Hamiltonian Annealed Importance Sampling for partition function estimation

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Abstract

We introduce an extension to annealed importance sampling that uses Hamiltonian dynamics to rapidly estimate normalization constants. We demonstrate this method by computing log likelihoods in directed and undirected probabilistic image models. We compare the performance of linear generative models with both Gaussian and Laplace priors, product of experts models with Laplace and Student’s t experts, the mc-RBM, and a bilinear generative model. We provide code to compare additional models.

1 Introduction

We would like to use probabilistic models to assign probabilities to data. Unfortunately, this innocuous statement belies an important, difficult problem: many interesting distributions used widely across sciences cannot be analytically normalized. Historically, the training of probabilistic models has been motivated in terms of maximizing the log probability of the data under the model or minimizing the KL divergence between the data and the model. However, for most models it is impossible to directly compute the log likelihood, due to the intractability of the normalization constant, or partition function. For this reason, performance is typically measured using a variety of diagnostic heuristics, not directly indicative of log likelihood. For example, image models are often compared in terms of their synthesis, denoising, inpainting, and classification performance. This inability to directly measure the log likelihood has made it difficult to consistently evaluate and compare models.

Recently, a growing number of researchers have given their attention to measures of likelihood in image models. Salakhutdinov & Murray (2008) use annealed importance sampling, and Murray & Salakhutdinov (2009) use a hybrid of annealed importance sampling and a Chib-style estimator to estimate the log likelihood of a variety of MNIST digits and natural image patches modeled using restricted Boltzmann machines and deep belief networks. Bethge (2006) measures the reduction in multi-information, or statistical redundancy, as images undergo various complete linear transformations. Chandler & Field (2007) and Stephens et al. (2008) produce estimates of the entropy inherent in natural scenes, but do not address model evaluation. Karklin (2007) uses kernel density estimates – essentially, vector quantization – to compare different image models, though that technique suffers from severe scaling problems except in specific contexts. Zoran & Weiss (2009) compare the true log likelihoods of a number of image models, but restricts their analysis to the rare cases where the partition function can be solved analytically.

In this work, we merge two existing ideas – annealed importance sampling and Hamiltonian dynamics – into a
single algorithm. To review, Annealed Importance Sampling (AIS) [Neal (2001)] is a sequential Monte Carlo method [Moral et al. (2006)] which allows the partition function of a non-analytically-normalizable distribution to be estimated in an unbiased fashion. This is accomplished by starting at a distribution with a known normalization, and gradually transforming it into the distribution of interest through a chain of Markov transitions. Its practicality depends heavily on the chosen Markov transitions. Hamiltonian Monte Carlo (HMC) [Neal (2010)] is a family of techniques for fast sampling in continuous state spaces, which work by extending the state space to include auxiliary momentum variables, and then simulating Hamiltonian dynamics from physics in order to traverse long iso-probability trajectories which rapidly explore the state space.

The key insight that makes our algorithm more efficient than previous methods is our adaptation of AIS to work with Hamiltonian dynamics. As in HMC, we extend the state space to include auxiliary momentum variables; however, we do this in such a way that the momenta change consistently through the intermediate AIS distributions, rather than resetting them at the beginning of each Markov transition. To make the practical applications of this work clear, we use our method, Hamiltonian Annealed Importance Sampling (HAIS), to measure the log likelihood of holdout data under a variety of directed distributions, rather than resetting them at the beginning of each Markov transition. To make the practical applications of this work clear, we use our method, Hamiltonian Annealed Importance Sampling (HAIS), to measure the log likelihood of holdout data under a variety of directed (generative) and undirected (analysis/feed-forward) probabilistic models of natural image patches.

The source code to reproduce our experiments is available.

2 Estimating Log Likelihood

2.1 Importance Sampling

Importance sampling [Kahn & Marshall (1953)] allows an unbiased estimate \( \hat{Z}_p \) of the partition function (or normalization constant) \( Z_p \) of a non-analytically-normalizable target distribution \( p(x) \) over \( x \in \mathbb{R}^M \),

\[
p(x) = \frac{e^{-E_p(x)}}{Z_p}, \quad Z_p = \int dx \ e^{-E_p(x)},
\]

(1)

\( \hat{Z}_p \) to be calculated. This is accomplished by averaging over samples \( S_q \) from a proposal distribution \( q(x) \),

\[
q(x) = \frac{e^{-E_q(x)}}{Z_q}
\]

(3)

\[
Z_p = \int dx \ q(x) \frac{e^{-E_p(x)}}{q(x)}
\]

(4)

\[
\hat{Z}_p = \frac{1}{|S_q|} \sum_{x \in S_q} e^{-E_p(x)} q(x),
\]

(5)

where \( |S_q| \) is the number of samples. \( q(x) \) is chosen to be easy both to sample from and to evaluate exactly, and must have support everywhere that \( p(x) \) does. Unfortunately, unless \( q(x) \) has significant mass everywhere \( p(x) \) does, it takes an impractically large number of samples from \( q(x) \) for \( \hat{Z}_p \) to accurately approximate \( Z_p \).

2.2 Annealed Importance Sampling

Annealed importance sampling [Neal (2001)] extends the state space \( x \) to a series of vectors, \( X = \{x_1, x_2 \ldots x_N\} \), \( x_n \in \mathbb{R}^M \). It then transforms the proposal distribution \( q(x) \) to a forward chain \( Q(X) \) over \( X \), by setting \( q(x) \) as the distribution over \( x_1 \) and then multiplying by a series of Markov transition distributions,

\[
Q(X) = q(x_1) \prod_{n=1}^{N-1} T_n(x_{n+1}|x_n),
\]

(6)

where \( T_n(x_{n+1}|x_n) \) represents a forward transition distribution from \( x_n \) to \( x_{n+1} \). The target distribution \( p(x) \) is similarly transformed to become a reverse chain \( P(X) \), starting at \( x_N \), over \( X \),

\[
P(X) = \frac{e^{-E_p(x_N)}}{Z_p} \prod_{n=1}^{N-1} \bar{T}_n(x_n|x_{n+1}),
\]

(7)

where \( \bar{T}_n(x_n|x_{n+1}) \) is a reverse transition distribution from \( x_{n+1} \) to \( x_n \). The transition distributions are, by definition, normalized (e.g., \( \int dx_{n+1} \bar{T}_n(x_{n+1}|x_n) = 1 \)).

In a similar fashion to Equations (4) and (5), samples \( S_Q \) from the forward proposal chain \( Q(X) \) can be used to

1 The expected variance of the estimate \( \hat{Z}_p \) is given by an \( \alpha \)-divergence between \( p(x) \) and \( q(x) \), times a constant and plus an offset - see Minka [2005].
estimate the partition function $Z_p$ (note that all integrals but the first in Equation [8] go to 1),

$$Z_p = \int dX_1 \cdots \int dX_{N-1} T_{N-1}(X_{N-1}|X_N)$$

$$= \int dX Q(X) \frac{e^{-E_p(x_1)}}{Q(x_1)} T_{N-1}(x_{N-1}|x_N) T_1(x_1|x_2)$$

$$= \frac{1}{|S_Q|} \sum_{x \in S_Q} e^{-E_p(x_1)} \frac{T_1(x_1|x_2)}{q(x_1)} \frac{T(x_{N-1}|x_N)}{T(x_{N-1}|x_{N-1})}$$

(9)

In order to further define the transition distributions, Neal introduces intermediate distributions $\pi_n(x)$ between $q(x)$ and $p(x)$,

$$\pi_n(x) = e^{-E_{\pi_n}(x)} Z_{\pi_n}$$

$$E_{\pi_n}(x) = (1 - \beta_n) E_q(x) + \beta_n E_p(x),$$

(12)

where the mixing fraction $\beta_n = \frac{n}{N}$ for all results reported here. $T_n(x_{n+1}|x_n)$ is then chosen to be any Markov chain transition for $\pi_n(x)$, meaning that it leaves $\pi_n(x)$ invariant

$$T_n \circ \pi_n = \pi_n.$$  

(13)

The reverse direction transition distribution $\tilde{T}_n(x_n|x_{n+1})$ is set to the reversal of $T_n(x_{n+1}|x_n)$,

$$\tilde{T}_n(x_n|x_{n+1}) = T_n(x_{n+1}|x_n) \frac{\pi_n(x_n)}{\pi_n(x_{n+1})}.$$  

(14)

Equation [10] thus reduces to

$$\tilde{Z}_p = \frac{1}{|S_Q|} \sum_{x \in S_Q} e^{-E_p(x_1)} \frac{\pi_1(x_1)}{\pi_1(x_2)} \frac{\pi_{N-1}(x_{N-1})}{\pi_{N-1}(x_N)} \cdots$$

$$e^{-E_{\pi_{N-1}}(x_{N-1})} e^{-E_{\pi_1}(x_1)} e^{-E_{\pi_2}(x_2)}$$

$$= \frac{1}{|S_Q|} \sum_{x \in S_Q} e^{-E_p(x_1)} \frac{\pi_1(x_1)}{\pi_1(x_2)} \frac{\pi_{N-1}(x_{N-1})}{\pi_{N-1}(x_N)} \cdots$$

$$e^{-E_{\pi_{N-1}}(x_{N-1})} e^{-E_{\pi_1}(x_1)} e^{-E_{\pi_2}(x_2)}$$

(15)

If the number of intermediate distributions $N$ is large, and the transition distributions $T_n(x_{n+1}|x_n)$ and $\tilde{T}_n(x_n|x_{n+1})$ mix effectively, then the distributions over intermediate states $x_n$ will be nearly identical to $\pi_n(x_n)$ in both the forward and backward chains. $P(X)$ and $Q(X)$ will then be extremely similar to one another, and the variance in the estimate $\tilde{Z}_p$ will be extremely low. If the transitions $T_n(x_{n+1}|x_n)$ do a poor job mixing, then the marginal distributions over $x_n$ under $P(X)$ and $Q(X)$ will look different from $\pi_n(x_n)$. The estimate $\tilde{Z}_p$ will still be unbiased, but with a potentially larger variance. Thus, to make AIS practical, it is important to choose Markov transitions $T_n(x_{n+1}|x_n)$ for the intermediate distributions $\pi_n(x)$ that mix quickly.

2.3 Hamiltonian Annealed Importance Sampling

Hamiltonian Monte Carlo [Neal (2010)] uses an analogy to the physical dynamics of particles moving with momentum under the influence of an energy function to propose Markov chain transitions which rapidly explore the state space. It does this by expanding the state space to include auxiliary momentum variables, and then simulating Hamiltonian dynamics to move long distances along iso-probability contours in the expanded state space. A similar technique is powerful in the context of annealed importance sampling. Additionally, by retaining the momenta variables across the intermediate distributions, significant momentum can build up as the proposal distribution is transformed into the target. This provides a mixing benefit that is unique to our formulation.

The state space $X$ is first extended to $Y = \{y_1, y_2 \ldots y_N\}, y_n = \{x_n, v_n\}$, where $v_n \in \mathbb{R}^M$ consists of a momentum associated with each position $x_n$. The momenta associated with both the proposal and target distributions is taken to be unit norm isotropic gaussian.

The proposal and target distributions $q(x)$ and $p(x)$ are extended to corresponding distributions $q(y)$ and $p(y)$.

\[2\] There is a direct mapping between annealed importance sampling and the Jarzynki equality in non-equilibrium thermodynamics - see Jarzynski (1997). It follows from this mapping, and the reversibility of quasistatic processes, that the variance in $\tilde{Z}_p$ can be made to go to 0 if the transition from $q(x_1)$ to $p(x_N)$ is sufficiently gradual.
over position and momentum \( y = \{ x, v \} \),

\[
p_{\cup}(y) = p(x) \Phi(v) = \frac{e^{-E_{\pi}(x)}}{Z_{\cup}} \quad (17)
\]

\[
q_{\cup}(y) = q(x) \Phi(v) = \frac{e^{-E_{\pi}(y)}}{Z_{\cup}} \quad (18)
\]

\[
\Phi(v) = \frac{-\frac{1}{2}v^Tv}{(2\pi)^{\frac{D}{2}}} \quad (19)
\]

\[
E_{p_{\cup}}(y) = E_p(x) + \frac{1}{2}v^Tv \quad (20)
\]

\[
E_{q_{\cup}}(y) = E_q(x) + \frac{1}{2}v^Tv \quad (21)
\]

The remaining distributions are extended to cover both position and momentum in a nearly identical fashion: the forward and reverse chains \( Q(X) \to Q_{\cup}(Y), P(X) \to P_{\cup}(Y), \) the intermediate distributions and energy functions \( \pi_n(x) \to \pi_{\cup n}(y), E_{\pi_n}(x) \to E_{\pi_{\cup n}}(y), \)

\[
E_{\pi_{\cup n}}(y) = (1 - \beta_n)E_q(y) + \beta_nE_p(y) \quad (22)
\]

\[
\text{and the forward and reverse Markov transition distributions} \quad T_n(x_{n+1}|x_n) \to T_{\cup n}(y_{n+1}|y_n) \text{ and } \bar{T}_n(x_n|x_{n+1}) \to \bar{T}_{\cup n}(y_n|y_{n+1}). \text{ Similarly, the samples } S_{Q_{\cup}} \text{ now each have both position } X \text{ and momentum } V, \text{ and are drawn from the forward chain described by } Q_{\cup}(Y).\]

The annealed importance sampling estimate \( \hat{Z}_p \) given in Equation 16 remains unchanged, except for a replacement of \( S_Q \) with \( S_{Q_{\cup}} \) – all the terms involving the momentum \( V \) conveniently cancel out, since the same momentum distribution \( \Phi(v) \) is used for the proposal \( q_{\cup}(y_1) \) and target \( p_{\cup}(y_N), \)

\[
\hat{Z}_p = \frac{1}{|S_{Q_{\cup}}|} \sum_{Y \in S_{Q_{\cup}}} \frac{e^{-E_p(x_0)}\Phi(v_N) e^{-E_{\pi_1}(x_1) + \frac{1}{2}v_1^Tv_1}}{q(x_1)\Phi(v_1) e^{-E_{\pi_2}(x_2) + \frac{1}{2}v_2^Tv_2} \cdots e^{-E_{\pi_{N-1}}(x_{N-1}) + \frac{1}{2}v_{N-1}^Tv_{N-1}}}
\]

\[
\hat{Z}_p = \frac{1}{|S_{Q_{\cup}}|} \sum_{Y \in S_{Q_{\cup}}} \frac{e^{-E_p(x_0)}e^{-E_{\pi_1}(x_1)}}{q(x_1) e^{-E_{\pi_2}(x_2)} \cdots e^{-E_{\pi_{N-1}}(x_{N-1})}} \quad (24)
\]

Thus, the momentum only matters when generating the samples \( S_{Q_{\cup}} \), by drawing from the initial proposal distribution \( p_{\cup}(y_1) \), and then applying the series of Markov transitions \( T_{\cup n}(y_{n+1}|y_n) \).

For the transition distributions, \( T_{\cup n}(y_{n+1}|y_n) \), we propose a new location by integrating Hamiltonian dynamics for a short time using a single leapfrog step, accept or reject the new location via Metropolis rules, and then partially corrupt the momentum. That is, we generate a sample from \( T_{\cup n}(y_{n+1}|y_n) \) by following the procedure:

1. \( \{ x^0_H, v^0_H \} = \{ x_n, v_n \} \)

2. leapfrog: \( x^1_H = x^0_H + \frac{1}{2}v^0_H \)

\[
v^1_H = v^0_H - \epsilon \frac{\partial E_{\pi_n}(x)}{\partial x}|_{x=x^1_H} \quad (23)
\]

\[
x^1_H = x^1_H + \frac{1}{2}v^1_H \]

where the step size \( \epsilon = 0.2 \) for all experiments in this paper.

3. accept/reject: \( \{ x', v' \} = \{ x^1_H, -v^1_H \} \) with probability \( P_{\text{accept}} = \min\left(1, \frac{e^{-E_{\pi_n}(x^1_H) - \frac{1}{2}v^1_H^Tv^1_H}}{e^{-E_{\pi_n}(x^0_H) - \frac{1}{2}v^0_H^Tv^0_H}} \right), \) otherwise \( \{ x', v' \} = \{ x^0_H, v^0_H \} \)

4. partial momentum refresh: \( \tilde{v}' = -\sqrt{1-\gamma}v' + \gamma r, \)

where \( r \sim N(0, I), \) and \( \gamma \in (0, 1) \) is chosen so as to randomize half the momentum power per unit simulation time Culpepper et al. (2011).

5. \( y_{n+1} = \{ x_{n+1}, v_{n+1} \} = \{ x', \tilde{v}' \} \)
This combines the advantages of many intermediate distributions, which can lower the variance in the estimated $\hat{Z}_p$, with the improved mixing which occurs when momentum is maintained over many update steps. For details on Hamiltonian Monte Carlo sampling techniques, and a discussion of why the specific steps above leave $\pi_n(x)$ invariant, we recommend Culpepper et al. (2011); Neal (2010).

Some of the models discussed below have linear constraints on their state spaces. These are dealt with by negating the momentum $v$ and reflecting the position $x$ across the constraint boundary every time a leapfrog half-step violates the constraint.

### 2.4 Log likelihood of analysis models

Analysis models are defined for the purposes of this paper as those which have an easy to evaluate expression for $E_p(x)$ when they are written in the form of Equation (1). The average log likelihood $\mathcal{L}$ of an analysis model $p(x)$ over a set of testing data $D$ is

$$\mathcal{L} = \frac{1}{|D|} \sum_{x \in D} \log p(x) = -\frac{1}{|D|} \sum_{x \in D} E_p(x) - \log Z_p,$$

(26)

where $|D|$ is the number of samples in $D$, and the $Z_p$ in the second term can be directly estimated by Hamiltonian annealed importance sampling.

### 2.5 Log likelihood of generative models

Generative models are defined here to be those which have a joint distribution,

$$p(x, a) = p(x|a)p(a) = \frac{e^{-E_{x|a}(x,a)}e^{-E_a(a)}}{Z_{x|a}Z_a},$$

(27)

over visible variables $x$ and auxiliary variables $a \in \mathbb{R}^L$ which is easy to exactly evaluate and sample from, but for which the marginal distribution over the visible variables $p(x) = \int da p(x,a)$ is intractable to compute. The average log likelihood $\mathcal{L}$ of a model of this form over a testing set $D$ is

$$\mathcal{L} = \frac{1}{|D|} \sum_{x \in D} \log Z_{a|x}$$

(28)

$$Z_{a|x} = \int da e^{-E_{x|a}(x,a)} - E_{x|a} - E_a - \log Z_a,$$

(29)

where each of the $Z_{a|x}$ can be estimated using HAIS. Generative models take significantly longer to evaluate than analysis models, as a separate HAIS chain must be run for each test sample.

### 3 Models

The probabilistic forms for all models whose log likelihood we evaluate are given below. In all cases, $x \in \mathbb{R}^M$ refers to the data vector.
1. linear generative:

\[ p(x|a) = \frac{\exp \left[ -\frac{1}{2\sigma_n^2}(x - \Phi a)^T(x - \Phi a) \right]}{(2\pi)^{\frac{M}{2}} \sigma_n^M} \]  

(30)

parameters: \( \Phi \in \mathbb{R}^{M \times L} \)

auxiliary variables: \( a \in \mathbb{R}^L \)

constant: \( \sigma_n = 0.1 \)

Linear generative models were tested with two priors, as listed:

(a) Gaussian prior:

\[ p(a) = \frac{\exp \left[ -\frac{1}{2} a^T a \right]}{(2\pi)^{\frac{1}{2}}} \]  

(31)

(b) Laplace prior \cite{OlshausenField1997}:

\[ p(a) = \frac{\exp \left[ -||a||_1 \right]}{2} \]  

(32)

2. bilinear generative \cite{CulpepperEtAl2011}: The form is the same as for the linear generative model, but with the coefficients \( a \) decomposed into 2 multiplicative factors,

\[ a = (\Theta c) \odot (\Psi d) \]  

(33)

\[ p(c) = \frac{\exp \left[ -||c||_1 \right]}{2} \]  

(34)

\[ p(d) = \frac{\exp \left[ -||d||_1 \right]}{2} \]  

(35)

where \( \odot \) indicates element-wise multiplication.

parameters: \( \Phi \in \mathbb{R}^{M \times L}, \Theta \in \mathbb{R}^{L \times K_c}, \Psi \in \mathbb{R}^{L \times K_d} \)

auxiliary variables: \( c \in \mathbb{R}^{K_c}, d \in \mathbb{R}^{K_d} \)

3. product of experts \cite{Hinton2002}: This is the analysis model analogue of the linear generative model,

\[ p(x) = \frac{1}{Z_{POE}} \prod_{i=1}^{L} \exp \left( -E_{POE}(\Phi_i x; \lambda_i) \right) \]  

(36)

parameters: \( \Phi \in \mathbb{R}^{L \times M}, \lambda \in \mathbb{R}_+^L \)

Product of experts models were tested with two experts, as listed:

(a) Laplace expert:

\[ E_{POE}(u; \lambda_l) = \lambda_l |u| \]  

(37)

(changing \( \lambda_l \) is equivalent to changing the length of the row \( \Phi_l \), so it is fixed to \( \lambda_l = 1 \))

(b) Student’s t expert:

\[ E_{POE}(u; \lambda_l) = \lambda_l \log (1 + u^2) \]  

(38)

4. Mean and covariance restricted Boltzmann machine (mcRBM) \cite{RanzatoHinton2010}: This is an analysis model analogue of the bilinear generative model. The exact marginal energy function \( E_{mcR} \) is taken from the released code rather than the paper.

\[ p(x) = \frac{\exp \left[ -E_{mcR}(x) \right]}{Z_{mcR}} \]  

(39)

\[ E_{mcR}(x) = -\sum_{k=1}^{K} \log \left[ 1 + e^{\lambda_k} \right] + e^{\lambda_k} x_k^2 \]  

(40)

parameters: \( P \in \mathbb{R}^{L \times K}, C \in \mathbb{R}^{L \times M}, W \in \mathbb{R}^{J \times M}, b_m \in \mathbb{R}^J, b_c \in \mathbb{R}^K, b^v \in \mathbb{R}^K, \sigma \in \mathbb{R} \)

4 Training

All models were trained on 10,000 16x16 pixel image patches taken at random from 4,112 linearized images of natural scenes from the van Hateren dataset \cite{vanHaterenVanDerSchaaf1998}. The extracted image patches were first logged, and then mean subtracted. They were then projected onto the top \( M \) PCA components, and whitened by rescaling each dimension to unit norm.

All generative models were trained using Expectation Maximization over the full training set, with a Hamiltonian Monte Carlo algorithm used during the expectation step to maintain samples from the posterior distribution. See \cite{CulpepperEtAl2011} for details. All analysis models were trained using LBFGS on the minimum probability flow learning objective function for the full training
5 Results

100 images from the van Hateren dataset were chosen at random and reserved as a test set for evaluation of log likelihood. The test data was preprocessed in an identical fashion to the training data. Unless otherwise noted, log likelihood is estimated on the same set of 100 patches drawn from the test images, using Hamiltonian annealed importance sampling with $N = 100,000$ intermediate distributions, and 200 particles. This procedure takes about 170 seconds for the 36 PCA component analysis models tested below. The generative models take approximately 4 hours, because models with unmarginalized auxiliary variables require one full HAIS run for each test datapoint.

5.1 Validating Hamiltonian annealed importance sampling

The log likelihood of the test data can be analytically computed for three of the models outlined above: linear generative with Gaussian prior (Section 3, model 1a), and product of experts with a complete representation ($M = L$) for both Laplace and Student’s t experts (Section 3, model 3). Figures 2, 3, and 4 show the convergence of Hamiltonian annealed importance sampling, with 200 particles, for each of these three models as a function of the number $N$ of intermediate distributions. Note that the Student’s t expert is a pathological case for sampling based techniques, as for several of the learned $\lambda_l$ even the first moment of the Student’s t-distribution was infinite.

Additionally, for all of the generative models, if $\Phi = 0$
and the log likelihood $L$ has a simple form that can be used to directly verify the estimate computed via HAIS. We performed this sanity check on all generative models, and found the HAIS estimated log likelihood converged to the true log likelihood in all cases.

5.2 Speed of convergence

In order to demonstrate the improved performance of HAIS, we compare against two alternate AIS learning methods. First, we compare to AIS with transition distributions $T_n(x_{n+1}|x_n)$ consisting of a Gaussian ($\sigma_{\text{diffusion}} = 0.1$) proposal distribution and Metropolis-Hastings rejection rules. Second, we compare to AIS with a single Hamiltonian leapfrog step per intermediate distribution $\pi_n(x_n)$, and unit norm isotropic Gaussian momentum. Unlike in HAIS however, in this case we randomize the momenta before each update step, rather than allowing them to remain consistent across intermediate transitions. As can be seen in Figures 2 and 3, HAIS requires fewer intermediate distributions by an order of magnitude or more.

5.3 Model size

By training models of different sizes and then using HAIS to compute their likelihood, we are able to explore how each model behaves in this regard, and find that three have somewhat different characteristics, shown in Figure 5. The POE model with a Laplace expert has relatively poor performance and we have no evidence that it is able to overfit the training data; in fact, due to the relatively weak sparsity of the Laplace prior, we tend to think the only thing it can learn is oriented, band-pass functions that more finely tile the space of orientation and frequency. In contrast, the Student-t expert model rises quickly to a high level of performance, then overfits dramatically. Surprisingly, the mcRBM performs poorly with a number of auxiliary variables that is comparable to the best performing POE model. One explanation for this is that we are testing it in a regime where the major structures de-
Table 1: Average log likelihood for the test data under each of the models. The model ‘size’ column denotes the number of experts in the POE models, the sum of the mean and covariance units for the mcRBM, and the total number of latent variables in the generative models.

| Model                         | Size  | Log Likelihood |
|-------------------------------|-------|----------------|
| LIN. generative, Gaussian     | 36    | -49.15 ± 2.31  |
| LIN. generative, Laplace      | 36    | -42.85 ± 2.41  |
| POE, Laplace experts          | 144   | -41.54 ± 2.46  |
| mcRBM                        | 432   | -36.01 ± 2.57  |
| POE, Student’s t experts      | 144   | -34.01 ± 2.68  |
| Bilinear generative           | 98    | -32.69 ± 2.56  |

signed into the model are not of great benefit. That is, the mcRBM is primarily good at capturing long range image structures, which are not sufficiently present in our data because we use only 36 PCA components. Although for computational reasons we do not yet have evidence that the mcRBM can overfit our dataset, it likely does have that power. We expect that it will fare better against other models as we scale up to more sizeable images. Finally, we are excited by the superior performance of the bilinear generative model, which outperforms all other models with only a small number of auxiliary variables. We suspect this is mainly due to the high degree of flexibility of the sparse prior, whose parameters (through $\Theta$ and $\Psi$) are learned from the data. The fact that for a comparable number of “hidden units” it outperforms the mcRBM, which can be thought of as the bilinear generative model’s ‘analysis counterpart’, highlights the power of this model.

6 Conclusion
By improving upon the available methods for partition function estimation, we have made it possible to directly compare large probabilistic models in terms of the likelihoods they assign to data. This is a fundamental measure of the quality of a model – especially a model trained in terms of log likelihood – and one which is frequently neglected due to practical and computational limitations. It is our hope that the Hamiltonian annealed importance sampling technique presented here will lead to better and more relevant empirical comparisons between models.

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