Debiasing Approximate Inference

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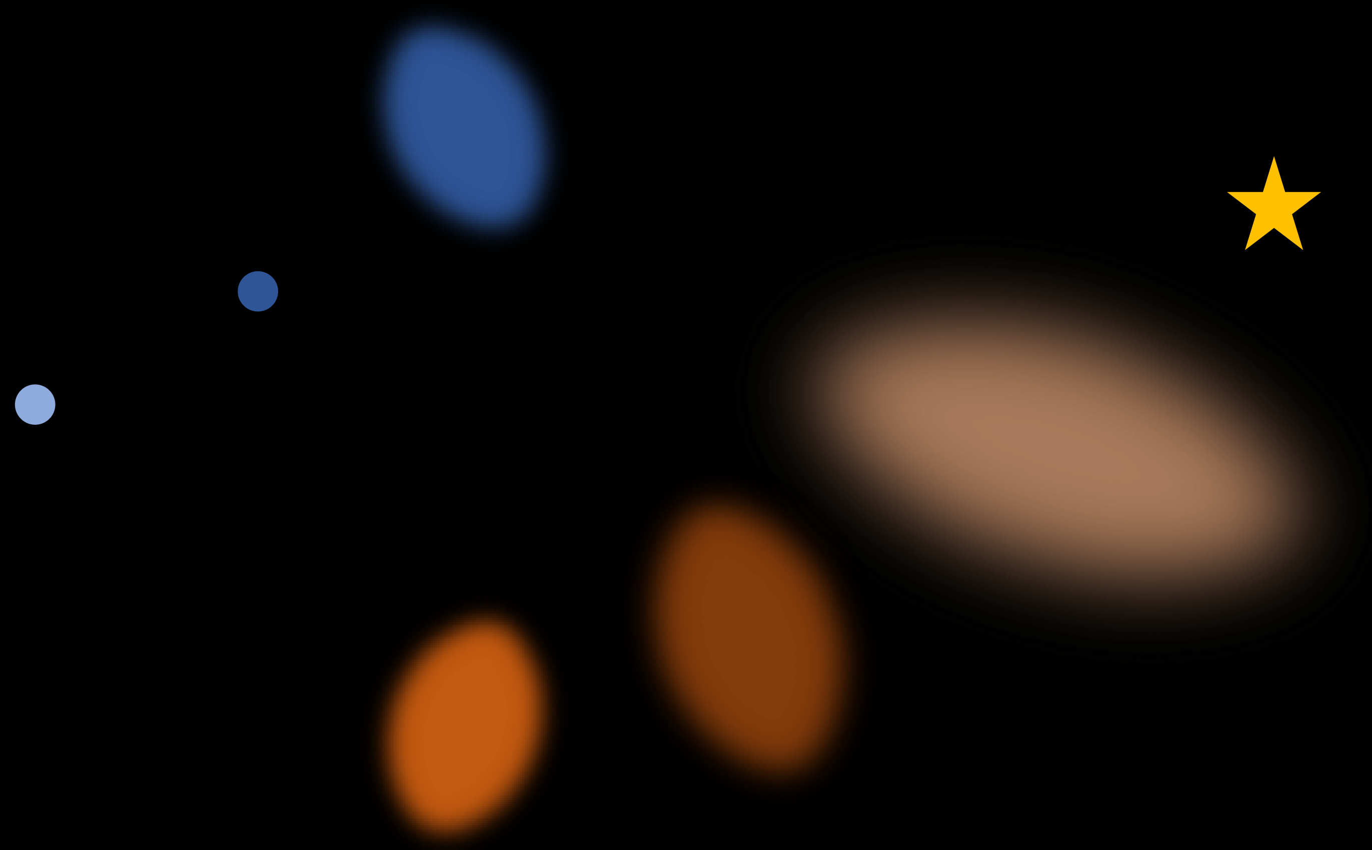


The Pattern

- "Consistent" approximate inference:
  consistent estimator of some quantity of interest ($k \to \infty$)
- Computationally constraints put limits on k

Example 1: Self-Normalized Importance Sampling

- Quantity of interest

$$\mathbb{E}_{x\sim p}[f(x)]$$

- Consistent estimator, unnormalized $\tilde{p}$

$$\hat{L}(\tilde{p},q,k)=\frac{1}{k}\sum_{i=1}^{k}\frac{1}{\sum\tilde{p}(x_i)}\frac{\tilde{p}(x_i)}{q(x_i)}f(x_i), \qquad x_i\sim q$$

Example 2: AIS Evidence Estimates

- Annealed Importance Sampling: unbiased estimates of

$$\hat{p}_k(x) \to p(x) = \int p(x|z)\, p(z)\, \mathrm{dz}$$

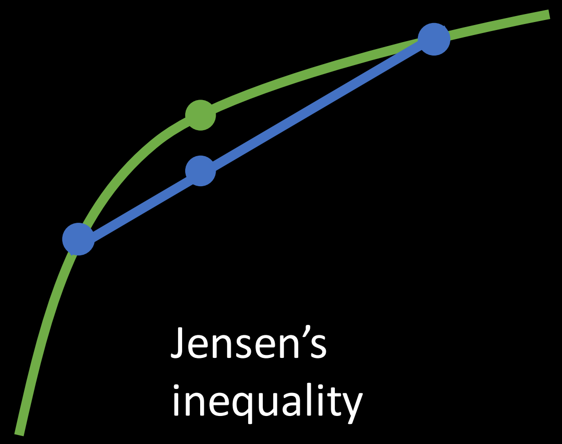
- However, in many applications we need to estimate (See [Salakhutdinov and Murray, 2008])

$$\log p(x)$$

- Naïve plug-in estimate, consistent,

$$\hat{L}_k = \log \hat{p}_k(x)$$

- Biased (“stochastic lower bound”, sounds better)



Example 3: Importance Weighted Autoencoder (IWAE)

- Family of tighter ELBO bounds [Burda et al., 2015]
- Intractable expectation

$$\log \mathbb{E}_{z\sim q_\omega(z|x)}\left[\frac{p_\theta(x|z)\,p(z)}{q_\omega(z|x)}\right]$$

- Approximate "naively" using empirical expectation

$$\hat{\mathcal{L}}_K \coloneqq \log \frac{1}{K}\sum_{i=1}^{K}\frac{p_\theta(x|z)\,p(z)}{q_\omega(z|x)}$$

$$z_i \sim q_\omega(z|x)$$

IWAE: known results [Burda et al., 2015]

- ELBO recovery

$$\mathrm{ELBO} = \hat{\mathcal{L}}_1$$

- Consistency

Corollary 2 (Consistency of $\hat{\mathcal{L}}_K$). *For $K \to \infty$ the estimator $\hat{\mathcal{L}}_K$ is* consistent, *that is, for all $\epsilon > 0$*

$$\lim_{K \to \infty} P(|\hat{\mathcal{L}}_K - \log p(x)| \geq \epsilon) = 0. \tag{12}$$

- Stochastic monotonicity (== bias)

$$\mathbb{E}\hat{\mathcal{L}}_1 \leq \mathbb{E}\hat{\mathcal{L}}_2 \leq \cdots \leq \mathbb{E}\hat{\mathcal{L}}_\infty = \log p(x)$$

Example 4: Markov Chain Monte Carlo

- Quantity of interest

$$\mathbb{E}_{x\sim p}[f(x)]$$

- Consistent estimator from truncated Markov chain samples

$$x_{t+1} \sim T(x_{t+1}|x_t), \qquad x_0 \sim T_0(x_0)$$

$$\hat{L}_k = \frac{1}{k}\sum_{t=1}^{k} f(x_t)$$

- Bias due to truncation

- See [Strathmann et al., ICML 2015]

Example 5: Stochastic Metropolis-Hastings Acceptance Rates

- Stochastic Gradient MCMC method omit accept-reject step in a Metropolis-Hastings chain (e.g. SGLD [Welling and Teh, ICML 2011]
- Problem: exact (MALA) acceptance rate is intractable

$$\alpha_n(x \to x') = \min\left\{1, \frac{\tilde{p}_n(x')}{\tilde{p}_n(x)} \frac{q_n(x|x')}{q_n(x'|x)}\right\}$$

- Consistent estimator by truncation

$$\alpha_k(x \to x')$$

- Biased due to exponentiation and min operation
- See [Lyne et al., Statistical Science, 2015] for pseudo-marginal MCMC

Debiasing Methods

Analytic Methods

Delta Method

Case-by-Case

Christopher G. Small, CRC Press, 2010

Resampling Methods

Jackknife Debiasing

[Schucany et al., JASA 1971] and [Sharot, JASA 1976]

Bootstrap Debiasing

Peter Hall's bootstrap lecture notes, 2016

Stochastic Methods

Russian Roulette, Debiasing Lemma

[Lyne et al., Statistical Science, 2015]

Analytic Methods

Delta Method

Importance Weighted Autoencoder (IWAE)

- Family of tighter ELBO bounds [Burda et al., 2015]
- Intractable expectation

$$\log \mathbb{E}_{z\sim q_\omega(z|x)}\left[\frac{p_\theta(x|z)\,p(z)}{q_\omega(z|x)}\right]$$

- Approximate "naively"

$$\hat{\mathcal{L}}_K := \log \frac{1}{K}\sum_{i=1}^{K}\frac{p_\theta(x|z)\,p(z)}{q_\omega(z|x)}$$

$$z_i \sim q_\omega(z|x)$$

Delta Method for Moments

- == Taylor expansion
- Here, Taylor expand log around $\mathbb{E}[w]$, evaluate at $Y_k = \frac{1}{k}\sum w_i$

$$\log Y_k = \log(\mathbb{E}[w] + (Y_k - \mathbb{E}[w]))$$
$$= \log \mathbb{E}[w] - \sum_{j=1}^{\infty} \frac{(-1)^j}{j\mathbb{E}[w]^j} \mathbb{E}\left[(Y_k - \mathbb{E}[w])^j\right]$$

Delta Method VI

$$\log Y_k = \log \mathbb{E}[w] - \sum_{j=1}^{\infty} \frac{(-1)^j}{j\mathbb{E}[w]^j} \mathbb{E}\left[(Y_k - \mathbb{E}[w])^j\right]$$

Naïve estimator

Quantity of interest (intractable)

Correction terms (intractable)

Delta Method VI

$$\log \mathbb{E}[w] = \log Y_k + \sum_{j=1}^{\infty} \frac{(-1)^j}{j\mathbb{E}[w]^j} \mathbb{E}\left[(Y_k - \mathbb{E}[w])^j\right]$$

Quantity of interest (intractable)

Naïve estimator

Correction terms (intractable)

Delta Method VI

$$\log \mathbb{E}[w] = \log Y_k + \frac{-1}{\mathbb{E}[w]} \mathbb{E}\big[Y_k - \mathbb{E}[w]\big] + \sum_{j=2}^{\infty} \frac{(-1)^j}{j\,\mathbb{E}[w]^j} \mathbb{E}\big[(Y_k - \mathbb{E}[w])^j\big]$$

Quantity of interest (intractable)

Naïve estimator

= 0

Remaining correction terms (intractable)

Delta Method VI [Teh et al., 2007]

$$\log \mathbb{E}[w] = \log Y_k + \frac{1}{2\mathbb{E}[w]^2}\mathbb{E}[(Y_k - \mathbb{E}[w])^2] + \sum_{j=3}^{\infty} \frac{(-1)^j}{j\mathbb{E}[w]^j}\mathbb{E}[(Y_k - \mathbb{E}[w])^j]$$

Quantity of interest (intractable)

Naïve estimator

Approximate using estimated moments

$$\frac{\hat{\mu}_2}{2\hat{\mu}^2}$$

Remaining correction terms (intractable)

Delta Method VI [Teh et al., 2007]

$$\log \mathbb{E}[w] \approx \log Y_k + \frac{\hat{\mu}_2}{2\hat{\mu}^2}$$

- Indeed reduces bias to $o(k^{-2})$, [Nowozin, 2018]

Proposition 5 (Bias of $\hat{\mathcal{L}}_K^D$). *We evaluate the bias of $\hat{\mathcal{L}}_K^D$ in (53) as follows.*

$$\mathbb{B}[\hat{\mathcal{L}}_K^D] = -\frac{1}{K^2}\left(\frac{\mu_3}{\mu^3} - \frac{3\mu_2^2}{2\mu^4}\right) + o(K^{-2}).$$

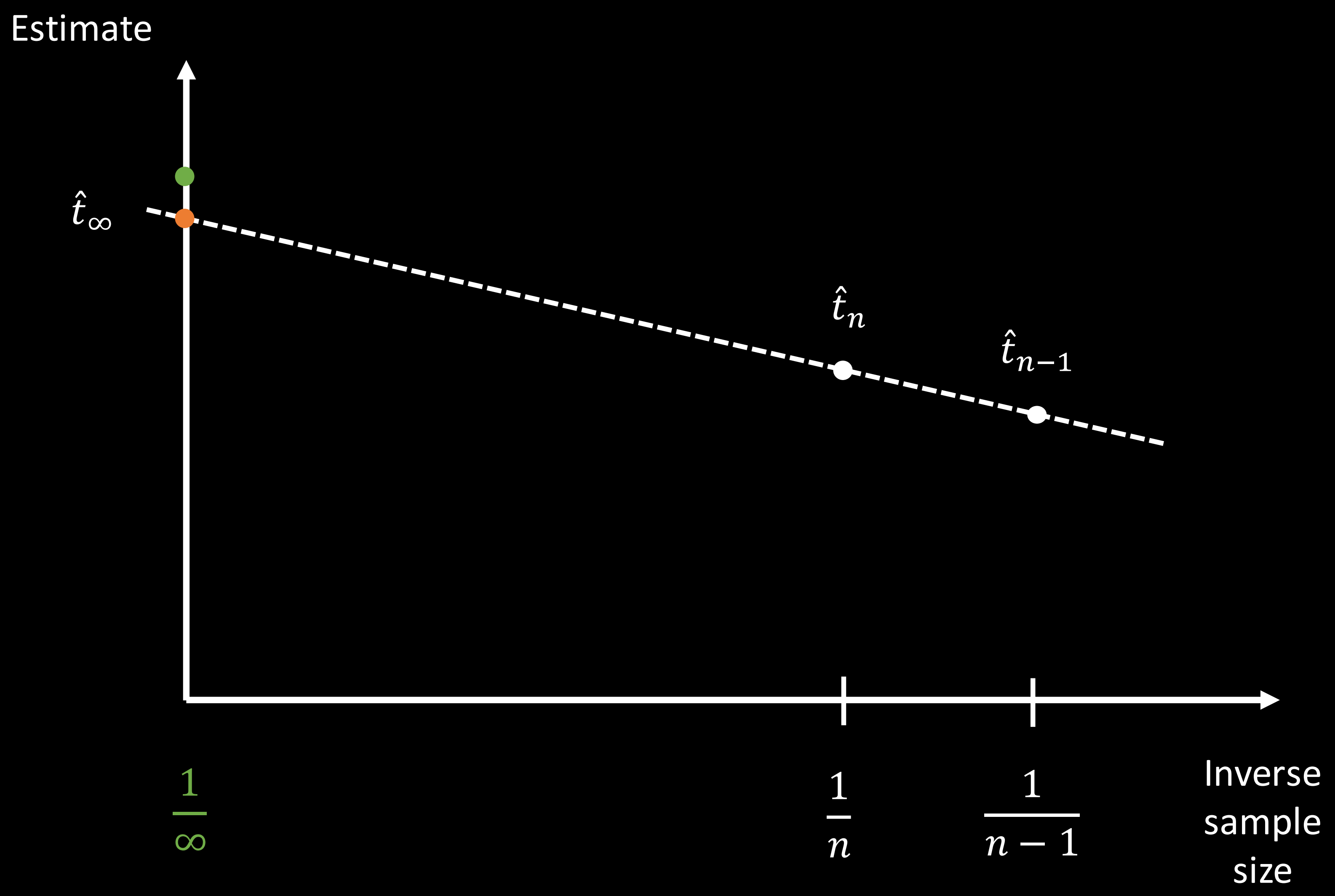
Analytic Methods

Resampling Methods

Delta Method

Jackknife Debiasing

[Nowozin, “Debiasing Evidence Approximations”, ICLR 2018]



Estimate
$\hat{t}_\infty$
$\hat{t}_n$
$\hat{t}_{n-1}$
$\frac{1}{\infty}$
$\frac{1}{n}$
$\frac{1}{n-1}$
Inverse sample size

Assume we have an asymptotic expansion

$$\mathbb{E}[\hat{T}_k] = T + \frac{a_1}{k} + \frac{a_2}{k^2} + \cdots$$

Then

$$\mathbb{E}[k\,\hat{T}_k - (k-1)\,\hat{T}_{k-1}] = k\left(T + \frac{a_1}{k} + \frac{a_2}{k^2}\right) - (k-1)\left(T + \frac{a_1}{k-1} + \frac{a_2}{(k-1)^2}\right) + O(k^{-2})$$

$$= T + a_1 + \frac{a_2}{k} - a_1 - \frac{a_2}{k-1} + O(k^{-2})$$

$$= T - \frac{a_2}{k(k-1)} + O(k^{-2})$$

$$= T + O(k^{-2})$$

Generalized Jackknife

- Original jackknife: [Quennouille, 1949]
  - Removes first order $O(n^{-1})$ bias
- Generalization to higher-order bias removal: [Schucany et al., 1974]
  - Eliminates bias to any order
  - Variance typically increases

Sharot form of the generalized Jackknife

$$\hat{T}_G^{(m)} = \sum_{j=0}^{m} c(n, m, j)\, \hat{T}_{n-j}.$$

$$c(n, m, j) = (-1)^j \frac{(n-j)^m}{(m-j)!\, j!}.$$

$$\hat{T}_G^{(0)} = \hat{T}_n$$

$$\hat{T}_G^{(1)} = n\hat{T}_n - (n-1)\hat{T}_{n-1}$$

$$\hat{T}_G^{(2)} = \frac{n^2}{2}\hat{T}_n - (n-1)^2\hat{T}_{n-1} + \frac{(n-2)^2}{2}\hat{T}_{n-2}$$

- [Sharot, 1976]
- n: sample size
- m: order of the jackknife, $m \geq 0$
- $\hat{T}_n$: original consistent estimator evaluated on n samples

Jackknife Variational Inference (JVI)

Definition 1 (Jackknife Variational Inference (JVI)). *Let $K \geq 1$ and $m < K$. The jackknife variational inference estimator of the evidence of order m with K samples is*

$$\hat{\mathcal{L}}_K^{J,m} \quad := \quad \sum_{j=0}^{m} c(K,m,j)\, \bar{\mathcal{L}}_{K-j}, \tag{20}$$

where $\bar{\mathcal{L}}_{K-j}$ is the empirical average of one or more IWAE estimates obtained from a subsample of size $K-j$, and $c(K,m,j)$ are the Sharot coefficients *defined in (18). In this paper we use all possible $\binom{K}{K-j}$ subsets, that is,*

$$\bar{\mathcal{L}}_{K-j} := \frac{1}{\binom{K}{K-j}} \sum_{i=1}^{\binom{K}{K-j}} \hat{\mathcal{L}}_{K-j}(Z_i^{(K-j)}), \tag{21}$$

where $Z_i^{(K-j)}$ is the i'th subset of size $K-j$ among all $\binom{K}{K-j}$ subsets from the original samples $Z = (z_1, z_2, \ldots, z_K)$. We further define $\mathcal{L}_K^{J,m} = \mathbb{E}_Z[\hat{\mathcal{L}}_K^{J,m}]$.

Higher-order Bias Reduction

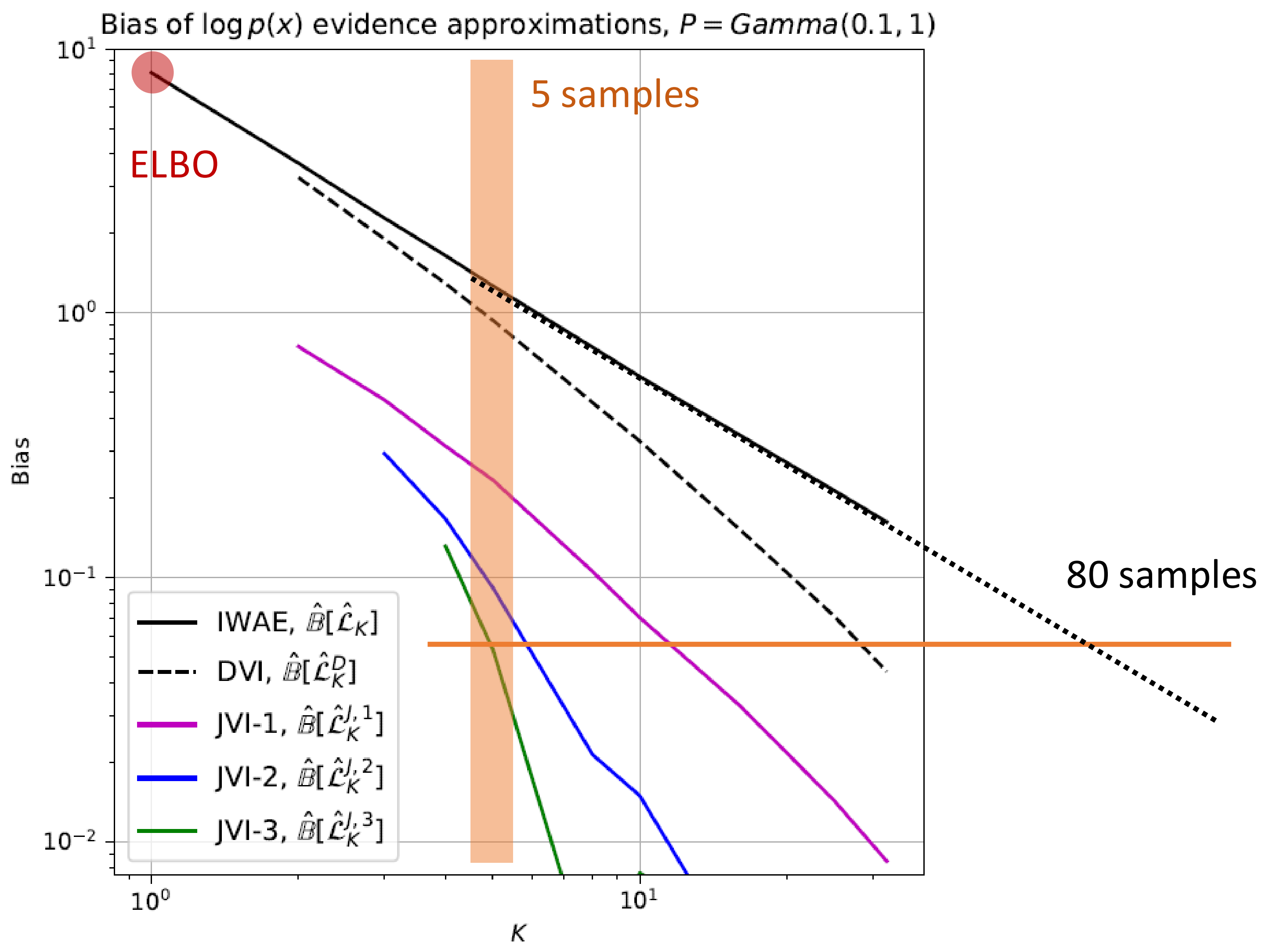
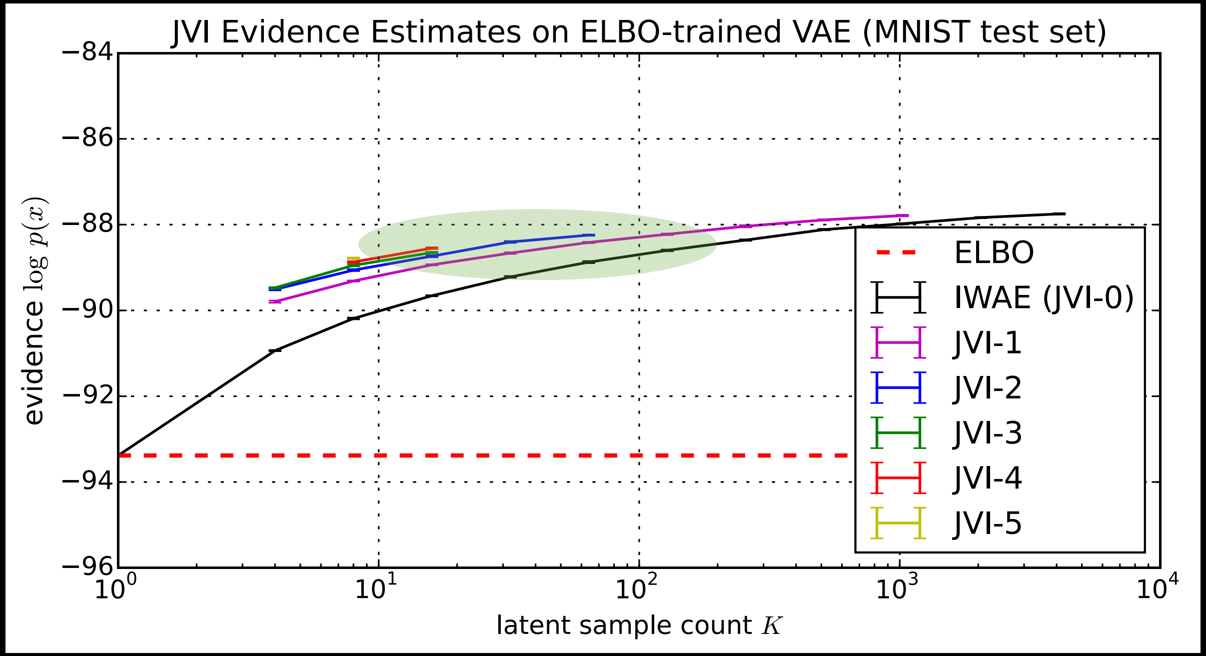
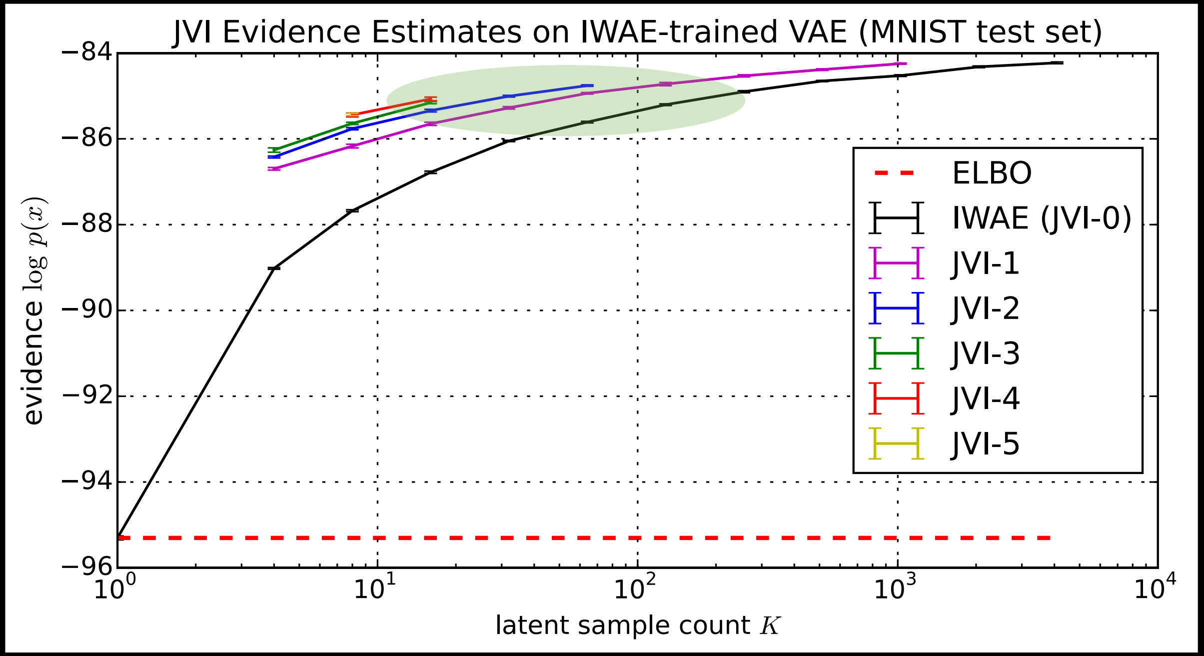


Figure 5: Absolute bias as a function of K.

Evidence Evaluations (VAE MNIST)



Trained with ELBO



Trained with IWAE

- Effective bias reduction
- Higher-order terms matter

Analytic Methods

Resampling Methods

Delta Method

Jackknife Debiasing

Case-by-Case

Example 5: Stochastic Metropolis-Hastings Acceptance Rates

- Stochastic Gradient MCMC method omit accept-reject step in a Metropolis-Hastings chain (e.g. SGLD [Welling and Teh, ICML 2011]
- Problem: exact (MALA) acceptance rate is intractable

$$\alpha_n(\theta \to \theta') = \min\left\{1, \frac{\tilde{p}_n(\theta')}{\tilde{p}_n(\theta)} \frac{q_n(\theta|\theta')}{q_n(\theta'|\theta)}\right\}$$

- Consistent estimator by truncation

$$\alpha_k(x \to x')$$

- Biased due to exponentiation and min operation

Stochastic Acceptance Rate (Ceperley and Dewing, “Penalty MCMC”, 1998)

$\log \frac{\tilde{p}_n(\theta')}{\tilde{p}_n(\theta)}$ is deterministic. Consider a random batch B of size $1 \ll m \ll n$, then approximately

$$\log \frac{\tilde{p}_B(\theta')}{\tilde{p}_B(\theta)} \sim \mathcal{N}(\mu(\theta,\theta'), v(\theta,\theta'))$$

Why? CLT:

$$\log \tilde{p}_B(\theta) = \log p(\theta) + \frac{n}{|B|} \sum\nolimits_{i \in B} \log p(x_i|\theta)$$

Ceperley-Dewing, Intuition, 1/2

- (Formal proof relies on relating Log-Normal distribution tail masses)
- Intuition:

$$\log \frac{\tilde{p}_B(\theta')}{\tilde{p}_B(\theta)} \sim \mathcal{N}(\mu(\theta,\theta'), v(\theta,\theta'))$$

- Then

$$\frac{\tilde{p}_B(\theta')}{\tilde{p}_B(\theta)} \sim \mathrm{LogNormal}\big(\mu(\theta,\theta'), v(\theta,\theta')\big)$$

- And

$$\mathbb{E}\left[\frac{\tilde{p}_B(\theta')}{\tilde{p}_B(\theta)}\right] = \exp\left(\mu(\theta,\theta') + \frac{1}{2}v(\theta,\theta')\right)$$

Ceperley-Dewing, Intuition, 2/2

$$\mathbb{E}\left[\frac{\tilde{p}_B(\theta')}{\tilde{p}_B(\theta)}\right] = \exp\left(\mu(\theta,\theta') + \frac{1}{2}v(\theta,\theta')\right)$$

$$\mathbb{E}\left[\frac{\tilde{p}_B(\theta')}{\tilde{p}_B(\theta)}\ \exp\left(-\frac{1}{2}v(\theta,\theta')\right)\right] = \exp(\mu(\theta,\theta')) = \frac{\tilde{p}_n(\theta')}{\tilde{p}_n(\theta)}$$

penalty factor, < 1

- Under assumptions of Normality: exact debiasing of stochastic MCMC
- The larger the variance, the worse the penalty

Langevin-Ceperley-Dewing (LCD)

Joint work with Alexander Gaunt (MSR Cambridge)

- Extension of Ceperley-Dewing to discretized Langevin dynamics
- Goal: Make SGLD valid for any stepsize via stochastic rejection

- Ceperley-Dewing assumes $q(\theta'|\theta) = q(\theta|\theta')$
- Simple extension using two batches B, B', one for q_B, and one for the likelihood ratio

Normal Experiment (1D)

- Simple 1D Normal mean experiment

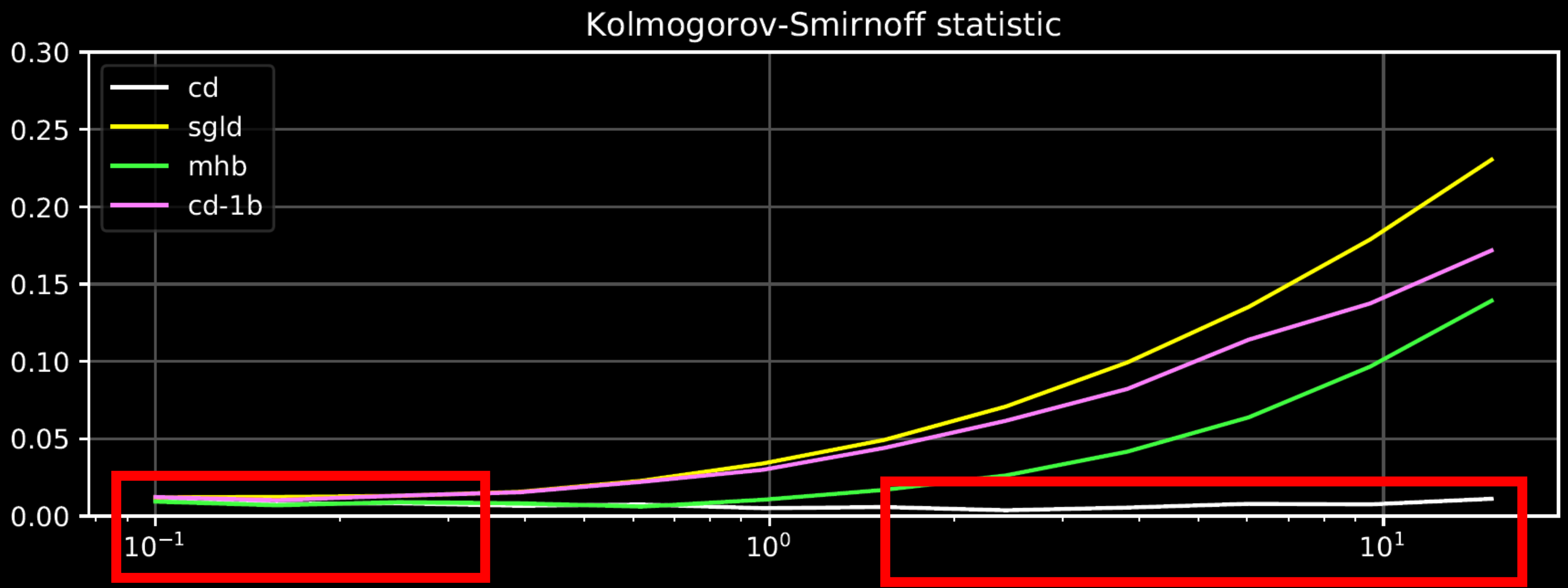
$$\mu \sim \mathcal{N}(\mu_0, \sigma_0^2)$$
$$x_i \sim \mathcal{N}(\mu, \sigma^2), \qquad i = 1, \ldots, 1000$$

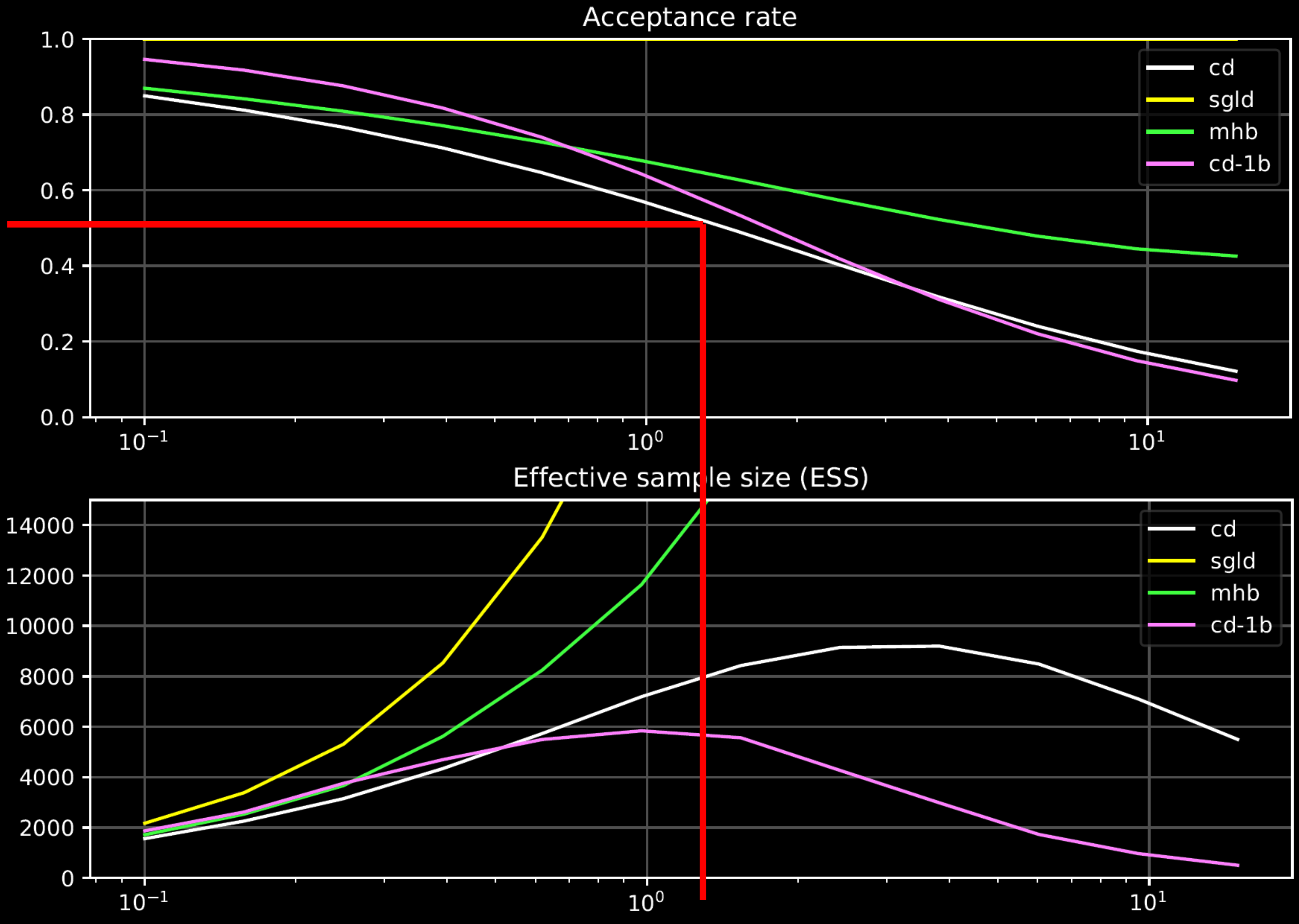
- Infer

$$p(\mu | x_1, \ldots, x_{1000})$$

- Compare SGLD and LCD for different stepsizes, batchsize 64
- Initialize using true posterior, no burn-in

Normal Experiment (1D)

- 



Acceptance rate
1.0
0.8
0.6
0.4
0.2
0.0
10^{-1}
10^{0}
10^{1}
cd
sgld
mhb
cd-1b
Effective sample size (ESS)
14000
12000
10000
8000
6000
4000
2000
0
10^{-1}
10^{0}
10^{1}
cd
sgld
mhb
cd-1b

Conclusions

- Approximate Inference is an estimation problem
- Let's use a broader toolbox of techniques to make bespoke tradeoffs in approximate inference

Analytic Methods	Resampling Methods		Stochastic Methods
Delta Method	Jackknife Debiasing	Bootstrap Debiasing	Russian Roulette, Debiasing Lemma
Case-by-Case			

Thanks!

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Code for JVI:

https://github.com/Microsoft/jackknife-variational-inference