Variational Inference: The Foundations

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https://vitutorial.github.io/tour/ua2020

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gourmet

This class is about approximate inference

- probabilistic models with latent variables often have intractable marginal and posterior
- inference in a probabilistic context means *computation*, it involves computing/inferring quantities by manipulation of probability calculus
- we will discuss one class of approximate inference algorithms known as *variational inference* (VI)

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

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

We can *invert* a conditional probability distribution.

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Bayes rule

We can *invert* a conditional probability distribution.

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

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)

Bayesian Inference

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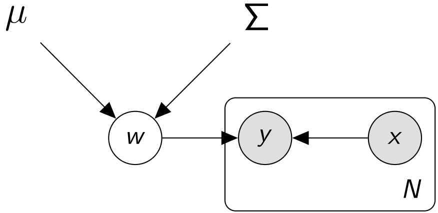
Today we will mostly focus on the frequentist case!

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 Model

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



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

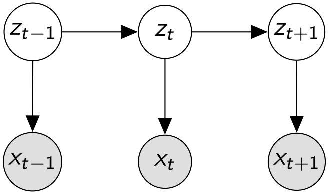
Bayesian Log-Linear Model

Intuition

Simply assume that the posterior is Gaussian.

Factorial HMMs

FHMMs have several Markov chains over latent variables.



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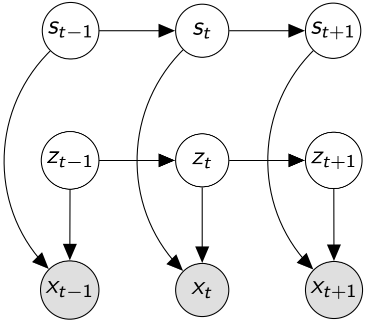

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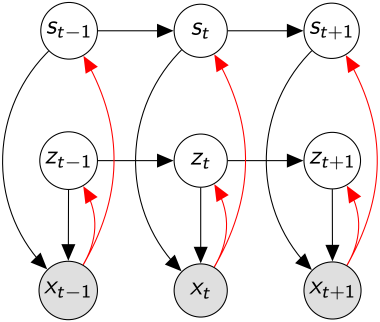

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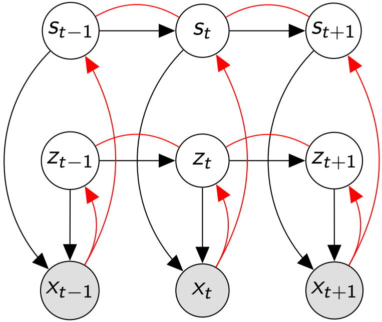

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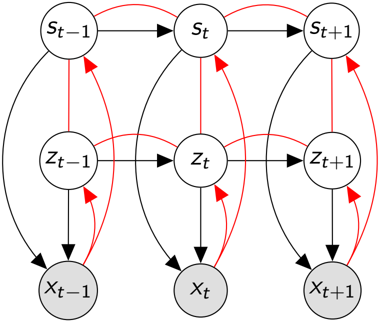
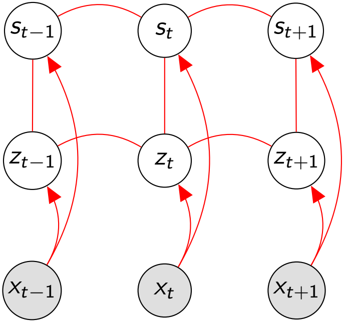


Factorial HMMs

Inference network for FHMMs.



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

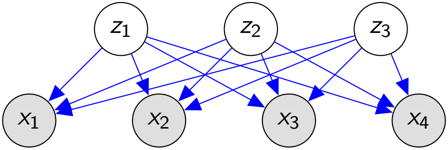
Intuition

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

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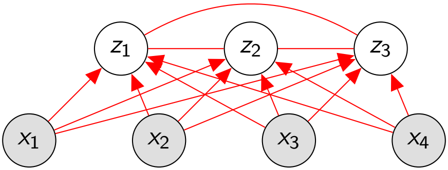

Posterior: latent variables are conditionally dependent

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: $\mathcal{O}(2^K)$.

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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.

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

Recap KL divergence

Properties

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

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Recap KL divergence

Properties

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

VI derivation I

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

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VI derivation I

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

This is a *lowerbound on the log-evidence*.
Crucially, it **does not require the true posterior**!

VI derivation I

Let's gain insight about this bound

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

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

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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

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Formal Objective

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VI derivation II

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Formal Objective

$$\begin{aligned}
&\arg\min_{q(z)} \; \mathrm{KL}\left(q(z) \,||\, p(z|x)\right) \\
&= \arg\max_{q(z)} -\mathrm{KL}\left(q(z) \,||\, p(z|x)\right)
\end{aligned}$$

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

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

Performing VI (Frequentist Case)

Variational Objective

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

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

Performing VI (Frequentist Case)

Variational Objective

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

Also optimize the model!

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

This optimises the posterior approximation and the **lowerbound** (not the evidence)

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.

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Performing VI (Frequentist Case)

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.

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

2. Optimise generative model.

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

Unconstrained (exact) optimisation

What's the solution to the following?

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

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

Unconstrained (exact) optimisation

What's the solution to the following?

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

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

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

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

Recap: EM Algorithm

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

$= p(z|x)$

Recap: EM Algorithm

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

$$\text{M-step} \quad \underset{p(x,z)}{\arg\max}\ \mathbb{E}_{p(z|x)}\left[\log p(x,z)\right] + \underbrace{\mathbb{H}\left(p(z|x)\right)}_{\text{constant}}$$

Recap: EM Algorithm

$$
\begin{aligned}
\text{E-step} \quad & \underset{q(z)}{\arg\max}\ \mathbb{E}_{q(z)}\left[\log p(x,z)\right] + \mathbb{H}\left(p(z|x)\right) \\
& = p(z|x) \\
\text{M-step} \quad & \underset{p(x,z)}{\arg\max}\ \mathbb{E}_{p(z|x)}\left[\log p(x,z)\right] + \underbrace{\mathbb{H}\left(p(z|x)\right)}_{\text{constant}}
\end{aligned}
$$

EM is variational inference!

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

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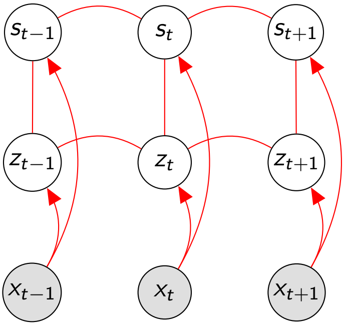
- Formal assumption: $q(z) = \prod_{i=1}^{N} q(z_i)$

Designing a tractable approximation

- Recall: The approximation $q(z)$ needs to be tractable.
- Common solution: make **all** latent variables independent under $q(z)$.
- Formal assumption: $q(z) = \prod_{i=1}^{N} q(z_i)$

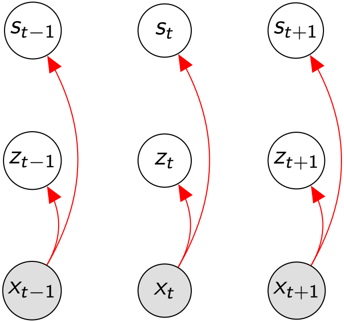
This approximation strategy is commonly known as **mean field** approximation.

Original FHMM Inference



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

Mean field FHMM Inference

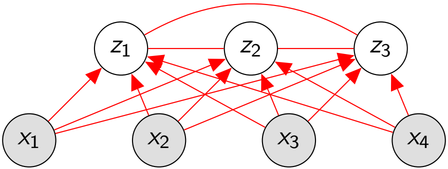


Approximate posterior $q(s, z) = \prod_{t=1}^{T} q(s_t)q(z_t)$

Original Latent Factor Model Inference

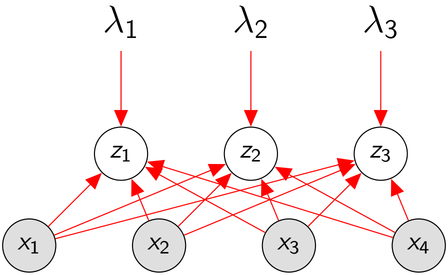
Joint distribution: latent variables are marginally independent a priori

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

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

Amortised variational inference

Amortise the cost of inference using NNs

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

still mean field

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

Amortised variational inference

Amortise the cost of inference using NNs

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

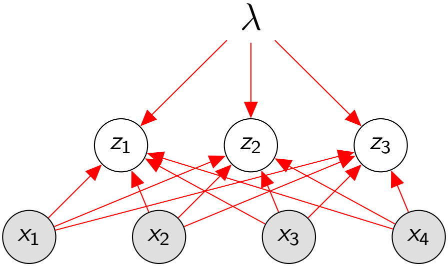
still mean field

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

but with a shared set of parameters

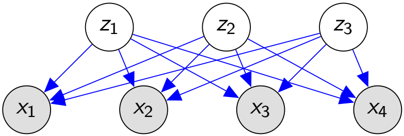
- where $b_1^K = \mathrm{NN}(x; \lambda)$

Amortised Mean Field Inference for Latent Factor Model

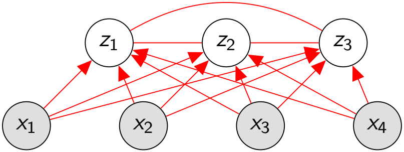


Overview

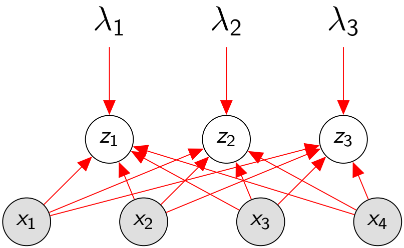
Joint distribution



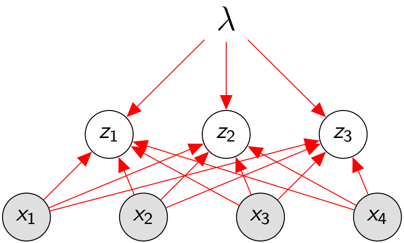
Posterior



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)**:

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

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

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

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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.