Massive Black Hole Binary parameter estimation using Masked Autoregressive Flows

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LISA Data Analysis: from Classical Methods to Machine Learning

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Towards a LISA DA pipeline

LISA L1 data $\rightarrow$???? $\rightarrow$ Posterior $p(\boldsymbol{\theta}|\mathbf{d})$

Bayesian inference

Likelihood $\log p(\,\mathbf{d} \mid \boldsymbol{\theta}\,) = \sum_{n=\{A,E,T\}} 2\,(\,\mathbf{h}(\boldsymbol{\theta}) \mid \mathbf{d}\,)_n - (\,\mathbf{h}(\boldsymbol{\theta}) \mid \mathbf{h}(\boldsymbol{\theta})\,)_n$

integrals!

forward simulations!

$$p(\,\boldsymbol{\theta} \mid \mathbf{d}\,) = \frac{p(\,\mathbf{d} \mid \boldsymbol{\theta}\,)\, p(\boldsymbol{\theta})}{p(\mathbf{d})}$$

Prior

Posterior

Evidence

even harder integrals!

$$p(\mathbf{d}) = \int p(\,\mathbf{d} \mid \boldsymbol{\theta}\,)\, d\boldsymbol{\theta}$$

Density estimation

- In practice, "classical" methods usually sample $p(\boldsymbol{\theta} \mid \mathbf{x}_{\text{obs}})$ with e.g. MCMC.
  - Use $p(\boldsymbol{\theta} \mid \mathbf{x}_{\text{obs}}) \propto p(\mathbf{x}_{\text{obs}} \mid \boldsymbol{\theta})\, p(\boldsymbol{\theta})$ to get posterior samples.
  - Sampling the likelihood can be tricky and take a long time…

- We'll try avoid computing $p(\mathbf{x} \mid \boldsymbol{\theta})$ at all using Machine Learning. Options:
  1. Estimate $p(\mathbf{x}, \boldsymbol{\theta})$, then substitute $\mathbf{x}_{\text{obs}}$ to find $p(\boldsymbol{\theta} \mid \mathbf{x}_{\text{obs}})$
  2. Estimate $p(\boldsymbol{\theta} \mid \mathbf{x})$ directly, then substitute $\mathbf{x}_{\text{obs}}$
  3. Estimate $p(\mathbf{x} \mid \boldsymbol{\theta})$ and use Bayes to find $p(\boldsymbol{\theta} \mid \mathbf{x}_{\text{obs}})$

Normalising Flows

Consider a complicated "target distribution" $q(x)$.
Can we find an invertible transformation $x = f(z)$ such that, starting from a simple "base distribution" $p(z)$, we recover $q(x)$ via change of variable?

$$\int q(x)\,dx = \int p(z)\,dz = 1$$

$$q(x) = p(z)\left|\frac{dz}{dx}\right| = p\big(f^{-1}(x)\big)\left|\frac{df^{-1}(x)}{dx}\right|$$

For multivariate distributions,

$$q(\mathbf{x}) = p(\mathbf{z})\,|\det \mathbf{J}[f^{-1}(x)]|$$

In practice, this determinant is generally **expensive** to compute!

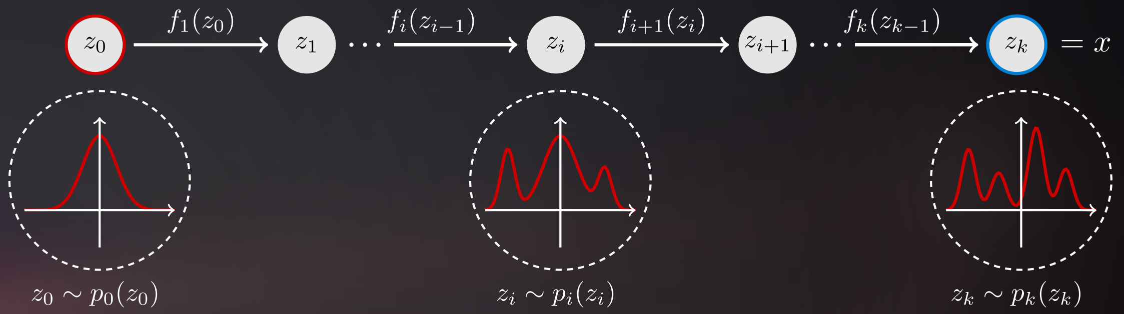


Image: Janosh Riebesell @ github

To create complex transformations, use compositions of simpler ones → a *flow* of transformations:

$$f(\mathbf{z}) = [f_k \circ f_{k-1} \circ \cdots \circ f_2 \circ f_1](\mathbf{z})$$

$$q(\mathbf{x}) = p(\mathbf{z}) \prod_{i=1}^{k} |\det \mathbf{J}[f_i(\mathbf{z}_{i-1})]|^{-1}$$

Masked Autoregressive Flows (MAF)

In summary: we will be chaining some transformation $f_i(\mathbf{z})$, which needs to be:

- Invertible
- Differentiable
- Easy-to-compute $\det \mathbf{J}$ (e.g., triangular $\mathbf{J}$)
- Expressive!

Several exist in the literature.

We choose: $x_j(\mathbf{z}) = \mu_j + z_j\,\sigma_j \quad \begin{cases} \mu_j = f_{\mu_j}(\mathbf{x}_{1,\dots,j-1}), \\ \sigma_j = f_{\sigma_j}(\mathbf{x}_{1,\dots,j-1}) \end{cases}$

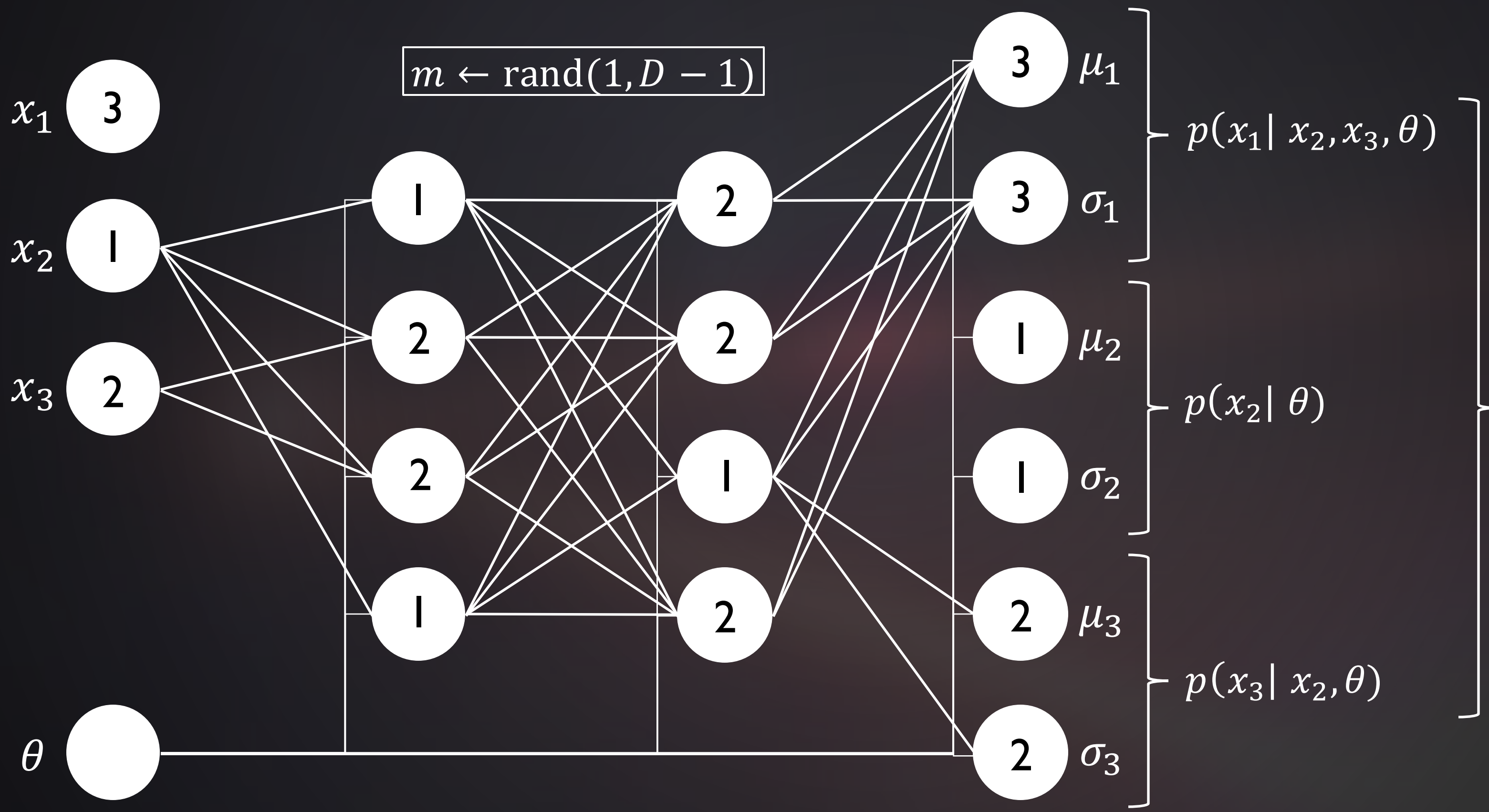
This is equivalent to modeling

$$q(\mathbf{x}) = \prod_{j=1}^{D} p(\, x_j \mid \mathbf{x}_{1,\dots,j-1}\,) = p(x_1)\, p(\, x_2 \mid x_1\,)\, p(\, x_3 \mid x_2, x_1\,) \dots \longrightarrow$$ This is our loss function!

$$\mathcal{N}(\, x_j \mid \mu_j(x_{1,\dots,j-1}), \sigma_j^2(x_{1,\dots,j-1})\,)$$

(Papamakarios et. al., arXiv: 1705.07057)

Masked Autoencoder for Distribution Estimation (MADE)



$$p(\mathbf{x} \mid \theta) = p(x_2 \mid \theta) \times p(x_3 \mid x_2; \theta) \times p(x_1 \mid x_2, x_3; \theta)$$

(Germain et. al., arXiv: 1502.03509)

MADE in practice: Masks

It is computationally easier to introduce masks $\mathbf{M}$ so that:

$$\mathbf{h}^l(\mathbf{h}^{l-1}) = g(\,(\mathbf{W}^l \odot \mathbf{M}^{\mathbf{W}^l})\mathbf{h}^{l-1} + \mathbf{b}^l + \mathbf{W}^l_\theta \boldsymbol{\theta})$$

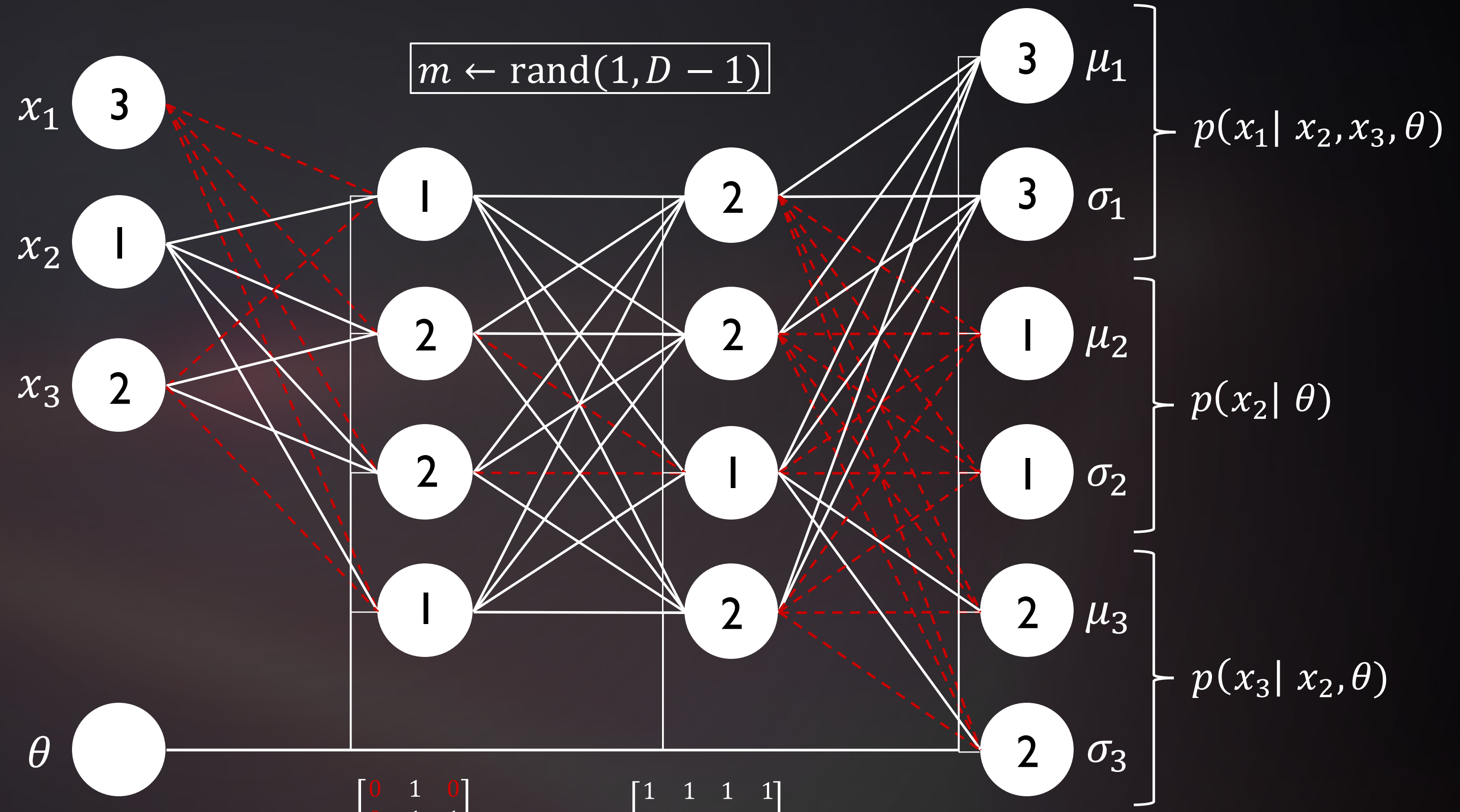
For hidden layers:

$$\mathbf{M}^{\mathbf{W}^l}_{k',k} = \begin{cases} 1 & \text{if } m^l(k') \geq m^{l-1}(k) \\ 0 & \text{otherwise.} \end{cases}$$

For the output layer:

$$\mathbf{M}^{\mathbf{W}^L}_{k',k} = \begin{cases} 1 & \text{if } m^L(k') > m^{L-1}(k) \\ 0 & \text{otherwise.} \end{cases}$$

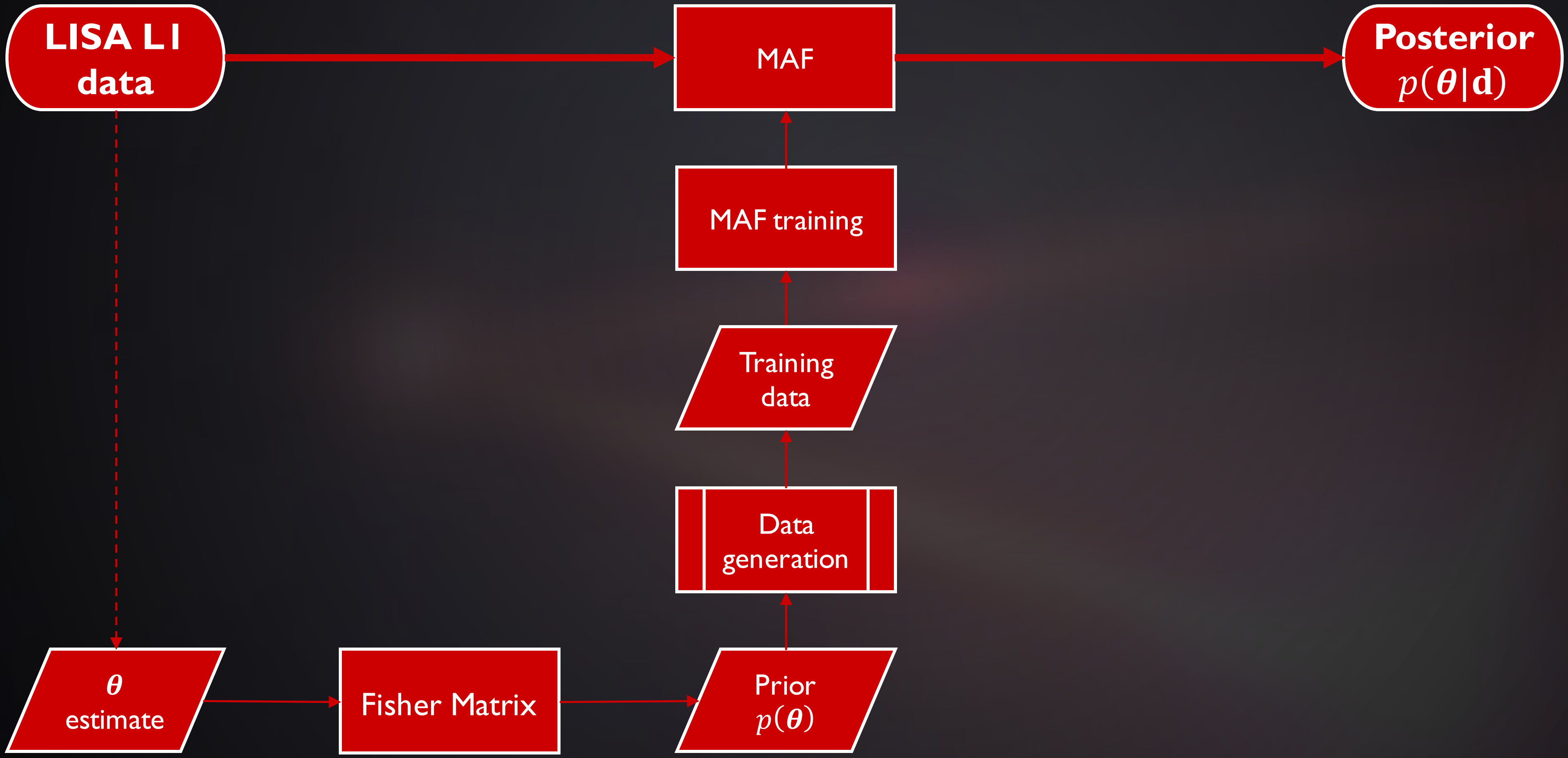
Stack several of these, with randomized ordering! ➡ **MAF**



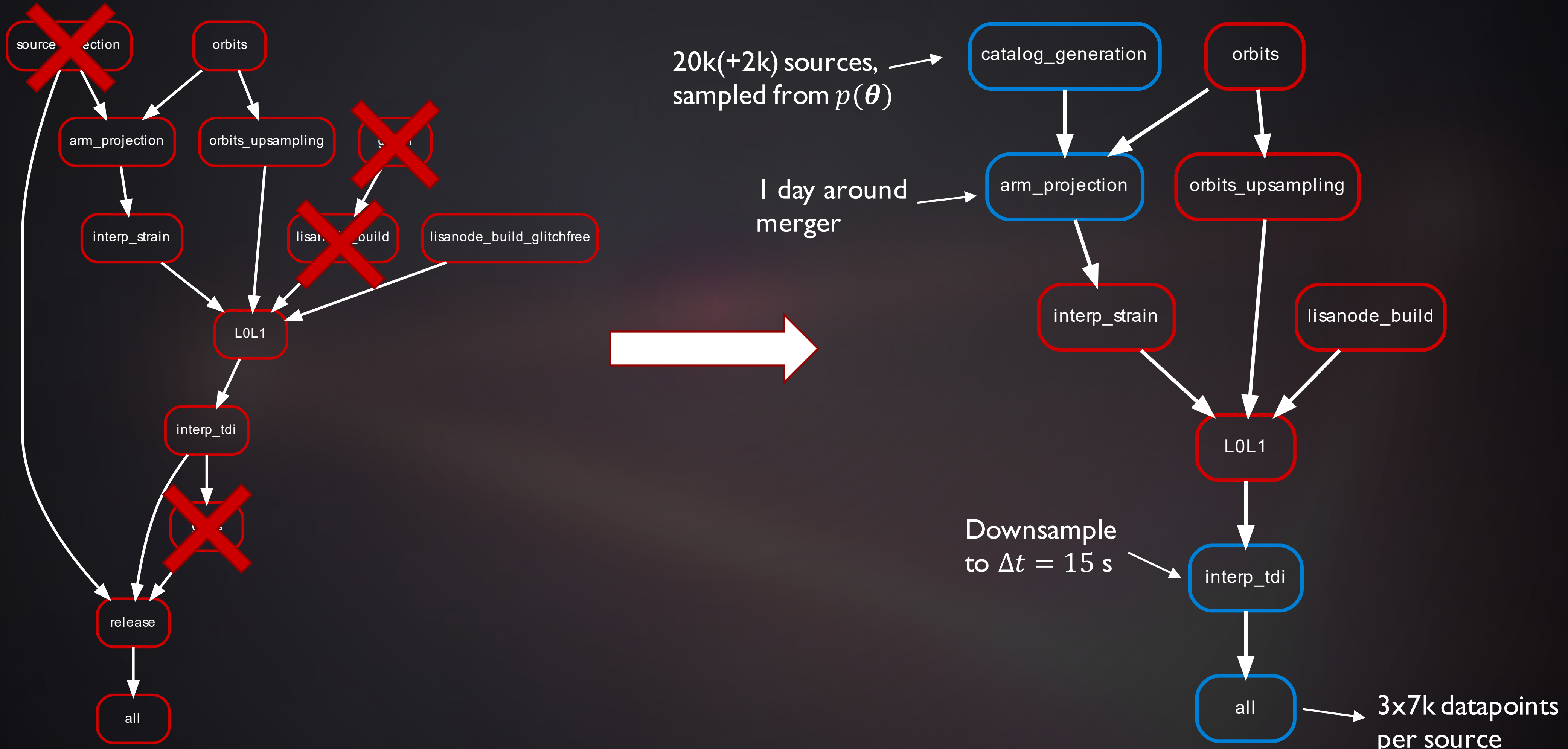
$$\mathbf{M}^{\mathbf{W}^1} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad \mathbf{M}^{\mathbf{W}^2} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \quad \mathbf{M}^{\mathbf{W}^3} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

(Germain et. al., arXiv: 1502.03509)

Towards a LISA DA pipeline



Data generation



Principal Component Analysis (PCA)

- Define

$$\mathrm{X} = \underbrace{\begin{bmatrix} | & | & \dots & | \\ \mathbf{d}_1 & \mathbf{d}_2 & \dots & \mathbf{d}_n \\ | & | & \dots & | \end{bmatrix}}_{(n \text{ columns})} \Bigg\} \text{(}m\text{ rows)} \qquad (m \geq n)$$

- One can decompose $\underset{(m,n)}{\mathrm{X}} = \underset{\substack{(m,m)\\ \text{unitary}}}{\mathrm{U}} \, \underset{\substack{(m,n)\\ \text{diag.}}}{\Sigma} \, \underset{\substack{(n,n)\\ \text{unitary}}}{\mathrm{V}^T} \longrightarrow \mathbf{d}_j = \mathrm{U}\,\Sigma\,\mathrm{V}_j^T$

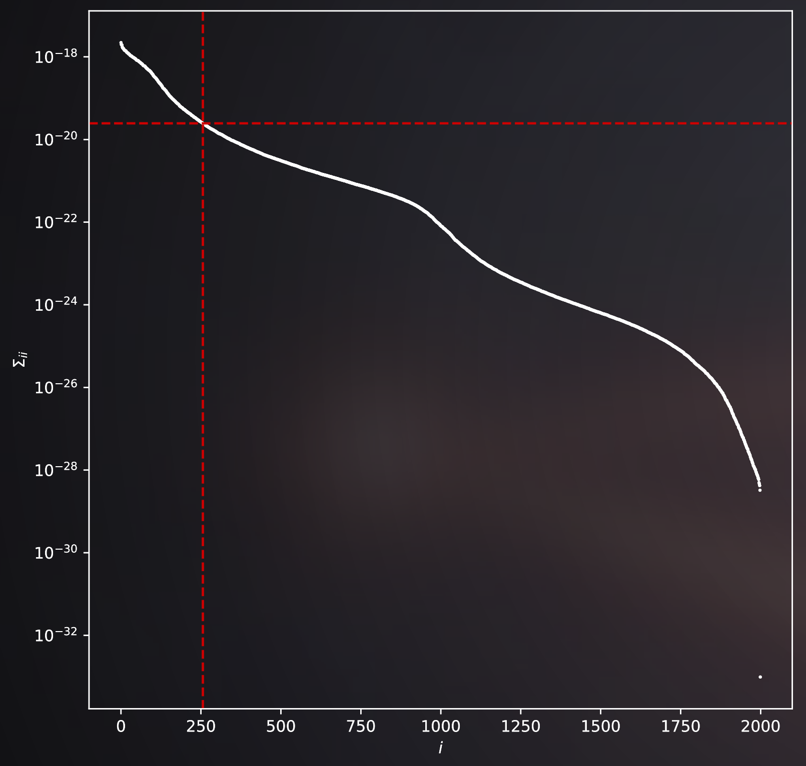
Singular Value Decomposition (SVD)

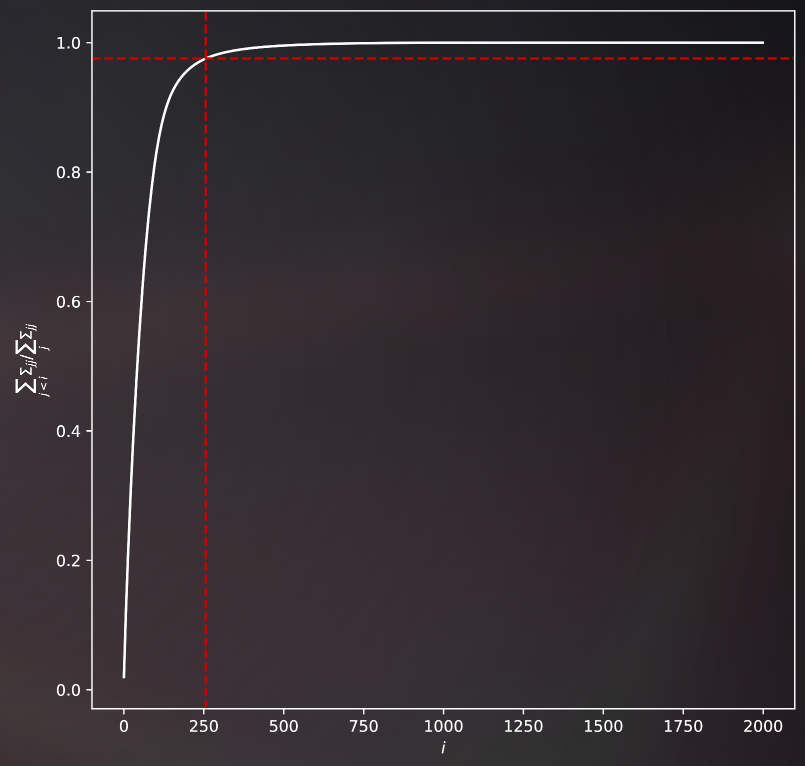
- Approximately, one can decompose

$$\mathrm{X} \approx \underset{(m,n)}{\widetilde{\mathrm{X}}_r} = \underset{(m,r)}{\widetilde{\mathrm{U}}} \, \underset{(r,r)}{\widetilde{\Sigma}} \, \underset{(r,n)}{\widetilde{\mathrm{V}}^T} \qquad (r < n)$$

- Then, for new $\underset{(m)}{\mathbf{d}} \rightarrow \underset{(r)}{\mathbf{x}} = \underset{(r,m)}{\widetilde{\mathrm{U}}^T} \underset{(m)}{\mathbf{d}}$ is a data summary!

Principal Component Analysis (PCA)





Some results

Validation

PRELIMINARY!!!

PRELIMINARY!!!

Some results

Spritz

PRELIMINARY!!!

PRELIMINARY!!!

Some results

"Spritz-like"

PRELIMINARY!!!

PRELIMINARY!!!

Conclusions

- We were able to successfully model the log-likelihood as a MAF

- Applications:
  - Very fast evaluation of the likelihood
  - GPU-accelerated MCMC, with gradients!
  - Fast waveform emulators, possibly?

- Caveats:
  - Tuned to narrow prior (but should be generalizable with enough compute power)
  - Issues with actual LDC data
  - Plenty of fine-tuning avenues