# BML lecture #3: variational Bayes

http://github.com/rbardenet/bml-course

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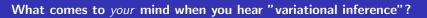




- 1 Introduction
- 2 Variational inference
- 3 Back to LDA
- 4 Generalizing VB

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- 2 Variational inference
- 3 Back to LDA
- 4 Generalizing VB



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- 2 Variational inference

- 3 Back to LDA
- 4 Generalizing VB

### When MCMC is intractable, variational inference comes to help

### Turning integration into optimization over measures

Variational Bayesian inference (VB) consists in approximating

$$\int f(\theta)\pi(\theta)\mathrm{d}\theta \approx \int f(\theta)q^{\star}(\theta)\mathrm{d}\theta$$

with  $q^* \in \arg\min_{q \in \mathcal{Q}} \operatorname{distance}(\pi, q)$ . Often we take

$$\mathsf{distance}(\pi,q) = \mathsf{KL}(q,\pi) := \int q(\theta) \log \frac{q(\theta)}{\pi(\theta)} \mathrm{d}\theta.$$

for computational convenience.

# But remember we can only evaluate $\pi_u = Z\pi...$

▶ Show that  $J(q) := \int q(\theta) \log \frac{q(\theta)}{\pi_n(\theta)} d\theta = \mathsf{KL}(q,\pi) - \log Z$ .

▶ In particular, 
$$L(q) = -J(q) \leqslant \log Z$$
. For

$$\pi_u(\theta) = p(\mathsf{data}|\theta)p(\theta),$$

L(q) is thus a lower bound for the evidence p(data) (ELBO).

# Choosing the approximating family $\mathcal Q$

▶ The most common approach is the mean-field approximation

$$Q = \{\theta \mapsto \prod_{d=1}^{D} q_d(\theta_d)\}.$$

Include all variables over which you integrate, e.g.

$$q(\theta, z_{1:n}) = \prod_{d=1}^{D} q_d(\theta_d) \prod_{i=1}^{N} q_i(z_i).$$

- ▶ Try to keep some dependence if it is key in your application.
- If your original model has NEF conditionals, coordinate-wise maximization of  $q \mapsto L(q)$  is easy.

# Mean-field yields closed-form updates

- 1 Introduction
- 2 Variational inference
- 3 Back to LDA
- 4 Generalizing VB

# Back to LDA 1/2

$$\begin{split} \log p(y, z, \pi, B) \\ &= \sum_{i=1}^{N} \left[ \log p(\pi_{i} | \alpha) + \sum_{\ell=1}^{L_{i}} \left( \log p(z_{i\ell} | \pi_{i}) + \log p(y_{i\ell} | z_{i\ell}, B) \right) \right] + p(B | \gamma) \\ &\propto \sum_{i=1}^{N} \left[ \sum_{k=1}^{K} \alpha_{k} \log \pi_{ik} + \sum_{\ell=1}^{L_{i}} \left( \sum_{k=1}^{K} \mathbf{1}_{z_{i\ell} = k} \log \pi_{ik} + \sum_{v=1}^{V} \sum_{k=1}^{K} \mathbf{1}_{y_{i\ell} = v} \mathbf{1}_{z_{i\ell} = k} \log b_{kv} \right) \right] \\ &+ \sum_{k=1}^{K} \sum_{v=1}^{V} \gamma_{k} \log b_{kv}. \end{split}$$

#### Lemma (exercise)

Let  $\Psi(\cdot) := \Gamma'(\cdot)/\Gamma(\cdot)$  be the digamma function. Then

$$\mathbb{E}_{\mathsf{Dir}(\theta|\eta)}\log\theta_i = \Psi(\eta_i) - \Psi(\|\eta\|_1).$$

# **VB** for **LDA**: singling out $\pi_i$

$$\log p(y, z, \pi, B)$$

$$\propto \sum_{i=1}^{N} \left[ \sum_{k=1}^{K} \alpha_k \log \pi_{ik} + \sum_{\ell=1}^{L_i} \left( \sum_{k=1}^{K} 1_{z_{i\ell}=k} \log \pi_{ik} + \sum_{v=1}^{V} \sum_{k=1}^{K} 1_{y_{i\ell}=v} 1_{z_{i\ell}=k} \log b_{kv} \right) \right] + \sum_{k=1}^{K} \sum_{v=1}^{V} \gamma_k \log b_{kv}.$$

# **VB** for **LDA**: singling out $z_{i\ell}$

$$\log p(y, z, \pi, B)$$

$$\propto \sum_{i=1}^{N} \left[ \sum_{k=1}^{K} \alpha_{k} \log \pi_{ik} + \sum_{\ell=1}^{L_{i}} \left( \sum_{k=1}^{K} 1_{z_{i\ell} = k} \log \pi_{ik} + \sum_{v=1}^{V} \sum_{k=1}^{K} 1_{y_{i\ell} = v} 1_{z_{i\ell} = k} \log b_{kv} \right) \right] + \sum_{k=1}^{K} \sum_{v=1}^{V} \gamma_{k} \log b_{kv}.$$

# **VB** for **LDA**: singling out $B_{k:}$

$$\log p(y, z, \pi, B)$$

$$\propto \sum_{i=1}^{N} \left[ \sum_{k=1}^{K} \alpha_k \log \pi_{ik} + \sum_{\ell=1}^{L_i} \left( \sum_{k=1}^{K} 1_{z_{i\ell}=k} \log \pi_{ik} + \sum_{v=1}^{V} \sum_{k=1}^{K} 1_{y_{i\ell}=v} 1_{z_{i\ell}=k} \log b_{kv} \right) \right] + \sum_{k=1}^{K} \sum_{v=1}^{V} \gamma_k \log b_{kv}.$$

### Using counts keeps space and time complexity low

▶ Storing  $\tilde{z}_{i\ell k}$  requires  $\mathcal{O}(NK \sum_i L_i)$  space. In practice, one works with (sparse) count data

 $n_{iv}$  = number of times word v appears in document i,

and variables  $c_{ivk}$ , thus reducing storage costs (and the dimension of the underlying integral!) to  $\mathcal{O}(NVK)$ .

Reparametrization+SGD vs mean-field+closed updates

# VB for deep networks

### Lots of variants of VB exist (Mur12)

For hidden variable models, EM is VB with

$$q(z,\theta) = \pi(z|\theta)\delta_{\tilde{\theta}}(\theta).$$

Variational EM is VB with

$$q(z,\theta) = q(z)\delta_{\tilde{\theta}}(\theta).$$

- ▶ VB for any PGMs with NEF arrows is variational message passing.
- Rather approximating

$$\pi( heta)pprox\prod_{f=1}^Fq_f( heta)$$

leads to expectation propagation.

► These days, ADVI with stochastic gradients is the default VI choice in probabilistic programming software like PyMC3, Stan, or PyRo.

1 Introduction

2 Variational inference

- 3 Back to LDA
- 4 Generalizing VB

### "Optimization-centric" Bayesian inference

Given a loss  $\ell$ , a divergence D, and a set of distributions Q, consider

$$q^{\star} \in \arg\min_{q \in \mathcal{Q}} \mathbb{E}_q \sum_{i=1}^N \ell(\theta, x_i) + D(q(\theta) \mathrm{d}\theta, p(\theta) d\theta).$$
  $(P(\ell, D, \mathcal{Q}))$ 

#### Conclusion on VB

- ► Computationally attractive alternative to MCMC.
- Lots of open questions on connecting VB and to the original SEU problem: is VB justified in itself or is it simply a computationally convenient backup option?
- Many partial answers, e.g. try to use VB in importance sampling, optimization-centric viewpoint.
- ► More meaningful alternatives to the KL: maximum mean discrepancy, etc.

# References I