Neural Simulation-Based Inference

November 2023

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Simulators

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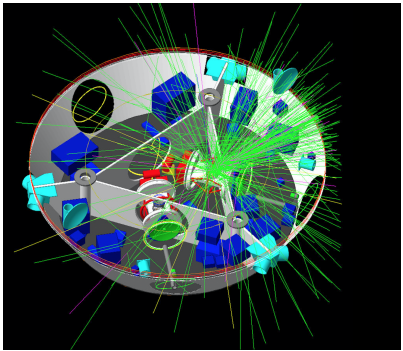
Thanks to modern computing, they can turn these into high-precision simulators.

Simulators: An Example

Geant4 - particle simulator (CERN 2023).



Science (like, most of it)

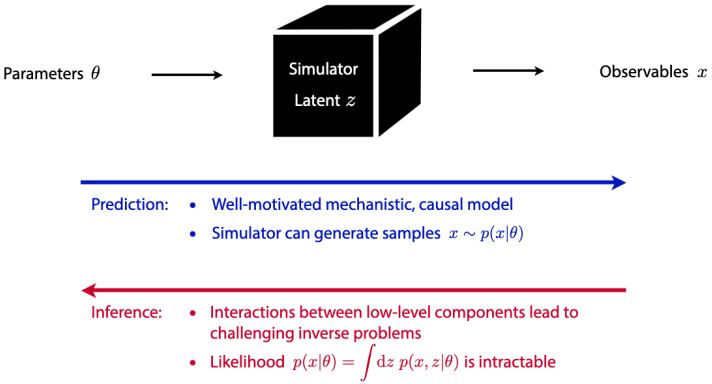


Figure: Credit: Johann Brehmer (Brehmer 2022).

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 $x \sim p(x|\theta)$.

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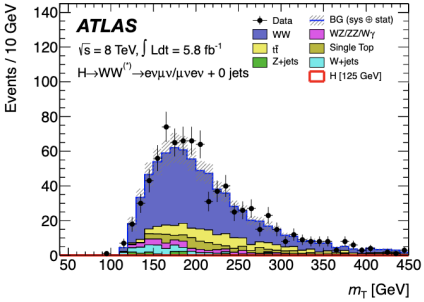

Essentially what was used for the Higgs boson discovery (ATLAS Collaboration 2012).

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 $\theta \sim p(\theta)$.

(Rubin 1984)

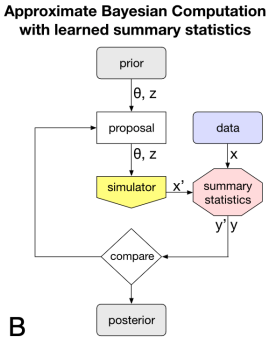

Figure: Cranmer, Brehmer, and Louppe 2020

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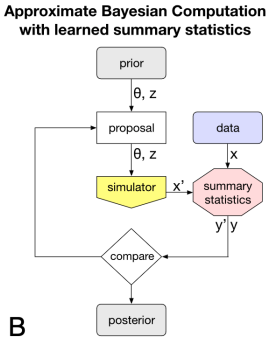

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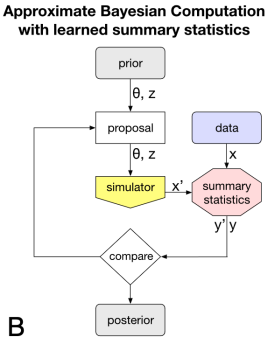

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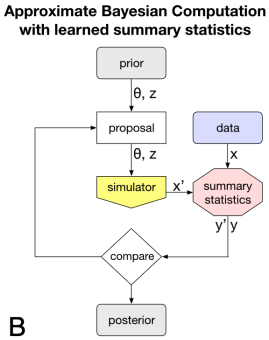

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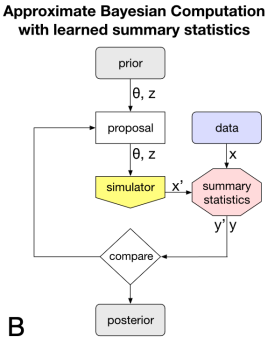

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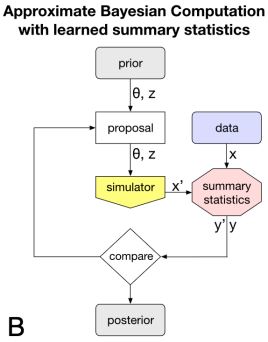

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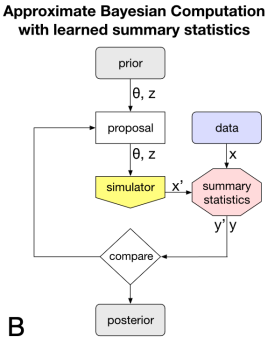

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Problems with ABC

Three main problems:

1. Choosing $s(x)$ to be informative and low-dimensional.

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Three main problems:

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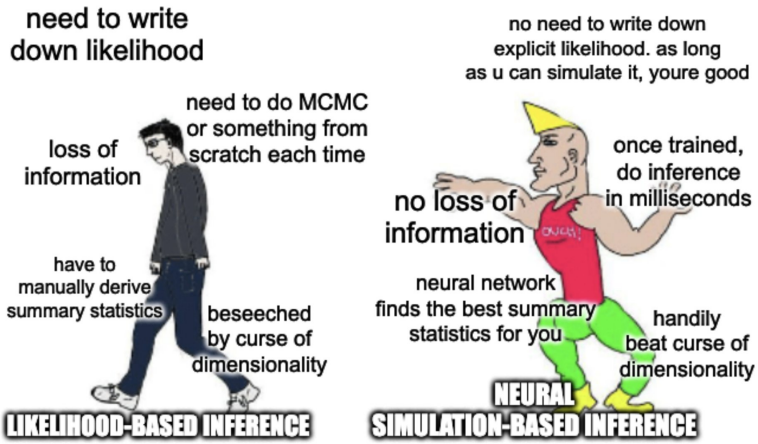
3. Tends to be very slow for small ϵ.
   - (Simulation is typically the bottleneck in SBI.)

Modern Simulation-Based Inference



Using Neural Networks

Two main approaches to Neural SBI:

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

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

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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 $\mathrm{d}(x)$ to distinguish between

- $x \sim p(x|\theta_0)$ with class label $y = 1$, and
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This has optimal classifier

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Which can be used to obtain the likelihood ratio

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

.

NRE: Parameterized Classifier

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

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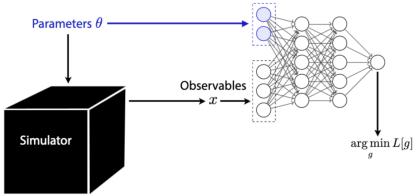

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*(Cranmer, Pavez, and Louppe 2016; Hermans, Begy, and Louppe 2020)

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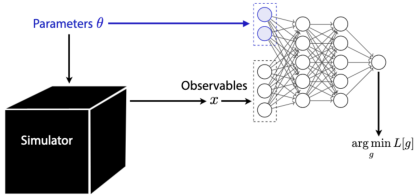
- So train a 'parameterised classifier'* $d(x, \theta)$ that takes in a proposed θ as input.
- Try to target the likelihood ratio against some reference $p_{\text{ref}}(x)$

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



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NRE: Parameterized Classifier

- In particular, train parameterised classifier $\mathrm{d}(x, \theta)$ 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 $y = 0$

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- This gives us the optimal classifier

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

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With this optimal classifier

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

the likelihood trick gives us:

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

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

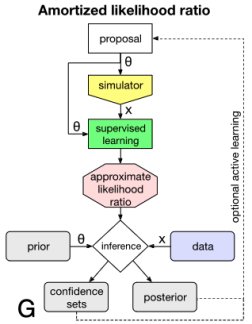
NRE: Algorithm Psuedocode

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

Inputs:	Criterion ℓ (e.g., BCE)
	Implicit generative model $p(\mathbf{x} \mid \boldsymbol{\theta})$
	Prior $p(\boldsymbol{\theta})$
Outputs:	Parameterized classifier $\mathbf{d}_\phi(\mathbf{x}, \boldsymbol{\theta})$
Hyperparameters:	Batch-size M

while not converged do
  Sample $\boldsymbol{\theta} \leftarrow \{\boldsymbol{\theta}_m \sim p(\boldsymbol{\theta})\}_{m=1}^{M}$
  Sample $\boldsymbol{\theta}' \leftarrow \{\boldsymbol{\theta}_m \sim p(\boldsymbol{\theta})\}_{m=1}^{M}$
  Simulate $\mathbf{x} \leftarrow \{\mathbf{x}_m \sim p(\mathbf{x} \mid \boldsymbol{\theta}_m)\}_{m=1}^{M}$
  $\mathcal{L} \leftarrow \ell(\mathbf{d}_\phi(\mathbf{x}, \boldsymbol{\theta}),\ 1) + \ell(\mathbf{d}_\phi(\mathbf{x}, \boldsymbol{\theta}'),\ 0)$
  $\phi \leftarrow \textbf{OPTIMIZER}(\phi,\ \nabla_\phi \mathcal{L})$
end while
return $\mathbf{d}_\phi$

Figure: Hermans, Begy, and Louppe 2020



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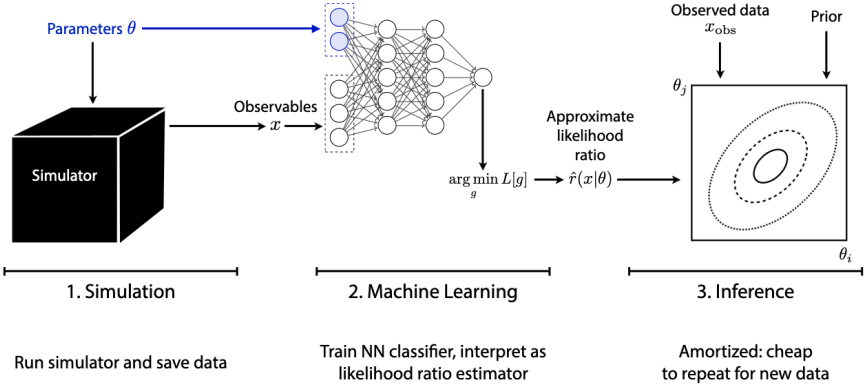
NRE: Algorithm Diagram



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- 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

- Mixure 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.

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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 $\mathcal{N}(0, \mathrm{I})$ through a series of K invertible, differentiable functions $f_1, \ldots, f_K$ which each depend on v, i.e.:

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

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- By a change of variables we get that

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

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- 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 $z_k^{(1)}, \ldots, z_k^{(j-1)}$:

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

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

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  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:

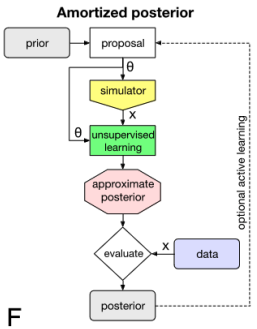
$$\det \left(\frac{\partial f_k}{\partial z_{k-1}} \right) = \prod_{j=1}^{M} \exp(\alpha_k^{(j)})$$

Neural Posterior Estimation (NPE)

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

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

(Papamakarios and Murray 2018)



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(Papamakarios and Murray 2018)

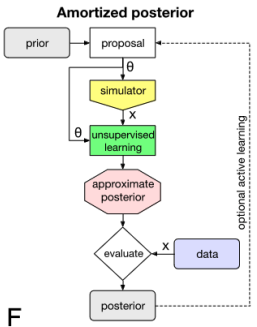

Figure: Cranmer, Brehmer, and Louppe 2020

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

(Papamakarios, Sterratt, and Murray 2019)

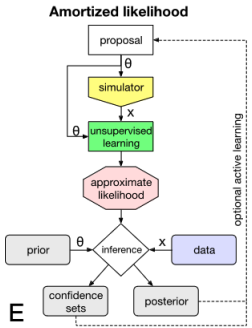

Figure: Cranmer, Brehmer, and Louppe 2020

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)

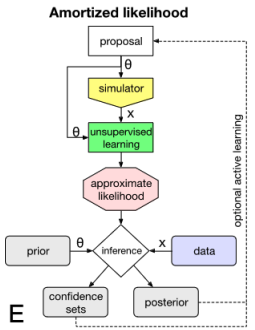

Figure: Cranmer, Brehmer, and Louppe 2020

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Problems with NPE & NLE

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- 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 $\tilde{p}(\theta)$.

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- 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).

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- 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)

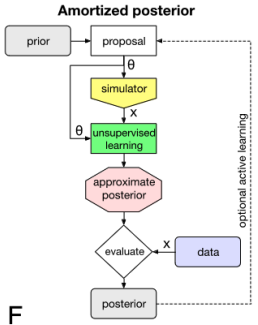
Algorithm 1: Training of proposal prior

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

Algorithm 2: Training of posterior

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

Figure: Hermans, Begy, and Louppe 2020



F

Figure: Cranmer, Brehmer, and Louppe 2020

SNPE (Type B)

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- Solution: use importance weights $w_i = \frac{p(\theta_i)}{\tilde{p}(\theta_i)}$ in your NN objective (Lueckmann, Goncalves, et al. 2017):

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

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- (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.

Algorithm 1: Sequential Neural Likelihood (SNL)

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

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

set $\hat{p}_0(\boldsymbol{\theta} \mid \mathbf{x}_o) = p(\boldsymbol{\theta})$ and $\mathcal{D} = \{\}$
for $r = 1 : R$ **do**
  for $n = 1 : N$ **do**
    sample $\boldsymbol{\theta}_n \sim \hat{p}_{r-1}(\boldsymbol{\theta} \mid \mathbf{x}_o)$ with MCMC
    simulate $\mathbf{x}_n \sim p(\mathbf{x} \mid \boldsymbol{\theta}_n)$
    add $(\boldsymbol{\theta}_n, \mathbf{x}_n)$ into $\mathcal{D}$
  (re-)train $q_{\boldsymbol{\phi}}(\mathbf{x} \mid \boldsymbol{\theta})$ on $\mathcal{D}$ and set $\hat{p}_r(\boldsymbol{\theta} \mid \mathbf{x}_o) \propto q_{\boldsymbol{\phi}}(\mathbf{x}_o \mid \boldsymbol{\theta})\, p(\boldsymbol{\theta})$
return $\hat{p}_R(\boldsymbol{\theta} \mid \mathbf{x}_o)$

Figure: Papamakarios, Sterratt, and Murray 2019

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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).

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SNLE

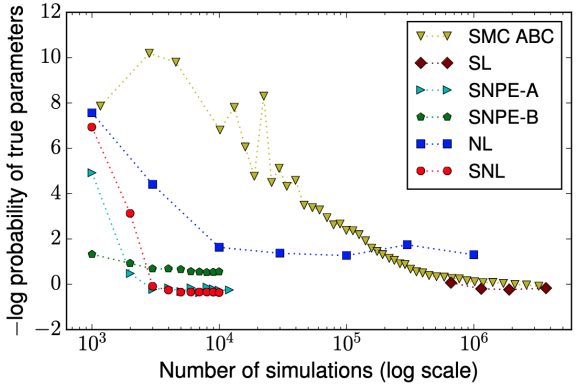

Figure: Papamakarios, Sterratt, and Murray 2019

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

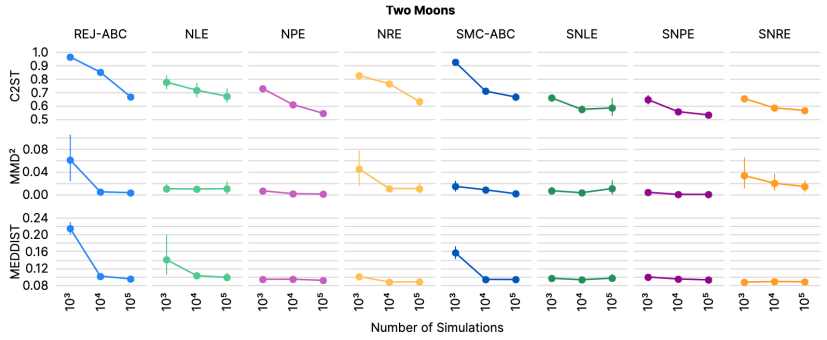

Figure 2: **Performance on Two Moons according to various metrics.** Best possible performance would be 0.5 for C2ST, 0 for MMD^2 and MEDDIST. Results for 10 observations each, means and 95% confidence intervals.

Figure: Lueckmann, Boelts, et al. 2021

Figure: Sharrock et al. 2022

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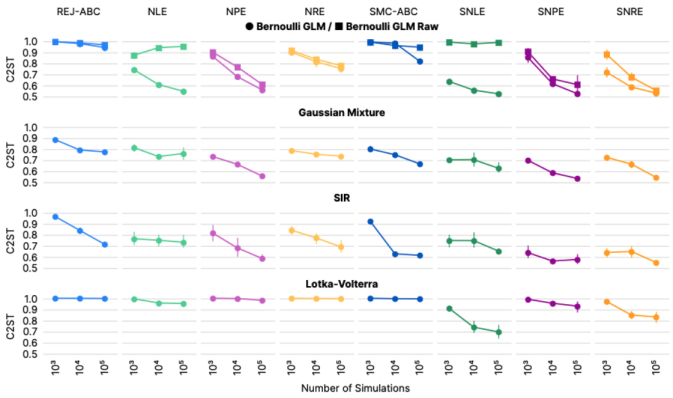

Figure 3: **Performance on other benchmark tasks.** Classification accuracy (C2ST) of REJ-ABC, SMC-ABC, NLE, SNLE, NPE, SNPE, NRE, SNRE for 10 observations each, means and 95% confidence intervals.

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    - 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 $x_{o_1}, x_{o_2} \ldots \sim p(x|\theta)$

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

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Conclusion

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  - Climate science — hydrology of river basins in Colorado Hull et al. 2022.

Useful Papers

The frontier of simulation-based inference

Kyle Cranmer[a,b,1], **Johann Brehmer**[a,b], and **Gilles Louppe**[c]

[a]Center for Cosmology and Particle Physics, New York University, New York, NY 10003; [b]Center for Data Science, New York University, New York, NY 10011; and [c]Montefiore Institute, University of Liège, B-4000 Liège, Belgium

Benchmarking Simulation-Based Inference

Jan-Matthis Lueckmann[1,2] **Jan Boelts**[2] **David S. Greenberg**[2,3]
Pedro J. Gonçalves[4] **Jakob H. Macke**[1,2,5]

[1]University of Tübingen [2]Technical University of Munich [3]Helmholtz Centre Geesthacht
[4]Research Center caesar [5]Max Planck Institute for Intelligent Systems, Tübingen

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