

# Variational Inference

Material adapted from David Blei

University of Maryland

Introduction

# Variational Inference

- Inferring hidden variables

# Variational Inference

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

Conjugacy: the joint distribution has special properties—we'll talk more about what that means in a second if you haven't heard that term before.

# Setup

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

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

# 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  $x_i \sim \mathcal{N}(\mu_{z_i}, \sigma_0^2)$

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- Posterior is intractable for large  $n$ , and we might want to add priors

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

Consider all means

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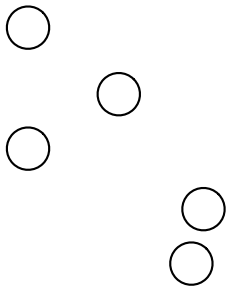
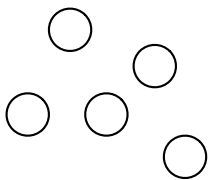
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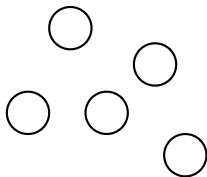
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Consider all assignments

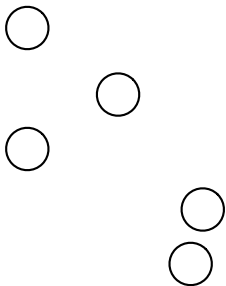




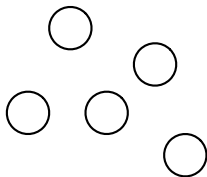
$\gamma_2$  +



$\gamma_1$  +



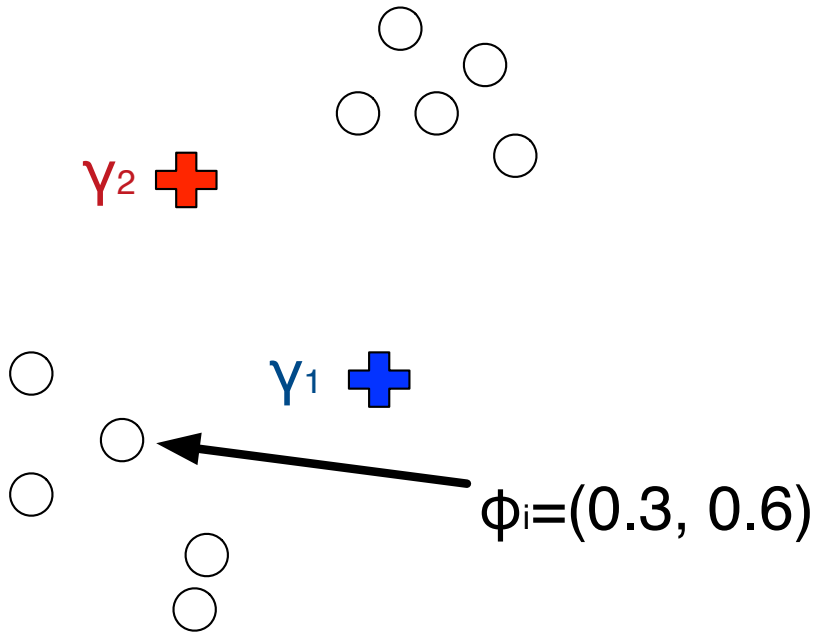
$\gamma_2 +$



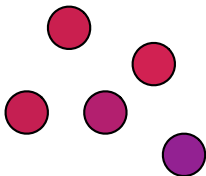
$\gamma_1 +$



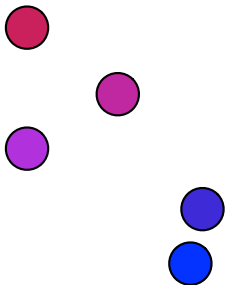
$\phi_i$

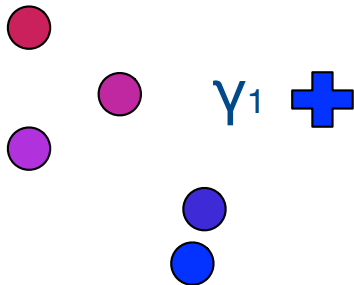
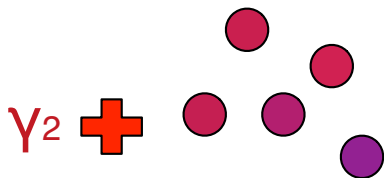


$\gamma_2 +$



$\gamma_1 +$





## Main Idea

- We create a **variational distribution** over the latent variables

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

- Find the settings of  $\nu$  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

$$\text{KL}(q||p) \equiv \mathbb{E}_q \left[ \log \frac{q(Z)}{p(Z|x)} \right] \quad (4)$$

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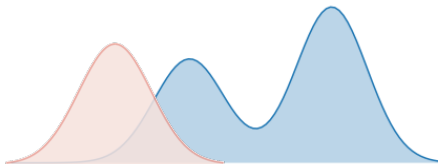
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This behavior is often called “mode splitting”: we want **a** good solution, not every solution.

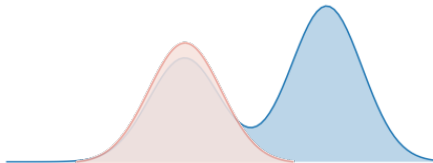
$KL(Q \parallel P)$

Bad



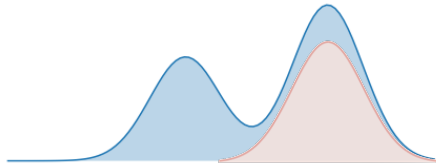
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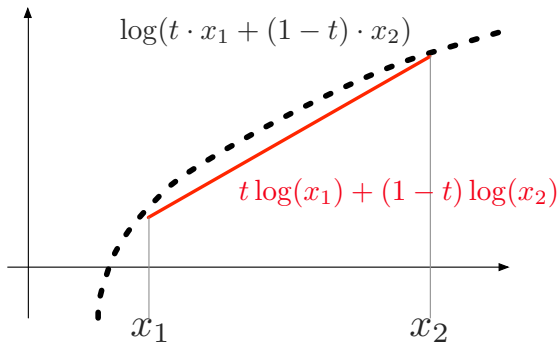


$KL(Q \parallel P)$

Equally Good



# Jensen's Inequality: Concave Functions and Expectations



When  $f$  is concave

$$f(\mathbb{E}[X]) \geq \mathbb{E}[f(X)]$$

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

## Evidence Lower Bound (ELBO)

- Apply Jensen's inequality on log probability of data

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Add a term that is equal to one

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Take the numerator to create an expectation

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Apply Jensen's equality and use log difference

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- Maximizing the ELBO gives as tight a bound on on log probability



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## Relation to KL Divergence

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Break quotient into difference

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Apply definition of conditional probability

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Reorganize terms



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



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P. DEBYE	M. KNUDSEN	W.L. BRAGG	H.A. KRAMERS	P.A.M. DIRAC	A.H. COMPTON	L. de BROGLIE	M. BORN	N. BOHR		
I. LANGMUIR	M. PLANCK	Mme CURIE	H.A. LORENTZ	A. EINSTEIN	P. LANGEVIN	Ch.E. GUYE	C.T.R. WILSON	O.W. RICHARDSON		

Absents : Sir W.H. BRAGG, H. DESLANDRES et E. VAN AUBEL



210 LE MAGNÉTISME.

parallèlement ou en sens opposés. On peut dire que l'énergie, ou la fonction d'Hamilton, est dans ce cas

$$\mathcal{H} = -A \sum_k (\sigma_k, \sigma_{k+1}),$$

où  $\sigma_k$  représente le vecteur de pivotement du  $k^{\text{ème}}$  électron. On a  $(\sigma, \sigma_{k+1}) = \pm 1$  suivant que les pivotements sont parallèles ou opposés. Ising n'a rien trouvé, dans les propriétés de ce modèle, qui corresponde au ferromagnétisme, mais une dépendance entre

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## Mean field variational inference

- Assume that your variational distribution factorizes

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

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

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# Gates

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**Tom Minka**

Microsoft Research Ltd.  
Cambridge, UK

**John Winn**

Microsoft Research Ltd.  
Cambridge, UK

## Abstract

Gates are a new notation for representing mixture models and context-sensitive independence in factor graphs. Factor graphs provide a natural representation for message-passing algorithms, such as expectation propagation. However, message passing in mixture models is not well captured by factor graphs unless the entire mixture is represented by one factor, because the message equations have a containment structure. Gates capture this containment structure graphically, allowing both the independences and the message-passing equations for a model to be readily visualized. Different variational approximations for mixture models can be understood as different ways of drawing the gates in a model. We present general equations for expectation propagation and variational message passing in the presence of gates.

# General Blueprint

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

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LDA Derivation



## Latent Dirichlet Allocation

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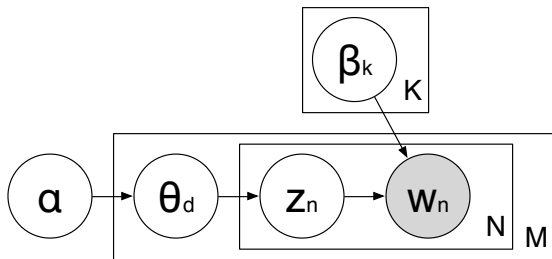
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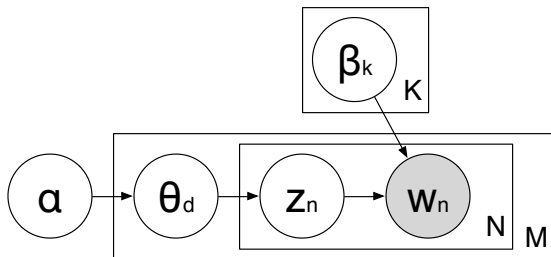
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## LDA Generative Model



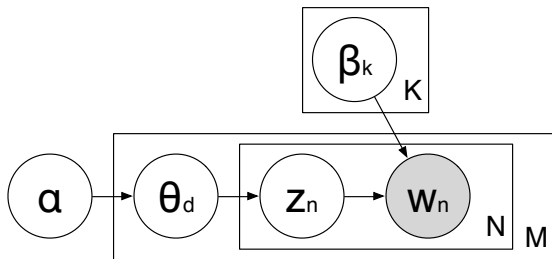
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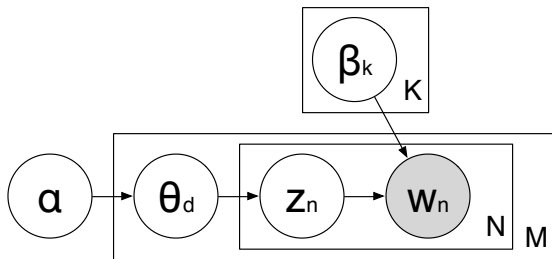
- For each topic  $k \in \{1, \dots, K\}$ , a multinomial distribution  $\beta_k$
- For each document  $d \in \{1, \dots, M\}$ , draw a multinomial distribution  $\theta_d$  from a Dirichlet distribution with parameter  $\alpha$

# LDA Generative Model



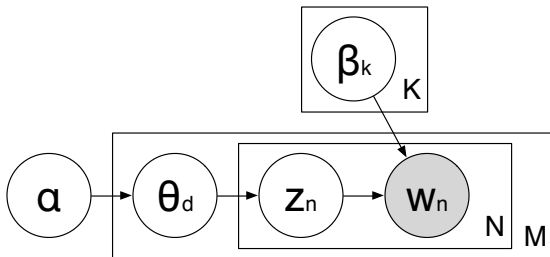
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Statistical inference uncovers most unobserved variables given data.

## Example: Latent Dirichlet Allocation

### TOPIC 1

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

### TOPIC 2

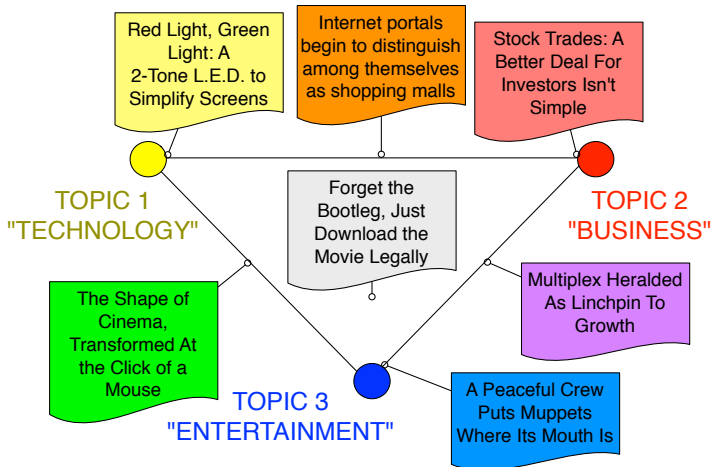
sell, sale,  
store, product,  
business,  
advertising,  
market,  
consumer

### TOPIC 3

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

Distribution over words given a topic  $i$ :  $\beta_i$

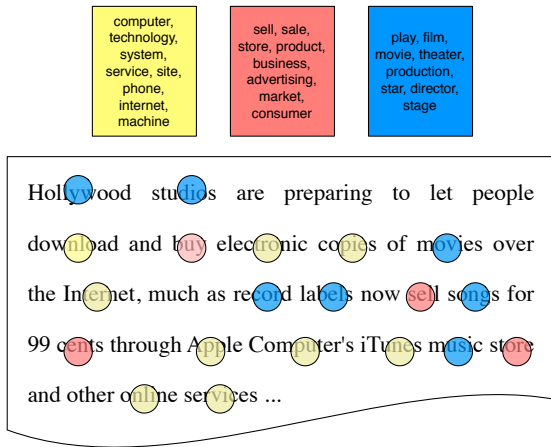
## Example: Latent Dirichlet Allocation



Distribution over topics given a document  $d$ :  $\theta_d$



## Example: Latent Dirichlet Allocation



Assignment of token to topic:  $z_{d,n}$

## Deriving Variational Inference for LDA

Joint distribution:

$$p(\theta, z, w | \alpha, \beta) = \prod_d p(\theta_d | \alpha) \prod_n p(z_{d,n} | \theta_d) p(w_{d,n} | \beta, z_{d,n}) \quad (7)$$

## Deriving Variational Inference for LDA

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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)

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- $p(z_{d,n} | \theta_d) = \theta_{d,z_{d,n}}$  (Draw from Multinomial)

# Deriving Variational Inference for LDA

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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)

## Deriving Variational Inference for LDA

Joint distribution:

$$p(\theta, z, w | \alpha, \beta) = \prod_d p(\theta_d | \alpha) \prod_n p(z_{d,n} | \theta_d) p(w_{d,n} | \beta, z_{d,n}) \quad (7)$$

Variational distribution:

$$q(\Theta, Z) = \prod_d q(\theta_d | \gamma_d) \prod_n q(z_{d,n} | \phi_{d,n}) \quad (8)$$

## Deriving Variational Inference for LDA

Joint distribution:

$$p(\theta, z, w | \alpha, \beta) = \prod_d p(\theta_d | \alpha) \prod_n p(z_{d,n} | \theta_d) p(w_{d,n} | \beta, z_{d,n}) \quad (7)$$

Variational distribution:

$$q(\Theta, Z) = \prod_d q(\theta_d | \gamma_d) \prod_n q(z_{d,n} | \phi_{d,n}) \quad (8)$$

ELBO:

$$\begin{aligned} L(\gamma, \phi; \alpha, \beta) = & \mathbb{E}_q [\log p(\theta | \alpha)] + \mathbb{E}_q [\log p(z | \theta)] + \mathbb{E}_q [\log p(w | z, \beta)] \\ & - \mathbb{E}_q [\log q(\theta)] - \mathbb{E}_q [\log q(z)] \end{aligned} \quad (9)$$

## What is the variational distribution?

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

- Variational document distribution over topics  $\gamma_d$ 
  - ▶ 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

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

### Reminders

- Gamma function

$$\Gamma(n) = (n-1)! = \int_0^{\infty} x^{n-1} e^{-x} dx \quad (12)$$

- Digamma function

$$\psi(x) = \frac{d}{dx} \ln(\Gamma(x)) = \frac{\Gamma'(x)}{\Gamma(x)} \quad (13)$$

## Expectation 1

$$\mathbb{E}_q[\log p(\theta \mid \alpha)] = \mathbb{E}_q \left[ \log \left\{ \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \prod_i \theta_i^{\alpha_i - 1} \right\} \right] \quad (14)$$

(15)

## Expectation 1

$$\mathbb{E}_q[\log p(\theta | \alpha)] = \mathbb{E}_q \left[ \log \left\{ \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \prod_i \theta_i^{\alpha_i - 1} \right\} \right] \quad (14)$$

$$= \mathbb{E}_q \left[ \log \left\{ \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \right\} + \sum_i \log \theta_i^{\alpha_i - 1} \right] \quad (15)$$

Log of products becomes sum of logs.

## Expectation 1

$$\mathbb{E}_q[\log p(\theta | \alpha)] = \mathbb{E}_q \left[ \log \left\{ \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \prod_i \theta_i^{\alpha_i - 1} \right\} \right] \quad (14)$$

$$\begin{aligned} &= \mathbb{E}_q \left[ \log \left\{ \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \right\} + \sum_i \log \theta_i^{\alpha_i - 1} \right] \\ &= \log \Gamma(\sum_i \alpha_i) - \sum_i \log \Gamma(\alpha_i) + \mathbb{E}_q \left[ \sum_i (\alpha_i - 1) \log \theta_i \right] \end{aligned} \quad (15)$$

Log of exponent becomes product, expectation of constant is constant

## Expectation 1

$$\begin{aligned}\mathbb{E}_q[\log p(\theta | \alpha)] &= \mathbb{E}_q \left[ \log \left\{ \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \prod_i \theta_i^{\alpha_i - 1} \right\} \right] \\ &= \mathbb{E}_q \left[ \log \left\{ \frac{\Gamma(\sum_i \alpha_i)}{\prod_i \Gamma(\alpha_i)} \right\} + \sum_i \log \theta_i^{\alpha_i - 1} \right] \\ &= \log \Gamma(\sum_i \alpha_i) - \sum_i \log \Gamma(\alpha_i) + \mathbb{E}_q \left[ \sum_i (\alpha_i - 1) \log \theta_i \right] \\ &= \log \Gamma(\sum_i \alpha_i) - \sum_i \log \Gamma(\alpha_i) \\ &\quad + \sum_i (\alpha_i - 1) \left( \Psi(\gamma_i) - \Psi\left(\sum_j \gamma_j\right) \right)\end{aligned}\tag{14}$$

Expectation of log Dirichlet

## Reminder: Indicator Function

$$\mathbb{1}[x] \equiv \begin{cases} 1 & \text{if } x \\ 0, & \text{otherwise} \end{cases} \quad (15)$$

## Expectation 2

$$\mathbb{E}_q[\log p(z|\theta)] = \mathbb{E}_q\left[\log \prod_n \prod_i \theta_i^{\mathbb{1}_{[z_n=i]}}\right] \quad (16)$$

$$(17)$$

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$$(18)$$

Products to sums



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$$(19)$$

Linearity of expectation

## Expectation 2

$$\mathbb{E}_q[\log p(z|\theta)] = \mathbb{E}_q \left[ \log \prod_n \prod_i \theta_i^{\mathbb{1}[z_n=i]} \right] \quad (16)$$

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$$= \sum_n \sum_i \phi_{ni} \mathbb{E}_q [\log \theta_i] \quad (19)$$

$$(20)$$

Independence of variational distribution, exponents become products

## Expectation 2

$$\mathbb{E}_q[\log p(z|\theta)] = \mathbb{E}_q\left[\log \prod_n \prod_i \theta_i^{\mathbb{1}[z_n=i]}\right] \quad (16)$$

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$$= \sum_n \sum_i \phi_{ni} \left( \Psi(\gamma_i) - \Psi\left(\sum_j \gamma_j\right) \right) \quad (20)$$

Expectation of log Dirichlet

## Expectation 3

$$\mathbb{E}_q[\log p(w|z, \beta)] = \mathbb{E}_q[\log \beta_{z_{d,n}, w_{d,n}}] \quad (21)$$

$$(22)$$

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$$= \mathbb{E}_q \left[ \log \prod_v^V \prod_i^K \beta_{i,v}^{\mathbb{1}[v=w_{d,n}, z_{d,n}=i]} \right] \quad (22)$$

$$(23)$$

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$$= \sum_v^V \sum_i^K \mathbb{E}_q[\mathbb{1}[v=w_{d,n}, z_{d,n}=i]] \log \beta_{i,v} \quad (23)$$

$$(24)$$

## Expectation 3

$$\mathbb{E}_q[\log p(w|z, \beta)] = \mathbb{E}_q[\log \beta_{z_{d,n}, w_{d,n}}] \quad (21)$$

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$$= \sum_v^V \sum_i^K \mathbb{E}_q[\mathbb{1}[v=w_{d,n}, z_{d,n}=i]] \log \beta_{i,v} \quad (23)$$

$$= \sum_v^V \sum_i^K \phi_{n,i} w_{d,n}^v \log \beta_{i,v} \quad (24)$$

# Entropies

## Entropy of Dirichlet

$$\begin{aligned}\mathbb{H}_q[\gamma] = & -\log \Gamma\left(\sum_j \gamma_j\right) + \sum_i \log \Gamma(\gamma_i) \\ & - \sum_i (\gamma_i - 1) \left( \Psi(\gamma_i) - \Psi\left(\sum_{j=1}^k \gamma_j\right) \right)\end{aligned}$$



# Entropies

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## Entropy of Multinomial

$$\mathbb{H}_q[\phi_{d,n}] = - \sum_i \phi_{d,n,i} \log \phi_{d,n,i} \quad (25)$$

## Complete objective function

$$\begin{aligned} L(\gamma, \phi; \alpha, \beta) = & \log \Gamma(\sum_{j=1}^k \alpha_j) - \sum_{i=1}^k \log \Gamma(\alpha_i) + \sum_{i=1}^k (\alpha_i - 1) (\Psi(\gamma_i) - \Psi(\sum_{j=1}^k \gamma_j)) \\ & + \sum_{n=1}^N \sum_{i=1}^k \phi_{ni} (\Psi(\gamma_i) - \Psi(\sum_{j=1}^k \gamma_j)) \\ & + \sum_{n=1}^N \sum_{i=1}^k \sum_{j=1}^V \phi_{ni} w_n^j \log \beta_{ij} \\ & - \log \Gamma(\sum_{j=1}^k \gamma_j) + \sum_{i=1}^k \log \Gamma(\gamma_i) - \sum_{i=1}^k (\gamma_i - 1) (\Psi(\gamma_i) - \Psi(\sum_{j=1}^k \gamma_j)) \\ & - \sum_{n=1}^N \sum_{i=1}^k \phi_{ni} \log \phi_{ni}, \end{aligned}$$

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

## Update for $\phi$

Derivative of ELBO:

$$\frac{\partial \mathcal{L}}{\partial \phi_{ni}} = \Psi(\gamma_i) - \Psi\left(\sum_j \gamma_j\right) + \log \beta_{i,v} - \log \phi_{ni} - 1 + \lambda \quad (26)$$

Solution:

$$\phi_{ni} \propto \beta_{iv} \exp\left(\Psi(\gamma_i) - \Psi\left(\sum_j \gamma_j\right)\right) \quad (27)$$

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Remind you of Gibbs?

How much the topic likes word  $v$

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Remind you of Gibbs?

How much document  $d$  likes topic  $i$

## Update for $\gamma$

Derivative of ELBO:

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \gamma_i} &= \Psi'(\gamma_i)(\alpha_i + \phi_{n,i} - \gamma_i) \\ &\quad - \Psi'\left(\sum_j \gamma_j\right) \sum_j \left(\alpha_j + \sum_n \phi_{nj} - \gamma_j\right)\end{aligned}$$

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Derivative of ELBO:

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Solution:

$$\gamma_i = \alpha_i + \sum_n \phi_{ni} \tag{28}$$

## Update for $\beta$

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

$$\beta_{ij} \propto \sum_d \sum_n \phi_{dni} w_{dn}^j \quad (29)$$

# Overall Algorithm

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

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# Online Learning for Latent Dirichlet Allocation

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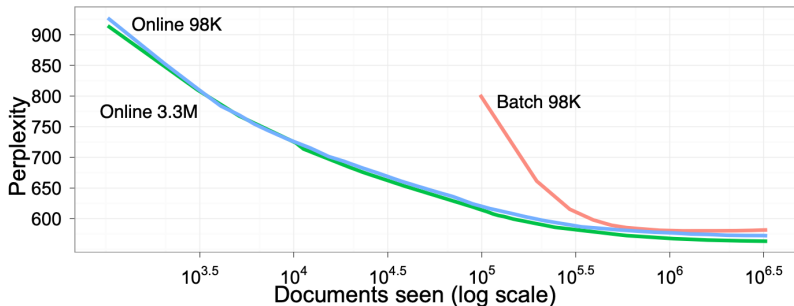
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## Implementation Tips

- Match derivation exactly at first
- Randomize initialization, but specify seed
- Use simple languages first

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- Write unit tests for each atomic update
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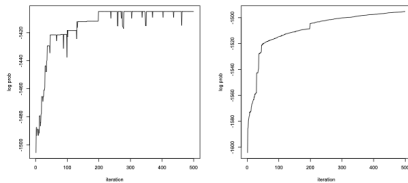
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- Visualize variational parameters



## Implementation Tips

- Match derivation exactly at first
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- Use simple languages first . . . then match implementation
- Check with synthetic data
- Try to match variables with paper
- Write unit tests for each atomic update
- Monitor variational bound (with asserts)
- Write the state (checkpointing and debugging)
- Visualize variational parameters
- Cache / memoize gamma / digamma functions

## Relationship with Gibbs Sampling



- Gibbs objective can jump around (left), variational always increases (right)
- Batch is sometimes a good fit for smaller datasets
- 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