

Variational Inference: The Basics

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VI Tutorial @ Host
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- 1 Generative Models
- 2 Examples
- 3 Variational Inference
 - Deriving VI with Jensen's Inequality
 - Deriving VI from KL Divergence
 - Relationship to EM
- 4 Mean Field Inference

1 Generative Models

2 Examples

3 Variational Inference

- Deriving VI with Jensen's Inequality
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4 Mean Field Inference

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

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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 , we write e.g. $p(z|\alpha)$ and 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

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

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!).

- $p(x|\theta) = \int p(x, z|\theta)dz$ (frequentist)
- $p(x) = \int \int p(x, z, \theta)dzd\theta$ (Bayesian)

Bayesian Inference

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Today we will mostly focus on the frequentist case!

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2 Examples

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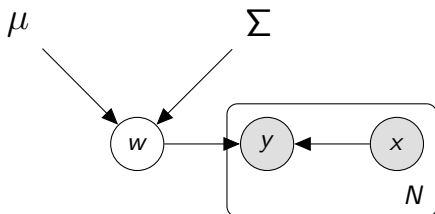
4 Mean Field Inference

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 Log-Linear Model

$$p(y|x, \mu, \Sigma) = \int \frac{\exp(w_y^\top x)}{\sum_c \exp(w_c^\top x)} \mathcal{N}(w|\mu, \Sigma) dw$$



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

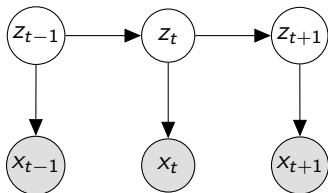
Bayesian Log-Linear Model

Intuition

Simply assume that the posterior is Gaussian.

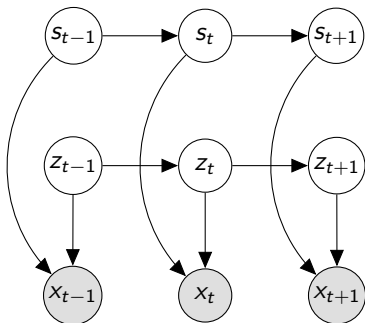
Factorial HMMs

FHMMs have several Markov chains over latent variables.



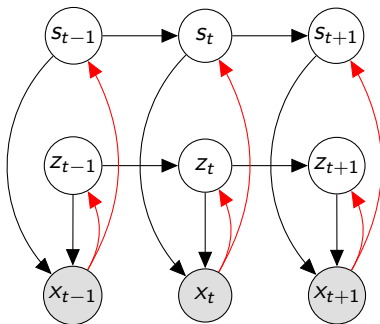
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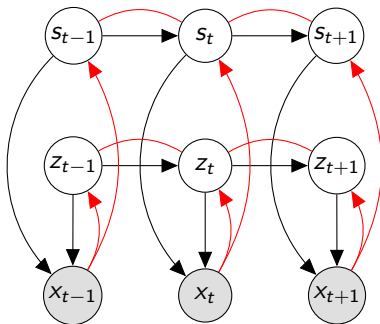
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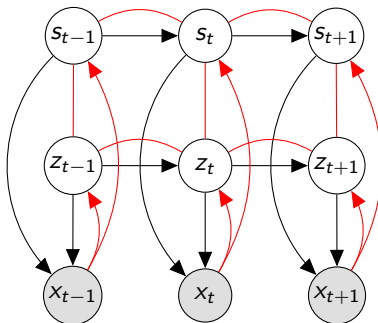
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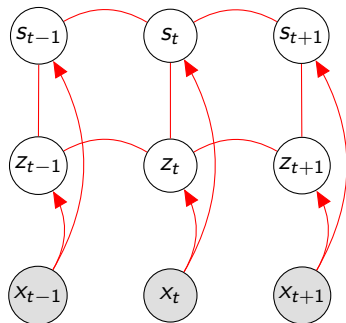
Factorial HMMs

FHMMs have several Markov chains over latent variables.



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

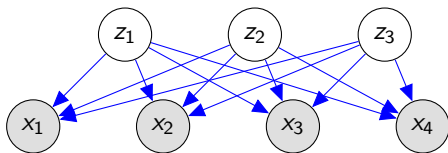
Intuition

Simply assume that the posterior consists of independent Markov chains.

Latent Factor Model

Joint distribution: latent variables are marginally independent a priori

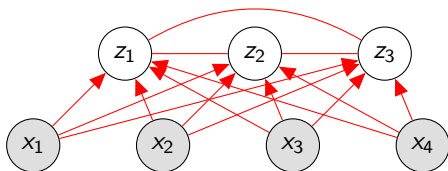
for example, $K = 3, N = 4$



Latent Factor Model

Joint distribution: latent variables are marginally independent a priori

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



Posterior: latent variables are conditionally dependent

Latent Factor Model

Latent binary variables that together produce an output.

- N output variables (e.g. pixels, words, sentences).
- K binary factors (usually much less than N).
- Complexity of inference: $\mathcal{O}(2^K)$.

Latent Factor Model

Intuition

Simply assume that the posterior consists of independent Bernoulli variables.

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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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Idea

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

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

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

Recap KL divergence

Properties

- $\text{KL}(q(z) \parallel p(z|x)) \geq 0$ with equality iff $q(z) = p(z|x)$.

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- $\text{KL}(q(z) \parallel p(z|x)) \geq 0$ with equality iff $q(z) = p(z|x)$.
- $-\text{KL}(q(z) \parallel p(z|x)) = \mathbb{E}_{q(z)} \left[\log \frac{p(z|x)}{q(z)} \right] \leq 0$.
- We want: $\text{supp}(q) \subseteq \text{supp}(p)$; otherwise $\text{KL}(q(z) \parallel p(z|x)) = \infty$

VI derivation I

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

VI derivation I

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

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

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

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

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

$$\arg \min_{q(z)} \text{KL}(q(z) \parallel p(z|x))$$

VI derivation II

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$$\begin{aligned} & \arg \min_{q(z)} \text{KL}(q(z) \parallel p(z|x)) \\ &= \arg \max_{q(z)} - \text{KL}(q(z) \parallel p(z|x)) \end{aligned}$$

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

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

Performing VI (Frequentist Case)

Variational Objective

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

This finds us the best posterior approximation for a **given model**.

Performing VI (Frequentist Case)

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Also optimize the model!

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

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

- 1 Maximize (regularised) expected log-density.

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

- 2 Optimise generative model.

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

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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What's the solution to the following?

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

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

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

Recap: EM Algorithm

$$\begin{aligned} \text{E-step} \quad & \arg \max_{q(z)} \mathbb{E}_{q(z)} [\log p(x, z)] + \mathbb{H}(p(z|x)) \\ & = p(z|x) \end{aligned}$$

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EM is variational inference!

$$\begin{aligned} q(z) &= p(z|x) \\ \text{KL}(q(z) || p(z|x)) &= 0 \end{aligned}$$

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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

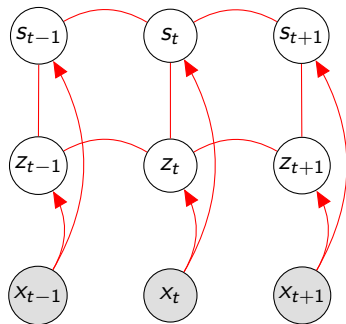
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- Formal assumption: $q(z) = \prod_{i=1}^N q(z_i)$

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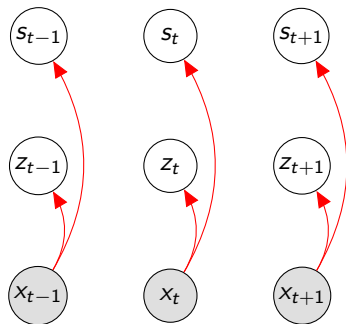
This approximation strategy is commonly known as **mean field** approximation.

Original FHMM Inference



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

Mean field FHHM Inference

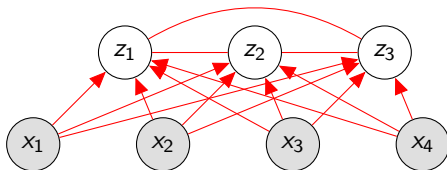


Approximate posterior $q(s, z) = \prod_{t=1}^T q(s_t)q(z_t)$

Original Latent Factor Model Inference

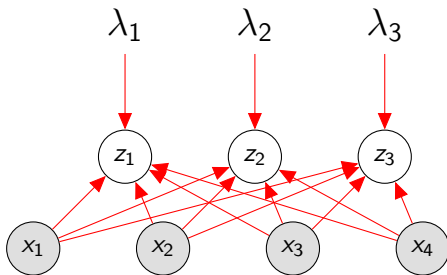
Joint distribution: latent variables are marginally independent a priori

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



Posterior: latent variables are marginally dependent given observations

Mean Field Latent Factor Model Inference



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

Amortised variational inference

Amortise the cost of inference using NNs

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

Amortised variational inference

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still mean field

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

Amortised variational inference

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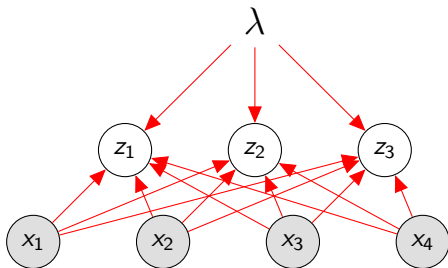
still mean field

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

but with a shared set of parameters

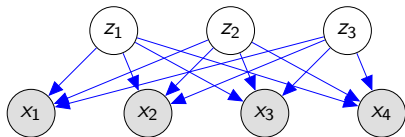
- where $b_1^K = \text{NN}(x; \lambda)$

Amortised Mean Field Inference for Latent Factor Model

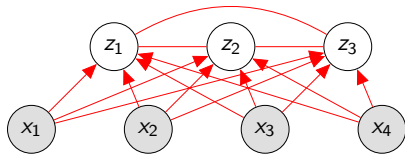


Overview

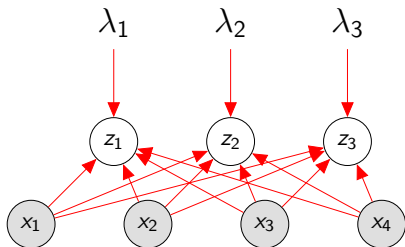
Joint distribution



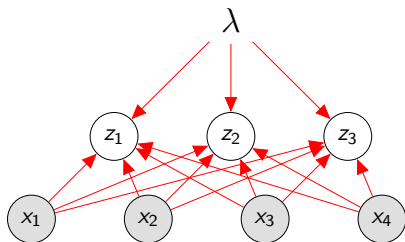
Posterior



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

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