Auto-encoding variational Bayes

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Mobile Robotics Lab Reading Group, McGill University

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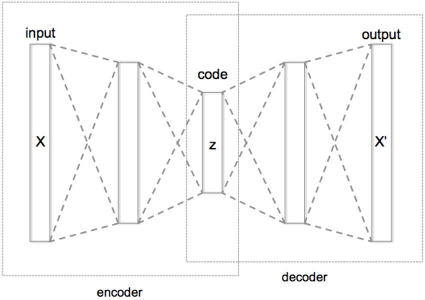
Overview

- Auto-encoders
- Variational Inference
- An example: data from mixture of Gaussians
- Evidence Lower Bound (ELBO)
- Mean-field approximation
- Optimization algorithms for VI and stochastic VI
- Auto-encoding variational Bayes

Auto-encoders



Unsupervised learning of efficient encodings $\mathbf{z}$ of observed data $\mathbf{x}$

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Variational Inference: definitions

- Latent variables $\mathbf{z} \in \mathbb{R}^m$ and observed data $\mathbf{x} = x_{1:n}$
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- Joint model is $p(\mathbf{z}, \mathbf{x}) = p(\mathbf{z})p(\mathbf{x}|\mathbf{z})$
- *Inference* means computing the posterior $p(\mathbf{z}|\mathbf{x})$
- *Inference* $=$ How do we encode the given data $\mathbf{x}$ using latent variables $\mathbf{z}$?

Some ways of computing $p(\mathbf{z}|\mathbf{x})$

- **MCMC**: Gibbs, Hamiltonian Monte Carlo, Metropolis-Hastings, etc.
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- **MCMC**: Gibbs, Hamiltonian Monte Carlo, Metropolis-Hastings, etc.
- Most of them slow (large mixing times)
- **Analytically**: $p(\mathbf{z}|\mathbf{x}) = p(\mathbf{z}, \mathbf{x})/p(\mathbf{x})$
- Computing the evidence $p(\mathbf{x})$ may be intractable

Variational Inference: main idea

- $q^*(\mathbf{z}) = \underset{q(\mathbf{z}) \in \mathcal{Q}}{\operatorname{argmin}} \, \mathsf{KL}(q(\mathbf{z}) \,||\, p(\mathbf{z}|\mathbf{x}))$
- $\mathcal{Q}$ is a family of "simpler" distributions q compared to p.

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- $\mathcal{Q}$ is a family of "simpler" distributions q compared to p.
- KL divergence is an asymmetric, nonnegative measure, not a norm. It doesn't obey the triangle inequality.
- It measures the extra bits you need to spend to compress samples from q using a code optimized for p.
- Difference measure between probability distributions.

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An example: data from mixture of Gaussians

- K mixture components, corresponding to normal distributions
- Means $\boldsymbol{\mu} = \{\mu_1, ..., \mu_K\} \sim \mathcal{N}(0, \sigma^2 \boldsymbol{I})$
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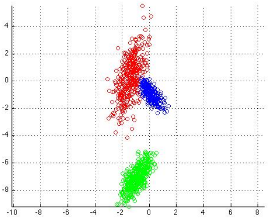

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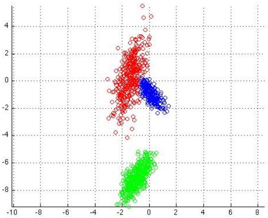

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- In this particular example we can use EM, but in general it assumes that you know $p(\mathbf{z}|\mathbf{x})$

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Variational Inference $\rightarrow$ find $q(\mathbf{z})$ that maximizes ELBO_q

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Mean-field approximation

- Simplification for posterior approximator $q(\mathbf{z})$:
- $q(\mathbf{z}) = \prod_j q_j(z_j)$
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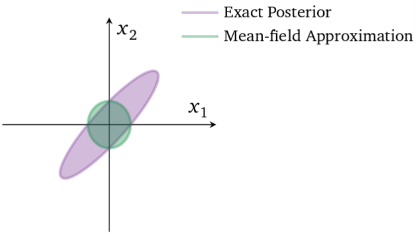

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- Algo $\#1$: coordinate ascent along each latent variable of ELBO
- Main problem is that it evaluates ELBO on the entire dataset (not great for big data)
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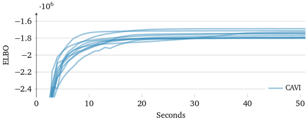

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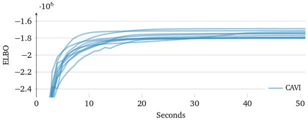

Figure 2: Different initializations may lead CAVI to find different local optima of the ELBO.

- Algo $\#2$: stochastic optimization over all latent variables
- Uses the natural gradient to account for manifold on which distributions live
- Evaluates ELBO on single data points, or minibatches

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Auto-encoding Variational Bayes: assumptions

- Data $x_i \in \mathbb{R}^d$ are i.i.d and generated from a parametric graphical model:
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- Large dataset, and intractable evidence $p_{\theta^*}(\mathbf{x})$ and posterior $p_{\theta^*}(\mathbf{z}|\mathbf{x})$ distributions

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- VI approximation of parametric evidence $p_{\theta^*}(\mathbf{x})$
- Usage of a reparametrization trick explained by Luc Devroye in 1986

Auto-encoding Variational Bayes: ELBO maximization

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Stochastic gradient ascent with minibatches to maximize ELBO w.r.t ϕ and θ

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- Joint optimization of ELBO over ϕ and θ implies training an autoencoder, the *variational autoencoder*
- They assume $q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}_1, \boldsymbol{\sigma}_1^2 \boldsymbol{I})$, $p_\theta(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_2, \boldsymbol{\sigma}_2^2 \boldsymbol{I})$, and $p_\theta(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mathbf{0}, \boldsymbol{I})$

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\text{ELBO}(q, \theta, \phi) &= \mathbb{E}_{q_\phi}[\log p_\theta(\mathbf{z}, \mathbf{x}) - \log q_\phi(\mathbf{z}|\mathbf{x})] \\
&= \mathbb{E}_{q_\phi}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p_\theta(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})] \\
&= \mathbb{E}_{q_\phi}[\log p_\theta(\mathbf{x}|\mathbf{z})] - \mathbb{E}_{q_\phi}[\log p_\theta(\mathbf{z}) + \log q_\phi(\mathbf{z}|\mathbf{x})] \\
&= \mathbb{E}_{q_\phi}[\log p_\theta(\mathbf{x}|\mathbf{z})] - \text{KL}(q_\phi(\mathbf{z}|\mathbf{x}) \mid\mid p_\theta(\mathbf{z})) \\
&= -\text{decoding error} - \text{encoding regularization error}
\end{aligned}$$

- Joint optimization of ELBO over ϕ and θ implies training an autoencoder, the *variational autoencoder*
- They assume $q_\phi(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}_1, \boldsymbol{\sigma}_1^2 \boldsymbol{I})$, $p_\theta(\mathbf{x}|\mathbf{z}) = \mathcal{N}(\mathbf{x}; \boldsymbol{\mu}_2, \boldsymbol{\sigma}_2^2 \boldsymbol{I})$, and $p_\theta(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mathbf{0}, \boldsymbol{I})$
- They use multi-layer perceptrons to represent $\boldsymbol{\mu}_1, \boldsymbol{\sigma}_1 = \text{MLP}_1(\mathbf{x}, \mathbf{z})$, $\boldsymbol{\mu}_2, \boldsymbol{\sigma}_2 = \text{MLP}_2(\mathbf{x}, \mathbf{z})$

MNIST results

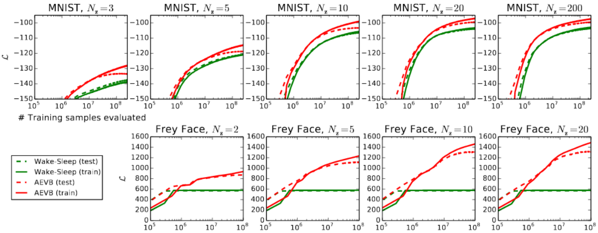
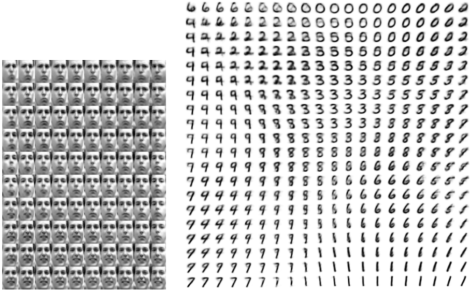


Figure 2: Comparison of our AEVB method to the wake-sleep algorithm, in terms of optimizing the lower bound, for different dimensionality of latent space ($N_\mathbf{z}$). Our method converged considerably faster and reached a better solution in all experiments. Interestingly enough, more latent variables does not result in more overfitting, which is explained by the regularizing effect of the lower bound. Vertical axis: the estimated average variational lower bound per datapoint. The estimator variance was small (< 1) and omitted. Horizontal axis: amount of training points evaluated. Computation took around 20-40 minutes per million training samples with a Intel Xeon CPU running at an effective 40 GFLOPS.

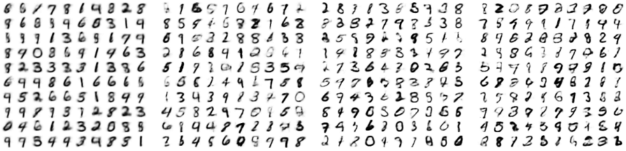
Frey Faces results



(a) Learned Frey Face manifold (b) Learned MNIST manifold

Figure 4: Visualisations of learned data manifold for generative models with two-dimensional latent space, learned with AEVB. Since the prior of the latent space is Gaussian, linearly spaced coordinates on the unit square were transformed through the inverse CDF of the Gaussian to produce values of the latent variables $\mathbf{z}$. For each of these values $\mathbf{z}$, we plotted the corresponding generative $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$ with the learned parameters $\boldsymbol{\theta}$.

Dimension of latent variables



(a) 2-D latent space (b) 5-D latent space (c) 10-D latent space (d) 20-D latent space

Figure 5: Random samples from learned generative models of MNIST for different dimensionalities of latent space.