# TTIC 31230, Fundamentals of Deep Learning

David McAllester, Winter 2019

Expectation Maximization (EM)

The Evidence Lower Bound (the ELBO)

Variational Autoencoders (VAEs)

# Latent Variable Models

We are often interested in models of the form

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

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

For example, CTC and probabilistic grammar models.

# Expectation Maximization (EM)

# Mixture of Gaussian Modeling

$$\Phi = (\pi_1, \mu_1, \Sigma_1, \ldots, \pi_k, \mu_k, \Sigma_k)$$

$$\begin{aligned} p_\Phi(y) &= \sum_i P(i)p(y|i) \\ &= \sum_i \pi_i \frac{1}{Z_i} \exp\left(-\frac{1}{2}(y-\mu_i)^\top \Sigma_i^{-1}(y-\mu_i)\right) \end{aligned}$$

$i$ is the latent variable.

# Expectation Maximization (EM)

## Mixture of Gaussian Modeling

$$\Phi = (\pi_1, \mu_1, \Sigma_1, \ldots, \pi_k, \mu_k, \Sigma_k)$$

$$\text{Train} = \{y_1, \ldots, y_N\}$$

Until Convergence:

$$P_\Phi(i|y_j) = \frac{\pi_i P(y_j|i)}{\sum_i \; \pi_i P(y_j|i)} \quad \text{Inference (E step)}$$

$$\left.\begin{array}{lcl} \pi_i^{t+1} & = & \frac{1}{N} \sum_j \; P_{\Phi^t}(i|y_j) \\ \mu_i^{t+1} & = & \frac{1}{N} \sum_j \; P_{\Phi^t}(i|y_j) y_j \\ \Sigma_i^{t+1} & = & \frac{1}{N} \sum_j P_{\Phi^t}(i|y_j) y_j y_j^\top \end{array}\right\} \text{Model Update (M step)}$$

## General EM

$$\Phi^* = \operatorname*{argmin}_{\Phi} E_{y \sim \text{Train}} - \ln P_\Phi(y)$$

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

$$\Phi^{t+1} = \underset{\substack{\Phi \\ \text{Update} \\ \text{(M Step)}}}{\operatorname{argmin}} \; E_{y \sim \text{Train}} \; \underset{\substack{\text{Inference} \\ \text{(E Step)}}}{E_{z \sim P_{\Phi^t}(z|y)}} - \ln P_\Phi(z, y)$$

# Colorization


$x$ $\hat{y}$ $y$

Larsson et al., 2016

$x$ is a black and white image.

$y$ is a color image drawn from $\mathrm{Pop}(y|x)$.

$\hat{y}$ is an arbitrary color image.

$P_\Phi(\hat{y}|x)$ is the probability that model $\Phi$ assigns to the color image $\hat{y}$ given black and white image $x$.

# Colorization with Latent Semantic Segmentation (TZ)


$x$ $\qquad\qquad$ $\hat{y}$ $\qquad\qquad$ $y$

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

$$\begin{aligned}
&\text{input } x \\
P_\Phi(z|x) &= \ldots \quad \text{semantic segmentation} \\
P_\Phi(\hat{y}|z,x) &= \ldots \quad \text{segment colorization}
\end{aligned}$$

## Maybe EM?

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

$$\Phi^{t+1} = \underset{\Phi}{\text{argmin}}\; E_{y\sim\text{Train}}\; E_{z\sim P_{\Phi^t}(z|y)}\; -\ln P_\Phi(z,y)$$

Update Inference

In most cases the inference is intractible!

# Variational Inference:
# The Evidence Lower Bound (The ELBO)

We introduce a friendly model $P_\Psi(z|y)$ to approximate $P_\Phi(z|y)$.

$$
\begin{aligned}
\ln P_\Phi(y) &= E_{z\sim P_\Psi(z|y)} \ln P_\Phi(y) \\
&= E_{z\sim P_\Psi(z|y)} \left( \ln P_\Phi(y) \frac{P_\Phi(z|y)}{P_\Psi(z|y)} + \ln \frac{P_\Psi(z|y)}{P_\Phi(z|y)} \right) \\
&= \left( E_{z\sim P_\Psi(z|y)} \ln \frac{P_\Phi(z,y)}{P_\Psi(z|y)} \right) + KL(P_\Psi(z|y), P_\Phi(z|y)) \\
&= \qquad\qquad \text{ELBO} \qquad\qquad + KL(P_\Psi(z|y), P_\Phi(z|y))
\end{aligned}
$$

# EM is Alternating Maximization of the ELBO

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

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

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

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

## Different Ways of Writing the ELBO

$$
\begin{aligned}
\text{ELBO} &= E_{z\sim P_\Psi(z|y)}\ \ln \frac{P_\Phi(z,y)}{P_\Psi(z|y)} \\
&= \ln\ P_\Phi(y) - KL(P_\Psi(z|y), P_\Phi(z|y)) \\
&= \left(E_{z\sim P_\Psi(z|y)} \ln P(y|z)\right) - KL(P_\Psi(z|x), P_\Phi(z)) \\
&= \left(E_{z\sim P_\Psi(z|y)}\ P_\Phi(z,y)\right) + H(P_\Psi(z|y))
\end{aligned}
$$

## Hard ELBO

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

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

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

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

# Measuring the ELBO

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

If $P_\Phi(z)$, $P_\Phi(y|z)$, and $P_\Psi(z|y)$ are friendly (even 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).

## We want $\Psi$ to adapt to $\Phi$

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

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

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

## However, $\Phi$ can ignore $\Psi$

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

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

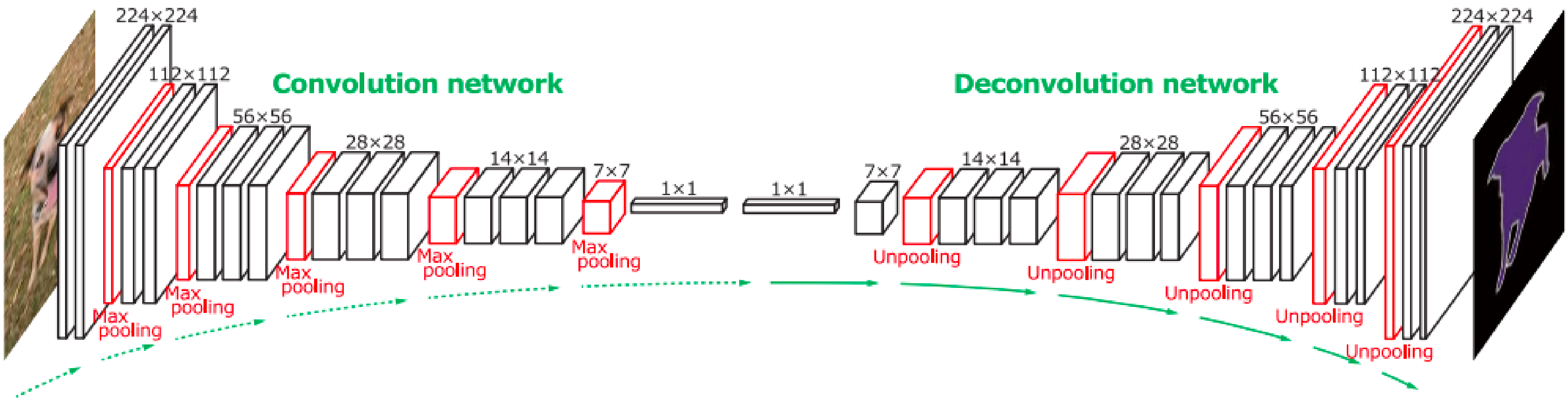
$$E_{y\sim\mathrm{Pop}}\ \mathcal{L}_{\mathrm{ELBO}}(y,P^*,\Psi) = H(\mathrm{Pop}, P_\Phi)$$

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

# A VAE for Images

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

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




[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

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

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

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 $\Psi$ to $\Psi'$ 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

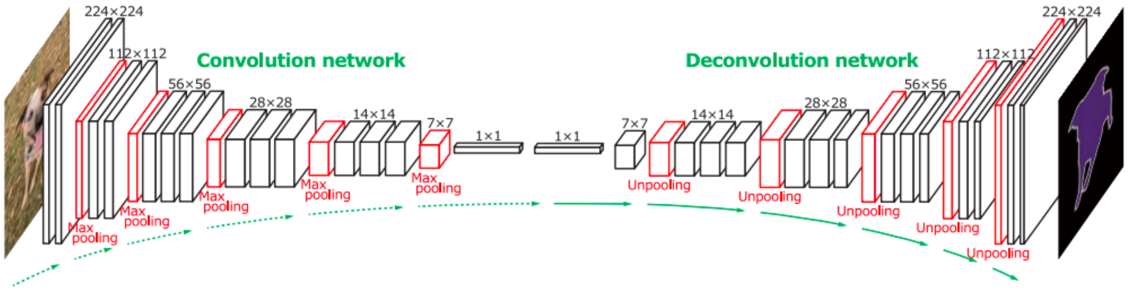
$$p_\Psi(z|y) \propto \exp\left(\sum_i (z[i] - z_\Psi(y)[i])^2/(2\sigma_\Psi(y)[i]^2)\right)$$

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

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

# Sampling

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




[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

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

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

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.

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

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.

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

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

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 $\gamma$ 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,

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

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

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

## Summary: ELBO and VAE

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

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

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

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

**END**