Latent Variable Models

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Lecture 5

4 Autoregressive models:

Recap of last lecture

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

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Plan for today

Latent Variable Models

- Mixture models
- Variational autoencoder
- Variational inference and learning

Latent Variable Models: Motivation

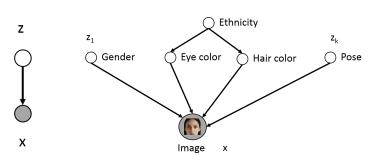


- Lots of variability in images **x** due to gender, eye color, hair color, pose, etc. However, unless images are annotated, these factors of variation are not explicitly available (latent).
- 2 Idea: explicitly model these factors using latent variables z

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Latent Variable Models: Motivation

Deep Latent Variable Models



- 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(x|z) could be much simpler than p(x)
 - If we had trained this model, then we could identify features via $p(\mathbf{z} \mid \mathbf{x})$, e.g., $p(EyeColor = Blue \mid \mathbf{x})$
- 3 Challenge: Very difficult to specify these conditionals by hand

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- Use neural networks to model the conditionals (deep latent variable models):
 - $\mathbf{0} \ \mathbf{z} \sim \mathcal{N}(\mathbf{0}, I)$
 - 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 $p(\mathbf{z} \mid \mathbf{x})$

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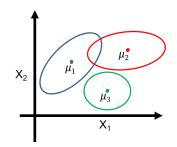
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Mixture of Gaussians: a Shallow Latent Variable Model

Mixture of Gaussians. Bayes net: $\mathbf{z} \rightarrow \mathbf{x}$.

- $\mathbf{z} \sim \text{Categorical}(1, \dots, K)$



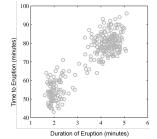
Generative process

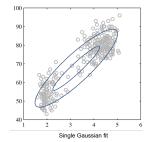
- \bigcirc Pick a mixture component k by sampling z
- Generate a data point by sampling from that Gaussian

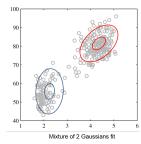
Mixture of Gaussians: a Shallow Latent Variable Model

Mixture of Gaussians:

- $\mathbf{z} \sim \text{Categorical}(1, \dots, K)$





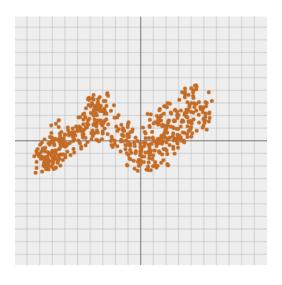


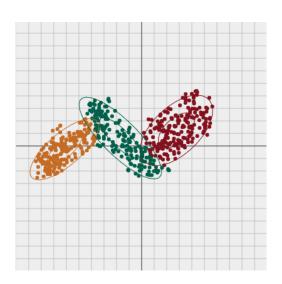
- Clustering: The posterior $p(\mathbf{z} \mid \mathbf{x})$ identifies the mixture component
- Unsupervised learning: We are hoping to learn from unlabeled data (ill-posed problem)

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Unsupervised learning

Unsupervised learning





Shown is the posterior probability that a data point was generated by the *i*-th mixture component, P(z = i|x)

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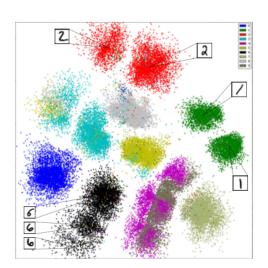
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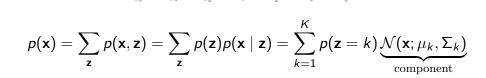
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Unsupervised learning

Mixture models



Alternative motivation: Combine simple models into a more complex and expressive one



Unsupervised clustering of handwritten digits.

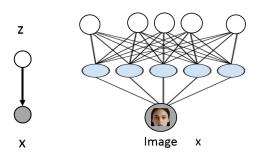
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Variational Autoencoder

Recap



A mixture of an infinite number of Gaussians:

- $\mathbf{0}$ $\mathbf{z} \sim \mathcal{N}(0, I)$
- $p(\mathbf{x} \mid \mathbf{z}) = \mathcal{N}(\mu_{\theta}(\mathbf{z}), \Sigma_{\theta}(\mathbf{z}))$ where $\mu_{\theta}, \Sigma_{\theta}$ are neural networks
 - $\mu_{\theta}(\mathbf{z}) = \sigma(A\mathbf{z} + c) = (\sigma(a_1\mathbf{z} + c_1), \sigma(a_2\mathbf{z} + c_2)) = (\mu_1(\mathbf{z}), \mu_2(\mathbf{z}))$
 - $\Sigma_{\theta}(\mathbf{z}) = diag(\exp(\sigma(B\mathbf{z} + d))) = \begin{pmatrix} \exp(\sigma(b_1\mathbf{z} + d_1)) & 0 \\ 0 & \exp(\sigma(b_2\mathbf{z} + d_2)) \end{pmatrix}$
 - $\theta = (A, B, c, d)$
- **3** Even though $p(\mathbf{x} \mid \mathbf{z})$ is simple, the marginal $p(\mathbf{x})$ is very complex/flexible

- Latent Variable Models
 - Allow us to define complex models $p(\mathbf{x})$ in terms of simpler building blocks $p(\mathbf{x} \mid \mathbf{z})$
 - Natural for unsupervised learning tasks (clustering, unsupervised representation learning, etc.)
 - No free lunch: much more difficult to learn compared to fully observed, autoregressive models

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Marginal Likelihood



- 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)

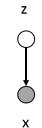
$$p(X, Z; \theta)$$

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)

Variational Autoencoder Marginal Likelihood



A mixture of an infinite number of Gaussians:

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

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

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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 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.

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Second attempt: Importance Sampling

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

$$p_{ heta}(\mathbf{x}) = \sum_{ ext{All possible values of } \mathbf{z}} p_{ heta}(\mathbf{x}, \mathbf{z}) = \sum_{\mathbf{z} \in \mathcal{Z}} rac{q(\mathbf{z})}{q(\mathbf{z})} p_{ heta}(\mathbf{x}, \mathbf{z}) = \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})} \left[rac{p_{ heta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})}
ight]$$

Monte Carlo to the rescue:

- **1** Sample $\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(k)}$ from $q(\mathbf{z})$
- 2 Approximate expectation with sample average

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

What is a good choice for $q(\mathbf{z})$? Intuitively, frequently sample \mathbf{z} (completions) that are likely given \mathbf{x} under $p_{\theta}(\mathbf{x}, \mathbf{z})$.

3 This is an unbiased estimator of $p_{\theta}(\mathbf{x})$

$$\mathbb{E}_{\mathsf{z}^{(j)}) \sim q(\mathsf{z})} \left[\frac{1}{k} \sum_{j=1}^k \frac{p_{\theta}(\mathsf{x}, \mathsf{z}^{(j)})}{q(\mathsf{z}^{(j)})} \right] = p_{\theta}(\mathsf{x})$$

First attempt: Naive Monte Carlo

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

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

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

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

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

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

Estimating log-likelihoods

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

$$p_{ heta}(\mathbf{x}) = \sum_{ ext{All possible values of } \mathbf{z}} p_{ heta}(\mathbf{x}, \mathbf{z}) = \sum_{\mathbf{z} \in \mathcal{Z}} rac{q(\mathbf{z})}{q(\mathbf{z})} p_{ heta}(\mathbf{x}, \mathbf{z}) = \mathbb{E}_{\mathbf{z} \sim q(\mathbf{z})} \left[rac{p_{ heta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})}
ight]$$

Monte Carlo to the rescue

- Sample $\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(k)}$ from $q(\mathbf{z})$
- 2 Approximate expectation with sample average (unbiased estimator):

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

Recall that for training, we need the *log*-likelihood log $(p_{\theta}(\mathbf{x}))$. We could estimate it as:

$$\log\left(p_{\theta}(\mathbf{x})\right) \approx \log\left(\frac{1}{k} \sum_{j=1}^{k} \frac{p_{\theta}(\mathbf{x}, \mathbf{z}^{(j)})}{q(\mathbf{z}^{(j)})}\right) \stackrel{k=1}{\approx} \log\left(\frac{p_{\theta}(\mathbf{x}, \mathbf{z}^{(1)})}{q(\mathbf{z}^{(1)})}\right)$$

However, it's clear that $\mathbb{E}_{\mathbf{z}^{(1)} \sim q(\mathbf{z})} \left[\log \left(\frac{p_{\theta}(\mathbf{x}, \mathbf{z}^{(1)})}{q(\mathbf{z}^{(1)})} \right) \right] \neq \log \left(\mathbb{E}_{\mathbf{z}^{(1)} \sim q(\mathbf{z})} \left[\frac{p_{\theta}(\mathbf{x}, \mathbf{z}^{(1)})}{q(\mathbf{z}^{(1)})} \right] \right)$

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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)

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

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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)

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

Choosing
$$f(\mathbf{z}) = \frac{p_{\theta}(\mathbf{x}, \mathbf{z})}{q(\mathbf{z})}$$

$$\log\left(\mathbb{E}_{\mathsf{z}\sim q(\mathsf{z})}\left[rac{p_{ heta}(\mathsf{x},\mathsf{z})}{q(\mathsf{z})}
ight]
ight) \geq \mathbb{E}_{\mathsf{z}\sim q(\mathsf{z})}\left[\log\left(rac{p_{ heta}(\mathsf{x},\mathsf{z})}{q(\mathsf{z})}
ight)
ight]$$

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

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

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

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

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

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

• (Aside: This is what we compute in the E-step of the EM algorithm)

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 $q(z) = p(z|x; \theta)$ the bound becomes:

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

$$= \sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x}; \theta) \log p(\mathbf{x}; \theta)$$

$$= \log p(\mathbf{x}; \theta) \sum_{\mathbf{z}} p(\mathbf{z}|\mathbf{x}; \theta)$$

$$= \log p(\mathbf{x}; \theta)$$

- Confirms our previous importance sampling intuition: we should choose likely completions.
- What if the posterior $p(\mathbf{z}|\mathbf{x};\theta)$ 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

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

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

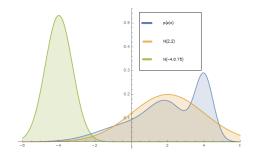
$$\log p(\mathbf{x}; \theta) = \sum_{\mathbf{z}} q(\mathbf{z}) \log p(\mathbf{z}, \mathbf{x}; \theta) + H(q)$$

• In general, $\log p(\mathbf{x}; \theta) = \text{ELBO} + D_{KL}(q(\mathbf{z}) || p(\mathbf{z} | \mathbf{x}; \theta))$. The closer q(z) is to $p(z|x;\theta)$, the closer the ELBO is to the true log-likelihood

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The Evidence Lower bound



- What if the posterior $p(\mathbf{z}|\mathbf{x};\theta)$ is intractable to compute?
- Suppose $q(\mathbf{z}; \phi)$ is a (tractable) probability distribution over the hidden variables parameterized by ϕ (variational parameters)
 - 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)

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A variational approximation to the posterior

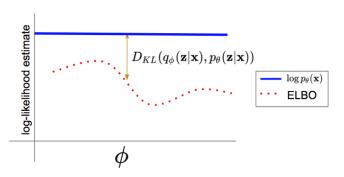


- Assume $p(\mathbf{x}^{top}, \mathbf{x}^{bottom}; \theta)$ assigns high probability to images that look like digits. In this example, we assume $z = x^{top}$ are unobserved (latent)
- Suppose $q(\mathbf{x}^{top}; \phi)$ is a (tractable) probability distribution over the hidden variables (missing pixels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

$$q(\mathbf{x}^{top}; \phi) = \prod_{\text{unobserved variables } \mathbf{x}_i^{top}} (\phi_i)^{\mathbf{x}_i^{top}} (1 - \phi_i)^{(1 - \mathbf{x}_i^{top})}$$

- Is $\phi_i = 0.5 \ \forall i$ 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

The Evidence Lower bound



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

The better $q(\mathbf{z}; \phi)$ can approximate the posterior $p(\mathbf{z}|\mathbf{x}; \theta)$, the smaller $D_{KI}(q(\mathbf{z};\phi)||p(\mathbf{z}|\mathbf{x};\theta))$ 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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Summary

- 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
- Alternative: give up on KL-divergence and likelihood (GANs)

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