Variational Inference: The Basics

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VI Tutorial @ IST
https://vitutorial.github.io/tour/ist2019

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

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, we write e.g. $p(z|\alpha)$ and call α a hyperparameter.

Bayes rule

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

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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

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

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

Bayesian Inference

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

- $p(x|\theta) = \int p(x, z|\theta)\mathrm{d}z$ (frequentist)
- $p(x) = \int \int p(x, z, \theta)\mathrm{d}z\mathrm{d}\theta$ (Bayesian)

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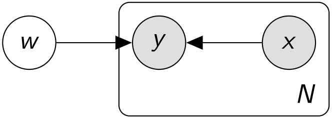
Today we will only treat the frequentist case!

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 Log-Linear POS Tagger



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

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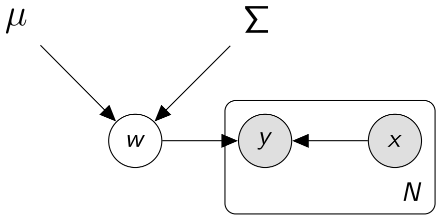

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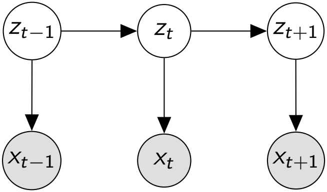
Bayesian Log-Linear POS Tagger

Intuition

Simply assume that the posterior is Gaussian.

Factorial HMMs

FHMMs have several Markov chains over latent variables.



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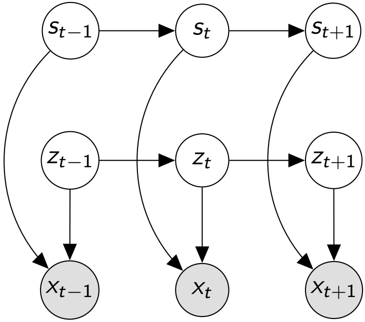

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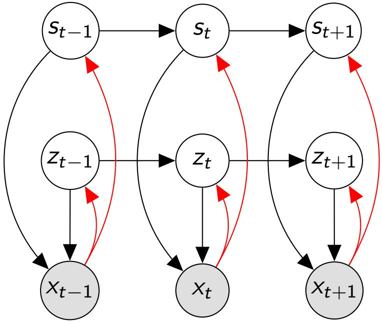

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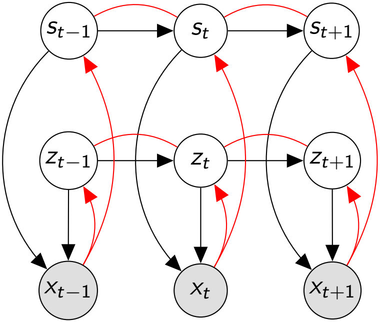

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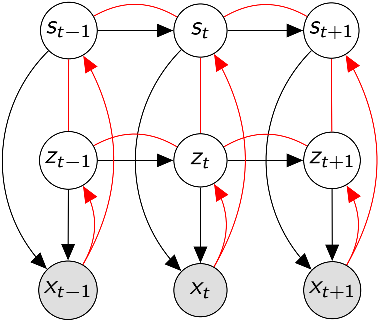
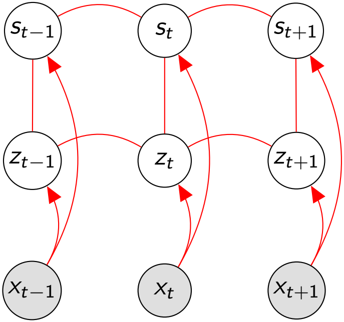


Factorial HMMs

Inference network for FHHMs.



Factorial HMMs

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- 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.

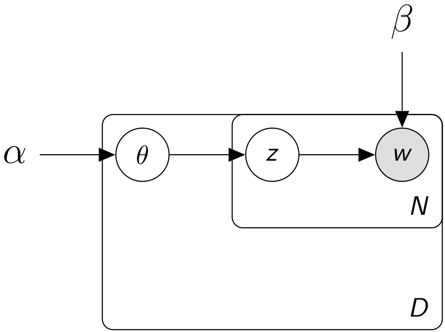
Factorial HMMs

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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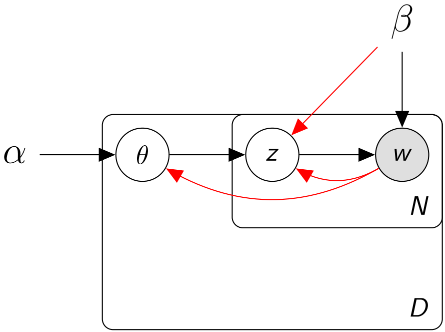

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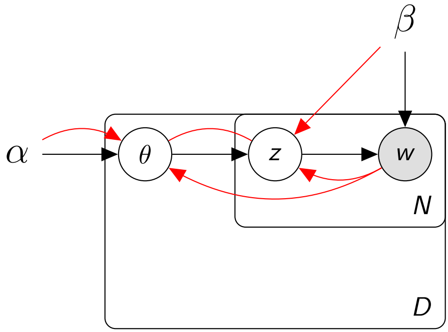
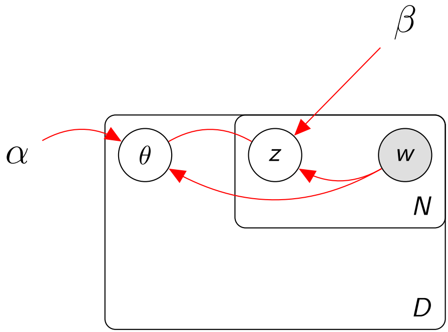


Latent Dirichlet Allocation

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: $\mathcal{O}(L^{DN})$.

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Intuition

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.

The Goal

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Idea

Let's approximate it by an auxiliary distribution $q(z)$ that is computable!

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Requirement

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

Recap KL divergence

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

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- $\mathrm{KL}\left(q(z) \mid\mid p(z|x)\right) = \sum_z q(z) \log \frac{q(z)}{p(z|x)}$ (discrete)

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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- $-\mathrm{KL}\left(q(z) \mid\mid p(z|x)\right) = \mathbb{E}_{q(z)}\left[\log \frac{p(z|x)}{q(z)}\right] \leq 0.$
- $\mathrm{KL}\left(q(z) \mid\mid p(z|x)\right) = \infty$ if $\exists z$ s.t. $p(z|x) = 0$ and $q(z) > 0$.

VI derivation I

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

VI derivation I

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

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\log p(x) &= \log\left(\int p(x,z)\mathrm{d}z\right) \\
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&= \mathbb{E}_{q(z)}\left[\log\frac{p(z|x)p(x)}{q(z)}\right]
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\end{aligned}$$

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 $\mathrm{KL}\left(q(z) \mid\mid p(z|x)\right)$ is small.

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&= \arg\max_{q(z)} \int q(z) \log p(z,x) \mathrm{d}z - \int q(z) \log q(z) \mathrm{d}z - \overbrace{\log p(x)}^{constant}
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&= \arg\max_{q(z)} \mathbb{E}_{q(z)} \left[\log p(x,z)\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

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

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.

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

2. Optimise generative model.

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

Unconstrained (exact) optimisation

What's the solution to the following?

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

(assume $\mathcal{Q}$ is large enough a family)

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The true posterior $p(z|x)$! Exactly because

$$\arg\max_{q(z)\in\mathcal{Q}} \text{ELBO} = \arg\min_{q(z)\in\mathcal{Q}} \text{KL}\left(q(z) \mid\mid p(z|x)\right)$$

and KL is never negative and 0 iff $q(z) = p(z|x)$.

Recap: EM Algorithm

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

$= p(z|x)$

Recap: EM Algorithm

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\text{E-step} \quad & \arg\max_{q(z)} \mathbb{E}_{q(z)} \left[\log p(x,z)\right] + \mathbb{H}\left(p(z|x)\right) \\
& = p(z|x) \\
\text{M-step} \quad & \arg\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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Recap: EM Algorithm

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EM is variational inference!

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

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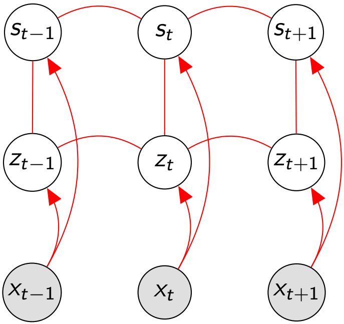
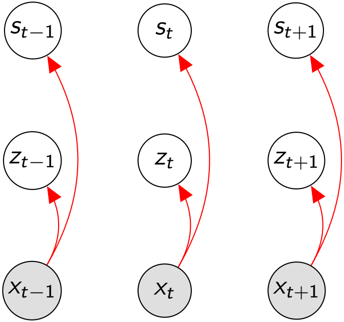
This approximation strategy is commonly known as **mean field** approximation.

Original FHHM Inference



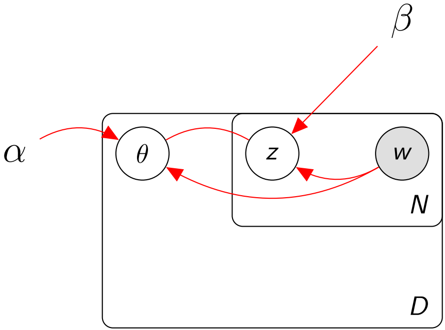
Exact posterior $p(s, z|x)$

Mean field FHHM Inference



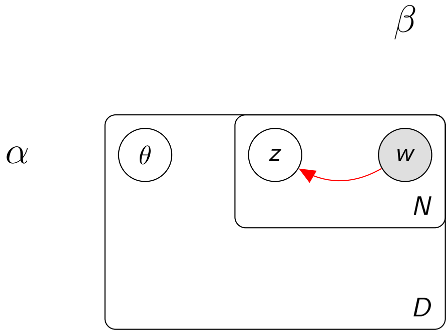
Approximate posterior $q(s, z) = \prod_{t=1}^{T} q(s_t)q(z_t)$

Original LDA Inference



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

Mean field LDA Inference



Approximate posterior

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

Latent Factor Document Model

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$$
\begin{aligned}
Z_j &\sim \mathrm{Bernoulli}(\alpha) && (1 \leq j \leq K) \\
X_i|z &\sim \mathrm{Categorical}\left(f(z;\theta)\right) && (1 \leq i \leq N)
\end{aligned}
$$

$f(\cdot)$ is computed by a NN

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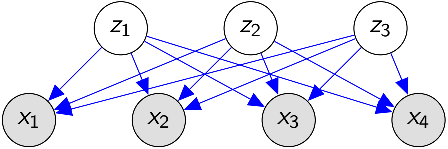
$$
\begin{aligned}
Z_j &\sim \text{Bernoulli}(\alpha) && (1 \leq j \leq K) \\
X_i|z &\sim \text{Categorical}\,(f\,(z;\theta)) && (1 \leq i \leq N)
\end{aligned}
$$

$f(\cdot)$ is computed by a NN with softmax output.

Original LFDM Inference

Joint distribution: latent variables are marginally independent a priori

for example, $K = 3, N = 4$



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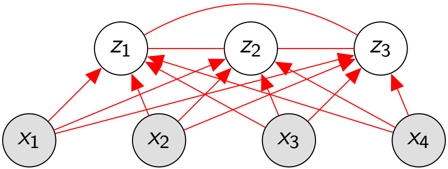

Posterior: latent variables are marginally dependent given observations

Mean field assumption

We have K latent variables

- assume the posterior factorises as K independent terms

$$q(z_1, \ldots, z_K) = \underbrace{\prod_{j=1}^{K} q_{\lambda_j}(z_j)}_{\text{mean field}}$$

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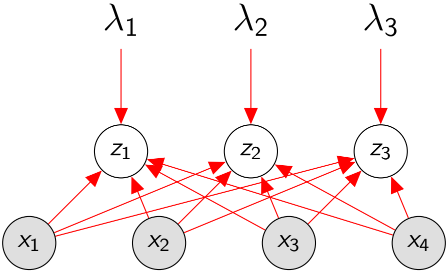
with independent sets of parameters $\lambda_j = \{b_j\}$

$$Z_j \sim \text{Bernoulli}(b_j)$$

Mean field: example



Amortised variational inference

Amortise the cost of inference using NNs

$$q(z_1, \ldots, z_K | x) = \prod_{j=1}^{K} q_{\lambda}(z_j | x)$$

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still mean field

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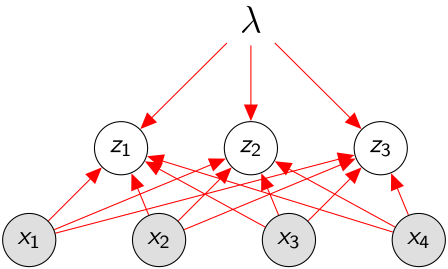
still mean field

$$Z_j|x \sim \text{Bernoulli}(b_j)$$

but with a shared set of parameters

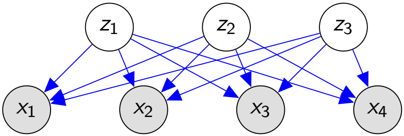
- where $b_1^K = g(x; \lambda)$

Amortised VI: example

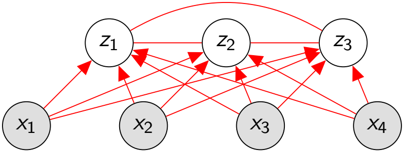


Overview

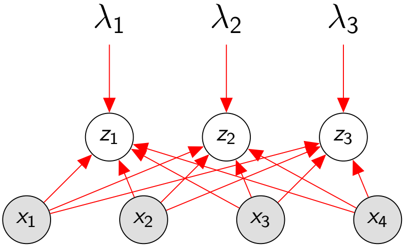
Joint distribution



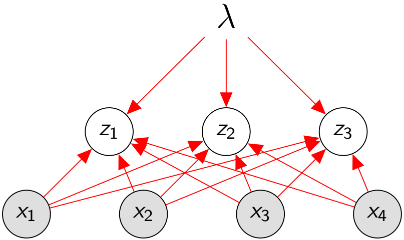
Posterior



Mean field



Amortised VI



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 $q(z)$.

Summary

- The variational objective is the **evidence lower bound (ELBO)**:

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

- The **ELBO** is a lower bound on the log-evidence.
- The solution to the ELBO minimises $\mathrm{KL}(q(z) \,||\, p(z|x))$
- When $q(z) = p(z|x)$ we recover EM.

Summary

- We design $q(z)$ to be simple
- 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. doi: 10.1162/jmlr.2003.3.4-5.993. URL http://dx.doi.org/10.1162/jmlr.2003.3.4-5.993.

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Literature II

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.