

Neural Simulation-Based Inference

November 2023

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Simulators

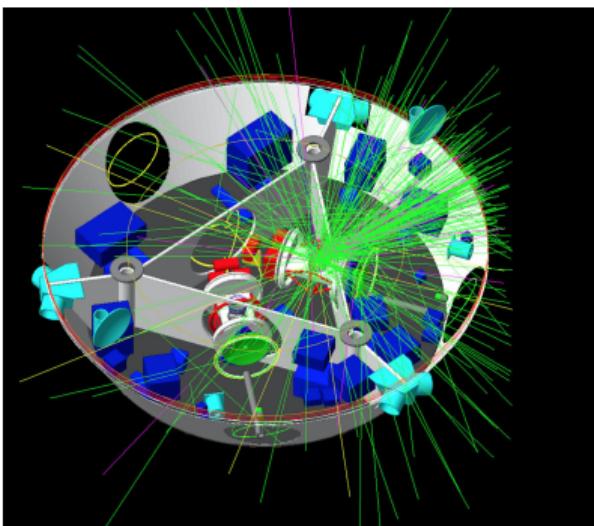
Scientists just love developing mechanistic models of phenomena:

- Particle physics
- Neuroscience
- Population genetics
- Epidemiology
- Climate/Earth sciences
- Astrophysics

Thanks to modern computing, they can turn these into high-precision simulators.

Simulators: An Example

Geant4 - particle simulator (CERN 2023).



Science (like, most of it)

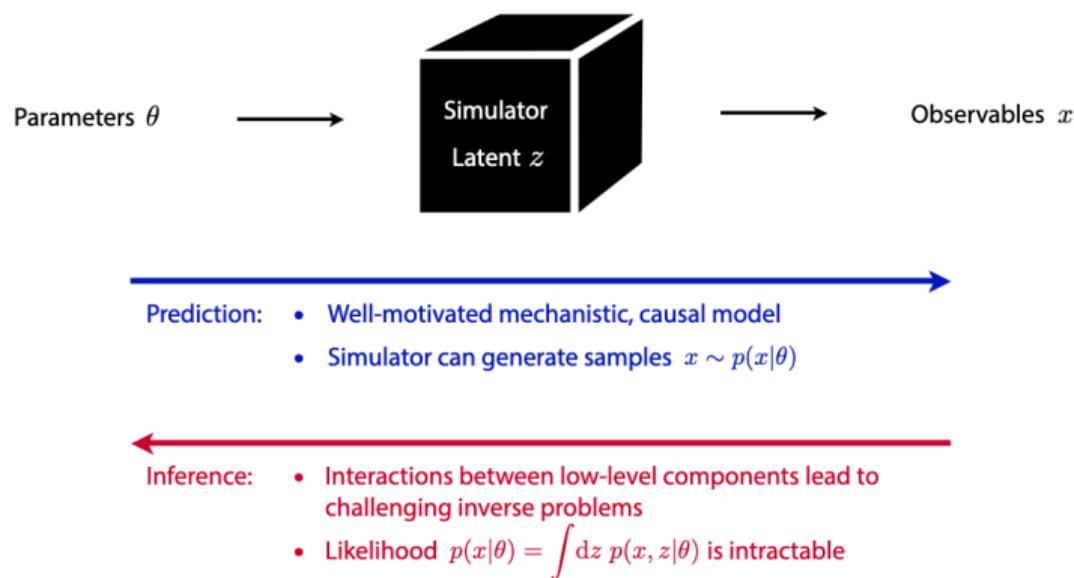


Figure: Credit: Johann Brehmer (Brehmer 2022).

Likelihood-Free Inference

The Problem: Performing inference over parameters θ with data x

$$p(\theta|x) = \frac{p(x|\theta)p(\theta)}{p(x)}$$

when we don't have access to the likelihood $p(x|\theta)$, but we can sample $x \sim p(x|\theta)$.

Motivation
ooooo

Traditional Methods
●ooooo

Using Classifiers (NRE)
oooooooo

Neural Density Estimation (NPE & NLE)
ooooooo

Sequential Algorithms
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Comparison
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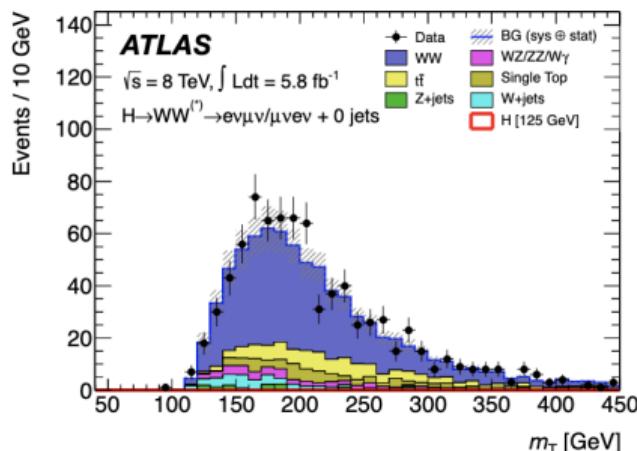
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Traditional Methods: Summary Statistics

- Choose a good summary statistic $s(x)$ based on domain knowledge (feature engineering)—this is *hard*.
- Approximate the likelihood $p(s|\theta)$ using histograms or kernel density estimation (e.g. Diggle and Gratton 1984).
- Does not scale well with the dimension of $s(x)$.



Essentially what was used for the Higgs boson discovery (ATLAS Collaboration 2012).

Traditional Methods: Approximate Bayesian Computation

Given true observed data x_o , want to find a set of suitable parameters $\theta \sim p(\theta|x_o)$.

- 1 Sample $\theta \sim p(\theta)$.
- 2 Simulate $x \sim p(x|\theta)$.
- 3 Calculate summary statistics $s(x_o)$ and $s(x)$.
- 4 Accept θ if the distance $\rho(s(x_o), s(x)) \leq \epsilon$, reject otherwise.
- 5 Repeat.

(Rubin 1984)

Approximate Bayesian Computation
with learned summary statistics

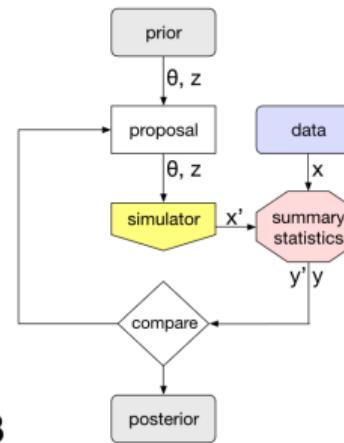


Figure: Cranmer, Brehmer, and Louppe 2020

Problems with ABC

Three main problems:

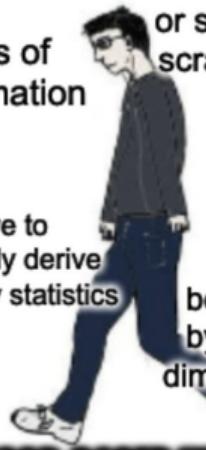
- 1 Choosing $s(x)$ to be informative and low-dimensional.
- 2 Choosing ρ and ϵ .
- 3 Tends to be very slow for small ϵ .
 - (Simulation is typically the bottleneck in SBI.)

Modern Simulation-Based Inference

need to write
down likelihood

loss of
information

have to
manually derive
summary statistics



beseeched
by curse of
dimensionality

LIKELIHOOD-BASED INFERENCE

no need to write down
explicit likelihood. as long
as u can simulate it, you're good

no loss of
information

neural network
finds the best summary
statistics for you



once trained,
do inference
in milliseconds

handily
beat curse of
dimensionality

**NEURAL
SIMULATION-BASED INFERENCE**

Using Neural Networks

Two main approaches to Neural SBI:

- 1 Supervised Learning: Use NN to model a likelihood ratio (NRE)

$$r(x|\theta) := \frac{p(x|\theta)}{p_{\text{ref}}(x)} \text{ or } r(x|\theta_0, \theta_1) := \frac{p(x|\theta_0)}{p(x|\theta_1)}$$

- 2 Unsupervised Learning: Use conditional neural density estimates (e.g. normalizing flows)
 - Neural Posterior Estimation (NPE): Model $p(\theta|x)$
 - Neural Likelihood Estimation (NLE): Model $p(x|\theta)$

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Neural Likelihood Ratio Estimation (NRE)

Neyman-Pearson lemma (Neyman, E. S. Pearson, and K. Pearson 1933): The most powerful test statistic to compare two hypotheses θ_0 and θ_1 for an observation x is the likelihood ratio:

$$r(x|\theta_0, \theta_1) := \frac{p(x|\theta_0)}{p(x|\theta_1)}$$

NRE: Likelihood Ratio Trick

Use supervised learning to obtain a classifier $d(x)$ to distinguish between

- $x \sim p(x|\theta_0)$ with class label $y = 1$, and
- $x \sim p(x|\theta_1)$ with class label $y = 0$.

This has optimal classifier

$$d^*(x) = p(y=1|x) = \frac{p(x|\theta_0)}{p(x|\theta_0) + p(x|\theta_1)}$$

Which can be used to obtain the likelihood ratio

$$r(x|\theta_0, \theta_1) = \frac{p(x|\theta_0)}{p(x|\theta_1)} = \frac{d^*(x)}{1 - d^*(x)}$$

NRE: Parameterized Classifier

Clearly we can't train a new classifier d for every possible pair of $\theta_0, \theta_1 \in \Theta$.

- So train a 'parameterised classifier'*
 $d(x, \theta)$ that takes in a proposed θ as input.
- Try to target the likelihood ratio against some reference $p_{\text{ref}}(x)$

$$r(x|\theta) = \frac{p(x|\theta)}{p_{\text{ref}}(x)}$$

*(Cranmer, Pavez, and Louppe 2016; Hermans, Begy, and Louppe 2020)

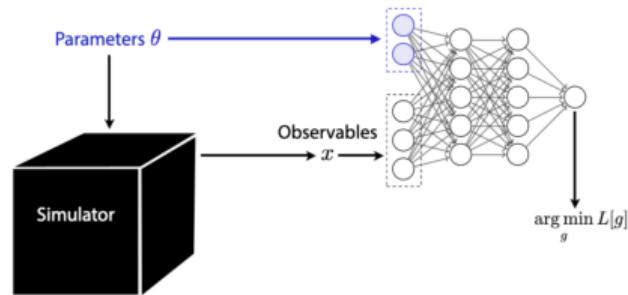


Figure: Credit: Johann Brehmer (Brehmer 2022).

NRE: Parameterized Classifier

- In particular, train parameterised classifier $d(x, \theta)$ to distinguish between
 - 1 dependent $(x, \theta) \sim p(x, \theta)$ pairs with class label $y = 1$,

$$\theta \sim p(\theta), \quad x \sim p(x|\theta)$$

- 2 independent (x, θ') pairs with class label $y = 0$

$$\theta' \sim p(\theta)$$

- This gives us the optimal classifier

$$d^*(x, \theta) = p(y = 1|x, \theta) = \frac{p(x, \theta)}{p(x, \theta) + p(x)p(\theta)}$$

NRE: Parameterized Classifier

With this optimal classifier

$$d^*(x, \theta) = p(y = 1|x, \theta) = \frac{p(x, \theta)}{p(x, \theta) + p(x)p(\theta)}$$

the likelihood trick gives us:

$$\frac{d^*(x, \theta)}{1 - d^*(x, \theta)} = \frac{p(x, \theta)}{p(x)p(\theta)} = \frac{p(x|\theta)}{p(x)} = r(x|\theta)$$

i.e. we're implicitly using $p_{\text{ref}}(x) = p(x)$.

NRE: Algorithm Psuedocode

Algorithm 1 Optimization of $\mathbf{d}_\phi(\mathbf{x}, \theta)$.

<i>Inputs:</i>	Criterion ℓ (e.g., BCE) Implicit generative model $p(\mathbf{x} \mid \theta)$ Prior $p(\theta)$
----------------	--

Outputs: Parameterized classifier $\mathbf{d}_\phi(\mathbf{x}, \theta)$

Hyperparameters: Batch-size M

```

1: while not converged do
2:   Sample  $\theta \leftarrow \{\theta_m \sim p(\theta)\}_{m=1}^M$ 
3:   Sample  $\theta' \leftarrow \{\theta'_m \sim p(\theta)\}_{m=1}^M$ 
4:   Simulate  $\mathbf{x} \leftarrow \{\mathbf{x}_m \sim p(\mathbf{x} | \theta_m)\}_{m=1}^M$ 
5:    $\mathcal{L} \leftarrow \ell(\mathbf{d}_\phi(\mathbf{x}, \theta), 1) + \ell(\mathbf{d}_\phi(\mathbf{x}, \theta'), 0)$ 
6:    $\phi \leftarrow \text{OPTIMIZER}(\phi, \nabla_\phi \mathcal{L})$ 
7: end while
8: return  $\mathbf{d}_\phi$ 

```

Figure: Hermans, Begy, and Louuppe 2020

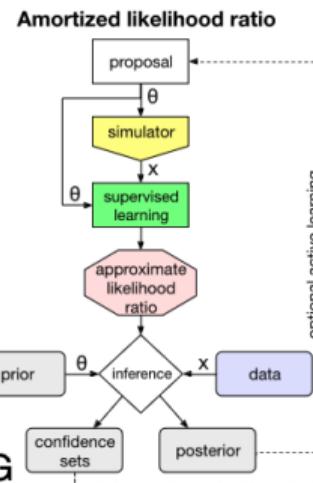


Figure: Cranmer, Brehmer, and Louppe
2020

NRE: Algorithm Diagram

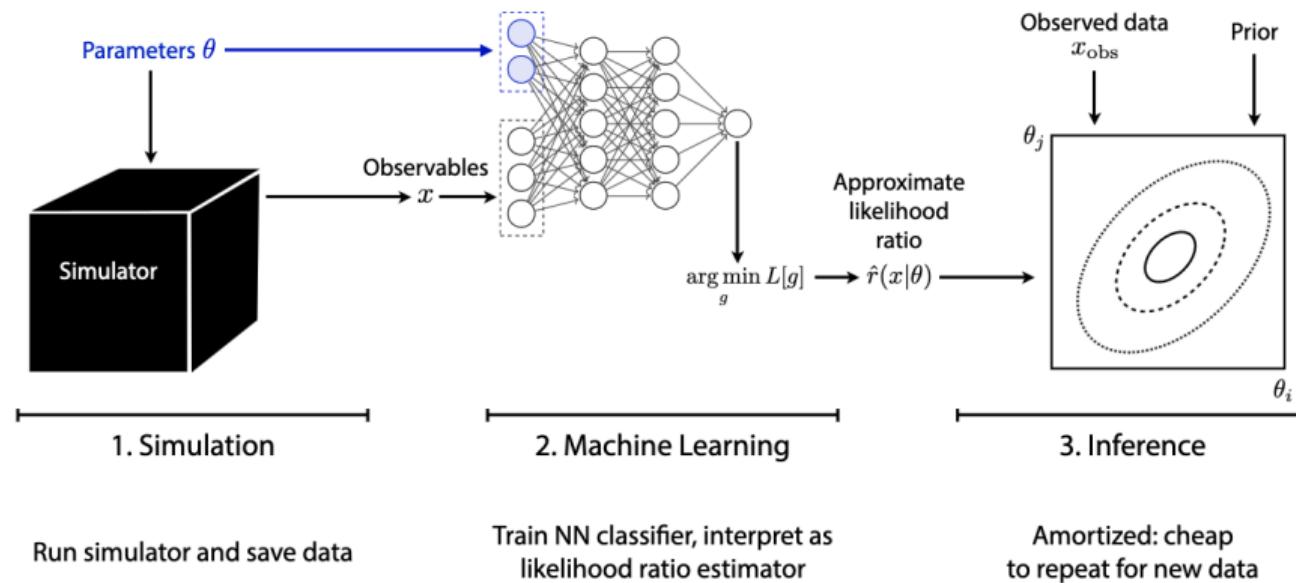


Figure: Hermans, Begy, and Louppe 2020

NRE: Inference

- Frequentist: Run for a whole lot of values of θ and get some confidence intervals.
- Bayesian:
 - Metropolis-Hastings MCMC

$$\alpha = \min \left(1, \frac{p(\theta') p(x|\theta') q(\theta'|\theta_t)}{p(\theta_t) p(x|\theta_t) q(\theta_t|\theta')} \right)$$

- Hamiltonian Monte Carlo

$$\nabla_{\theta} U(\theta) = -\frac{\nabla_{\theta} p(x|\theta)}{p(x|\theta)}$$

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Conditional Neural Density Estimation

- Train a NN q_ϕ to learn a density $p(u|v)$, given iid pairs $\{(u_i, v_i)\}_{i=1}^n$ from the joint distribution $p(u, v)$ by maximising the total log probability w.r.t. ϕ

$$\sum_{i=1}^n \log q_\phi(u_i|v_i)$$

Conditional Neural Density Estimation: Mixture Density Networks

- Mixture Density Network (MDN): $q_\phi(u|v)$ is a mixture of K Gaussians:

$$q_\phi(u|v) = \sum_{k=1}^K \alpha_k \mathcal{N}(u|\mu_k, \Sigma_k)$$

where $\{\alpha_k\}$, $\{\mu_k\}$, $\{\Sigma_k\}$ are computed by a feed-forward NN.

- Not very popular anymore (used in Papamakarios and Murray 2018), but nice and simple (and easily normalised).

Conditional Neural Density Estimation: Normalising Flows

- Normalising Flow: $q_\phi(u|v)$ is a transformation of a standard Gaussian density $\mathcal{N}(0, I)$ through a series of K invertible, differentiable functions f_1, \dots, f_K which each depend on v , i.e.:

$$z_0 \sim \mathcal{N}(0, I), \quad z_k = f_k(z_{k-1}, v) \in \mathbb{R}^M, \quad u = z_K$$

- By a change of variables we get that

$$q_\phi(u|v) = \mathcal{N}(z_0|0, I) \prod_{k=1}^K \left| \det \left(\frac{\partial f_k}{\partial z_{k-1}} \right) \right|^{-1}.$$

- One choice is a Masked Autoregressive Flow (MAF) (Papamakarios, Pavlakou, and Murray 2018).

Normalising Flows: MAF

- Each component $z_k^{(j)}$ is computed depending on the previous components $z_k^{(1)}, \dots, z_k^{(j-1)}$:

$$p(z_k^{(j)} | z_k^{(1:j)}) = \mathcal{N}(z_k^{(j)} | \mu_k^{(j)}, (\exp \alpha_k^{(j)})^2)$$

where $\mu_k^{(j)}$ and $\alpha_k^{(j)}$ come from the NN receiving $z_k^{(1:j-1)}$ and v as input.

- The autoregressive nature of each f_k ensures their jacobians are all triangular:

$$\det \left(\frac{\partial f_k}{\partial z_{k-1}} \right) = \prod_{j=1}^M \exp(\alpha_k^{(j)})$$

Neural Posterior Estimation (NPE)

- 1 Generate n pairs $(x_i, \theta_i) \sim p(x_i, \theta_i)$ from the joint by drawing

$$\theta_i \sim p(\theta)$$

$$x_i \sim p(x|\theta_i)$$

- 2 Train a neural network q_ϕ to approximate $p(\theta|x)$ by maximising $\sum_{i=1}^n \log q_\phi(\theta_i|x_i)$.
(Papamakarios and Murray 2018)

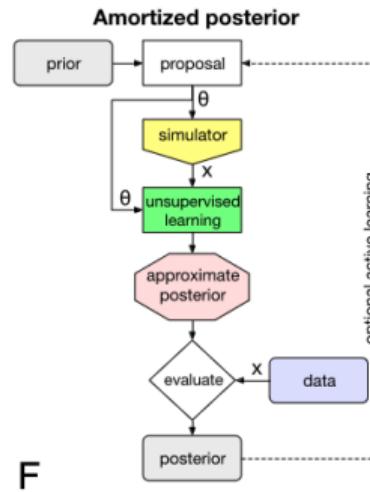


Figure: Cranmer, Brehmer, and Louppe 2020

Neural Likelihood Estimation (NLE)

Model the likelihood rather than the posterior.

- 1 Train a neural network q_ϕ to approximate $p(x|\theta)$ by maximising $\sum_{i=1}^n \log q_\phi(x_i|\theta_i)$.
- 2 Once q_ϕ is trained, proceed by using your likelihood in MCMC to obtain posterior samples.

(Papamakarios, Sterratt, and Murray 2019)

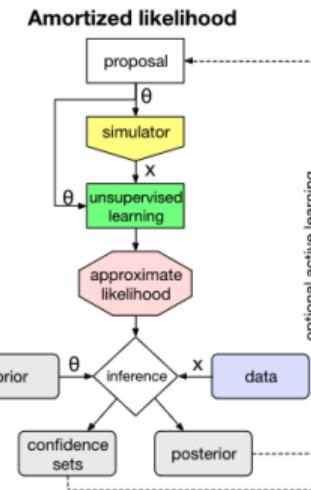


Figure: Cranmer, Brehmer, and Louppe 2020

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Problems with NPE & NLE

- NPE & NLE require a lot of data to accurately describe the posterior everywhere.
- But we might only want to learn the posterior in parameter- and data-space relevant to our real-world observations x_o .
- **Solution:** sequentially choose where in Θ our next training pair (θ_i, x_i) should come from so as to be maximally informative.

SNPE (Type A)

- Instead of drawing $\theta \sim p(\theta)$ for each training example, draw from some other proposal distribution $\tilde{p}(\theta)$.
 - Such as the current posterior approximation $q_\phi(\theta|x_o)$!
 - (Update this proposal every $N \in \mathbb{N}$ samples.)
- **Problem:** This would end up biasing us away from the true posterior $p(\theta|x_o) \propto p(x_o|\theta)p(\theta)$ and toward $p(\theta|x_o)\tilde{p}(\theta)$ (ignoring normalisation).
- **Solution:** Model the posterior as $p(\theta|x = x_o) \approx \frac{p(\theta)}{\tilde{p}(\theta)} q_\phi(\theta|x_o)$. (Papamakarios and Murray 2018)

SNPE (Type A)

Algorithm 1: Training of proposal prior

```

initialize  $q_\phi(\theta | \mathbf{x})$  with one component
 $\tilde{p}(\theta) \leftarrow p(\theta)$ 
repeat
    for  $n = 1..N$  do
        sample  $\theta_n \sim \tilde{p}(\theta)$ 
        sample  $\mathbf{x}_n \sim p(\mathbf{x} | \theta_n)$ 
    end
    retrain  $q_\phi(\theta | \mathbf{x})$  on  $\{\theta_n, \mathbf{x}_n\}$ 
     $\tilde{p}(\theta) \leftarrow \frac{p(\theta)}{\tilde{p}(\theta)} q_\phi(\theta | \mathbf{x}_o)$ 
until  $\tilde{p}(\theta)$  has converged;

```

Algorithm 2: Training of posterior

```

initialize  $q_\phi(\theta | \mathbf{x})$  with K components
// if  $q_\phi$  available by Algorithm 1
// initialize by replicating its
// one component K times
for  $n = 1..N$  do
    sample  $\theta_n \sim \tilde{p}(\theta)$ 
    sample  $\mathbf{x}_n \sim p(\mathbf{x} | \theta_n)$ 
end
train  $q_\phi(\theta | \mathbf{x})$  on  $\{\theta_n, \mathbf{x}_n\}$ 
 $\hat{p}(\theta | \mathbf{x} = \mathbf{x}_o) \leftarrow \frac{p(\theta)}{\tilde{p}(\theta)} q_\phi(\theta | \mathbf{x}_o)$ 

```

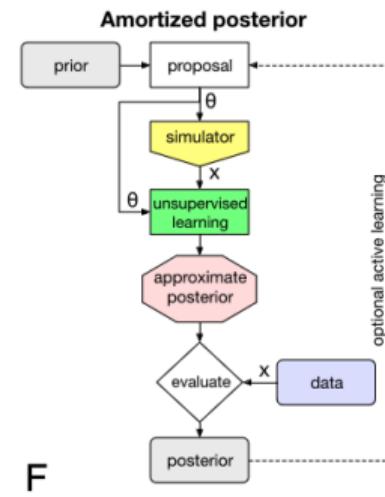


Figure: Hermans, Begy, and Louppe 2020

Figure: Cranmer, Brehmer, and Louppe 2020

SNPE (Type B)

- SNPE-A works, but the division $\frac{p(\theta)}{\tilde{p}(\theta)}$ can be numerically unstable.
- **Solution:** use importance weights $w_i = \frac{p(\theta_i)}{\tilde{p}(\theta_i)}$ in your NN objective (Lueckmann, Goncalves, et al. 2017):

$$\sum_{i=1}^n w_i \log q_\phi(\theta_i | x_i)$$

- (Though often w_i have high variance \rightarrow NN gradients have high variance \rightarrow training instability.)

SNLE

- Essentially the same thing but have q_ϕ model the likelihood.
 - Avoids the posterior-bias problems.
- Note: q_ϕ is no longer a posterior, so we have to sample our $\theta_i \sim \tilde{p}(\theta|x_o)$ using MCMC (using $q_\phi(x_o|\theta)$ as our likelihood).

Algorithm 1: Sequential Neural Likelihood (SNL)

Input : observed data \mathbf{x}_o , estimator $q_\phi(\mathbf{x}|\boldsymbol{\theta})$, number of rounds R , simulations per round N

Output: approximate posterior $\hat{p}(\boldsymbol{\theta}|\mathbf{x}_o)$

set $\hat{p}_0(\boldsymbol{\theta}|\mathbf{x}_o) = p(\boldsymbol{\theta})$ and $\mathcal{D} = \{\}$

for $r = 1 : R$ **do**

- for** $n = 1 : N$ **do**
 - sample $\boldsymbol{\theta}_n \sim \hat{p}_{r-1}(\boldsymbol{\theta}|\mathbf{x}_o)$ with MCMC
 - simulate $\mathbf{x}_n \sim p(\mathbf{x}|\boldsymbol{\theta}_n)$
 - add $(\boldsymbol{\theta}_n, \mathbf{x}_n)$ into \mathcal{D}
- (re-)train $q_\phi(\mathbf{x}|\boldsymbol{\theta})$ on \mathcal{D} and set $\hat{p}_r(\boldsymbol{\theta}|\mathbf{x}_o) \propto q_\phi(\mathbf{x}_o|\boldsymbol{\theta}) p(\boldsymbol{\theta})$

return $\hat{p}_R(\boldsymbol{\theta}|\mathbf{x}_o)$

Figure: Papamakarios, Sterratt, and Murray
 2019

SNLE

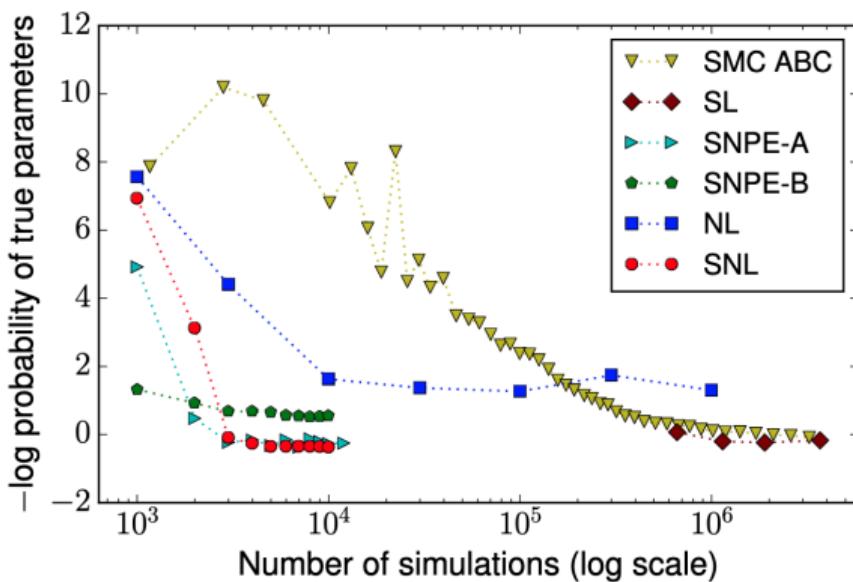


Figure: Papamakarios, Sterratt, and Murray 2019

SNRE

We can use this idea of sampling from the current approximation to the posterior to help us generate training data for NRE too! (Durkan, Murray, and Papamakarios 2020)

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Comparison of Algorithms

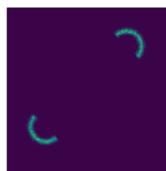
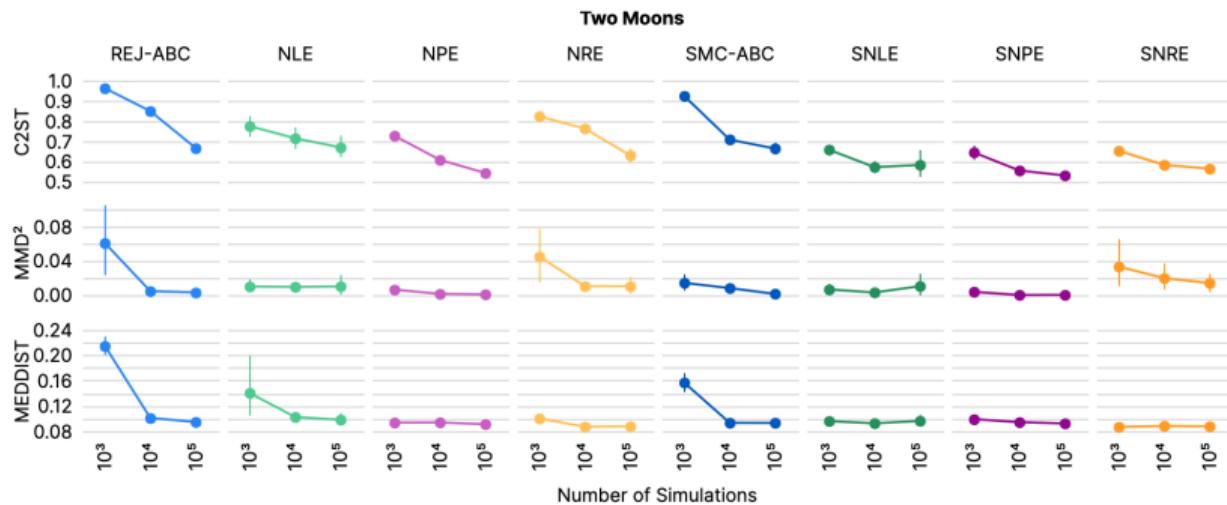


Figure:
Sharrock
et al.
2022

Figure 2: Performance on Two Moons according to various metrics. Best possible performance would be 0.5 for C2ST, 0 for MMD² and MEDDIST. Results for 10 observations each, means and 95% confidence intervals.

Figure: Lueckmann, Boelts, et al. 2021

Comparison of Algorithms

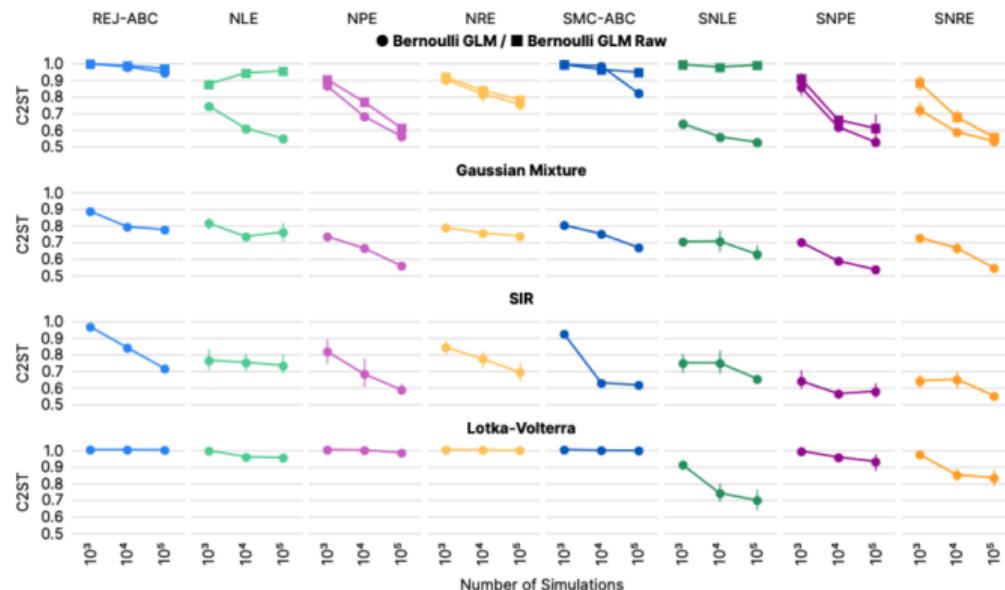


Figure 3: Performance on other benchmark tasks. Classification accuracy (C2ST) of REJ-ABC, SMC-ABC, NLE, SNLE, NPE, SNPE, NRE, SNRE for 10 observations each, means and 95% confidence intervals.

Comparison of Algorithms

What each algorithm gives you:

- ABC:
 - Samples from posterior $\theta \sim q(\theta|x_o)$.
- (S)NLE + (S)NRE:
 - Samples from posterior $\theta \sim q(\theta|x_o)$ via MCMC.
 - Unnormalised evaluations $q(\theta|x_o)$.
- (S)NPE:
 - Samples from posterior $\theta \sim q(\theta|x_o)$ directly.
 - Normalised evaluations $q(\theta|x_o)$.

Comparison of Algorithms

- Different problems lend themselves to different algorithms as solutions...
- Sequential algorithms might not always be best:
 - Not needed if simulation is cheap.
 - Performing SBI separately for many data points:
 - Better to have an amortized likelihood/posterior that is accurate everywhere in the data-space $x_o \in \mathcal{X}$.
 - E.g. for iid data $x_{o_1}, x_{o_2} \dots \sim p(x|\theta)$

$$p(\theta|x_{o_1}, x_{o_2} \dots) \propto p(\theta) \prod_i \left[\underbrace{p(x_{o_i}|\theta)}_{\text{amortized likelihood}} \right].$$

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Conclusion

- SNPE/SNLE/SNRE are all pretty popular, but there are other methods out there too, e.g.:
 - GATSBI (Ramesh et al. 2022) — GAN-inspired approach.
 - 'Grey-box' approaches (Brehmer, Louppe, et al. 2020) — try to squeeze as much information out of the simulator as possible.
- SBI is pretty promising for a whole range of scientific subjects
 - Particle physics (Brehmer and Cranmer 2020).
 - Astrophysics — gravitational waves (Delaunoy et al. 2020), dark matter (Hermans, Banik, et al. 2021).
 - Climate science — hydrology of river basins in Colorado Hull et al. 2022.

Useful Papers

The frontier of simulation-based inference

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Benchmarking Simulation-Based Inference

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⁴Research Center caesar ⁵Max Planck Institute for Intelligent Systems, Tübingen

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[slides/2022/simulation_based_inference_rodem_sinergia_2022.pdf](https://github.com/johannbrehmer/slides/blob/master/slides/2022/simulation_based_inference_rodem_sinergia_2022.pdf) at master · johannbrehmer/slides. en. URL:

https://github.com/johannbrehmer/slides/blob/master/2022/simulation_based_inference_rodem_sinergia_2022.pdf (visited on 11/06/2023).

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