

Variational Inference

Material adapted from David Blei University of Maryland

Variational Inference

- Inferring hidden variables
- Unlike MCMC:
 - Deterministic
 - Easy to gauge convergence
 - Requires dozens of iterations
- Doesn't require conjugacy
- Slightly hairier math

Setup

- $\vec{x} = x_{1:n}$ observations
- $\vec{z} = z_{1 \cdot m}$ hidden variables
- α fixed parameters
- Want the posterior distribution

$$p(z|x,\alpha) = \frac{p(z,x|\alpha)}{\int_{z} p(z,x|\alpha)}$$
(1)

Motivation

Can't compute posterior for many interesting models

GMM (finite)

- 1. Draw $\mu_k \sim \mathcal{N}(0, \tau^2)$
- 2. For each observation $i = 1 \dots n$:
 - 2.1 Draw $z_i \sim \text{Mult}(\pi)$
 - 2.2 Draw $x_i \sim \mathcal{N}(\mu_{z_i}, \sigma_0^2)$
- Posterior is intractable for large n, and we might want to add priors

$$p(\mu_{1:K}, z_{1:n} | x_{1:n}) = \frac{\prod_{k=1}^{K} p(\mu_k) \prod_{i=1}^{n} p(z_i) p(x_i | z_i, \mu_{1:K})}{\int_{\mu_{1:K}} \sum_{z_{1:n}} \prod_{k=1}^{K} p(\mu_k) \prod_{i=1}^{n} p(z_i) p(x_i | z_i, \mu_{1:K})}$$
(2

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Consider all means

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(2

Consider all assignments

Main Idea

We create a variational distribution over the latent variables

$$q(z_{1:m}|\nu) \tag{3}$$

- Find the settings of v so that q is close to the posterior
- If q == p, then this is vanilla EM

What does it mean for distributions to be close?

 We measure the closeness of distributions using Kullback-Leibler Divergence

$$KL(q||p) \equiv \mathbb{E}_q \left[\log \frac{q(Z)}{p(Z|x)} \right]$$
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- Characterizing KL divergence
 - If q and p are high, we're happy
 - If q is high but p isn't, we pay a price
 - If q is low, we don't care
 - If KL = 0, then distribution are equal

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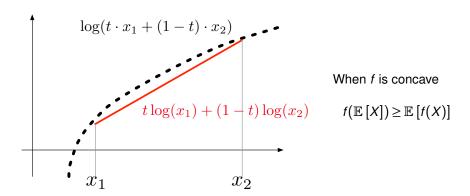
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This behavior is often called "mode splitting": we want **a** good solution, not every solution.

Jensen's Inequality: Concave Functions and Expectations



If you haven't seen this before, spend fifteen minutes to convince yourself that it's true

Material adapted from David Blei | UMD

Apply Jensen's inequality on log probability of data

$$\log p(x) = \log \left[\int_{z} p(x,z) \right]$$

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$$\log p(x) = \log \left[\int_{z} p(x, z) \right]$$
$$= \log \left[\int_{z} p(x, z) \frac{q(z)}{q(z)} \right]$$

Add a term that is equal to one

Apply Jensen's inequality on log probability of data

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$$= \log \left[\int_{z} p(x, z) \frac{q(z)}{q(z)} \right]$$

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

Take the numerator to create an expectation

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

Apply Jensen's equality and use log difference

Apply Jensen's inequality on log probability of data

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- Fun side effect: Entropy
- Maximizing the ELBO gives as tight a bound on on log probability

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Conditional probability definition

$$\rho(z|x) = \frac{p(z,x)}{p(x)} \tag{5}$$

Conditional probability definition

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Plug into KL divergence

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Break quotient into difference

Conditional probability definition

$$p(z|x) = \frac{p(z,x)}{p(x)}$$
 (5)

Plug into KL divergence

$$\begin{aligned} \mathsf{KL}(q(z) || \, p(z | \, x)) = & \mathbb{E}_q \bigg[\log \frac{q(z)}{p(z | \, x)} \bigg] \\ = & \mathbb{E}_q \big[\log q(z) \big] - \mathbb{E}_q \big[\log p(z | \, x) \big] \\ = & \mathbb{E}_q \big[\log q(z) \big] - \mathbb{E}_q \big[\log p(z, x) \big] + \log p(x) \end{aligned}$$

Apply definition of conditional probability

Conditional probability definition

$$p(z|x) = \frac{p(z,x)}{p(x)} \tag{5}$$

Plug into KL divergence

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Reorganize terms

Conditional probability definition

$$p(z|x) = \frac{p(z,x)}{p(x)} \tag{5}$$

Plug into KL divergence

$$\begin{split} \mathsf{KL}(q(z) || \, p(z | \, x)) = & \mathbb{E}_q \bigg[\log \frac{q(z)}{p(z | \, x)} \bigg] \\ = & \mathbb{E}_q \big[\log q(z) \big] - \mathbb{E}_q \big[\log p(z | \, x) \big] \\ = & \mathbb{E}_q \big[\log q(z) \big] - \mathbb{E}_q \big[\log p(z, x) \big] + \log p(x) \\ = & - \Big(\mathbb{E}_q \big[\log p(z, x) \big] - \mathbb{E}_q \big[\log q(z) \big] \Big) + \log p(x) \end{split}$$

 Negative of ELBO (plus constant); minimizing KL divergence is the same as maximizing ELBO

Mean field variational inference

Assume that your variational distribution factorizes

$$q(z_1,...,z_m) = \prod_{j=1}^m q(z_j)$$
 (6)

- You may want to group some hidden variables together
- Does not contain the true posterior because hidden variables are dependent

General Blueprint

- Choose q
- Derive ELBO
- Coordinate ascent of each q_i
- Repeat until convergence

Material adapted from David Blei | UMD

Example: Latent Dirichlet Allocation

TOPIC 1

computer, technology, system, service, site, phone, internet, machine

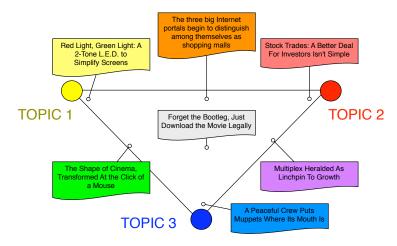
TOPIC 2

sell, sale, store, product, business, advertising, market, consumer

TOPIC 3

play, film, movie, theater, production, star, director, stage

Example: Latent Dirichlet Allocation



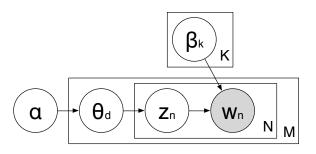
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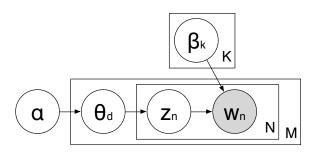
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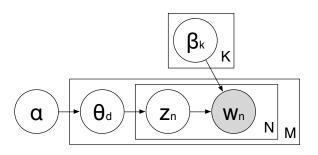
Holwood studies are preparing to let people download and buy electronic copies of movies over the Internet, much as record laters now sell songs for 99 cents through Apple Computer's iTunes music store and other online services ...



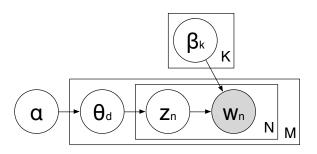
■ For each topic $k \in \{1, ..., K\}$, a multinomial distribution β_k



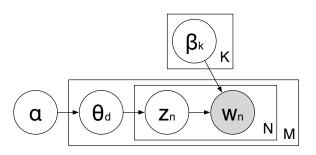
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- Choose the observed word w_n from the distribution β_{z_n} .



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Deriving Variational Inference for LDA

Joint distribution:

$$p(\theta, z, w | \alpha, \beta) = \prod_{d} p(\theta_{d} | \alpha) \prod_{n} p(z_{d,n} | \theta_{d}) p(w_{d,n} | \beta, z_{d,n})$$
(7)

Deriving Variational Inference for LDA

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(7)

•
$$p(\theta_d | \alpha) = \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \prod_k \theta_{d,k}^{\alpha_k - 1}$$
 (Dirichlet)

Joint distribution:

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- $p(\theta_d | \alpha) = \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \prod_k \theta_{d,k}^{\alpha_k 1}$ (Dirichlet)
- $p(z_{d,n}|\theta_d) = \theta_{d,z_{d,n}}$ (Draw from Multinomial)

Joint distribution:

$$p(\theta, z, w | \alpha, \beta) = \prod_{d} p(\theta_{d} | \alpha) \prod_{n} p(z_{d,n} | \theta_{d}) p(w_{d,n} | \beta, z_{d,n})$$
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- $p(z_{d,n}|\theta_d) = \theta_{d,z_{d,n}}$ (Draw from Multinomial)
- $p(w_{d,n} | \beta, z_{d,n}) = \beta_{z_{d,n}, w_{d,n}}$ (Draw from Multinomial)

Joint distribution:

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(7)

Variational distribution:

$$q(\theta, z) = q(\theta | \gamma)q(z | \phi)$$
 (8)

Joint distribution:

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Variational distribution:

$$q(\theta, z) = q(\theta | \gamma)q(z | \phi)$$
 (8)

ELBO:

$$L(\gamma, \phi; \alpha, \beta) = \mathbb{E}_{q}[\log p(\theta \mid \alpha)] + \mathbb{E}_{q}[\log p(z \mid \theta)] + \mathbb{E}_{q}[\log p(w \mid z, \beta)] - \mathbb{E}_{q}[\log q(\theta)] - \mathbb{E}_{q}[\log q(z)]$$
(9)

What is the variational distribution?

$$q(\vec{\theta}, \vec{z}) = \prod_{d} q(\theta_d | \gamma_d) \prod_{n} q(z_{d,n} | \phi_{d,n})$$
 (10)

- Variational document distribution over topics γ_d
 - Vector of length K for each document
 - Non-negative
 - Doesn't sum to 1.0
- Variational token distribution over topic assignments $\phi_{d,n}$
 - Vector of length K for every token
 - Non-negative, sums to 1.0

Expectation of log Dirichlet

- Most expectations are straightforward to compute
- Dirichlet is harder

$$\mathbb{E}_{\mathsf{dir}}[\log p(\theta_i | \alpha)] = \Psi(\alpha_i) - \Psi\left(\sum_j \alpha_j\right) \tag{11}$$

$$\mathbb{E}_{q}\left[\log p(\theta \mid \alpha)\right] = \mathbb{E}_{q}\left[\log \left\{\frac{\Gamma(\sum_{i} \alpha_{i})}{\prod_{i} \Gamma(\alpha_{i})} \prod_{i} \theta_{i}^{\alpha_{i}-1}\right\}\right]$$
(12)

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$$= \mathbb{E}_{q}\left[\log \left\{\frac{\Gamma(\sum_{i} \alpha_{i})}{\prod_{i} \Gamma(\alpha_{i})}\right\} + \sum_{i} \log \theta_{i}^{\alpha_{i}-1}\right]$$
(12)

Log of products becomes sum of logs.

$$\mathbb{E}_{q}[\log p(\theta \mid \alpha)] = \mathbb{E}_{q}\left[\log\left\{\frac{\Gamma(\sum_{i}\alpha_{i})}{\prod_{i}\Gamma(\alpha_{i})}\prod_{i}\theta_{i}^{\alpha_{i}-1}\right\}\right]$$

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$$= \log\Gamma(\sum_{i}\alpha_{i}) - \sum_{i}\log\Gamma(\alpha_{i}) + \mathbb{E}_{q}\left[\sum_{i}(\alpha_{i}-1)\log\theta_{i}\right]$$

$$(13)$$

Log of exponent becomes product, expectation of constant is constant

$$\mathbb{E}_{q}[\log p(\theta \mid \alpha)] = \mathbb{E}_{q}\left[\log\left\{\frac{\Gamma(\sum_{i}\alpha_{i})}{\prod_{i}\Gamma(\alpha_{i})}\prod_{i}\theta_{i}^{\alpha_{i}-1}\right\}\right]$$

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$$= \log\Gamma(\sum_{i}\alpha_{i}) - \sum_{i}\log\Gamma(\alpha_{i})$$

$$+ \sum_{i}(\alpha_{i}-1)\left(\Psi(\gamma_{i}) - \Psi\left(\sum_{i}\gamma_{i}\right)\right)$$

$$(12)$$

Expectation of log Dirichlet

$$\mathbb{E}_{q}[\log p(z|\theta)] = \mathbb{E}_{q}\left[\log \prod_{n} \prod_{i} \theta_{i}^{\mathbb{1}[z_{n}==i]}\right]$$
(13)

$$\mathbb{E}_{q}[\log p(z|\theta)] = \mathbb{E}_{q} \left[\log \prod_{n} \prod_{i} \theta_{i}^{\mathbb{I}[z_{n}==i]} \right]$$
 (13)

$$= \mathbb{E}_q \left[\sum_{n} \sum_{i} \log \theta_i^{\mathbb{1}[z_n = -i]} \right]$$
 (14)

(15)

Products to sums

$$\mathbb{E}_{q}[\log p(z|\theta)] = \mathbb{E}_{q}\left[\log \prod_{n} \prod_{i} \theta_{i}^{\mathbb{I}[z_{n}==i]}\right]$$
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(16)

Linearity of expectation

$$\mathbb{E}_{q}[\log p(z|\theta)] = \mathbb{E}_{q}\left[\log \prod_{n} \prod_{i} \theta_{i}^{\mathbb{1}[z_{n}=-i]}\right]$$
(13)

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 (15)

$$= \sum_{n} \sum_{i} \phi_{ni} \mathbb{E}_{q} [\log \theta_{i}]$$
 (16)

(17)

Independence of variational distribution, exponents become products

$$\mathbb{E}_{q}\left[\log p(z|\theta)\right] = \mathbb{E}_{q}\left[\log \prod_{n} \prod_{i} \theta_{i}^{\mathbb{1}\left[z_{n}=-i\right]}\right]$$
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$$= \sum_{n} \sum_{i} \phi_{ni} \left(\Psi(\gamma_{i}) - \Psi\left(\sum_{j} \gamma_{j}\right) \right) \tag{17}$$

Expectation of log Dirichlet

$$\mathbb{E}_{q}\left[\log p(w|z,\beta)\right] = \mathbb{E}_{q}\left[\log \beta_{z_{d,n},w_{d,n}}\right]$$
(18)

(19)

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(18)

$$= \mathbb{E}_q \left[\log \prod_{v}^{V} \prod_{i}^{K} \beta_{i,v}^{\mathbb{1}[v = w_{d,n}, z_{d,n} = i]} \right]$$
 (19)

(20)

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$$(19)$$

$$= \sum_{v}^{V} \sum_{i}^{K} \mathbb{E}_{q} [\mathbb{1} [v = w_{d,n}, z_{d,n} = i]] \log \beta_{i,v}$$
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 (20)

$$=\sum_{v}^{V}\sum_{i}^{K}\phi_{n,i}w_{d,n}^{v}\log\beta_{i,v}$$
 (21)

Entropies

Entropy of Dirichlet

$$\mathbb{H}_{q}[\gamma] = -\log\Gamma\left(\sum_{j}\gamma_{j}\right) + \sum_{i}\log\Gamma(\gamma_{i})$$
$$-\sum_{i}(\gamma_{i}-1)\left(\Psi(\gamma_{i}) - \Psi\left(\sum_{j=1}^{k}\gamma_{j}\right)\right)$$

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$$-\sum_{i}(\gamma_{i}-1)\left(\Psi(\gamma_{i}) - \Psi\left(\sum_{j=1}^{k}\gamma_{j}\right)\right)$$

Entropy of Multinomial

$$\mathbb{H}_{q}[\phi_{d,n}] = -\sum_{i} \phi_{d,n,i} \log \phi_{d,n,i} \tag{22}$$

Complete objective function

$$\begin{split} L(\mathbf{y}, \mathbf{\phi}; \mathbf{\alpha}, \mathbf{\beta}) &= \log \Gamma \left(\sum_{j=1}^k \alpha_j \right) - \sum_{i=1}^k \log \Gamma(\alpha_i) + \sum_{i=1}^k \left(\alpha_i - 1 \right) \left(\Psi(\mathbf{y}_i) - \Psi \left(\sum_{j=1}^k \mathbf{y}_j \right) \right) \\ &+ \sum_{n=1}^N \sum_{i=1}^k \phi_{ni} \left(\Psi(\mathbf{y}_i) - \Psi \left(\sum_{j=1}^k \mathbf{y}_j \right) \right) \\ &+ \sum_{n=1}^N \sum_{i=1}^k \sum_{j=1}^V \phi_{ni} w_n^j \log \beta_{ij} \\ &- \log \Gamma \left(\sum_{j=1}^k \mathbf{y}_j \right) + \sum_{i=1}^k \log \Gamma(\mathbf{y}_i) - \sum_{i=1}^k (\mathbf{y}_i - 1) \left(\Psi(\mathbf{y}_i) - \Psi \left(\sum_{j=1}^k \mathbf{y}_j \right) \right) \\ &- \sum_{n=1}^N \sum_{i=1}^k \phi_{ni} \log \phi_{ni}, \end{split}$$

Note the entropy terms at the end (negative sign)

Deriving the algorithm

- Compute partial wrt to variable of interest
- Set equal to zero
- Solve for variable

Material adapted from David Blei | UMD Variationa

Update for ϕ

Derivative of ELBO:

$$\frac{\partial \mathcal{L}}{\partial \phi_{ni}} = \Psi(\gamma_i) - \Psi\left(\sum_j \gamma_j\right) + \log \beta_{i,v} - \log \phi_{ni} - 1 + \lambda \tag{23}$$

Solution:

$$\phi_{ni} \propto \beta_{iv} \exp\left(\Psi(\gamma_i) - \Psi\left(\sum_j \gamma_j\right)\right)$$
 (24)

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Update for γ

Derivative of ELBO:

$$\frac{\partial \mathcal{L}}{\partial \gamma_{i}} = \Psi'(\gamma_{i}) (\alpha_{i} + \phi_{n,i} - \gamma_{i})$$

$$-\Psi'\left(\sum_{j} \gamma_{j}\right) \sum_{j} \left(\alpha_{j} + \sum_{n} \phi_{nj} - \gamma_{j}\right)$$

Update for γ

Derivative of ELBO:

$$\frac{\partial \mathcal{L}}{\partial \gamma_{i}} = \Psi'(\gamma_{i}) \left(\alpha_{i} + \phi_{n,i} - \gamma_{i}\right)$$

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Update for γ

Derivative of ELBO:

$$\frac{\partial \mathcal{L}}{\partial \gamma_{i}} = \Psi'(\gamma_{i}) \left(\alpha_{i} + \phi_{n,i} - \gamma_{i}\right)$$
$$-\Psi'\left(\sum_{j} \gamma_{j}\right) \sum_{j} \left(\alpha_{j} + \sum_{n} \phi_{nj} - \gamma_{j}\right)$$

Solution:

$$\gamma_i = \alpha_i + \sum_n \phi_{ni} \tag{25}$$

Update for β

Slightly more complicated (requires Lagrange parameter), but solution is obvious:

$$\beta_{ij} \propto \sum_{d} \sum_{n} \phi_{dni} w_{dn}^{j} \tag{26}$$

Overall Algorithm

- 1. Randomly initialize variational parameters (can't be uniform)
- 2. For each iteration:
 - **2.1** For each document, update γ and ϕ
 - 2.2 For corpus, update β
 - 2.3 Compute $\mathcal L$ for diagnostics
- Return expectation of variational parameters for solution to latent variables

Relationship with Gibbs Sampling

- Gibbs sampling: sample from the conditional distribution of all other variables
- Variational inference: each factor is set to the exponentiated log of the conditional
- Variational is easier to parallelize, Gibbs faster per step
- Gibbs typically easier to implement

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- Randomize initialization, but specify seed
- Use simple languages first

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- Visualize variational parameters
- Cache / memoize gamma / digamma functions

Next class

- Example on toy LDA problem
- Current research in variational inference

Material adapted from David Blei | UMD