Differentiable SMC Samplers for Fast Bayesian Deep Learning

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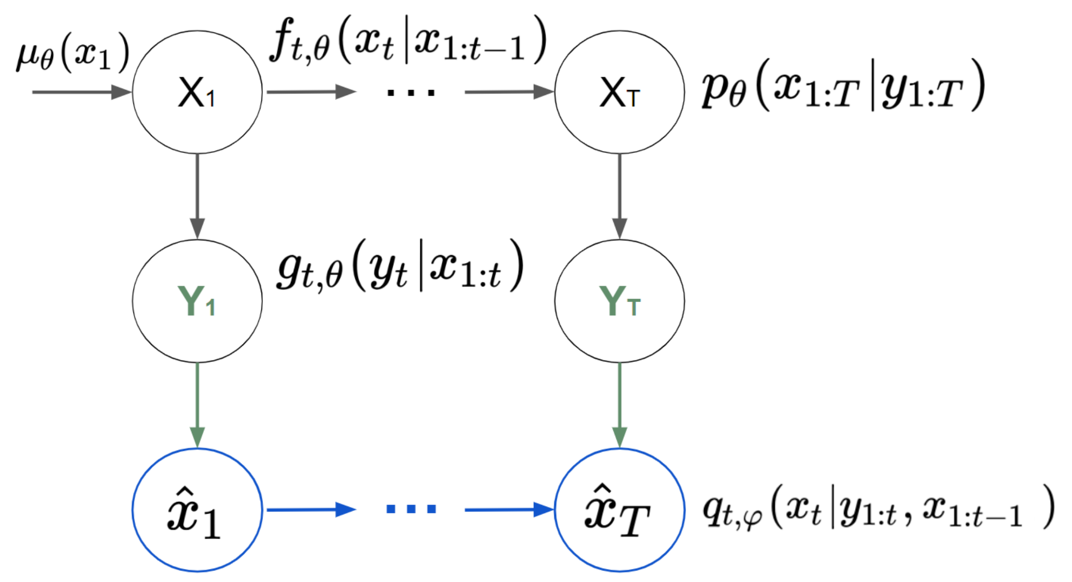
Motivation and Summary

- Provide a **Bayesian solution** to neural networks to obtain uncertainty.
- Build a Bayesian Neural network that can deal with **stationary distributions** with a **scalable convergence**.
- Make a clear differentiation of SMC samplers.
- SMC samplers combine benefits from MCMC methods and Particle Filters.

Background

We want to infer a target distribution. We use a proposal distribution to generate samples and use **Importance sampling** to weight them proportionally to our target. Using these weighted samples we can infer our target.

- **MCMC methods** have offered state-of-the-art sampling methods to infer stationary distributions.
- **Particle filters** are sequential Bayesian samplers that are used in wide range of fields involving state-space models, they offer unbiased Bayesian estimates and are parallelisable.



Algorithm 1 Bootstrap Particle Filter

> Sample initial N particles $x_1^{(i)} \sim q_{1,\phi}(y_1)$
> Compute the weights $\widetilde{\mathbf{w}}_1^{(i)} = \frac{p_{1,\theta}(x_1^{(i)}, y_1)}{q_{1,\phi}(x_1^{(i)}|y_1)} = \frac{\mu_\theta(x_t^{(i)}) g_{1,}(y_1|x_t^{(i)})}{q_{1,\phi}(x_1^{(i)}|y_1)}$
> Set $t = 2$
> **for** $k \leq$ iter **do**
>   Normalise weights, $\mathbf{w}_t^{(i)} = \frac{\widetilde{\mathbf{w}}_k^{(i)}}{\sum_j (\widetilde{\mathbf{w}}_t^{(j)})}$
>   Calculate $N_{eff} = \frac{1}{\sum_i (\mathbf{w}_t^{(i)})^2}$
>   **if** $N_{eff} < \frac{N}{2}$ **then**
>   Resample the particles $\widetilde{x}_t^{(i)} \sim \sum_i^N \mathbf{w}_t^{(i)} \delta_{x_t^{(i)}}$
>   Set $\mathbf{w}_t^{(i)} = \frac{1}{N}$
>   **end if**
>   t = t+1
>   Propagate the particles $x_t^{(i)} \sim q_\phi(x_t|x_{t-1}^{(i)})$
>   Calculate $\widetilde{\mathbf{w}}_t^{(i)} = \mathbf{w}_{t-1}^{(i)} \frac{p_{t,\theta}\left(x_k^{(i)}, y_t\right)}{q_{t,\phi}\left(x_t^{(i)}|x_{k-1}^{(i)}, y_t\right)} = \mathbf{w}_{t-1}^{(i)} \frac{f_{t,\theta}(x_t^{(i)}|x_{1:t1}) g_{t,\theta}(y_t|x_{1:t})}{qt,\phi\left(x_k^{(i)}|x_{k-1}^{(i)}, y_t\right)}$
> **end for**

We just give our filer/sampler the measurements generated by the target and likelihood dist.

Here we aim to infer the **posterior distribution:**

$p_\theta(x_{1:T}|y_{1:T})$

θ, ϕ are fixed , the weights give us the likelihood based on the measurements.

Differentiable Particle Filter:

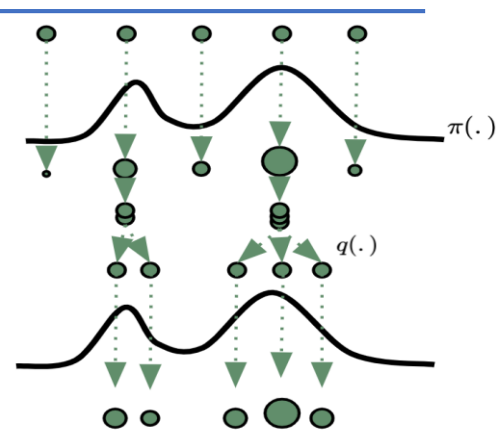
We can differentiate the PF and **learn the parameters** of all the **distributions** by maximising the normalising constant, therefore minimising: $-\frac{1}{T}\sum_{t=1}^{T} \nabla_{\theta,\phi} log(\sum_{i=1}^{N} \widetilde{w}_t^i)$. However:

- **Differentiable Resampling**: Resampling avoids weight degeneracy and low variance estimates. But it can't be differentiated as it's multinomial. Therefore several solutions have been proposed, [1] [2] [3] [4] , it seems that it exists a trade-off between biased-likelihood and biased-gradient.
- **Confusion in the literature:** What loss do we use ? Belief ? Semi supervised ? Optimising the normalising constant yields to a minimisation of the ELBO, therefore, optimisation of all the distributions/functions: the transition, likelihood, proposals and prior.

SMC Samplers

An SMC sampler targets a distribution $\pi(x)$ over T iterations using N samples. Importance sampling assigns each sample a weight, like in MCMC, at iteration t which is used to estimate $\pi(x)$.

$$\widetilde{\mathbf{w}}_t^{(i)} = \mathbf{w}_{t-1}^{(i)} \frac{p_{t,\theta}\left(x_t^{(i)}, y_t\right) \mathcal{L}_{t,\psi}\left(x_{t-1}^{(i)}|x_t^{(i)}, y_t\right)}{p_{t,\theta}\left(x_{t-1}^{(i)}, y_t\right) q_{t,\phi}\left(x_t^{(i)}|x_{t-1}^{(i)}, y_t\right)}$$



- **Backward Kernel (L-kernel):** The L-Kernel, $\mathcal{L}$, is commonly underexploited. The literature uses the proposal kernel as the backward kernel but it has been proven that it doesn't necessarily has to be the case [5]. A good choice of a backward kernel can improve the exploration of the parameter space and then **speed up convergence**.
- **Parallelisable:** SMC samplers can benefit from all the parallelisation techniques that are applied in the PF literature, even the resampling step [6].
- **Other Benefits**: **No burn-in steps**, handle multimodality, recycling.

Prior Proposals

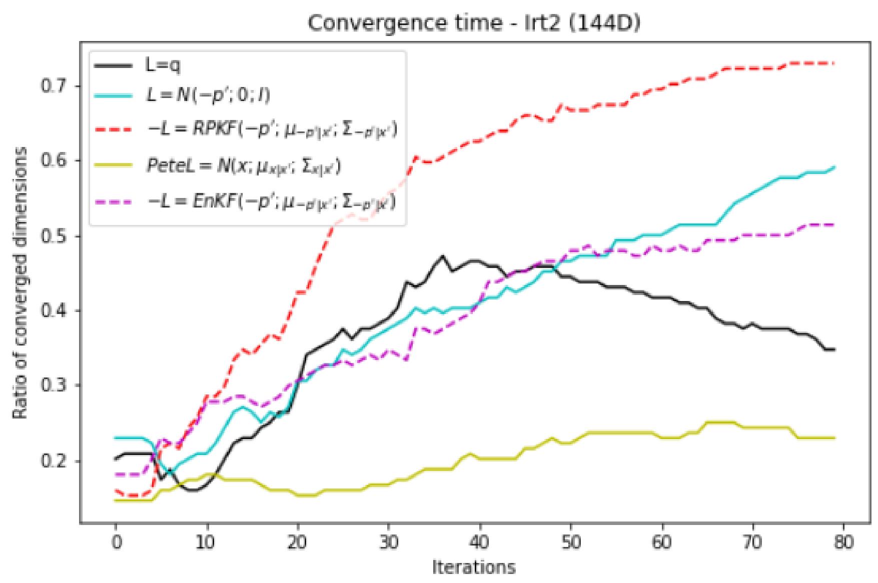
- **Proposal Kernel:** Even though a significant portion of the literature focuses on the impact of the resampling gradient bias. It has been shown in a submitted paper that the **choice of the proposal as a bigger impact** on the quality of the parameter estimation.

$$\widetilde{\mathbf{w}}_t^{(i)} = \mathbf{w}_{t-1}^{(i)} \frac{p_{t,\theta}\left(x_t^{(i)}, y_t\right) \mathcal{L}_{t,\psi}\left(-p_t^{(i)}|x_t^{(i)}, y_t\right)}{p_{t,\theta}\left(x_{t-1}^{(i)}, y_t\right) q_{t,\phi}\left(p_{t-1}^{(i)}|x_{t-1}^{(i)}, y_t\right)}$$

Weight update using **NUTS** [7] as a proposal. Where p is the momentum in the leapfrog algorithm.

- **L-Kernel:** It is possible to directly compute an optimal L-Kernel [5]. However its computational complexity remains $O(N^2)$ which might be a non negligible bottleneck.
  - **Near optimal-l Kernel using Kalman Filtering** [5]. Therefore we can choose to use a Ensemble Kalman Filter (to tackle non-linearity and high dimensions) as a decent backward kernel instead of learning it through optimisation.

We proposed a new high dimensional Kalman filter (RPKF). We show here a comparison of convergence depending on the choice of L-Kernel on a 144 dimensional model (irt2) [8]. We compare against L=q (forward kernel), a suboptimal L-kernel, RPKF, regular KF (Pete), EnKF.



Future Work & References

- **VAE:** We will try to compete against the current state of the art methods for the inference of latent space.
- **Fully Parallelised SMC Network:** We will try to exploit the inherent parallelisation of the sampler to speed up inference.

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