Deep Generative Models

Philip Schulz and Wilker Aziz

Generative Models

First Attempt: Log-linear Models

Second Attempt: Wake-Sleep

This is how we do: Variational Autoencoders

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Recap: Generative Models

Joint distribution over observed data x and latent variables Z.

$$p(x, z | \alpha) = \overbrace{p(x | z, \alpha)}^{\text{likelihood}} \underbrace{p(z | \alpha)}_{\text{prior}}$$

The likelihood and prior are often standard distributions (Gaussian, Bernoulli) with simple dependence on conditioning information.

Recap: Variational Inference

Objective

$$\max_{q(z)} \mathbb{E}\left[\log p(x,z)\right] + \mathbb{H}\left(q(z)\right)$$

- ▶ The ELBO is a lower bound on log p(x)
- Mean field assumption: $q(z) = \prod_{i=1}^{N} q(z_i)$

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Feature-rich Generative Models

Let us assume that z has internal structure (features). How can we exploit that?

First Idea

Make $p(x|z, \alpha)$ a log-linear model.

- Only discrete data
- ► Trainable with EM if we can efficiently enumerate \mathcal{X} and \mathcal{Z} .

Log-linear Model

Let us treat z as observed.

$$p(x|z, \alpha = w) = \frac{\exp\left(w^{\top}f(x, z)\right)}{\sum_{x \in \mathcal{X}} \exp\left(w^{\top}f(x, z)\right)}$$

Log-linear Model

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$$\frac{d}{dw}\log p(x|z,w) = f(x,z) - \mathbb{E}\left[f(X,z)|z,w\right]$$

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Weight Gradient

$$\frac{d}{dw}\log p(x|z,w) = f(x,z) - \mathbb{E}\left[f(X,z)|z,w\right]$$

Updates need to be performed iteratively.

Now let us treat z as latent.

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Model

$$p(x, z | w) = \underbrace{\frac{\exp\left(w^{\top} f(x, z)\right)}{\sum_{x \in \mathcal{X}} \exp\left(w^{\top} f(x, z)\right)}}_{p(x | z, w)} \times \underbrace{p(z)}_{arbitrary}$$

Posterior

$$p(z|x, w) = \frac{p(x, z|w)}{p(x|w)} = \frac{p(x, z|w)}{\sum_{z} p(x, z|w)} = \frac{\exp(w^{T}f(x,z))}{\frac{\sum_{x \in \mathcal{X}} \exp(w^{T}f(x,z))}{\sum_{z} \frac{\exp(w^{T}f(x,z))}{\sum_{x \in \mathcal{X}} \exp(w^{T}f(x,z))} \times p(z)}}$$

$$\frac{d}{dw} \mathbb{E}_{p(z|x,w)} \left[\log p(x,z|w) \right] =$$

$$\frac{d}{dw} \sum_{z} p(z|x,w) \log p(x,z|w) =$$

$$\sum_{z} p(z|x,w) \frac{d}{dw} \log p(x,z|w)$$

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$$\sum_{z} p(z|x,w) \underbrace{\frac{d}{dw} \log p(x,z|w)}_{\text{We've already solved this!}}$$

$$\frac{d}{dw} \mathbb{E}_{\rho(z|x,w)} \left[\log \rho(x,z|w) \right] = \\ \mathbb{E}_{\rho(z|x,w)} \left[f(x,Z)|x,w \right] - \mathbb{E}_{\rho(z|x,w)} \left[\mathbb{E} \left[(f(X,Z)|Z,w) \right] \right]$$

Weight Gradient

$$\frac{d}{dw} \mathbb{E}_{\rho(z|x,w)} \left[\log \rho(x,z|w) \right] = \\ \mathbb{E}_{\rho(z|x,w)} \left[f(x,Z)|x,w \right] - \mathbb{E}_{\rho(z|x,w)} \left[\mathbb{E} \left[(f(X,Z)|Z,w) \right] \right]$$

Procedurally

$$\mathsf{E}_{\mathsf{-}}\mathsf{count}(x,z)$$
 - $\mathsf{E}_{\mathsf{-}}\mathsf{count}(x,z)$ $\times \mathbb{E}\left[X|z,w\right]$

EM

E-step
$$p(z|x, w) = \frac{p(x,z|w)}{\sum_{z} p(x,z|w)}$$
 in $\mathcal{O}(|\mathcal{X}| \times |\mathcal{Z}|)$
M-step Iteratively optimise w to match $\mathsf{E}_\mathsf{count}(x,z)$ with $\mathsf{E}_\mathsf{count}(x,z) \times \mathbb{E}[X|z,w]$

Restrictions

- Only log-linear models
- Scales badly

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Wake-sleep Algorithm

- Generalise latent variables to Neural Networks
- Train generative neural model
- Use variational inference! (kind of)

2 Neural Networks:

▶ A generation network to model the data (the one we want to optimise) – parameters: θ

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- A generation network to model the data (the one we want to optimise) parameters: θ
- An inference (recognition) network (to model the latent variable) – parameters: λ
- Original setting: binary hidden units
- ▶ Training is performed in a "hard EM" fashion

Wake-sleep Training

Wake Phase

- Use inference network to sample hidden unit setting z from $q(z|x,\lambda)$
- ▶ Update generation parameters θ to maximize liklelihood of data given latent state $p(x|z,\theta)$

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Sleep Phase

- Produce dream sample \tilde{x} from random hidden unit z
- ▶ Update inference parameters λ to maximize probability of latent state $q(z|\tilde{x}, \lambda)$

Wake Phase Objective

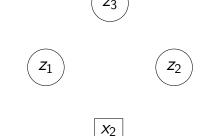
Assumes latent state z to be fixed random draws from $q(z|x, \lambda)$.

$$\max_{\theta} \log p(x|z, \theta)$$

This is simply supervised learning with imputed latent data!

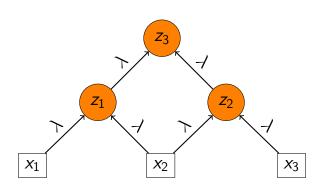
Wake Phase Sampling

 x_1

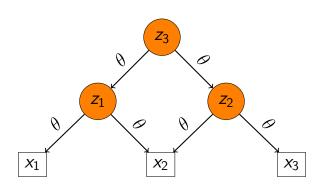


*X*3

Wake Phase Sampling



Wake Phase Update



Sleep Phase Objective

Assumes fake data \tilde{x} and latent variables z to be fixed random draw from $p(x, z|\theta)$.

$$\min_{\lambda} \ \mathbb{E}_{q(z|\tilde{x},\lambda)} \left[\log p(\tilde{x},z|\theta) \right] + \mathbb{H} \left(q(z|\tilde{x},\lambda) \right)$$

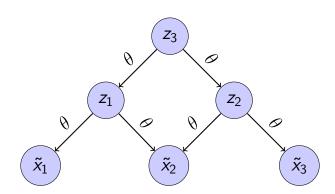
Sleep Phase Sampling



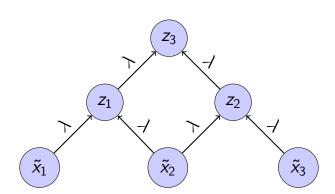




Sleep Phase Sampling



Sleep Phase Update



Wake-sleep Algorithm

Advantages

- Simple layer-wise updates
- Amortised inference: all latent variables are inferred from the same weights λ

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Drawbacks

- Inference and generative networks are trained on different objectives
- Inference weights \(\lambda \) are updated on fake data \(\tilde{x} \)
- Generative weights are bad initially, giving wrong signal to the updates of λ

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Define model $p(x, z|\theta) = p(x|z, \theta)p(z)$ where the likelihood $p(x|z, \theta)$ is given by a neural network. (We fix p(z) for simplicity.)

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Problem

 $p(x) = \int p(x|z,\theta)p(z)dz$ is hard to compute.

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Define model $p(x, z|\theta) = p(x|z, \theta)p(z)$ where the likelihood $p(x|z, \theta)$ is given by a neural network. (We fix p(z) for simplicity.)

Problem

$$p(x) = \int \underbrace{p(x|z,\theta)}_{\substack{\text{highly} \\ \text{non-linear!}}} p(z) dz$$
 is hard to compute.

$$\log p(x) \geq \underbrace{\mathbb{E}_{q(z|x,\lambda)} \left[\log p(x,z|\theta)\right] + \mathbb{H}\left(q(z|x,\lambda)\right)}_{ ext{ElBO}}$$

$$\begin{split} \log p(x) & \ge \overbrace{\mathbb{E}_{q(z|x,\lambda)} \left[\log p(x,z|\theta) \right] + \mathbb{H} \left(q(z|x,\lambda) \right)}^{\mathsf{ELBO}} \\ & = \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) p(z) \right] + \mathbb{H} \left(q(z|x,\lambda) \right) \end{split}$$

$$\begin{split} \log p(x) &\geq \underbrace{\mathbb{E}_{q(z|x,\lambda)} \left[\log p(x,z|\theta) \right] + \mathbb{H} \left(q(z|x,\lambda) \right)}_{\text{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) p(z) \right] + \mathbb{H} \left(q(z|x,\lambda) \right)} \\ &= \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \right] - \mathsf{KL} \left(p(z) \mid\mid q(z|x,\lambda) \right) \end{split}$$

$$\begin{split} \log p(x) &\geq \underbrace{\mathbb{E}_{q(z|x,\lambda)} \left[\log p(x,z|\theta) \right] + \mathbb{H} \left(q(z|x,\lambda) \right)}_{\text{essume analytical}} \\ &= \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) p(z) \right] + \mathbb{H} \left(q(z|x,\lambda) \right) \\ &= \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \right] - \underbrace{\mathsf{KL} \left(p(z) \mid\mid q(z|x,\lambda) \right)}_{\text{assume analytical}} \\ & \text{(true for exponential families)} \end{split}$$

$$\log p(x) \geq \underbrace{\mathbb{E}_{q(z|x,\lambda)} \left[\log p(x,z|\theta)\right] + \mathbb{H}\left(q(z|x,\lambda)\right)}_{\text{elements}}$$

$$= \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta)p(z)\right] + \mathbb{H}\left(q(z|x,\lambda)\right)$$

$$= \underbrace{\mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta)\right]}_{\text{approximate by sampling}} - \underbrace{\mathsf{KL}\left(p(z)\mid\mid q(z|x,\lambda)\right)}_{\text{assume analytical (true for exponential families)}}$$

$$\frac{d}{d\theta} \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \right] - \overbrace{\mathsf{KL} \left(p(z) \mid\mid q(z|x,\lambda) \right)}^{constant}$$

$$\frac{d}{d\theta} \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \right] - \overbrace{\mathsf{KL} \left(p(z) \mid \mid q(z|x,\lambda) \right)}^{constant}$$

$$= \mathbb{E}_{q(z|x,\lambda)} \left[\frac{d}{d\theta} \log p(x|z,\theta) \right]$$

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$$= \mathbb{E}_{q(z|x,\lambda)} \left[\frac{d}{d\theta} \log p(x|z,\theta) \right]$$

$$\stackrel{\mathsf{MC}}{\approx} \frac{1}{S} \sum_{i=1}^{S} \frac{d}{d\theta} \log p(x|z_i,\theta)$$

$$\frac{d}{d\theta} \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \right] - \overbrace{\mathsf{KL} \left(p(z) \mid \mid q(z|x,\lambda) \right)}^{constant}$$

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Note: $q(z|x,\lambda)$ does not depend on θ .

$$\frac{d}{d\lambda} \left[\mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \right] - \mathsf{KL} \left(p(z) \mid\mid q(z|x,\lambda) \right) \right]$$

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The first term again requires approximation by sampling

$$\frac{d}{d\lambda} \mathbb{E}_{q(z|x,\lambda)} \left[\log p(x|z,\theta) \right] \\
= \frac{d}{d\lambda} \int q(z|x,\lambda) \log p(x|z,\theta) dz$$

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MC estimator non-differentiable

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MC estimator non-differentiable

• Sampling z neglects $\frac{d}{d\lambda}q(z|x,\lambda)$

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MC estimator non-differentiable

- ▶ Sampling z neglects $\frac{d}{d\lambda}q(z|x,\lambda)$
- ▶ Differentiating $q(z|x, \lambda)$ breaks the expectation

$$= \frac{d}{d\lambda} \int q(z|x,\lambda) \log p(x|z,\theta) dz$$

$$= \frac{d}{d\lambda} \int q(z|x,\lambda) \log p(x|z,\theta) dz$$
$$= \frac{d}{d\lambda} \int q(\epsilon) \log p(x|h(\epsilon,\lambda),\theta) d\epsilon$$

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$$\stackrel{\text{MC}}{\approx} \frac{1}{S} \sum_{i=1}^{S} \frac{d}{d\lambda} \log p(x|h(\epsilon_{i},\lambda),\theta) \times \frac{d}{d\lambda} h(\epsilon,\lambda)$$

Reparametrisation Trick

- Find transformation $h(\epsilon, \lambda)$ of parameter-free variable ϵ
- $h(\epsilon, \lambda)$ needs to be invertible
- $h(\epsilon, \lambda)$ needs to be differentiable

Gaussian Transformation

Affine property

$$Ax + b \sim \mathcal{N}\left(\mu + b, A\Sigma A^{T}\right) \text{ for } x \sim \mathcal{N}\left(\mu, \Sigma\right)$$

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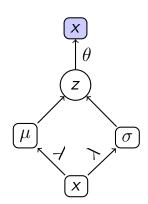
Gaussian transformation

$$h(\epsilon, \lambda) = \mu(x, \lambda) + \sigma(x, \lambda) \odot \epsilon \quad \epsilon \sim \mathcal{N}(0, 1)$$

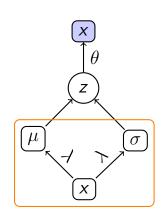
Gaussian KL

Analytical computation of $- KL(q(z|x, \lambda) || p(z))$:

$$-\frac{1}{2}\sum_{i=1}^{N}\left(1+\log\left(\sigma_{i}^{2}\right)-\mu_{i}-\sigma_{i}^{2}\right)$$

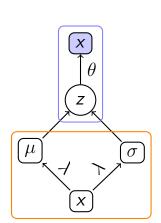


inference model



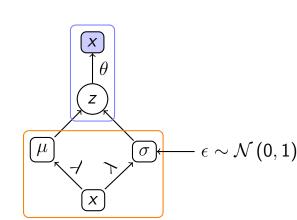
generation model

inference model



generation model

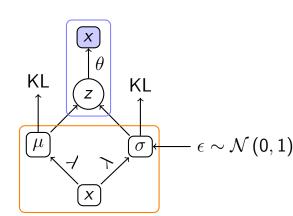
inference model



Computation Graph

generation model

inference model



Example

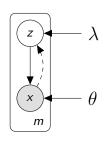
- Data: binary mnist
- Likelihood: product of Bernoullis
 - Let $\phi = \sigma(NN(z))$
- ▶ Prior over z: $\mathcal{N}(0,1)$
- $q(z|x,\lambda) = \mathcal{N}\left(\mu(x,\lambda), \sigma(x,\lambda)^2\right)$
- $\mu(x,\lambda) = \mathsf{NN}_{\mu}(x;\lambda)$

Example

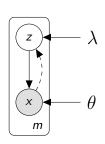
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Mean Field assumption

Variational approximation factorises over latent dimensions

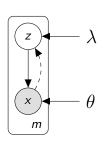


▶ approximate posterior $q(z|x,\lambda) = \mathcal{N}(\mu(x,\lambda), \sigma(x,\lambda)^2)$



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- where

$$\mu(x,\lambda) = \mathsf{NN}_{\mu}(x;\lambda)$$
 e.g. $\mu(x,\lambda) = W^{(u)}x + b^{(u)}$

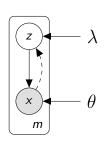


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e.g. $\mu(x,\lambda) = W^{(u)}x + b^{(u)}$

$$\sigma(x,\lambda) = \exp(\mathsf{NN}_{\sigma}(x;\lambda))$$
e.g. $\sigma(x,\lambda) = \log(1 + \exp(W^{(v)}x + b^{(v)}))$



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•
$$\sigma(x,\lambda) = \exp(\mathsf{NN}_{\sigma}(x;\lambda))$$

e.g. $\sigma(x,\lambda) = \log(1 + \exp(W^{(v)}x + b^{(v)}))$

$$\lambda = (W^{(u)}, \dot{W}^{(v)}, b^{(u)}, b^{(v)})$$

Variational Autoencoder

Advantages

- Backprop training
- Easy to implement
- Posterior inference possible
- One objective for both NNs

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Drawbacks

- Discrete latent variables are difficult
- Optimisation may be difficult with several latent variables

Summary

- ▶ When $|\mathcal{X}|$ and $|\mathcal{Z}|$ are not too large, we can do EM with features
- Otherwise use VI with simple approximation
- Wake-Sleep: train inference and generation networks with separate objectives
- VAE: train both networks with same objective
- Reparametrisation
 - ▶ Transform parameter-free variable ϵ into latent value z
 - Update parameters with stochastic gradient estimates

Literature I

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Literature II

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