A Variational Sequential Monte Carlo – Supplementary Material

A.1 Proof of Proposition 1

We start by noting that the distribution of all random variables generated by the VSMC algorithm is given by

$$\widetilde{\phi}(x_{1:T}^{1:N}, a_{1:T-1}^{1:N}, b_T; \lambda) = \frac{w_T^{b_T}}{\sum_{\ell} w_T^{\ell}} \prod_{i=1}^{N} r(x_1^i; \lambda) \cdot \prod_{t=2}^{T} \prod_{i=1}^{N} \frac{w_{t-1}^{a_{t-1}^i}}{\sum_{\ell} w_{t-1}^{\ell}} r(x_t^i | x_{t-1}^{a_{t-1}^i}; \lambda).$$

$$(12)$$

We are interested in the marginal distribution $q(x_{1:T}; \lambda) \triangleq \widetilde{\phi}(x_{1:T}; \lambda) = \mathbb{E}_{b_{1:T}}[\widetilde{\phi}(x_{1:T}^{b_{1:T}}, b_{1:T}; \lambda)]$. A key observation is that the distribution of $b_{1:T} \mid x_{1:T}$, the conditional distribution of the ancestral path of the returned particle, is uniform on $\{1, \ldots, N\}^T$. Thus we get

$$q(x_{1:T};\lambda) = \frac{\widetilde{\phi}(x_{1:T}^{b_{1:T}}, b_{1:T};\lambda)}{\widetilde{\phi}(b_{1:T} \mid x_{1:T};\lambda)} = \frac{1}{N^{-T}} \sum_{\substack{a_{1:T-1}^{-b_{1:T-1}} \\ a_{1:T-1}^{-b_{1:T-1}}}} \int \widetilde{\phi}(x_{1:T}^{b_{1:T}}, x_{1:T}^{\neg b_{1:T}}, a_{1:T-1}^{\neg b_{1:T-1}};\lambda) \, \mathrm{d}x_{1:T}^{\neg b_{1:T}},$$
(13)

where

$$\begin{split} &\frac{1}{N^{-T}}\widetilde{\phi}(x_{1:T}^{b_{1:T}},x_{1:T}^{\neg b_{1:T}},a_{1:T-1}^{\neg b_{1:T-1}};\lambda) \\ &= N^{T}\frac{w_{1}^{b_{1}}}{\sum_{\ell}w_{1}^{\ell}}r(x_{1}^{b_{1}};\lambda)\prod_{t=2}^{T}\frac{w_{t}^{b_{t}}}{\sum_{\ell}w_{t}^{\ell}}r(x_{t}^{b_{t}}\mid x_{t-1}^{b_{t-1}};\lambda) \cdot \prod_{\substack{i=1\\i\neq b_{1}}}^{N}r(x_{1}^{i};\lambda) \cdot \prod_{t=2}^{T}\prod_{\substack{i=1\\i\neq b_{t}}}^{N}\frac{w_{t-1}^{a_{t-1}}}{\sum_{\ell}w_{t-1}^{\ell}}r(x_{t}^{i}|x_{t-1}^{a_{t-1}};\lambda) \\ &= p(x_{1}^{b_{1}},y_{1})\prod_{t=2}^{T}\frac{p(x_{1:t}^{b_{1:t}},y_{1:t})}{p(x_{1:t-1}^{b_{1:t-1}},y_{1:t-1})}\prod_{t=1}^{T}\frac{1}{\frac{1}{N}\sum_{\ell}w_{t}^{\ell}} \cdot \prod_{\substack{i=1\\i\neq b_{1}}}^{N}r(x_{1}^{i};\lambda) \cdot \prod_{t=2}^{T}\prod_{\substack{i=1\\i\neq b_{t}}}^{N}\frac{w_{t-1}^{a_{t-1}}}{\sum_{\ell}w_{t-1}^{\ell}}r(x_{t}^{i}|x_{t-1}^{a_{t-1}};\lambda) \\ &= p(x_{1:T}^{b_{1:T}},y_{1:T})\prod_{t=1}^{T}\frac{1}{\frac{1}{N}\sum_{\ell}w_{t}^{\ell}} \cdot \widetilde{\phi}(x_{1:T}^{\neg b_{1:T}},a_{1:T-1}^{\neg b_{1:T-1}};\lambda). \end{split}$$

We insert the above expression in (13) and we get

$$q(x_{1:T}; \lambda) = p(x_{1:T}^{b_{1:T}}, y_{1:T}) \sum_{\substack{a_{1:T-1}^{-b_{1:T-1}}}} \int \left(\prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} w_t^i \right)^{-1} \cdot \widetilde{\phi}(x_{1:T}^{\neg b_{1:T}}, a_{1:T-1}^{\neg b_{1:T-1}}; \lambda) \, dx_{1:T}^{\neg b_{1:T}}$$

$$= p(x_{1:T}^{b_{1:T}}, y_{1:T}) \mathbb{E}_{\widetilde{\phi}(x_{1:T}^{\neg b_{1:T}}, a_{1:T-1}^{\neg b_{1:T-1}}; \lambda)} \left[\left(\prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} w_t^i \right)^{-1} \right]. \tag{14}$$

A.2 Proof of Theorem 1

The evidence lower bound (ELBO), using the above result about the distribution of $q(x_{1:T}; \lambda)$, is given by

$$\mathcal{L}(\lambda) = \mathbb{E}_{q(x_{1:T};\lambda)} \left[\log p(x_{1:T}, y_{1:T}) - \log q(x_{1:T};\lambda) \right]$$

$$= -\int \left\{ p(x_{1:T}^{b_{1:T}}, y_{1:T}) \mathbb{E}_{\widetilde{\phi}(x_{1:T}^{-b_{1:T}}, a_{1:T-1}^{-b_{1:T}-1};\lambda)} \left[\frac{1}{\prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} w_{t}^{i}} \right] \cdot \log \mathbb{E}_{\widetilde{\phi}(x_{1:T}^{-b_{1:T}}, a_{1:T-1}^{-b_{1:T}-1};\lambda)} \left[\frac{1}{\prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} w_{t}^{i}} \right] \right\} dx_{1:T}^{b_{1:T}}.$$
(15)

Note that $-t \log t$ is a concave function for t > 0, this means by the conditional Jensen's inequality we have $-\mathbb{E}[t] \log \mathbb{E}[t] \ge -\mathbb{E}[t \log t]$. If we apply this to (15) we get

$$\mathcal{L}(\lambda) \geq \int \mathbb{E}_{\widetilde{\phi}(x_{1:T}^{-b_{1:T}}, a_{1:T-1}^{-b_{1:T}-1}; \lambda)} \left[\frac{p(x_{1:T}^{b_{1:T}}, y_{1:T})}{\prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} w_{t}^{i}} \sum_{t=1}^{T} \log \left(\frac{1}{N} \sum_{i=1}^{N} w_{t}^{i} \right) \right] dx_{1:T}^{b_{1:T}}$$

$$= \mathbb{E}_{\widetilde{\phi}(x_{1:T}^{1:N}, a_{1:T-1}^{1:N}; \lambda)} \left[\sum_{t=1}^{T} \log \left(\frac{1}{N} \sum_{i=1}^{N} w_{t}^{i} \right) \right] = \widetilde{\mathcal{L}}(\lambda),$$

where the last step follows because $q(x_{1:T}; \lambda)$ is the marginal of $\widetilde{\phi}(x_{1:T}^{1:N}, a_{1:T-1}^{1:N}; \lambda)$.

A.3 Stochastic Optimization

For the control variates we use

$$\sum_{t=2}^{T} c_{t} \mathbb{E}_{s(\cdot)\widetilde{\phi}(\cdot|\cdot\;;\lambda)} \left[\sum_{i=1}^{N} \nabla \log w_{t-1}^{a_{t-1}^{i}} - \sum_{\ell=1}^{N} \frac{w_{t-1}^{\ell}}{\sum_{m} w_{t-1}^{m}} \nabla \log w_{t-1}^{\ell} \right]$$

where

$$c_t = \mathbb{E}_{s(\cdot)\widetilde{\phi}(\cdot|\cdot;\lambda)} \left[\sum_{t'=t}^{T} \log \left(\frac{1}{N} \sum_{i=1}^{N} w_{t'}^{i} \right) \right].$$

In practice we use a stochastic estimate of c_t .

For T=2 we can use a leave-one-out estimator of the ancestor variable score function gradient

$$\sum_{i=1}^N \mathbb{E}_{s(\cdot)\widetilde{\phi}(\cdot|\cdot\;;\lambda)} \left[\log \left(\frac{N-1}{N} \frac{\sum_{\ell=1}^N w_2^\ell}{\sum_{j\neq i} w_2^j} \right) \left(\nabla \log w_1^{a_1^i} - \sum_{\ell=1}^N \frac{w_1^\ell}{\sum_m w_1^m} \nabla \log w_1^\ell \right) \right].$$

Score Function Gradient Below we provide the derivation of a score function-like estimator that is applicable in very general settings. However, we have found that in practice the variance tends to be quite high.

$$\begin{split} \nabla \widetilde{\mathcal{L}}(\lambda) &= \nabla \mathbb{E}_{\widetilde{\phi}(x_{1:T}^{1:N}, a_{1:T-1}^{1:N}; \lambda)} \left[\log \widehat{p}(y_{1:T}) \right] \\ &= \mathbb{E}_{\widetilde{\phi}(x_{1:T}^{1:N}, a_{1:T-1}^{1:N}; \lambda)} \left[\nabla \log \widehat{p}(y_{1:T}) + \log \widehat{p}(y_{1:T}) \nabla \log \widetilde{\phi}(x_{1:T}^{1:N}, a_{1:T-1}^{1:N}; \lambda) \right], \end{split}$$

with

$$\nabla \log \widehat{p}(y_{1:T}) = \nabla \sum_{t=1}^{T} \log \left(\frac{1}{N} \sum_{i=1}^{N} w_t^i \right) = \sum_{t=1}^{T} \sum_{i=1}^{N} \frac{w_t^i}{\sum_{\ell} w_t^{\ell}} \nabla \log w_t^i,$$

and

$$\begin{split} & \nabla \log \widetilde{\phi}(x_{1:T}^{1:N}, a_{1:T-1}^{1:N}; \lambda) \\ & = \sum_{i=1}^{N} \left[\nabla \log r(x_1^i; \lambda) + \sum_{t=2}^{T} \left[\nabla \log r(x_t^i | x_{t-1}^{a_{t-1}^i}; \lambda) + \nabla \log w_{t-1}^{a_{t-1}^i} - \sum_{\ell=1}^{N} \bar{w}_{t-1}^{\ell} \nabla \log w_{t-1}^{\ell} \right] \right]. \end{split}$$

A.4 Scaling With Dimension

In this section we study how the methods compare on a simple toy model defined by

$$p(x_{1:T}, y_{1:T}) = \prod_{t=1}^{T} \mathcal{N}(x_t; 0, 1) \mathcal{N}(y_t; x_t^2, 1).$$

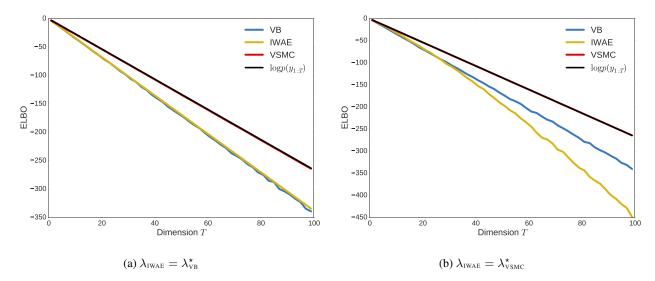


Figure 6: ELBO, for standard VB, IWAE, and VSMC, as a function of the dimension T of a toy problem. Here we set the number of samples in IWAE and VSMC to be N=2T.

We study the data set $y_t=3, \forall t$. Figure 6 shows the result when we let the number of samples in importance weighted auto-encoder (IWAE) (variational importance sampling (VIS)) and VSMC grow with the dimension N=2T. For low T the optimal parameters for IWAE are close to $\lambda_{\text{VSMC}}^{\star}$. On the other hand for high T, the optimal parameters for IWAE are close to those of standard variational Bayes (VB), i.e. $\lambda_{\text{VB}}^{\star}$. Figure 6 indicates that just by letting $N \propto T$, VSMC can achieve arbitrarily good approximation of $p(x_{1:T} \mid y_{1:T})$ even if $T \to \infty$. This holds, under some regularity conditions, even if $p(x_{1:T}, y_{1:T})$ is a state space model [Bérard et al., 2014]. This asymptotic approximation property is not satisfied by VIS, we see in Figure 6 that the approximation deteriorates as T increases. Note that this does not hold if the dimension of the latent space, i.e. $\dim(x_t)$, tends to infinity rather than the number of time points T.