Variational Inference: The Basics

Philip Schulz and Wilker Aziz

https: //github.com/philschulz/VITutorial

Generative Models

Examples

Variational Inference
    Deriving VI with Jensen's Inequality
    Deriving VI from KL Divergence
    Relationship to EM
    Variational Bayes

Mean Field Inference

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Joint Distribution

Let X and Z be random variables. A generative model is any model that defines a joint distribution over these variables.

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3 Examples of Generative Models

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

Likelihood and prior

From here on, x is our observed data. On the other hand, z is an unobserved outcome.

- $p(x|z)$ is the **likelihood**
- $p(z)$ is the **prior** over Z

Notice: both distributions may depend on a non-random quantity α (write e.g. $p(z|\alpha)$). In that case, we call α a hyperparameter.

Bayes rule

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$$\underbrace{p(z|x)}_{\text{posterior}} = \frac{\overbrace{p(x|z)}^{\text{likelihood}} \overbrace{p(z)}^{\textit{prior}}}{p(x)}$$

Bayes rule

We can *invert* a conditional probability distribution.

$$\underbrace{p(z|x)}_{\text{posterior}} = \frac{\overbrace{p(x|z)}^{\text{likelihood}} \overbrace{p(z)}^{\text{prior}}}{\underbrace{p(x)}_{\text{marginal likelihood/evidence}}}$$

The Basic Problem

We want to compute the posterior over latent variables $p(z|x)$. This involves computing the marginal likelihood

$$p(x) = \int p(x, z)\mathrm{d}z$$

which is often **intractable**. This problem motivates the use of **approximate inference** techniques.

Bayesian Inference

Model parameters θ are also random. The generative model becomes

- $p(x, \theta)$ for fully observed data (supervised learning)
- $p(x, z, \theta)$ for observed and latent data (unsupervised learning)

Bayesian Inference

The evidence becomes even harder to compute
because θ is often high-dimensional (just think of
neural nets!).

- $p(x) = \int p(x, \theta)\mathrm{d}\theta$ (supervised learning)
- $p(x) = \int \int p(x, z, \theta)z\mathrm{d}\theta$ (unsupervised learning)

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Again, approximate inference is needed.

Generative Models

Examples

Variational Inference
    Deriving VI with Jensen's Inequality
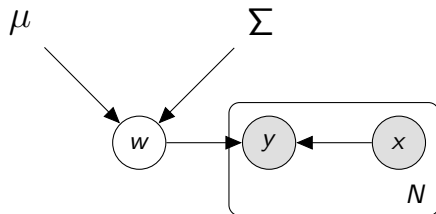   Deriving VI from KL Divergence
    Relationship to EM
    Variational Bayes

Mean Field Inference

We cannot compute the posterior when

1. The functional form of the posterior is unknown (we don't know which parameters to infer)
2. The functional form is known but the computation is intractable

Bayesian Logistic Regression

The Normal distribution is not conjugate to the Gibbs distribution. The form of the posterior is unknown.
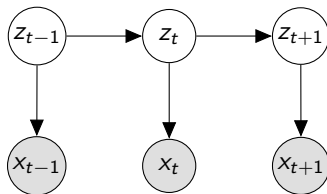
Bayesian Logistic Regression

Intuition

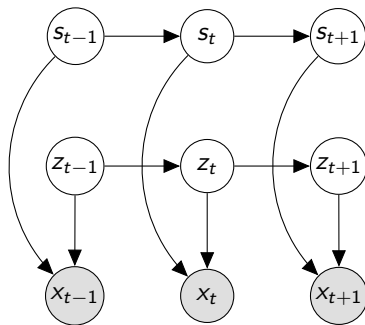Simply assume that the posterior is Gaussian.

Factorial HMMs

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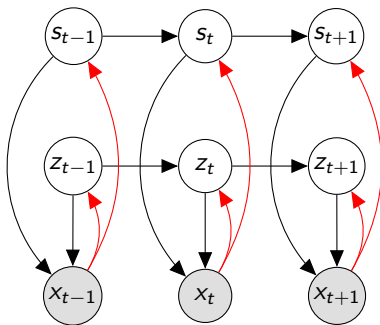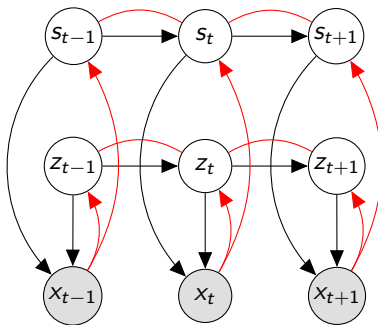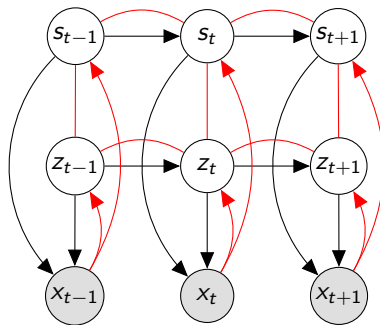
Factorial HMMs

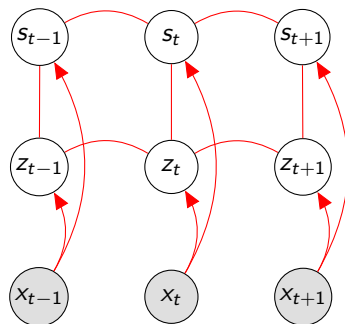FHMMs have several Markov chains over latent variables.

Factorial HMMs

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Factorial HMMs

Inference network for FHHMs.

Factorial HMMs

FHMMs have several Markov chains over latent variables.

- M Markov chains over latent variables.
- L outcomes per latent variable.
- Sequence of length T.
- Complexity of inference: $\mathcal{O}(L^{2M}T)$.

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Intractable

Exponential dependency on the number of hidden Markov chains.

Factorial HMMs

Intuition

Simply assume that the posterior consists of independent Markov chains.

Latent Dirichlet Allocation

An admixture model that changes its mixture
weights per document. We assume that the mixture
components are fixed.
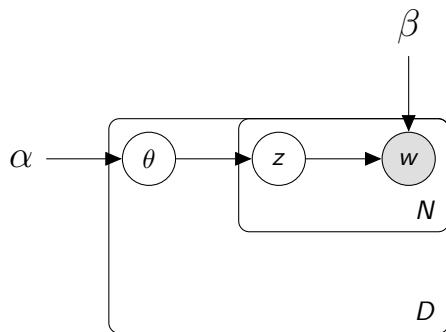
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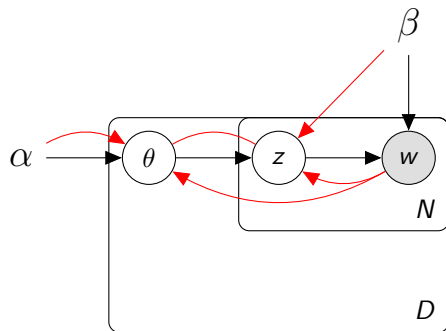
Latent Dirichlet Allocation

Inference network for LDA.
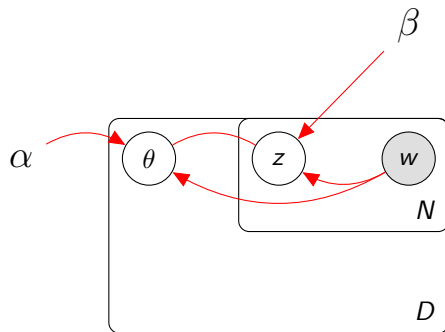
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mixture components are fixed.

- D documents.
- N tokens and latent variables per document.
- L outcomes per latent variable.
- Complexity of inference: $\mathcal{O}(L^{DN})$.
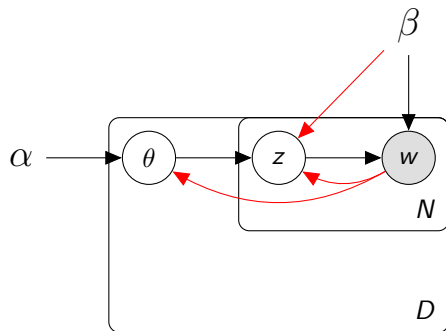
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Simply assume that the posterior consists of independent categorical and Dirichlet distributions.

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Rule of Thumb
Simply assume that the posterior is in the same family as the prior.

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The Goal

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Requirement
Choose $q(z|x)$ as close as possible to $p(z|x)$ to obtain a faithful approximation.

Recap KL divergence

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- $\mathrm{KL}\left(q(z|x) \;||\; p(z|x)\right) = \mathbb{E}_{q(z|x)}\left[\log\left(\frac{q(z|x)}{p(z|x)}\right)\right]$ (both)

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Originally known as relative entropy. Read
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Expand KL $(q \parallel p)$

$$\mathbb{E}_{q(z|x)}\left[\log\left(\frac{q(z|x)}{p(z)}\right)\right] = -\mathbb{E}_{q(z|x)}\left[\log p(z)\right] + \mathbb{E}_{q(z|x)}\left[\log q(z|x)\right]$$

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Bits needed to encode p once we know q.

Recap KL divergence

Properties

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- $\mathrm{KL}\left(q(z|x) \| p(z|x)\right) = \infty$ if $\exists z$ s.t. $p(z|x) = 0$ and $q(z|x) > 0$.

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- $\text{KL}\left(q(z|x) \,||\, p(z|x)\right) = \infty$ if $\exists z$ s.t. $p(z|x) = 0$ and $q(z|x) > 0$.
- In general $\text{KL}\left(q(z|x) \,||\, p(z|x)\right) \neq \text{KL}\left(p(z|x) \,||\, q(z|x)\right)$.

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$$= - \mathrm{KL} \left(q(z|x) \,||\, p(z|x) \right) + \log p(x)$$

We have derived a lower bound on the log-evidence whose gap is exactly $\mathrm{KL} \left(q(z|x) \,||\, p(z|x) \right)$.

VI derivation II

Recall that we want to find $q(z|x)$ such that $\text{KL}\left(q(z|x) \,||\, p(z|x)\right)$ is small.

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$$\min_{q(z|x)} \text{KL}\left(q(z|x) \,||\, p(z|x)\right) = \max_{q(z|x)} -\text{KL}\left(q(z|x) \,||\, p(z|x)\right)$$

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

As before, we have derived a lower bound on the log-evidence. This **evidence lower bound** or **ELBO** is our optimisation objective.

ELBO

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

Performing VI (Frequentist Case)

VI in its basic form can be performed via coordinate ascent. This can be done as a 2-step procedure.

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1. Maximize (regularised) expected log-density.

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2. Optimise generative model.

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

Recap: EM Algorithm

E-step Compute: $\mathbb{E}_{p(z|x)}\left[\log\left(p(x,z)\right)\right]$.

Same as: $\max_{p(z|x)} \mathbb{E}_{p(z|x)}\left[\log p(x,z)\right]$

M-step $\max_{p(x,z)} \mathbb{E}_{p(z|x)}\left[\log p(x,z)\right] + \underbrace{\mathbb{H}\left(p(z|x)\right)}_{\text{constant}}$

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EM is variational inference!

$$q(z|x) = p(z|x)$$
$$\text{KL}\left(q(z|x) \,||\, p(z|x)\right) = 0$$

Performing VI (Bayesian Case)

We have latent variables z (e.g. POS tags) and θ (e.g. model parameters).

1. Maximise over local variables z.

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

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2. Maximise over global variables θ.

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

Differences between frequentist VI and VB (Variational Bayes)

- ▶ Frequentist VI optimises two sets of parameters, VB only optimises variational parameters
- ▶ Entropy term matters in the M-step for VB but not for VI

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Mean Field Inference

Designing a tractable approximation

▶ Recall: The approximation $q(z|x)$ needs to be tractable.

▶ Common solution: make **all** latent variables independent under $q(z|x)$.

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► Formal assumption: $q(z|x) = \prod_{i=1}^{N} q(z_i)$

Designing a tractable approximation

- Recall: The approximation $q(z|x)$ needs to be tractable.
- Common solution: make **all** latent variables independent under $q(z|x)$.
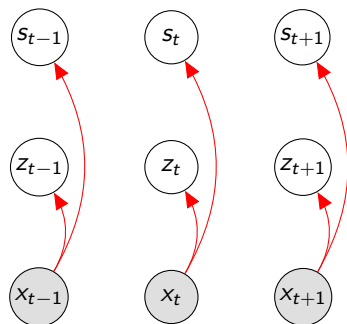- Formal assumption: $q(z|x) = \prod_{i=1}^{N} q(z_i)$

This approximation strategy is commonly known as **mean field** approximation.
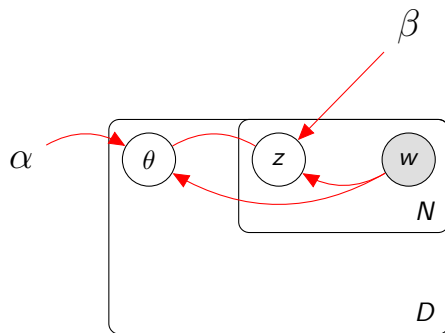
Original FHHM Inference
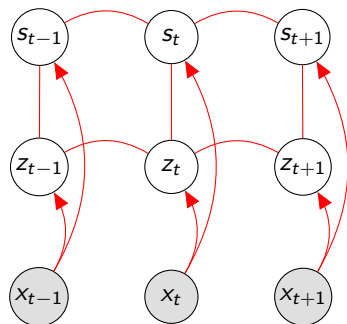
Exact posterior $p(s, z|x)$
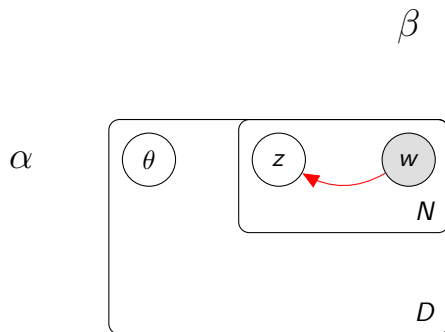
Mean field FHHM Inference

Approximate posterior $q(s, z) = \prod_{t=1}^{T} q(s_t) q(z_t)$

Original LDA Inference

Exact posterior $p(z, \theta | w, \alpha, \beta)$

Mean field LDA Inference

$$\beta$$

$$\alpha$$

Approximate posterior
$$q(z, \theta | w, \alpha, \beta) = \prod_{d=1}^{D} q(\theta_d) \prod_{i=1}^{N} q(z_i | w)$$

Summary

- Posterior inference is often **intractable** because the marginal likelihood (or **evidence**) $p(x)$ cannot be computed efficiently.
- Variational inference approximates the posterior $p(z|x)$ with a simpler distribution $q(z|x)$.
- The variational objective is the **evidence lower bound (ELBO)**:

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

Summary

- The **ELBO** is a lower bound on the log-evidence.
- When $q(z|x) = p(z|x)$ we recover EM.
- A common approximation is the **mean field** approximation which assumes that all latent variables are independent:

$$q(z|x) = \prod_{i=1}^{N} q(z_i)$$

Literature I

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