# Variational Sequential Monte Carlo

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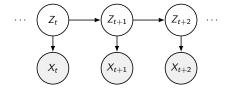
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#### Overview

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  - State space models
  - Inference in SSM
- 2 Importance Sampling
  - Basic Monte Carlo
- Sequential Monte Carlo
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# State-Space Models



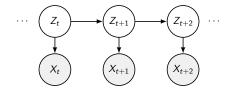
 $\{Z_t\}_{t\geq 1}$  is a hidden Markov process

$$Z_1 \sim \mu(\cdot)$$
  $Z_t \mid (Z_{t-1} = z) \sim f_{\theta}(\cdot | z)$  (1)

 $\{X_t\}_{t\geq 1}$  is Markov observation process

$$X_t \mid (Z_t = z) \sim g_{\theta}(\cdot \mid z)$$
 (2)

# State-Space Models: Examples



- Hidden Markov Model:  $\{Z_t\}$  is a finite Markov Chain
- 2 Linear Gaussian SSM:

$$Z_{t} = A_{t}Z_{t-1} + B_{t}V_{t} \qquad V_{t} \stackrel{iid}{\sim} \mathcal{N}(0, I)$$

$$X_{t} = B_{t}Z_{t} + D_{t}W_{t} \qquad W_{t} \stackrel{iid}{\sim} \mathcal{N}(0, I)$$
(3)

Non-linear non-Gaussian model – stochastic volatility model

$$Z_{t} = \phi Z_{t-1} + \sigma V_{t} \qquad V_{t} \stackrel{iid}{\sim} \mathcal{N}(0, I)$$

$$X_{t} = \beta \exp(Z_{t}/2)W_{t} \qquad W_{t} \stackrel{iid}{\sim} \mathcal{N}(0, I)$$
(4)

### Inference in SSM

#### Goals:

- $\theta$  is known: infer  $\{z_t\}_{t\geq 1}$  from  $\{x_t\}_{t\geq 1}$ 
  - Filtering:  $p(z_t|x_{1:t})$ ,  $p(x_{1:t})$
  - Smoothing:  $p(z_t|x_{1:T}), p(z_{1:T}|x_{1:T})$
- $\theta$  is unknown: identify dynamics, i.e.  $\log p(x_{1:T}|\theta) \to \max_{\theta}$

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$$p(z_{1:T}|x_{1:T}) = \frac{p(x_{1:T}, z_{1:T})}{p(x_{1:T})}$$
 (5)

$$p(x_{1:T}, z_{1:T}) = \underbrace{\mu(z_1) \prod_{t=2}^{T} f(z_t | z_{t-1}) \prod_{t=1}^{T} g(x_t | z_t)}_{p(x_{1:T} | z_{1:T})}$$
(6)

$$p(x_{1:T}) = \int p(x_{1:T}, z_{1:T}) dz_{1:T}$$
 (7)

## Analytic Inference

Posterior

$$p(z_{1:t}|x_{1:t}) = \frac{p(z_{1:t}, x_{1:t})}{p(x_{1:t})} = \frac{p(z_{1:t-1}, x_{1:t-1})g(x_t|z_t)f(z_t|z_{t-1})}{p(x_{1:t})}$$

$$= p(z_{1:t-1}|x_{1:t-1})\frac{g(x_t|z_t)f(z_t|z_{t-1})}{p(x_t|x_{1:t-1})}$$
(8)

Denominator

$$p(x_t|x_{1:t-1}) = \int g(x_t|z_t)f(z_t|z_{t-1})p(z_{t-1}|x_{1:t-1})dz_{t-1:t}$$
 (9)

Marginal likelihood decomposes naturally

$$p(x_{1:t}) = p(x_1) \prod_{k=2}^{t} p(x_k | x_{1:k-1})$$
 (10)

Non-Gaussian non-linear dynamics?

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Non-Gaussian non-linear dynamics? No way!

# Monte Carlo Integration

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Let us for the moment review the basic Monte Carlo methods.

$$\gamma_t(z_{1:t}) \stackrel{\triangle}{=} p(z_{1:t}, x_{1:t})$$

$$C_t \stackrel{\triangle}{=} p(x_{1:t})$$

$$\pi_t(z_{1:t}) \stackrel{\triangle}{=} \frac{\gamma_t(z_{1:t})}{C_t}$$
(12)

#### Basic Monte Carlo

Assuming we can sample  $z_{1:t}^i \sim \pi_t(z_{1:t})$ 

$$\pi_t(z_{1:t}) = \frac{\gamma(z_{1:t})}{C_t} \approx \frac{1}{N} \sum_{i=1}^N \delta(z_{1:t} - Z_{1:t}^i) \stackrel{\triangle}{=} \widehat{\pi}_t(z_{1:t})$$

$$I_{t}(\varphi) = \int \varphi(z_{1:t}) \pi(z_{1:t}) dz_{1:t} \approx \frac{1}{N} \sum_{i=1}^{N} \varphi(Z_{1:t}^{i}) \qquad \triangleq I_{t}^{MC}(\varphi)$$

This estimate is unbiased and have a variance of

$$\mathbb{V}\mathrm{ar}\left[I_t^{MC}(\varphi)\right] = \frac{1}{N}\left(\int \varphi^2(z_{1:t})\pi(z_{1:t})dz_{1:t} - I_t(\varphi)^2\right) \tag{13}$$

## Variance of MC estimate

#### Problems of basic Monte Carlo

- We cannot sample from high dimensional complex  $\pi(z_{1:t})$
- ② We dont want to resample  $z_{1:t}$  on increment of t

#### Variance of MC estimate

#### Problems of basic Monte Carlo

- **1** We cannot sample from high dimensional complex  $\pi(z_{1:t})$
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#### We are going to address

- the first problem with Importance Sampling (IS)
- 2 the second problem with Sequential IS

# Importance Sampling

- choose a proposal distribution  $q: \pi(z_{1:t}) > 0 \Rightarrow q(z_{1:t}) > 0$
- 2 sample from q, i.e.  $z_{1:t}^i \sim q(z_{1:t})$ ,
- 3 reweight samples with importance weights  $w(z_{1:t}) = \frac{\gamma(z_{1:t})}{q(z_{1:t})}$

Then we can

- renormalize the weights  $W_t^i = \frac{w(z_{1:t}^i)}{\sum_j w(z_{1:t}^j)}$
- ullet and approximate  $\pi$  with

$$\widehat{\pi}(z_{1:t}) = \sum_{i=1}^{N} W_t^i \delta(z_{1:t} - z_{1:t}^i)$$

estimate of the normalizing constant

$$\widehat{C}_t = \frac{1}{N} \sum_{i=1}^N w(z_{1:t}^i)$$

## Properties of IS estimation

#### Estimate of $C_t$

is unbiased

$$\mathbb{E}\left[\widehat{C}_{t}\right] = \frac{1}{N} \sum_{i=1}^{N} \mathbb{E}_{z_{1:t} \sim q} \left[\frac{\gamma_{t}(z_{1:t})}{q(z_{1:t})}\right] = \frac{N}{N} C_{t}$$

• has relative variance of  $\mathcal{O}(\frac{1}{N})$ 

$$\frac{\mathbb{V}\mathrm{ar}\left[\widehat{C}_{t}\right]}{C_{t}^{2}} = \frac{1}{N} \left( \int \frac{\pi^{2}(z_{1:t})}{q(z_{1:t})} dz_{1:t} - 1 \right)$$

To address the second problem we introduce Sequential IS

# Sequential Importance Sampling

- lacksquare choose a proposal of the form  $q(z_{1:t}) = q(z_t|z_{1:t-1})q(z_{1:t-1})$
- 2 on increment of t, sample  $z_t^i \sim q(z_t|z_{1:t-1}^i)$
- recompute IS weights according to the recurrence

$$w(z_{1:t}) \stackrel{\triangle}{=} \frac{\gamma(z_{1:t})}{q(z_{1:t})} = \frac{\gamma(z_{1:t})}{q(z_t|z_{1:t-1})\gamma(z_{1:t-1})} \cdot \frac{\gamma(z_{1:t-1})}{q(z_{1:t-1})}$$

$$\stackrel{\triangle}{=} \alpha(z_{1:t}) \cdot w(z_{1:t-1}) = w_1(z_1) \prod_{k=2}^t \alpha(z_{1:k})$$

We have mitigated both problems.

So what could go wrong?

#### Enormous variance

Consider the simplest example possible

$$\pi_t(z_{1:t}) = \prod_{k=1}^t \mathcal{N}(z_k|0,1) = \frac{\gamma_t(z_{1:t})}{C_t} = \frac{\prod_{k=1}^t \exp\left(-\frac{z_k^2}{2}\right)}{(2\pi)^{t/2}}$$
 $q_t(z_{1:t}) = \prod_{k=1}^t \mathcal{N}(z_k|0,\sigma^2)$ 

Then

$$\frac{\mathbb{V}\mathrm{ar}\left[\widehat{C}_{t}\right]}{C_{t}^{2}} = \frac{1}{N}\left(\int \frac{\pi^{2}(z_{1:t})}{q(z_{1:t})}dz_{1:t} - 1\right) = \left[\left(\frac{\sigma^{4}}{2\sigma^{2} - 1}\right)^{t/2} - 1\right]$$

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For almost perfect q with  $\sigma=1.2$  to obtain relative variance of 0.01 for t=1000 we would need  $N\approx 2\times 10^{23}$  particles. SMC in the same setting will require only  $N\approx 10^4$ 

Sequential Monte Carlo

## Definition of SMC

### SMC = Sequential IS + Resampling

SMC is a family of methods for sampling from a sequence of distributions  $\{\pi_t(z_{1:t})\}$  of increasing dimension t.

Note:  $\pi_t$  may not be nested, i.e.  $\pi_t(z_{1:t-1}) \neq \pi_{t-1}(z_{1:t-1})$ 

At each time step SMC provides

- **1** approximation  $\widehat{\pi}_t$  of  $\pi_t$
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At each time step SMC provides

- **1** approximation  $\widehat{\pi}_t$  of  $\pi_t$
- 2 estimates normalization constant  $C_t$ 
  - simple technique, hard to analyze due to resampling
  - very strong theoretical guarantees
  - well explored field (over 20 years of thorough investigation)
  - very good in practice

# SMC procedure: Bootstrap filter (Gordon, 1993)

At t=1

- **1** Sample *N* particles  $z_1^i \sim q(z_1)$
- Compute weights  $w_1(z_1^i) = \frac{\gamma(z_1^i)}{q(z_1^i)}$   $W_1^i = \frac{w_1(z_1^i)}{\sum_i w_1(z_1^i)}$

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At  $t \ge 2$ 

- Sample ancestor indices  $a_{t-1}^i \sim \operatorname{Cat}(W_{t-1}^1, ..., W_{t-1}^N)$
- Sample N particles  $z_t^i \sim q(z_t|z_{1:t-1}^{a_{t-1}^i})$
- Compute weights

$$w_t(z_{1:t}^i) = \frac{\gamma(z_{1:t-1}^i)}{q(z_{1:t}^i)} \qquad W_t^i = \frac{w_t(z_{1:t}^i)}{\sum_i w_t(z_{1:t}^i)}$$

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At t > 2

- Sample ancestor indices  $a_{t-1}^i \sim \operatorname{Cat}(W_{t-1}^1, ..., W_{t-1}^N)$
- 2 Sample N particles  $z_t^i \sim q(z_t|z_{1:t-1}^{a_{t-1}'})$
- Compute weights

$$w_t(z_{1:t}^i) = \frac{\gamma(z_{1:t-1}^i)}{q(z_{1:t}^i)} \qquad W_t^i = \frac{w_t(z_{1:t}^i)}{\sum_i w_t(z_{1:t}^i)}$$

Estimate normalization constant and target distribution

$$\widehat{C}_t = \frac{1}{N} \sum_{i=1}^t w_t(z_{1:t}^i) \qquad \widehat{\pi}_t(z_{1:t}) = \sum_{i=1}^N W_t^i \delta(z_{1:t} - z_{1:t}^i)$$

## Resampling reduces variance of final estimates

$$N \frac{\mathbb{V}\text{ar}\left[\widehat{C}_{t}^{SIS}\right]}{C_{t}^{2}} = \int \frac{\pi_{t}^{2}(z_{1:t})}{q(z_{1:t})} dz_{1:t} - 1$$

$$N \frac{\mathbb{V}\text{ar}\left[\widehat{C}_{t}^{SMC}\right]}{C_{t}^{2}} \approx \int \frac{\pi_{t}^{2}(z_{1})}{q_{1}(z_{1})dz_{1}} - 1$$

$$+ \sum_{l=0}^{t} \int \frac{\pi_{t}^{2}(z_{1:k})}{\pi_{k-1}(z_{1:k-1})q_{k}(z_{k}|z_{1:k})} dz_{k-1:k} - 1$$

Resampling "resets" the system – splits the integral into parts.

## Particle impoverishment

No free lunch: (Doucet, 2011)

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At each step we can only reduce the particle set!

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Many techniques to partially mitigate impoverishment

- Controlled resampling: the variance of weights (ESS, ent.)
- Advanced resampling: Systematic / Residual resampling, etc.
- Look-aheads: Block Sampling, Auxiliary Particle Filter
- Resample-Move: MCMC / Gibbs steps to "jitter" particles

# SMC for Filtering – Particle Filter

Recall

$$\pi_t(z_{1:t}) \stackrel{\Delta}{=} \frac{\gamma_t(z_{1:t})}{C_t} = \frac{p(z_{1:t}, x_{1:t})}{p(x_{1:t})} = p(z_{1:t}|x_{1:t})$$

$$p(z_{1:t}|x_{1:t}) = p(z_{1:t-1}|x_{1:t-1}) \frac{g(x_t|z_t)f(z_t|z_{t-1})}{p(x_t|x_{1:t-1})}$$

- We have  $\widehat{p}(z_{1:t-1}|x_{1:t-1}) = \sum_{i} W_{i}^{t-1} \delta(z_{1:t-1} z_{1:t-1}^{i})$
- Can marginalize  $\widehat{p}(z_{t-1}|x_{1:t-1}) = \sum_{i} W_{i}^{t-1} \delta(z_{t-1} z_{t-1}^{i})$
- Resample, i.e. sample from  $\widehat{p}(z_{t-1}|x_{1:t-1})$ :

$$\overline{p}(z_{t-1}|x_{1:t-1}) \triangleq \frac{1}{N} \sum_{i=1}^{N} \delta(z_{t-1} - z_{t-1}^{i})$$

# The marginal likelihood estimate

Sampling  $z_t^i$  from proposal  $q(z_t|z_{t-1}^i)$  we obtain

$$p(x_t|x_{1:t-1}) \approx \int \frac{g(x_t|z_t)f(z_t|z_{t-1})}{q(z_t|z_{t-1}^i)} q(z_t|z_{t-1}^i) \overline{p}(z_{t-1}|x_{1:t-1}) dz_{t-1:t}$$

$$= \frac{1}{N} \sum_{i}^{N} \frac{g(x_t|z_t^i)f(z_t^i|z_{t-1}^i)}{q(z_t^i|z_{t-1}^i)}$$

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$$\begin{aligned} p(x_t|x_{1:t-1}) &\approx \int \frac{g(x_t|z_t)f(z_t|z_{t-1})}{q(z_t|z_{t-1}^i)} q(z_t|z_{t-1}^i) \overline{p}(z_{t-1}|x_{1:t-1}) dz_{t-1:t} \\ &= \frac{1}{N} \sum_{i}^{N} \frac{g(x_t|z_t^i)f(z_t^i|z_{t-1}^i)}{q(z_t^i|z_{t-1}^i)} \end{aligned}$$

We can model f, g, q with complex models:

$$w_t^i = \frac{f(z_t|z_{1:t-1}^{a_{t-1}^i})g(x_t|z_{1:t}^k)}{q(z_t^k|x_{1:t},z_{1:t-1}^{a_{t-1}^i})}$$

And still easily estimate marginal likelihood (unbiasedly)

$$\widehat{p}(x_{1:t}) \stackrel{\triangle}{=} \prod_{t=1}^{T} \frac{1}{N} \sum_{i=1}^{N} w_t^i,$$

#### Some of the theoretical results

**Assumption**: exponential stability –  $\forall z_1, z'_1$ 

$$\int |p(z_t|x_{2:t}, \mathbf{z_1}) - p(z_t|x_{2:t}, \mathbf{z_1'})| dx_t \leq \alpha^t, \qquad 0 \leq \alpha < 1$$

• L1 distance. Bias increases linearly with  $t: \exists B_1 < \infty$ 

$$\int \left| \mathbb{E}\left[\widehat{p}(z_{1:t}|x_{1:t})\right] - p(z_{1:t}|x_{1:t}) \right| \leq \frac{B_1 \cdot t}{N}$$

• Central Limit Theorem. Approximate Normality:  $\exists B_2 < \infty$ 

$$\lim_{N\to\infty} \sqrt{N}(\log \widehat{p}(x_{1:t}) - \log p(x_{1:t})) \to \mathcal{N}(0, \sigma_t^2), \quad \sigma_t^2 \leq B_2 t$$

• **Relative Variance** increases linearly with  $t: \exists B_3 < \infty$ 

$$\mathbb{E}\left[\left(\frac{\widehat{p}(x_{1:t})}{p(x_{1:t})}-1\right)^2\right] \leq \frac{B_3t}{N}$$

## Improvements over standard SMC

#### Proposal improvements:

- Estimating the mode of a true posterior  $p(z_t|x_{1:t})$
- Local approximations: local linearization of system dynamics (EKF), Unscented KF, etc.
- Implicit proposals (Chorin, 2012)

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Can we improve upon the fixed proposal?

Variational Sequential Monte Carlo

## High level overview

- $\bullet$  We can parametrise our proposal distribution q
- ② And optimize KL between q and true posterior  $p(z_{1:t}|x_{1:t})$
- To sample from variational posterior
  - Run SMC and pick one of the particles
- Applicable to any sequence of probabilistic models
- VSMC allows for model learning, proposal adaptation and inference amortization

# Unifying view on ELBO

For any unnormalized target density  $\gamma(z)$  with normalizing constant C,  $\pi(z) = \frac{\gamma(z)}{C}$  and a proposal density q

$$\mathrm{ELBO} = \int Q(z) \log \frac{\gamma(z)}{Q(z)} dz = \log C - \mathrm{KL}(Q||\pi)$$

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- Assume  $\widehat{C}(z)$  is nonnegative and  $\int Q(z)\widehat{C}(z) = C$
- Then we can plug  $\gamma(z) = Q(z)\widehat{C}(z)$  into ELBO

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ELBO = 
$$\int Q(z) \log \frac{Q(z)\widehat{C}(z)}{Q(z)} dz = \int Q(z) \log \widehat{C}(z) dz$$

• For example  $\widehat{C}(z)$  may be one of these

$$\widehat{C}(z)^{VAE} = \frac{p(x,z)}{q(z|x)}, \qquad \widehat{C}(z^{1:K})^{IWAE} = \frac{1}{K} \sum_{k=1}^{K} \frac{p(x,z^k)}{q(z^k|x)}$$

## **VSMC**

Based on sampling distribution of SMC

$$Q_{SMC}(z_{1:T}^{1:K}, a_{1:T-1}^{1:K}) = \left(\prod_{k=1}^{K} q_{\phi}(z_{1}^{k})\right) \left(\prod_{t=2}^{T} \prod_{k=1}^{K} q_{\phi}(z_{t}^{k}|z_{1:t-1}^{a_{t-1}^{k}}) \operatorname{Cat}(a_{t-1}^{k}|W_{t-1}^{1:K})\right)$$

and unbiased estimator of marginal likelihood

$$\widehat{C}_{SMC}(z_{1:T}^{1:K}, a_{1:T-1}^{1:K}) = \prod_{t=1}^{T} \left[ \frac{1}{N} \sum_{i=1}^{N} w_{t}^{i} \right] \quad w_{t}^{i} = \frac{f_{\theta}(z_{t} | z_{1:t-1}^{a_{t-1}^{i}}) g_{\theta}(x_{t} | z_{1:t}^{k})}{q_{\phi}(z_{t}^{k} | x_{1:t}, z_{1:t-1}^{a_{t-1}^{i}})}$$

**3** we can form and optimize ELBO on  $\log p(x_{1:T})$ 

ELBO<sub>SMC</sub>(
$$\theta$$
,  $\phi$ ,  $x_{1:T}$ ) =

$$\int Q_{SMC}(z_{1:T}^{1:K}, a_{1:T-1}^{1:K}) \log C_{SMC}(z_{1:T}^{1:K}, a_{1:T-1}^{1:K}) \ dz_{1:T}^{1:K} \ da_{1:T-1}^{1:K}$$

# Optimization

$$\mathrm{ELBO}_{SMC}(\theta, \phi, x_{1:T}) \rightarrow \max_{\phi, \theta}$$

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$$\text{ELBO}_{SMC}(\theta, \phi, x_{1:T}) \rightarrow \max_{\phi, \theta}$$

- make proposal  $q(z_t|z_{1:t-1}^k)$  reparametrizable
- ignore gradient with respect to categorical sampling

## Theoretical benefits

• We can bound the KL in N

$$\mathrm{KL}(q_{\phi}(z_{1:t})||p(z_{1:T}|x_{1:T})) \leq \frac{c(\phi)}{N}$$

② We can bound the KL in T if N = bT

$$\mathrm{KL}(q_{\phi}(z_{1:t})||p(z_{1:T}|x_{1:T})) \leq -\mathbb{E}\left[\log\frac{\widehat{p}(x_{1:T})}{p(x_{1:T})}\right] \stackrel{T \to \infty}{\longrightarrow} \frac{\sigma^2(\phi)}{2b} < \infty$$

**3** In general cannot achieve the marginal likelihood on optimal proposal  $q^*$ . Though, it is possible if p admits independence structure, i.e. if

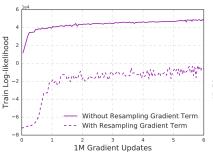
$$p(z_{1:t-1}|x_{1:t}) = p(z_{1:t-1}|x_{1:t-1})$$

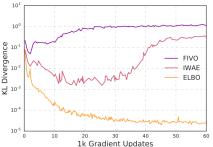
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# Experiments

N	Bound	TIMIT	
		64 units	256 units
4	ELBO	0	10,438
	<b>IWAE</b>	-160	11,054
	FIVO	5,691	17,822
8	ELBO	2,771	9,819
	<b>IWAE</b>	3,977	11,623
	FIVO	6,023	21,449
16	ELBO	1,676	9,918
	<b>IWAE</b>	3,236	13,069
	FIVO	8,630	21,536

## Experiments





# Thank you!

#### References I

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