

Variational Inference: The Basics

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Joint Distribution

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2 Examples of Generative Models

- ▶ $p(x, z) = p(x)p(z|x)$
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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.

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

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$$p(z|x) = \frac{\overbrace{p(x|z)}^{\text{likelihood}} \overbrace{p(z)}^{\text{prior}}}{p(x)} \quad (2)$$

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

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

The Basic Problem

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

$$p(x) = \int p(x, z) dz$$

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

Bayesian Inference

Under the Bayesian view, 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. This is because θ is often high-dimensional (just think of neural nets!).

- ▶ $p(x) = \int p(x, \theta) d\theta$ (supervised learning)
- ▶ $p(x) = \int \int p(x, z, \theta) dz d\theta$ (unsupervised learning)

Bayesian Inference

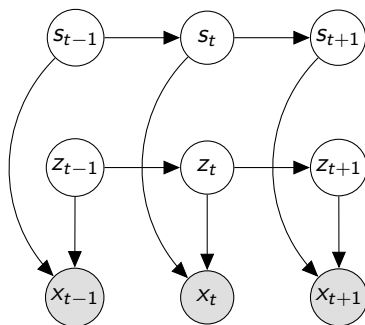
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Again, approximate inference is needed.

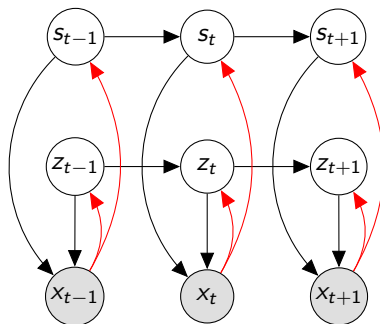
Factorial HMMs

FHMMs have several Markov chains over latent variables.



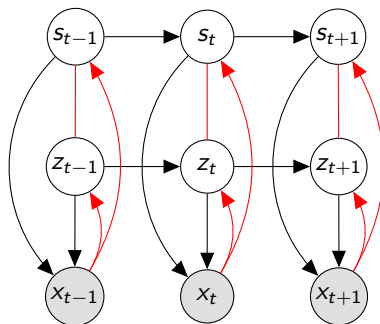
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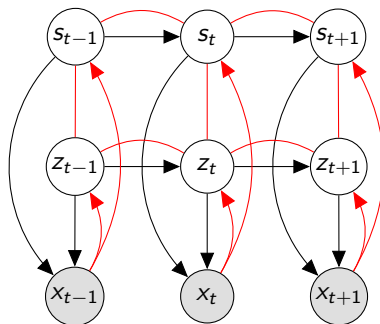
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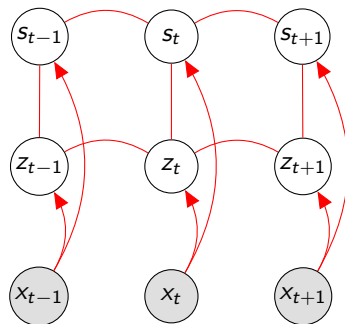
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Factorial HMMs

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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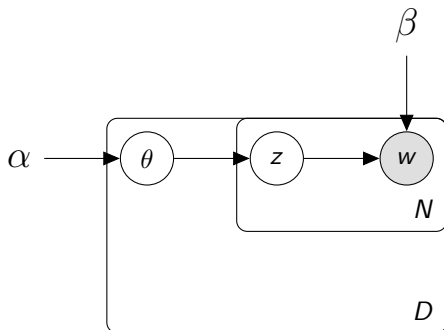
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This model is **intractable** because of the exponential dependence on the number of hidden Markov chains.

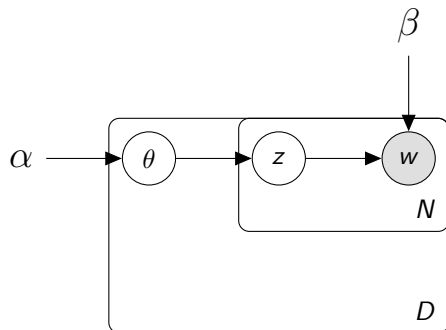
Latent Dirichlet Allocation

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



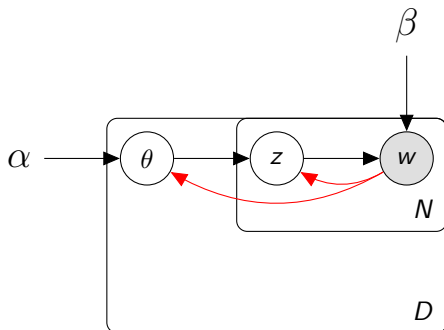
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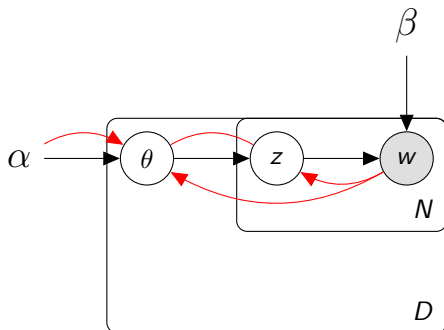
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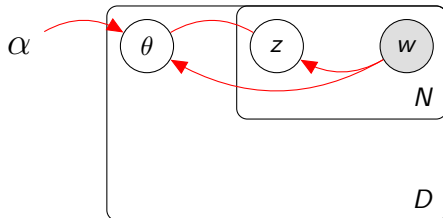
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β 

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- ▶ 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 $\text{KL}(q(z) || p(z|x))$.

Recap KL divergence

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

- ▶ $\text{KL}(q(z) \parallel p(z|x)) = \int q(z) \log \left(\frac{q(z)}{p(z|x)} \right) dz$
(continuous)
- ▶ $\text{KL}(q(z) \parallel p(z|x)) = \sum_z q(z) \log \left(\frac{q(z)}{p(z|x)} \right)$
(discrete)

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Properties

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- ▶ In general
 $\text{KL}(q(z) \parallel p(z|x)) \neq \text{KL}(p(z|x) \parallel q(z))$.

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- ▶ In general
 $\text{KL}(q(z) \parallel p(z|x)) \neq \text{KL}(p(z|x) \parallel q(z))$.
- ▶ $-\text{KL}(q(z) \parallel p(z|x)) = \int q(z) \frac{p(z|x)}{q(z)} dz \leq 0$.

VI derivation I

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

VI derivation I

Notice that

$$\begin{aligned} \int q(z) \log \left(\frac{p(z|x)}{q(z)} \right) dz + \log(p(x)) \\ = -\text{KL}(q(z) \parallel p(z|x)) + \log(p(x)) \end{aligned}$$

confirming that we have derived a lower bound on the log-evidence. The gap in the bound is exactly the KL divergence between the model posterior $p(z|x)$ and its approximation $q(z)$.

VI derivation II

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

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Formal Objective

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

VI derivation II

$$\max_{q(z)} -\text{KL}(q(z) \parallel p(z|x))$$

$$= \max_{q(z)} \int q(z) \log \left(\frac{p(z|x)}{q(z)} \right) dz$$

$$= \max_{q(z)} \int q(z) \log \left(\frac{p(z, x)}{p(x)q(z)} \right) dz$$

$$= \max_{q(z)} \int q(z) \log(p(z, x)) dz - \int q(z) \log(q(z)) dz - \overbrace{\log(p(x))}^C$$

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

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

ELBO

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

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

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

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

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

1. Compute the expected log-density $\mathbb{E}_{p(z|x)} [\log(p(x, z))]$.
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$$\max_{p(z|x)} \mathbb{E}_{p(z|x)} [\log(p(x, z))] + \mathbb{H}(p(z|x)) \quad (6)$$

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

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

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

Relationship to EM

- ▶ Variational Inference where $q(z) = p(z|x)$ is EM!
- ▶ The implementation of the M-step does not change.
- ▶ The implementation of the E-step changes when $q(z) \neq p(z|x)$ because the expectation term changes.

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

Designing a tractable approximation

- ▶ Recall: The approximation $q(z)$ needs to be tractable.
- ▶ Common solution: make **all** latent variables independent under $q(z)$.

Designing a tractable approximation

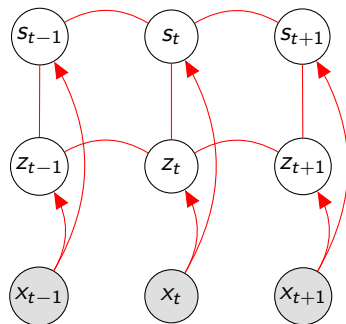
- ▶ Recall: The approximation $q(z)$ needs to be tractable.
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- ▶ Formal assumption: $q(z) = \prod_{i=1}^N q(z_i)$

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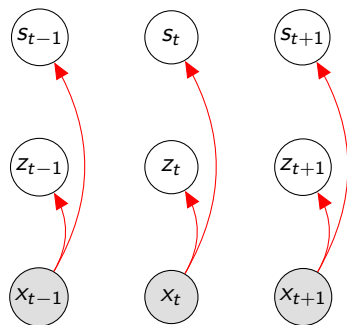
This approximation strategy is commonly known as **mean field** approximation.

Original FHMM Inference



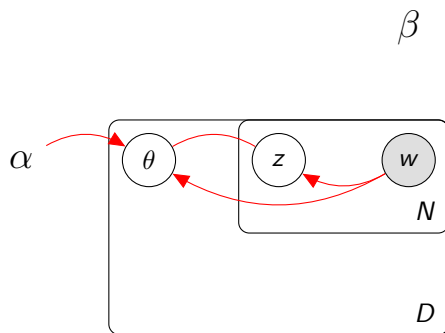
Exact posterior $p(s, z|x)$

Mean field FHMM Inference



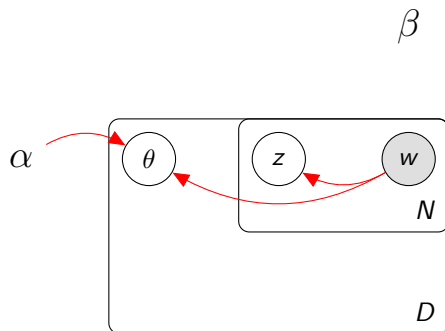
Approximate posterior $q(s, z) = q(s)q(z)$

Original LDA Inference



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

Mean field LDA Inference



Approximate posterior

$$q(z, \theta | w, \alpha, \beta) = q(z | w, \beta) q(\theta | w, \alpha)$$

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)**:

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

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

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Literature II

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