Latent Variable Models

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Lecture 5

- Glitches with Google Hangout link should be resolved. Will be checking email at the beginning of each office hours session to make sure there are no more glitches.
- Homework template is available.
- Extra lecture notes have been posted.
- Good luck with ICML deadline!

Autoregressive models:

- Chain rule based factorization is fully general
- Compact representation via *conditional independence* and/or *neural parameterizations*
- Autoregressive models Pros:
 - Easy to evaluate likelihoods
 - Easy to train
- Output Autoregressive models Cons:
 - Requires an ordering
 - Generation is sequential
 - Cannot learn features in an unsupervised way

Latent variable models

- Definition
- Motivation
- Warm-up: Shallow mixture models
- Oeep latent-variable models
 - Representation: Variational autoencoder
 - Learning: Variational inference

Latent Variable Models: Motivation



- Lots of variability in images x due to gender, eye color, hair color, pose, etc. However, unless images are annotated, these factors of variation are not explicitly available (latent).
- Idea: explicitly model these factors using latent variables z

Latent Variable Models: Definition



Х

A latent variable model defines a probability distribution

$$p(x,z) = p(x|z)p(z)$$

containing two sets of variables:

- Observed variables x that represent the high-dimensional object we are trying to model.
- 2 Latent variables z that are not in the training set, but that are associated with the x via p(z|x) and can encode the structure of the data.

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Latent Variable Models: Example



Only shaded variables x are observed in the data (pixel values)

- 2 Latent variables z correspond to high level features
 - If z chosen properly, $p(\mathbf{x}|\mathbf{z})$ could be much simpler than $p(\mathbf{x})$
 - If we had trained this model, then we could identify features via p(z | x), e.g., p(EyeColor = Blue|x)

Ohallenge: Very difficult to specify these conditionals by hand

Deep Latent Variable Models: Example



- $z \sim \mathcal{N}(0, I)$
- 2 $p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mu_{\theta}(\mathbf{z}), \Sigma_{\theta}(\mathbf{z}))$ where $\mu_{\theta}, \Sigma_{\theta}$ are neural networks
- Hope that after training, z will correspond to meaningful latent factors of variation (*features*). Unsupervised representation learning.
- As before, features can be computed via p(z | x). In practice, we will need to use approximate inference.

Mixture of Gaussians: a Shallow Latent Variable Model



Generative process

- Pick a mixture component k by sampling z
- Q Generate a data point by sampling from that Gaussian

Mixture of Gaussians: a Shallow Latent Variable Model

Mixture of Gaussians:



Clustering: The posterior p(z | x) identifies the mixture component
 Unsupervised learning: We are hoping to learn from unlabeled data (ill-posed problem)

Representational Power of Mixture models

Combine simple models into a more complex and expressive one



The likelihood is non-convex: this increases representational power, but makes inference more challenging.

Example: Unsupervised learning over hand-written digits



Unsupervised clustering of handwritten digits.

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Example: Unsupervised learning over DNA sequence data



Example: Unsupervised learning over face images



Latent variable models

- Definition
- Motivation
- Warm-up: Shallow mixture models

Open latent-variable models

- Representation: Variational autoencoder
- Learning: Variational inference

Variational Autoencoder



A mixture of an infinite number of Gaussians:

•
$$\mathbf{z} \sim \mathcal{N}(0, I)$$

• $p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mu_{\theta}(\mathbf{z}), \Sigma_{\theta}(\mathbf{z}))$ where $\mu_{\theta}, \Sigma_{\theta}$ are neural networks
• $\mu_{\theta}(\mathbf{z}) = \sigma(A\mathbf{z} + c) = (\sigma(a_1\mathbf{z} + c_1), \sigma(a_2\mathbf{z} + c_2)) = (\mu_1(\mathbf{z}), \mu_2(\mathbf{z}))$
• $\Sigma_{\theta}(\mathbf{z}) = diag(\exp(\sigma(B\mathbf{z} + d))) = \begin{pmatrix} \exp(\sigma(b_1\mathbf{z} + d_1)) & 0 \\ 0 & \exp(\sigma(b_2\mathbf{z} + d_2)) \end{pmatrix}$
• $\theta = (A, B, c, d)$

Seven though p(x | z) is simple, the marginal p(x) is very complex/flexible

- Allow us to define complex models p(x) in terms of simple building blocks p(x | z)
- Natural for unsupervised learning tasks (clustering, unsupervised representation learning, etc.)
- No free lunch: much more difficult to learn compared to fully observed, autoregressive models

Partially observed data

• Suppose that our joint distribution is

 $p(\mathbf{X}, \mathbf{Z}; \theta)$

- We have a dataset \mathcal{D} , where for each datapoint the **X** variables are observed (e.g., pixel values) and the variables **Z** are never observed (e.g., cluster or class id.). $\mathcal{D} = \{\mathbf{x}^{(1)}, \cdots, \mathbf{x}^{(M)}\}.$
- Maximum likelihood learning:

$$\log \prod_{\mathbf{x} \in \mathcal{D}} p(\mathbf{x}; \theta) = \sum_{\mathbf{x} \in \mathcal{D}} \log p(\mathbf{x}; \theta) = \sum_{\mathbf{x} \in \mathcal{D}} \log \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}; \theta)$$

• Evaluating
$$\log \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}; \theta)$$
 can be hard!

Example: Learning with Missing Values



- Suppose some pixel values are missing at train time (e.g., top half)
- Let **X** denote observed random variables, and **Z** the unobserved ones (also called hidden or latent)
- Suppose we have a model for the joint distribution (e.g., PixelCNN)

$$p(\mathbf{X}, \mathbf{Z}; \theta)$$

What is the probability $p(\mathbf{X} = \bar{\mathbf{x}}; \theta)$ of observing a training data point $\bar{\mathbf{x}}$?

$$\sum_{\mathbf{z}} p(\mathbf{X} = \bar{\mathbf{x}}, \mathbf{Z} = \mathbf{z}; \theta) = \sum_{\mathbf{z}} p(\bar{\mathbf{x}}, \mathbf{z}; \theta)$$

Need to consider all possible ways to complete the image (fill green part)

Example: Variational Autoencoder



A mixture of an infinite number of Gaussians:

- $z \sim \mathcal{N}(0, I)$. $p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mu_{\theta}(\mathbf{z}), \Sigma_{\theta}(\mathbf{z}))$ where $\mu_{\theta}, \Sigma_{\theta}$ are neural networks
- Z are unobserved at train time (also called hidden or latent)
- Suppose we have a model for the joint distribution. What is the probability p(X = x̄; θ) of observing a training data point x̄?

$$\int_{z} p(\mathbf{X} = \bar{\mathbf{x}}, \mathbf{Z} = \mathbf{z}; \theta) d\mathbf{z} = \int_{z} p(\bar{\mathbf{x}}, \mathbf{z}; \theta) d\mathbf{z}$$

Partially observed data

• Suppose that our joint distribution is

 $p(\mathbf{X}, \mathbf{Z}; \theta)$

- We have a dataset D, where for each datapoint the X variables are observed (e.g., pixel values) and the variables Z are never observed (e.g., cluster or class id.). D = {x⁽¹⁾, ..., x^(M)}.
- Maximum likelihood learning:

$$\log \prod_{\mathbf{x} \in \mathcal{D}} p(\mathbf{x}; \theta) = \sum_{\mathbf{x} \in \mathcal{D}} \log p(\mathbf{x}; \theta) = \sum_{\mathbf{x} \in \mathcal{D}} \log \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}; \theta)$$

- Evaluating $\log \sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}; \theta)$ can be intractable. Suppose we have 30 binary latent features, $\mathbf{z} \in \{0, 1\}^{30}$. Evaluating $\sum_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}; \theta)$ involves a sum with 2^{30} terms. For continuous variables, $\log \int_{\mathbf{z}} p(\mathbf{x}, \mathbf{z}; \theta) d\mathbf{z}$ is often intractable. Gradients ∇_{θ} also hard to compute.
- Need **approximations**. One gradient evaluation per training data point $\mathbf{x} \in \mathcal{D}$, so approximation needs to be cheap.

First attempt: Naive Monte Carlo

Likelihood function $p_{\theta}(\mathbf{x})$ for Partially Observed Data is hard to compute:

$$p_{\theta}(\mathbf{x}) = \sum_{\text{All values of } \mathbf{z}} p_{\theta}(\mathbf{x}, \mathbf{z}) = |\mathcal{Z}| \sum_{\mathbf{z} \in \mathcal{Z}} \frac{1}{|\mathcal{Z}|} p_{\theta}(\mathbf{x}, \mathbf{z}) = |\mathcal{Z}| \mathbb{E}_{\mathbf{z} \sim \textit{Uniform}(\mathcal{Z})} [p_{\theta}(\mathbf{x}, \mathbf{z})]$$

We can think of it as an (intractable) expectation. Monte Carlo to the rescue:

- **(**) Sample $\mathbf{z}^{(1)}, \cdots, \mathbf{z}^{(k)}$ uniformly at random
- Approximate expectation with sample average

$$\sum_{\mathbf{z}} p_{\theta}(\mathbf{x}, \mathbf{z}) pprox |\mathcal{Z}| rac{1}{k} \sum_{j=1}^{k} p_{\theta}(\mathbf{x}, \mathbf{z}^{(j)})$$

Works in theory but not in practice. For most \mathbf{z} , $p_{\theta}(\mathbf{x}, \mathbf{z})$ is very low (most completions don't make sense). Some are very large but will never "hit" likely completions by uniform random sampling. Need a clever way to select $\mathbf{z}^{(j)}$ to reduce variance of the estimator.

Second attempt: Importance Sampling

Likelihood function $p_{\theta}(\mathbf{x})$ for Partially Observed Data is hard to compute:

$$p_{\theta}(\mathbf{x}) = \sum_{\text{All possible values of } \mathbf{z}} p_{\theta}(\mathbf{x}, \mathbf{z}) = \sum_{\mathbf{z} \in \mathcal{Z}} \frac{q(\mathbf{z})}{q(\mathbf{z})} p_{\theta}(\mathbf{x}, \mathbf{z}) = \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})} \left[\frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} \right]$$

Monte Carlo to the rescue:

1 Sample
$$z^{(1)}, \cdots, z^{(k)}$$
 from $q(z)$

Approximate expectation with sample average

$$p_{ heta}(\mathbf{x}) pprox rac{1}{k} \sum_{j=1}^k rac{p_{ heta}(\mathbf{x}, \mathbf{z}^{(j)})}{q(\mathbf{z}^{(j)})}$$

What is a good choice for q(z)? Intuitively, choose likely completions. Challenges: deriving algorithms for choosing q and extending this approximation to the marginal log-likelihood.

Approximating the Marginal Log LIkelihood

We can approximate marginal probabilities with importance sampling:

$$p_{ heta}(\mathbf{x}) pprox rac{1}{k} \sum_{j=1}^k rac{p_{ heta}(\mathbf{x}, \mathbf{z}^{(j)})}{q(\mathbf{z}^{(j)})}$$

However, what we want to approximate is the marginal log-likelihood:

$$\log\left(\sum_{\mathbf{z}\in\mathcal{Z}}p_{\theta}(\mathbf{x},\mathbf{z})\right) = \log\left(\sum_{\mathbf{z}\in\mathcal{Z}}\frac{q(\mathbf{z})}{q(\mathbf{z})}p_{\theta}(\mathbf{x},\mathbf{z})\right) = \log\left(\mathbb{E}_{\mathbf{z}\sim q(\mathbf{z})}\left[\frac{p_{\theta}(\mathbf{x},\mathbf{z})}{q(\mathbf{z})}\right]\right)$$

It's clear that

$$\mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})} \left[\log \left(\frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} \right) \right] \neq \log \left(\mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})} \left[\frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} \right] \right)$$

Jensen's Inequality

What we want to approximate is the marginal log-likelihood:

$$\log\left(\sum_{\mathbf{z}\in\mathcal{Z}}p_{\theta}(\mathbf{x},\mathbf{z})\right) = \log\left(\sum_{\mathbf{z}\in\mathcal{Z}}\frac{q(\mathbf{z})}{q(\mathbf{z})}p_{\theta}(\mathbf{x},\mathbf{z})\right) = \log\left(\mathbb{E}_{\mathbf{z}\sim q(\mathbf{z})}\left[\frac{p_{\theta}(\mathbf{x},\mathbf{z})}{q(\mathbf{z})}\right]\right)$$

- log() is a concave function. log $(px + (1-p)x') \ge p \log(x) + (1-p) \log(x')$.
- Idea: use Jensen Inequality (for concave functions)

$$\log \left(\mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})} \left[f(\mathbf{z}) \right] \right) = \log \left(\sum_{\mathbf{z}} q(\mathbf{z}) f(\mathbf{z}) \right) \ge \sum_{\mathbf{z}} q(\mathbf{z}) \log f(\mathbf{z})$$

Evidence Lower Bound

Log-Likelihood function for Partially Observed Data is hard to compute:

$$\log\left(\sum_{\mathbf{z}\in\mathcal{Z}}p_{\theta}(\mathbf{x},\mathbf{z})\right) = \log\left(\sum_{\mathbf{z}\in\mathcal{Z}}\frac{q(\mathbf{z})}{q(\mathbf{z})}p_{\theta}(\mathbf{x},\mathbf{z})\right) = \log\left(\mathbb{E}_{\mathbf{z}\sim q(\mathbf{z})}\left[\frac{p_{\theta}(\mathbf{x},\mathbf{z})}{q(\mathbf{z})}\right]\right)$$

- log() is a concave function. $\log(px + (1-p)x') \ge p\log(x) + (1-p)\log(x')$.
- Idea: use Jensen Inequality (for concave functions)

$$\log\left(\mathbb{E}_{\mathsf{z}\sim q(\mathsf{z})}\left[f(\mathsf{z})\right]\right) = \log\left(\sum_{\mathsf{z}} q(\mathsf{z})f(\mathsf{z})\right) \geq \sum_{\mathsf{z}} q(\mathsf{z})\log f(\mathsf{z})$$

Choosing $f(\mathbf{z}) = \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})}$ $\log\left(\mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})}\left[\frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})}\right]\right) \ge \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})}\left[\log\left(\frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})}\right)\right]$

Called Evidence Lower Bound (ELBO).

Variational inference

Suppose q(z) is any probability distribution over the hidden variables
Evidence lower bound (ELBO) holds for any q

$$\log p(\mathbf{x}; \theta) \geq \sum_{\mathbf{z}} q(\mathbf{z}) \log \left(\frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})} \right)$$

=
$$\sum_{\mathbf{z}} q(\mathbf{z}) \log p_{\theta}(\mathbf{x}, \mathbf{z}) - \sum_{\mathbf{z}} q(\mathbf{z}) \log q(\mathbf{z})$$

Entropy $H(q)$ of q
=
$$\sum_{\mathbf{z}} q(\mathbf{z}) \log p_{\theta}(\mathbf{x}, \mathbf{z}) + H(q)$$

• Equality holds if
$$q = p(\mathbf{z} | \mathbf{x}; \theta)$$

$$\log p(\mathbf{x}; \theta) = \sum_{\mathbf{z}} q(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}; \theta) + H(q)$$

• Variational Inference: Optimize over the possible *q*'s to make bound as tight as possible.

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Why is the bound tight

• We derived this lower bound that holds holds for any choice of q(z):

$$\log p(\mathbf{x}; \theta) \geq \sum_{\mathbf{z}} q(\mathbf{z}) \log \frac{p(\mathbf{x}, \mathbf{z}; \theta)}{q(\mathbf{z})}$$

• If $q(\mathbf{z}) = p(\mathbf{z}|\mathbf{x}; \theta)$ the bound becomes:

$$\sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x};\theta) \log \frac{p(\mathbf{x},\mathbf{z};\theta)}{p(\mathbf{z}|\mathbf{x};\theta)} = \sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x};\theta) \log \frac{p(\mathbf{z}|\mathbf{x};\theta)p(\mathbf{x};\theta)}{p(\mathbf{z}|\mathbf{x};\theta)}$$
$$= \sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x};\theta) \log p(\mathbf{x};\theta)$$
$$= \log p(\mathbf{x};\theta) \underbrace{\sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x};\theta)}_{=1}$$
$$= \log p(\mathbf{x};\theta)$$

- Confirms our previous importance sampling intuition: we should choose likely completions.
- In practice, the posterior p(z|x; θ) is intractable to compute. How loose is the bound?

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Variational inference continued

• Suppose q(z) is **any** probability distribution over the hidden variables. A little bit of algebra reveals

$$D_{KL}(q(\mathbf{z}) \| p(\mathbf{z} | \mathbf{x}; \theta)) = -\sum_{\mathbf{z}} q(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}; \theta) + \log p(\mathbf{x}; \theta) - H(q) \ge 0$$

• Rearranging, we re-derived the Evidence lower bound (ELBO)

$$\log p(\mathbf{x}; \theta) \geq \sum_{\mathbf{z}} q(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}; \theta) + H(q)$$

• Equality holds if $q = p(\mathbf{z}|\mathbf{x}; \theta)$ because $D_{KL}(q(\mathbf{z}) || p(\mathbf{z}|\mathbf{x}; \theta)) = 0$

$$\log p(\mathbf{x}; \theta) = \sum_{\mathbf{z}} q(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}; \theta) + H(q)$$

• Suppose q(z) is **any** probability distribution over the hidden variables. A little bit of algebra reveals

$$D_{KL}(q(\mathbf{z}) \| p(\mathbf{z} | \mathbf{x}; \theta)) = -\sum_{\mathbf{z}} q(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}; \theta) + \log p(\mathbf{x}; \theta) - H(q) \ge 0$$

• Rearranging, we get that

$$\log p(\mathbf{x}; \theta) = \text{ELBO} + D_{KL}(q(\mathbf{z}) \| p(\mathbf{z} | \mathbf{x}; \theta)).$$

The closer $q(\mathbf{z})$ is to $p(\mathbf{z}|\mathbf{x};\theta)$, the closer the ELBO is to the true log-likelihood

Variational Inference Optimizes the Evidence Lower Bound



- Variational inference: Optimize q to approximate the intractable posterior p(z|x; θ).
- Suppose q(z; φ) is a (tractable) probability distribution over the hidden variables parameterized by φ (variational parameters)
 - ${\, \bullet \,}$ For example, a Gaussian with mean and covariance specified by ϕ

$$q(\mathbf{z};\phi) = \mathcal{N}(\phi_1,\phi_2)$$

• Variational inference: pick ϕ so that $q(\mathbf{z}; \phi)$ is as close as possible to $p(\mathbf{z}|\mathbf{x}; \theta)$. In the figure, the posterior $p(\mathbf{z}|\mathbf{x}; \theta)$ (blue) is better approximated by $\mathcal{N}(2, 2)$ (orange) than $\mathcal{N}(-4, 0.75)$ (green)

Example: Optimizing Likelihood with Missing Data



- Assume p(x^{top}, x^{bottom}; θ) assigns high probability to images that look like digits. In this example, we assume z = x^{top} are unobserved (latent)
- Suppose q(x^{top}; φ) is a (tractable) probability distribution over the hidden variables (missing pixels in this example) x^{top} parameterized by φ (variational parameters)

$$q(\mathbf{x}^{top};\phi) = \prod_{i \neq j \neq j} (\phi_i)^{\mathbf{x}_i^{top}} (1-\phi_i)^{(1-\mathbf{x}_i^{top})}$$

unobserved variables \mathbf{x}_{i}^{top}

- Is $\phi_i = 0.5 \forall i \text{ a good approximation to the posterior } p(\mathbf{x}^{top} | \mathbf{x}^{bottom}; \theta)$? No
- Is $\phi_i = 1 \ \forall i$ a good approximation to the posterior $p(\mathbf{x}^{top} | \mathbf{x}^{bottom}; \theta)$? No
- Is $\phi_i \approx 1$ for pixels *i* corresponding to the top part of digit **9** a good approximation? Yes

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Summary: The Evidence Lower bound



 $\log p(\mathbf{x}; \theta) \geq \sum_{\mathbf{z}} q(\mathbf{z}; \phi) \log p(\mathbf{z}, \mathbf{x}; \theta) + H(q(\mathbf{z}; \phi)) = \underbrace{\mathcal{L}(\mathbf{x}; \theta, \phi)}_{\text{ELBO}}$ $\log p(\mathbf{x}; \theta) = \mathcal{L}(\mathbf{x}; \theta, \phi) + D_{\mathcal{K}I}(q(\mathbf{z}; \phi) || p(\mathbf{z} | \mathbf{x}; \theta))$

The better $q(\mathbf{z}; \phi)$ can approximate the posterior $p(\mathbf{z}|\mathbf{x}; \theta)$, the smaller $D_{KL}(q(\mathbf{z}; \phi)||p(\mathbf{z}|\mathbf{x}; \theta))$ we can achieve, the closer ELBO will be to $\log p(\mathbf{x}; \theta)$. Next: jointly optimize over θ and ϕ to maximize the ELBO over a dataset

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- Latent Variable Models Pros:
 - Easy to build flexible models
 - Suitable for unsupervised learning
- Latent Variable Models Cons:
 - Hard to evaluate likelihoods
 - Hard to train via maximum-likelihood
 - Fundamentally, the challenge is that posterior inference $p(\mathbf{z} \mid \mathbf{x})$ is hard. Typically requires variational approximations
- Next steps: scale-up variational inference to large datasets and neural networks
 - Amortized variational inference
 - Low variance gradient estimators and the reparametrization trick
- Alternative: give up on KL-divergence and likelihood (GANs)