Denoising Autoencoders

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The idea of a denoising autoencoder [Vincent et al., 2010] is to recover a data point $x \sim p$ given a noisy observation, for example $\tilde{x} = x + \varepsilon$ where $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$. These models were initially introduced to provide an objective for unsupervised pre-training of deep networks. While that training methodology has become less relevant over time, the denoising autoencoder has been adapted as a means of constructing generative models [Bengio et al., 2013] leading to recent spectacular results [Ho et al., 2020].

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Formally, let $x \sim p$, $\tilde{x} \sim p(\cdot|x)$, which together define a joint distribution $p(x, \tilde{x}) = p(\tilde{x}|x)p(x)$. A denoising autoencoder is a model of the posterior distribution

$$p(x|\tilde{x}) = \frac{p(\tilde{x}|x)p(x)}{\int_{\mathcal{X}} p(\tilde{x}|y)p(y)\,dy}. \tag{1}$$

Specifically, we model $p_\theta(x|\tilde{x}) = \mathcal{N}(g_\theta(f_\varphi(\tilde{x})), \sigma^2 I)$, where $f_\varphi : \mathcal{X} \to \mathcal{Z}$ and $g_\theta : \mathcal{Z} \to \mathcal{X}$ are neural networks work parameters φ and θ respectively. Fitting this model using the maximum likelihood estimator leads to the reconstruction objective

$$\theta^*, \varphi^* = \underset{\theta,\varphi}{\arg\min} \mathop{\mathbb{E}}_{(x,\tilde{x})\sim p} \|x - g_\theta(f_\varphi(\tilde{x}))\|^2. \tag{2}$$

We can think of the composition $g_\theta \circ f_\varphi(\tilde{x})$ as projecting a corrupted data point $\tilde{x} \sim p(\cdot|x)$ back onto the support of p (the data manifold) and we can think of the latent space $\mathcal{Z}$ as a coordinate system on the data manifold. Previewing the work of Bengio et al. [2013] and [Ho et al., 2020], we can imagine constructing a Markov chain of denoising autoencoders that guides us from samples $x_0 = \varepsilon \sim \mathcal{N}(0, I)$ through a sequence of denoising operations $x_s \sim p_{s,\theta}(\cdot|x_{s-1})$ to produce a final sample x_t distributed approximately according to p.

Denoising Score Matching

We can use a denoising autoencoder to construct an explicit score matching estimator, following Vincent [2011]. Recall that the score function estimator given by minimization of the Fisher divergence

$$\hat{\theta} = \underset{\theta}{\arg\min} \mathop{\mathbb{E}}_{x\sim p} \left[\frac{1}{2}\|s_\theta(x) - \nabla_x \log p(x)\|_2^2\right]. \tag{3}$$

This expression requires that we evaluate gradients of the unknown density $p(x)$, which are not accessible to us. Previously, we saw an implicit score matching estimator [Hyvärinen, 2005] for estimating this quantity using samples. Denoising autoencoders offer another alternative.

Suppose we are willing to settle for samples of an estimate of the density $p(x)$ given by the noisy distribution

$$q(\tilde{x}) = \int_{\mathcal{X}} p(\tilde{x}|x)p(x)\,dx. \tag{4}$$

For example, if $p(\tilde{x}|x) = p_\sigma(\tilde{x}|x) = \mathcal{N}(\tilde{x}; x, \sigma^2 I)$ for small variance σ^2, then $q(\tilde{x}) = q_\sigma(\tilde{x})$ is a Gaussian convolution corresponding to a mildly-smoothed version of $p(x)$, with $D(q_\sigma \parallel p) \to 0$ as $\sigma^2 \to 0$. Suppose we want to calculate the score matching estimator for this noisy distribution q_σ. The following proposition shows that this is much easier than score matching with p.

Proposition 1. *(Denoising Score Matching) [Vincent, 2011]*

$$\arg\min_\theta \mathop{\mathbb{E}}_{\tilde{x}\sim q_\sigma}\left[\frac{1}{2}\|s_\theta(\tilde{x}) - \nabla_{\tilde{x}} \log q_\sigma(\tilde{x})\|_2^2\right] = \arg\min_\theta \mathop{\mathbb{E}}_{\substack{x\sim p\\ \tilde{x}\sim p_\sigma(\cdot|x)}}\left[\frac{1}{2}\|s_\theta(\tilde{x}) - \nabla_{\tilde{x}} \log p_\sigma(\tilde{x}|x)\|_2^2\right]. \tag{5}$$

Proof. Expanding the quadratic and dropping the constant term, we have

$$\arg\min_\theta \mathop{\mathbb{E}}_{\tilde{x}\sim q_\sigma}\left[\frac{1}{2}\|s_\theta(\tilde{x}) - \nabla_{\tilde{x}} \log q_\sigma(\tilde{x})\|_2^2\right] = \arg\min_\theta \mathop{\mathbb{E}}_{\tilde{x}\sim q_\sigma}\left[\frac{1}{2}\|s_\theta(\tilde{x})\|^2 - s_\theta(\tilde{x})^T\nabla_{\tilde{x}} \log q_\sigma(\tilde{x})\right]. \tag{6}$$

And with routine algebraic calcuations,

$$\begin{aligned}
\mathop{\mathbb{E}}_{\tilde{x}\sim q_\sigma}\left[s_\theta(\tilde{x})^T\nabla_{\tilde{x}} \log q_\sigma(\tilde{x})\right] &= \int_{\mathcal{X}} s_\theta(\tilde{x})^T\nabla_{\tilde{x}} \log q_\sigma(\tilde{x}) q_\sigma(\tilde{x})\,d\tilde{x} && (7)\\
&= \int_{\mathcal{X}} s_\theta(\tilde{x})^T\nabla_{\tilde{x}} q_\sigma(\tilde{x})\,d\tilde{x} && (8)\\
&= \int_{\mathcal{X}} s_\theta(\tilde{x})^T\nabla_{\tilde{x}} \int_{\mathcal{X}} p(x)p_\sigma(\tilde{x}|x)\,dx\,d\tilde{x} && (9)\\
&= \int_{\mathcal{X}} s_\theta(\tilde{x})^T \int_{\mathcal{X}} \nabla_{\tilde{x}} p(x)p_\sigma(\tilde{x}|x)\,dx\,d\tilde{x} && (10)\\
&= \int_{\mathcal{X}} s_\theta(\tilde{x})^T \int_{\mathcal{X}} p(x)p_\sigma(\tilde{x}|x)\nabla_{\tilde{x}} \log p_\sigma(\tilde{x}|x)\,dx\,d\tilde{x} && (11)\\
&= \iint_{\mathcal{X}\times\mathcal{X}} p(x)p_\sigma(\tilde{x}|x)s_\theta(\tilde{x})^T\nabla_{\tilde{x}} \log p_\sigma(\tilde{x}|x)\,d(x,\tilde{x}) && (12)\\
&= \mathop{\mathbb{E}}_{\substack{x\sim p\\ \tilde{x}\sim p_\sigma(\tilde{x}|x)}}\left[s_\theta(\tilde{x})^T\nabla_{\tilde{x}} \log p_\sigma(\tilde{x}|x)\right]. && (13)
\end{aligned}$$

From this and Equation 6, completing the square gives us

$$\begin{aligned}
&\arg\min_\theta \mathop{\mathbb{E}}_{\tilde{x}\sim q_\sigma}\left[\frac{1}{2}\|s_\theta(\tilde{x})\|^2 - s_\theta(\tilde{x})^T\nabla_{\tilde{x}} \log q_\sigma(\tilde{x})\right] && (14)\\
&= \arg\min_\theta \mathop{\mathbb{E}}_{\substack{x\sim p\\ \tilde{x}\sim p_\sigma(\tilde{x}|x)}}\left[\frac{1}{2}\|s_\theta(\tilde{x})\|^2 - s_\theta(\tilde{x})^T\nabla_{\tilde{x}} \log p_\sigma(\tilde{x}|x)\right] && (15)\\
&= \arg\min_\theta \mathop{\mathbb{E}}_{\substack{x\sim p\\ \tilde{x}\sim p_\sigma(\tilde{x}|x)}}\left[\frac{1}{2}\|s_\theta(\tilde{x})\|^2 - s_\theta(\tilde{x})^T\nabla_{\tilde{x}} \log p_\sigma(\tilde{x}|x) + \frac{1}{2}\|\nabla_{\tilde{x}} \log p_\sigma(\tilde{x}|x)\|^2\right] && (16)\\
&= \arg\min_\theta \mathop{\mathbb{E}}_{\substack{x\sim p\\ \tilde{x}\sim p_\sigma(\cdot|x)}}\left[\frac{1}{2}\|s_\theta(\tilde{x}) - \nabla_{\tilde{x}} \log p_\sigma(\tilde{x}|x)\|_2^2\right] && (17)
\end{aligned}$$

$\square$

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