Sequential Monte Carlo For Amortized Variational Inference

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Collaborators

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Outline

1. Background
   - Variational Inference
   - Amortized Variational Inference
2. SMC-Wake
   - Forward KL Objective
   - Experiments

Background

Bayesian Inference

- Given a generative model $p(\theta, x)$, the posterior distribution (density) can be computed by Bayes' rule via

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- The *evidence* $p(x) = \int p(\theta, x) d\theta$ is usually computationally intractable, so we resort to approximate Bayesian methods.

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Variational Inference

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- The choice of the objective function L is an area of active research.
- What if we want to perform VI for $x_1, \ldots, x_n$, for n large?

Amortized Inference

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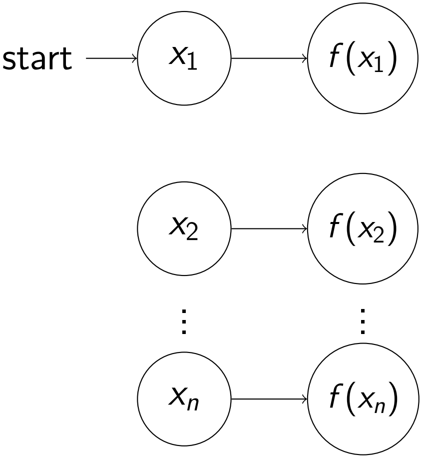
- Ideally, $f(x)$ defines a distribution "close" to the posterior $p(\theta \mid x)$ for each $x \in \mathcal{X}$.

Amortized Inference



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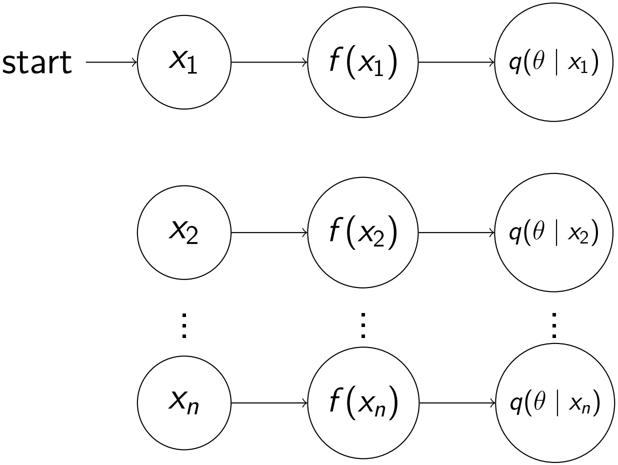

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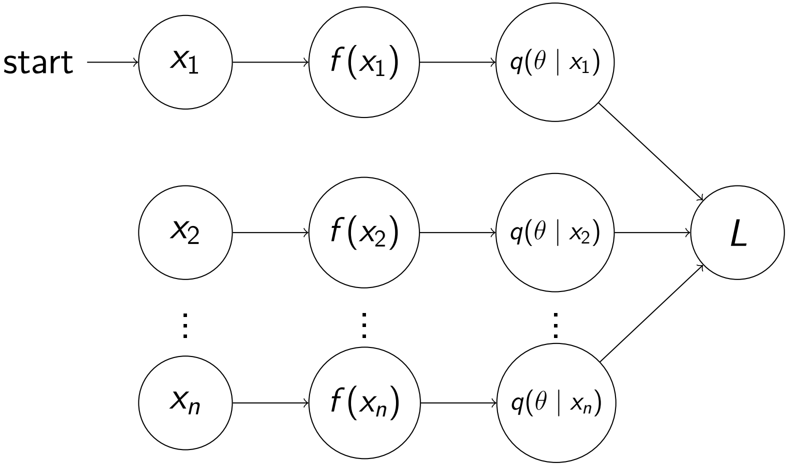

Example

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- For each observation x, a neural network f would have 5 scalar outputs that define a distribution on θ,

$$f(x) = (\mu_1, \mu_2, \sigma_1, \sigma_2, \rho) \mapsto \mathcal{N}\left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{bmatrix} \right)$$

Objectives

We let $q_\phi(\theta \mid x)$ denote an amortized variational posterior, corresponding to a neural network with parameters ϕ.

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$$q^{\mathrm{VI}}(\theta) = \underset{q \in \mathcal{Q}}{\operatorname{argmin}} \; L(q(\theta), \pi(\theta), p(x \mid \theta))$$

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$$\downarrow$$

$$q_{\phi}^{\mathrm{AVI}}(\theta) = \operatorname*{argmin}_{\phi \in \Phi} \; \frac{1}{n} \sum_{i=1}^{n} L(q_{\phi}(\theta \mid x_i), \pi(\theta), p(x_i \mid \theta))$$

SMC-Wake

The Forward KL Divergence

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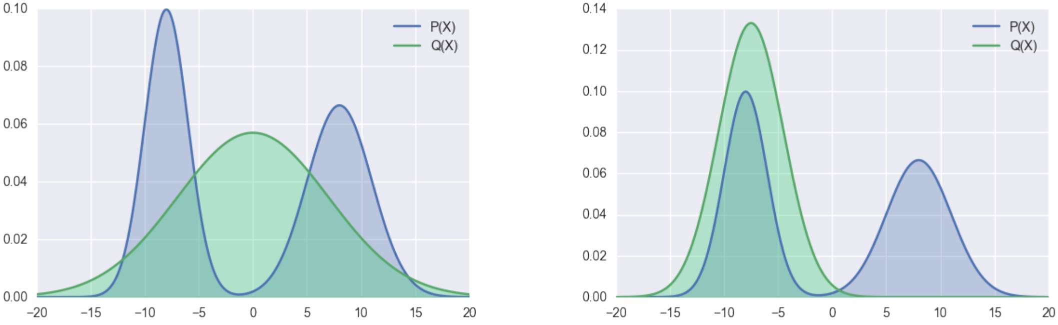
$$L(q, \pi, p) = \mathrm{KL}\left[p(\theta \mid x) || q(\theta \mid x)\right].$$

- VI often uses the evidence lower bound (ELBO) to target the reverse KL divergence.

Forward vs. Reverse KL



(a) Forward KL (b) Reverse KL

Image source: `https://agustinus.kristia.de/techblog/2016/12/21/forward-reverse-kl/`

Particle Approximations

- Estimating the forward KL objective

$$\mathbb{E}_{p(\theta|x)} \log \frac{p(\theta \mid x)}{q_\phi(\theta \mid x)}$$

or its gradient

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- The "Wake" algorithm uses self-normalized importance sampling (IS) to estimate the objective.

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- We propose using tools from the Sequential Monte Carlo (SMC) literature to estimate this objective.

SMC

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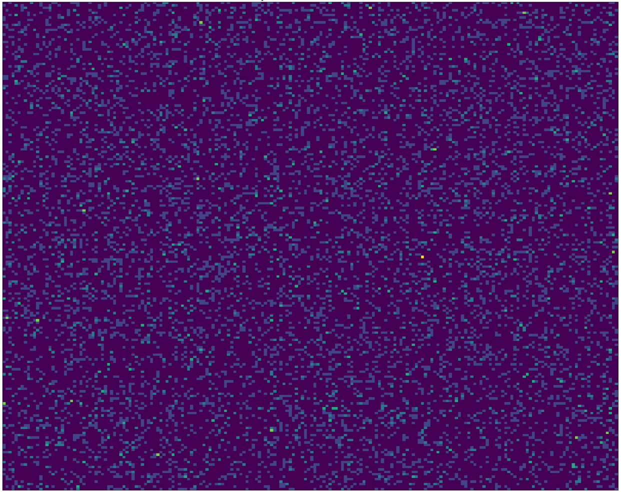
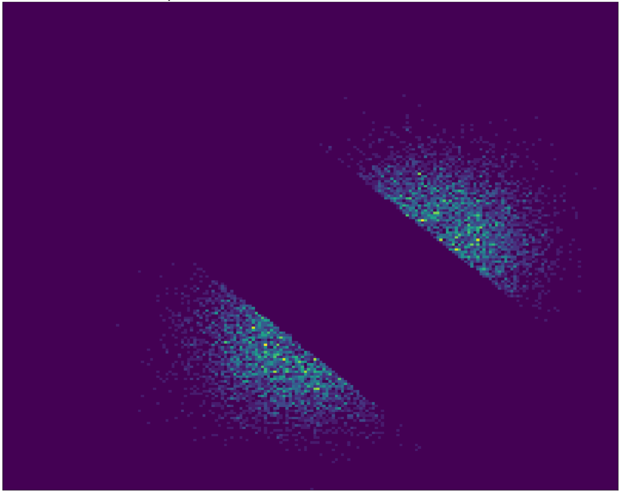
- Weighted samples from the base distribution are resampled, extended, and reweighted.
- While SMC is commonly used for state-space models, it can be used to target *any* distribution.

Temperature $\tau = 0.0$



Temperature $\tau = 0.005289797269164934$



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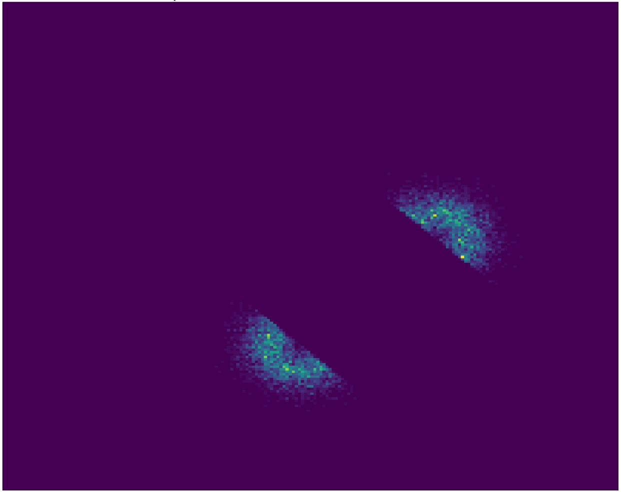

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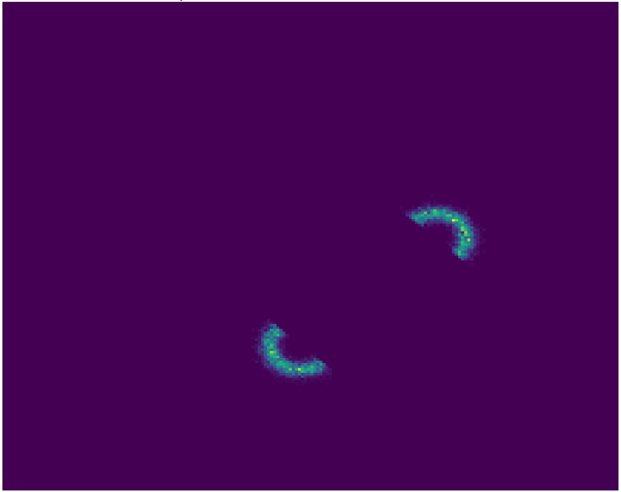
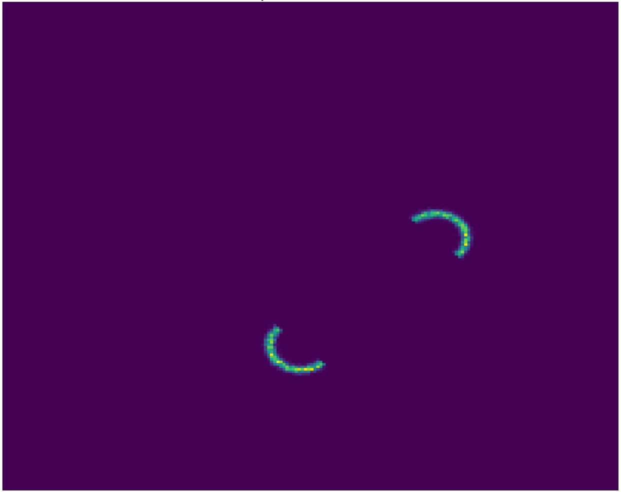


Temperature $\tau = 1.0$



Likelihood-Tempered SMC

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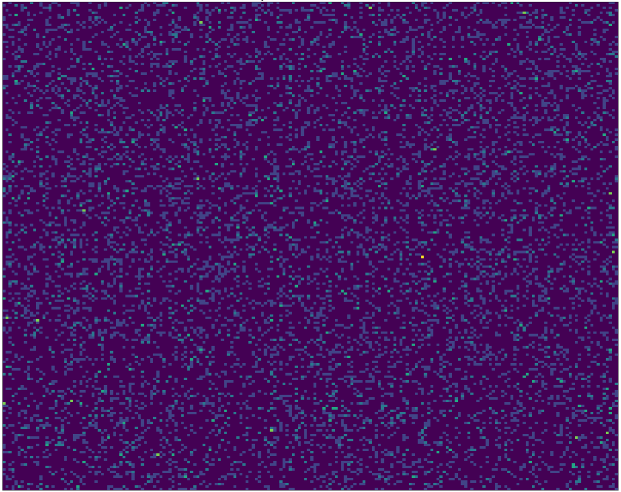
- Temperatures satisfy $0 = \tau_1 < \cdots < \tau_T = 1$.

Temperature $\tau = 0.0$



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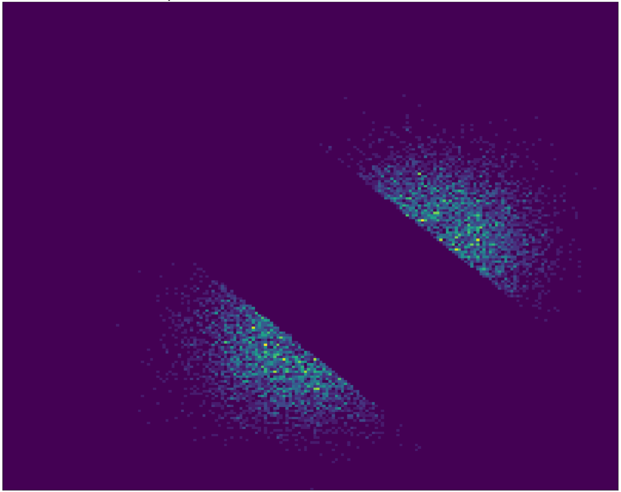

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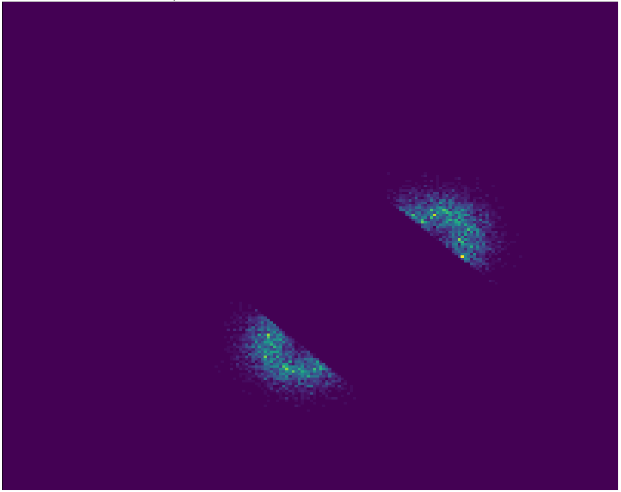

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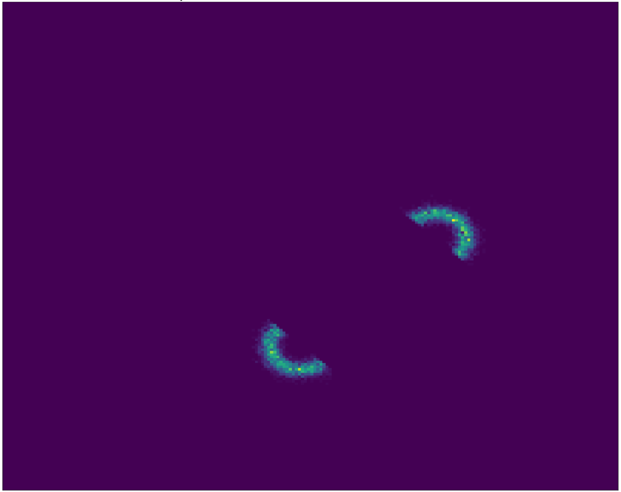

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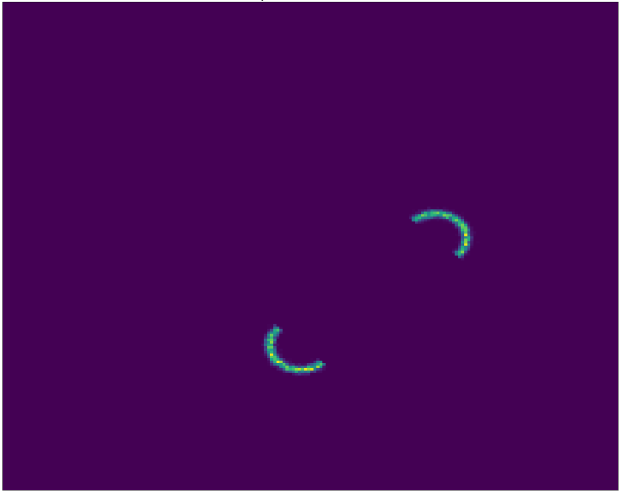

SMC-Wake

- Our proposed algorithm, SMC-Wake, trains the inference network using gradient updates

$$-\frac{1}{n}\sum_{i=1}^{n}\mathbb{E}_{p(\theta|x_i)}\nabla_\phi \log q_\phi(\theta \mid x_i).$$

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- Each expectation is estimated using particles sets constructed by SMC.
- Gradients estimated in this way are *consistent* as the number of particles $K \to \infty$.

Convergence

Lemma (Del Moral, 2004)

Let K be the number of particles used by likelihood-tempered SMC, and $\hat{P}(\theta_T)$ the empirical distribution at the final step. Then as $K \to \infty$,

$$\mathrm{KL}(\mathbb{E}\left[\hat{P}(\theta_T)\right] \;||\; p(\theta \mid x)) \to 0$$

Consistent Gradient Estimation

Theorem

Let

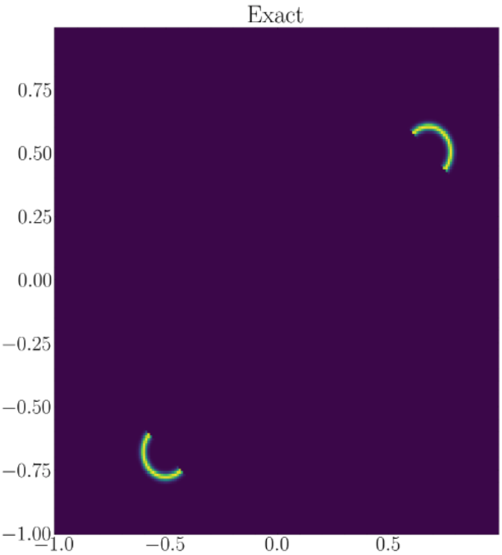
$$\psi = \mathbb{E}_{p(\theta|x)} \nabla_\phi \log q_\phi(\theta \mid x),$$
$$\hat{\psi} = \mathbb{E}_{\hat{P}(\theta_T)} \nabla_\phi \log q_\phi(\theta \mid x),$$

where $\hat{P}$ is a (random) discrete distribution resulting from an instance of SMC-Wake. Suppose that $|\nabla_\phi \log q_\phi(\theta \mid x)| \leq M$ (in each dimension), and that $\mathbb{E}(\hat{P}(\theta_T))$ is absolutely continuous with respect to $p(\theta \mid x)$. Then $\mathbb{E}(\hat{\psi}) - \psi \to 0$ as $K \to \infty$.

Experiment – Two Moons

$$
\begin{aligned}
\theta_1, \theta_2 &\overset{iid}{\sim} U(-1, 1), \\
a &\sim U\left(-\frac{\pi}{2}, \frac{\pi}{2}\right), \\
r &\sim \mathcal{TN}\left(0.1, 0.01^2; 0\right), \\
p &= (r\cos(a) + 0.25, r\sin(a)), \\
\text{and } x^\top &= p + \left(-\frac{|\theta_1 + \theta_2|}{\sqrt{2}}, \frac{-\theta_1 + \theta_2}{\sqrt{2}}\right).
\end{aligned}
$$

Two Moons Posterior



Experiments – Two Moons

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- We sample 100 iid data points from the “two-moons” model.
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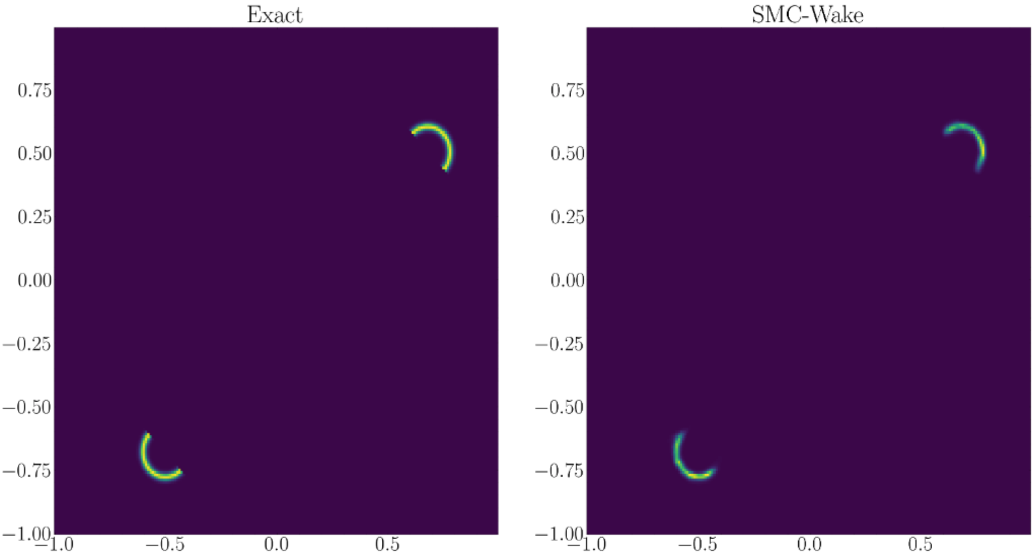
- We use the class Neural Spline Flows (NSP) as the variational family $\mathcal{Q}$.

Results – SMC-Wake



Competing Methods

Wake-phase training

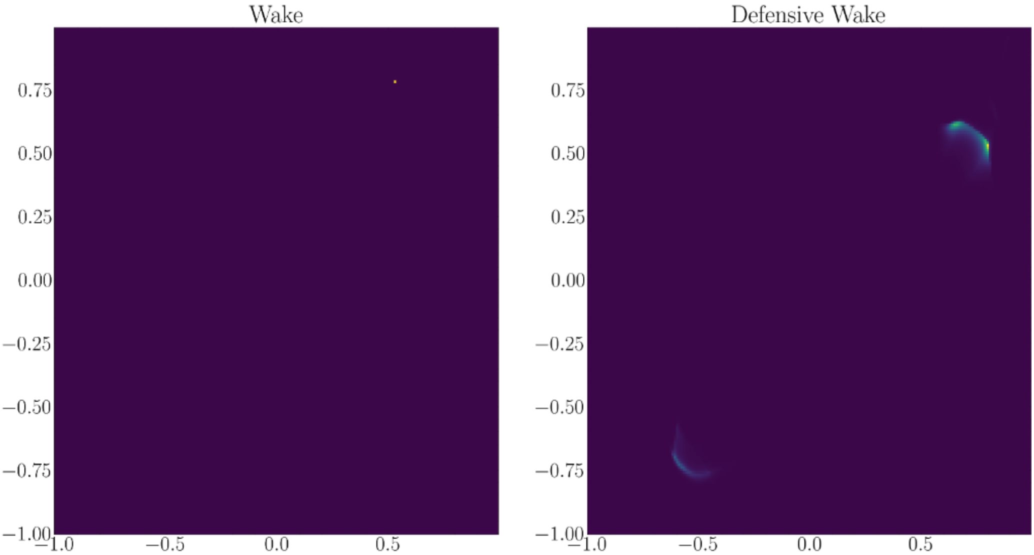
- Uses self-normalized importance sampling with q_ϕ as a proposal to estimate the gradient

$$-\mathbb{E}_{p(\theta|x)} \nabla_\phi \log q_\phi(\theta \mid x)$$

Defensive-Wake

- A variant that proposes with equal probability from either q_ϕ or the prior for importance sampling.

Results – Competitors



Discussion

SMC-Wake improves on wake-phase training by

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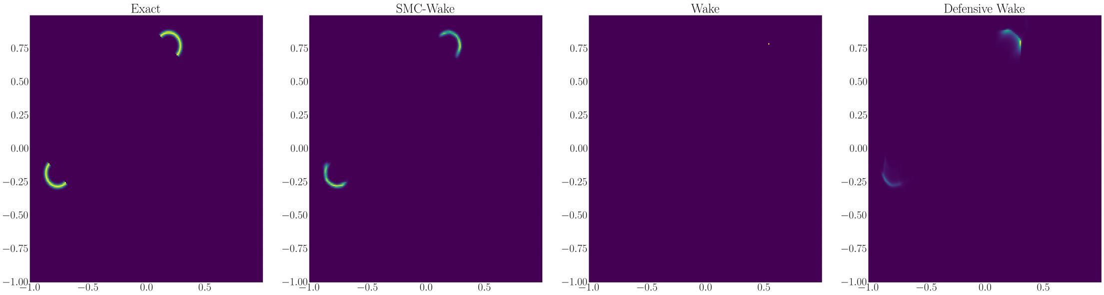
- Removing the pathology of proposing from and optimizing q_ϕ.
- Utilizing the likelihood more effectively via tempering to construct high-quality particle approximations.

Additional Results



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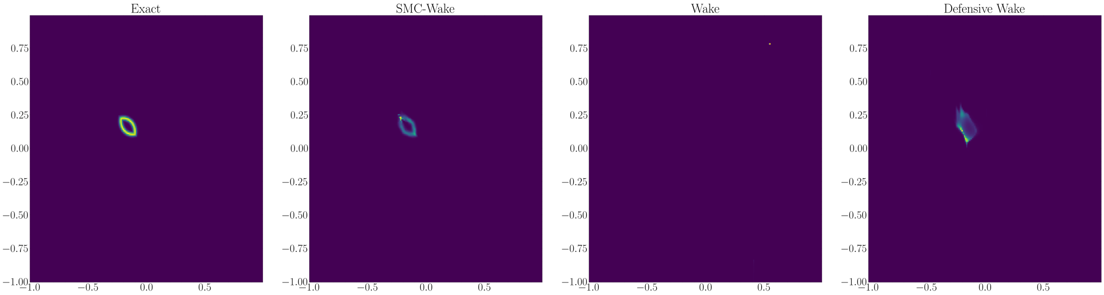

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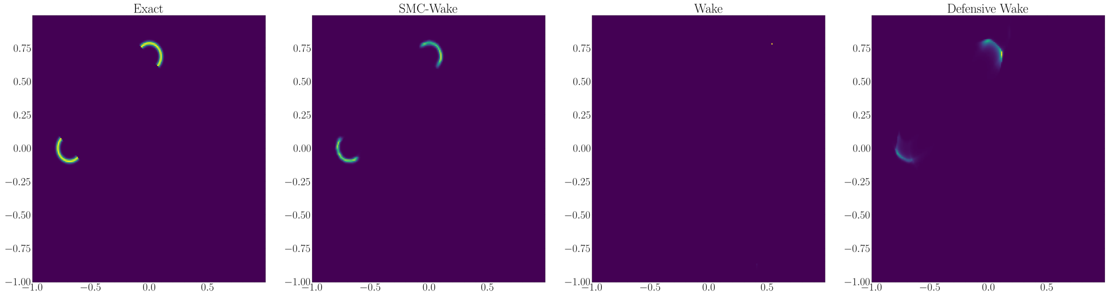

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- We simulate from this forward model by sampling from a prior on the parameters, and subsequently
  - Add realistic noise.
  - Normalize out a magnitude parameter.

Inference For Galaxy Spectra

- Our PROVABGS emulator thus generates galaxy spectra from 11 distinct cosmological parameters.

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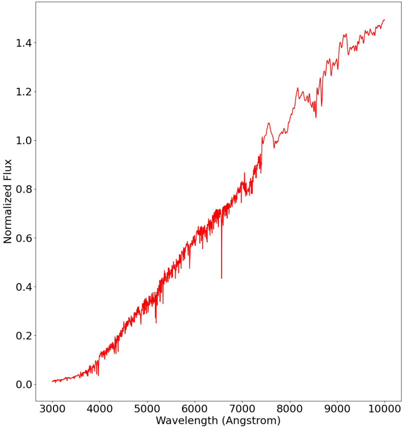
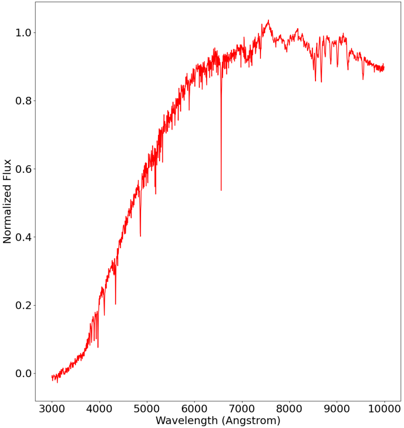
- We add Gaussian noise to the emulator outputs, and aim to perform inference over these parameters using SMC-Wake.

PROVABGS


Normalized Flux
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
3000
4000
5000
6000
7000
8000
9000
10000
Wavelength (Angstrom)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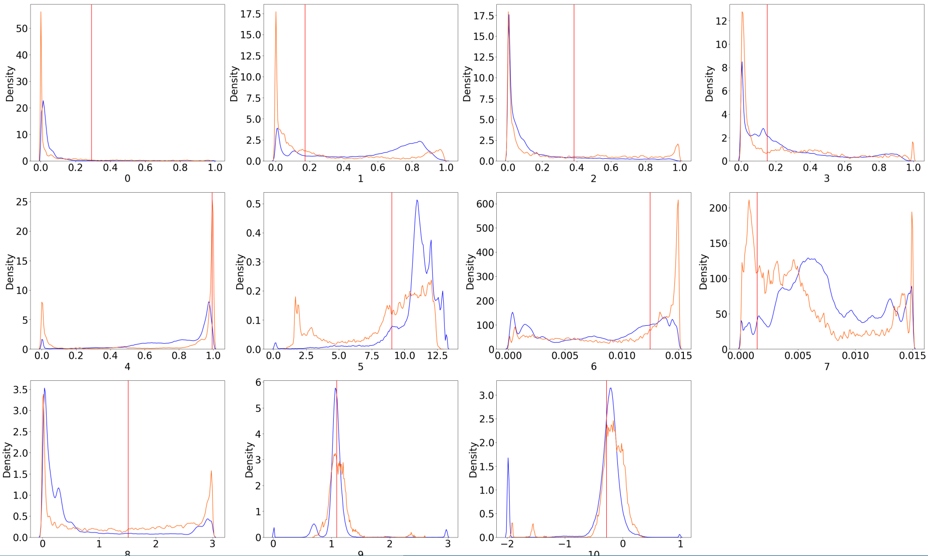
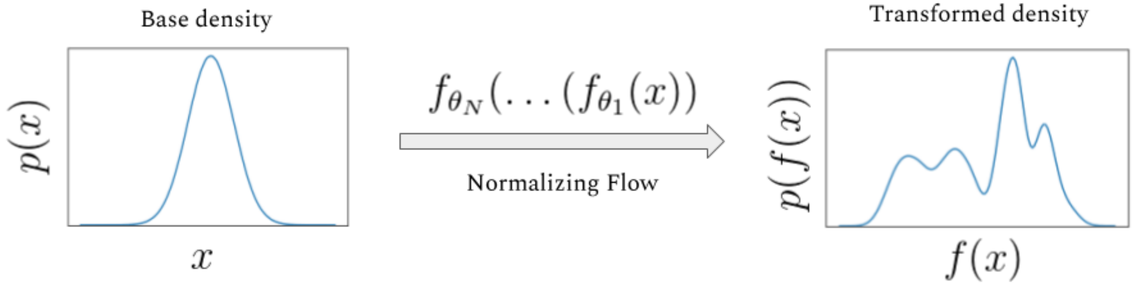
Results



Normalizing Flows



Source: https://gebob19.github.io/normalizing-flows/