## Trans-dimensional sampling methods for LISA Data Analysis: Current status and future prospects

Nikolaos Karnesis
Aristotle University of Thessaloniki
karnesis@auth.gr
LIDa Workshop
32/10/2022


## Outline

- Why do we choose to use sampling methods?
- Trans-dimensional sampling: What, why, how, limits?
- Future usage for LISA Data Analysis?


## What do we expect for LISA?



## So, what is in the future?

## Way too many events to be measured!

- LISA: $\sim 10^{6}$ DWD ( $\sim 10^{4}$ resolvable), ( $\sim 10^{1}$ ) SMBHB/year, ? EMRIs/year, $\sim 10^{6}$ SOBBHs ( $\sim 10^{1}$ resolvable) ? Stochastic GW backgrounds.
- In some cases, we'll have so many sources, that they will generate a stochastic GW signal above the detector noise!


## Why sampling methods \& Global fit for LISA DA?

## Matched filtering

this is what we normally do, first assume $y=h(\vec{\theta})+n$







## In practice, we define a likelihood function,

 form a posterior, which we then need to investigate.$$
\pi(y \mid \vec{\theta})=C \times e^{-\frac{1}{2}(y-h(\vec{\theta}) \mid y-h(\vec{\theta}))}=C \times e^{-\chi^{2} / 2}
$$

## Defining the parameter space

## Way too many events to be measured!

- Focusing on LISA, we get to measure thousands of overlapping signals of different types.

$$
N_{\vec{\theta}}=N_{\mathrm{ucbs}}+N_{\mathrm{smbhb}}+N_{\mathrm{sobhbs}}+N_{\mathrm{emris}}+N_{\mathrm{stoch}}+N_{\mathrm{noise}} \approx \mathcal{O}\left(10^{5}\right)
$$

## Defining the parameter space

## Way too many events to be measured!

- Focusing on LISA, we get to measure thousands of overlapping signals of different types.

$$
N_{\vec{\theta}}=N_{\mathrm{ucbs}}+N_{\mathrm{smbhb}}+N_{\mathrm{sobhbs}}+N_{\mathrm{emris}}+N_{\mathrm{stoch}}+N_{\mathrm{noise}} \approx \mathcal{O}\left(10^{5}\right)
$$

## LISA Global Fit

- Computational reasons: sequential fits are inefficient
- Grid searches are almost impossible
- Correlations between sources become important for that many signals
- Imperfect source subtraction yields imperfect residuals
- Uncertainties propagation
- Not fixed dimensions!

Trans-dimensional MCMC

## Start with fixed dimensionality

Markov chains

mu

## https://blog.stata.com/

https://blog.revolutionanalytics.com/

- Start from theta_0
- Propose a new point from proposal distribution q
- Accept, or reject with a probability $\alpha=\min \left[1, \frac{p\left(\overrightarrow{\theta_{1}} \mid y\right) q\left(\overrightarrow{\theta_{0}}, \overrightarrow{\theta_{1}}\right)}{p\left(\overrightarrow{\theta_{0}} \mid y\right) q\left(\overrightarrow{\theta_{1}}, \overrightarrow{\theta_{0}}\right)}\right]$


## Continue with non-fixed dimensionality

Assume a model with a changing dimensionality...


## Continue with non-fixed dimensionality

Assume a model with a changing dimensionality...


- Same procedure, now generalized for $\boldsymbol{k}$-order of model. It is organized in two steps.
- Before all, we begin with $\boldsymbol{\theta}_{\mathbf{k}}$ for model $\boldsymbol{k}$.

1. In-Model Step: The usual MH step, for model $\boldsymbol{k}$.
2. Outer-Model Step:

- Propose new $\boldsymbol{\theta}_{\boldsymbol{m}}$ for model $\boldsymbol{m}$ from a given proposal distribution $q$.
- Essentially propose the "birth" or "death" of dimensions at each iteration.
- Accept, or reject with a probability:

$$
\alpha=\min \left[1, \frac{p\left(y \mid \vec{\theta}_{k}\right) p\left(\vec{\theta}_{k}\right) q\left(\left\{k, \vec{\theta}_{k}\right\},\left\{m, \theta_{m}\right\}\right)}{p\left(y, \vec{\theta}_{m}\right) p\left(\vec{\theta}_{m}\right) q\left(\left\{m, \vec{\theta}_{m}\right\},\left\{k, \theta_{k}\right\}\right)}\right]
$$

## Continue with non-fixed dimensionality

## Assume a model with a changing dimensionality...



- Same procedure, now generalized for $\boldsymbol{k}$-order of model. It is organized in two steps.
- Before all, we begin with $\boldsymbol{\theta}_{\mathbf{k}}$ for model $\boldsymbol{k}$.

1. In-Model Step: The usual MH step, for model $\boldsymbol{k}$.
2. Outer-Model Step:

- Propose new $\boldsymbol{\theta}_{\mathbf{m}}$ for model $\boldsymbol{m}$ from a given proposal distribution $q$.
- Essentially propose the "birth" or "death" of dimensions at each iteration.
- Accept, or reject with a probability:

$$
\alpha=\min \left[1, \frac{p\left(y \mid \vec{\theta}_{k}\right) p\left(\vec{\theta}_{k}\right) q\left(\left\{k, \vec{\theta}_{k}\right\},\left\{m, \theta_{m}\right\}\right)}{p\left(y, \vec{\theta}_{m}\right) p\left(\vec{\theta}_{m}\right) q\left(\left\{m, \vec{\theta}_{m}\right\},\left\{k, \theta_{k}\right\}\right)}\right]
$$

## Continue with non-fixed dimensionality

## Assume a model with a changing dimensionality...

- Usually, this means that we have to compute a Jacobian term at each iteration, which is given by:
- Same procedure, now generalized for $\boldsymbol{k}$-order of model. It is organized in two steps.
- Before all, we begin with $\boldsymbol{\theta}_{\mathrm{k}}$ for model $\boldsymbol{k}$.

$$
|\mathbf{J}|=\left|\frac{\partial\left(\vec{\theta}_{m}, u_{m}\right)}{\partial\left(\vec{\theta}_{k}, u_{k}\right)}\right|
$$

1. In-Model Step: The usual MH step, for model $\boldsymbol{k}$.
2. Outer-Model Step:

- Propose new $\boldsymbol{\theta}_{\mathbf{m}}$ for model $\boldsymbol{m}$ from a given proposal distribution $q$.
" Essentially propose the "birth" or "death" of dimensions at each iteration.
- Accept, or reject with a probability:
- Use independent proposals for each k.
- Very useful for multiple signals detection.
- Then, we get:

$$
|\mathbf{J}|=1
$$

$$
\alpha=\min \left[1, \frac{p\left(y \mid \vec{\theta}_{k}\right) p\left(\vec{\theta}_{k}\right) q\left(\left\{k, \vec{\theta}_{k}\right\},\left\{m, \theta_{m}\right\}\right)}{p\left(y, \vec{\theta}_{m}\right) p\left(\vec{\theta}_{m}\right) q\left(\left\{m, \vec{\theta}_{m}\right\},\left\{k, \theta_{k}\right\}\right)}\right]
$$

## A simple example.

## Searching for Gaussian pulses.






Video source: https://www.youtube.com/watch?v=wBTGoA dllo

## What about the LISA Data Analysis?

 It really sounds quite painful to achieve convergence...
## Two ways to improve

## One focusing on the sampler, the second on the waveforms/likelihoods.

-Ensemble Walkers.
-CPU parallelization.

- GPU accelerated Waveforms.
-Delayed Rejection.
-Advanced Search techniques.
>Efficient proposals.


## On the sampler side

- Ensemble Walkers.
- Delayed Rejection.
- Multiple Try.
- Parallel Tempering.


## On the sampler side

D. Foreman-Mackey +, 2013

- Run multiple walkers in parallel.
- Sample a transform of the parameters:

$$
\begin{gathered}
\vec{\zeta}=A \vec{\theta}+b \\
p_{A, b}(\vec{\zeta} \mid y)=p_{A, b}(A \vec{\theta}+b \mid y) \propto p(\vec{\theta} \mid y)
\end{gathered}
$$

- Less sensitive to covariance "features".
- Use walkers to draw candidates (stretch proposal).

A Allows for locating secondary maxima.

- Healthier chains, good mixing.
- Parallelizable.


## On the sampler side

- Ensemble Walkers.
- Delayed Rejection.
- Multiple Try.
- Parallel Tempering.

$$
1 \wedge\left\{\frac{p\left(\vec{\theta}_{2} \mid y\right) q\left(\vec{\theta}_{1}, \vec{\theta}_{0}\right) q\left(\vec{\theta}_{2}, \vec{\theta}_{1}, \vec{\theta}_{0}\right)\left[1-\alpha_{1}\left(\vec{\theta}_{2}, \vec{\theta}_{1}\right)\right]}{p\left(\vec{\theta}_{0} \mid y\right) q\left(\vec{\theta}_{0}, \vec{\theta}_{1}\right) q\left(\vec{\theta}_{0}, \vec{\theta}_{1}, \vec{\theta}_{2}\right)\left[1-\alpha_{1}\left(\vec{\theta}_{0}, \vec{\theta}_{1}\right)\right]}\right\}
$$

A Allows for locating secondary maxima.
A Healthier chains, good mixing.
$\nabla$ Serial calculations

## On the sampler side

- Ensemble Walkers.
- Delayed Rejection.
- Multiple Try.
- Parallel Tempering.


$$
\alpha\left(\vec{\theta}_{t-1}, \vec{\theta}_{t}\right)=1 \wedge\left\{\frac{w\left(\vec{\theta}_{t}^{j}\right)+\sum_{n, n \neq j}^{N} w\left(\vec{\theta}_{t}^{n}\right)}{w\left(\vec{\theta}_{t-1}\right)+\sum_{n, n \neq j}^{N} w\left(\vec{\theta}_{t}^{n}\right)}\right\}
$$

A Allows for mapping the posterior surface.
A Healthier chains, good mixing.
V Many likelihood evaluations.

## On the sampler side



- Ensemble Walkers.
- Delayed Rejection.
- Multiple Try.
- Parallel Tempering.



## Adaptive Parallel Tempering in action

As presented in Vousden et al 2016


## Simple applications

## Usually encountered in data analysis





## Simple applications

## Usually encountered in data analysis




## A realization

## All of the above methods for improving, have one requirement:

V Many likelihood evaluations.

- Running this machinery with limited resources requires a long convergence time.
- Parallelizing really helps!
- Analyze the data in segments.
- Parallelize MCMC processes.
- GPU waveforms/likelihoods change the game!


## Erebor!

## A proposal for a pipeline

- M. Katz, J Gair (AEI), \& N. Korsakova (APC Paris), N Stergioulas, NK (AUTh). -https://github.com/mikekatz04/Eryn
- Using Eryn plus:


1. GPU accelerated Waveforms.
2. Advanced Search techniques.
3. Efficient proposals.
4. Ability to search for multiple models.


And yet...

## Tuning this type of algorithms is hard!

- The scale of the problem of LISA DA is huge!
- The algorithm needs to be exactly fine-tuned to the specific problem, also depending on the frequency band, also accounting for other types of sources, also ...
- Convergence greatly depends on efficiently sampling:
- Need to improve acceptance rate.
- This is where different improvements/enhancements can enter.


## Proposal distributions are crucial

## An example application, part of Erebor, led by N. Korsakova

- First run a search phase on the data.
- Subtract "loudest" sources.
- Get an estimate of residuals,
- and then run a set of RJ MCMC on those residuals, looking for the "harder-to-get" lower SNR signals.
- Use those samples we to construct efficient proposals!


## Proposal distributions are crucial

## An example application, part of Erebor, led by N. Korsakova

- First run a search phase on the data.
- Subtract "loudest" sources.
- Get an estimate of residuals,
- and then run a set of RJ MCMC on those residuals, looking for the "harder-to-get" lower SNR signals.
- Use those samples we to construct efficient proposals!
- Fit probability distribution function from the samples.
- Use Normalising Flows as a density estimator.
- Train network by optimising Kullback-Leibler divergence between samples and transformed base distribution.

$$
K L(p \| q)=\sum_{x} p(x) \log \left[\frac{p(x)}{q(x)}\right]
$$

- Use estimated distribution for proposals.


## Proposal distributions are crucial

## An example application, part of Erebor, led by N. Korsakova



## Proposal distributions are crucial

## An example application, part of Erebor, led by N. Korsakova



## Proposal distributions are crucial

## An example application, part of Erebor, led by N. Korsakova



## Proposal distributions are crucial

## An example application, part of Erebor, led by N. Korsakova



- Trans-dimensional methods for LISA global fit are extremely useful.
- But also very hard to tune and scale them to the problem.
- We are in a good state though! [See next talk by K. Lackeos]
- Novel methods can help ease the burden of stochastic methods, or in some cases replace them entirely.
- The scale of the problem is so large, that any improvement counts!


## 'E६tpa Matépıa入



$$
\text { Posterior: } \quad p(k \mid y)=\frac{p(y \mid k) p(k)}{p(y)}=\frac{\int_{\Theta_{k}} p\left(y \mid \theta_{k}, k\right) p\left(\theta_{k} \mid k\right) d \theta_{k} p(k)}{p(y)}
$$

$$
\text { Acceptance ratio: } \quad \alpha=\min \left(1, \frac{p\left(k^{\prime}, \theta_{k^{\prime}} \mid y\right) q_{1}\left(k ; k^{\prime}\right) q_{2}(u)}{p\left(k, \theta_{k} \mid y\right) q_{1}\left(k^{\prime} ; k\right) q_{2}\left(u^{\prime}\right)}\left|\frac{\partial\left(\theta_{k^{\prime}}, u\right)}{\partial\left(\theta_{k}, u^{\prime}\right)}\right|\right)
$$

Proposal distributions for dimension matching parameters:

Map functions for different k :
Jacobian is Unity when we use independent proposals:

$$
q_{2}(u) \text { and } q_{2}\left(u^{\prime}\right)
$$

$$
\theta_{k^{\prime}}=g\left(\theta_{k}, u^{\prime}\right) \quad \theta_{k}=g\left(\theta_{k^{\prime}}, u\right)
$$

$$
\theta_{k}=g\left(\theta_{k^{\prime}}, u\right)=u \text { and } \theta_{k^{\prime}}=g\left(\theta_{k}, u^{\prime}\right)=u^{\prime}
$$

