# Sequential Importance Sampling Resampling 

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## Sequential Importance Sampling

- We use a structured IS distribution

$$
\begin{aligned}
q_{n}\left(x_{1: n}\right) & =q_{n-1}\left(x_{1: n-1}\right) q_{n}\left(x_{n} \mid x_{1: n-1}\right) \\
& =q_{1}\left(x_{1}\right) q_{2}\left(x_{2} \mid x_{1}\right) \cdots q_{n}\left(x_{n} \mid x_{1: n-1}\right)
\end{aligned}
$$

so if $X_{1: n-1}^{(i)} \sim q_{n-1}\left(x_{1: n-1}\right)$ then we only need to sample $X_{n}^{(i)} \mid X_{1: n-1}^{(i)} \sim q_{n}\left(x_{n} \mid X_{1: n-1}^{(i)}\right)$ to obtain $X_{1: n}^{(i)} \sim q_{n}\left(x_{1: n}\right)$

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- The importance weights are updated according to

$$
w_{n}\left(x_{1: n}\right)=\frac{\gamma_{n}\left(x_{1: n}\right)}{q_{n}\left(x_{1: n}\right)}=w_{n-1}\left(x_{1: n-1}\right) \underbrace{\frac{\gamma_{n}\left(x_{1: n}\right)}{\gamma_{n-1}\left(x_{1: n-1}\right) q_{n}\left(x_{n} \mid x_{1: n-1}\right)}}_{\alpha_{n}\left(x_{1: n}\right)}
$$

## Sequential Importance Sampling

- At time $n=1$, sample $X_{1}^{(i)} \sim q_{1}(\cdot)$ and set $w_{1}\left(X_{1}^{(i)}\right)=\frac{\gamma_{1}\left(X_{1}^{(i)}\right)}{q_{1}\left(X_{1}^{(i)}\right)}$.


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- It follows that

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\begin{aligned}
\widehat{\pi}_{n}\left(d x_{1: n}\right) & =\sum_{i=1}^{N} W_{n}^{(i)} \delta_{x_{1: n}^{(i)}}\left(d x_{1: n}\right) \\
\widehat{Z}_{n} & =\frac{1}{N} \sum_{i=1}^{N} w_{n}\left(x_{1: n}^{(i)}\right)
\end{aligned}
$$

## Sequential Importance Sampling for State-Space Models

- State-space models

Hidden Markov process: $X_{1} \sim \mu, X_{k} \mid\left(X_{k-1}=x_{k-1}\right) \sim f\left(\cdot \mid x_{k-1}\right)$
Observation process: $Y_{k} \mid\left(X_{k}=x_{k}\right) \sim g\left(\cdot \mid x_{k}\right)$

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- Assume we have received $y_{1: n}$, we are interested in sampling from

$$
\pi_{n}\left(x_{1: n}\right)=p\left(x_{1: n} \mid y_{1: n}\right)=\frac{p\left(x_{1: n}, y_{1: n}\right)}{p\left(y_{1: n}\right)}
$$

and estimating $p\left(y_{1: n}\right)$ where

$$
\begin{aligned}
& \gamma_{n}\left(x_{1: n}\right)=p\left(x_{1: n}, y_{1: n}\right)=\mu\left(x_{1}\right) \prod_{k=2}^{n} f\left(x_{k} \mid x_{k-1}\right) \prod_{k=1}^{n} g\left(y_{k} \mid x_{k}\right) \\
& Z_{n}=p\left(y_{1: n}\right)=\int \cdots \int \mu\left(x_{1}\right) \prod_{k=2}^{n} f\left(x_{k} \mid x_{k-1}\right) \prod_{k=1}^{n} g\left(y_{k} \mid x_{k}\right) d x_{1: n}
\end{aligned}
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## Locally Optimal Importance Distribution

- The optimal IS distribution $q_{n}\left(x_{n} \mid x_{1: n-1}\right)$ at time $n$ minimizing the variance of $w_{n}\left(x_{1: n}\right)$ is given by

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q_{n}^{\text {opt }}\left(x_{n} \mid x_{1: n-1}\right)=\pi_{n}\left(x_{n} \mid x_{1: n-1}\right)
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and yields an incremental importance weight of the form

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\alpha_{n}\left(x_{1: n}\right)=\frac{\gamma_{n}\left(x_{1: n-1}\right)}{\gamma_{n-1}\left(x_{1: n-1}\right)}
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- For state-space models, we have

$$
\begin{aligned}
q_{n}^{\mathrm{opt}}\left(x_{n} \mid x_{1: n-1}\right)= & p\left(x_{n} \mid y_{n}, x_{n-1}\right)=\frac{g\left(y_{n} \mid x_{n}\right) f\left(x_{n} \mid x_{n-1}\right)}{p\left(y_{n} \mid x_{n-1}\right)} \\
& \alpha_{n}\left(x_{1: n}\right)=p\left(y_{n} \mid x_{n-1}\right)
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- Importance Sampling only works decently for moderate size problems.
- Today, we discuss how to partially fix this problem.


## Resampling

- Intuitive KEY idea: As the time index $n$ increases, the variance of the unnormalized weights $\left\{w_{n}\left(X_{1: n}^{(i)}\right)\right\}$ tend to increase and all the mass is concentrated on a few random samples/particles. We propose to reset the approximation by getting rid in a principled way of the particles with low weights $W_{n}^{(i)}$ (relative to $1 / N$ ) and multiply the particles with high weights $W_{n}^{(i)}$ (relative to $1 / N$ ).


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- The main reason is that if a particle at time $n$ has a low weight then typically it will still have a low weight at time $n+1$ (though I can easily give you a counterexample).
- You want to focus your computational efforts on the "promising" parts of the space.


## Multinomial Resampling

- At time $n$, IS provides the following approximation of $\pi_{n}\left(x_{1: n}\right)$

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- The simplest resampling schemes consists of sampling $N$ times $\widetilde{X}_{1: n}^{(i)} \sim \widehat{\pi}_{n}\left(d x_{1: n}\right)$ to build the new approximation

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\widetilde{\pi}_{n}\left(d x_{1: n}\right)=\frac{1}{N} \sum_{i=1}^{N} \delta_{\widetilde{x}_{1: n}^{(i)}}\left(d x_{1: n}\right)
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- The new resampled particles $\left\{\widetilde{X}_{1: n}^{(i)}\right\}$ are approximately distributed according to $\pi_{n}\left(x_{1: n}\right)$ but statistically dependent. This is theoretically more difficult to study.
- Note that we can rewrite

$$
\tilde{\pi}_{n}\left(d x_{1: n}\right)=\sum_{i=1}^{N} \frac{N_{n}^{(i)}}{N} \delta_{X_{1: n}^{(i)}}\left(d x_{1: n}\right)
$$

where $\left(N_{n}^{(1)}, \ldots, N_{n}^{(N)}\right) \sim \mathcal{M}\left(N ; W_{n}^{(1)}, \ldots, W_{n}^{(N)}\right)$ thus
$\mathbb{E}\left[N_{n}^{(i)}\right]=N W_{n}^{(i)}, \operatorname{var}\left[N_{n}^{(1)}\right]=N W_{n}^{(i)}\left(1-W_{n}^{(i)}\right)$.

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- It follows that the resampling step is an unbiased operation

$$
\mathbb{E}\left[\widetilde{\pi}_{n}\left(d x_{1: n}\right) \mid \widehat{\pi}_{n}\left(d x_{1: n}\right)\right]=\widehat{\pi}_{n}\left(d x_{1: n}\right)
$$

but clearly it introduces some errors "locally" in time. That is for any test function, we have

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\operatorname{var}_{\tilde{\pi}_{n}}\left[\varphi\left(X_{1: n}\right)\right] \geq \operatorname{var}_{\hat{\pi}_{n}}\left[\varphi\left(X_{1: n}\right)\right]
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- Resampling is beneficial for future time steps (sometimes).


## Stratified Resampling

- Better resampling steps can be designed such that $\mathbb{E}\left[N_{n}^{(i)}\right]=N W_{n}^{(i)}$ but $\mathbb{V}\left[N_{n}^{(i)}\right]<N W_{n}^{(i)}\left(1-W_{n}^{(i)}\right)$.


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- A popular alternative to multinomial resampling consists of selecting

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U_{1} \sim \mathcal{U}\left[0, \frac{1}{N}\right]
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and for $i=2, \ldots, N$

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U_{i}=U_{1}+\frac{i-1}{N}=U_{i-1}+\frac{1}{N}
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- Then we set

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N_{n}^{(i)}=\#\left\{U_{j}: \sum_{m=1}^{i-1} W_{n}^{(m)} \leq U_{j}<\sum_{m=1}^{i} W_{n}^{(m)}\right\}
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where $\sum_{m=1}^{0}=0$.

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- It is trivial to check that $\mathbb{E}\left[N_{n}^{(i)}\right]=N W_{n}^{(i)}$.


## An alternative approach to resampling

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= & \alpha_{n}\left(x_{1: n}\right) q_{n}\left(x_{n} \mid x_{1: n-1}\right) \pi_{n-1}\left(x_{1: n-1}\right) \\
& +\left(1-\int \alpha_{n}\left(x_{1: n}\right) q_{n}\left(d x_{n} \mid x_{1: n-1}\right) \pi_{n-1}\left(d x_{1: n-1}\right)\right) \\
& \times \frac{\alpha_{n}\left(x_{1: n}\right) q_{n}\left(x_{n} \mid x_{1: n-1}\right) \pi_{n-1}\left(x_{1: n-1}\right)}{\int \alpha_{n}\left(x_{1: n}\right) q_{n}\left(d x_{n} \mid x_{1: n-1}\right) \pi_{n-1}\left(d x_{1: n-1}\right)}
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\end{aligned}
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- Looks like measure-valued Metropolis-Hastings algorithm.


## Probabilistic interpretation

- We have

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\begin{gathered}
\pi_{n}\left(x_{1: n}\right)=\underbrace{\alpha_{n}\left(x_{1: n}\right)}_{\text {accept with proba } w_{n}} \underbrace{q_{n}\left(x_{n} \mid x_{1: n-1}\right) \pi_{n-1}\left(x_{1: n-1}\right)}_{\text {trial distribution }}+ \\
\underbrace{\left(1-\int \alpha_{n}\left(x_{1: n}\right) q_{n}\left(d x_{n} \mid x_{1: n-1}\right) \pi_{n-1}\left(d x_{1: n-1}\right)\right)}_{\text {rejection probability }} \pi_{n}\left(x_{1: n}\right)
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- With probability $\alpha_{n}\left(X_{n}^{(i)}\right)$, set $\widetilde{X}_{1: n}^{(i)}=X_{1: n}^{(i)}$ otherwise $\widetilde{X}_{1: n}^{(i)} \sim \sum_{i=1}^{N} W_{n}^{(i)} \delta_{X_{1: n}^{(i)}}\left(d x_{1: n}\right)$.


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- Remark: Allows to decrease variance if $\alpha_{n}\left(x_{1: n}\right)$ "flat" over $E_{n}$; e.g. filtering with large observation noise.


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- We have $E S S=N$ and $C V=0$ if $W_{n}^{(i)}=1 / N$ for any $i$.


## Degeneracy Measures

- Resampling at each time step is harmful. We should resample only when necessary.
- To measure the variation of the weights, we can use the Effective Sample Size (ESS) or the coefficient of variation CV

$$
E S S=\left(\sum_{i=1}^{N}\left(W_{n}^{(i)}\right)^{2}\right)^{-1}, C V=\left(\frac{1}{N} \sum_{i=1}^{N}\left(N W_{n}^{(i)}-1\right)^{2}\right)^{1 / 2}
$$

- We have $E S S=N$ and $C V=0$ if $W_{n}^{(i)}=1 / N$ for any $i$.
- We have $E S S=1$ and $C V=\sqrt{N-1}$ if $W_{n}^{(i)}=1$ and $W_{n}^{(j)}=1$ for $j \neq i$.
- We can also use the entropy

$$
E n t=-\sum_{i=1}^{N} W_{n}^{(i)} \log _{2}\left(W_{n}^{(i)}\right)
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- Dynamic Resampling: If the variation of the weights as measured by ESS, CV or Ent is too high, then resample the particles.


## Generic Sequential Monte Carlo Scheme

- At time $n=1$, sample $X_{1}^{(i)} \sim q_{1}(\cdot)$ and set $w_{1}\left(X_{1}^{(i)}\right)=\frac{r_{1}\left(X_{1}^{(i)}\right)}{q_{1}\left(X_{1}^{(i)}\right)}$.


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- At time $n=1$, sample $X_{1}^{(i)} \sim q_{1}(\cdot)$ and set $w_{1}\left(X_{1}^{(i)}\right)=\frac{\gamma_{1}\left(X_{1}^{(i)}\right)}{q_{1}\left(X_{1}^{(i)}\right)}$.
- Resample $\left\{X_{1}^{(i)}, W_{1}^{(i)}\right\}$ to obtain new particles also denoted $\left\{X_{1}^{(i)}\right\}$


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- Resample $\left\{X_{1: n}^{(i)}, W_{n}^{(i)}\right\}$ to obtain new particles also denoted $\left\{X_{1: n}^{(i)}\right\}$
- At any time $n$, we have two approximation of $\pi_{n}\left(x_{1: n}\right)$

$$
\begin{aligned}
& \widehat{\pi}_{n}\left(d x_{1: n}\right)=\sum_{i=1}^{N} W_{n}^{(i)} \delta_{X_{1: n}^{(i)}}\left(d x_{1: n}\right) \text { (before resampling) } \\
& \widetilde{\pi}_{n}\left(d x_{1: n}\right)=\frac{1}{N} \sum_{i=1}^{N} \delta_{X_{1: n}^{(i)}}\left(d x_{1: n}\right) \text { (after resampling). }
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- We also have

$$
\frac{\widehat{Z_{n}}}{Z_{n-1}}=\frac{1}{N} \sum_{i=1}^{N} w_{n}\left(X_{1: n}^{(i)}\right)
$$

## Sequential Monte Carlo for Hidden Markov Models

- At time $n=1$, sample $X_{1}^{(i)} \sim q_{1}(\cdot)$ and set

$$
w_{1}\left(X_{1}^{(i)}\right)=\frac{\mu\left(X_{1}^{(i)}\right) g\left(y_{1} \mid X_{1}^{(i)}\right)}{q\left(X_{1}^{(i)} \mid y_{1}\right)} .
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- Resample $\left\{X_{1: n}^{(i)}, W_{n}^{(i)}\right\}$ to obtain new particles also denoted $\left\{X_{1: n}^{(i)}\right\}$
- Example: Linear Gaussian model

$$
\begin{aligned}
& X_{1} \sim \mathcal{N}(0,1), X_{n}=\alpha X_{n-1}+\sigma_{v} V_{n}, \\
& Y_{n}=X_{n}+\sigma_{w} W_{n}
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- We know that $p\left(x_{1: n} \mid y_{1: n}\right)$ is Gaussian and its parameters can be computed using Kalman techniques. In particular $p\left(x_{n} \mid y_{1: n}\right)$ is also a Gaussian which can be computed using the Kalman filter.
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- We apply the SMC method with
$q\left(x_{n} \mid y_{n}, x_{n-1}\right)=f\left(x_{n} \mid x_{n-1}\right)=\mathcal{N}\left(x_{n} ; \alpha x_{n-1}, \sigma_{v}^{2}\right)$.


Figure: Histograms of the base 10 logarithm of $W_{n}^{(i)}$ for $n=1$ (top), $n=50$ (middle) and $n=100$ (bottom).

- By itself this graph does not mean that the procedure is efficient!
- This SMC strategy performs remarkably well in terms of estimation of the marginals $p\left(x_{k} \mid y_{1: k}\right)$. This is what is only necessary in many applications thankfully.
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- The same conclusion holds for most sequences of distributions $\pi_{k}\left(x_{1: k}\right)$.
- Resampling only solves partially our problems.


## Another Illustration of the Degeneracy Phenomenon

- For the linear Gaussian state-space model described before, we can compute in closed form

$$
S_{n}=\frac{1}{n} \sum_{k=1}^{n} \mathbb{E}\left[X_{k}^{2} \mid Y_{1: n}\right]
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- This estimate can be updated sequentially using our SMC approximation.


Figure: Sufficient statistics computed exactly through the Kalman smoother (blue) and the SMC method (red).

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- It looks like a nice result but it is rather useless as $C_{n}$ increases polynomially/exponentially with time.
- To achieve a fixed precision, this would require to use a time-increasing number of particles $N$.
- You cannot hope to estimate with a fixed precision a target distribution of increasing dimension.
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- At best, you can expect results of the following form

$$
\begin{aligned}
& \mathbb{E}\left[\left|\int \varphi\left(x_{n-L+1: n}\right)\left(\widehat{\pi}_{n}\left(d x_{n-L+1: n}\right)-\pi_{n}\left(d x_{n-L+1: n}\right)\right)\right|^{p}\right]^{1 / p} \\
& \quad \leq \frac{M_{L}\|\varphi\|_{\infty}}{N}
\end{aligned}
$$

if the model has nice forgetting/mixing properties, i.e.

$$
\int\left|\pi_{n}\left(x_{n} \mid x_{1}\right)-\pi_{n}\left(x_{n} \mid x_{1}^{\prime}\right)\right| d x_{n} \leq 2 \lambda^{n-1}
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$$

with $0 \leq \lambda<1$.

- In the HMM case, it means that

$$
\int\left|p\left(x_{n} \mid y_{1: n}, x_{1}\right)-p\left(x_{n} \mid y_{1: n}, x_{1}^{\prime}\right)\right| d x_{n} \leq \lambda^{n-1}
$$

## Central Limit Theorems

- For SIS we have

$$
\sqrt{N}\left(\mathbb{E}_{\widehat{\pi}_{n}}\left(\varphi_{n}\left(X_{1: n}\right)\right)-\mathbb{E}_{\pi_{n}}\left(\varphi_{n}\left(X_{1: n}\right)\right)\right) \Rightarrow \mathcal{N}\left(0, \sigma_{I S}^{2}\left(\varphi_{n}\right)\right)
$$

where

$$
\sigma_{I S}^{2}\left(\varphi_{n}\right)=\int \frac{\pi_{n}^{2}\left(x_{1: n}\right)}{q_{n}\left(x_{1: n}\right)}\left(\left(\varphi_{n}\left(x_{1: n}\right)\right)-\mathbb{E}_{\pi_{n}}\left(\varphi\left(x_{1: n}\right)\right)\right)^{2} d x_{1: n}
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$$

- We also have

$$
\sqrt{N}\left(\hat{Z}_{n}-Z_{n}\right) \Rightarrow \mathcal{N}\left(0, \sigma_{I S}^{2}\right)
$$

where

$$
\sigma_{I S}^{2}=\int \frac{\pi_{n}^{2}\left(x_{1: n}\right)}{q_{n}\left(x_{1: n}\right)} d x_{1: n}-1
$$

- For SMC, we have

$$
\begin{aligned}
& \sigma_{S M C}^{2}\left(\varphi_{n}\right)=\int \frac{\pi_{n}^{2}\left(x_{1}\right)}{q_{1}\left(x_{1}\right)}\left(\int \varphi_{n}\left(x_{2: n}\right) \pi_{n}\left(x_{2: n} \mid x_{1}\right) d x_{2: n}-\mathbb{E}_{\pi_{n}}\left(\varphi_{n}\left(X_{1: n}\right)\right)\right)^{2} d x_{1} \\
& +\sum_{k=2}^{n-1} \int \frac{\pi_{n}\left(x_{1: k}\right)^{2}}{\pi_{k-1}\left(x_{1: k-1}\right) q_{k}\left(x_{k} \mid x_{k-1}\right)} \\
& \times\left(\int \varphi_{n}\left(x_{1: n}\right) \pi_{n}\left(x_{k+1: n} \mid x_{k}\right) d x_{k+1: n}-\mathbb{E}_{\pi_{n}}\left(\varphi_{n}\left(X_{1: n}\right)\right)\right)^{2} d x_{1: k} \\
& +\int \frac{\pi_{n}\left(x_{1: n}\right)^{2}}{\pi_{n-1}\left(x_{1: n-1}\right) q_{n}\left(x_{n} \mid x_{n-1}\right)}\left(\varphi_{n}\left(x_{1: n}\right)-\mathbb{E}_{\pi_{n}}\left(\varphi_{n}\left(X_{1: n}\right)\right)\right)^{2} d x_{1: n} .
\end{aligned}
$$

and

$$
\sigma_{S M C}^{2}=\int \frac{\pi_{n}^{2}\left(x_{1}\right)}{q_{1}\left(x_{1}\right)} d x_{1}+\sum_{k=2}^{n} \int \frac{\pi_{n}\left(x_{1: k}\right)^{2}}{\pi_{k-1}\left(x_{1: k-1}\right) q_{k}\left(x_{k} \mid x_{k-1}\right)} d x_{1: k}-n
$$

## Back to our toy example

- Consider the case where the target is defined on $\mathbb{R}^{n}$ and

$$
\begin{aligned}
& \pi\left(x_{1: n}\right)=\prod_{n=1}^{n} \mathcal{N}\left(x_{k} ; 0,1\right), \\
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\end{aligned}
$$

- We select an importance distribution

$$
q\left(x_{1: n}\right)=\prod_{k=1}^{n} \mathcal{N}\left(x_{k} ; 0, \sigma^{2}\right)
$$

- For SMC, the asymptotic variance is finite only when $\sigma^{2}>\frac{1}{2}$ and

$$
\begin{aligned}
\frac{\mathbb{V}_{\mathrm{SMC}}\left[\hat{Z}_{n}\right]}{Z_{n}^{2}} & \approx \frac{1}{N}\left[\int \frac{\pi_{n}^{2}\left(x_{1}\right)}{q_{1}\left(x_{1}\right)} d x_{1}-1+\sum_{k=2}^{n} \int \frac{\pi_{n}^{2}\left(x_{k}\right)}{q_{k}\left(x_{k}\right)} d x_{k}-1\right] \\
& =\frac{n}{N}\left[\left(\frac{\sigma^{4}}{2 \sigma^{2}-1}\right)^{1 / 2}-1\right]
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$$

compared to

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\frac{\mathbb{V}_{\mathrm{IS}}\left[\widehat{Z}_{n}\right]}{Z_{n}^{2}}=\frac{1}{N}\left[\left(\frac{\sigma^{4}}{2 \sigma^{2}-1}\right)^{n / 2}-1\right]
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- If select $\sigma^{2}=1.2$ then we saw that it is necessary to employ $N \approx 2 \times 10^{23}$ particles in order to obtain $\frac{\mathbb{V}_{15}\left[\hat{Z}_{n}\right]}{Z_{n}^{2}}=10^{-2}$ for $n=1000$.
- For SMC, the asymptotic variance is finite only when $\sigma^{2}>\frac{1}{2}$ and

$$
\begin{aligned}
\frac{\mathbb{V}_{\mathrm{SMC}}\left[\hat{Z}_{n}\right]}{Z_{n}^{2}} & \approx \frac{1}{N}\left[\int \frac{\pi_{n}^{2}\left(x_{1}\right)}{q_{1}\left(x_{1}\right)} d x_{1}-1+\sum_{k=2}^{n} \int \frac{\pi_{n}^{2}\left(x_{k}\right)}{q_{k}\left(x_{k}\right)} d x_{k}-1\right] \\
& =\frac{n}{N}\left[\left(\frac{\sigma^{4}}{2 \sigma^{2}-1}\right)^{1 / 2}-1\right]
\end{aligned}
$$

compared to

$$
\frac{\mathbb{V}_{\mathrm{IS}}\left[\widehat{Z}_{n}\right]}{Z_{n}^{2}}=\frac{1}{N}\left[\left(\frac{\sigma^{4}}{2 \sigma^{2}-1}\right)^{n / 2}-1\right]
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for SIS.

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- To obtain the same performance, $\frac{\mathbb{V}_{\text {SMC }}\left[\hat{Z}_{n}\right]}{Z_{n}^{2}}=10^{-2}$, SMC requires the use of just $N \approx 10^{4}$ particles: an improvement by 19 orders of magnitude.
- If you have nice mixing properties, then you can obtain

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- Under the same assumptions, you can also obtain

$$
\sigma_{S M C}^{2} \leq \frac{D \cdot T}{N}
$$

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- The SMC approximation of $\pi_{n}\left(x_{1: n}\right)$ is only reliable for 'small' $n$.

