Sandwiching the marginal likelihood using bidirectional Monte Carlo

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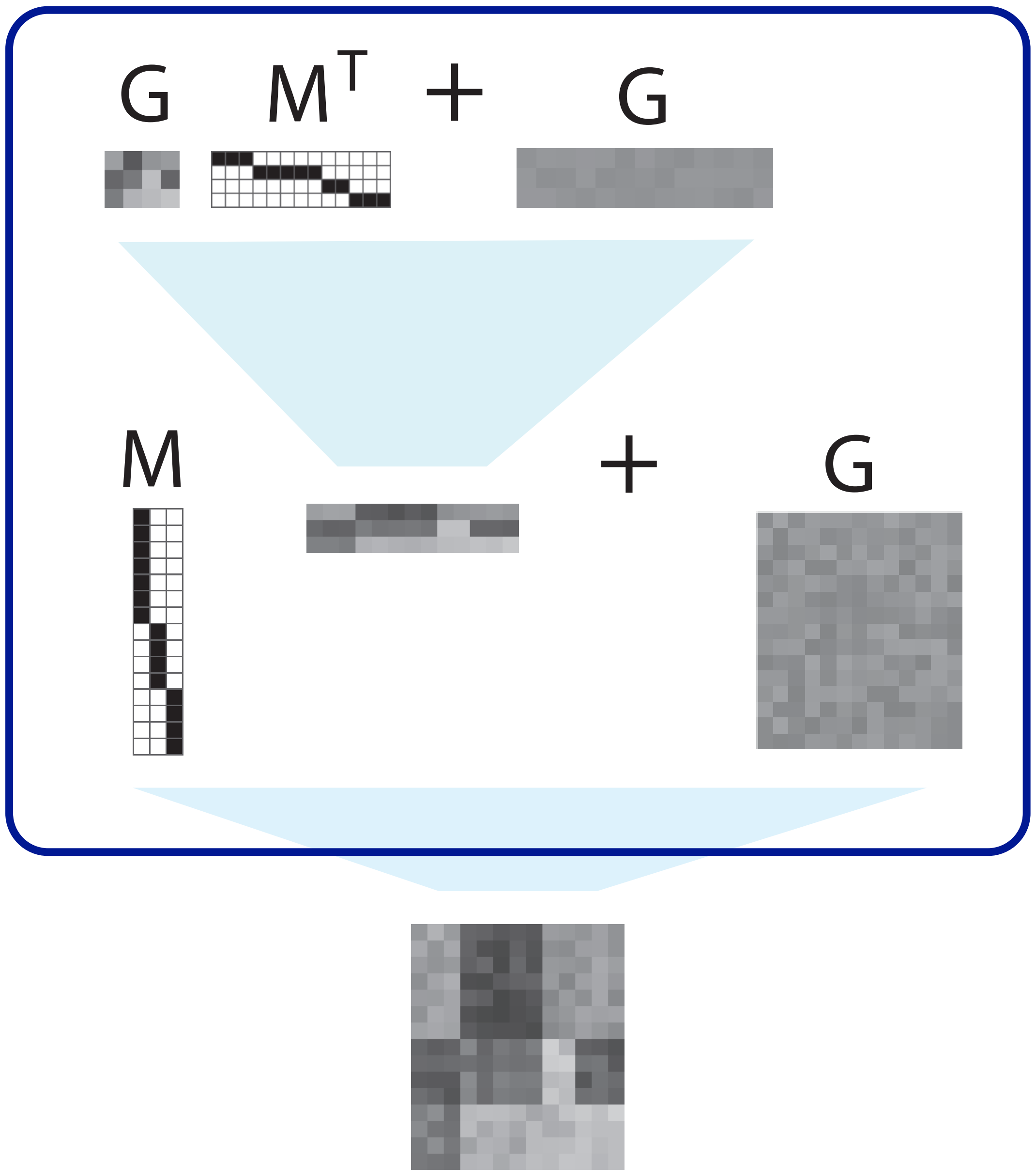
Introduction

- When comparing different statistical models, we'd like a quantitative criterion which trades off model complexity and fit to the data
- In a Bayesian setting, we often use marginal likelihood
  - Defined as the probability of the data, with all parameters and latent variables integrated out
- Motivation: plug into Bayes' Rule

$$p(\mathcal{M}_i \,|\, \mathcal{D}) = \frac{p(\mathcal{M}_i)\, p(\mathcal{D} \,|\, \mathcal{M}_i)}{\sum_j p(\mathcal{M}_j)\, p(\mathcal{D}|\mathcal{M}_j)}$$

Introduction: marginal likelihood



need to integrate out all of the component matrices and their hyperparameters

Introduction

- Advantages of marginal likelihood (ML)
  - Accounts for model complexity in a sophisticated way
  - Closely related to description length
  - Measures the model's ability to generalize to unseen examples
- ML is used in those rare cases where it is tractable
  - e.g. Gaussian processes, fully observed Bayes nets
- Unfortunately, it's typically very hard to compute because it requires a very high-dimensional integral
- While ML has been criticized on many fronts, the proposed alternatives pose similar computational difficulties

Introduction

- Focus on latent variable models
  - parameters $\boldsymbol{\theta}$, latent variables $\mathbf{z}$, observations $\mathbf{y}$
  - assume i.i.d. observations
- Marginal likelihood requires summing or integrating out latent variables and parameters

$$p(\mathbf{y}) = \int p(\boldsymbol{\theta}) \prod_{i=1}^{N} \sum_{\mathbf{z}_i} p(\mathbf{z}_i \,|\, \boldsymbol{\theta})\, p(\mathbf{y}_i \,|\, \mathbf{z}_i, \boldsymbol{\theta})\, \mathrm{d}\boldsymbol{\theta}$$

- Similar to computing the partition function

$$\mathcal{Z} = \sum_{\mathbf{x} \in \mathcal{X}} f(\mathbf{x})$$

Introduction

- Problem: exact marginal likelihood computation is intractable
- There are many algorithms to approximate it, but we don't know how well they work

Why evaluating ML estimators is hard

The answer to life, the universe, and everything is...

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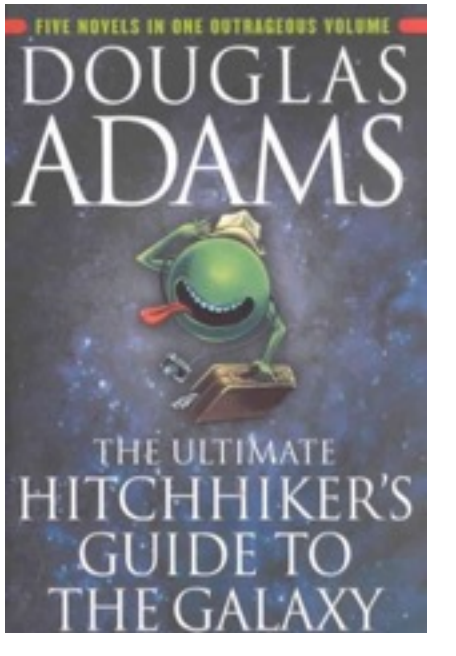
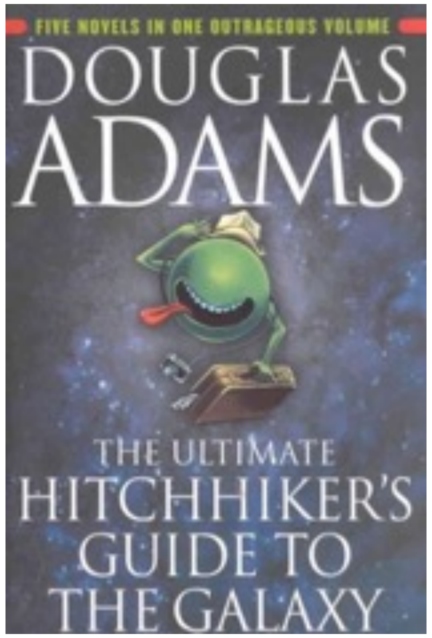


Why evaluating ML estimators is hard

The marginal likelihood is…

$$\log p(\mathcal{D}) = -23814.7$$



Why evaluating ML estimators is hard

- How does one deal with this in practice?
  - polynomial-time approximations for partition functions of ferromagnetic Ising models
  - test on very small instances which can be solved exactly
  - run a bunch of estimators and see if they agree with each other

Log-ML lower bounds

- One marginal likelihood estimator is simple importance sampling:

$$\{\boldsymbol{\theta}^{(k)}, \mathbf{z}^{(k)}\}_{k=1}^{K} \sim q \qquad \hat{p}(\mathcal{D}) = \frac{1}{K} \sum_{k=1}^{K} \frac{p(\boldsymbol{\theta}^{(k)}, \mathbf{z}^{(k)}, \mathcal{D})}{q(\boldsymbol{\theta}^{(k)}, \mathbf{z}^{(k)})}$$

- This is an unbiased estimator

$$\mathbb{E}[\hat{p}(\mathcal{D})] = p(\mathcal{D})$$

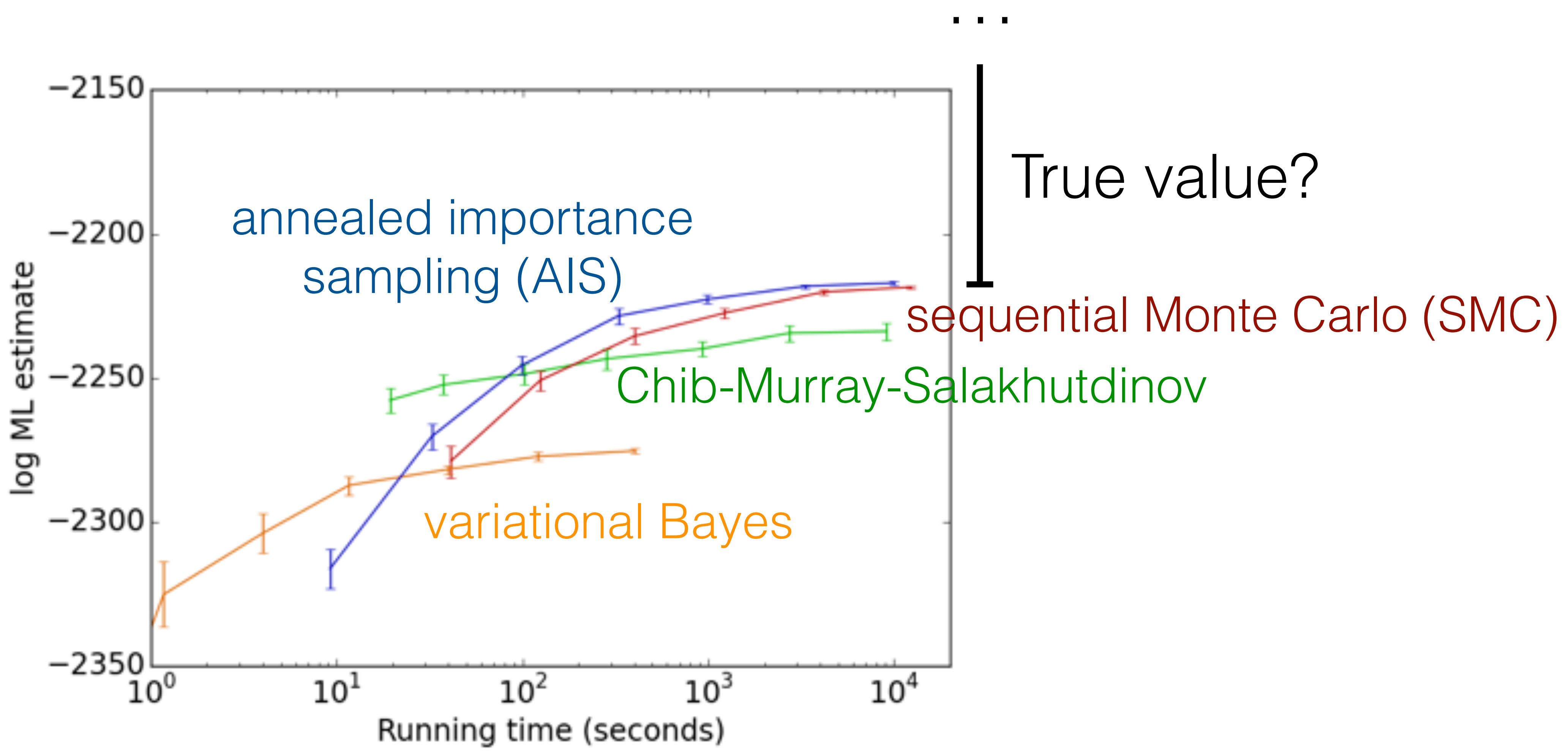
- Unbiased estimators are stochastic lower bounds

(Jensen's inequality) $$\mathbb{E}[\log \hat{p}(\mathcal{D})] \leq \log p(\mathcal{D})$$

(Markov's inequality) $$\Pr(\log \hat{p}(\mathcal{D}) > \log p(\mathcal{D}) + b) \leq e^{-b}$$

- Many widely used algorithms have the same property!

Log-ML lower bounds



How to obtain an upper bound?

- Harmonic Mean Estimator:

$$\{\boldsymbol{\theta}^{(k)}, \mathbf{z}^{(k)}\}_{k=1}^{K} \sim p(\boldsymbol{\theta}, \mathbf{z} \,|\, \mathcal{D}) \qquad \hat{p}(\mathcal{D}) = \frac{K}{\sum_{k=1}^{K} 1/p(\mathcal{D} \,|\, \boldsymbol{\theta}^{(k)}, \mathbf{z}^{(k)})}$$

- Equivalent to simple importance sampling, but with the role of the proposal and target distributions reversed

- Unbiased estimate of the *reciprocal* of the ML

$$\mathbb{E}\left[\frac{1}{\hat{p}(\mathcal{D})}\right] = \frac{1}{p(\mathcal{D})}$$

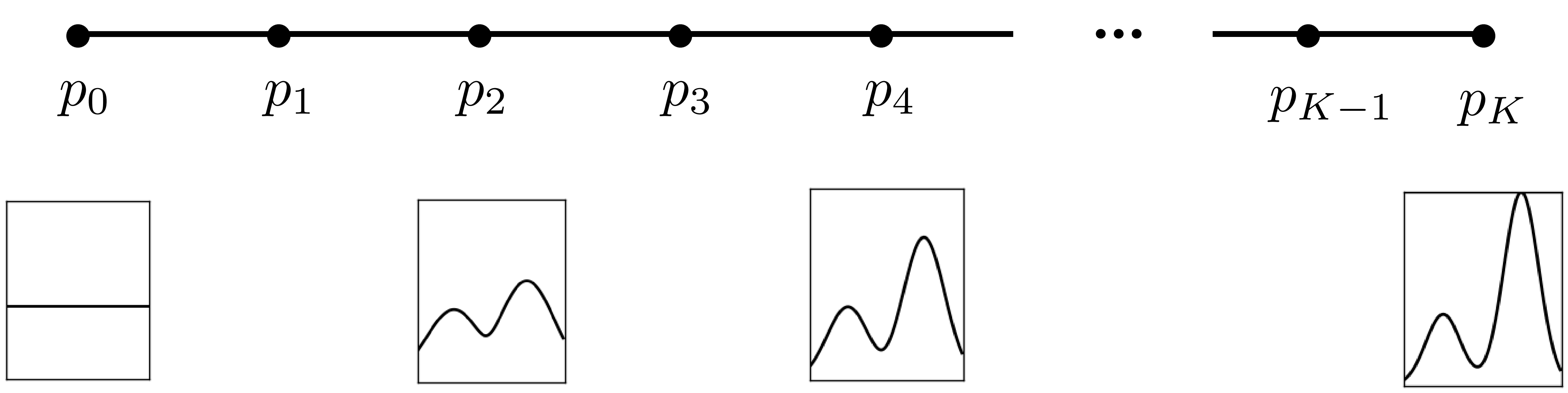
- Gives a stochastic *upper* bound on the log-ML

- Caveat 1: only an upper bound if you sample *exactly* from the posterior, which is generally intractable

- Caveat 2: this is the Worst Monte Carlo Estimator (Neal, 2008)

Annealed importance sampling

(Neal, 2001)



tractable initial distribution (e.g. prior)

intractable target distribution (e.g. posterior)

Annealed importance sampling
(Neal, 2001)

Given:

unnormalized distributions $f_0, \ldots, f_K$

MCMC transition operators $\mathcal{T}_0, \ldots, \mathcal{T}_K$

f_0 easy to sample from, compute partition function of

$\mathbf{x} \sim f_0$

$w = 1$

For $i = 0, \ldots, K-1$

$w := w \frac{f_{i+1}(\mathbf{x})}{f_i(\mathbf{x})}$

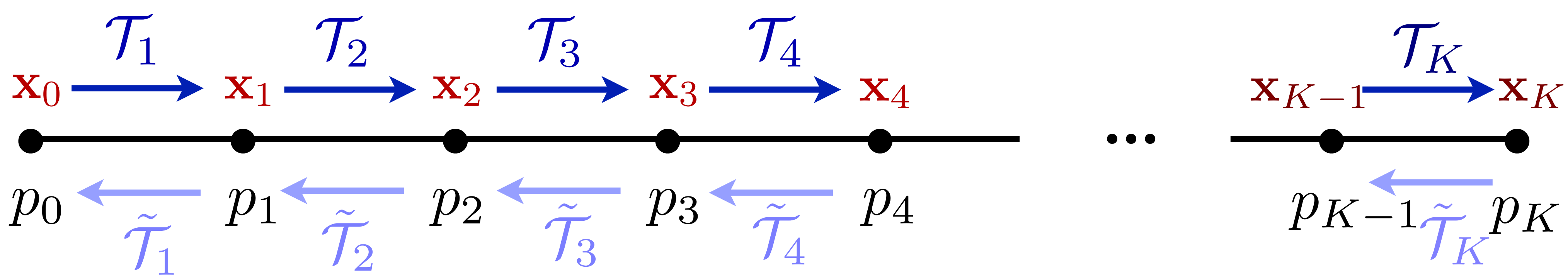
$\mathbf{x} :\sim \mathcal{T}_{i+1}(\mathbf{x})$

Then, $\mathbb{E}[w] = \frac{\mathcal{Z}_K}{\mathcal{Z}_0}$

$$\hat{\mathcal{Z}}_K = \frac{\mathcal{Z}_0}{S} \sum_{s=1}^{S} w^{(s)}$$

Annealed importance sampling

(Neal, 2001)



Forward: $$w := \prod_{i=1}^{K} \frac{f_i(\mathbf{x}_{i-1})}{f_{i-1}(\mathbf{x}_{i-1})} = \frac{\mathcal{Z}_K}{\mathcal{Z}_0} \frac{q_{\text{back}}(\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_K)}{q_{\text{fwd}}(\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_K)} \qquad \mathbb{E}[w] = \frac{\mathcal{Z}_K}{\mathcal{Z}_0}$$

Backward: $$w := \prod_{i=1}^{K} \frac{f_{i-1}(\mathbf{x}_i)}{f_i(\mathbf{x}_i)} = \frac{\mathcal{Z}_0}{\mathcal{Z}_K} \frac{q_{\text{fwd}}(\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_K)}{q_{\text{back}}(\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_K)} \qquad \mathbb{E}[w] = \frac{\mathcal{Z}_0}{\mathcal{Z}_K}$$

Bidirectional Monte Carlo

- Initial distribution: prior $p(\boldsymbol{\theta}, \mathbf{z})$
- Target distribution: posterior $p(\boldsymbol{\theta}, \mathbf{z} \,|\, \mathcal{D}) = \dfrac{p(\boldsymbol{\theta}, \mathbf{z}, \mathcal{D})}{p(\mathcal{D})}$
- Partition function: $\mathcal{Z} = \int p(\boldsymbol{\theta}, \mathbf{z}, \mathcal{D}) \, \mathrm{d}\boldsymbol{\theta} \, \mathrm{d}\mathbf{z} = p(\mathcal{D})$
- Forward chain

$$\mathbb{E}[w] = \frac{\mathcal{Z}_K}{\mathcal{Z}_0} = p(\mathcal{D})$$

stochastic lower bound

- Backward chain (requires exact posterior sample!)

$$\mathbb{E}[w] = \frac{\mathcal{Z}_0}{\mathcal{Z}_K} = \frac{1}{p(\mathcal{D})}$$

stochastic upper bound

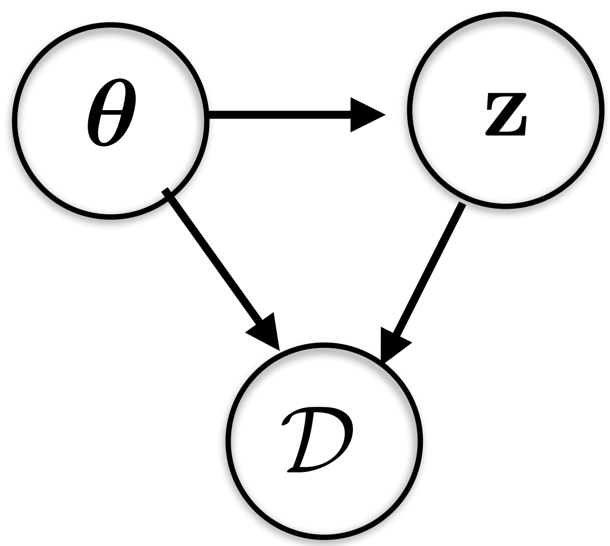
Bidirectional Monte Carlo

How to get an exact sample?

Two ways to sample from $p(\boldsymbol{\theta}, \mathbf{z}, \mathcal{D})$

$p(\boldsymbol{\theta}, \mathbf{z})\, p(\mathcal{D} \,|\, \boldsymbol{\theta}, \mathbf{z})$

forward sample



$p(\mathcal{D})\, p(\boldsymbol{\theta}, \mathbf{z} \,|\, \mathcal{D})$

generate data, then perform inference

Therefore, the parameters and latent variables used to generate the data are an exact posterior sample!

Bidirectional Monte Carlo

Summary of algorithm:

$$\boldsymbol{\theta}^\star, \mathbf{z}^\star \sim p_{\boldsymbol{\theta},\mathbf{z}}$$

$$\mathbf{y} \sim p_{\mathbf{y}\,|\,\boldsymbol{\theta},\mathbf{z}}(\cdot\,|\,\boldsymbol{\theta}^\star, \mathbf{z}^\star)$$

Obtain a stochastic lower bound on $\log p(\mathbf{y})$ by running AIS forwards

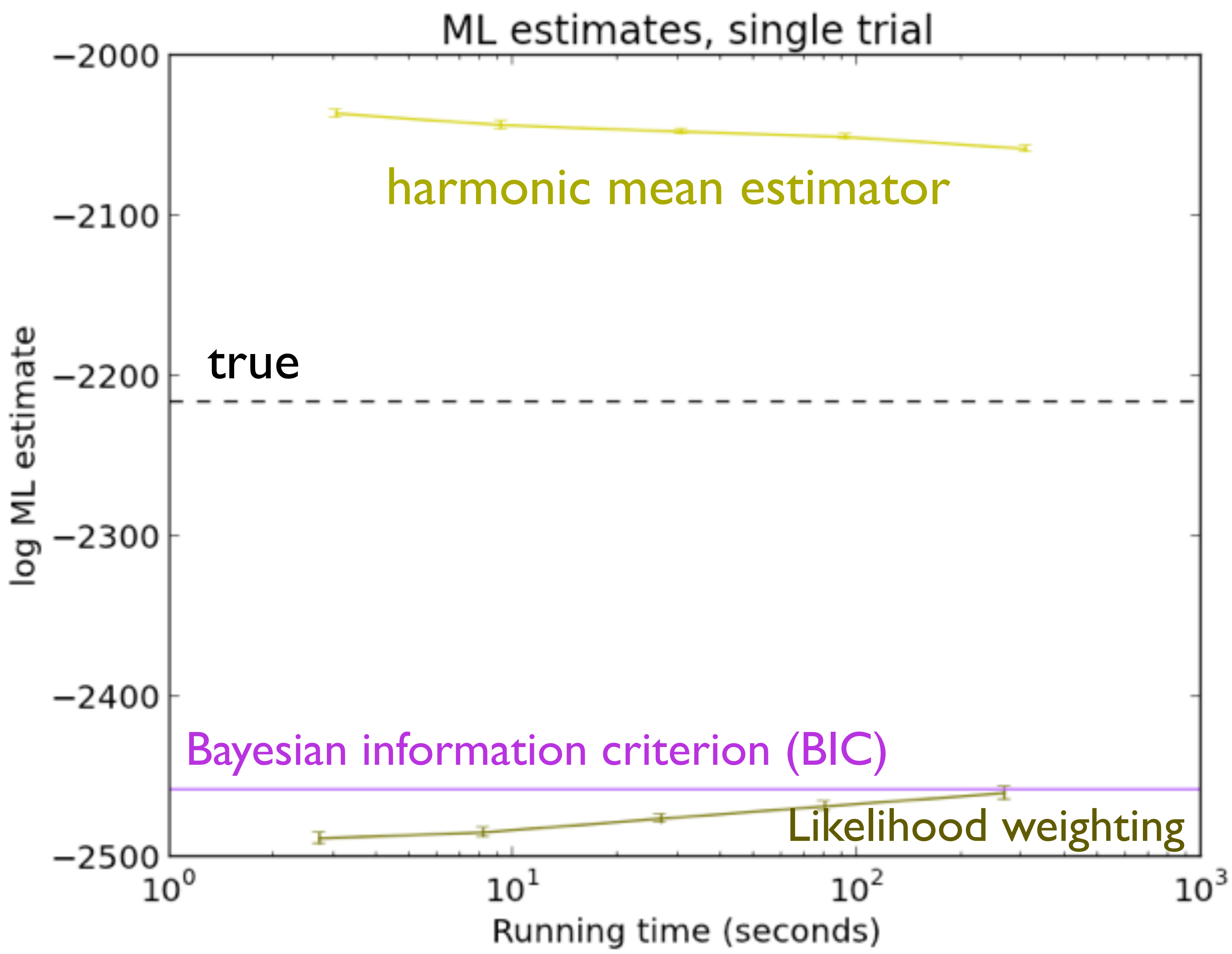
Obtain a stochastic upper bound on $\log p(\mathbf{y})$ by running AIS backwards, starting from $(\boldsymbol{\theta}^\star, \mathbf{z}^\star)$

The two bounds will converge given enough intermediate distributions.

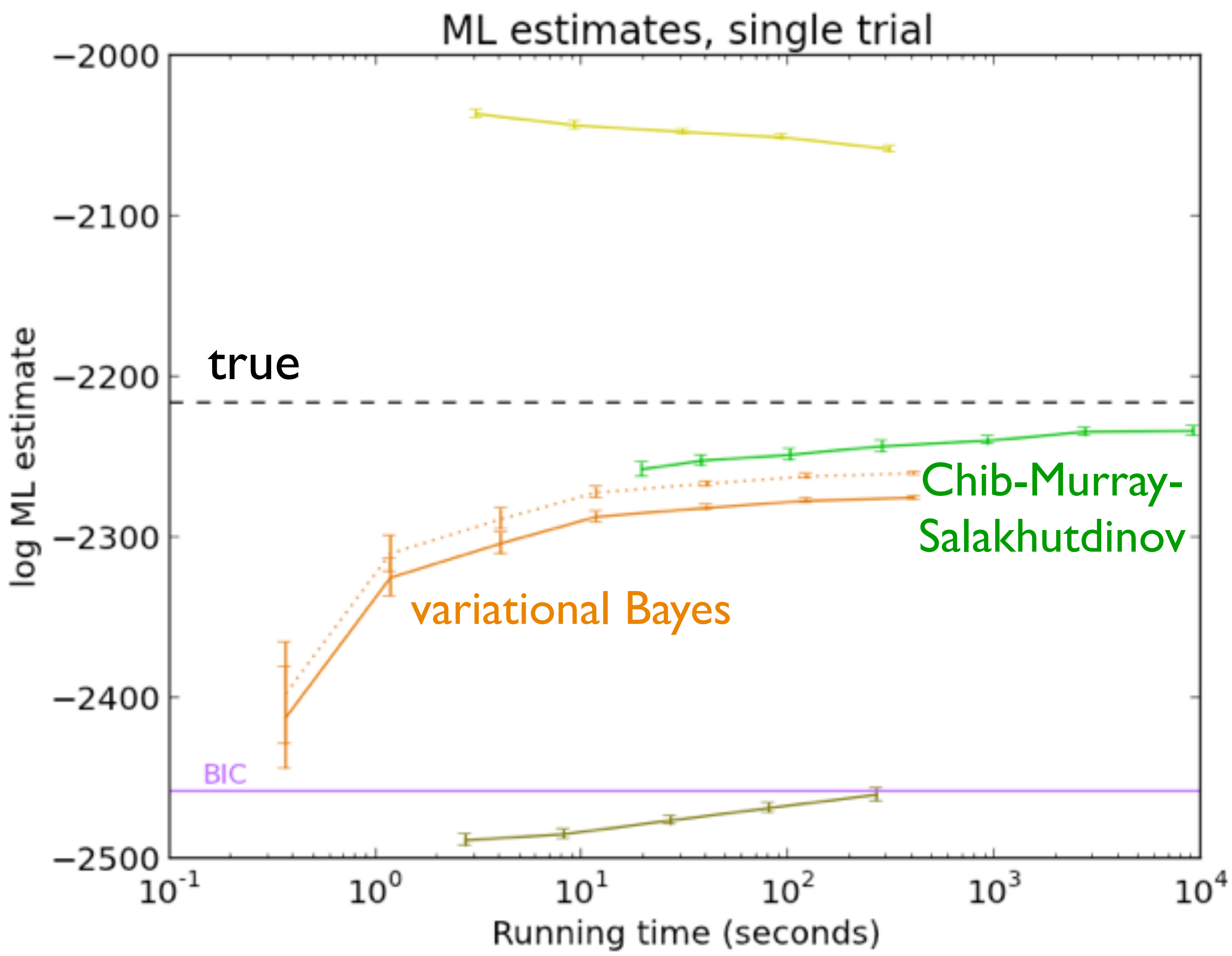
Experiments

- BDMC lets us compute ground truth log-ML values for data simulated from a model
  - We can use these ground truth values to benchmark log-ML estimators!
- Obtained ground truth ML for simulated data for
  - clustering
  - low rank approximation
  - binary attributes
- Compared a wide variety of ML estimators
- MCMC operators shared between all algorithms wherever possible

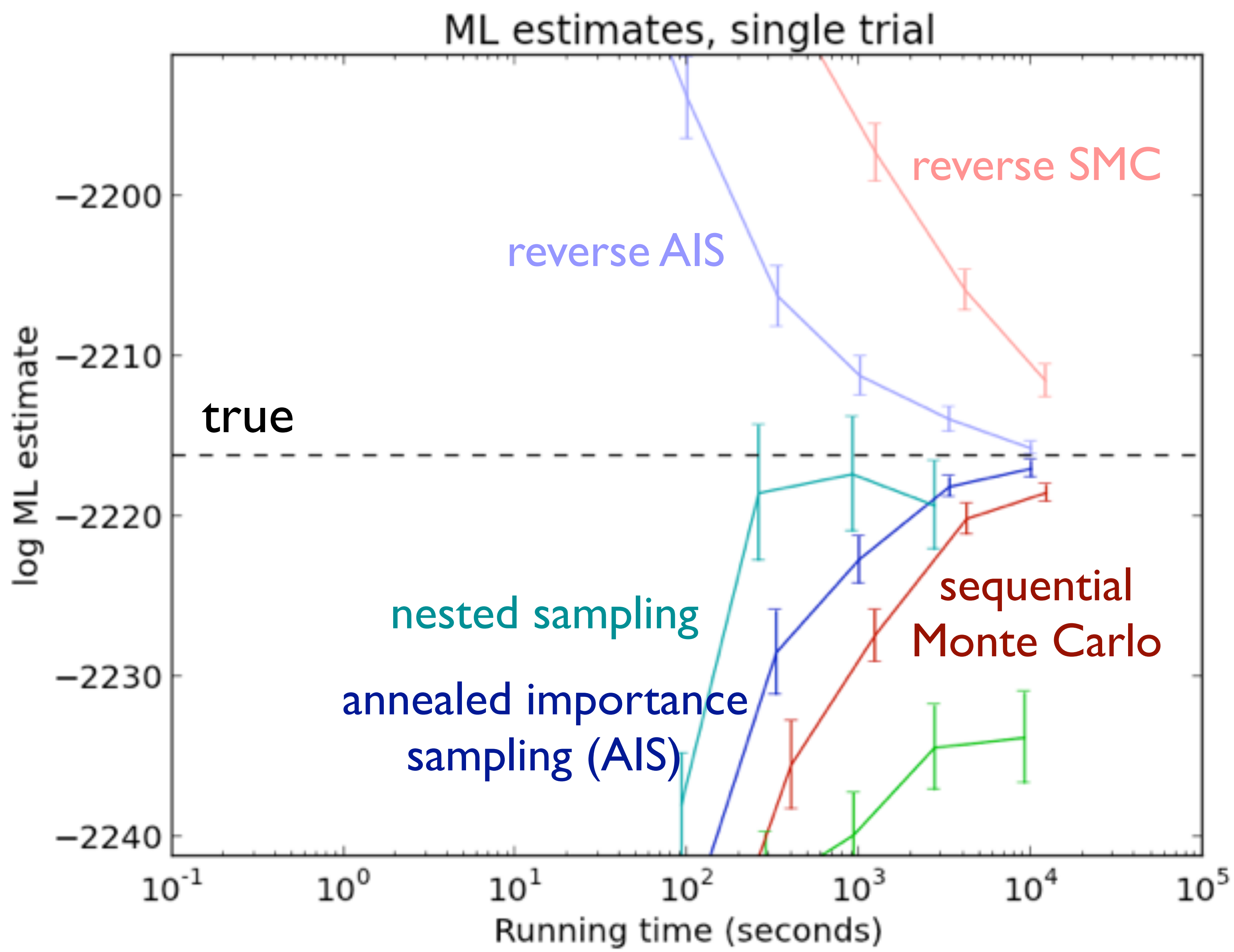
Results: binary attributes



Results: binary attributes

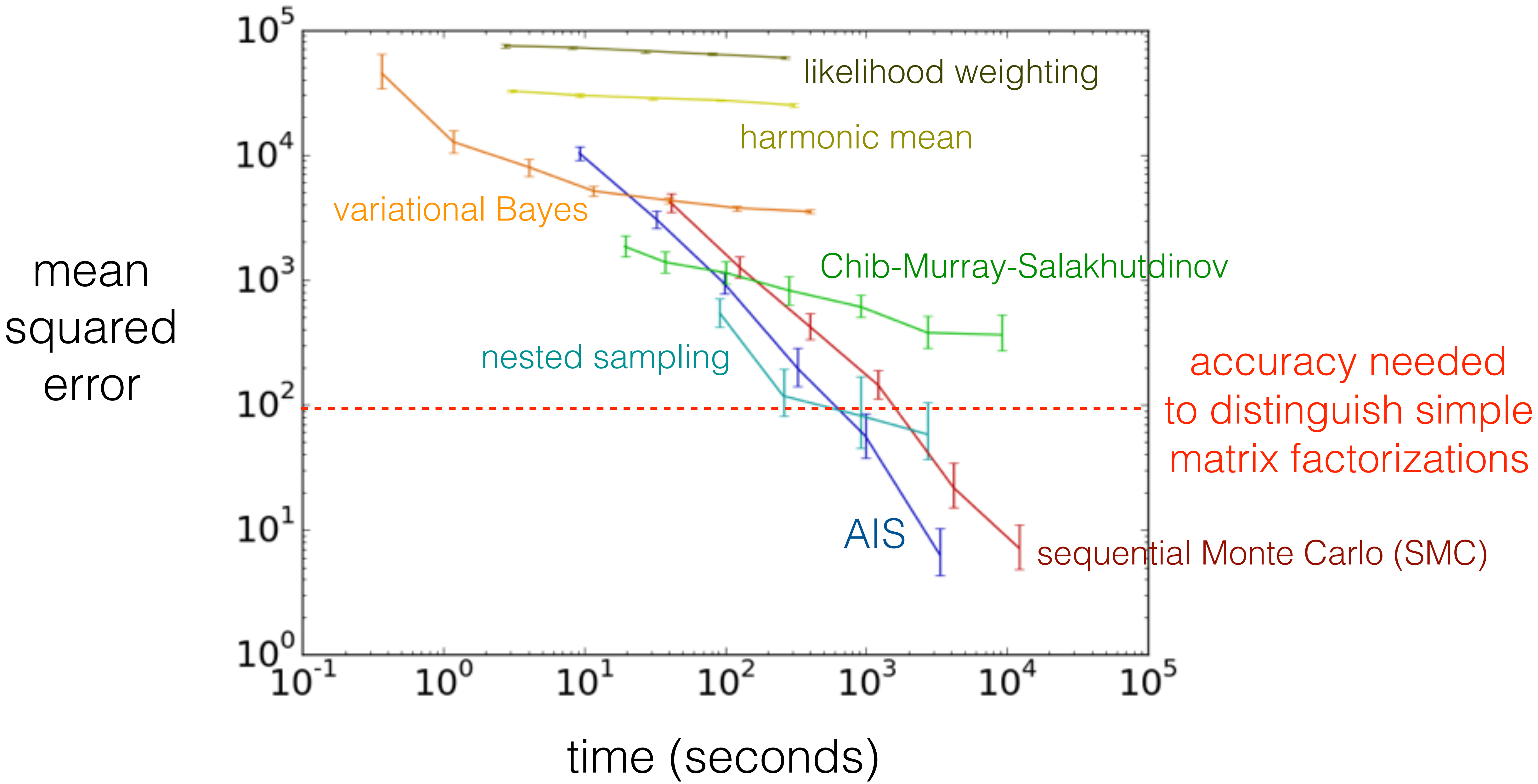


Results: binary attributes (zoomed in)

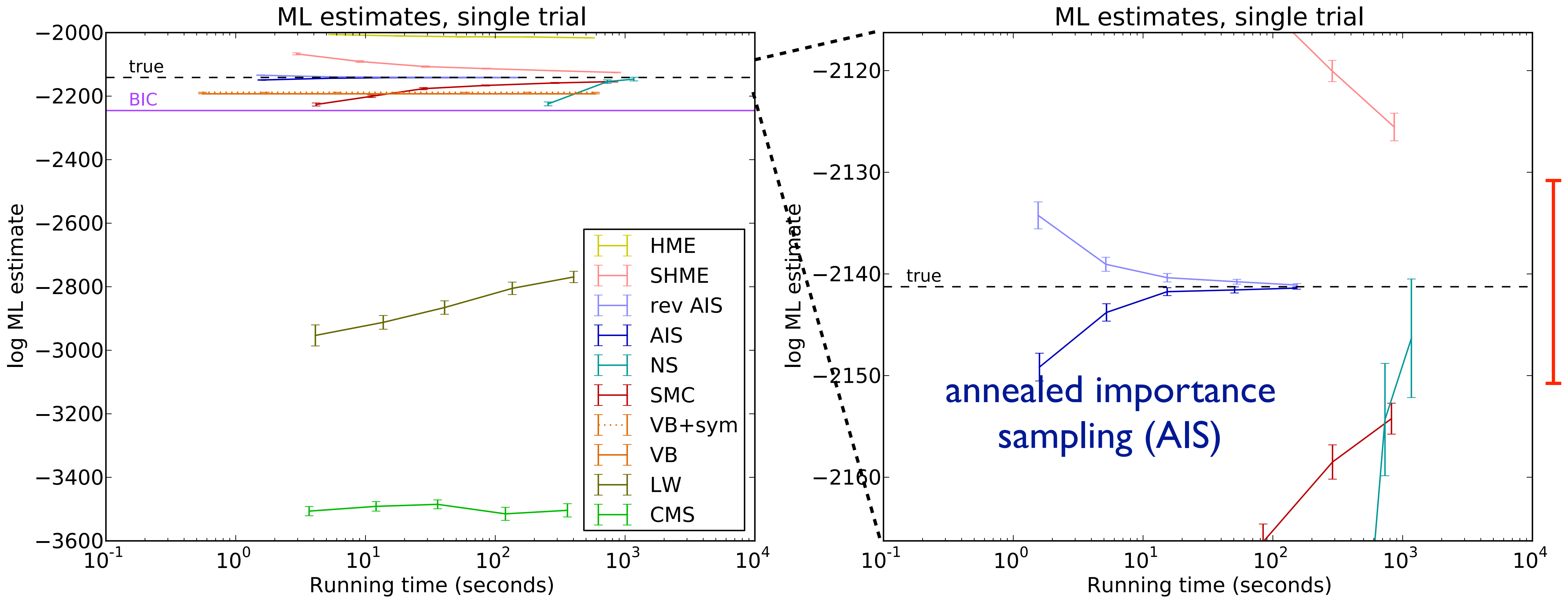


Results: binary attributes

Which estimators give accurate results?



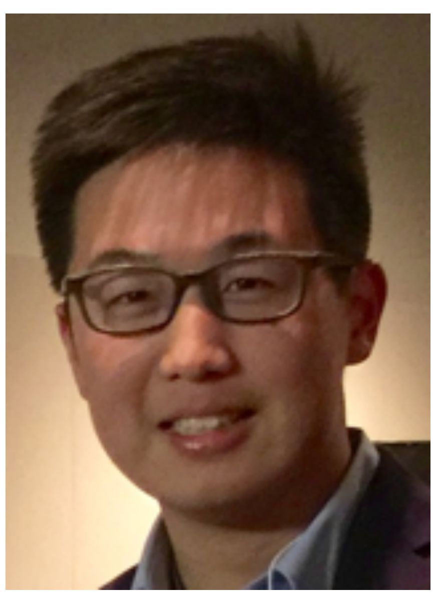
Results: low rank approximation



Recommendations

- Try AIS first
- If AIS is too slow, try sequential Monte Carlo or nested sampling
- Can’t fix a bad algorithm by averaging many samples
- Don’t trust naive confidence intervals -- need to evaluate rigorously

On the quantitative evaluation of decoder-based generative models



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Decoder-based generative models

- Define a generative process:
  - sample latent variables z from a simple (fixed) prior p(z)
  - pass them through a decoder network to get x = f(z)
- Examples:
  - variational autoencoders (Kingma and Welling, 2014)
  - generative adversarial networks (Goodfellow et al., 2014)
  - generative moment matching networks (Li et al., 2015; Dziugaite et al., 2015)
  - nonlinear independent components estimation (Dinh et al., 2015)

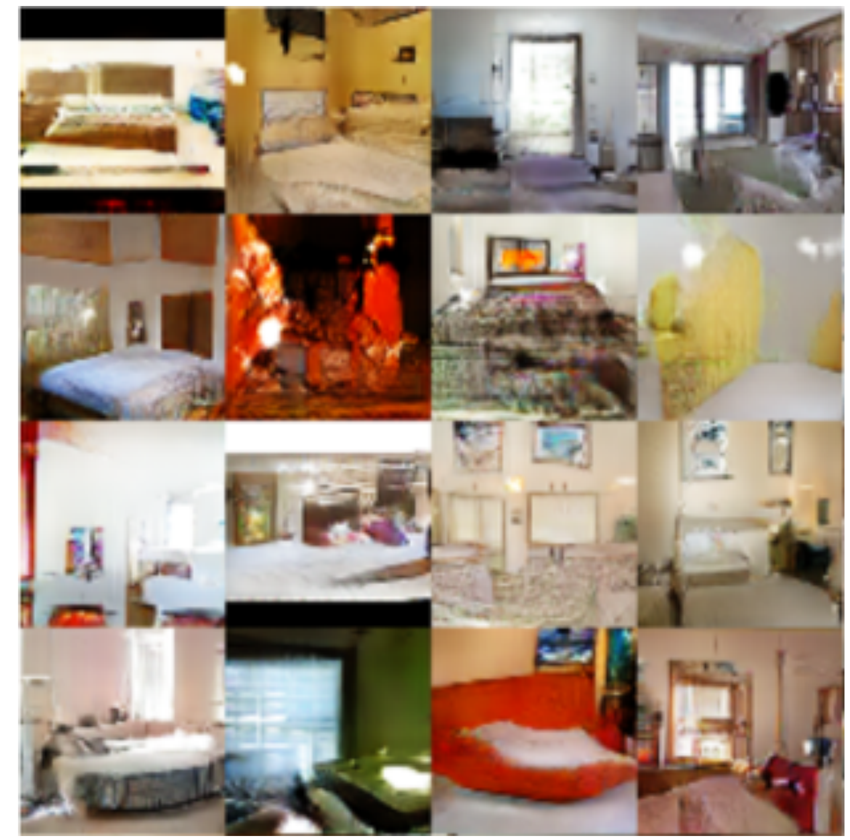
Decoder-based generative models

- Variational autoencoder (VAE)
  - Train both a generator (decoder) and a recognition network (encoder)
  - Optimize a variational lower bound on the log-likelihood
- Generative adversarial network (GAN)
  - Train a generator (decoder) and a discriminator
  - Discriminator wants to distinguish model samples from the training data
  - Generator wants to fool the discriminator
- Generative moment matching network (GMMN)
  - Train a generative network such that certain statistics match between the generated samples and the data

Decoder-based generative models

Some impressive-looking samples:

Denton et al. (2015)



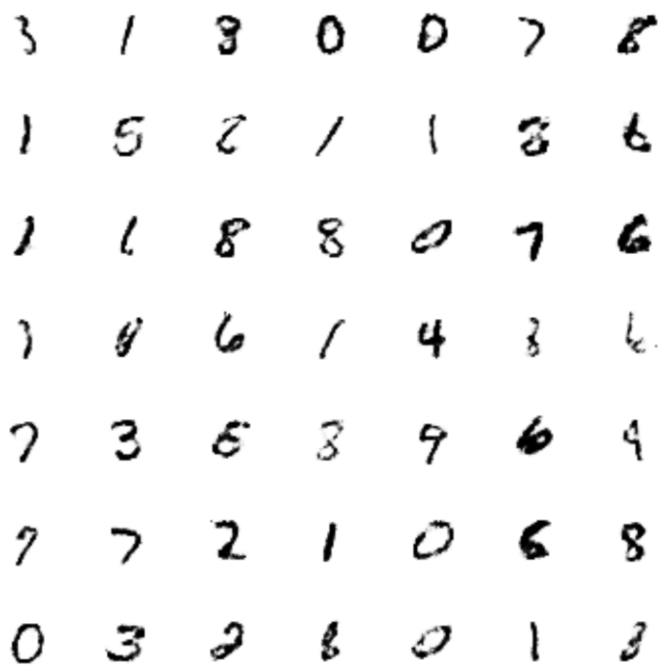
Radford et al. (2016)

But how well do these models capture the distribution?

Decoder-based generative models

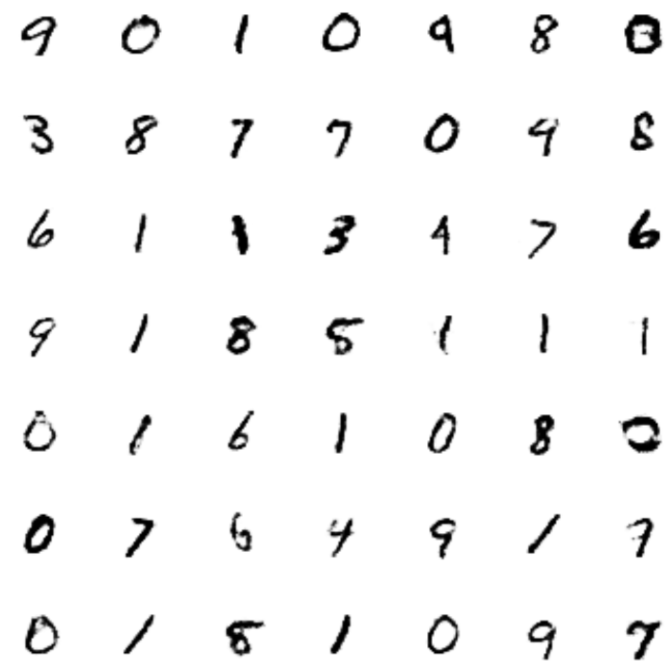
Looking at samples can be misleading:

Decoder-based generative models



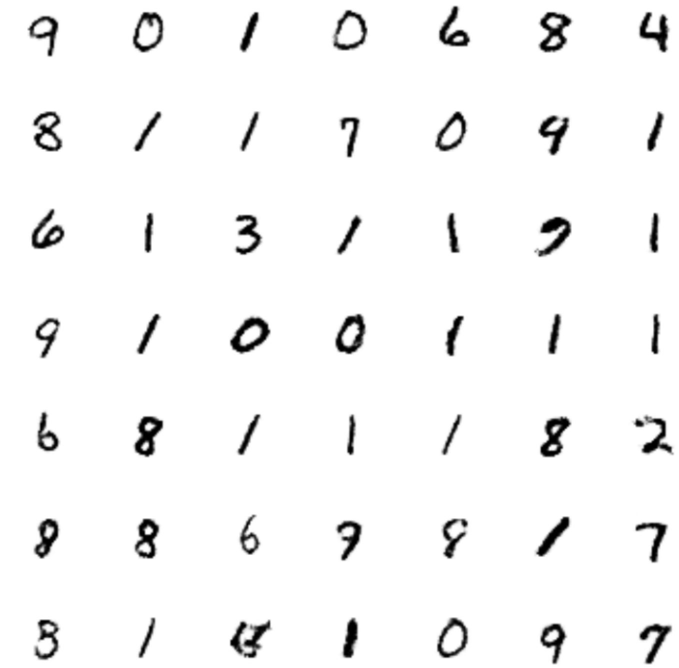
GAN, 10 dim

LLD = 328.7



GAN, 50 dim, 200 epochs

LLD = 543.5



GAN, 50 dim, 1000 epochs

LLD = 625.5

Evaluating decoder-based models

- Want to quantitatively evaluate generative models in terms of the probability of held-out data
- Problem: a GAN or GMMN with k latent dimensions can only generate within a k-dimensional submanifold!
- Standard (but unsatisfying) solution: impose a spherical Gaussian observation model

$$p_\sigma(\mathbf{x} \,|\, \mathbf{z}) = \mathcal{N}(f(\mathbf{z}), \sigma \mathbf{I})$$

  - tune σ on a validation set
- Problem: this still requires computing an intractable integral:

$$p_\sigma(\mathbf{x}) = \int p(\mathbf{z})\, p_\sigma(\mathbf{x} \,|\, \mathbf{z})\, \mathrm{d}\mathbf{z}$$

Evaluating decoder-based models

- For some models, we can tractably compute log-likelihoods, or at least a reasonable lower bound

- Tractable likelihoods for models with reversible decoders (e.g. NICE)

- Variational autoencoders: ELBO lower bound

$$\log p(\mathbf{x}) \geq \mathbb{E}_{q(\mathbf{z} \,|\, \mathbf{x})}[\log p(\mathbf{x} \,|\, \mathbf{z})] - \mathrm{D}_{\mathrm{KL}}(q(\mathbf{z} \,|\, \mathbf{x}) \,\|\, p(\mathbf{z}))$$

- Importance Weighted Autoencoder

$$\log p(\mathbf{x}) \geq \mathbb{E}_{q(\mathbf{z} \,|\, \mathbf{x})}\left[\log \frac{p(\mathbf{x}, \mathbf{z})}{q(\mathbf{z} \,|\, \mathbf{x})}\right]$$

- In general, we don't have accurate and tractable bounds
  - Even in the cases of VAEs and IWAEs, we don't know how accurate the bounds are

Evaluating decoder-based models

- Currently, results reported using kernel density estimation (KDE)

$$\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(S)} \sim p(\mathbf{z})$$

$$\hat{p}_\sigma(\mathbf{x}) = \frac{1}{S} \sum_{s=1}^{S} p_\sigma(\mathbf{x} \,|\, \mathbf{z}^{(s)})$$

  - Can show this is a stochastic lower bound:

$$\mathbb{E}[\log \hat{p}_\sigma(\mathbf{x})] \leq \log p_\sigma(\mathbf{x})$$

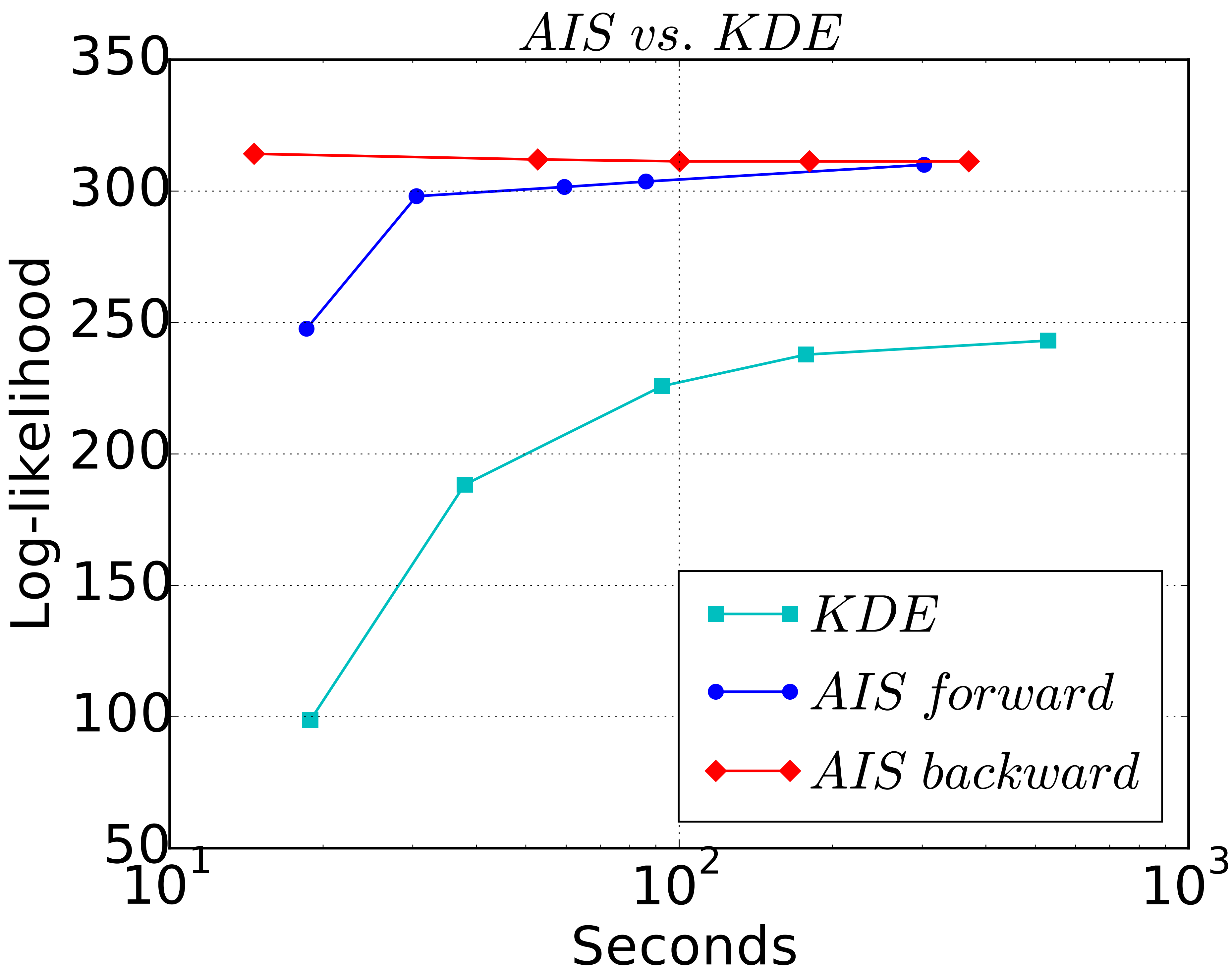
  - Unlikely to perform well in high dimensions
  - Papers caution the reader not to trust the results

Evaluating decoder-based models

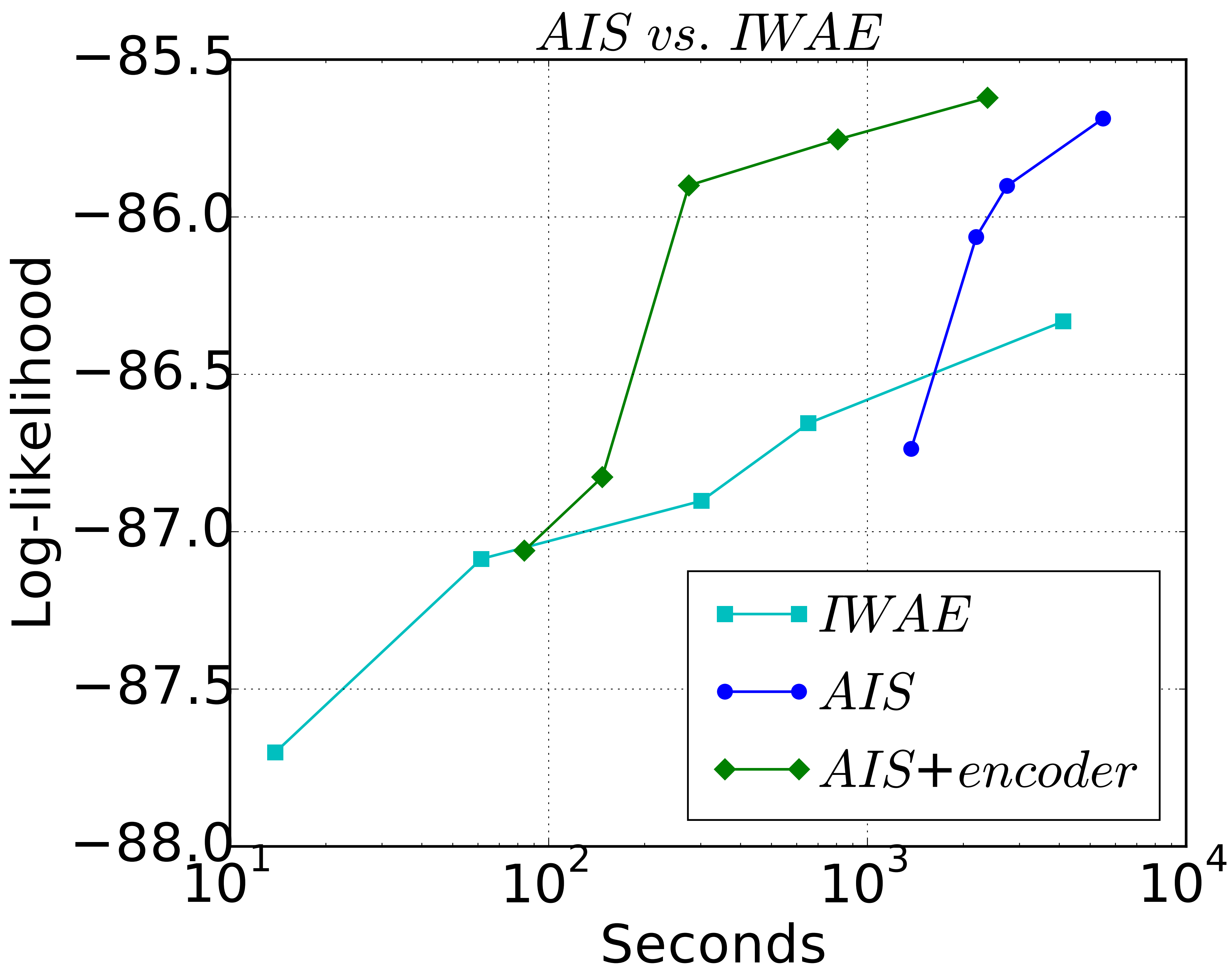
- Our approach: integrate out latent variables using AIS, with Hamiltonian Monte Carlo (HMC) as the transition operator
- Validate the accuracy of the estimates on simulated data using BDMC
- Experiment details
  - Real-valued MNIST dataset
  - VAEs, GANs, GMMNs with the following decoder architectures:
    - 10-64-256-256-1024-784
    - 50-1024-1024-1024-784
  - Spherical Gaussian observations imposed on all models (including VAE)

How accurate are AIS and KDE?

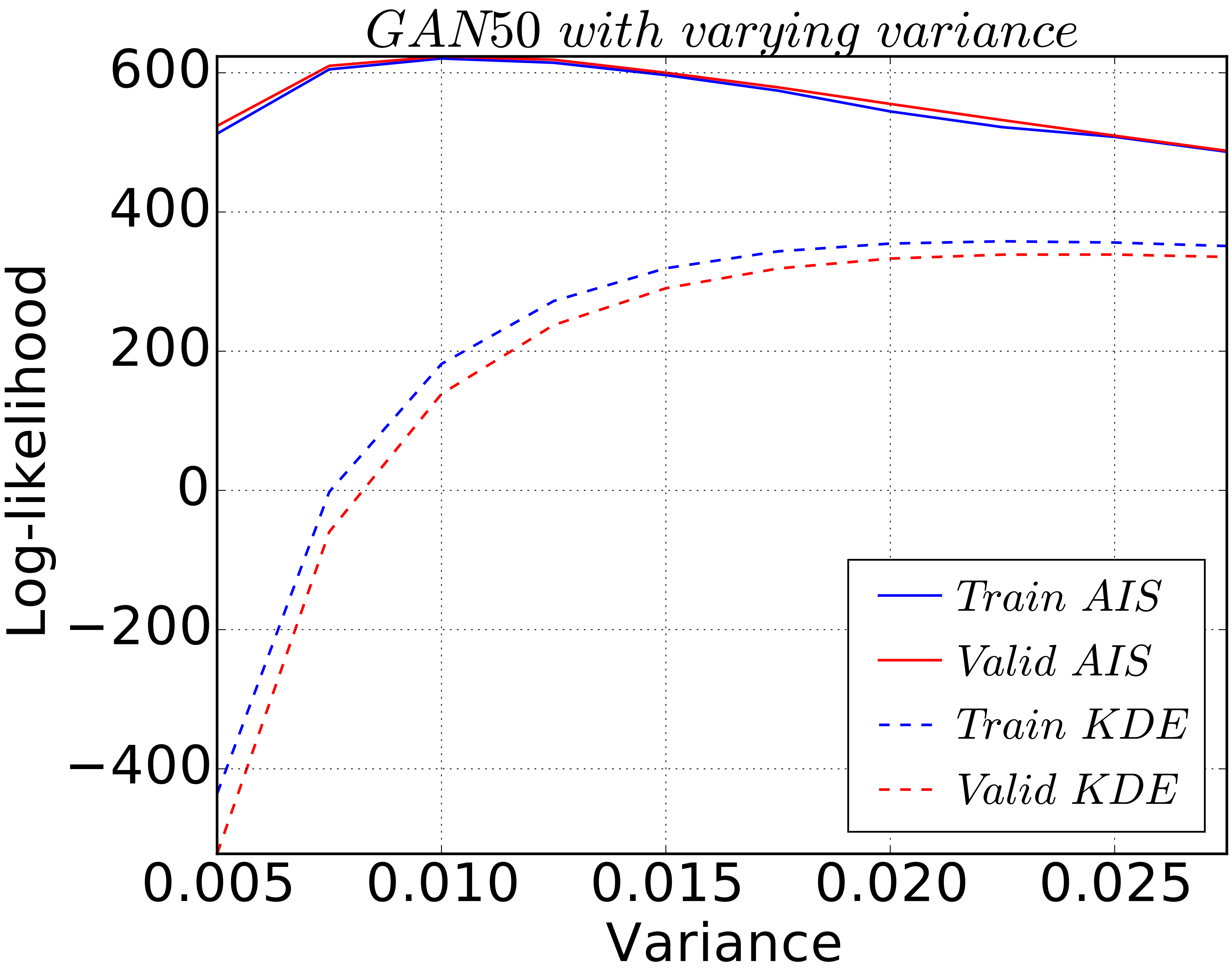
(GMMN-50)



How accurate is the IWAE bound?



Estimation of variance parameter



Comparison of different models

(Nats)	AIS Test (1000ex)	AIS Train (100ex)	BDMC gap	KDE Test	IWAE Test
VAE-50	991.435±6.477	1272.586±6.759	1.540	351.213	826.325
GAN-50	627.297±8.813	620.498±31.012	10.045	300.331	/
GMMN-50	593.472±8.591	571.803±30.864	1.146	277.193	/
VAE-10	705.375±7.411	780.196±19.147	0.832	408.659	486.466
GAN-10	328.772±5.538	318.948±22.544	0.934	259.673	/
GMMN-10	346.679±5.860	345.176±19.893	0.605	262.73	/

AIS estimates are accurate (small BDMC gap)

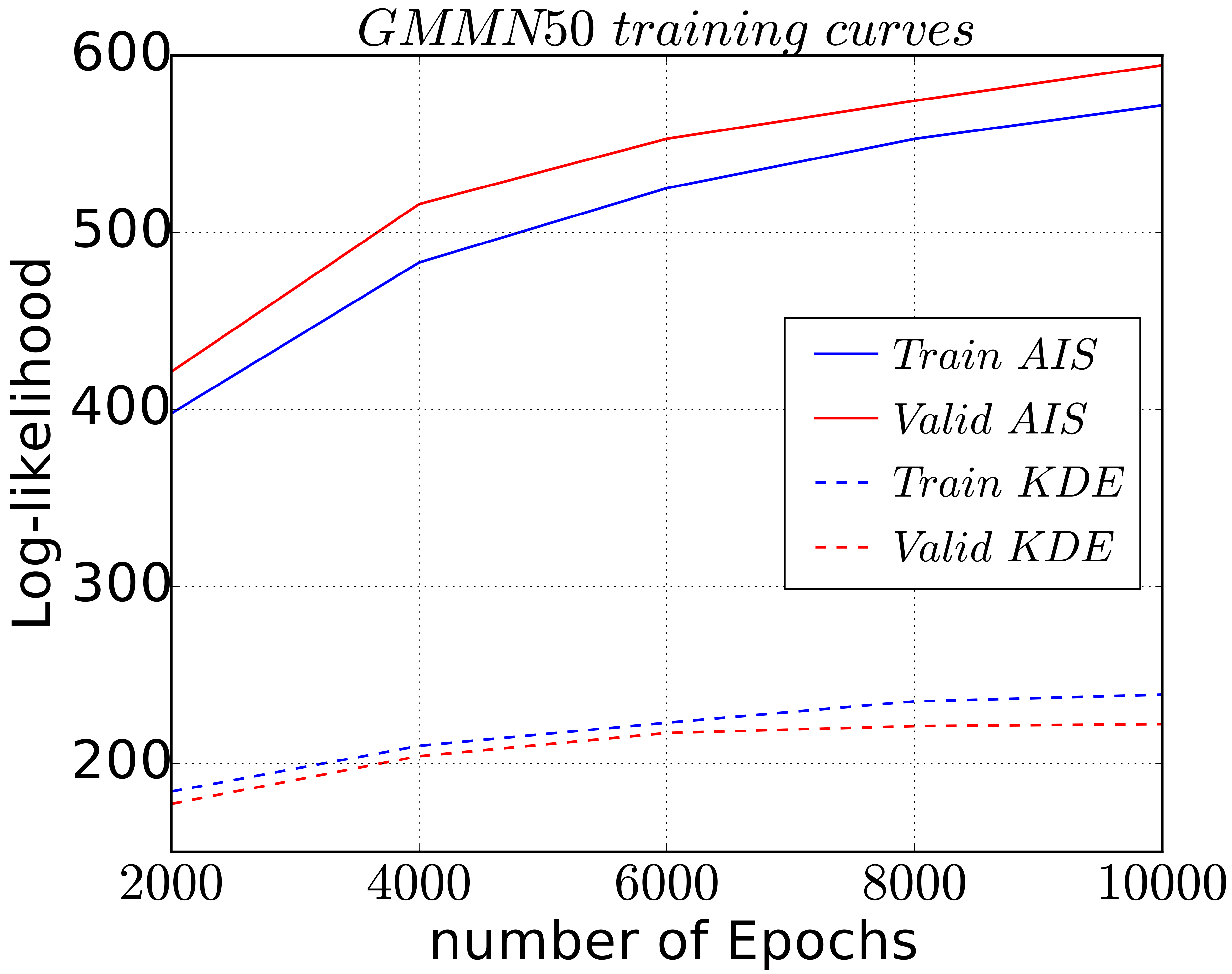
Larger model ==> much higher log-likelihood

VAEs achieve much higher log-likelihood than GANs and GMMNs

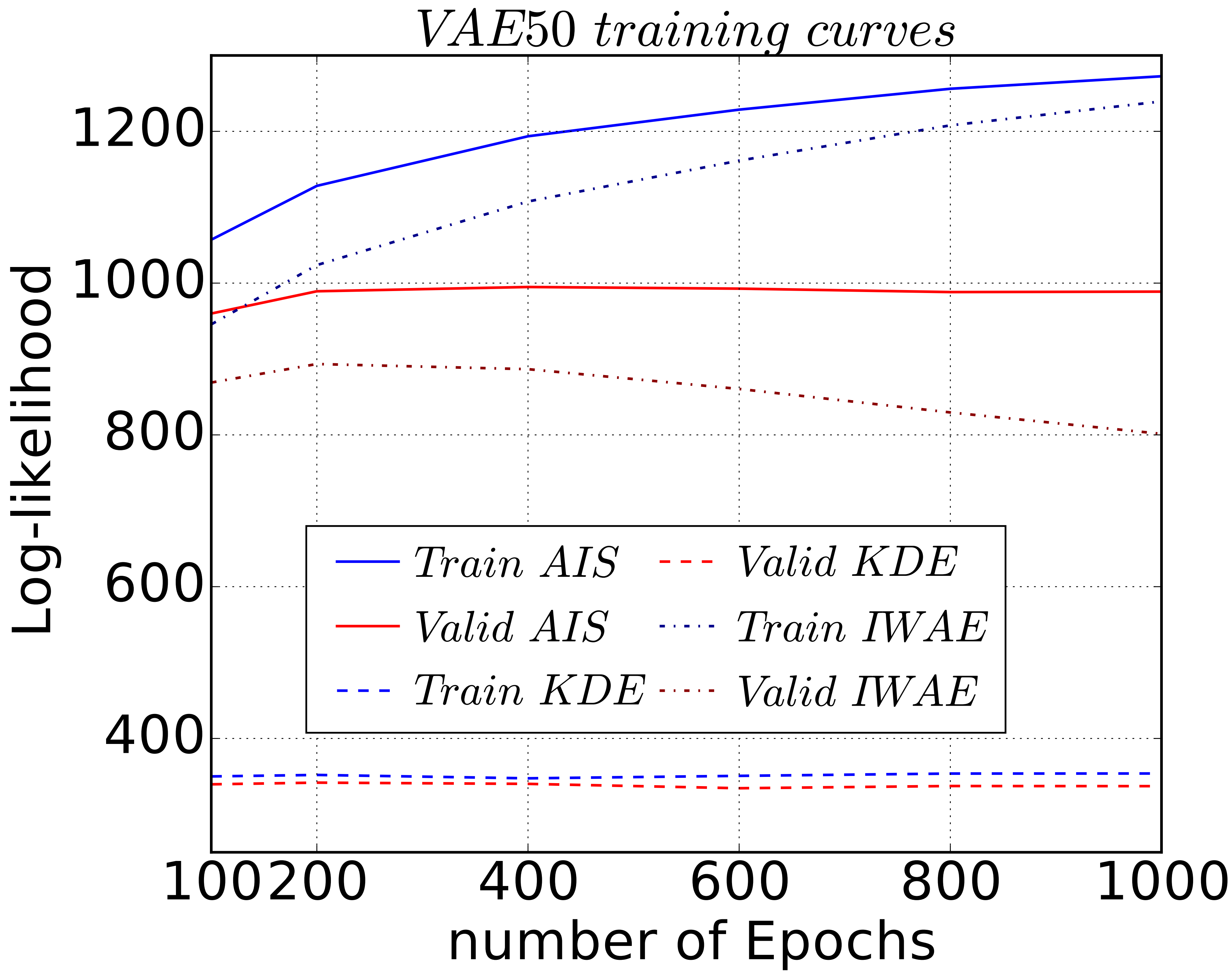
For GANs and GMMNs, no statistically significant difference between training and test log-likelihoods!

These models are not just memorizing training examples.

Training curves for a GMMN

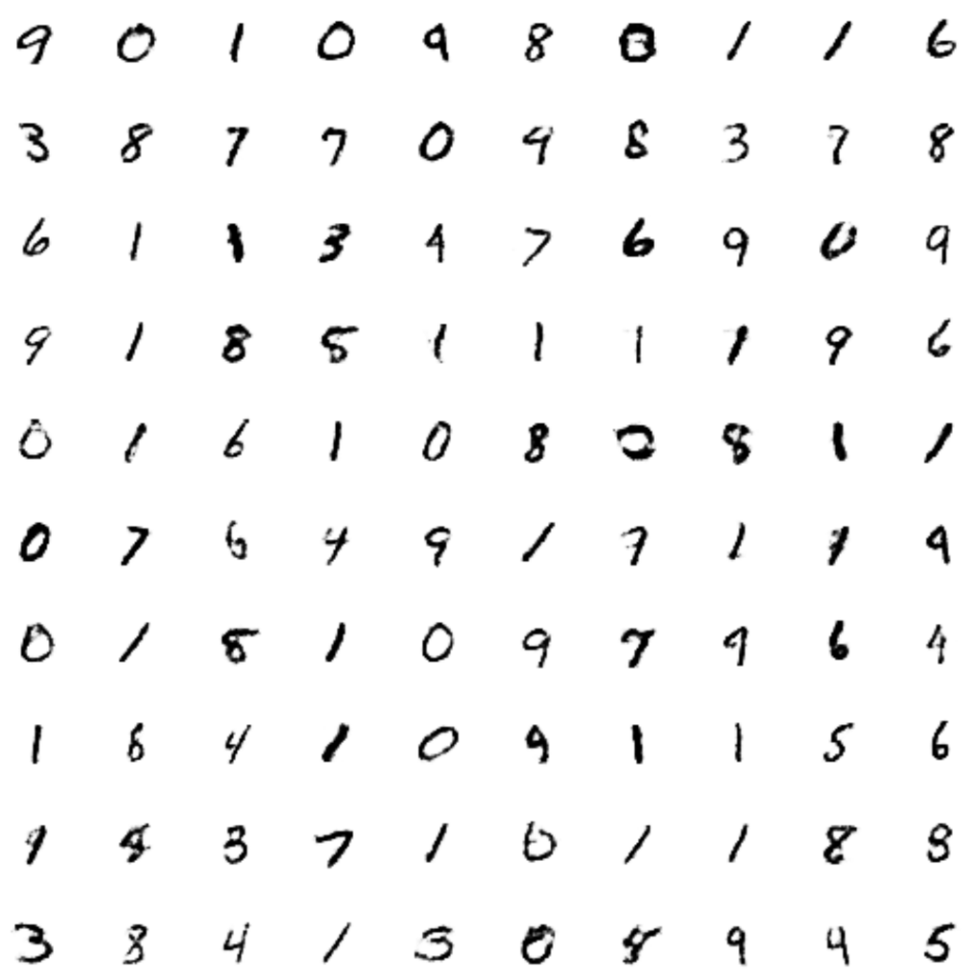


Training curves for a VAE

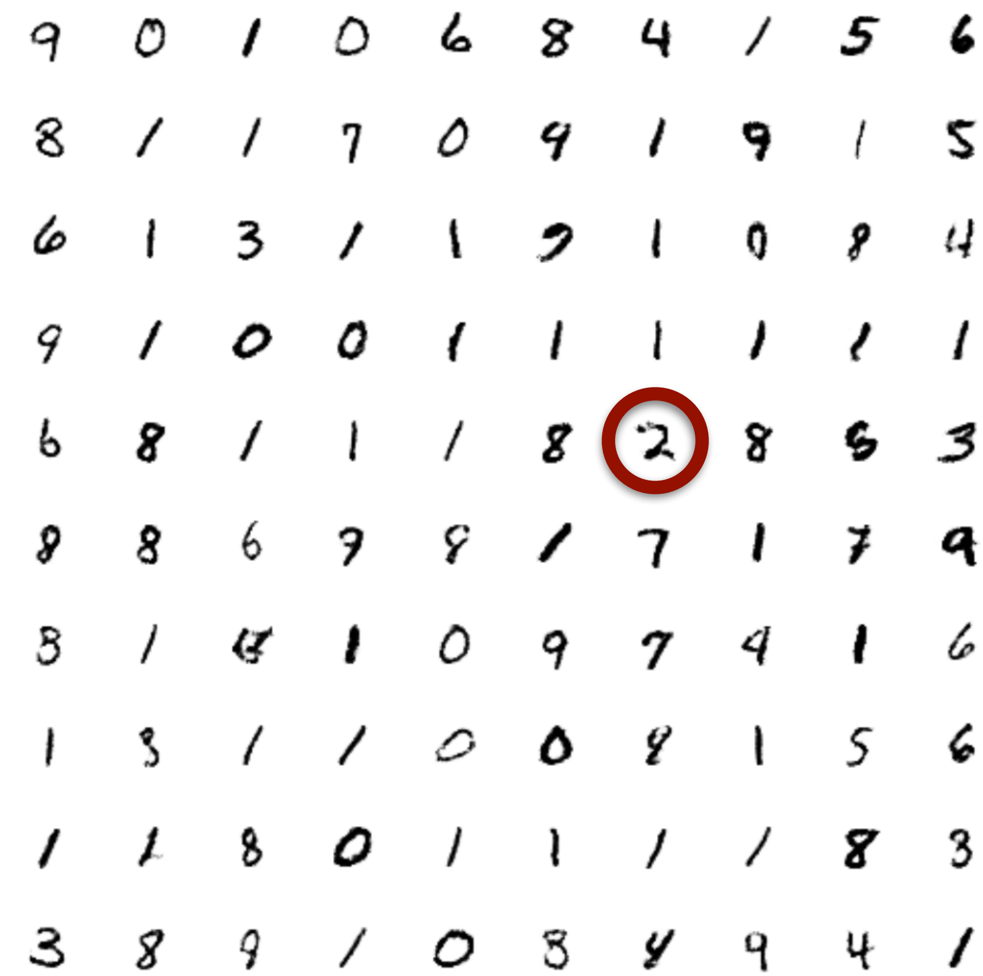


Missing modes

The GAN seriously misallocates probability mass between modes:



200 epochs



1000 epochs

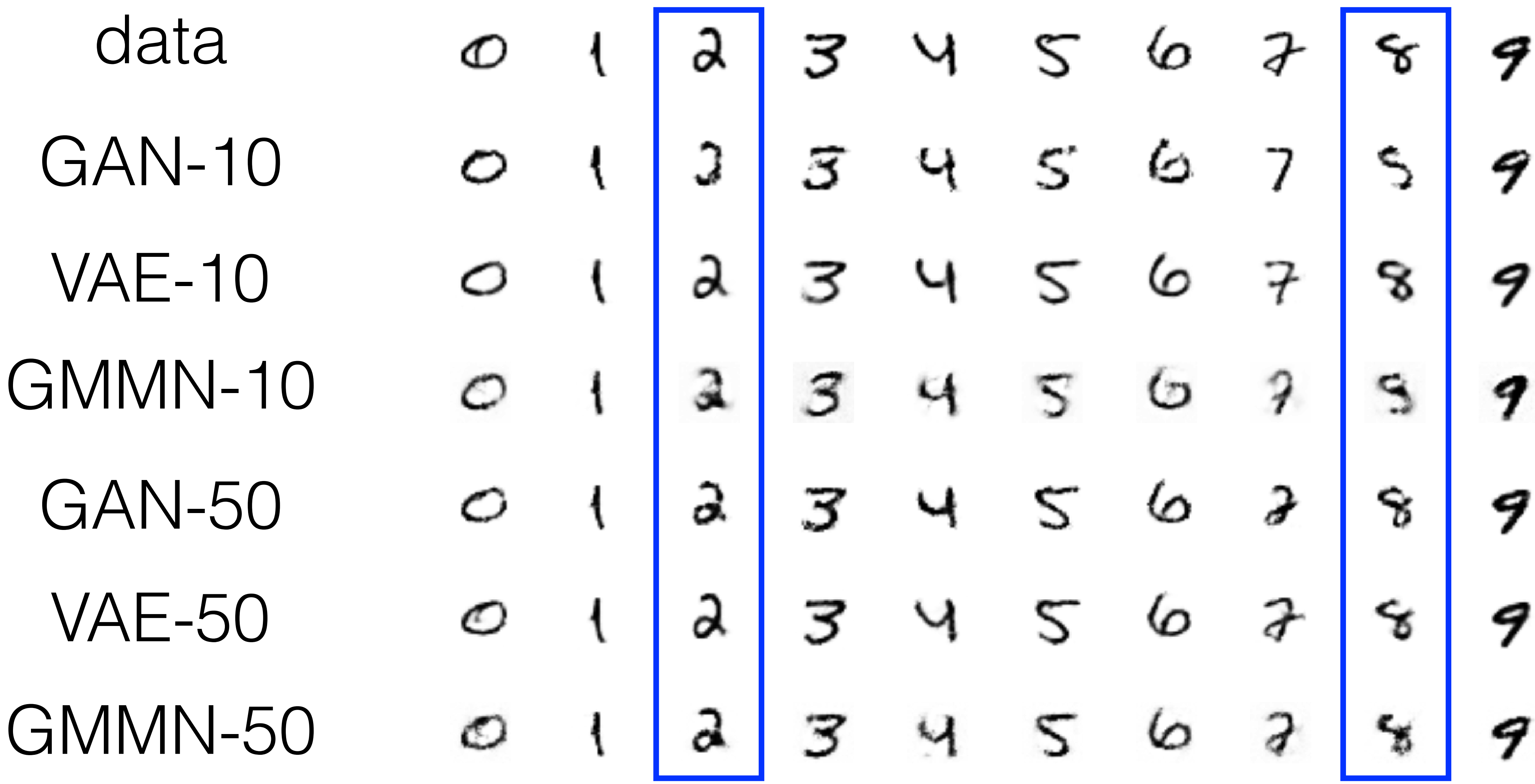
But this effect by itself is too small to explain why it underperforms the VAE by over 350 nats

Missing modes

- To see if the network is missing modes, let's visualize posterior samples given observations.
- Use AIS to approximately sample z from p(z | x), then run the decoder
- Using BDMC, we can validate the accuracy of AIS samples on simulated data

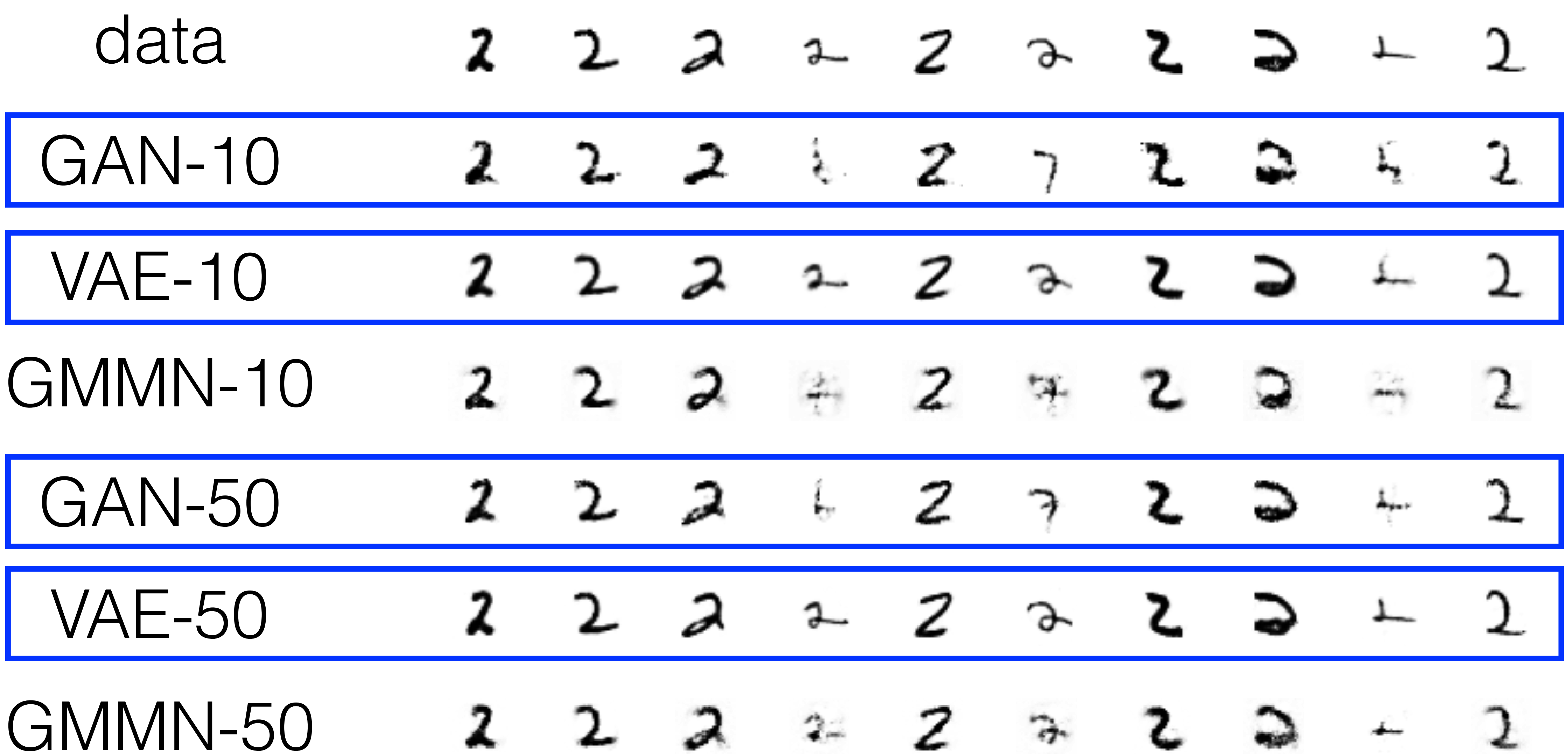
Missing modes

Visualization of posterior samples for validation images



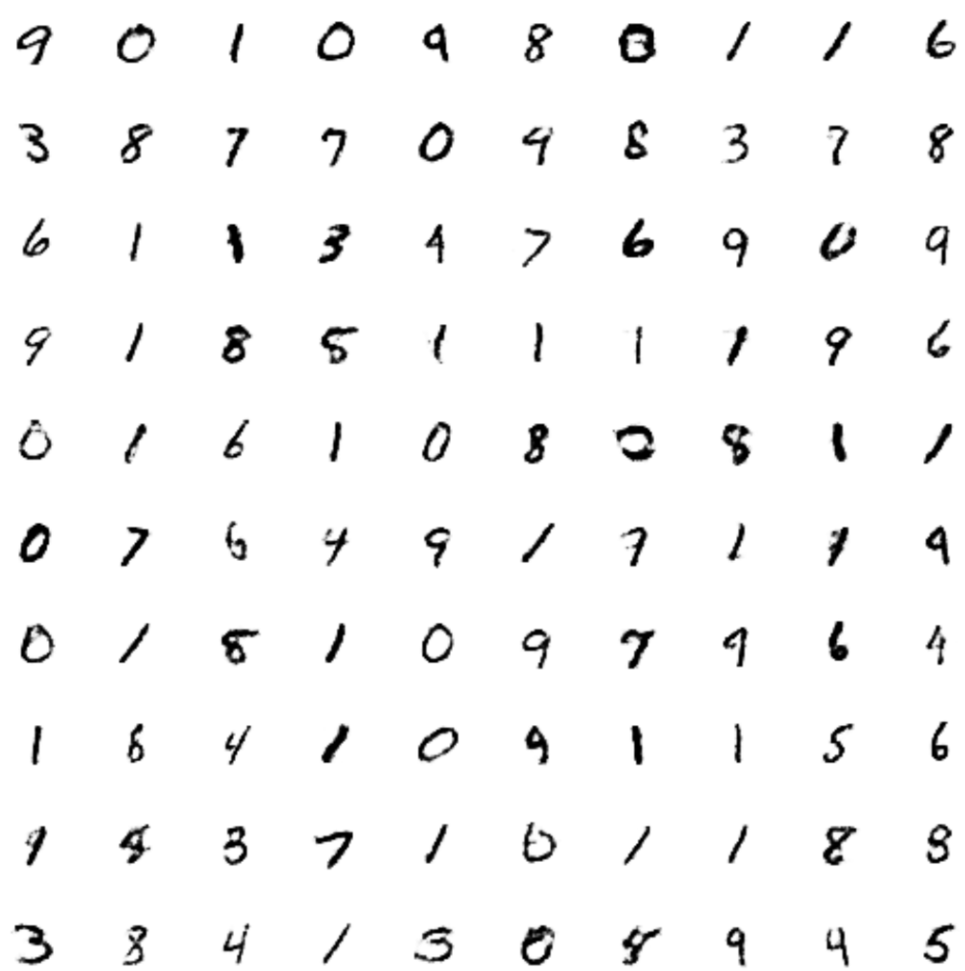
Missing modes

Posterior samples on *training* set

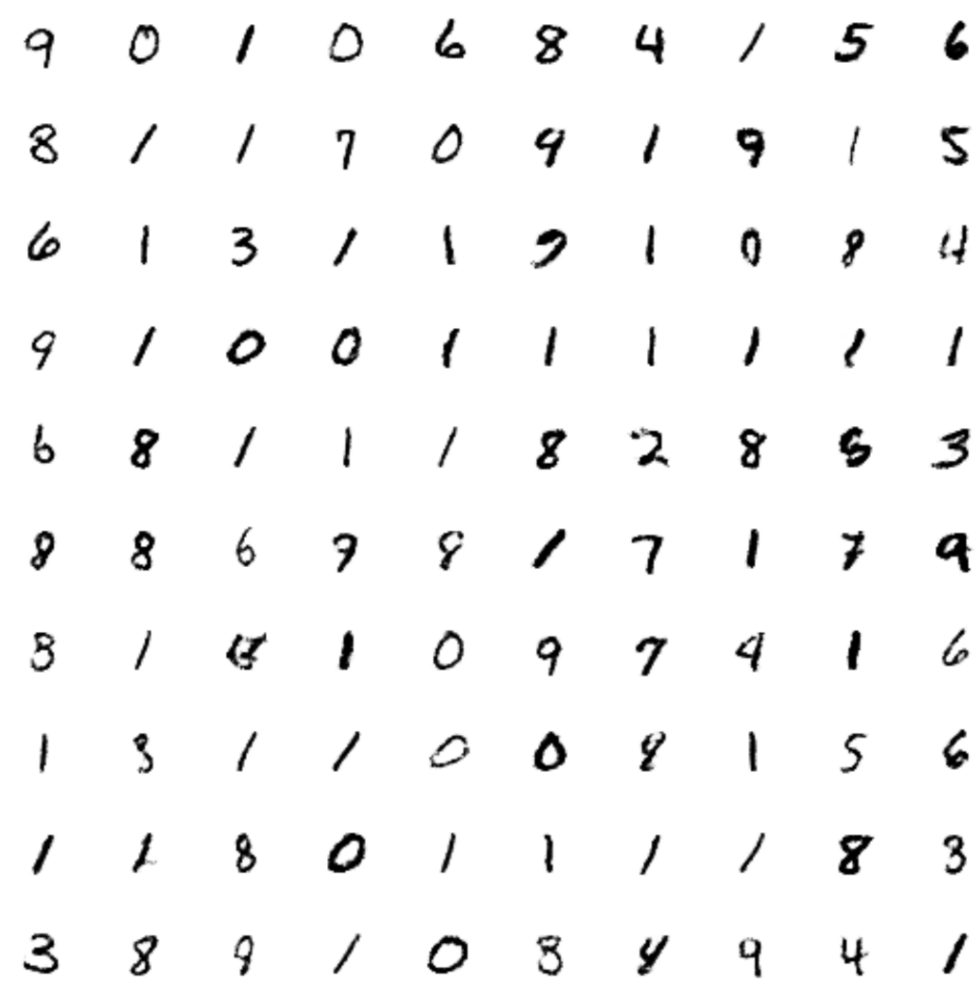


Missing modes

Conjecture: the GAN acts like a frustrated student



200 epochs



1000 epochs

Conclusions

- AIS gives high-accuracy log-likelihood estimates on MNIST (as validated by BDMC)
- This lets us observe interesting phenomena that are invisible to KDE
- GANs and GMMNs are not just memorizing training examples
- VAEs achieve substantially higher log-likelihoods than GANs and GMMNs
  - This appears to reflect failure to model certain modes of the data distribution
- Recognition nets can overfit
- Networks may continue to improve during training, even if KDE estimates don't reflect that
- Will be interesting to measure the effects of other algorithmic improvements to these networks