Likelihood- free Inference for Large Forward Models in Astrophysics/ Cosmology

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Timeline of the Universe



Structure Formation in the Universe

Time since the Big Bang: 0.4 billion years



21st century cosmology



Overview

- Large Forward Models
- Inverse Problems
- Solving inverse problems with Neural Networks
- Examples

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Large Forward Models



- ~ 6 Gamma-ray sources
- Diffuse emission

- 188 Gamma-ray sources
- Extended point sources
- Resolved gas emission

- 6658 Gamma-ray sources
- Highly resolved gas
- Many extended sources
- Fermi bubbles
- GeV excess
- Dark gas
- .

More data leads to more objects. More objects lead to more parameters. More parameters lead to more complicated statistical analyses.

Binary black hole merger Bravitational waves



Livingston, Louisiana (L1)



- Computationally expensive numerical relativity simulations.
- Many parameters (masses or merging objects, positions in the sky etc...)

Characteristics of Large Forward Models

A forward model generates samples $x, z \sim p(x|z)p(z)$. Why it could be large? simulator

- 1. Model Complexity: Number of parameters with complex interactions between them
- 2. Amount of Data: Different data sources, volume of data
- 3. Computational Recourses: Computational power, memory or time to run

In Physics and Astronomy

Forward models are usually principled. They implement specific physical laws. Parameters z typically have an interpretation in terms of specific physical quantities.

Inverse Problems



Bayes Theorem



where $p(\mathbf{x}) = \int d\mathbf{z} \ p(\mathbf{x}|\mathbf{z})p(\mathbf{z})$

Evidence

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Likelihood-based Inference



Image credit: Wikipedia

Ex: Metropolis Hastings Algorithm

$$p(\boldsymbol{z}|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})}{p(\boldsymbol{x})}$$

• MC methods sample from the joint highdimensional posterior for all parameters

 $\boldsymbol{z} \sim p(\boldsymbol{z} | \boldsymbol{x}), \boldsymbol{z} \in \mathbb{R}^{D}$

D: Number of parameters

Obtain marginals by projection onto parameters of interest

 $\boldsymbol{z} \equiv (\boldsymbol{z}_1, \boldsymbol{z}_2, \dots, \boldsymbol{z}_D)^T \to (zi, zj)^T \in \mathbb{R}^2$

Expensive!

• Require an explicit likelihood

Likelihood-based Inference



Likelihood-based Inference vs high dimensional models



Slide credit: Christoph Weniger

Making problems tractable



Slide credit: Christoph Weniger

A thought experiment



Simulated images:



1, 3, 2, 1 , 5, 4, 3, 1, 6, 7, 9,
6, 2, 5, <mark>8</mark> , 6, 8, 4, 3, 2, 1, 3,
3, 4, 2, <mark>3</mark> , 1, 7, 8, 9, 5, 3, 2,
4, 2, 1, <mark>4</mark> , 6, 8, 6, 4, 3, 2, 4,
1, 3, 2, <mark>9</mark> , 5, 4, 3, 1, 6, 7, 9,
6, 2, 5, <mark>8</mark> , 6, 8, 4, 3, 1, 3, 4,
2, 3, 4, 1 , 1, 7, 8, 9, 5, 3, 2,
4, 2, 1, 2 , 6, 8, 6, 4, 3, 2, 4,
1, 3, 2, <mark>4</mark> , 5, 4, 3, 1, 6, 7, 9,

?

Red (position of moon): parameter of interest

Black: **Nuisance parameters** (parametrizing *all* possible background images)

A thought experiment



1, 3, 2, **1**, 5, 4, 3, 1, 6, 7, 9, ... 6, 2, 5, **8**, 6, 8, 4, 3, 2, 1, 3, ... 3, 4, 2, 3, 1, 7, 8, 9, 5, 3, 2, ... 4, 2, 1, 4, 6, 8, 6, 4, 3, 2, 4, ... 1. 3. 2. 9. 5. 4. 3. 1. 6. 7. 9. ... 6, 2, 5, **8**, 6, 8, 4, 3, 1, 3, 4, ... 2, 3, 4, **1**, 1, 7, 8, 9, 5, 3, 2, ... 4, 2, 1, **2**, 6, 8, 6, 4, 3, 2, 4, ... 1, 3, 2, 4, 5, 4, 3, 1, 6, 7, 9, ...

-, -, -, **8**, -,-, -, -, -, -, -, ...

Red (position of moon): parameter of interest

Black: **Nuisance parameters** (parametrizing *all* possible background images)

Observed data:

Simulated images:



A thought experiment



You learned from a few examples to recognize the pattern related to the parameter of interest.

Simulation efficient: Just 8 examples are enough!

How can we achieve efficiency and precision?

Neural simulation-based inference (SBI)

Numerous methods exist with various pros/cons



Fig. 3. Overview of different approaches to simulation-based inference.

[Cranmer, Brehmer, Louppe 1911.01429]

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General goal: obtain *neural network approximator* for one of the following:

• Posterior*



- Likelihood*
- Ratios of posteriors and priors = ratios of likelihood and evidence



• Various variations of the above quantities ...

Neural Ratio Estimation (NRE)

Estimating the joint-vs-marginal ratio estimates the posterior

Bayes theorem

$$r(\mathbf{x}, \mathbf{z}) = \frac{p(\mathbf{x}, \mathbf{z})}{p(\mathbf{x})p(\mathbf{z})} = \frac{p(\mathbf{x}|\mathbf{z})p(\mathbf{z})}{p(\mathbf{x})p(\mathbf{z})} = \frac{p(\mathbf{z}|\mathbf{x})}{p(\mathbf{z})}$$

Strategy: We train a neural network $d_{\varphi}(x, z)$ as a binary classifier to be able to distinguish

- dependent sample-parameter pairs: $x, z \sim p(x|z) p(z)$ with class label Y=1 from
- independent ones: $x, z \sim p(x) p(z)$ with class label Y=0.

[Cranmer, Begy, Louppe 1903.04057]

Neural Ratio Estimation (NRE)

We want the output of the NN to be the probability of class Y=1, i.e.,

$$d_{\varphi}(x,z) = p(y = 1 | x, z) = \frac{p(x,z|Y=1)p(Y=1)}{p(x,z|Y=1)p(Y=1) + p(x,z|Y=0)p(Y=0)} = \frac{p(x,z)}{p(x,z) + p(x)p(z)}$$

The corresponding loss function is the binary cross-entropy loss function:

$$L[d_{\varphi}(\boldsymbol{x},\boldsymbol{z})] = -\int d\boldsymbol{x} \, d\boldsymbol{z} \, p(\boldsymbol{x},\boldsymbol{z})[-\ln(d_{\varphi}(\boldsymbol{x},\boldsymbol{z})]) + p(\boldsymbol{x})p(\boldsymbol{z})[\ln(1-d_{\varphi}(\boldsymbol{x},\boldsymbol{z}))]$$

z={cats, donkeys}



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Cat

Cat

Minimizing this function w.r.t. the network parameters ϕ yields

$$d_{\varphi}^{*}(\boldsymbol{x},\boldsymbol{z}) = \frac{p(\boldsymbol{x},\boldsymbol{z})}{p(\boldsymbol{x},\boldsymbol{z}) + p(\boldsymbol{x})p(\boldsymbol{z})} \quad \text{and thus} \quad r(\boldsymbol{x},\boldsymbol{z}) = \frac{d_{\varphi}^{*}(\boldsymbol{x},\boldsymbol{z})}{d_{\varphi}^{*}(\boldsymbol{x},\boldsymbol{z}) - 1} \quad \begin{bmatrix} \text{Cranmer, Brehmer,} \\ \text{Louppe 1911.01429} \end{bmatrix}$$

Using the result of the NN we have access to posteriors

$$p(\boldsymbol{z}|\boldsymbol{x}) = r(\boldsymbol{x}, \boldsymbol{z}) \cdot p(\boldsymbol{z})$$



• Estimates:

 $p(\mathbf{z}_1|\mathbf{x}), p(\mathbf{z}_2|\mathbf{x}), p(\mathbf{z}_3,\mathbf{z}_4|\mathbf{x})$

 $p(z_1, z_2 | x), p(z_1, z_2, z_3 | x)$

Does not estimate

Pros

- Implicit likelihood → Cherry-picking marginal posteriors!
- No need to retrain to look at a different observation (Amortization)
- Ability to focus on a single observation through truncation
- Easy network architecture

Cons

 Difficult to sample from high-dim posteriors

Example 1:

A toy model for N-body simulations

[AD, Camila Correa, Christoph Weniger 2206.11312]

- Goal: reconstruction of halo clustering and halo mass function of DM-only cosmological simulations generated by the EAGLE project
- Approach: an analytical halo model based on a toy implementation of two body correlation functions
- The EAGLE project





- > The **first parameter of interest** is the number, *N* , of the haloes
- ➤ The masses of the haloes, $M_h \in (10^9, 10^{12})$ M_☉, can be sampled from a halo mass function

$$rac{dn}{dM} \propto M^{-a}$$

> The second parameter of interest is the slope, *a*, of the halo mass function

Adding Clustering to the Model

> We will sample the positions according to distributions generated from 2D realizations of gaussian random fields, δ

 $P(k) \propto \frac{1}{k^n}$

> The gaussian fields will be specified by a power-law power spectrum

> The slope of the power spectrum, *n*, is the **third parameter of interest** of our model



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Adding Clustering to the Model

- > We transform the field δ to a probability distribution function to sample from it:
 - We first multiply δ with a fourth parameter of interest ε ,
 - We exponentiate $\boldsymbol{\delta} \cdot \boldsymbol{\varepsilon}$,
 - We normalize the field $f = e^{\delta \cdot \varepsilon}$, s.t., its values sum to 1



> We sample the positions of the haloes according to this distribution

• The toy halo model

> We calculate the logarithmic surface density

> We add all the images of the individual haloes together to obtain the total surface density field



Thousands of nuisance parameters: positions of haloes, masses



Training NRE

Parameters of interest:

- > N: Number of halos, where $N \in (100, 2100)$
- > a : Inner slope of the halo mass function, $a \in (1, 3)$

 ε : Exponent of the density field, where $\varepsilon \in (0,2)$

n: Slope of the power spectrum, where $n \in (0, 10)$

• We define a CNN:



• We train using 200.000 mock images

Results on actual N body simulations



Results on actual N body simulations

Box 4 orientations 4 simulation boxes Box 3 ٠ and 3 rotations of them Box 2 interval 68.45% **94.74%** Box 1 correct value 1.5 1000 1200 1400 1600 1800 2000 1.0 2.0 2.5 3.0 800 slope of halo mass function (a) number of haloes (N) Box 4 Box 3 Box 2 Box 1 1.5 0.0 0.5 1.0 2.0 10 6 Ó 2 4 8 exponent of density field (ε) slope of power spectrum (*n*)

different box

•

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N-body simulation image vs mock image



Neural Posterior Estimation (NPE)

Approximate $p(\mathbf{z}|\mathbf{x_0})$ with a NN $q_{\varphi}(\mathbf{z}|\mathbf{x_0})$. How can we compare the two pdfs?

$$D_{KL}(p||q_{\phi}) = \int d\mathbf{z} \ p(\mathbf{z}|\mathbf{x}_{0}) \ln \left[\frac{p(\mathbf{z}|\mathbf{x}_{0})}{q_{\phi}(\mathbf{z}|\mathbf{x}_{0})}\right] = \mathbb{E}_{\mathbf{z} \sim p(\mathbf{z}|\mathbf{x}_{0})} \ln \left[\frac{p(\mathbf{z}|\mathbf{x}_{0})}{q_{\phi}(\mathbf{z}|\mathbf{x}_{0})}\right] \text{ intractable}$$

Problem: How to avoid sampling from the intractable posterior?

Solution: Amortize (average) over simulation data. The loss is now the expected KL divergence, where we have exploited Bayes theorem, i.e., p(x|z)p(z) = p(z|x)p(x).

$$\mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x})} \Big[D_{\boldsymbol{KL}}(\boldsymbol{p} | | \boldsymbol{q}_{\phi}) \Big] = \mathbb{E}_{\boldsymbol{x} \sim p(\boldsymbol{x})} \mathbb{E}_{\boldsymbol{z} \sim p(\boldsymbol{z} | \boldsymbol{x})} \Big[\ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \Big] = \mathbb{E}_{\boldsymbol{x}, \boldsymbol{z} \sim p(\boldsymbol{x}, \boldsymbol{z})} \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \Big] = \mathbb{E}_{\boldsymbol{x}, \boldsymbol{z} \sim p(\boldsymbol{x}, \boldsymbol{z})} \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \Big] \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \\ \mathbf{x} = p(\boldsymbol{x}, \boldsymbol{z}) \begin{bmatrix} \ln \frac{p(\boldsymbol{z} | \boldsymbol{x})}{\boldsymbol{q}_{\varphi}(\boldsymbol{z} | \boldsymbol{x})} \end{bmatrix} \end{bmatrix}$$

Neural Posterior Estimation (NPE)

$$\mathbb{E}_{x \sim p(x)} \Big[D_{KL}(p \, | \, | \, q_{\phi}) \Big] = \mathbb{E}_{x, z \sim p(x, z)} \Big[\ln \frac{p(z \, | \, x)}{q_{\varphi}(z \, | \, x)} \Big] = -\mathbb{E}_{x, z \sim p(x, z)} \ln q_{\varphi}(z \, | \, x) + \mathbb{E}_{x, z \sim p(x, z)} \ln p(z \, | \, x)$$

Training inference networks with forward KL leads to posteriors that minimize the posterior entropy:

$$\mathcal{L} = -\mathbb{E}_{\mathbf{x},\mathbf{z} \sim p(\mathbf{x},\mathbf{z})} \ln q_{\varphi}(\mathbf{z}|\mathbf{x}) \longrightarrow \varphi^{*} \text{ (optimum parameters)} \quad \begin{bmatrix} \text{Papamakarios, Murray} \\ 1605.06376 \end{bmatrix}$$

Pros

- Implicit likelihood → Cherry-picking marginal posteriors!
- No need to retrain to look at a different observation (Amortization)
- Ability to focus on a single observation
 with multi-round inference
- Obtain samples and evaluate the posterior

Cons

q_φ should be a PDF, i.e. normalizing flow or Gaussian mixture model, sometimes difficult to train

Example 2: Reconstruction of Gravitational Wave Backgrounds

[AD, Daniel G. Figueroa, Bryan Zaldivar 2309.08430]

- Goal: Reconstructing the spectral shape Ω_{GW}(f) of an unknown Stochastic Gravitational Wave Background (SGWB) with LISA:
 - will consist of a constellation of three
 satellites forming a nearly equilateral triangle
 with ~ 2.5 million km length arms
 - will perform three correlated interferometric measurements (X, Y and Z data streams)
 - X, Y and Z data streams can be transformed into three uncorrelated ones (A, E, and T), which diagonalise the signal and noise covariance matrices
 - will cover frequencies from 3×10⁻⁵Hz to 0.5
 Hz



- Approach: A model for data as close as possible to the real data-taking procedure of LISA
 - ➤ We assume that the LISA mission will last 4 years.
 - The data will be collected 75% of the time and will be clean of noise glitches and transient signals.
 - > Due to the need for regular operational breaks, the data will be collected in 94 time chunks (N_c).

Data

α, β: given channels	GW signal	Noise
	$D_{i,j}^{lphaeta} = S_{i,j}$ +	$\mathcal{N}_{i,j}^{lphaeta}$
$i \in \{1, 2,, N_c\}$ time chunks	$f_i \in \{3 \times 10^{-3}, 0.5\}$	

> Data

 \succ For each frequency f_i , we obtain channel

$$\mathcal{N}_{i,j}^{\alpha\beta} = \left| \frac{G_3\left(0, \sqrt{\Omega_{\text{noise}}^{\alpha\beta}(f_j)}\right) + iG_4\left(0, \sqrt{\Omega_{\text{noise}}^{\alpha\beta}(f_j)}\right)}{\sqrt{2}} \right|^2$$
, we obtain the mean across time chunks for each char

Gs samples from Gaussian distributions

where

$$S_{i,j} = \left| \frac{G_1\left(0, \sqrt{\Omega_{\text{GW}}(f_j)}\right) + iG_2\left(0, \sqrt{\Omega_{\text{GW}}(f_j)}\right)}{\sqrt{2}} \right|^2$$

Noise

GW signal

 $D_{i,j}^{lphaeta} = S_{i,j} + \mathcal{N}_{i,j}^{lphaeta}$

$$ar{D}_j^{lphaeta} = rac{1}{N_c}\sum_{i=1}^{N_c}D_{i,j}^{lphaeta}$$

Noise power spectra

> We model the LISA noise spectra in the A, E, and T channel basis,



GW power spectrum

We define a GW signal with an unknown frequency profile by approximating it in a piece-wise manner as power-laws in 27 intervals (27 *bins*).



> Given a dataset $D_0 = \{D_0^{AA}, D_0^{EE}, D_0^{TT}\}$ we want to reconstruct and plot,

$$\Omega_{\rm GW}(f;\mathbf{s}) = \Omega_p^{(*)} \cdot \begin{cases} \vdots \\ F_{-2}(f) & \text{if } f_{-2} \le f < f_1 \\ F_{-1}(f) & \text{if } f_{-1} \le f < f_0 \\ F_0(f) & \text{if } f_0 \le f < f_1 \\ F_{1}(f) & \text{if } f_1 \le f < f_2 \\ F_{+1}(f) & \text{if } f_1 \le f < f_2 \\ F_{+2}(f) & \text{if } f_2 \le f < f_3 \\ \vdots \end{cases}$$
 with $F_{-1}(f) \equiv F_0(f_1) \left(\frac{f}{f_1}\right)^{\gamma_1}, \quad F_{-2}(f) \equiv F_{-1}(f_{-1}) \left(\frac{f}{f_{-1}}\right)^{\gamma_{-2}}, \quad \dots$

i.e., we need to sample from $p(\Omega_p(*), ..., \gamma_{-1}, \gamma_0, \gamma_1, ..., A_P, A_{acc} | \boldsymbol{D}_0)$

- **30 parameters of interest:** 2 noise + 28 GW parameters
- thousands of nuisance parameters: G's
- non-gaussian likelihood



GWBackFinder pipeline



GWBackFinder pipeline

Test coverage on mock data

 Compare analysis with MCMC for mock data using a non-gaussian likelihood:

$$\ln \mathcal{L} = rac{1}{3}\ln \mathcal{L}_G + rac{2}{3}\ln \mathcal{L}_{LN}$$

 $\mathcal{O}(10^5)$ likelihood evaluations to obtain the posterior of only one observation

slow & NOT Amortized !

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GWBackFinder pipeline

 10^{-9}

0-10

C 0⁻¹¹

0-12

0-13

- Reconstruct template signals, e.g.,
 - ➤ single power-law
 - broken power-law \succ

single bump signal



Accurate & fast reconstruction!



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Frequency [Hz]

SBI appears to be broadly applicable

Supernova cosmology



arxiv: 2209.06733

CMB physics



arxiv: 1911.01429

Stellar streams

Gravitational waves



arxiv: 2308.06318

Strong Lensing



arxiv: 2211.04365

Conclusions

- Large forward models are omnipresent in physics/astronomy and pose challenges for analysing current and future data.
- Deep learning opens many new powerful ways for tackling these inference problems.
- There is a large variety of different methods and algorithms, both simulation- and likelihood-based, which differ in applicability, scaling and requirements for the forward model.
- There are many open research questions, both in physics/ astronomy and computer science.

Thank you!