TTIC 31230, Fundamentals of Deep Learning

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The Evidence Lower Bound (the ELBO)

Variational Autoencoders

Big Picture: Latent Variables

We are often interested in models of the form

$$P_\Phi(y) = \sum_z P_\Phi(z) P_\Phi(y|z).$$

Note that CTC has this form.

Probabilistic grammar models also have this form where y is a sentence and z is a parse tree.

Rate-Distortion Autoencoders also have this form where z is the compression of y.

In the first two cases, and for lossless compression, the sum over z can be computed exactly.

Big Picture: Friendly Distributions

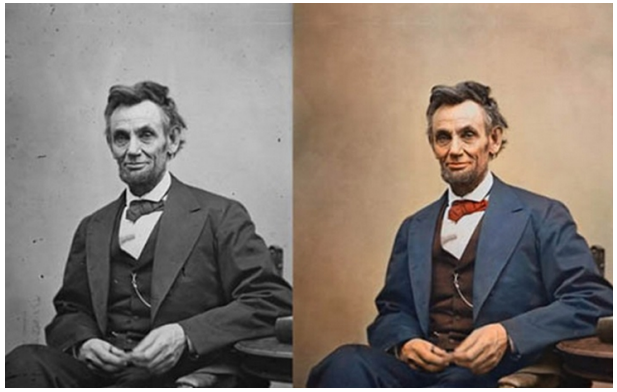
A distribution $P(u)$ will be called **friendly** if we can both draw samples from it and compute $P(u)$ for any value u.

$$P_\Phi(y) = \sum_z P_\Phi(z) P_\Phi(y|z).$$

It is often the case that $P_\Phi(z)$ is friendly, and $P_\Phi(y|z)$ is friendly, but $P_\Phi(y)$ is not friendly (the sum over z is intractible).

For example z might be an assignment of truth values to Boolean variables and y might be the value of a fixed Boolean formula Φ. In this case determining if $P_\Phi(y) > 0$ is the SAT problem which is NP hard.

Colorization



x is a black and white image, y a color image, and z a semantic segmentation.

$$P_\Phi(y|x) = \sum_z P_\Phi(z|x) P_\Phi(y|z,x).$$

Colorization

$P_\Phi(z|x)$ is defined by a deep network computing a friendly graphical model on semantic segmentations – perhaps each pixel is assigned a distribution over material categories such as "face", "shirt", "shirt-color1" or "shirt-color2".

$P_\Phi(y|z,x)$ is a deep network taking a particular semantic segmentation (a particular semantic material label at each pixel) and computing a distribution on a discrete color space for each material label.

Although $P(z|x)$ is friendly, and $P_\Phi(y|z,x)$ is friendly, $P(y|x)$ not friendly (similar to the SAT example).

Big Picture: ELBO Replaces Search with Generation

$$
\begin{aligned}
P_\Phi(y) &= E_{z\sim P_\Phi(z)} P_\Phi(y|z) \quad \text{sampling } z \text{ is ineffective} \\
\ln P_\Phi(y) &= E_{z\sim P_\Psi(z|y)} \ln P_\Phi(y) \quad \text{introduce } z \text{ generator using } y \\
&= E_{z\sim P_\Psi(z|y)} \left(\ln P_\Phi(y) P_\Phi(z|y) + \ln \frac{P_\Psi(z|y)}{P_\Phi(z|y)} + \ln \frac{1}{P_\Psi(z|y)} \right) \\
&= \left(E_{z\sim P_\Psi(z|y)} \ \ln \ P_\Phi(z,y) \right) + KL(P_\Psi(z|y), P_\Phi(z|y)) + H(P_\Psi(z|y)) \\
&\geq E_{z\sim P_\Psi(z|y)} \ (\ \ln \ P_\Phi(z) P_\Phi(y|z) - \ln P_\Psi(z|y) \ ) \quad \text{ELBO}
\end{aligned}
$$

Measuring the ELBO

$$\text{ELBO}(y, \Phi, \Psi) = E_{z \sim P_\Psi(y)} \ \ln P_\Phi(z) P_\Phi(y|z) - \ln P_\Psi(z)$$

If $P_\Phi(z)$, $P_\Phi(y|z)$, and $P_\Psi(z|y)$ are friendly (even whwn when $P_\Phi(y)$ is not friendly) we can measure ELBO loss through sampling.

If we can measure it, we can do gradient descent on it (but perhaps with difficulty).

Colorization

x is a black and white image, y a color image, and z a semantic segmentation.

$P_\Phi(z|x)$ is friendly and $P_\Phi(y|z,x)$ is friendly but $P(y|x)$ is not friendly.

$P_\Psi(z|y,x)$ computes a friendly graphical model for z given y.

A General ELBO Architecture

$P_\Phi(y|x)$

intput x

$\vdots$

$z = \underset{z}{\text{expsoftmax}} \ldots$

input z

$\vdots$

$y = \underset{y}{\text{expsoftmax}} \ldots$

$P_\Psi(z|y,x)$

intput x, y

$\vdots$

$z = \underset{z}{\text{expsoftmax}} \ldots$

The exponential softmaxes are friendly (they produce a friendly graphical model).

Two Expressions for the ELBO

$$\ln P_\Phi(y) = ELBO(y, \Phi, \Psi) + KL(P_\Psi(z|y), P_\Phi(z|y))$$

$$ELBO = E_{z \sim P_\Psi(z|y)} \ln P_\Phi(z, y) + H(P_\Psi(z|y)) \quad (1)$$

$$= \ln P_\Phi(y) - KL(P_\Psi(z|y), P_\Phi(z|y)) \quad (2)$$

EM is Alternating Maximization of the ELBO

Forward-backward EM for HMMs and inside-outside EM for PCFGs (or any EM) can be written as

$$\text{ELBO} = E_{z \sim P_\Psi(z|y)} \ln P_\Phi(z, y) + H(P_\Psi(z|y)) \quad (1)$$

$$= \ln P_\Phi(y) - KL(P_\Psi(z|y), P_\Phi(z|y)) \quad (2)$$

$$\text{by (2)} \quad \Psi^{t+1} = \operatorname*{argmin}_\Psi E_{y \sim \text{Train}} KL(P_\Psi(z|y), P_{\Phi^t}(z|y)) = \Phi^t$$

$$\text{by (1)} \quad \Phi^{t+1} = \operatorname*{argmax}_\Phi E_{y \sim \text{Train}} E_{z \sim P_{\Phi^t}(z|y)} \ln P_\Phi(z, y)$$

We want Ψ to adapt to Φ

$$\mathcal{L}_{\text{ELBO}}(y, \Phi, \Psi) = KL(P_\Psi(z|y), P_\Phi(z|y)) - \ln\ P_\Phi(y)$$

$$Q^*(z|y) = P_\Phi(z|y)$$

$$E_{y \sim \text{Pop}}\, \mathcal{L}_{\text{ELBO}}(y, \Phi, Q^*) = H(\text{Pop}, P_\Phi)$$

However, Φ can ignore Ψ

$$\mathcal{L}_{\text{ELBO}}(y, \Phi, \Psi) = KL(P_\Psi(z|y), P_\Phi(z|y)) - \ln\ P_\Phi(y)$$

$$P^*(z) = P_\Psi(z)$$
$$P^*(y|z) = P_\Phi(y)$$

$$E_{y\sim\text{Pop}}\, \mathcal{L}_{\text{ELBO}}(y, P^*, \Psi) = H(\text{Pop}, P_\Phi)$$

It seems important that $P_\Phi(y|z)$ have limited expressive power.

Hard ELBO

Hard ELBO is to ELBO as hard EM is to EM.

$$\mathcal{L}_{\text{ELBO}}(y, \Phi, \Psi) = KL(P_\Psi(z|y), P_\Phi(z|y)) - \ln P_\Phi(y)$$

$$\mathcal{L}_{\text{ELBO}}(y, \Phi, \Psi) = E_{z \sim P_\Psi(z|y)} - \ln P_\Phi(z, y) + \ln P_\Psi(z|y)$$

$$\mathcal{L}_{\text{HELBO}}(y, \Phi, \Psi) = E_{z \sim P_\Psi(z|y)} - \ln P_\Phi(z, y)$$

Hard ELBO and Rate-Distortion Autoencoding

$$\mathcal{L}_{\mathrm{HELBO}}(y, \Phi, \Psi) = E_{z \sim P_\Psi(z|y)} - \ln P_\Phi(z, y)$$

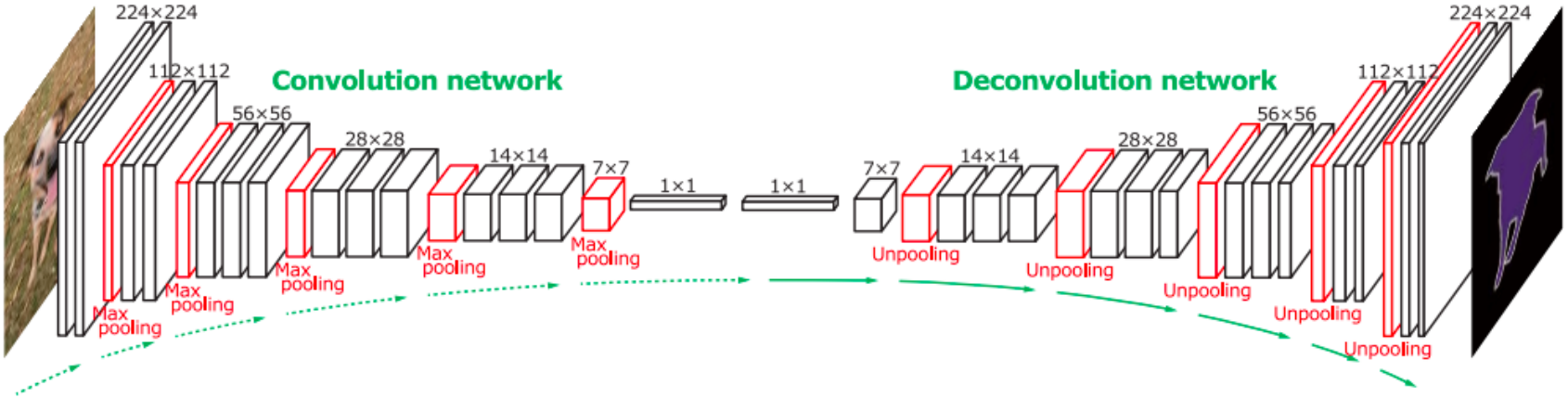
$$\min_{P,Q} E_{y \sim \mathrm{Pop}}\, \mathcal{L}_{\mathrm{HELBO}}(y, P, Q) \leq H(\mathrm{Pop}) + \ln 2$$

This can be proved from Shannon's source coding theorem where z is the code for y.

A VAE for Images

Auto-Encoding Variational Bayes, Diederik P Kingma, Max Welling, 2013.

y $z_\Psi(y, \epsilon)$ $z\ p_\Phi(z)$ $\hat{y}_\Phi(z)$ $||y - \hat{y}||^2$



[Hyeonwoo Noh et al.]

Gaussian Distributions

$$p_\Phi(z) \propto \exp\left(\sum_i (z[i] - \mu[i])^2/(2\sigma[i]^2)\right)$$

$$p_\Phi(y|z) \propto \exp\left(\sum_j (y[j] - y_\Phi(z)[j])^2/(2\gamma[j]^2)\right)$$

$$p_\Psi(z|y) \propto \exp\left(\sum_i (z[i] - z_\Psi(y)[i])^2/(2\sigma_\Psi(y)[i]^2)\right)$$

KL-Divergence Form for the ELBO

$$E_{z \in p_\Psi(z|y)} \ \ln \ p_\Psi(z|y) - \ln \ p_\Phi(z) p_\Phi(y|z) \quad \mathcal{L}_{\text{ELBO}}$$

$$= KL(p_\Psi(z|y), p_\Phi(z)) + E_{z \in P_\Psi(z|y)} - \ln p_\Phi(y|z)$$

The ELBO is a KL-divergence + a cross entropy

Continuous KL-divergence is ok.

Continuous cross-entropy has issues — we will come back to that later.

Closed Form KL-Divergence

$$KL(p_\Psi(z|y), p_\Phi(z))$$

$$= \sum_i \frac{\sigma_\Psi(y)[i]^2 + (z_\Psi(y)[i] - \mu[i])^2}{2\sigma[i]^2} + \ln \frac{\sigma[i]}{\sigma_\Psi(y)[i]} - \frac{1}{2}$$

Standardizing $p_\Phi(z)$

The KL-divergence term is

$$\sum_i \frac{\sigma_\Psi(y)[i]^2 + (z_\Psi(y)[i] - \mu[i])^2}{2\sigma[i]^2} + \ln \frac{\sigma[i]}{\sigma_\Psi(y)[i]} - \frac{1}{2}$$

We can adjust Ψ to Ψ' such that

$$\begin{aligned} z_{\Psi'}(y)[i] &= z_\Psi(y)[i]/\sigma[i] + \mu[i] \\ \sigma_{\Psi'}(y)[i] &= \sigma_\Psi(y)/\sigma[i] \end{aligned}$$

We then get $KL(p_\Psi(z|y), p_\Phi(z)) = KL(p_{\Psi'}(z|y), \mathcal{N}(0, I))$.

Standardizing $p_\Phi(z)$

Without loss of generality the VAE becomes.

$$\min_{\Phi,\Psi} \; E_y \; KL(P_\Psi(z|y), \mathcal{N}(0, I)) + E_{z \in P_\Psi(z|y)} - \ln p_\Phi(y|z)$$

Reparameterization Trick for the Cross-Entropy

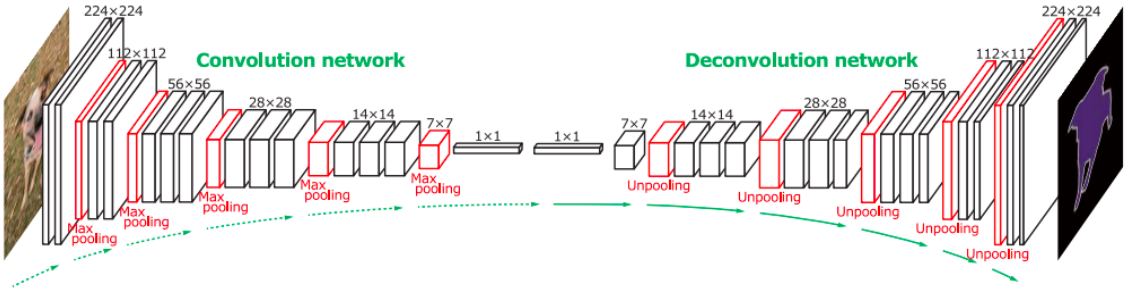
$$p_\Psi(z|y) \propto \exp\left(\sum_i (z[i] - z_\Psi(y)[i])^2/(2\sigma_\Psi(y)[i]^2)\right)$$

$$E_{z\in p_\Psi(z|y)} \ln p_\Phi(y|z)$$

$$= E_{\epsilon\sim\mathcal{N}(0,I)} z[i] = z_\Psi(y)[i] + \sigma_\Psi(y)[i]\epsilon[i]; \quad \ln p_\Phi(y|z)$$

Sampling

$$P_\Psi(z|y) \quad z \quad P_\Phi(z, y)$$



[Hyeonwoo Noh et al.]

Sampling uses just the second half $P_\Phi(z, y)$.

Sampling

[Alec Radford]

Why Blurry?

A common explanation for the blurryness of images generated from VAEs is the use of L_2 as the distortion measure.

It does seem that L_1 works better.

However, training on L_2 distortion can produce sharp images in rate-distortion autoencoders.

Noisy-Channel Rate-Distortion Autoencoders

The twilight zone is material for which I do not know of a reference.

Differential Entropy and Cross-Entropy are Ill-Defined

$$\mathcal{L}_{\text{VAE}} = \sum_j \frac{E_{z\sim P_\Psi(z|y)}\left(y[j] - \hat{y}_\Phi(z)[j]\right)^2}{2\gamma[j]^2} + \ln \gamma[j]$$
$$+KL(p_\Psi(z|y), p_\Phi(z))$$

Consider a probability density on light intensity.

While the first term is dimensionless, $\gamma[j]$ is an intensity.

The cross-entropy term can be assigned any numerical value depending on the choice units (metric, English, or martian).

Differential Entropy and Cross-Entropy are Ill-Defined

There are also other problems with continuous entropy and cross-entropy.

- Finite continuous entropy violates the source coding theorem — it takes an infinite number of bits to code a real number.
- Finite continuous entropy violates the data processing inequality that $H(f(x)) \leq H(x)$. For a continuous random variable x under finite continuous entropy we can have $H(f(x)) > H(x)$.

For these reasons it seems best to avoid using finite continuous entropy and finite continuous cross entropy.

Distortion

A stochastic encoder $p_\Phi(z|y)$, a decoder $y_\Phi(z)$, and distortion function D define a quantity of distortion.

$$E_{y\sim\text{Pop},\, z\sim p_\Phi(z|y)}\, D(y, y_\Phi(z))$$

For L_2 distortion we can use

$$D(y, y') = ||y - y'||_2$$

Distortion can typically be given the same units as y.

Rate

A stochastic encoder defines a rate.

$$p_\Phi(z) \doteq \sum_y \text{Pop}(y) p_\Phi(z|y)$$

$$I_\Phi(y,z) = E_y \; KL(p_\Phi(z|y), p_\Phi(z))$$

By Shannon's channel capacity theorem, $I_\Phi(y,z)$ is the channel capacity when sending y across the noisy channel z.

For z continuous, a deterministic encoder has an infinite rate.

Here $p_\Phi(z)$ is not friendly.

Bounding the Rate

$$
\begin{aligned}
I_\Phi(y,z) &= E_{y\sim \mathrm{Pop}}\, KL(p_\Phi(z|y), p_\Phi(z)) \\
&= E_{y,z} \ln p_\Phi(z|y) - \ln p_\Psi(z) + \ln p_\Psi(z) - \ln p_\Phi(z) \\
&= E_y\, KL(p_\Phi(z|y), p_\Psi(z)) - KL(p_\Phi(z), p_\Psi(z)) \\
&\leq E_y\, KL(p_\Phi(z|y), p_\Psi(z))
\end{aligned}
$$

We can take $p_\Psi(z)$ to be friendly, and WLOG, fixed at $\mathcal{N}(0, I)$.

The Noisy-Channel Rate-Distortion Autoencoder

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\ E_y\ KL(p_\Phi(z|y), \mathcal{N}(0, I)) + \frac{1}{\gamma}\ E_{z\sim p_\Phi(z|y)}\ D(y,\ y_\Phi(z))$$

Here γ has the same units as distortion and controls the trade-off between rate and distortion.

Summary: Rate-Distortion

Rate-Distortion: y, continuous, $\tilde{z}$ a bit string,

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_y \, |\tilde{z}_\Phi(y)| + \lambda D(y, y_\Phi(\tilde{z}_\Phi(y)))$$

Noisy Channel: $\tilde{z} = z_\Phi(y) + \sigma_\Phi(y) \odot \epsilon, \qquad \epsilon \sim \mathcal{N}(0, I)$

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}}\, E_y \;\; KL(p_\Phi(\tilde{z}|y), \mathcal{N}(0, I)) + E_{\tilde{z} \sim p_\Phi(\tilde{z}|y)} \, \lambda D(y, y_\Phi(\tilde{z}))$$

Summary: ELBO and VAE

ELBO: $P_\Phi(z)$, $P_\Phi(y|z)$, $P_\Psi(z|y)$ friendly graphical models:

$$\Phi^*, \Psi^* = \underset{\Phi,\Psi}{\operatorname{argmin}} \; E_{y\sim \mathrm{Pop},\, z\sim P_\Psi(z|y)} \; \ln P_\Psi(z|y) - \ln P_\Phi(z) P_\Phi(y|z)$$

VAE: $p_\Phi(z|y)$, $p_\Phi(y|z)$ Gaussian:

$$\Phi^* = \underset{\Phi}{\operatorname{argmin}} \, E_{y\sim \mathrm{Pop}} \; KL(p_\Phi(z|y), \mathcal{N}(0, I)) - E_{z\sim p_\Phi(z|y)} \; \ln p_\Phi(y|z)$$

END