Variational Inference: The Basics

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Joint Distribution

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2 Examples of Generative Models

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

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: the prior may depend on a non-random quantity α (write $p(z|\alpha)$). In that case, we call α a hyperparameter.

Bayes' rule

Bayes rule asserts that we can *invert* a conditional probability distribution.

$$p(z|x) = \frac{p(x|z)p(z)}{p(x)} \tag{1}$$

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$$\underbrace{p(z|x)}_{\text{posterior}} = \frac{\overbrace{p(x|z)}^{\text{likelihood}}\ \overbrace{p(z)}^{\textit{prior}}}{p(x)} \tag{3}$$

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$$\underbrace{p(z|x)}_{\text{posterior}} = \frac{\overbrace{p(x|z)}^{\text{likelihood}}\,\overbrace{p(z)}^{\text{prior}}}{\underbrace{p(x)}_{\text{marginal likelihood/evidence}}} \tag{4}$$

The Basic Problem

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

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

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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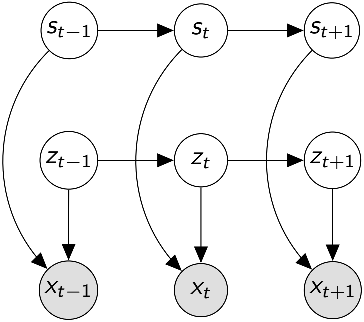
Again, approximate inference is needed.

Factorial HMMs

FHMMs have several Markov chains over latent variables.



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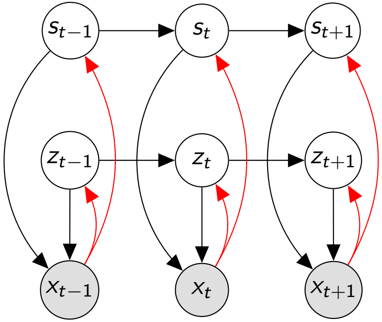

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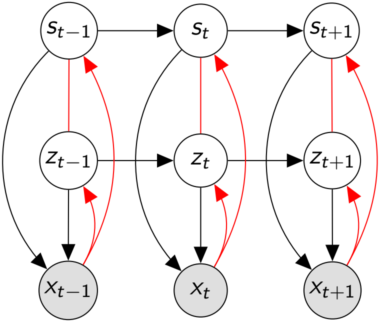

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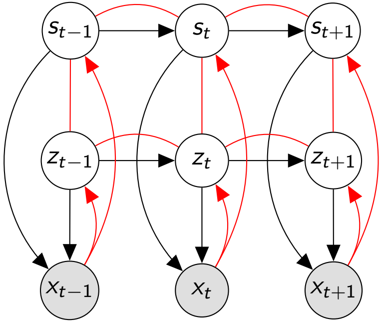
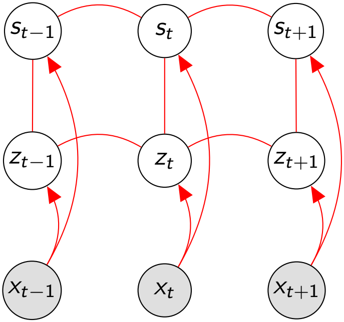


Factorial HMMs

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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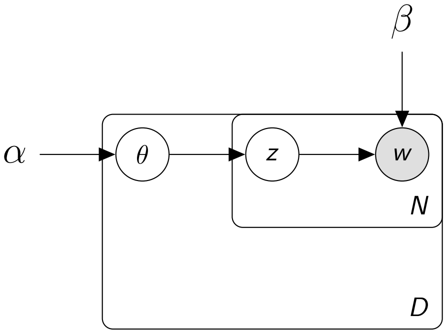
Intractable

Exponential dependency on the number of hidden Markov chains.

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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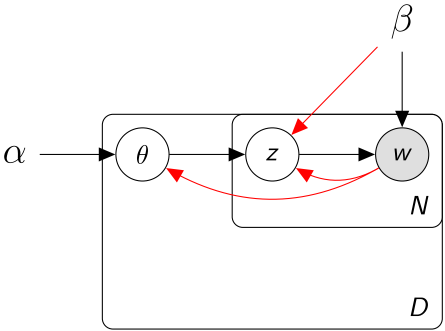

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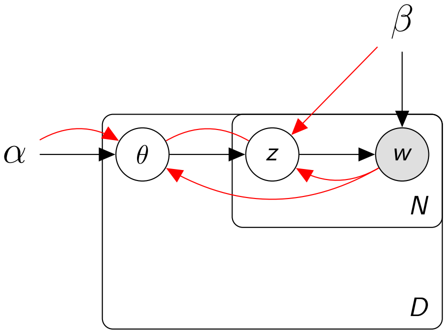
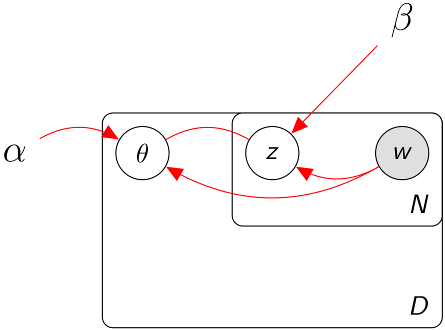


Latent Dirichlet Allocation

Inference network for LDA.



Latent Dirichlet Allocation

An admixture model that changes its mixture weights per document. Here we assume that the mixture components are fixed.

- D documents.
- N tokens and latent variables per document.
- L outcomes per latent variable.
- Complexity of inference: $\mathcal{O}(L^{DN})$.

The Goal

Assume $p(z|x)$ is intractable.

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Implementation

Minimize $\mathrm{KL}\left(q(z) \,||\, p(z|x)\right)$.

Recap KL divergence

The Kullback-Leibler divergence (or relative entropy) measures the divergence of a distribution q from a distribution q.

- $\mathrm{KL}\left(q(z) \,||\, p(z|x)\right) = \int q(z) \log\left(\frac{q(z)}{p(z|x)}\right) \mathrm{d}z$ (continuous)
- $\mathrm{KL}\left(q(z) \,||\, p(z|x)\right) = \sum_z q(z) \log\left(\frac{q(z)}{p(z|x)}\right)$ (discrete)
- $\mathrm{KL}\left(q(z) \,||\, p(z|x)\right) = \mathbb{E}_{q(z)}\left[\log\left(\frac{q(z)}{p(z|x)}\right)\right]$ (both)

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Properties

- $\mathrm{KL}\left(q(z) \,||\, p(z|x)\right) \geq 0$ with equality iff $q(z) = p(z|x)$.

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

VI derivation I

$$
\begin{aligned}
\log p(x) &= \log \left(\int p(x, z) \mathrm{dz} \right) \\
&= \log \left(\int q(z) \frac{p(x, z)}{q(z)} \mathrm{dz} \right) \\
&\geq \int q(z) \log \left(\frac{p(x, z)}{q(z)} \right) \mathrm{dz} \\
&= \int q(z) \log \left(\frac{p(z|x) p(x)}{q(z)} \right) \mathrm{dz} \\
&= \int q(z) \log \left(\frac{p(z|x)}{q(z)} \right) \mathrm{dz} + \log p(x)
\end{aligned}
$$

VI derivation I

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

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

VI derivation II

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

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Formal Objective

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

VI derivation II

$$
\begin{aligned}
&\max_{q(z)} - \mathrm{KL}\left(q(z) \;||\; p(z|x)\right) \\
&= \max_{q(z)} \int q(z) \log\left(\frac{p(z|x)}{q(z)}\right) \mathrm{dz} \\
&= \max_{q(z)} \int q(z) \log\left(\frac{p(z,x)}{p(x)q(z)}\right) \mathrm{dz} \\
&= \max_{q(z)} \int q(z) \log\left(p(z,x)\right) \mathrm{dz} - \int q(z) \log\left(q(z)\right) \mathrm{dz} - \overbrace{\log(p(x))}^{constant} \\
&= \max_{q(z)} \mathbb{E}_{q(z)}\left[\log\left(p(x,z)\right)\right] + \mathbb{H}\left(q(z)\right)
\end{aligned}
$$

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

ELBO

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

Performing VI

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. Compute the expected log-density $\mathbb{E}_{q(z)}\left[\log\left(p(x,z)\right)\right]$.
2. Maximize with respect to $q(z)$ and while trying to keep $q(z)$ as broad as possible (through entropy regularisation):

$$\max_{q(z)} \mathbb{E}_{q(z)}\left[\log\left(p(x,z)\right)\right] + \mathbb{H}\left(q(z)\right) \tag{5}$$

What if $q(z) = p(z|x)$?

If $q(z) = p(z|x)$ then $\mathrm{KL}\left(q(z) \,||\, p(z|x)\right) = 0$ and thus we are directly optimising the log-evidence.

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

M-step Maximize with respect to $p(z|x)$ and while trying to keep $p(z|x)$ as broad as possible (through entropy regularisation):

$$\max_{p(z|x)} \mathbb{E}_{p(z|x)}\left[\log\left(p(x,z)\right)\right] + \mathbb{H}\left(p(z|x)\right) \tag{7}$$

Relationship to EM

- Variational Inference where $q(z) = p(z|x)$ is EM!
- The E-step does not change except that we are using $q(z)$ to compute the expected density.

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

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- The M-step depends on what family we chose for $q(z)$. This may be a different family than $p(z|x)$!

Designing a tractable approximation

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

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- Common solution: make **all** latent variables independent under $q(z)$.
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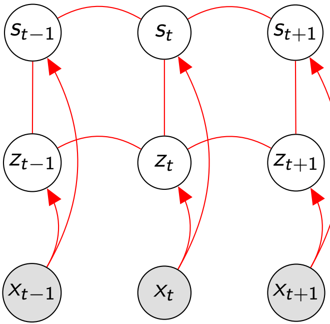
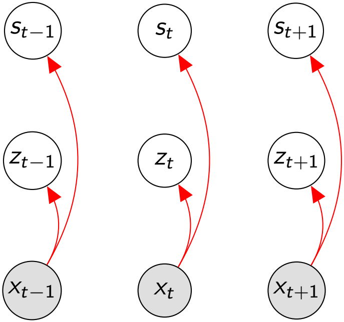
This approximation strategy is commonly known as **mean field** approximation.

Original FHHM Inference



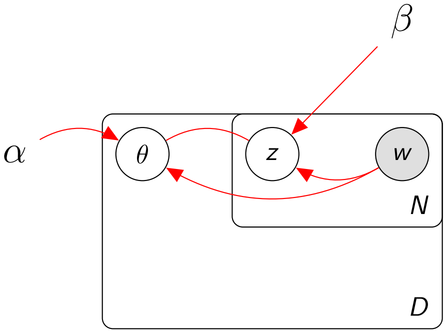
Exact posterior $p(s, z|x)$

Mean field FHHM Inference



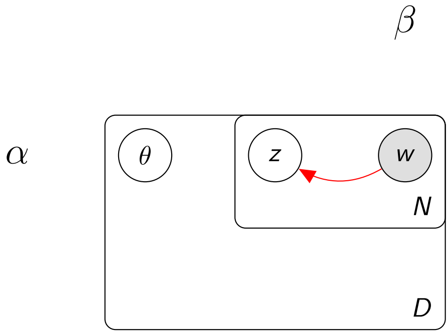
Approximate posterior $q(s, z) = \prod_{t=1}^{T} q(s_t)q(z_t)$

Original LDA Inference



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

Mean field LDA Inference



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 $q(z)$.
- The variational objective is the **evidence lower bound (ELBO)**:

$$\mathbb{E}_{q(z)}\left[\log\left(p(x,z)\right)\right]+\mathbb{H}\left(q(z)\right) \tag{8}$$

Summary

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

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

Literature I

David Blei, Andrew Ng, and Michael Jordan. Latent dirichlet allocation. *Journal of Machine Learning Research*, 3(4-5): 993–1022, 2003. ISSN 1532-4435. doi: 10.1162/jmlr.2003.3.4-5.993. URL http://dx.doi.org/10.1162/jmlr.2003.3.4-5.993.

David M. Blei, Alp Kucukelbir, and Jon D. McAuliffe. Variational inference: A review for statisticians. 01 2016. URL https://arxiv.org/abs/1601.00670.

Literature II

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