TTIC 31230, Fundamentals of Deep Learning

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Variational Auto-Encoders (VAEs)

Widely Used VAEs

Diffusion Models: A diffusion model is a hierarchical Gaussian VAE.

Vector Quantized VAEs: A VQ-VAE defines $P_{\mathrm{enc}}(z|y)$ in terms of vector quantization analogous to K-means clustering. VQ-VAEs provide a translation from continuous data, such as images, to token data that can be modelled with a transformer. This is done in GPT-4o.

Auto-Regressive Language Models: An auto-regressive language model, such as a transformer, is mathematically equivalent to a hierarchical VAE.

VAEs

A variational autoencoder (VAE) is defined by three parts:

- An encoder distribution $P_{\mathrm{enc}}(z|y)$.

- A decoder distribution $P_{\mathrm{dec}}(y|z)$

- A "prior" distribution $P_{\mathrm{pri}}(z)$

VAE generation uses $P_{\mathrm{pri}}(z)$ and $P_{\mathrm{dec}}(y|z)$.

VAE training uses the encoder $P_{\mathrm{enc}}(z|y)$.

Two Joint Distributions

A VAE defines two joint distributions on y and z, namely $P_{\mathrm{gen}}(y,z)$ and $P_{\mathrm{enc}}(y,z)$ defined by

$$P_{\mathrm{gen}}(y,z) = P_{\mathrm{pri}}(z)P_{\mathrm{dec}}(y|z)$$

$$P_{\mathrm{enc}}(y,z) = \mathrm{Pop}(y)P_{\mathrm{enc}}(z|y)$$

Training the Generator

Fix the encoder arbitrarily and train P_{gen} by cross entropy.

$$\text{gen}^* = \underset{\text{gen}}{\text{argmin}}\ E_{(y,z)\sim P_{\text{enc}}(y,z)}\left[-\ln P_{\text{gen}}(y,z)\right]$$

Under universality we have $P_{\text{gen}^*} = P_{\text{enc}}$ and hence the generator distribution on y defined by gen^* matches the population distribution.

In a diffusion model the encoder just adds noise. The encoder is not trained.

The ELBO Loss

$$\mathrm{Pop}(y) \;=\; \frac{\mathrm{Pop}(y)P_{\mathrm{enc}}(z|y)}{P_{\mathrm{enc}}(z|y)} \;=\; \frac{P_{\mathrm{enc}}(y,z)}{P_{\mathrm{enc}}(z|y)}$$

$$E_{(y,z)\sim P_{\mathrm{enc}}}\left[-\ln \mathrm{Pop}(y)\right] \;=\; E_{(y,z)\sim P_{\mathrm{enc}}}\left[-\ln \frac{P_{\mathrm{enc}}(y,z)}{P_{\mathrm{enc}}(z|y)}\right]$$

$$H(y) \;\leq\; E_{(y,z)\sim P_{\mathrm{enc}}}\left[-\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{enc}}(z|y)}\right]$$

The right hand side of the last line is called the **ELBO Loss**.

The Variational Bayes Interpretation

The generator is interpreted as a Bayesian model where y is evidence for z.

$$
\begin{aligned}
\ln P_{\mathrm{gen}}(y) &= \ln \frac{P_{\mathrm{gen}}(y)P_{\mathrm{gen}}(z|y)}{P_{\mathrm{gen}}(z|y)} \\
&= E_{z\sim P_{\mathrm{enc}}(z|y)}\left[\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{gen}}(z|y)}\right] \\
&\geq E_{z\sim P_{\mathrm{enc}}(z|y)}\left[\ln \frac{P_{\mathrm{gen}(y,z)}}{P_{\mathrm{enc}}(z|y)}\right]
\end{aligned}
$$

Hence the name **evidence lower bound** or **ELBO**.

Fundamental Equations of Deep Learning

- Cross Entropy Loss: $\Phi^* =$

$$\operatorname*{argmin}_{\Phi} E_{(x,y)\sim \mathrm{Pop}} \left[-\ln P_\Phi(y|x)\right]$$

- GAN: $\mathrm{gen}^* =$

$$\operatorname*{argmax}_{\mathrm{gen}} \min_{\mathrm{disc}} E_{i\sim\{-1,1\},y\sim P_i} \left[-\ln P_{\mathrm{disc}}(i|y)\right]$$

- VAE: $\mathrm{pri}^*, \mathrm{dec}^*, \mathrm{enc}^* =$

$$\operatorname*{argmin}_{\mathrm{pri,dec,enc}} \; E_{(y,z)\sim P_{\mathrm{enc}}} \left[-\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{enc}}(z|y)}\right]$$

Training the Encoder

In diffusion models the encoder simply adds noise and is not trained.

In a VQ-VAE the encoder is trained. A naive approach to training the encoder is to optimize the ELBO loss.

$$\mathrm{enc}^* = \operatorname*{argmin}_{\mathrm{enc}} E_{(y,z)\sim P_{\mathrm{enc}}}\left[-\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{enc}}(z|y)}\right]$$

Training the Encoder

$$\mathrm{enc}^* = \operatorname*{argmin}_{\mathrm{enc}} E_{(y,z)\sim P_{\mathrm{enc}}}\left[-\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{enc}}(z|y)}\right]$$

Unfortunately this optimization involves optimizing a sampling distribution (the encoder). As with GANs, optimizing a sampling distribution (such as a GAN generator) is subject to mode collapse — the loss function is very forgiving of a failure of the sampling distribution to cover the desired space of values.

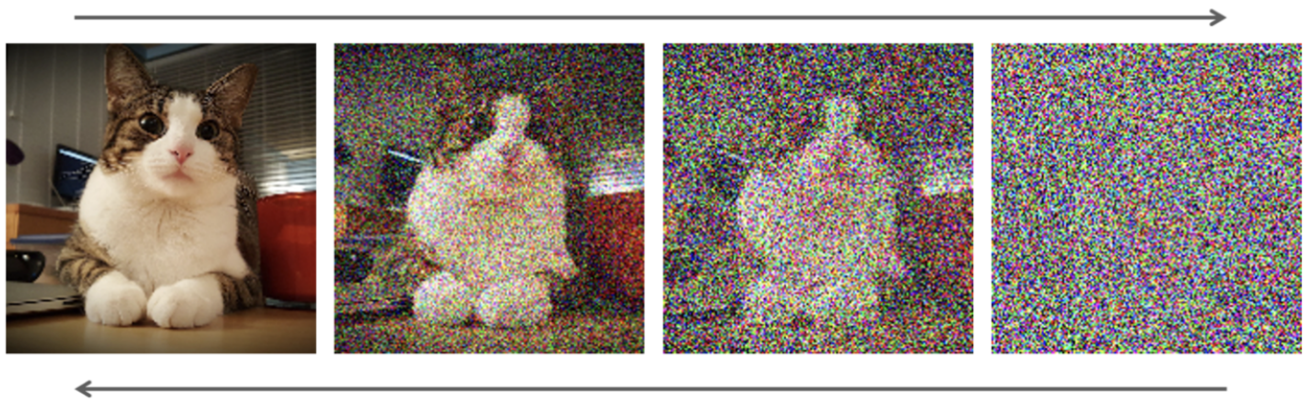
Training the Encoder

In a VQ-VAE the encoder is traned jointly with the decoder $P_{\mathrm{dec}}(y|z)$ but is trained independently of $P_{\mathrm{pri}}(z)$. $P_{\mathrm{pri}}(z)$ is trained later using a transformer model. The encoder of a VQ-VAE is closely related to K-means clustering. In a VQ-VAE the encoder converts vectors to tokens so that a transformer can be applied.

This minimal training of the encoder again exploits the fact that under universality $\mathrm{Pop}(y)$ can be modelled fully for any encoder.

A different approach to training the encoder, an ME-VAE, is discussed below.

Hierarchical VAEs



[Sally talked to John] $\rightleftarrows$ [Sally talked to] $\rightleftarrows$ [Sally talked] $\rightleftarrows$ [Sally] $\rightleftarrows$ []

$$y \rightleftarrows z_1 \rightleftarrows \cdots \rightleftarrows z_N$$

Hierarchical VAEs

$$y \overset{\rightarrow}{\leftarrow} z_1 \overset{\rightarrow}{\leftarrow} \cdots \overset{\rightarrow}{\leftarrow} z_N$$

Encoder: $\mathrm{Pop}(y)$, $P_{\mathrm{enc}}(z_1|y)$,$P_{\mathrm{enc}}(z_2|z_1), \ldots, P(z_N|Z_{N-1})$.

Generator: $P_{\mathrm{pri}}(z_N), P_{\mathrm{dec}}(z_{N-1}|z_N), \ldots, P_{\mathrm{dec}}(z_1|z_2), P_{\mathrm{dec}}(y|z_1)$

The encoder and the decoder define distributions $P_{\mathrm{enc}}(y, z_1, \ldots, z_N)$ and $P_{\mathrm{gen}}(y, z_1, \ldots, z_N)$ respectively.

Hierarchical VAEs

$$y \rightleftarrows z_1 \rightleftarrows \cdots \rightleftarrows z_N$$

- autoregressive models

- diffusion models

Hierarchical ELBO Loss

$$H(y) \;=\; E_{(y,z_1,\ldots,z_n)\sim P_{\mathrm{enc}}}\left[-\ln \frac{P_{\mathrm{gen}}(y,z_1,\ldots,z_n)}{P_{\mathrm{enc}}(z_1,\ldots,z_N|y)}\right]$$

EM-VAEs

The use of minimal encoder training may reflect the mode collapse problem of training a sampling distribution, such as a GAN generator or a VAE encoder.

The situation might be different if a better method were available for training the encoder. Here I will propose a method for training the encoder that avoids the mode collapse problem.

EM-VAEs

We start with the following "optimum encoder" inequality.

$$E_{y \sim \mathrm{Pop}, z \sim P_{\mathrm{gen}}(z|y)} \left[-\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{gen}}(z|y)} \right] \leq E_{(y,z) \sim P_{\mathrm{enc}}} \left[-\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{enc}}(z|y)} \right]$$

This implies $P^*_{\mathrm{enc}}(z|y) = P_{\mathrm{gen}}(z|y)$ and universality gives

$$\mathrm{enc}^* = \operatorname*{argmin}_{\mathrm{enc}} E_{(y,z) \sim P_{\mathrm{gen}}} - \ln P_{\mathrm{enc}}(z|y)$$

EM-VAE

$$\text{E: enc}^* = \operatorname*{argmin}_{\text{enc}} E_{(y,z)\sim P_{\text{gen}}} - \ln P_{\text{enc}}(z|y)$$

$$\text{M: gen}^* = \operatorname*{argmin}_{\text{gen}} \; E_{(y,z)\sim P_{\text{enc}}(y,z)} \left[-\ln P_{\text{gen}}(y,z)\right]$$

The classical EM algorithm is the case where we alternate optimizing the encoder (the E step) and the generator (the M step) and where the E step yields $P_{\text{enc}}(z|y) = P_{\text{gen}}(z|y)$ exactly and where the M step cannot fully fit the population.

Here we can use SGD on these two objectives independent of details of the models.

Derivation of the Encoder Optimum

$$
\begin{aligned}
& E_{(y,z)\sim P_{\mathrm{enc}}}\left[-\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{enc}}(z|y)}\right] \\
= \;& E_{(y,z)\sim P_{\mathrm{enc}}}\left[-\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{gen}}(z|y)}\right] + E_{y\sim \mathrm{Pop}}\; KL(P_{\mathrm{enc}}(z|y), P_{\mathrm{gen}}(z|y)) \\
\geq \;& E_{(y,z)\sim P_{\mathrm{enc}}}\left[-\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{gen}}(z|y)}\right] \\
= \;& E_{(y,z)\sim P_{\mathrm{enc}}}\left[-\ln P_{\mathrm{gen}}(y)\right] \\
= \;& E_{y\sim \mathrm{Pop},\, z\sim P_{\mathrm{gen}}(z|y)}\left[-\ln P_{\mathrm{gen}}(y)\right] \\
= \;& E_{y\sim \mathrm{Pop},\, z\sim P_{\mathrm{gen}}(z|y)}\left[-\ln \frac{P_{\mathrm{gen}}(y,z)}{P_{\mathrm{gen}}(z|y)}\right]
\end{aligned}
$$

END