combination of precession, obliquity and eccentricity.

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Embed these models within a statistical state space model relating climate to observations

$$\begin{aligned} \mathrm{d}X_t &= g(X_t, \theta)\mathrm{d}t + F(t, \gamma)\mathrm{d}t + \Sigma \mathrm{dW} \\ Y_t &= d + sX_{1,t} + \epsilon_t \end{aligned}$$

where we have 'noised-up' the models turning them into SDEs to account for model discrepancies.
Typically these models have 10-15 parameters that need to be estimated from the data.

Bayesian basics

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$$= \frac{\int \pi(y|x)\pi(x|\theta)\mathrm{d}x\ \pi(\theta)}{\iint \pi(y|x)\pi(x|\theta)\pi(\theta)\mathrm{d}x\mathrm{d}\theta}$$

Added difficulty: $\pi(x|\theta)$ is usually unknown!

Bayesian basics

The quantities we need to calculate are

- Climate reconstruction (filtering)

$$\pi(x_{1:T}|y_{1:T},\theta_m,\mathcal{M}_m) \propto \pi(x_{1:T-1}|y_{1:T-1},\theta)\pi(x_T|x_{T-1},\theta)\pi(y_T|x_T)$$

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$$\pi(y_{1:T}|\mathcal{M}_m)$$

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These are progressively more difficult to calculate, particularly as

$$\pi(X_{t+1}|X_t, \theta_m, \mathcal{M}_m)$$

is unknown.

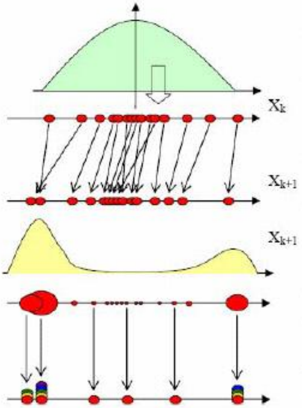
Filtering

Sequential Monte Carlo (SMC) methods are the natural approach for finding the filtering distributions $\pi(x_{1:T}|y_{1:T}, \theta)$

- Represent all distributions by collection of weighted particles $\{x^{(i)}, w^{(i)}\}$, e.g.,

$$p(x) \approx \sum w_0^{(i)} \delta_{x^{(i)}}(x)$$

- Sequentially build up approximation to $\pi(x_{1:t}|y_{1:t}, \theta)$ one step at a time.



SMC

At time $t-1$, suppose $(X_{1:t-1}^n, W_{t-1}^n)_{n=1}^N$ is a collection of weighted particles approximating $\pi(X_{1:t-1}|Y_{1:t-1},\theta)$

- Sample ancestor particle index $\mathcal{A}_{t-1}^n \sim \mathcal{F}(W_{t-1}^n)$
- Propagate state particles $X_t^n \sim q_t(\cdot|X_{t-1}^{\mathcal{A}_{t-1}^n}, \theta, Y_t)$
- Weight state particles

$$w_t^n(X_{1:t}^n) = \frac{\pi(X_t^n|X_{t-1}^{\mathcal{A}_{t-1}^n},\theta)\pi(Y_t|X_t^n)}{q_t(X_t^n|X_{t-1}^{\mathcal{A}_{t-1}^n},\theta, Y_t)}, \qquad W_t^n = \frac{w_t^n(X_{1:t}^n)}{\sum_n w_t^n(X_{1:t}^n)}$$

SMC

At time $t-1$, suppose $(X^n_{1:t-1}, W^n_{t-1})^N_{n=1}$ is a collection of weighted particles approximating $\pi(X_{1:t-1}|Y_{1:t-1}, \theta)$

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$$w^n_t(X^n_{1:t}) = \frac{\pi(X^n_t|X^{\mathcal{A}^n_{t-1}}_{t-1}, \theta)\pi(Y_t|X^n_t)}{q_t(X^n_t|X^{\mathcal{A}^n_{t-1}}_{t-1}, \theta, Y_t)}, \qquad W^n_t = \frac{w^n_t(X^n_{1:t})}{\sum_n w^n_t(X^n_{1:t})}$$

We need $\pi(X_t|X_{t-1}, \theta)$ to cancel, but setting $q = \pi$ can lead to extreme degeneracy, as too many proposals are in regions of low-posterior probability

We use the Golightly and Wilkinson (2006) approach to nudge the proposals towards the data.

Parameter estimation

SMC provides an unbiased estimate of the marginal likelihood

$$\pi(y_{1:T}|\theta) = \pi(y_1|\theta) \prod_{t=2}^{T} \pi(y_t|y_{1:t-1}, \theta)$$

when we substitute the estimate

$$\tilde{\pi}(y_t|y_{1:t-1}, \theta) = \frac{1}{M} \sum w_t^n$$

for $\pi(y_t|y_{1:t-1}, \theta)$.

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for $\pi(y_t|y_{1:t-1},\theta)$.
We can then use these estimates in a pseudo marginal scheme such as PMCMC (Andrieu *et al.* 2010) to estimate

$$\pi(\theta, x_{1:T}|y_{1:T})$$

and

$$\pi(\theta|y_{1:T})$$

SMC^2

We've found that SMC^2 (Chopin *et al.* 2011) works well for our problem

Basic idea:

- Introduce M parameter particles $\theta_1, \ldots, \theta_M$
- For $t = 1, \ldots, T$
  - For each θ_i run a particle filter targeting $\pi(X_{1:t}|y_{1:t}, \theta_i)$
  - Recalculate all the importance weights and resample if necessary

Note that to avoid particle degeneracy, it is still usually necessary to run a PMCMC sampler targeting $\pi(\theta, X_{1:t}|y_{1:t})$ at each resampling step.

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This takes 3-4 days on a standard server, or 4-6 hours on a GPU (2500 processors) with 1000 θ particles and 1000 X particles.

SMC^2 to sample from $\pi(\theta, X_{1:T}|y_{1:T})$

Assume that at stage t we have particles $\{\theta^i, X_{1:t}^{1:N_x,i}\}_{i=1}^{N_\theta}$ with weights $\{W_t^i\}$ that approximates $\pi(\theta, X_{1:t}|y_{1:t})$
For $t = 1, \ldots, T$:

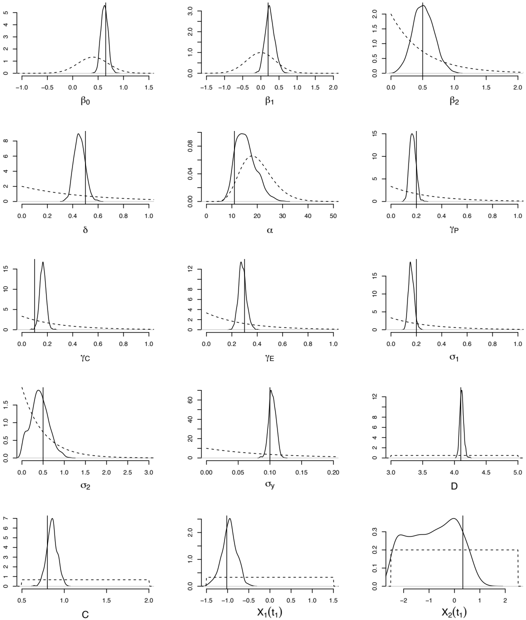
- If effective sample size is too small, resample by running a PMCMC algorithm targeting $\pi(\theta, X_{1:t}|y_{1:t})$
- Sample $\{\theta^i, X_{1:t+1}^{1:N_x,i}\}$ by performing iteration $t+1$ of the PF
- Estimate $\hat{\pi}(y_{t+1}|y_t, \theta^i)$
- Reweight by setting

$$w_{t+1}^i = w_t^i \hat{\pi}(y_{t+1}|y_t, \theta^i)$$

and $W_{t+1}^i = \frac{w_{t+1}^i}{\sum_i w_{t+1}^i}$

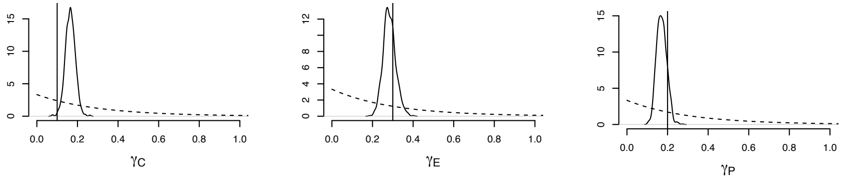
In total, this requires the use of $N_\theta \times N_x$ particles.

Results



Results

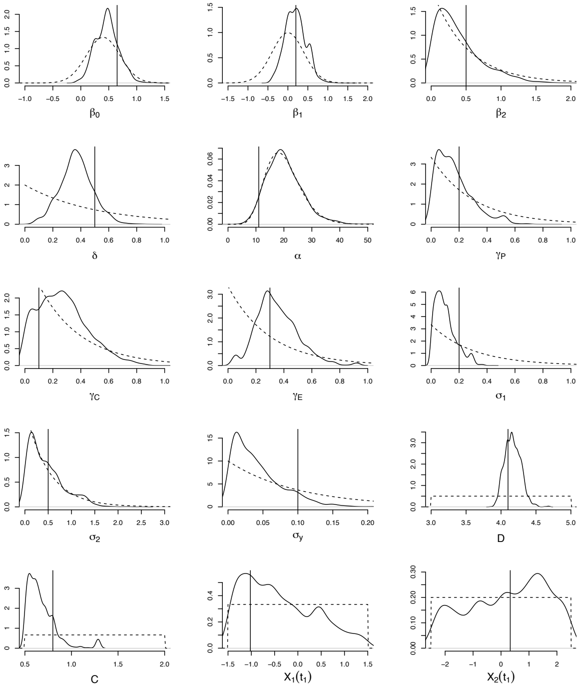
$\gamma = (\gamma_P, \gamma_E, \gamma_C)$ controls the relative contribution of the three components of the orbital variations in the forcing.



Alternative approaches

ABC

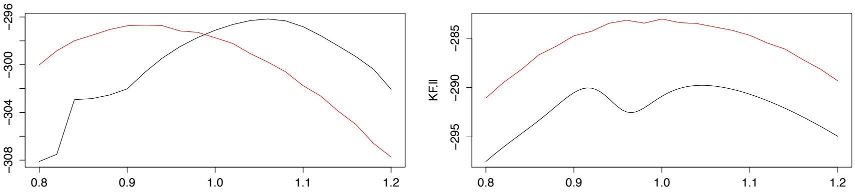
- Instead of approximating the likelihood (as in SMC^2), we try to find θ that give good match between observed and simulated data
- Allows us to calibrate on carefully chosen aspects of the system (period, volatility, etc), rather than just on the data.
- The loss of information from the ABC approximation is large, so the posteriors are usually much wider than with SMC^2.


β0
β1
β2
δ
α
γP
γC
γE
σ1
σ2
σy
D
C
X1(t1)
X2(t1)

Alternative approaches

Instead of using the particle filter (SMC) to do the filtering, we would like to use the unscented Kalman filter (UKF) or EnKF.

- Assumes $\pi(x_t|y_{1:t})$ is Gaussian and uses Sigma-point particles to estimate mean and variance.
- Much cheaper than *SMC* or *MCMC* approaches.
- We found the UKF works well for filtering (location), less well for parameter estimation, and terribly for model selection.



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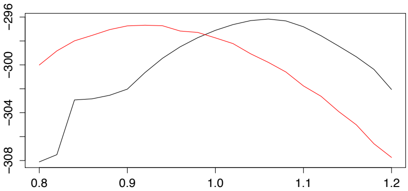

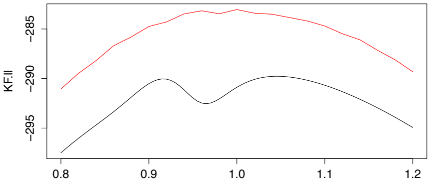

A further discredited alternative is the idea of augmenting the state vector with the parameter, and inferring the joint distribution using the particle filter.

Bayes factors

Consider comparing two models, $\mathcal{M}_1$ and $\mathcal{M}_2$.

Bayes factors (BF) are the Bayesian approach to model selection.

$$\frac{\mathbb{P}(\mathcal{M}_1|\mathcal{D})}{\mathbb{P}(\mathcal{M}_2|\mathcal{D})} = \frac{\pi(\mathcal{M}_1)}{\pi(\mathcal{M}_2)} \frac{\mathbb{P}(\mathcal{D}|\mathcal{M}_1)}{\mathbb{P}(\mathcal{D}|\mathcal{M}_2)}$$

$$\text{posterior odds} = \text{prior odds} \times \text{Bayes factor}$$

where

$$B_{12} = \frac{\mathbb{P}(\mathcal{D}|\mathcal{M}_1)}{\mathbb{P}(\mathcal{D}|\mathcal{M}_2)} = \frac{\int \pi(\theta_1|\mathcal{M}_1)\mathbb{P}\ (\mathcal{D}|\theta_1, \mathcal{M}_1)d\theta_1}{\int \pi(\theta_2|\mathcal{M}_2)\mathbb{P}(\mathcal{D}|\theta_2, \mathcal{M}_2)d\theta_2}$$

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B_{12} range	$\mathbb{P}(\mathcal{M}_1\|D)$ range	Interpretation
1–3	0.5-0.75	Barely worth mentioning
3–10	0.75 - 0.91	Substantial
10–30	0.91-0.97	Strong
30–100	0.97- 0.99	Very strong
> 100	0.99-1	Decisive

Bayes factors

Advantages:

- Provide evidence in favour of a model
- Provides an automatic form of Occam's razor.
- Do not require models to be nested
- Asymptotic consistency

Disadvantages

- **Hard** to calculate
- Sensitive to choice of prior
- Integrated likelihood may not be desirable treatment
  - predictive evaluation via scoring rules? (not p-values)

Model selection

To compare models $\mathcal{M}_1$ and $\mathcal{M}_2$, we want to find the Bayes factor

$$B_{12} = \frac{\pi(y_{1:T}|\mathcal{M}_1)}{\pi(y_{1:T}|\mathcal{M}_2)}$$

Values of $B_{12} > 100$ indicate 'decisive' evidence in favour of $\mathcal{M}_1$.

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SMC^2 can be used to provide an unbiased estimate of

$$\pi(y_{1:T}|\mathcal{M})$$

for any model.

However, the variance of our estimates are typically an order of magnitude, so don't consider B_{12} to be large until we see values > 1000.

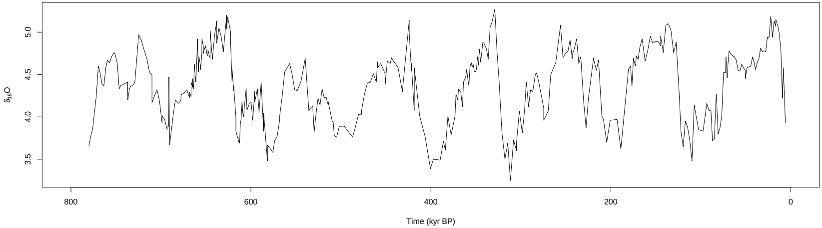
Results

We generate simulated data from SM91, using both the astronomically forced and unforced version of the model

Model		Evidence $\pi(y_{1:N}\|\mathcal{M}_m)$	
		SM91-unforced	SM91-forced
SM91	Forced	5.6×10^{28}	1.4×10^{41}
	Unforced	1.1×10^{30}	2.4×10^{18}
T06	Forced	3.6×10^{20}	2.6×10^{30}
	Unforced	1.1×10^{22}	2.9×10^{14}
PP12	Forced	2.8×10^{8}	2.1×10^{18}

- Strongest evidence for the true model found each time
- Unforced model is special case of forced model with 3 parameters set to zero, so we expect it to be harder to select the unforced model.
- For the data generated from the forced model, the forced version of the wrong model is preferred.

Results: ODP677



We use the ODP677 stack (a composite record from multiple cores), which has been dated by two authors:

- Lisiecki and Raymo (2005) used orbital tuning
- Huybers 2007 used a depth-derived age model (no orbital tuning)

Results: ODP677

Model		Evidence	
		ODP677: H07(unforced)	ODP677: LR04(forced)
SM91	Forced	4.0×10^{24}	1.1×10^{28}
	Unforced	3.5×10^{26}	1.6×10^{18}
T06	Forced	3.3×10^{25}	4.5×10^{29}
	Unforced	1.7×10^{28}	3.3×10^{21}
PP12	Forced	1.5×10^{22}	1.8×10^{34}

The dating method applied changes the answer

- Using Huybers' non-orbitally tuned data, we find evidence in favour of the unforced T06 model.
- Using Lisiecki's orbitally tuned data, we find strong evidence for PP12 a tuned model (PP12)

Moreover, orbitally tuned data leads us to strongly prefer the orbitally tuned version of each model (and vice versa)

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The age model used to date the stack (often taken as a given) has a strong effect on model selection conclusions

Age model

Can we also quantify chronological uncertainty?

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Target

$$\pi(\theta, T_{1:N}, X_{1:N} | y_{1:N})$$

where $T_{1:N}$ are the times of the observation $Y_{1:N}$, which were previously taken as given.

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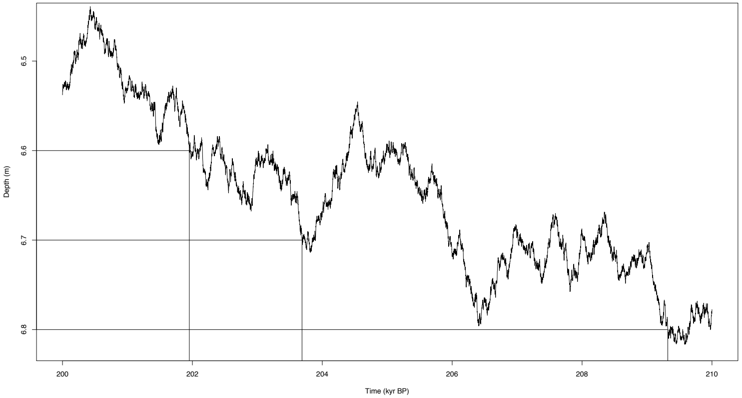
Propose a simple age model for sediment accumulation:
Let H be the depth in the core, with $H_N = 0$ at $T_N = 0$

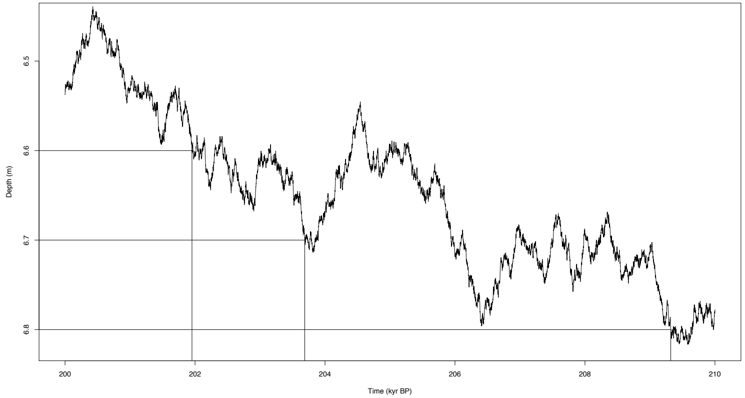
$$\mathrm{d}H = -\mu_s \mathrm{d}T + \sigma \mathrm{d}W$$

Slices are then taken through the core at specific depths $H_1, \ldots, H_N$.



There may have been multiple times when a certain depth was reached: the most recent time is the age of that slice, i.e., it is a first passage problem. Given (T_m, H_m), then T_{m-1} is the first passage time of H_{m-1} with

$$T_{m-1} | T_m \sim IG\left(T_m - \frac{H_{m-1} - H_m}{\mu_s}, \frac{(H_{m-1} - H_m)^2}{\sigma_s^2}\right)$$



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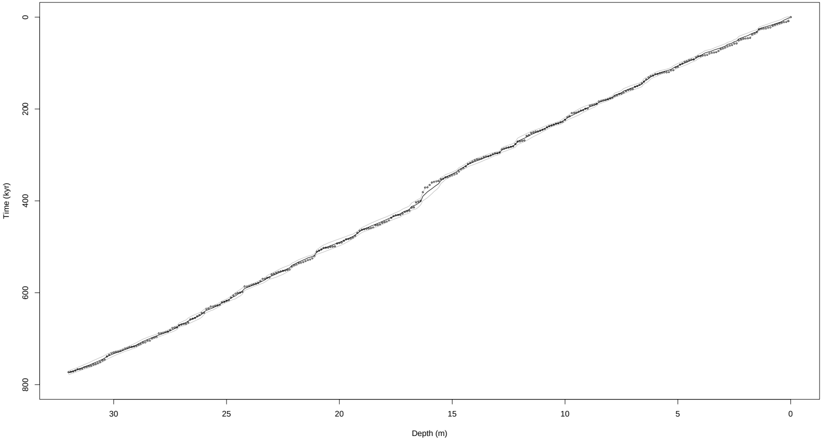
We then add a model to account for compaction in the core, and apply Bayes theorem to find $\pi(T_m|T_{m-1})$ so that we can run the model forward in time

Simulation study results ($n = 321$) - age vs depth

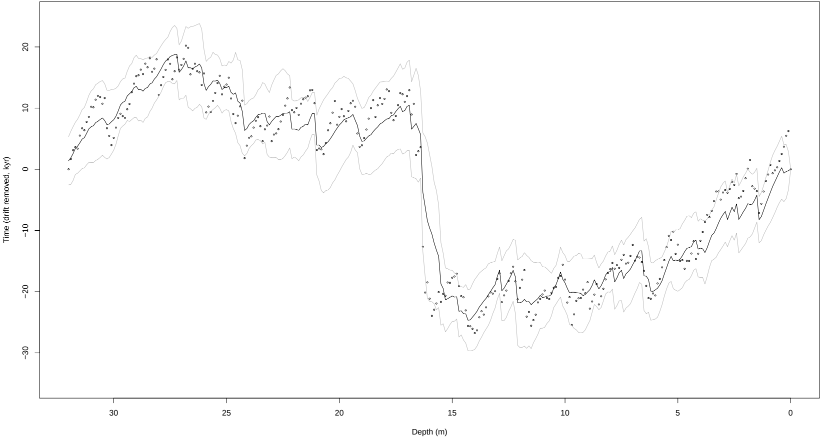
Dots = truth, black line = estimate, grey = 95% CI

We use simulated data from the CR12 model, with parameter values, and initial conditions comparable to real data. We consider the period 780 kyr to the present.



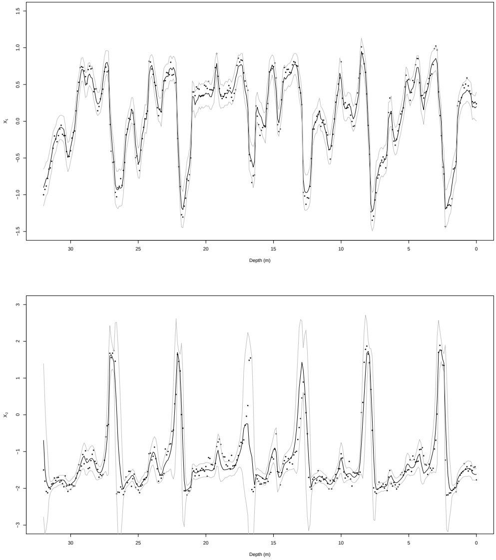
Simulation study results - age vs depth (trend removed)

Dots = truth, black line = estimate, grey = 95% CI

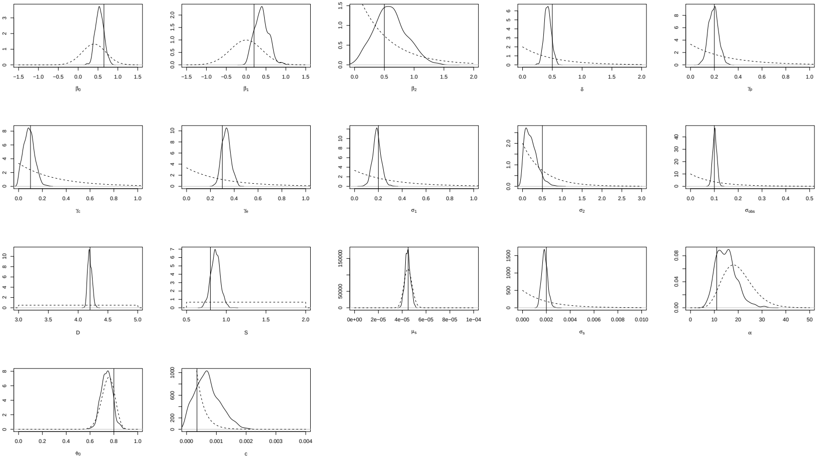


Simulation study results - climate reconstruction

Dots = truth, black line = estimate, grey = 95% CI



Simulation study results - parameter estimation

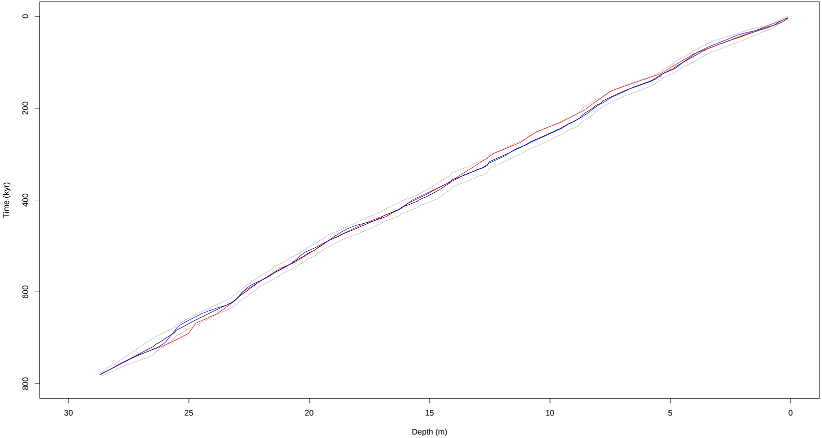


Results for ODP846 core

- ODP846 contains a marker for the Brunhes-Matuyama magnetic reversal at 780kyr, allowing us to give a strong prior for T_1 ($\pm$2kyr).
- Has again been dated by two groups
  - Lisiekci and Raymo (LR04): graphical correlation of 57 cores. The stack is then orbitally tuned
  - Huybers and Wunsch 2004 (HW04) use a depth-derived age model. They decompact each core, fit a linear age model, then average over many several realisations and to get a distribution for 17 age control points(ACPS) , such as terminations. Average ages for the the ACP events are then found, and a linear age model is fitted between consecutive ACPs

Results for ODP846 - age vs depth

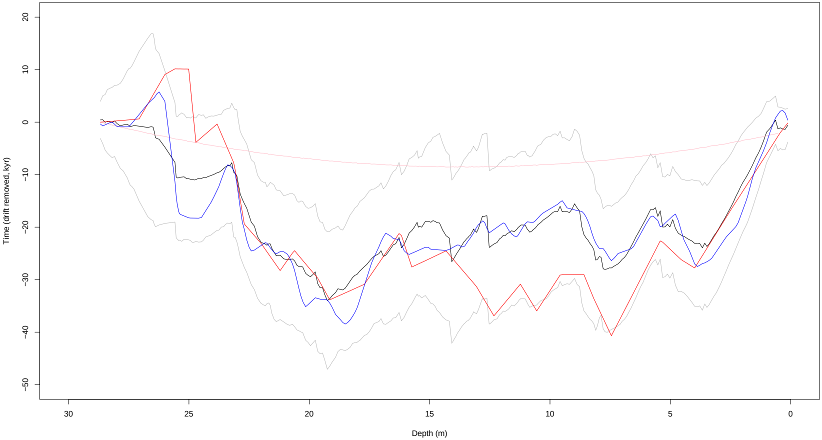
Black = posterior mean, grey = 95%CI, red = H07, blue = LR04



Our results come with uncertainty bounds (HW04 estimate accuracy of ±9kyr for all ages). Moreover, the full joint distribution for all quantities is available if required.

Results for ODP846 - age vs depth (trend removed)

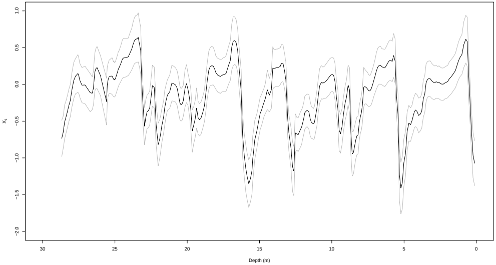
Black = posterior mean, grey = 95%CI, red = H07, blue = LR04

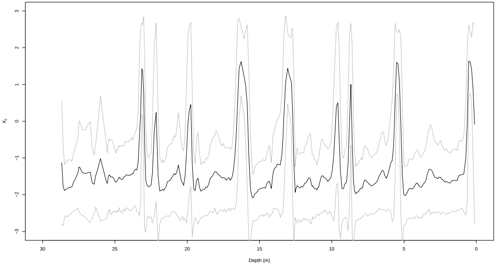


Note that these age estimates now depend explicitly on the model CR12.

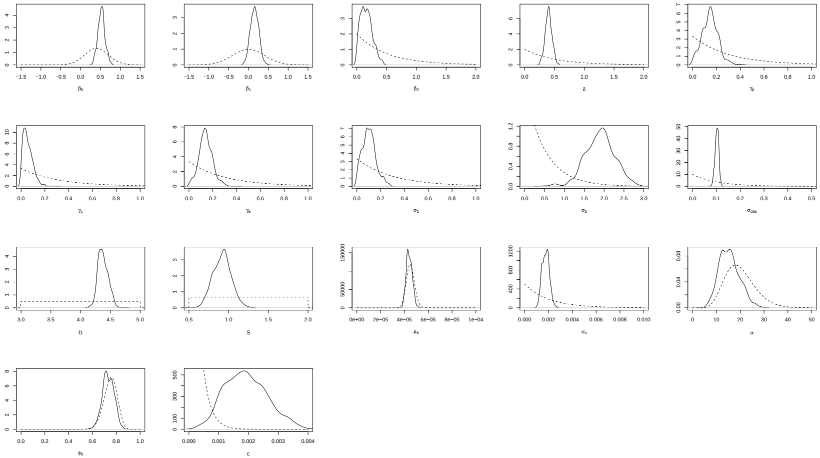
Results for ODP846 - climate reconstruction

We can now give climate reconstructions that account for age uncertainty.





Results for ODP846 - parameter estimates



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- The data do contain enough information to partially discriminate between models
- However, the results are very sensitive to the age model applied to the data.
    - If we don't do joint estimation of all uncertain quantities, the results are over confident and can lead to contradictory conclusions.
- Monte Carlo methodology and computer power are now sufficiently advanced that we can tackle the joint reconstruction, age model, and model selection problems in a fully Bayesian manner
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Thank you for listening!