Spectral Subsampling MCMC for Stationary Multivariate Time Series

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Overview

- **Background: Subsampling MCMC/HMC**
- **Spectral subsampling for multivariate time series**
- **Application to vector ARTFIMA**

- **Slides**: http://mattiasvillani.com/news (soon).

Joint work with some Aussies

- **Robert Kohn**, UNSW Sydney
- **Matias Quiroz**, UTS Sydney
- **Robert Salomone**, QUT Brisbane
- Other subsampling MCMC/HMC papers:
  - **Minh-Ngoc Tran**, Univ of Sydney
  - **Khue-Dung Dang**, Univ of Melbourne

Motivation

- **Long time series** are increasingly **common**:
  - high frequency financial transaction data
  - neuroimaging data with high temporal resolution
  - sensor data from robots
  - meteorological weather stations
  - GPS data used in urban traffic monitoring.
- Often **multivariate observations**.
- Automatic **decision making under uncertainty**.
- **Bayesian decisions**: maximize **posterior expected utility**.
- Posteriors by Markov Chain Monte Carlo (**MCMC**) simulation.
- **MCMC is slow** on large datasets.

The Metropolis-Hastings (MH) algorithm

- **Bayesian inference**

$$p(\boldsymbol{\theta}|\mathbf{y}) \propto L(\boldsymbol{\theta})p(\boldsymbol{\theta})$$

- Initialize $\boldsymbol{\theta}^{(0)}$ and iterate for $k = 1, 2, ..., N$

  1. Sample $\boldsymbol{\theta}_p \sim q\left(\cdot|\boldsymbol{\theta}^{(k-1)}\right)$ (the **proposal distribution**)
  2. Accept $\boldsymbol{\theta}_p$ with **acceptance probability**

$$\alpha = \min\left(1, \frac{L(\boldsymbol{\theta}_p)p(\boldsymbol{\theta}_p)}{L\left(\boldsymbol{\theta}^{(k-1)}\right)p\left(\boldsymbol{\theta}^{(k-1)}\right)} \frac{q\left(\boldsymbol{\theta}^{(k-1)}|\boldsymbol{\theta}_p\right)}{q\left(\boldsymbol{\theta}_p|\boldsymbol{\theta}^{(k-1)}\right)}\right)$$

- **Costly** to evaluate $L(\boldsymbol{\theta}_p)$ when n is large. **Big data**.

Naive Subsampling MH

- Independent data - **log-likelihood** is a **sum**

$$\ell(\boldsymbol{\theta}) \stackrel{\text{def}}{=} \log L(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log \ell_i(\boldsymbol{\theta}), \text{ with } \ell_i(\boldsymbol{\theta}) \stackrel{\text{def}}{=} p(y_i|\boldsymbol{\theta})$$

- **Unbiased estimate** of $\ell(\boldsymbol{\theta})$ from **subsample** of size $m \ll n$

$$\hat{\ell}(\boldsymbol{\theta}, \mathbf{u}) = \frac{n}{m} \sum_{i \in \mathbf{u}} \log \ell_i(\boldsymbol{\theta})$$

- Unbiased log-likelihood: $\mathbb{E}_{\mathbf{u}}[\hat{\ell}(\boldsymbol{\theta}, \mathbf{u})] = \ell(\boldsymbol{\theta})$.
- Run **Pseudo-marginal MH** with $\hat{L}(\boldsymbol{\theta}, \mathbf{u}) = \exp(\hat{\ell}(\boldsymbol{\theta}, \mathbf{u}))$.

- Initialize $(\boldsymbol{\theta}^{(0)}, \mathbf{u}^{(0)})$ and iterate for $k = 1, 2, ..., N$
  1. Sample $\boldsymbol{\theta}_p \sim q(\cdot|\boldsymbol{\theta}^{(k-1)})$ and subsample $\mathbf{u}_p \sim p(\mathbf{u})$
  2. Accept $(\boldsymbol{\theta}_p, \mathbf{u}_p)$ with **acceptance probability**

$$\alpha = \min\left(1, \frac{\hat{L}\big(\boldsymbol{\theta}_p, \mathbf{u}_p\big) p(\boldsymbol{\theta}_p)}{\hat{L}\big(\boldsymbol{\theta}^{(k-1)}, \mathbf{u}^{(i-1)}\big) p(\boldsymbol{\theta}^{(k-1)})} \frac{q\big(\boldsymbol{\theta}^{(k-1)}|\boldsymbol{\theta}_p\big)}{q\big(\boldsymbol{\theta}_p|\boldsymbol{\theta}^{(k-1)}\big)}\right)$$

Fixing Naive Subsampling MH - Bias

- **If $\hat{L}$ unbiased** then samples are from $p(\boldsymbol{\theta}|\boldsymbol{y})$ [1]
- **Approximate bias correction of** $\exp\left(\hat{\ell}(\boldsymbol{\theta},\mathbf{u})\right)$ [2]

  Theorem: Error in posterior approximation is $O\left(\frac{1}{m^2 n}\right)$ [3]
- **Unbiased Block-Poisson estimator** + **Signed PMMH** [4]

Fixing Naive Subsampling MH - Variance

- **Low** $\mathbb{V}\left(\hat{L}\left(\boldsymbol{\theta},\mathbf{u}\right)\right)$ is crucial for **efficient sampling**.
- **Difference estimator** with control variates [3]

$$\widehat{\ell}_{\mathrm{diff}}(\boldsymbol{\theta},\mathbf{u}) := \sum_{k=1}^{n} q_k(\boldsymbol{\theta}) + \frac{n}{m}\sum_{i=1}^{m}\left(\ell_{u_i}(\boldsymbol{\theta}) - q_{u_i}\left(\boldsymbol{\theta}\right)\right)$$

- **Control variates** $q_{u_i}\left(\boldsymbol{\theta}\right)$ by Taylor expansion around $\tilde{\boldsymbol{\theta}}$. [3, 5]
- **Optimal tuning** of subsample size m [6, 3, 4]
- **Blocking**: only refresh part of the subsample [7, 8]
- **Grouping observations** for improved control variates [9]
- **High-dim θ**: **Subsampling HMC**. [10]

Beyond independent data

- Subsampling methods **assume** the **log-likelihood is a sum**

$$\ell(\boldsymbol{\theta}) = \sum_{i=1}^{n} \log p(y_i|\boldsymbol{\theta})$$

- Estimating $\ell(\theta)$ is like estimating a **population total**

$$\hat{\ell}(\boldsymbol{\theta}, \mathbf{u}) = \frac{n}{m} \sum_{i \in \mathbf{u}} \log p(y_i|\boldsymbol{\theta})$$

- **Log-likelihood is a sum:**
  - for conditionally independent y_i
  - for longitudinal data when subjects are independent.
  - for special time series, e.g. AR processes. Sample (x_t, x_{t-1}).
- General **time series** dependence? Spatial dependence?

Spectral density of a stationary process

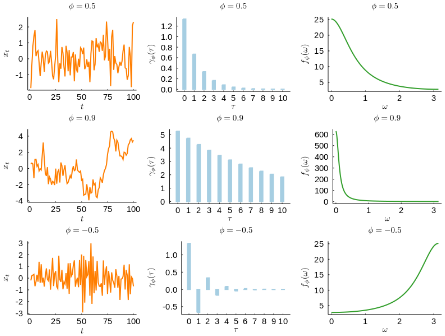
- **Autocovariance function**

$$\gamma(\tau) = \mathbb{E}\left[(x_t - \mu)(x_{t-\tau} - \mu)\right], \quad \tau = 0, 1, \ldots$$

- **Spectral density**

$$f(\omega) \equiv \frac{1}{2\pi} \sum_{\tau=-\infty}^{\infty} \gamma(\tau) \exp(-\mathrm{i}\omega\tau) \text{ for } \omega \in (-\pi, \pi].$$

- **AR(1) process:** $x_t = \phi x_{t-1} + \varepsilon_t, \quad \varepsilon_t \overset{iid}{\sim} N(0, \sigma_\varepsilon^2)$



Multivariate Fourier analysis

- **Autocovariance matrix function** for time series $\boldsymbol{x}_t \in \mathbb{R}^r$

$$\gamma_{\boldsymbol{x}}(\tau) = \mathrm{Cov}(\boldsymbol{x}_t, \boldsymbol{x}_{t-\tau}) = \left[\gamma_{jk}(\tau)\right]_{i,j=1,\ldots,r}$$

- **Spectral density matrix**

$$f_{\boldsymbol{x}}(\omega) = \frac{1}{2\pi} \sum_{\tau=-\infty}^{\infty} \gamma_{\boldsymbol{x}}(\tau) \exp(-i\omega\tau)$$

where off-diagonal elements are the **cross-spectral densities**

$$f_{jk}(\omega) = \sum_{\tau=-\infty}^{\infty} \gamma_{jk}(\tau) \exp(-i\omega\tau), \text{ for } \omega \in (-\pi, \pi]$$

- **Multivariate** discrete Fourier transform (**DFT**)

$$J(\omega_k) = \sum_{t=0}^{n-1} \boldsymbol{x}_t \exp(-i\omega_k t)$$

Subsampling MCMC for multivariate time series

- DFT are asymptotically independent complex normal [11]

$$n^{-1/2} J(\omega_k) \overset{\text{indep}}{\sim} \mathrm{CN}(0, 2\pi f_{\mathbf{x}}(\omega_k)) \text{ as } n \to \infty.$$

- **Multivariate periodogram** is complex singular Wishart

$$I_T(\omega) = (2\pi n)^{-1} J(\omega) J_T(\omega)^H \sim \mathrm{CW}(1, f_{\mathbf{x}}(\omega))$$

- **Multivariate Whittle** log-likelihood [12]

$$\ell_{\mathcal{W}}(\boldsymbol{\theta}) = -\sum_{\omega_k \in \Omega_n} \left(\log |f_{\mathbf{x}}(\omega_k)| + \mathrm{tr}\left[f_{\mathbf{x}}(\omega_k)^{-1} I_T(\omega)\right]\right)$$

- **Whittle log-likelihood is a sum**. **Subsample frequencies!**
- Whittle **biased for small** n
- ... but **subsampling** only relevant for **large** n.

Improved control variates by grouping

- Difference estimator:

$$\widehat{\ell}_{\text{diff}}(\boldsymbol{\theta}, \mathbf{u}) := \sum_{k=1}^{n} q_k(\boldsymbol{\theta}) + \frac{n}{m} \sum_{j=1}^{m} \left(\ell_{u_j}(\boldsymbol{\theta}) - q_{u_j}(\boldsymbol{\theta}) \right)$$

- Need $q_i(\boldsymbol{\theta}) \approx \ell_i(\boldsymbol{\theta})$ to have small $Var(\widehat{\ell}_{\text{diff}}(\boldsymbol{\theta}, \mathbf{u}))$.
- $q_i(\boldsymbol{\theta})$ by second order Taylor approximation of $\ell_i(\boldsymbol{\theta})$.
- **Group observations**. Treat partial sum as a sampling unit: [9]

$$\ell(\boldsymbol{\theta}) = \underbrace{\ell_{\omega_1}(\boldsymbol{\theta}) + \ell_{\omega_2}(\boldsymbol{\theta}) + \ldots \ell_{\omega_K}(\boldsymbol{\theta})}_{\text{group 1}} + \underbrace{\ell_{\omega_{K+1}}(\boldsymbol{\theta}) + \ell_{\omega_2}(\boldsymbol{\theta}) + \ldots \ell_{\omega_{2K}}(\boldsymbol{\theta})}_{\text{group 2}} + \ldots$$

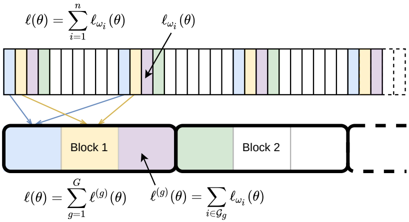
- **Bernstein-von Mises**: partial sums quadratic as $K \to \infty$.
- Each group spans the whole spectral domain.

Blocking

- What really matters for MH is the variance of

$$\log \frac{\hat{p}\left(\mathbf{y}|\theta_p, \mathbf{u}_p\right)}{\hat{p}\left(\mathbf{y}|\theta^{(i-1)}, \mathbf{u}^{(i-1)}\right)}$$

- **Blocking**: [7]
  - partition the groups in blocks
  - **update only a single block** at each iteration.



Univariate ARTFIMA

- **ARFIMA**(p, d, q) with fractional differencing d

$$\phi_p(L)(1-L)^d x_t = \theta_q(L)\varepsilon_t$$

- **Long memory**. $\sum_{\tau=-\infty}^{\infty} |\gamma(\tau)| = \infty$. But stationary if $|d| < 1/2$.

$$(1-L)^d \stackrel{\text{def}}{=} \sum_{j=0}^{\infty} (-1)^j \frac{\Gamma(1+d)}{\Gamma(1+d-j)j!} L^j$$

- **ARTFIMA** adds **tempering** parameter $\lambda \geq 0$ [13]

$$(1-e^{-\lambda}L)^d x_t \stackrel{\text{def}}{=} \sum_{j=0}^{\infty} (-1)^j \frac{\Gamma(1+d)}{\Gamma(1+d-j)j!} e^{-\lambda j} x_{t-j}$$

  - long range dependence in $\gamma(\tau)$ for small τ
  - exponential decay for larger τ
  - Stationary for all d and $\lambda > 0$.

Vector ARTFIMA(p, d, λ, q)

- Multivariate extension of ARTFIMA for r-dim $\boldsymbol{x}_t$ [12]

$$\Phi_p(L)\Delta^{\boldsymbol{d},\boldsymbol{\lambda}}(\boldsymbol{x}_t - \boldsymbol{\mu}) = \Theta_q(L)\boldsymbol{\varepsilon}_t, \quad \boldsymbol{\varepsilon}_t \overset{\text{iid}}{\sim} N(0, \Sigma_\varepsilon)$$

where

$$\Delta^{\boldsymbol{d},\boldsymbol{\lambda}} \equiv \mathrm{Diag}\Big((1 - e^{-\lambda_1}L)^{d_1}, \ldots, (1 - e^{-\lambda_r}L)^{d_r}\Big)$$

- VARTFIMA is **stationary** and causal for all $\boldsymbol{d}$ and $\boldsymbol{\lambda} > \mathbf{0}$.
- **Spectral density matrix**

$$f_{\boldsymbol{x}}(\omega) = \frac{1}{2\pi}\boldsymbol{B}\Phi_p^{-1}(e^{-i\omega})\Theta_q(e^{-i\omega})\Sigma_\varepsilon\Theta_q(e^{-i\omega})\Phi_p^{-H}(e^{-i\omega})^H\boldsymbol{B}^H$$

$$\boldsymbol{B} = \mathrm{Diag}\Big((1 - e^{-(\lambda_1 + i\omega)})^{-d_1}, \ldots, (1 - e^{-(\lambda_r + i\omega)})^{-d_r}\Big).$$

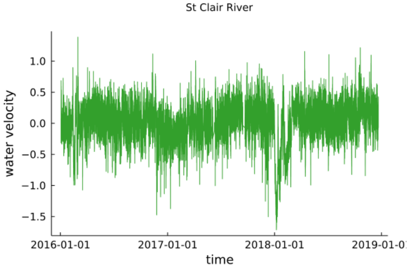
- **Ansley-Kohn parametrization** of both Φ and Θ to ensure stationarity and invertibility.
- Aim: joint posterior

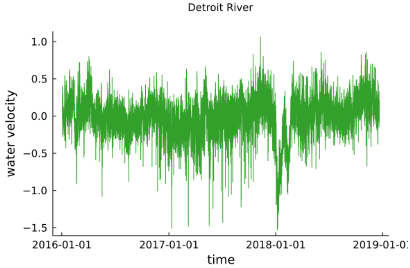
$$p(\Phi, \Theta, \boldsymbol{d}, \boldsymbol{\lambda} | \boldsymbol{x}_{1:n})$$

Three datasets for evaluation

- **Swedish temperatures**
  - Three locations: Arlanda, Bromma and Landvetter.
  - Hourly data from February 1, 2008 until May 1, 2022.
- **Water velocity**
  - Mean water velocity every 12th minute at two locations on opposite sides of Lake St Clair.
  - 130,001 observations from Jan 3, 2016 until Dec 21, 2018.
- **Air pollution** in Stockholm
  - Nitrogen dioxide (NO2) and particulate matter (PM10) pollution at two streets in central Stockholm.
  - Hourly data for the time period February 16, 2010 until October 31, 2015.
- **Subsample**: **1%** of sample, using control variates for groups.

Water velocity data





Model selection via BIC approximation

		Water Velocity		Temperature		Pollution	
AR	MA	No TFI	TFI	No TFI	TFI	No TFI	TFI
1	0	737079	759123	327097	334122	363760	366022
0	1	588297	759457	61320	332888	306068	365658
2	0	749650	761200	335201	**335757**	365522	**366266**
0	2	621765	**761786**	93256	333948	325717	366142
1	1	758838	761305	333582	335647	365762	**366267**

Computional times

- **Computational Time (CT)**

$$\text{CT} = \text{Inefficiency factor} \times \text{Compute time for single draw}$$

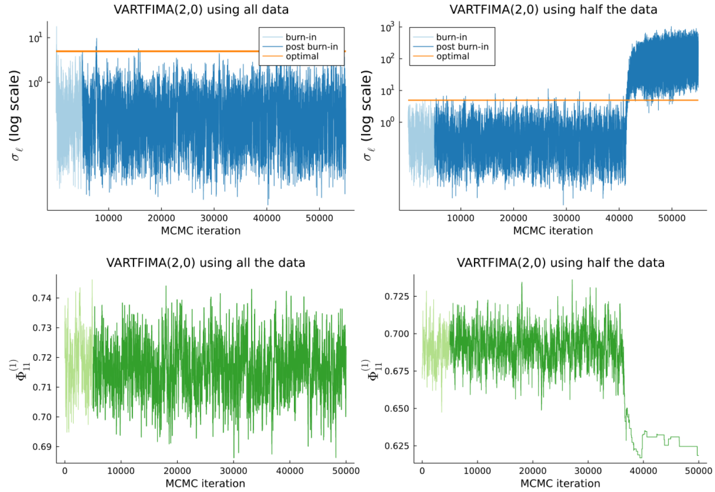
- **Relative Computational Time (RCT)**:

$$\text{RCT} = \frac{\text{CT MCMC full data sample}}{\text{CT Spectral subsampling MCMC}}$$

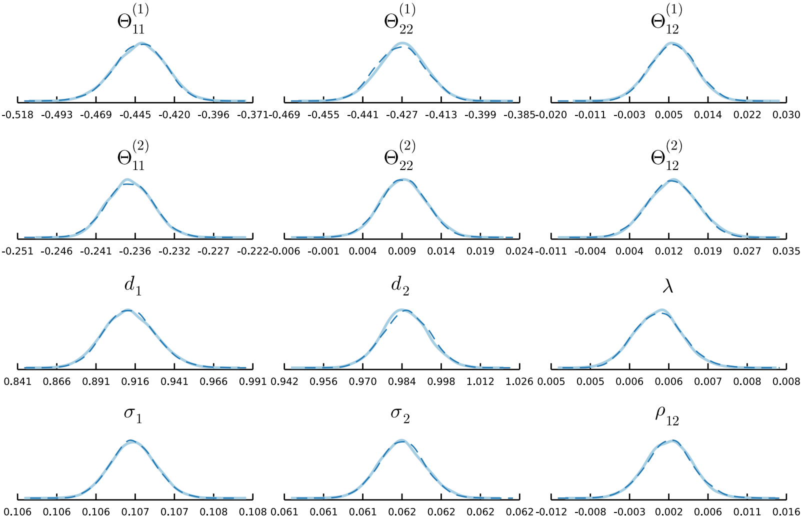
Dataset	Model	Min	Mean	Max
Water velocity	VARTFIMA(0,2)	87	98	125
Temperature	VARTFIMA(2,0)	68	89	114

Variance of log-likehood estimator is crucial

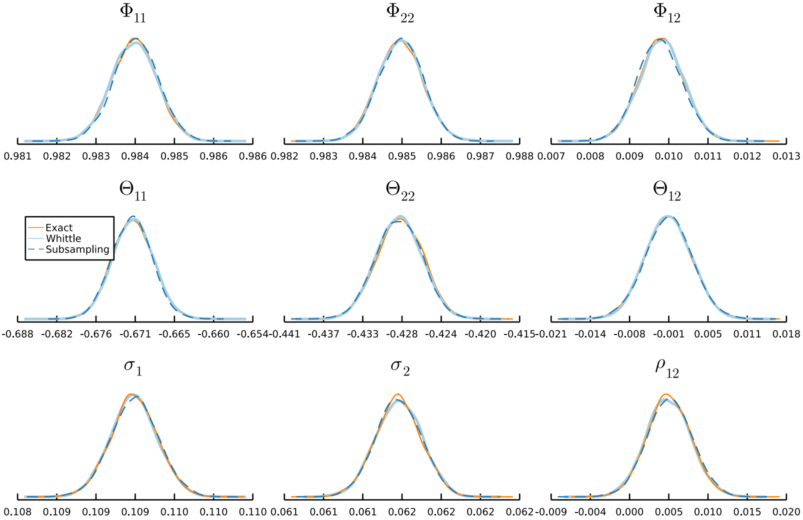
- Spectral subsampling can fail when $Var(\hat{\ell})$ is too large.
- VARTFIMA(2,0) for Swedish temperature data:



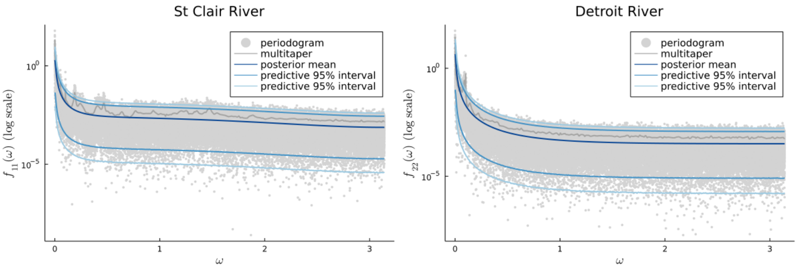
VARTFIMA(0,2) - Subsampling is accurate



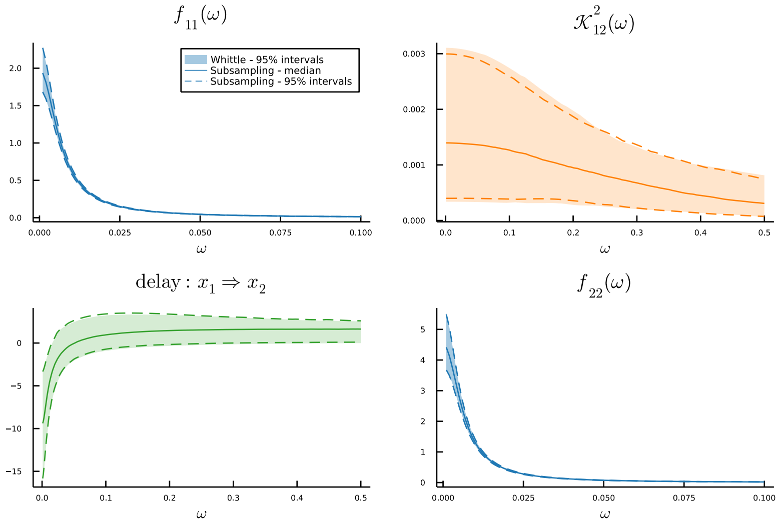
VARMA(1,1) - Whittle is accurate



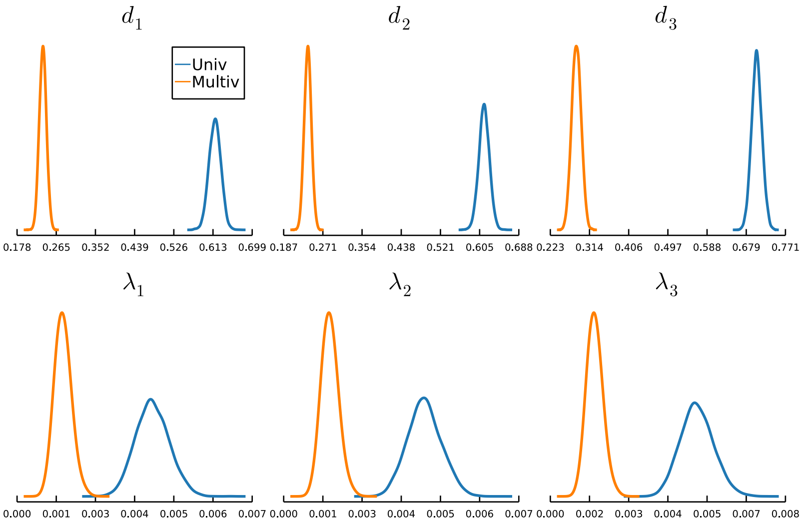
VARTFIMA(0,2) - good model fit



VARTFIMA(0,2) - coherence and delay (phase)



Swedish temperature data



Conclusions

- **Whittle log-likelihood** is fast to compute and is a sum.
- **Whittle enables subsampling** for time series.
- **Subsampling of matrix periodogram** data to speed up MCMC/HMC for multivariate time series.
- **Very large speed-ups** compared to regular MCMC/HMC.
- Future extensions:
  - Better **control variates for high-dim $\boldsymbol{\theta}$**
  - **Spatial data**
  - **Better Whittle**

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