Variational Inference: The Basics

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https://github.com/philschulz/VITutorial

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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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

We can *invert* a conditional probability distribution.

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

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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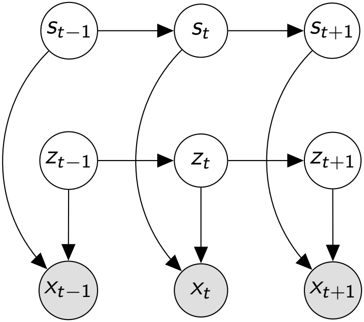
Again, approximate inference is needed.

Factorial HMMs

FHMMs have several Markov chains over latent variables.



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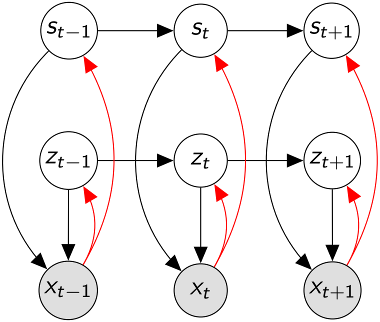

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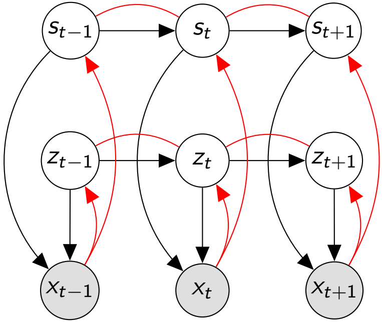

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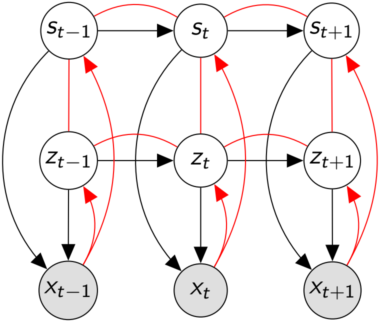
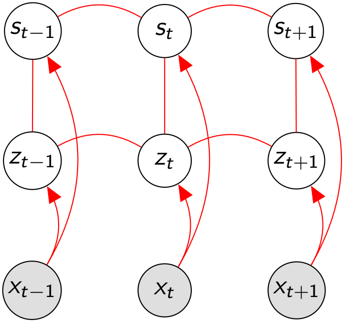


Factorial HMMs

Inference network for FHHMs.



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

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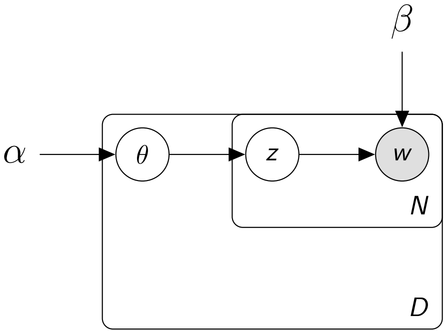
Intractable

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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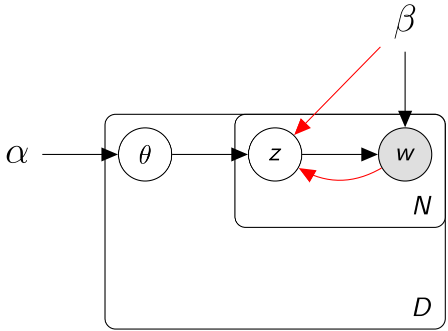

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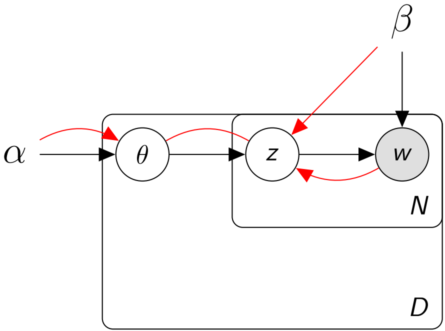
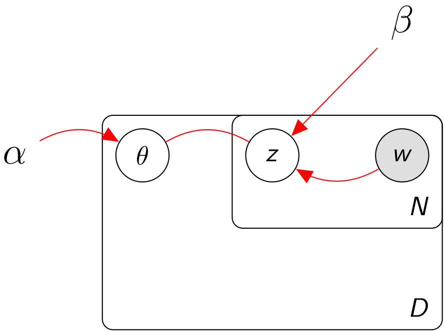


Latent Dirichlet Allocation

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.

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

Recap KL divergence

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 $q(z) > 0$.

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

VI derivation I

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

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

VI derivation I

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

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$$

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

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&= \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}
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&= \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

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

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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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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M-step Maximize with respect to $p(z|x)$ with entropy regularisation:

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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

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

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Designing a tractable approximation

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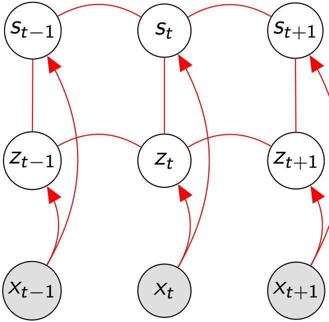
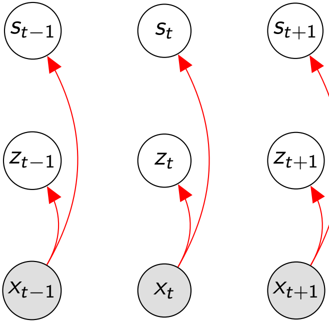
This approximation strategy is commonly known as **mean field** approximation.

Original FHHM Inference



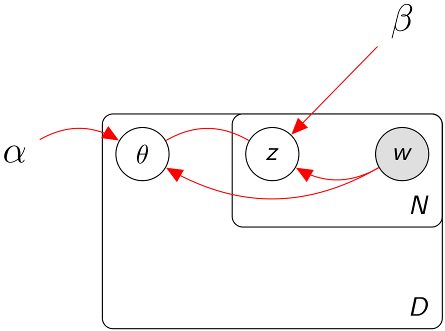
Exact posterior $p(s, z|x)$

Mean field FHHM Inference



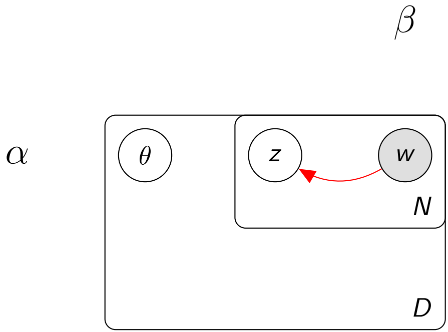
Approximate posterior $q(s, z) = \prod_{t=1}^{T} q(s_t)q(z_t)$

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)**:

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

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

Zoubin Ghahramani and Michael I Jordan. Factorial hidden markov models. In *Advances in Neural Information Processing Systems*, pages 472–478, 1996. URL http://papers.nips.cc/paper/1144-factorial-hidden-markov-models.pdf.

Radford M Neal and Geoffrey E Hinton. A view of the em algorithm that justifies incremental, sparse, and other variants. In *Learning in graphical models*, pages 355–368. Springer, 1998. URL http://www.cs.toronto.edu/~fritz/absps/emk.pdf.