Implicit Density Estimation by Local Moment Matching to Sample from Auto-Encoders

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Abstract
Recent work suggests that some auto-encoder variants do a good job of capturing the local manifold structure of the unknown data generating density. This paper contributes to the mathematical understanding of this phenomenon and helps define better justified sampling algorithms for deep learning based on auto-encoder variants. We consider an MCMC where each step samples from a Gaussian whose mean and covariance matrix depend on the previous state, defines through its asymptotic distribution a target density. First, we show that good choices (in the sense of consistency) for these mean and covariance functions are the local expected value and local covariance under that target density. Then we show that an auto-encoder with a contractive penalty captures estimators of these local moments in its reconstruction function and its Jacobian. A contribution of this work is thus a novel alternative to maximum-likelihood density estimation, which we call local moment matching. It also justifies a recently proposed sampling algorithm for the Contractive Auto-Encoder and extends it to the Denoising Auto-Encoder.

1 Introduction
Machine learning is about capturing aspects of the unknown distribution from which the observed data are sampled (the data-generating distribution). For many learning algorithms and in particular in manifold learning, the focus is on identifying the regions (sets of points) in the space of examples where this distribution concentrates, i.e., which configurations of the observed variables are plausible.

Unsupervised representation-learning algorithms attempt to characterize the data-generating distribution through the discovery of a set of features or latent variables whose variations capture most of the structure of the data-generating distribution. In recent years, a number of unsupervised feature learning algorithms have been proposed that are based on minimizing some form of reconstruction error, such as auto-encoder and sparse coding variants (Bengio et al., 2007; Ranzato et al., 2007; Jain and Seung, 2008; Vincent et al., 2008; Kavukcuoglu et al., 2009; Rifai et al., 2008).
An auto-encoder reconstructs the input through two stages, an encoder function $f$ (which outputs a learned representation $h = f(x)$ of an example $x$) and a decoder function $g$, such that $g(f(x)) \approx x$ for most $x$ sampled from the data-generating distribution. These feature learning algorithms can be stacked to form deeper and more abstract representations. There are arguments and much empirical evidence to suggest that when they are well-trained, such deep learning algorithms (Hinton et al., 2006; Bengio, 2009; Lee et al., 2009; Salakhutdinov and Hinton, 2009) can perform better than their shallow counterparts, both in terms of learning features for the purpose of classification tasks and for generating higher-quality samples.

Here we restrict ourselves to the case of continuous inputs $x \in \mathbb{R}^d$ with the data-generating distribution being associated with an unknown target density function, denoted $p$. Manifold learning algorithms assume that $p$ is concentrated in regions of lower dimension (Cayton, 2005; Narayanan and Mitter, 2010), i.e., the training examples are by definition located very close to these high-density manifolds. In that context, the core objective of manifold learning algorithms is to identify the local directions of variation, such that small movement in input space along these directions stays on or near the high-density manifold.

Some important questions remain concerning many of these feature learning algorithms. What is their training criterion learning about the input density? Do these algorithms implicitly learn about the whole density or only some aspect? If they capture the essence of the target density, then can we formalize that link and in particular exploit it to sample from the model? This would turn these algorithms into implicit density models, which only define a density indirectly, e.g., through a generative procedure that converges to it. These are the questions to which this paper contributes.

A crucial starting point for this work is very recent work (Rifai et al., 2012) proposing a sampling algorithm for Contractive Auto-Encoders, detailed in the next section. This algorithm was motivated on geometrical grounds, based on the observation and intuition that the leading singular vectors of the Jacobian of the encoder function specify those main directions of variation (i.e., the tangent plane of the manifold, the local directions that preserve the high-probability nature of training examples). Here we make a formal link between the target density and models minimizing reconstruction error through a contractive mapping, such as the Contractive Auto-Encoder (Rifai et al., 2011a) and the Denoising Auto-Encoder (Vincent et al., 2008). This allows us to justify sampling algorithms similar to that proposed by (Rifai et al., 2012), and apply these ideas to Denoising Auto-Encoders as well.

We define a novel alternative to maximum likelihood training, local moment matching, which we find that Contractive and Denoising Auto-Encoders perform. This is achieved by optimizing a criterion (such as a regularized reconstruction error) such that the optimal learned reconstruction function (and its derivatives) provide estimators of the local moments (and local derivatives) of the target density. These local moments can be used to define an implicit density, the asymptotic distribution of a particular Markov chain, which can also be seen as corresponding to an uncountable Gaussian mixture, with one Gaussian component at each possible location in input space.

The main novel contributions of this paper are the following. First, we show in Section 2 that the Denoising Auto-Encoder with small Gaussian perturbations and squared error loss is actually a Contractive Auto-Encoder whose contraction penalty is the mag-
agnitude of the perturbation, making the theory developed here applicable to both, and in particular extending the sampling procedure used for the Contractive Auto-Encoder to the Denoising Auto-Encoder as well. Second, we present in Section 3.3 consistency arguments justifying the use of the first and second estimated local moments to sample from a chain. Such a sampling algorithm has successfully been used in Rifai et al. (2012) to sample from a Contractive Auto-Encoder. With small enough steps, we show that the asymptotic distribution of the chain has the same similar (smoothed) first and second local moments as those estimated. Third, we show in Section 3.4 that non-parametrically minimizing reconstruction error with a contractive regularizer yields a reconstruction function whose value and Jacobian matrix estimate respectively the first and second local moments, i.e., up to a scaling factor, are the right functions to use in the Markov chain. Finally, although the sampling algorithm was already empirically verified in Rifai et al. (2012), we include in Section 4 an experimental validation for the case when the model is trained with the denoising criterion.

2 Contractive and Denoising Auto-Encoders

The Contractive Auto-Encoder or CAE (Rifai et al., 2011a) is trained to minimize the following regularized reconstruction error:

$$\mathcal{L}_{CAE} = \mathbb{E} \left[ \ell(x, r(x)) + \alpha \left\| \frac{\partial f(x)}{\partial x} \right\|_F^2 \right]$$  (1)

where $$r(x) = g(f(x))$$ and $$\|A\|_F^2$$ is the sum of the squares of the elements of $$A$$. Both the squared loss $$\ell(x, r) = \frac{1}{2} \|x - r\|^2$$ and the cross-entropy loss $$\ell(x, r) = -x \log r - (1 - x) \log(1 - r)$$ have been used, but here we focus our analysis on the squared loss because of the easier mathematical treatment it allows. Note that success of minimizing the above criterion strongly depends on the parametrization of $$f$$ and $$g$$ and in particular on the tied weights constraint used, with $$f(x) = \text{sigmoid}(W x + b)$$ and $$g(h) = \text{sigmoid}(W^T h + c)$$. The above regularizing term forces $$f$$ (as well as $$g$$, because of the tied weights) to be contractive, i.e., to have singular values less than 1. Larger values of $$\alpha$$ yielding more contraction (smaller singular values) where it hurts reconstruction error the least, i.e., in the local directions where there are only little or no variations in the data.

The Denoising Auto-Encoder or DAE (Vincent et al., 2008) is trained to minimize the following denoising criterion:

$$\mathcal{L}_{DAE} = \mathbb{E} \left[ \ell(x, r(N(x))) \right]$$  (2)

where $$N(x)$$ is a stochastic corruption of $$x$$ and the expectation is over the training distribution. Here we consider mostly the squared loss and Gaussian noise corruption, again because it is easier to handle them mathematically. In particular, if $$N(x) = x + \epsilon$$ with $$\epsilon$$ a small zero-mean isotropic Gaussian noise vector of variance $$\sigma^2$$, then a Taylor

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1Note that an auto-encoder without any regularization would tend to find many leading singular values near 1 in order to minimize reconstruction error, i.e., preserve input norm in all the directions of variation present in the data.
expansion around $x$ gives $r(x + \epsilon) \approx r(x) + \partial r(x) / \partial x \epsilon$, which when plugged into $L_{DAE}$ gives

$$L_{DAE} \approx \frac{1}{2} \left( x - \left( r(x) + \frac{\partial r(x)}{\partial x} \epsilon \right) \right)^T \left( x - \left( r(x) + \frac{\partial r(x)}{\partial x} \epsilon \right) \right)$$

$$= \frac{1}{2} \left( \mathbb{E} \left[ \|x - r(x)\|^2 \right] - 2 \mathbb{E}[\epsilon]^T \mathbb{E} \left[ \frac{\partial r(x)}{\partial x} (x - r(x)) \right] + \text{Tr} \left( \mathbb{E}[\epsilon \epsilon^T] \mathbb{E} \left[ \frac{\partial r(x)}{\partial x} \frac{\partial r(x)}{\partial x} \right] \right) \right)$$

$$= \frac{1}{2} \left( \mathbb{E} \left[ \|x - r(x)\|^2 \right] \right) + \sigma^2 \mathbb{E} \left[ \left\| \frac{\partial r(x)}{\partial x} \right\|^2 \right] \right)$$

(3)

where in the second line we used the independance of the noise from $x$ and properties of the trace, while in the last line we used $\mathbb{E} \left[ \epsilon \epsilon^T \right] = \sigma^2 I$ and $\mathbb{E}[\epsilon] = 0$ by definition of $\epsilon$. This derivation shows that the DAE is also a Contractive Auto-Encoder but where the contraction is imposed explicitly on the whole reconstruction function $r(\cdot) = g(f(\cdot))$ rather than on $f(\cdot)$ alone (and $g(\cdot)$ as a side effect of the parametrization).

### 2.1 A CAE Sampling Algorithm

Consider the following coupled Markov chains with elements $M_t$ and $X_t$ respectively:

$$M_{t+1} = \mu(X_t)$$

$$X_{t+1} = M_{t+1} + Z_{t+1}.$$  

(4)

where $M_t, X_t, \mu(X_t) \in \mathbb{R}^d$ and $Z_{t+1}$ is a sample from a zero-mean Gaussian with covariance $\Sigma(X_t)$.

The basic algorithm for sampling from the CAE, proposed in Rifai et al. (2012), is based on the above Markov chain operating in the space of hidden representation $h = f(x)$, with $\mu(h) = f(g(h))$ and $Z_{t+1} = \left( \frac{\partial f(x_t)}{\partial x_t} \right)^T \epsilon$, where $\epsilon$ is zero-mean isotropic Gaussian noise vector in $h$-space. This defines a chain of hidden representations $h_t$, and the corresponding chain of input-space samples is given by $x_t = g(h_t)$. Slightly better results are obtained with this $h$-space than with the corresponding $x$-space chain which defines $\mu(x) = g(f(x))$ and $Z_{t+1} = \left( \frac{\partial f(x_t)}{\partial x_t} \right)^T \epsilon$ where $\epsilon$ is zero-mean isotropic Gaussian noise in $x$-space. We conjecture that this advantage stems from the fact that moves in $h$-space are done in a more abstract, more non-linear space.

### 3 Local Moment Matching as an Alternative to Maximum Likelihood

#### 3.1 Previous Related Work

Well-known manifold learning (“embedding”) algorithms include Kernel PCA (Schölkopf et al., 1998), LLE (Roweis and Saul, 2000), Isomap (Tenenbaum et al., 2000), Laplacian Eigenmap (Belkin and Niyogi, 2003), Hessian Eigenmaps (Donoho and Grimes, 2003), Semidefinite Embedding (Weinberger and Saul, 2004), SNE (Hinton and Roweis...
and t-SNE (van der Maaten and Hinton 2008) that were primarily developed and used for data visualization through dimensionality reduction. These algorithms optimize the hidden representation associated with training points in order to best preserve certain properties of an input-space neighborhood graph.

The properties that we are interested in here are the local mean and local covariance. They are defined as the mean and covariance of a density restricted to a small neighborhood. For example, if we have lots of samples and we only consider the samples around a point \( x_0 \), the local mean at \( x_0 \) would be estimated by the mean of these neighbors and the local covariance at \( x_0 \) by the empirical covariance among these neighbors. There are previous machine learning algorithms that have been proposed to estimate these local first and second moments by actually using local neighbors (Brand 2003; Vincent and Bengio 2003; Bengio et al. 2006). In Manifold Parzen Windows (Vincent and Bengio 2003) this is literally achieved by estimating for each test point the empirical mean and empirical covariance of the neighboring points, with a regularization of the empirical covariance that sets a floor value for the eigenvalues of the covariance matrix. In Non-Local Manifold Parzen Windows (Bengio et al. 2006) the mean and covariance are predicted by a neural network that takes \( x_0 \) as input and outputs the estimated mean along with a basis for the leading eigenvectors and eigenvalues of the estimated covariance. The predictor is trained to maximize the likelihood of the near neighbors under the Gaussian with the predicted mean and covariance parameters. Both algorithms are manifold learning algorithms motivated by the objective to discover the local manifold structure of the data, and in particular predict the manifold tangent planes around any given test point. Besides the computational difficulty of having to find the \( k \) nearest neighbors of each training example, these algorithms, especially Manifold Parzen Windows, heavily rely on the smoothness of the target manifolds, so that there are enough samples to teach the model how and where the manifolds bend.

Note that the term local moment matching was already used by Gerber (1982) in an actuarial context to match moments of a discretized scalar distribution. Here we consider the more general problem of modeling a multivariate density from data, by estimating the first and second multivariate moments at every possible input point.

### 3.2 A Sampling Procedure From Local Moment Estimators

We first show that mild conditions suffice for the chain to converge\(^2\) and then that if local first and second moments have been estimated, then one can define a plausible sampling algorithm based on a Markov chain that exploits these local moments at each step.

**Convergence of the Chain**

This Markov chain \( X_1, X_2, \ldots, X_t, \ldots \) is precisely the one that samples a new point by sampling from the Gaussian with these local first and second moments:

\[
X_{t+1} \sim N(\mu(X_t), \Sigma(X_t))
\]  

\(^2\)This is also shown in Rifai et al. (2012).
as in Eq.(4), but where we propose to choose $\mu(X_t) - X_t$ proportional to the local mean at $x_0 = X_t$ minus $X_t$, and $\Sigma(X_t)$ proportional to the local covariance at $x_0 = X_t$. The functions $\mu(\cdot)$ and $\Sigma(\cdot)$ thus define a Markov chain.

Let us sketch a proof that it converges under mild hypotheses, using the decomposition into the chains of $M_t$’s and of $X_t$’s. Assuming that $\forall x$, $\mu(x) \in B$ for some bounded ball $B$, then $M_t \in B \ \forall t$. If we further assume that $\Sigma(X_t)$ is always full rank, then there is a non-zero probability of jumping from any $M_t \in B$ to any $M_{t+1} \in B$, which is sufficient for ergodicity of the chain and its convergence. Then if $M_t$’s converge, so do their noisy counterparts $X_t$’s.

**Uncountable Gaussian Mixture**

If the chain converges, let $\pi$ be the asymptotic distribution of the $X_t$’s. It is interesting to note that $\pi$ satisfies the operator equation

$$\pi(x) = \int \pi(\tilde{x}) \mathcal{N}(x; \mu(\tilde{x}), \Sigma(\tilde{x}))d\tilde{x}$$

where $\mathcal{N}(x; \mu(\tilde{x}), \Sigma(\tilde{x}))$ is the density of $x$ under a normal multivariate distribution with mean $\mu(\tilde{x})$ and covariance $\Sigma(\tilde{x})$. This can be seen as a kind of uncountable Gaussian mixture $\pi$ where the weight of each component $\tilde{x}$ is given by $\pi(\tilde{x})$ itself and the functions $\mu(\cdot)$ and $\Sigma(\cdot)$ specify the mean and covariance of each component.

**3.3 Consistency**

From the point of view of learning, what we would like is that the $\mu(\cdot)$ and $\Sigma(\cdot)$ functions used in a sampling chain such as Eq. (5) be such that they yield an asymptotic density $\pi$ close to some target density $p$. Because the Markov chain makes noisy finite steps, one would expect that the best one can hope for is that $\pi$ be a smooth approximation of $p$.

What we show below is that, in the asymptotic regime of very small steps (i.e. $\Sigma(x)$ is small in magnitude), a good choice is just the intuitive one, where $\mu(x_0) - x_0 \propto \mathbb{E}[x|x_0] - x_0$ and $\Sigma(x_0) \propto \text{Cov}(x|x_0)$.

For this purpose, we formally define the local density $p_\delta(x|x_0)$ of points $x$ in the $\delta$-neighborhood of an $x_0$, as

$$p_\delta(x|x_0) = \frac{p(x)1_{||x-x_0||<\delta}}{Z(x_0)}$$

where $Z(x_0)$ is the appropriate normalizing constant. Then we respectively define the local mean and covariance around $x_0$ as simply being

$$m_0 \overset{def}{=} \mathbb{E}[x|x_0] = \int xp_\delta(x|x_0)dx$$

$$C_0 \overset{def}{=} \text{Cov}(x|x_0) = \int (x - m_0)(x - m_0)^T p_\delta(x|x_0)dx.$$  

Note that we have two scales here, the scale $\delta$ at which we take the local mean and covariance, and the scale $\sigma = ||\Sigma(x_0)||$ of the Markov chain steps. To prove
consistency we assume here that \( \sigma \ll \delta \) and that both are small. Furthermore, we assume that \( \mu \) and \( \Sigma \) are somehow calibrated, so that the steps \( \mu(x) - x \) are comparable in size to \( \sigma \). This means that \( ||\mu(x) - x|| \ll \delta \), which we use below.

We want to compute the local mean obtained when we follow the Markov chain, i.e., in Eq. (7) we choose a \( p \) equal to \( \pi \) (which is defined in Eq. (6)), and we obtain the following:

\[
m_{\pi} \overset{\text{def}}{=} E_{\pi}[x|x_0] = \frac{1}{Z(x_0)} \int x \int \tilde{x} p(\tilde{x}) \mathcal{N}(x; \mu(\tilde{x}), \Sigma(\tilde{x})) d\tilde{x} \ 1_{||x-x_0||<\delta} dx
\]

\[
= \frac{1}{Z(x_0)} \int \tilde{x} p(\tilde{x}) \int x \mathcal{N}(x; \mu(\tilde{x}), \Sigma(\tilde{x})) dx d\tilde{x}. \tag{9}
\]

Because the Gaussian sample of the inner integral must be in a small region inside the \( \delta \)-ball, the inner integral is approximately the Gaussian mean if \( \mu(\tilde{x}) \) is in the \( \delta \)-ball, and 0 otherwise:

\[
\int 1_{||x-x_0||<\delta} x \mathcal{N}(x; \mu(\tilde{x}), \Sigma(\tilde{x})) dx \approx \mu(\tilde{x}) 1_{||\mu(\tilde{x})-x_0||<\delta}. \tag{10}
\]

which gives

\[
m_{\pi} \approx \int \mu(\tilde{x}) \frac{p(\tilde{x})}{Z(x_0)} 1_{||\mu(\tilde{x})-x_0||<\delta} d\tilde{x}. \tag{11}
\]

Now we use the above assumptions, which give \( ||\mu(x) - x|| \ll \delta \), to conclude that integrating under the region defined by \( 1_{||\mu(\tilde{x})-x_0||<\delta} \) is equivalent to integrating under the region defined by \( 1_{||\tilde{x}-x_0||<\delta} \). Hence the above approximation is rewritten

\[
m_{\pi} \approx \int \tilde{x} \frac{p(\tilde{x})}{Z(x_0)} 1_{||\tilde{x}-x_0||<\delta} \mu(\tilde{x}) d\tilde{x} \tag{12}
\]

which by the definition of \( E[\cdot|x_0] \) gives the final result:

\[
m_{\pi} \approx \mathbb{E}[\mu(x)|x_0], \tag{13}
\]

It means that the local mean under the small-steps Markov chain is a local mean of the chain’s \( \mu \)’s. This justifies choosing \( \mu(x) \) equal to the local mean of the target density to be represented by the chain, so that the Markov chain will yield an asymptotic distribution that has local moments that are close but smooth versions of those of the target density.

A similar result can be shown for the covariance by observing that the \( x \) term in Eq. (10) produced the first moment of the Gaussian and that the same reasoning would apply with \( xx^T \) instead.

Alternatively, we can follow a shortened version of the above starting with

\[
C_{\pi} \overset{\text{def}}{=} E_{\pi}[(x - m_{\pi})(x - m_{\pi})^T|x_0] \tag{14}
\]

\[
= \frac{1}{Z(x_0)} \int \tilde{x} p(\tilde{x}) \int (x - m_{\pi})(x - m_{\pi})^T \mathcal{N}(x; \mu(\tilde{x}), \Sigma(\tilde{x})) dx d\tilde{x}. \tag{15}
\]
where
\[ \int_{||x-x_0||<\delta} (x-m_\pi)(x-m_\pi)^T \mathcal{N}(x; \mu(\tilde{x}), \Sigma(\tilde{x})) dx \approx (\Sigma(\tilde{x}) + (\mu(\tilde{x}) - m_\pi)(\mu(\tilde{x}) - m_\pi)^T) 1_{||\mu(\tilde{x})-x_0||<\delta}. \] (16)

By construction the magnitude of the covariance \( \Sigma(\tilde{x}) \) was made very small, so the following term vanishes
\[ \int p(\tilde{x}) \frac{1_{||\tilde{x}-x_0||<\delta \Sigma(\tilde{x})}}{Z(x_0)} d\tilde{x} \to 0 \] (18)
and we are left with the desired result
\[ C_\pi \approx \mathbb{E} \left[ (\mu(x) - m_\pi)(\mu(x) - m_\pi)^T | x_0 \right]. \] (19)

### 3.4 Local Moment Matching By Minimizing Regularized Reconstruction Error

We consider here an alternative to using nearest neighbors for estimating local moments, by showing that minimizing reconstruction error with a contractive penalty yields estimators of the local mean and covariance.

We start from a training criterion similar to the CAE’s but penalizing the contraction of the whole auto-encoder’s reconstruction function, which is also equivalent to the DAE’s training criterion in the case of small Gaussian corruption noise (as shown in Eq. (3)):
\[ L_{\text{global}} = \int p(x_0) \left( \|x_0 - r(x_0)\|^2 + \alpha \left\| \frac{\partial r(x_0)}{\partial x_0} \right\|_F^2 \right) dx_0 \] (20)

where \( p \) is the target or training distribution. We prove that in a non-parametric setting (where \( r \) is completely free), the optimal \( r \) is such that the local mean \( m_0 \) is estimated by \( r_0 \) defined by \( r_0 \overset{\text{def}}{=} r(x_0) \) while the local covariance \( C_0 \) is estimated by \( J_0 \) defined by \( J_0 \) defined by \( \frac{\partial r}{\partial x}|_{x_0} \).

To find out what the auto-encoder estimates we follow an approach which has already been used, e.g., to show that minimizing squared prediction error \( \mathbb{E}[(f(X) - Y)^2] \) is equivalent to estimating the conditional expectation, \( f(X) \to \mathbb{E}[Y|X] \). For this purpose we consider an asymptotic and non-parametric setting corresponding to the limit where the number of examples goes to infinity (we actually minimize the expected error) and the capacity goes to infinity: we allow the value \( r_0 \) and the derivative \( J_0 \) of \( r \) at every point \( x_0 \), to be different, i.e., we “parametrize” \( r(x) \) in every neighborhood around \( x_0 \) by
\[ r(x) = r(x_0) + \frac{\partial r}{\partial x}|_{x_0} (x - x_0) = r_0 + J_0(x - x_0) \] (21)

In practice, i.e., the parametric case, there is no guarantee that the estimator be symmetric, but this is easily fixed by symmetrizing it, i.e., using \( \frac{J_0 + J_0^T}{2} \).
which is like a Taylor expansion only valid in the neighborhood of \(x\)'s around \(x_0\), but where we actually consider \(r_0\) and \(J_0\) to be parameters free to be chosen separately for each \(x_0\).

Armed with this non-parametric formulation, we consider an infinity of such neighborhoods and the local density \(p_\delta(x|x_0)\) (Eq. 7) which approaches a Dirac delta function in the limit of \(\delta \to 0\), and we rewrite \(L_{\text{global}}\) as follows:

\[
L_{\text{global}} = \lim_{\delta \to 0} \int p(x_0) \left( \left( \int_x ||x - r(x)||^2 p_\delta(x|x_0) dx \right) + \alpha \left\| \frac{\partial r(x_0)}{\partial x_0} \right\|^2_F \right) dx_0.
\]

The reason for choosing \(p_\delta(x|x_0)\) that turns into a Dirac is that the expectations of \(x\) and \(xx^T\) arising in the above inner integral will give rise to the local mean \(m_0\) and local covariance \(C_0\). If in the above equation we define \(r(x)\) non-parametrically (as per Eq. (21)), the minimum can be achieved by considering the separate minimization in each \(x_0\) neighborhood with respect to \(r_0\) and \(J_0\). We can express the local contribution to the loss at \(x_0\) as

\[
L_{\text{local}}(x_0, \delta) = \int_x ||x - (r_0 + J_0(x - x_0))||^2 p_\delta(x|x_0) dx + \alpha \left\| J_0 \right\|^2_F
\]

so that

\[
L_{\text{global}} = \lim_{\delta \to 0} \int p(x_0) L_{\text{local}}(x_0, \delta) dx_0.
\]

We take the gradient of the local loss with respect to \(r_0\) and \(J_0\) and set it to 0 (detailed derivation in Appendix) to get

\[
\begin{align*}
\frac{\partial L_{\text{local}}(x_0, \delta)}{\partial r_0} &= 2(r_0 - m_0) + 2J_0(m_0 - x_0) \\
\frac{\partial L_{\text{local}}(x_0, \delta)}{\partial J_0} &= 2\alpha J_0 - 2 \left( R - m_0x_0^T - r_0(m_0 - x_0)^T \right) \\
&\quad + 2J_0 \left( R - m_0x_0^T - x_0m_0^T + x_0x_0^T \right).
\end{align*}
\]

Solving these equations (detailed derivation in Appendix) gives us the solutions

\[
\begin{align*}
r_0 &= (I - J_0)m_0 + J_0x_0 \\
J_0 &= C_0(\alpha I + C_0)^{-1}.
\end{align*}
\]

Note that these quantities \(m_0, C_0\) are defined through \(p_\delta(x|x_0)\) so they depend implicitly on \(\delta\) and we should consider what happens when we take the limit \(\delta \to 0\).

In particular, when \(\delta \to 0\) we have that \(\|C_0\| \to 0\) and we can see from the solutions (26) that this forces \(\|J_0\| \to 0\). In a practical numerical application, we fix \(\delta > 0\) to be small and it becomes interesting to see how these quantities relate asymptotically (in terms of \(\delta\) decreasing). In such a situation, we have the following
asymptotically:

\[ r_0 \approx m_0 \]
\[ J_0 \approx \alpha^{-1} C_0. \]  \hspace{1cm} (27)

Thus, we have proved that the value of the reconstruction and its Jacobian immediately give us estimators of the local mean and local covariance, respectively.

4 Experimental Validation

In the above analysis we have considered the limit of a non-parametric case with an infinite amount of data. In that limit, unsurprisingly, reconstruction is perfect, i.e.,

\[ r(x) \rightarrow x, \quad \mathbb{E}[x|x_0] \rightarrow x_0, \quad \text{and} \quad \| \frac{\partial r(x)}{\partial x} \|_F \rightarrow 0 \quad \text{and} \quad \| \text{Cov}(x|x_0) \|_F \rightarrow 0, \]

at a speed that depends on the scale \( \delta \), as we have seen above. We do not care so much about the magnitudes but instead care about the directions indicated by \( r(x) - x \) (which indicate where to look for increases in probability density) and by the singular vectors and relative singular values of \( \frac{\partial r(x)}{\partial x} \), which indicate what directions preserve high density. In a practical sampling algorithm such as described in Section 2.1 one wants to take non-infinitesimal steps. Furthermore, in the practical experiments of Rifai et al. (2012), in order to get good generalization with a limited training set, one typically works with a parametrized model which cannot perfectly reconstruct the training set (but can generalize). This means that the learned reconstruction is not equal to the input, even on training examples, and nor is the Jacobian of the reconstruction function tiny (as it would be in the asymptotic non-parametric case). The mathematical link between the two situations needs to be clarified in future work, but a heuristic approach which we found to work well is the following: control the scale of the Markov chain with a hyper-parameter that sets the magnitude of the Gaussian noise (the variance of \( \epsilon \) in Section 2.1). That hyper-parameter can be optimized by visual inspection or by estimating the log-likelihood of the samples, using a technique introduced in Breuleux et al. (2011) and also used in Rifai et al. (2012). The basic idea is to generate many samples from the model, train a non-parametric density estimator (Parzen Windows) using these samples as a training set, and evaluate the log-likelihood of the test set using that density estimator. If the sample generator does not mix well, then some test examples will be badly covered (far from any of the generated samples), thus incurring a high price in log-likelihood. If the generator mixes well but smoothes too much the true density, then the automatically selected bandwidth of the Parzen Windows will be chosen larger, incurring again a penalty in test log-likelihood.

In Fig. 4 we show samples of DAEs trained and sampled similarly as in Rifai et al. (2012) on both MNIST digits images and the Toronto Face Dataset (TFD) (Susskind et al., 2010). These results and those already obtained in Rifai et al. (2012) confirm that the auto-encoder trained either as a CAE or a DAE estimates local moments that can be followed in a Markov chain to generate likely-looking samples (and which have been shown quantitatively to be of high quality in Rifai et al. (2012)).

Here, to avoid confusion with the overloaded \( \sim \) notation for sampling, we instead use the \( \equiv \) notation to denote that the ratio of any coefficient on the left with its corresponding coefficient on the right goes to 1 as \( \delta \rightarrow 0 \).
Figure 1: Samples generated by a DAE trained on TFD (top 2 rows) and MNIST (bottom 2 rows).

5 Conclusion

This paper has contributed a novel approach to modeling densities: indirectly, through the estimation of local moments. It has shown that local moments can be estimated by auto-encoders with contractive regularization. It has justified a sampling algorithm based on a simple Markov chain when estimators of the local moments are available. Whereas auto-encoders are unsupervised learning algorithms that have been known for many decades, it has never been clear if they captured everything that can be captured from a distribution. For the first time, this paper presents a theoretical justification showing that they do implicitly perform density estimation (provided some appropriate regularization is used, and assuming the training criterion can be minimized). This provides a more solid footing to the recently proposed algorithm for sampling Contractive Auto-Encoders (Rifai et al., 2012) and opens the door to other related learning and sampling algorithms. In particular, it shows that this sampling algorithm can be applied to Denoising Auto-Encoders as well.

An interesting advantage of modeling data through such training criteria is that there is no need to estimate an untractable partition function or its gradient, and that there is no difficult inference problem associated with these types of models either. Future work following up on this paper should try to answer the more difficult mathematical questions of what happens (e.g., with the consistency arguments presented here) if the Markov chain steps are not tiny, and when we consider a learner that has parametric constraints, rather than the asymptotic non-parametric limit considered here. We believe that the approach presented here can also be applied to energy-based models (for which the free energy can be computed), and that the local moments are directly related to the first and second derivative of the estimated density. Future work should clarify that relationship, possibly giving rise to new sampling algorithms for energy-based models (since we have shown here that one can sample from the estimated density if one can compute the local moments). Finally, it would be interesting to extend this work in the direction of analysis that explicitly takes into account the decomposition of the auto-encoder into an encoder and a decoder. Indeed, we have found experimentally that sampling in the representation space gives better results than sampling in the original input space, but a more solid mathematical treatment of such algorithms is still missing.
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A Derivation of the local training criterion gradient

We want to obtain the derivative of the local training criterion,

\[ L_{\text{local}} = \lim_{\delta \to 0} \int_x \| x - (r_0 + J_0(x - x_0)) \|^2 \tilde{p}_\delta(x|x_0) dx + \alpha \| J_0 \|^2_F. \]  

(28)

We use the definitions

\[ \mu_0 = \mathbb{E}[x|x_0] = \int_x x \tilde{p}_\delta(x|x_0) dx \]
\[ R_0 = \mathbb{E}[xx^T|x_0] \]
\[ C_0 = \text{Cov}(x|x_0) = \mathbb{E}[(x - \mu_0)(x - \mu_0)^T|x_0] = R - \mu_0 \mu_0^T. \]
We first expand the expected square error:

\[ \text{MSE} = \mathbb{E}[|x - (r_0 + J_0(x - x_0))|^2|x_0] = \mathbb{E}[(x - (r_0 + J_0(x - x_0))(x - (r_0 + J_0(x - x_0))^T] \]

\[ = \mathbb{E}[(x - r_0)(x - r_0)^T - 2(x - r_0)^T J_0(x - x_0)] \]

\[ = \mathbb{E}[(x - x_0)^T J_0^T J_0(x - x_0)]. \]

Differentiating this with respect to \( r_0 \) yields

\[ \frac{\partial \text{MSE}}{\partial r_0} = -2(\mu_0 - r_0) + 2J_0(\mu - x_0) \]

corresponding to Eq.(25) of the paper.

For differentiating with respect to \( J_0 \), we use the trace properties

\[ ||A||_F^2 = \text{Tr}(AA^T) \]

\[ \text{Tr}(ABC) = \text{Tr}(BCA) \]

\[ \frac{\partial \text{Tr}(A^T XAZ)}{\partial A} = XAZ + X^T AZ^T \]

\[ \frac{\partial \text{Tr}(XA)}{\partial A} = X^T \]

\[ \frac{\partial \text{Tr}(X^T A^T)}{\partial A} = X. \]

We obtain for the regularizer,

\[ \frac{\partial \alpha ||J_0||_F^2}{\partial J_0} = 2\alpha J_0 \]

and for the MSE:

\[ \frac{\partial \text{MSE}}{\partial J_0} = -2\mathbb{E} \left[ \frac{\partial}{\partial J_0} \text{tr}(J_0(x - x_0)(x - r_0)^T) \right] + \mathbb{E} \left[ \frac{\partial}{\partial J_0} \text{tr}(J_0^T J_0(x - x_0)(x - x_0)^T) \right] \]

\[ = -2\mathbb{E} \left[ (x - r_0)(x - x_0)^T \right] + 2J_0\mathbb{E} \left[ (x - x_0)(x - x_0)^T \right] \]

\[ = -2(R - \mu_0 x_0^T - r_0(\mu_0 - x_0)^T) + 2J_0 \left( R - \mu_0 x_0^T - x_0\mu_0^T + x_0 x_0^T \right) \]

B  Detailed derivation of the minimizers of the local training criterion

Starting with \( r_0 \), we solve when the gradient is 0 to obtain

\[ \frac{\partial \text{MSE}}{\partial r_0} = (\mu - r_0) - J_0(\mu - x_0) = 0 \]

\[ \mu - r_0 = J_0(\mu - x_0) \]

\[ r_0 = \mu - J_0(\mu - x_0) \]

\[ r_0 = (I - J_0)\mu + J_0x_0. \]
Substituting that value for \( r_0 \) into the expression for the gradient with respect to \( J_0 \), we get

\[
\frac{\partial \text{MSE}}{\partial J_0} = -2 \left( R - \mu_0 x_0^T - (\mu_0 - J_0(\mu_0 - x_0))(\mu_0 - x_0)^T \right) + 2J_0 \left( R - \mu_0 x_0^T - x_0 \mu_0^T + x_0 x_0^T \right)
\]

Adding the regularizer term and setting the gradient to 0, we get

\[
\frac{\partial (\text{MSE} + \alpha \|J_0\|^2_F)}{\partial J_0} = -2(I - J_0)C_0 + 2\alpha J_0 = 0
\]

which altogether gives us Eq.(26) from the main text:

\[
\begin{align*}
    r_0 &= (I - J_0)\mu_0 + J_0 x_0 \\
    J_0 &= \alpha I + C_0^{-1} C_0
\end{align*}
\]

Note that we can also solve for \( \mu_0 \)

\[
\mu = (I - J_0)^{-1} (r_0 - J_0 x_0)
\]

and for \( C_0 \):

\[
\begin{align*}
(I - J_0)C_0 &= \alpha J_0 \\
C_0 &= \alpha (I - J_0)^{-1} J_0
\end{align*}
\]

However, we still have to take the limit as \( \delta \to 0 \). Noting that the magnitude of \( C_0 \) goes to 0 as \( \delta \to 0 \), it means that \( J_0 \) also goes to 0 in magnitude. Plugging in the above equations gives the final results:

\[
\begin{align*}
r_0 &= \mu_0 \\
C_0 &= J_0
\end{align*}
\]