Attention as a Latent Variable Model

February 20, 2018

VAEs

- Describes how the observed data are generated
- You've seen one example already:
  Language modeling : Given $x_1, \ldots, x_T$, fit $p_\theta(x_1, \ldots, x_T)$ to the data.

Conditional VAEs

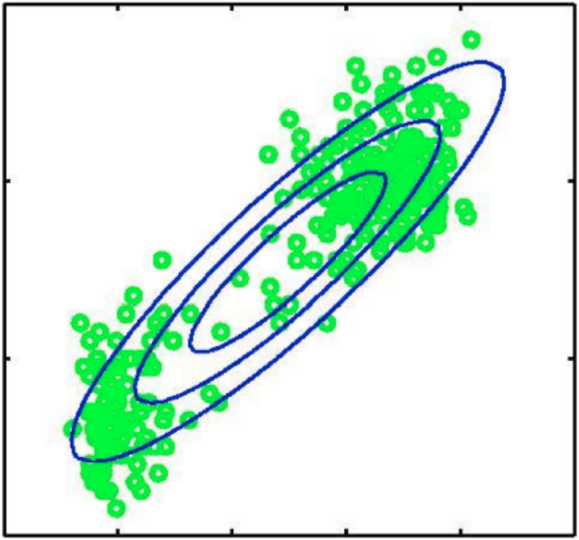
Often helpful to think of the underlying **generative story** (i.e. how one could generate data according to the model). E.g. for a bigram language model,

1. Draw $x_1 \sim p(X|Y = \langle \mathsf{s} \rangle)$
2. Draw $x_2 \sim p(X|Y = x_1)$
3. Draw $x_3 \sim p(X|Y = x_2)$
4. ...

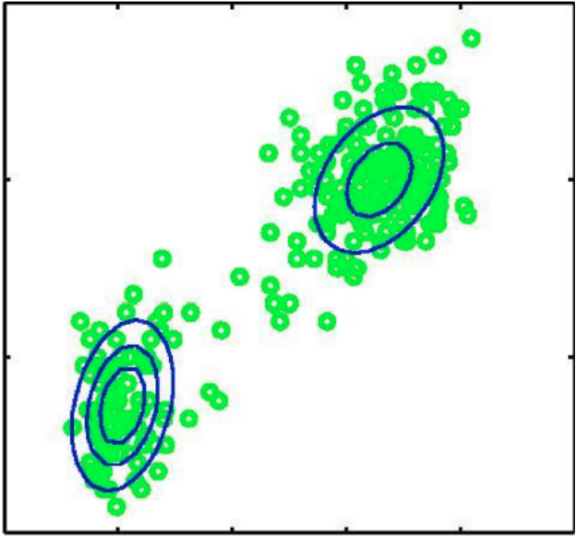
Variational RNN

- Language model: no latent variables, factorize $p(\mathbf{x})$ according to chain rule
- Latent variable models: Assumes **observed** data $\mathbf{x}$ are generated from **unobserved** latent variables $\mathbf{z}$
- Simplest case:
  1. Draw $\mathbf{z}$ from prior $p(\mathbf{z})$
  2. Draw $\mathbf{x}$ from conditional $p(\mathbf{x}|\mathbf{z})$
- Our setup:
  1. $p(\mathbf{z})$ usually simple
  2. $p_\theta(\mathbf{x}|\mathbf{z})$ parameterized with a deep model θ

Example: Mixture of Gaussians



Example: Mixture of Gaussians



Example: Mixture of Gaussians

Generative process for GMM with K mixture components:

For each data point,

1. Sample $z^{(i)} \sim \text{Categorical}(\frac{1}{K})$
2. Sample $\mathbf{x}^{(i)} \sim \mathcal{N}(\mu_{z^{(i)}}, \Sigma_{z^{(i)}})$

What is the prior? What is θ? What is $p_\theta(\mathbf{x})$? How do we learn?

Example: Deep Generative Models

MNIST digits, $\mathbf{x} \in \mathbb{R}^{784}$

1. Sample $\mathbf{z}^{(i)} \sim \mathcal{N}(0, I), \mathbf{z} \in \mathbb{R}^n$
2. Feed $\mathbf{z}^{(i)}$ through a one-layer feed-forward network

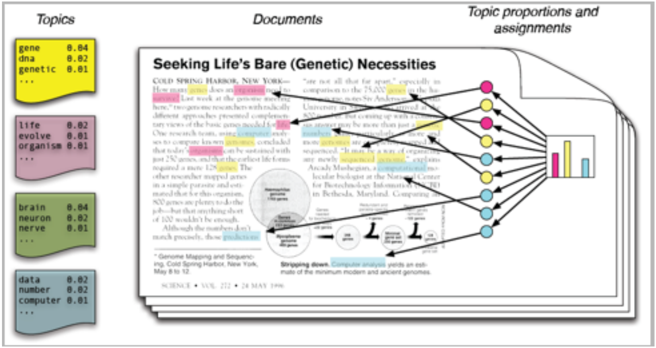
$$\mathbf{h} = \text{ReLU}(\mathbf{W}_1 \mathbf{z})$$

3. Sample $\mathbf{x}^{(i)} \sim \sigma(\mathbf{W}_2 \mathbf{h})$

Why Latent Variable Models?

- Learn useful representations from unlabeled data (unsupervised learning)
- Natural way of incorporating multimodality
- Able to capture complex, hierarchical generative processes

Why Latent Variable Models?



Learning in Latent Variable Models

Given data $\mathbf{x}^{(i)}, i = 1, \ldots, N$, want to maximize log-likelihood, i.e.

$$\max_\theta \sum_{i=1}^{N} \log p(\mathbf{x}^{(i)})$$

- No latent variables: usual setup
- Latent variables:

$$\max_\theta \sum_{i=1}^{N} \log \int_{\mathbf{z}} p_\theta(\mathbf{x}^{(i)}|\mathbf{z}^{(i)}) p(\mathbf{z}^{(i)}) d\mathbf{z}$$

(replace $\int$ with sum if $\mathbf{z}$ discrete)

Learning in Latent Variable Models

Variational Inference:

- Idea: Introduce a **variational** distribution $q_\lambda(\mathbf{z})$ parameterized by λ for each data point. Then,

$$\log p_\theta(\mathbf{x}) \geq \mathbb{E}_{q_\lambda(\mathbf{z})}[\log p_\theta(\mathbf{x}|\mathbf{z})] - KL[q_\lambda(\mathbf{z}) \| p(\mathbf{z})]$$

  (Derive on board)

- This is called the **evidence lower bound** or **ELBO**

- Running example: Gaussian variational family

$$q_\lambda(\mathbf{z}) = \mathcal{N}(\mu, \Sigma)$$

  i.e. $\lambda = [\mu, \Sigma]$

Evidence Lower Bound

Learning problem: Find $\lambda^{(i)}, \theta$ that maximize

$$\sum_{i=1}^{N} \mathbb{E}_{q_\lambda^{(i)}(\mathbf{z})}[\log p_\theta(\mathbf{x}^{(i)}|\mathbf{z}^{(i)})] - KL[q_{\lambda^{(i)}}(\mathbf{z})\|p(\mathbf{z}^{(i)})]$$

Coordinate ascent:

1. Hold θ fixed, maximize ELBO with respect to $\lambda^{(i)}$'s
2. Hold $\lambda^{(i)}$'s fixed, maximize ELBO with respect to θ
3. Repeat

In certain cases coordinate ascent admits analytic update formulas

Examining the ELBO

Consider a single point

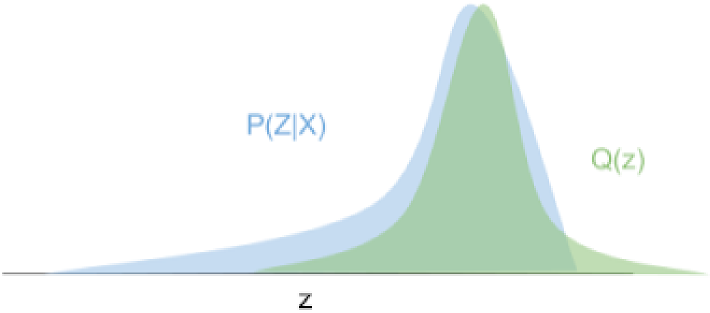
$$ELBO = \log p_\theta(\mathbf{x}) - KL[q_\lambda(\mathbf{z}) \| p_\theta(\mathbf{z}|\mathbf{x}))]$$

Claim: Setting $q_\lambda(\mathbf{z}) = p_\theta(\mathbf{z}|\mathbf{x})$ makes the bound tight, i.e.

$$ELBO = \log p_\theta(\mathbf{x})$$

- Justifies why optimizing the ELBO is a good idea
- But why can't we do this all the time?

Posterior vs Variational Family



Examining the ELBO

$$ELBO = \log p_\theta(\mathbf{x}) - KL[q_\lambda(\mathbf{z}) \| p_\theta(\mathbf{z}|\mathbf{x}))]$$

- Usually, we will be learning the generative model θ
- But if we are just interested in inference (e.g. at test time), we can minimize with respect to $q_\lambda(\mathbf{z})$

$$KL[q_\lambda(\mathbf{z}) \| p_\theta(\mathbf{z}|\mathbf{x})]$$

- "Inference as optimization"

Yet another view of ELBO

Rearranging some terms, we also get that

$$\begin{aligned} ELBO &= \log p_\theta(\mathbf{x}) - KL[q_\lambda(\mathbf{z}) \| p_\theta(\mathbf{z}|\mathbf{x})) \\ &= \mathbb{E}_{q_\lambda(\mathbf{z})}[\log p_\theta(\mathbf{x}, \mathbf{z})] + \mathbb{H}[q_\lambda(\mathbf{z})] \end{aligned}$$

1. Hold θ fixed, set $q_\lambda(\mathbf{z}) = p_\theta(\mathbf{z}|\mathbf{x})$ (suppose this is tractable)
2. Hold $q_\lambda(\mathbf{z})$ fixed, maximize

$$\mathbb{E}_{q_\lambda(\mathbf{z})}[\log p_\theta(\mathbf{x}, \mathbf{z})]$$

   ($\mathbb{H}[q_\lambda(\mathbf{z})]$ constant with respect to θ)

(This is exactly the EM algorithm)

Stochastic Variational Inference

$$\sum_{i=1}^{N} \mathbb{E}_{q_{\lambda}^{(i)}(\mathbf{z})}[\log p_\theta(\mathbf{x}^{(i)}|\mathbf{z}^{(i)})] - KL[q_{\boldsymbol{\lambda}^{(i)}}(\mathbf{z})\|p(\mathbf{z}^{(i)})]$$

- Coordinate ascent is impractical on large datasets (need to find optimal $\lambda^{(i)}$ for all i, then update θ)
- Idea: Just use minibatches (or single datum) $\implies$ Stochastic Variational Inference

Stochastic Variational Inference (Hoffman et al. 2013)

Define ELBO with respect to single datum

$$ELBO(\mathbf{x}, \lambda, \theta) = \mathbb{E}_{q_\lambda(\mathbf{z})}[\log p_\theta(\mathbf{x}|\mathbf{z})] - KL[q_\lambda(\mathbf{z}) \| p(\mathbf{z})]$$

1. Sample $\mathbf{x} \sim p_{\mathcal{D}}(\mathbf{x})$
2. Randomly initialize λ_0
3. For number of steps, optimize ELBO wrt λ with gradient ascent, i.e. for $k = 1, \dots, K$

$$\lambda_k \leftarrow \lambda_{k-1} + \alpha \nabla_\lambda ELBO(\mathbf{x}, \theta, \lambda_0)$$

4. Optimize ELBO wrt θ, i.e.

$$\theta \leftarrow \theta + \alpha \nabla_\theta ELBO(\mathbf{x}, \theta, \lambda_K)$$

Stochastic Variational Inference

Need to compute: $\nabla_\lambda ELBO(\mathbf{x}, \theta, \lambda)$, $\nabla_\theta ELBO(\mathbf{x}, \theta, \lambda)$

- Easy:
  $\nabla_\theta ELBO(\mathbf{x}, \theta, \lambda) = \mathbb{E}_{q_\lambda(\mathbf{z})}[\nabla_\theta \log p_\theta(\mathbf{x}|\mathbf{z})]$

- Hard:
  $\nabla_\lambda ELBO(\mathbf{x}, \theta, \lambda) = \nabla_\lambda \mathbb{E}_{q_\lambda(\mathbf{z})}[\log p_\theta(\mathbf{x}|\mathbf{z})] - \nabla_\lambda KL[q_\lambda(\mathbf{z}) \| p(\mathbf{z})]$

In the fully general case, need score function (i.e. policy gradients/ REINFORCE) from last lecture

The Reparameterization Trick

- Until now: $p(\mathbf{z}), q_\lambda(\mathbf{z})$ arbitrary distributions
- From hereon: $p(\mathbf{z}) = N(0, I)$, $q_\lambda(\mathbf{z}) = N(\mu, \Sigma)$
- The variational family is given by Gaussian with mean vector μ and covariances Σ (i.e. $\lambda = [\mu, \Sigma]$)
- Σ usually diagonal
- This allows low-variance estimators for $\nabla_\lambda ELBO(\mathbf{x}, \theta, \lambda)$

The Reparameterization Trick

$$\underbrace{\mathbb{E}_{q_\lambda(\mathbf{z})}[\log p_\theta(\mathbf{x}|\mathbf{z})]}_{\text{1. Reparameterization trick}} \quad - \quad \underbrace{KL[q_\lambda(\mathbf{z})\|p(\mathbf{z})]}_{\text{2. Analytic formula for Gaussian family}}$$

- Reparameterization trick (pathwise derivatives): Exploit the fact that Gaussians are **reparameterizable**
- Drawing $\mathbf{z}$ from $N(\mu, \Sigma)$ is the same as drawing $\epsilon \sim N(0, I)$ and applying the transformation

  $$\mathbf{z} = \mu + A\epsilon$$

  where $AA^\top = \Sigma$ (obtained from, for example, Cholesky decomposition)
- If Σ is diagonal, $\text{diag}(A) = [\sigma_1, \ldots, \sigma_n]$

The Reparameterization Trick

$\lambda = [\mu, \sigma^2]$

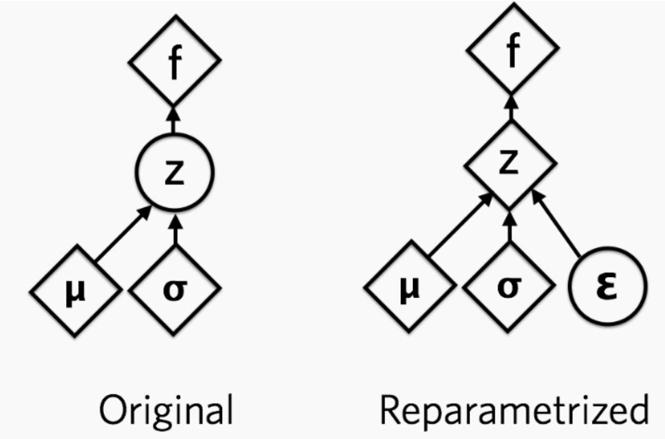
$$
\begin{aligned}
&\nabla_\lambda \mathbb{E}_{q_\lambda(\mathbf{z})}[\log p_\theta(\mathbf{x}|\mathbf{z})] \\
=&\nabla_\lambda \mathbb{E}_{\epsilon \sim N(0,I)}[\log p_\theta(\mathbf{x}|\mu + \epsilon\sigma)] \\
=&\mathbb{E}_{\epsilon \sim N(0,I)}[\nabla_\lambda \log p_\theta(\mathbf{x}|\mu + \epsilon\sigma)]
\end{aligned}
$$

- Now we just need samples from a **fixed** distribution $\epsilon \sim N(0, I)$
- Empirically this has lower variance than REINFORCE estimator

$$\mathbb{E}_{q_\lambda(\mathbf{z})}[\log p_\theta(\mathbf{x}|\mathbf{z}) \nabla_\lambda \log q_\lambda(\mathbf{z})]$$

- (But both are unbiased estimators)

The Reparameterization Trick



(Circles are stochastic nodes)

Variational Autoencoders/Amortized Inference

Amortized variational inference (Mnih et al. 2014, Kingma and Welling 2014, Rezende et al. 2014):

- **Predict** the variational parameters to be a function of the input

$$\lambda(\mathbf{x}) = enc_{\phi}(\mathbf{x})$$

- The **inference network** (or encoder/recognition network), parameterized by ϕ, is shared (i.e. amortized) across all $\mathbf{x}$
- "Inference as prediction"

Variational Autoencoders/Amortized Inference

Learning problem

$$\max_{\phi,\theta} \; \mathbb{E}_{q_{enc_\phi(\mathbf{x})}}[\log p_\theta(\mathbf{x}|\mathbf{z})] - KL[q_{enc_\phi(\mathbf{x})}(\mathbf{z}) \| p(\mathbf{z})]$$

Why Variational "Autoencoder"

$$\min_{\phi,\theta} \; \underbrace{\mathbb{E}_{q_{enc_\phi(\mathbf{x})}}[-\log p_\theta(\mathbf{x}|\mathbf{z})]}_{\text{Reconstruction loss}} + \underbrace{KL[q_{enc_\phi(\mathbf{x})}(\mathbf{z}) \| p(\mathbf{z})]}_{\text{Regularizer}}$$

Variational Autoencoders/Amortized Inference

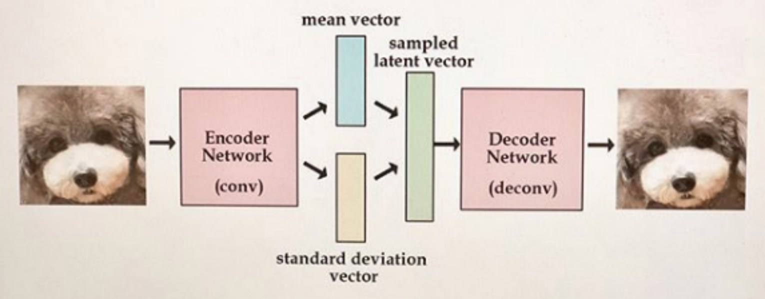
End-to-end training with backprop (no coordinate ascent)

1. Sample $\mathbf{x} \sim p_{\mathcal{D}}(\mathbf{x})$
2. Run inference network

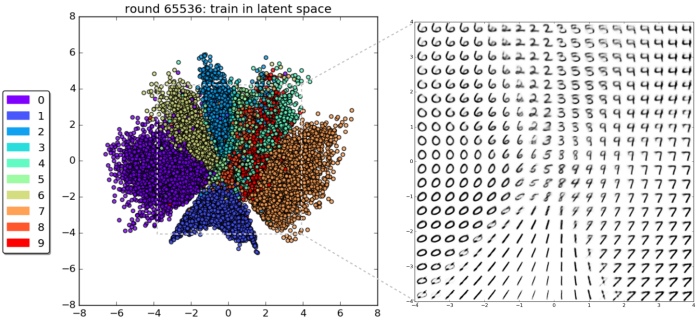
$$\mu(\mathbf{x}), \sigma^2(\mathbf{x}) = enc_{\phi}(\mathbf{x})$$

3. Sample $\epsilon \sim N(0, I)$, reparameterize $\mathbf{z} = \mu(\mathbf{x}) + \sigma(\mathbf{x})\epsilon$
4. Calculate loss $\mathcal{L} = -\log p_{\theta}(\mathbf{x}|\mathbf{z}) + KL(q_{\lambda}(\mathbf{z})\|p(\mathbf{z}))$
5. Update θ, ϕ based on $\nabla_{\theta}\mathcal{L}, \nabla_{\phi}\mathcal{L}$

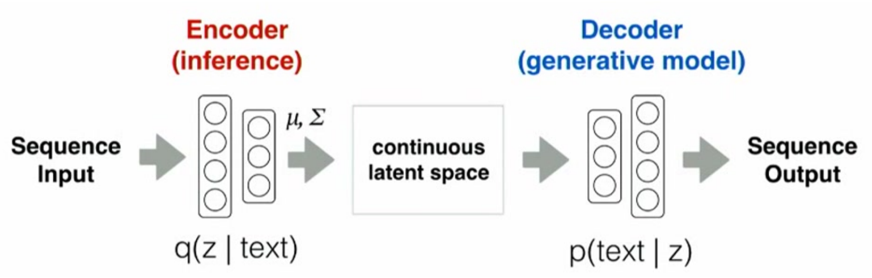
Variational Autoencoders for Images



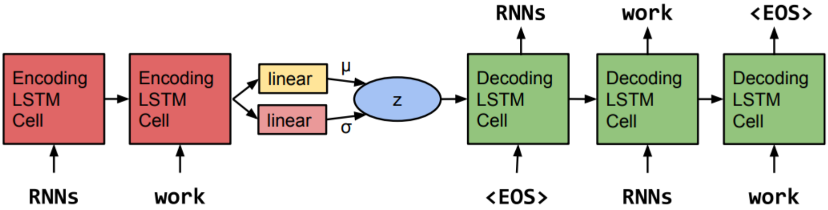
Variational Autoencoders for Images



Variational Autoencoders for Text Processing



Variational Autoencoders for Text Processing



Practical Issues

- Parameterization: Use $\log \sigma^2$ instead of σ^2
- Tricks: KL-annealing, word-dropout

Takeaways

- Variational Inference: “Inference as Optimization”
- Amortized Inference: “Optimization as Prediction”