PETUUM

Carnegie Mellon University
School of Computer Science

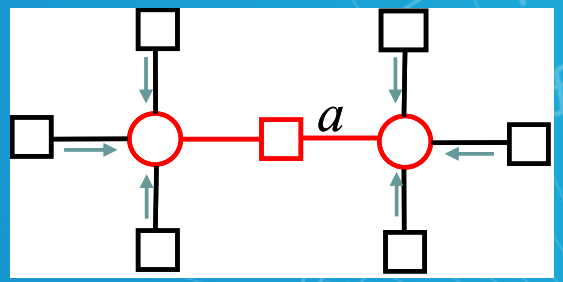
Probabilistic Graphical Models

Variational Inference: Loopy Belief Propagation

Eric Xing

Lecture 11a, February 20, 2019

Reading: see class homepage



Inference Problems

- Compute the likelihood of observed data $p(x_A)$
- Compute the marginal distribution $p(x_A|x_B)$ over a particular subset of nodes $A \subset V$
- Compute the conditional distribution $\hat{x} = \arg\max_{x \in \mathcal{X}^m} p(x)$ for disjoint subsets *A* and *B*
- Compute a mode of the density

- Methods we have

Brute force **Elimination**

Message Passing

(Forward-backward , Max-product /BP, Junction Tree)

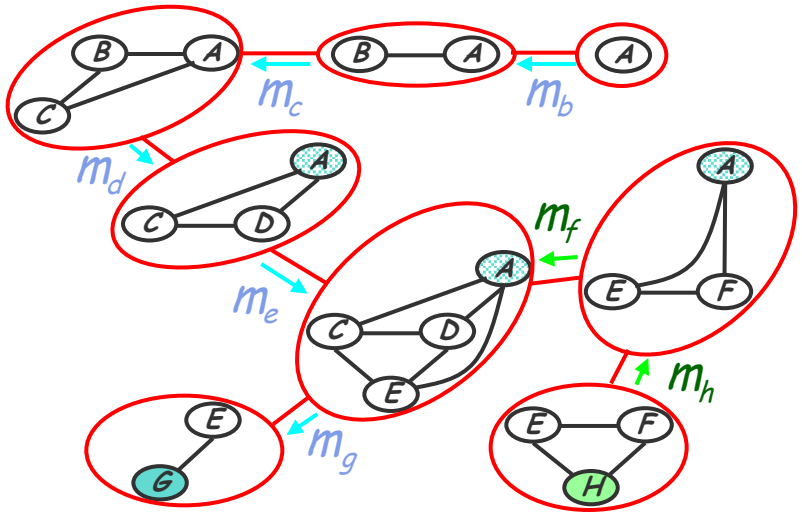
Individual computations independent

Sharing intermediate terms

From Elimination to Message Passing

- Recall that Induced dependency during marginalization is captured in elimination cliques
  - Summation <-> elimination
  - Intermediate term <-> elimination clique

$$
\begin{aligned}
& P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)P(h|e,f) \\
\Rightarrow\ & P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)P(g|e)\phi_h(e,f) \\
\Rightarrow\ & P(a)P(b)P(c|b)P(d|a)P(e|c,d)P(f|a)\phi_g(e)\phi_h(e,f) \\
\Rightarrow\ & P(a)P(b)P(c|b)P(d|a)P(e|c,d)\phi_f(a,e) \\
\Rightarrow\ & P(a)P(b)P(c|b)P(d|a)\phi_e(a,c,d) \\
\Rightarrow\ & P(a)P(b)P(c|b)\phi_d(a,c) \\
\Rightarrow\ & P(a)P(b)\phi_c(a,b) \\
\Rightarrow\ & P(a)\phi_b(a) \\
\Rightarrow\ & \phi(a)
\end{aligned}
$$



- Elimination ≡ message passing on a clique tree

Complexity

- The overall complexity is determined by the number of the largest elimination clique
  - What is the largest elimination clique? – a pure graph theoretic question
  - Tree-width *k*: one less than the smallest achievable value of the cardinality of the largest elimination clique, ranging over all possible elimination ordering
  - "good" elimination orderings lead to small cliques and hence reduce complexity (what will happen if we eliminate "e" first in the above graph?)
  - Find the best elimination ordering of a graph --- NP-hard

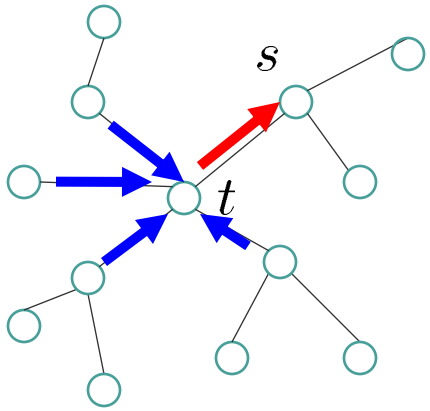
→ Inference is NP-hard

- But there often exist "obvious" optimal or near-opt elimination ordering

Sum-Product Algorithm

- Tree-structured GMs

$$p(x_1, \cdots, x_m) = \frac{1}{Z} \prod_{s \in V} \psi_s(x_s) \prod_{(s,t) \in E} \psi_{st}(x_s, x_t)$$



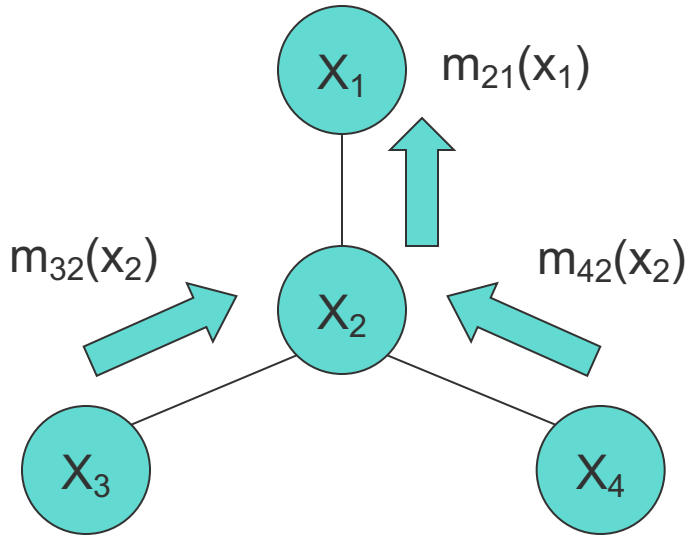
- Message Passing on Trees:

$$M_{t \to s}(x_s) \leftarrow \kappa \sum_{x'_t} \left\{ \psi_{st}(x_s, x'_t) \psi_t(x'_t) \prod_{u \in N(t) \setminus s} M_{u \to t}(x'_t) \right\}$$

  - On trees, converge to a unique fixed point after a finite number of iterations

The message passing protocol:

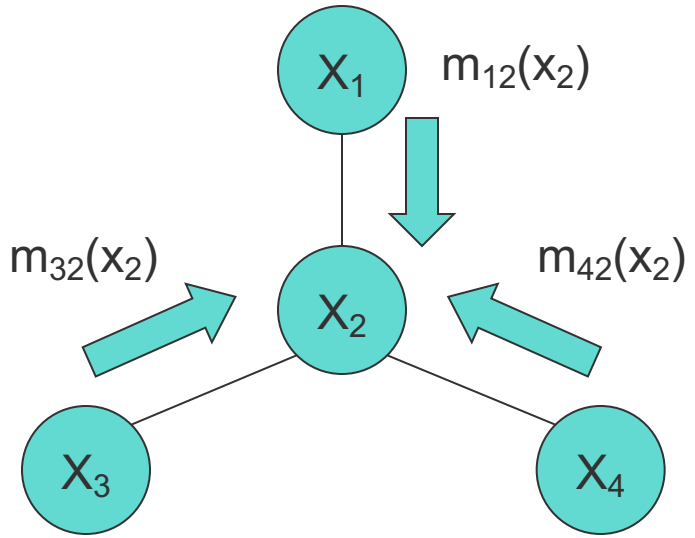
- A node can send a message to its neighbors when (and only when) it has received messages from all its *other* neighbors.
- Computing node marginals:
  - Naïve approach: consider each node as the root and execute the message passing algorithm



Computing $P(X_1)$

The message passing protocol:

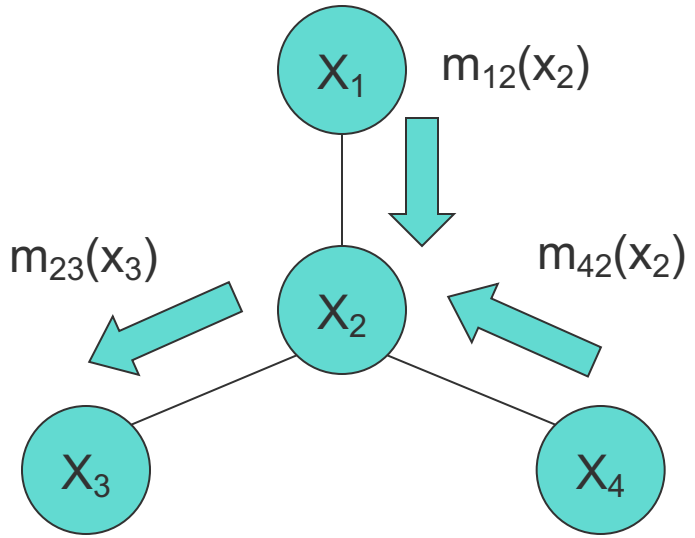
- A node can send a message to its neighbors when (and only when) it has received messages from all its *other* neighbors.
- Computing node marginals:
  - Naïve approach: consider each node as the root and execute the message passing algorithm



Computing $P(X_2)$

The message passing protocol:

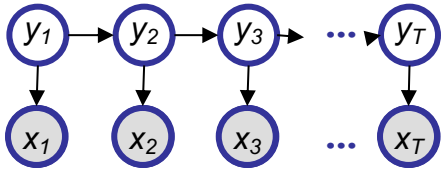
- A node can send a message to its neighbors when (and only when) it has received messages from all its *other* neighbors.
- Computing node marginals:
  - Naïve approach: consider each node as the root and execute the message passing algorithm

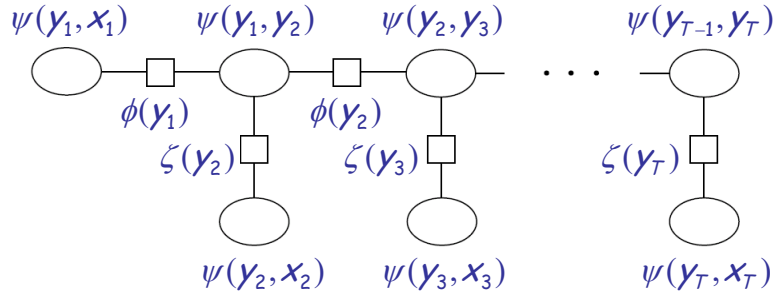


Computing $P(X_3)$

Message Passing for HMMs

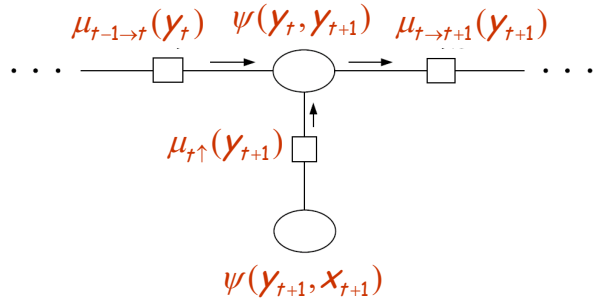
- A "click tree" for the HMM





- Rightward pass

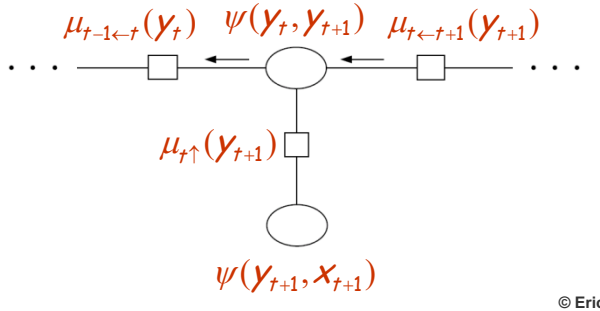
$$\mu_{t\to t+1}(y_{t+1}) = \sum_{y_t} \psi(y_t, y_{t+1}) \mu_{t-1\to t}(y_t) \mu_{t\uparrow}(y_{t+1})$$
$$= \sum_{y_t} p(y_{t+1} \mid y_t) \mu_{t-1\to t}(y_t) p(x_{t+1} \mid y_{t+1})$$
$$= p(x_{t+1} \mid y_{t+1}) \sum_{y_t} a_{y_t, y_{t+1}} \mu_{t-1\to t}(y_t)$$



  - This is exactly the *forward algorithm*!

- Leftward pass …

$$\mu_{t-1\leftarrow t}(y_t) = \sum_{y_{t+1}} \psi(y_t, y_{t+1}) \mu_{t\leftarrow t+1}(y_{t+1}) \mu_{t\uparrow}(y_{t+1})$$
$$= \sum_{y_{t+1}} p(y_{t+1} \mid y_t) \mu_{t\leftarrow t+1}(y_{t+1}) p(x_{t+1} \mid y_{t+1})$$



  - This is exactly the *backward algorithm*!

Correctness of BP on tree

- Collollary: the synchronous implementation is "non-blocking"
- Thm: The Message Passage Guarantees obtaining all marginals in the tree

$$m_{ji}(x_i) \quad = \quad \sum_{x_j} \left(\psi(x_j)\psi(x_i,x_j) \prod_{k \in N(j)\setminus i} m_{kj}(x_j) \right)$$

Local Consistency → Global Consistency

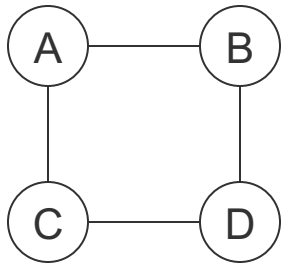
- Given a set of functions $\{\tau_C,\ C \in \mathcal{C}\}$ and $\{\tau_S,\ S \in \mathcal{S}\}$ associated with the cliques and separator sets
- They are locally consistent if:

$$\sum_{x'_S} \tau_S(x'_S) = 1,\ \forall S \in \mathcal{S}$$

$$\sum_{x'_C | x'_S = x_S} \tau_C(x'_C) = \tau_S(x_S),\ \forall C \in \mathcal{C},\ S \subset C$$

- For junction trees, local consistency is equivalent to global consistency!
- What about non-tree?

A problem



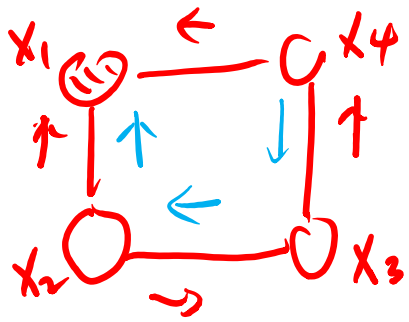
$p(x_1) \propto \phi_1 m_{41} m_{21}$

$= \phi_1$

$p(x_1 \dots x_4)$

$= \frac{1}{Z} \phi(x_1) \phi(x_2) \phi(x_3) \phi(x_4)$

$\phi(x_1, x_4)\ \phi_{14}\ \phi_{43}\ \phi_{23}$



$p(x_1) \propto \phi_1 m_{41} m_{21}$

$= \phi_1 \left(\sum_4 \phi_4 \phi_{41} m_{34}\right) \sum_2 \phi_2 \phi_{21}$

$= \phi_1 \sum_4 \phi_4 \phi_{41} \left(\sum_3 \phi_3 \phi_{34} m_{23}\right)$

$\sum_2 \phi_2 \phi_{21}$

$=$

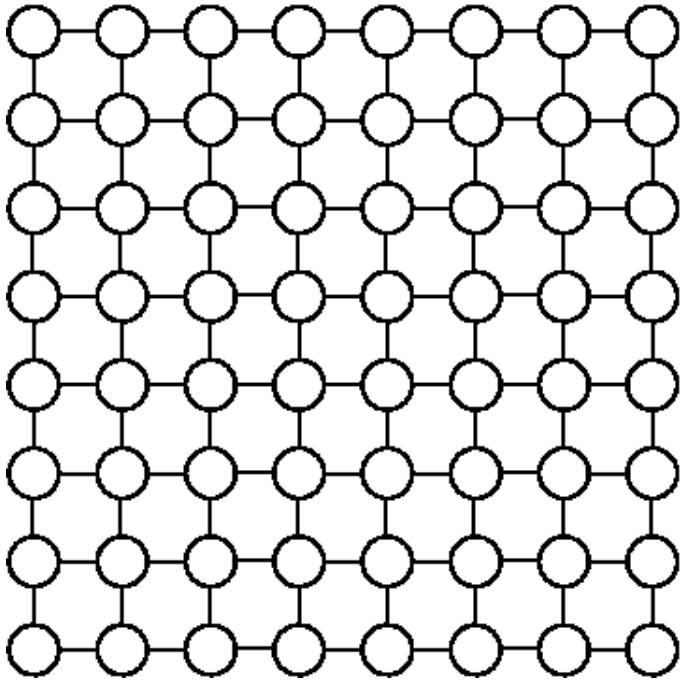
A problem

- Consider the following graph and a corresponding clique tree

  - Note that C appears in two non-neighboring cliques
- *Question*: with the previous message passage, can we ensure that the probability associated with C in these two (non-neighboring) cliques consistent?
- Answer: No. It is not true that in general local consistency implies global consistency
- What else do we need to get such a guarantee?

Why Approximate Inference?

- Why can't we just run "clique tree" on this graph?



$$p(X) = \frac{1}{Z}\exp\left\{\sum_{i<j}\theta_{ij}X_iX_j + \sum_i \theta_{i0}X_i\right\}$$

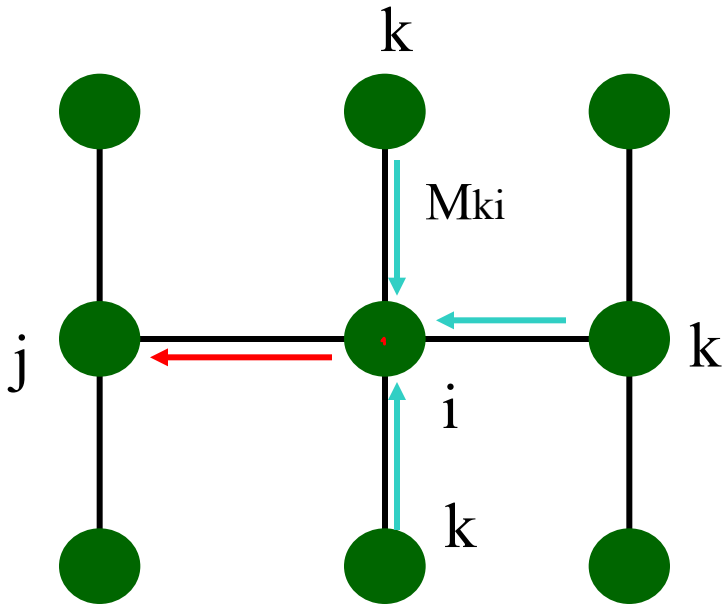
- If NxN grid, tree width at least N
- N can be a huge number(~1000s of pixels)
  - If N~O(1000), we have a clique with 2^{100} entries

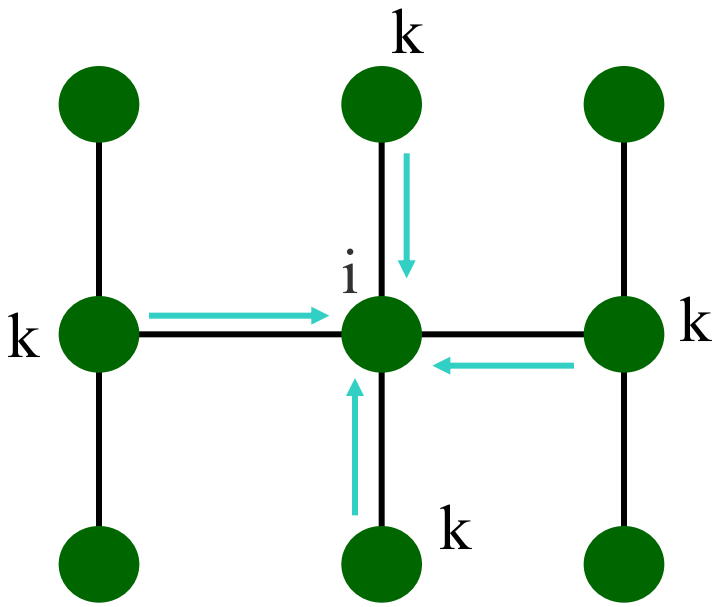
Approaches to inference

- Exact inference algorithms
  - The elimination algorithm
  - Message-passing algorithm (sum-product, belief propagation)
  - The junction tree algorithms

- Approximate inference techniques
  - Variational algorithms
    - Loopy belief propagation
    - Mean field approximation
  - Stochastic simulation / sampling methods
  - Markov chain Monte Carlo methods

Recap: Belief Propagation





- BP Message-update Rules

$$M_{i\to j}(x_j) \propto \sum_{x_i} \psi_{ij}(x_i, x_j)\psi_i(x_i)\prod_k M_{k\to i}(x_i)$$

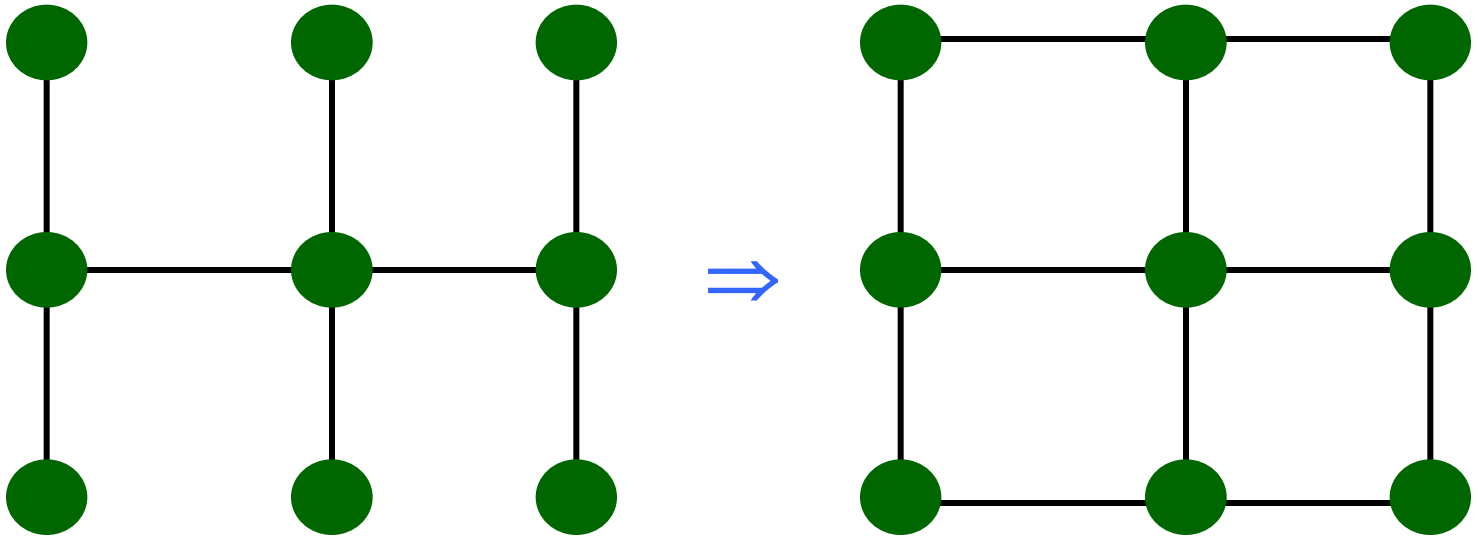
Compatibilities (interactions)

external evidence

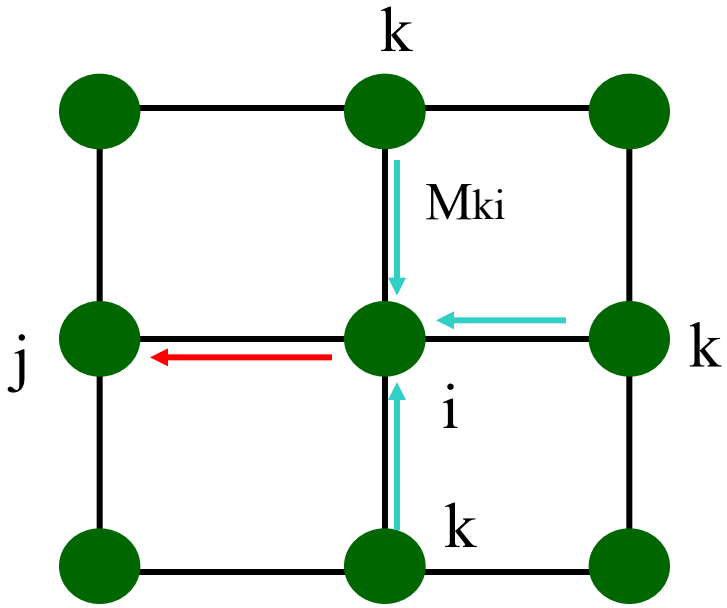
$$b_i(x_i) \propto \psi_i(x_i)\prod_k M_k(x_k)$$

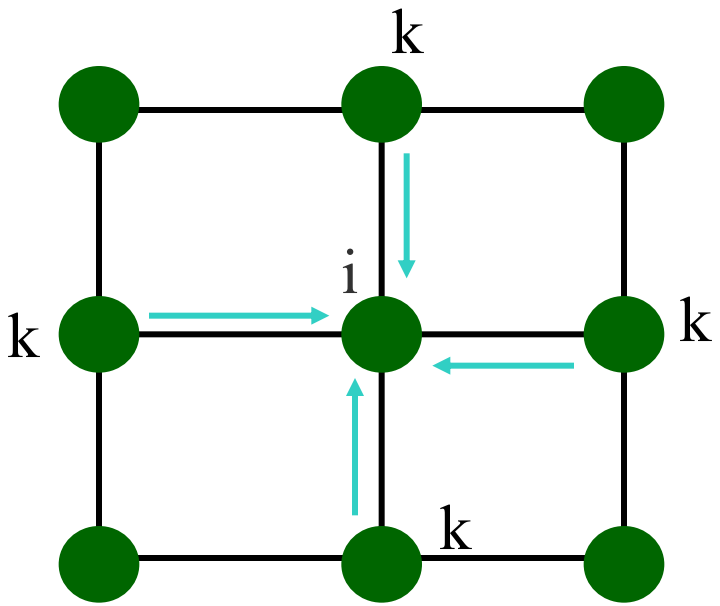
- BP on trees always converges to exact marginals (cf. Junction tree algorithm)

What if the graph is loopy?



Belief Propagation on loopy graphs





- BP Message-update Rules

$$M_{i\to j}(x_j) \propto \sum_{x_i} \psi_{ij}(x_i, x_j)\psi_i(x_i)\prod_k M_{k\to i}(x_i)$$

Compatibilities (interactions)

external evidence

$$b_i(x_i) \propto \psi_i(x_i)\prod_k M_k(x_k)$$

- May not converge or converge to a wrong solution

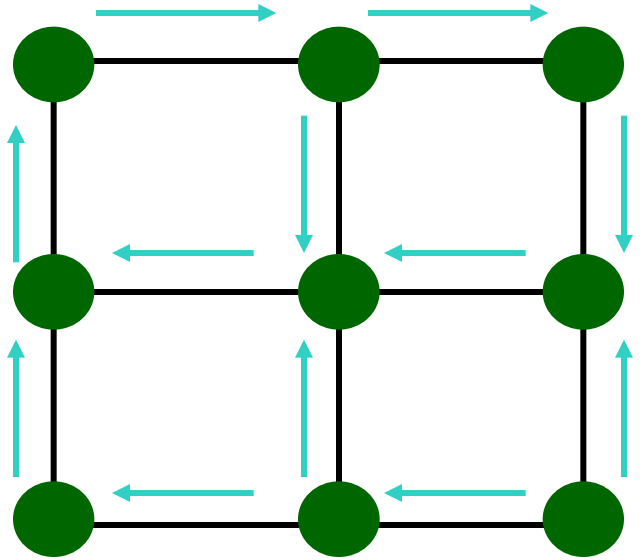
Loopy Belief Propagation

- If BP is used on graphs with loops, messages may circulate indefinitely
- But let's run it anyway and hope for the best … ☺
- Empirically, a good approximation is still achievable
  - Stop after fixed # of iterations
  - Stop when no significant change in beliefs
  - If solution is not oscillatory but converges, it usually is a good approximation

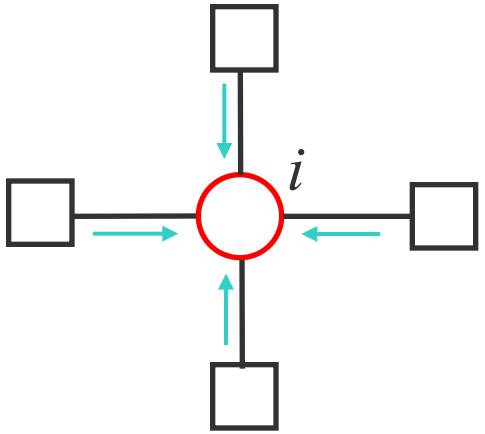
Loopy-belief Propagation for Approximate Inference: An Empirical Study
Kevin Murphy, Yair Weiss, and Michael Jordan.
UAI '99 (Uncertainty in AI). **]**

So what is going on?

- Is it a dirty hack that you bet your luck?

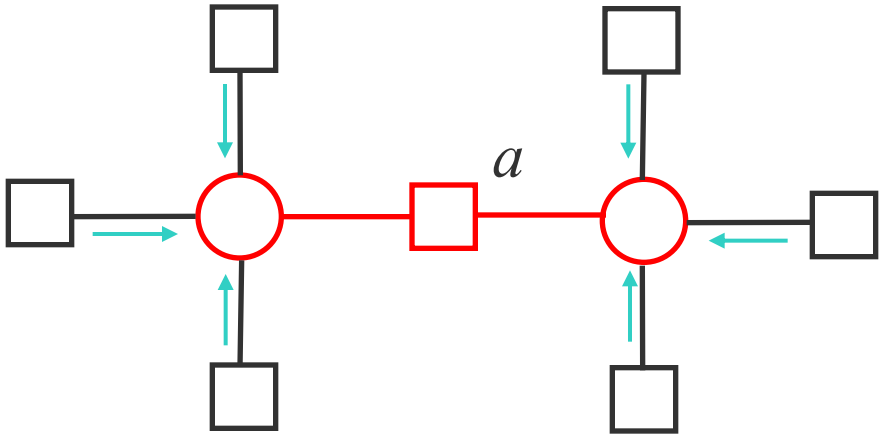


Beliefs and messages in "Factored Graphs"



$$b_i(x_i) \propto f_i(x_i) \prod_{a \in N(i)} m_{a \to i}(x_i)$$

"beliefs" "messages"



$$m_{i \to a}(x_i) = \prod_{c \in N(i) \setminus a} m_{c \to i}(x_i)$$

$$b_a(X_a) \propto f_a(X_a) \prod_{i \in N(a)} m_{i \to a}(x_i)$$

$$m_{a \to i}(x_i) = \sum_{X_a \setminus x_i} f_a(X_a) \prod_{j \in N(a) \setminus i} m_{j \to a}(x_j)$$

Approximate Inference

- For the actual distribution P: $P(X) = 1/Z \prod_{f_a \in F} f_a(X_a)$
- We wish to find a distribution Q such that Q is a "good" approximation to P
- The quality of the approximation can be measured by:

$$KL(Q \| P) = \sum_X Q(X) \log(\frac{Q(X)}{P(X)})$$

$$= \sum_X Q(X) \log Q(X) - \sum_X Q(X) \log P(X)$$

$$= -H_Q(X) - E_Q \log P(X)$$

$$= -H_Q(X) - \log 1/Z - \sum_{f_a \in F} E_Q \log f_a(X_a) = -\underbrace{H_Q(X) - \sum_{f_a \in F} E_Q \log f_a(X_a)}_{F(P,Q)} + \log Z$$

- $F(P,Q)$ is called the "Free energy" *

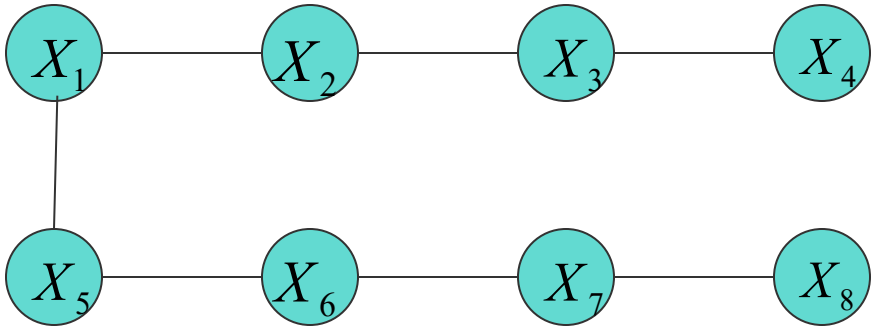
Mean Field: we have seen it last lecture

Maximize the variational lower bound:

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) = \mathbb{E}_{q_\phi(\boldsymbol{x}|\boldsymbol{e})}[\log p_\theta(e|x)] + KL\left(q_\phi(x|e)||p(x)\right)$$
$$= \log p(\boldsymbol{e}) - KL(q_\phi(\boldsymbol{x}|\boldsymbol{e}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{e}))$$

Tree Energy Functionals

- Consider a tree-structured distribution



- The probability can be written as: $b(\mathbf{x}) = \prod_a b_a(\mathbf{x}_a) \prod_i b_i(x_i)^{1-d_i}$

$$H_{tree} = -\sum_a \sum_{\mathbf{x}_a} b_a(\mathbf{x}_a) \ln b_a(\mathbf{x}_a) + \sum_i (d_i - 1) \sum_{\mathbf{x}_i} b_i(\mathbf{x}_i) \ln b_i(\mathbf{x}_i)$$

$$F_{Tree} = \sum_a \sum_{\mathbf{x}_a} b_a(\mathbf{x}_a) \ln \frac{b_a(\mathbf{x}_a)}{f_a(\mathbf{x}_a)} + \sum_i (1 - d_i) \sum_{\mathbf{x}_i} b_i(\mathbf{x}_i) \ln b_i(\mathbf{x}_i)$$

$$= F_{12} + F_{23} + .. + F_{67} + F_{78} - F_1 - F_5 - F_2 - F_6 - F_3 - F_7$$

  - involves summation over edges and vertices and is therefore easy to compute

Bethe Approximation to Gibbs Free Energy

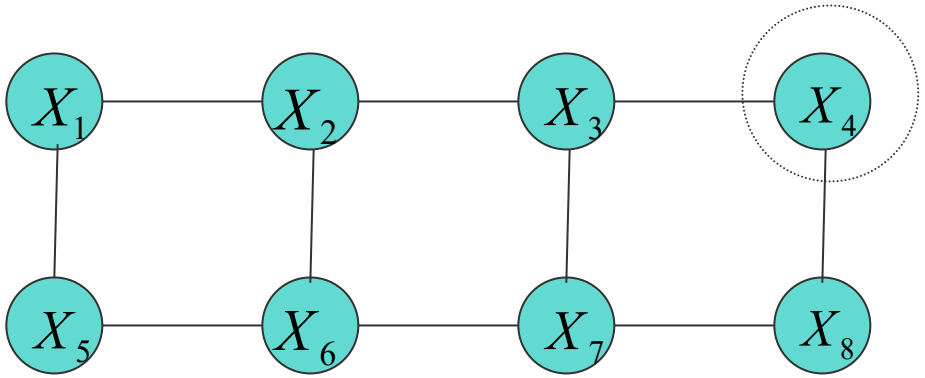
- For a general graph, choose $\hat{F}(P,Q) = F_{Betha}$

$$H_{Bethe} = -\sum_a \sum_{\mathbf{x}_a} b_a(\mathbf{x}_a)\ln b_a(\mathbf{x}_a) + \sum_i (d_i - 1)\sum_{\mathbf{x}_i} b_i(\mathbf{x}_i)\ln b_i(\mathbf{x}_i)$$

$$F_{Bethe} = \sum_a \sum_{\mathbf{x}_a} b_a(\mathbf{x}_a)\ln \frac{b_a(\mathbf{x}_a)}{f_a(\mathbf{x}_a)} + \sum_i (1 - d_i)\sum_{\mathbf{x}_i} b_i(\mathbf{x}_i)\ln b_i(\mathbf{x}_i) = -\langle f_a(\mathbf{x}_a)\rangle - H_{betha}$$

  - Called the "Bethe approximation" after the physicist Hans Bethe
  - Equal to the exact Gibbs free energy when the factor graph is a tree
  - In general, H_{Bethe} is **not** the same as the H of a tree

- For a "loopy graph like this:



$$F_{bethe} = F_{12} + F_{23} + .. + F_{67} + F_{78} - F_1 - F_5 - 2F_2 - 2F_6 .. - F_8$$

Constrained Minimization of the Bethe Free Energy

$$L = F_{Bethe} + \sum_i \gamma_i \{ \sum_{x_i} b_i(x_i) - 1 \}$$

$$+ \sum_a \sum_{i \in N(a)} \sum_{x_i} \lambda_{ai}(x_i) \left\{ \sum_{X_a \setminus x_i} b_a(X_a) - b_i(x_i) \right\}$$

$$\frac{\partial L}{\partial b_i(x_i)} = 0 \quad \Longrightarrow \quad b_i(x_i) \propto \exp\left(\frac{1}{d_i - 1} \sum_{a \in N(i)} \lambda_{ai}(x_i) \right)$$

$$\frac{\partial L}{\partial b_a(X_a)} = 0 \quad \Longrightarrow \quad b_a(X_a) \propto \exp\left(-E_a(X_a) + \sum_{i \in N(a)} \lambda_{ai}(x_i) \right)$$

Bethe = BP on FG

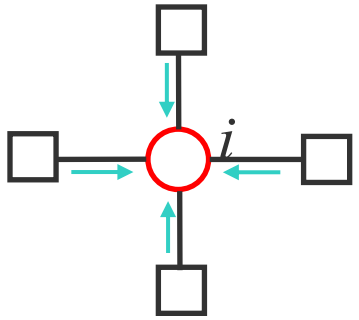
- We had:

$$b_i(x_i) \propto \exp\left(\frac{1}{d_i - 1}\sum_{a\in N(i)}\lambda_{ai}(x_i)\right) \qquad b_a(X_a) \propto \exp\left(-\log f_a(X_a) + \sum_{i\in N(a)}\lambda_{ai}(x_i)\right)$$

- Identify

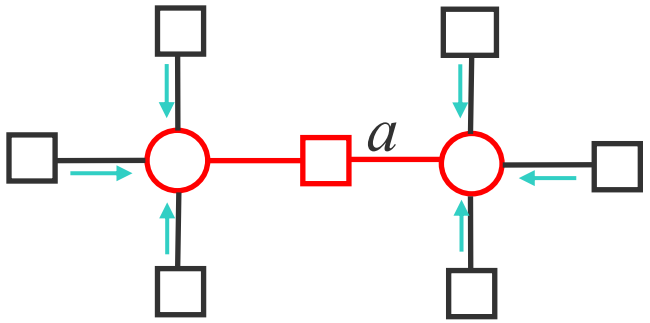
$$\lambda_{ai}(x_i) = \log(m_{i\to a}(x_i)) = \log \prod_{b\in N(i)\neq a} m_{b\to i}(x_i)$$

- to obtain BP equations:



$$b_i(x_i) \propto f_i(x_i)\prod_{a\in N(i)} m_{a\to i}(x_i)$$

"beliefs" "messages"



$$b_a(X_a) \propto f_a(X_a)\prod_{i\in N(a)}\prod_{c\in N(i)\setminus a} m_{c\to i}(x_i)$$

The "belief" is the BP approximation of the marginal probability.

Summary

- We defined an objective function (F) for approximate inference
- However, we found that optimizing this function was hard
- We first approximated objective function F to simpler F_{bethe}
  - Minima of F_{bethe} turned out to be fixed points of BP
- Then we extended this to more complicated approximations
  - The resulting algorithms come under a family called Generalized Belief Propagation
- Next class, we will cover other methods of approximations

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School of Computer Science

Probabilistic Graphical Models

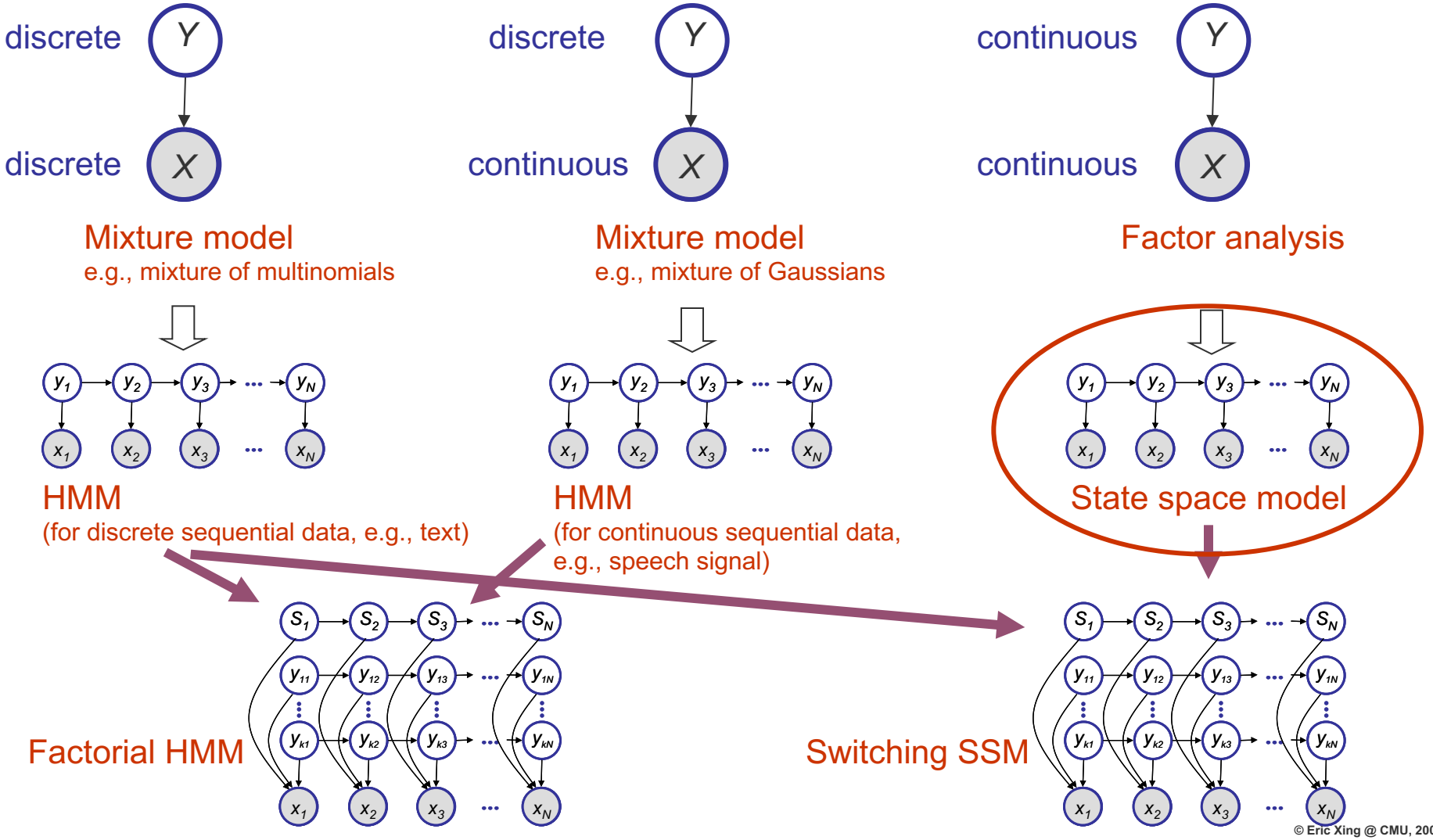
Approximate Inference and Topic Models: Mean Field and Loopy Belief Prop

Eric Xing

Lecture 11b, February 20, 2019

Reading: see class homepage

A road map to more complex dynamic models



Probabilistic Topic Models

- Humans cannot afford to deal with (e.g., search, browse, or measure similarity) a huge number of text documents
- We need computers to help out …

How to get started for a new modeling task?

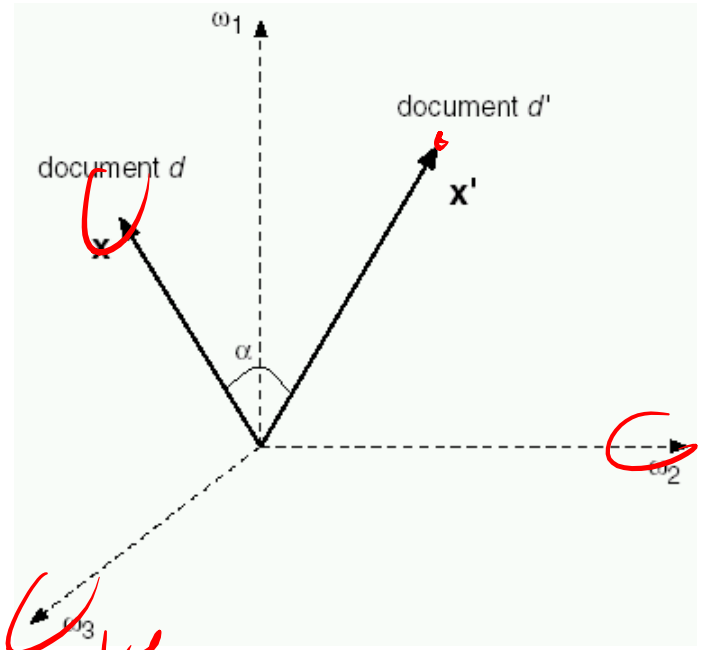
Here are some important elements to consider before you start:

- Task:
  - Embedding? Classification? Clustering? Topic extraction? …
- Data representation:
  - Input and output (e.g., continuous, binary, counts, …)
- Model:
  - BN? MRF? Regression? SVM?
- Inference:
  - Exact inference? MCMC? Variational?
- Learning:
  - MLE? MCLE? Max margin?
- Evaluation:
  - Visualization? Human interpretability? Perperlexity? Predictive accuracy?

It is better to consider one element at a time!

Tasks: document embedding

- Say, we want to have a mapping …, so that

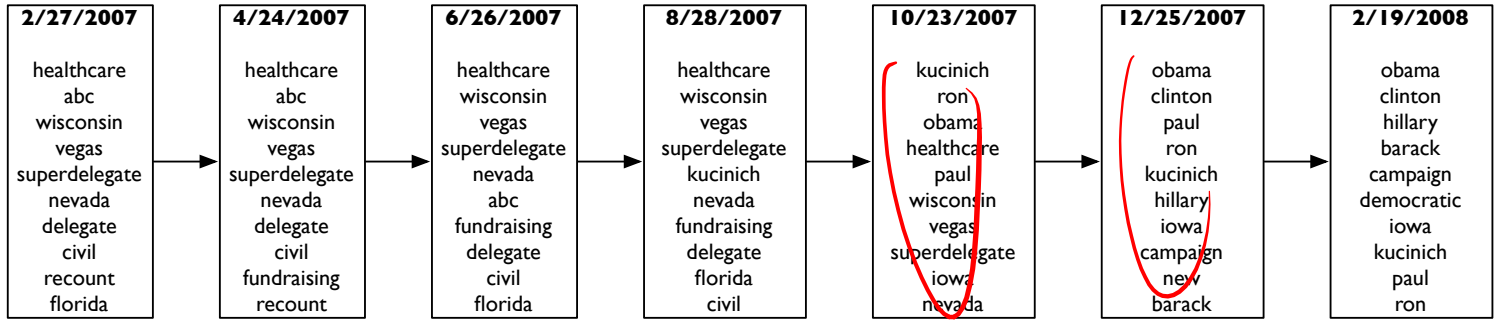


- Compare simil
- Classify conten
- Cluster/group/categorizing
- Distill semantics and perspectives
- ..

Summarizing the data using topics

Bayesian modeling	Visual cortex	Education	Market
Bayesian	cortex	students	market
model	cortical	education	economic
inference	areas	learning	financial
models	visual	educational	economics
probability	area	teaching	markets
probabilistic	primary	school	returns
Markov	connections	student	price
prior	ventral	skills	stock
hidden	cerebral	teacher	value
approach	sensory	academic	investment

See how data changes over time



User interest modeling using topics

User interest profile (adjustable with sliders---Changing these changes recommendations.)

Weight	User preferred topics
	1: learning machine training vector learn machines kernel learned classifiers classifier
	2: online classification digital library libraries browsing classify classifying labels catalog
	3: two differences active hypothesis arise difference evolved morphological modify morphology
	4: experiments ability demonstrated produced contexts situations instances fail recognize string
	5: features class classes subset java characteristic earlier represented defines separate
	6: process making presents objective steps reports distinguish exploit maintaining select
	7: algorithm signal input signals output exact performs music sound iterative
	8: database databases contains version list comprehensive release stored update curated
	9: applications application provide built numerous proven providing discusses tremendous presents
	10: text literature discovery mining biomedical full extract discovering texts themes

http://cogito-demos.ml.cmu.edu/cgi-bin/recommendation.cgi

Representation: Bag of Words Representation

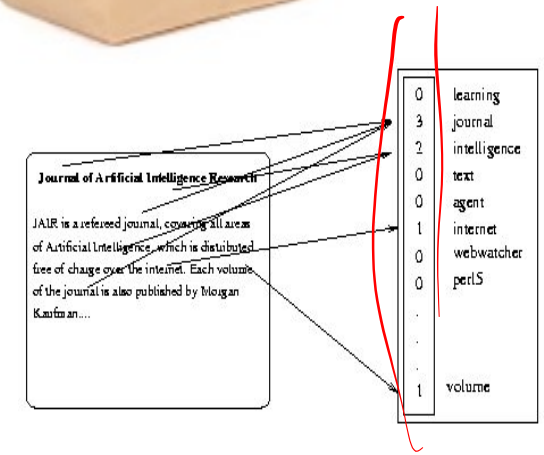
- Data:

> As for the Arabian and Palestinean voices that are against the current negotiations and the so-called peace process, they are not against peace per se, but rather for their well-founded predictions that Israel would NOT give an inch of the West bank (and most probably the same for Golan Heights) back to the Arabs. An 18 months of "negotiations" in Madrid, and Washington proved these predictions. Now many will jump on me saying why are you blaming israelis for no-result negotiations. I would say why would the Arabs stall the negotiations, what do they have to loose ?

- Each document is a vector in the word space
- Ignore the order of words in a document. Only count matters!

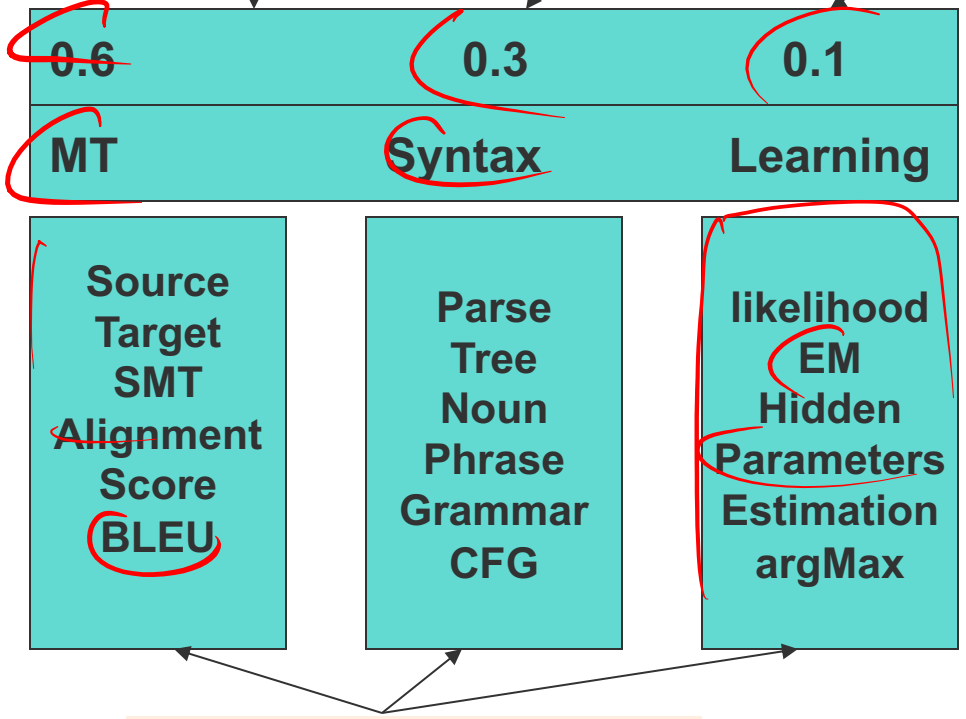
- A high-dimensional and sparse representation
  - Not efficient text processing tasks, e.g., search, document classification, or similarity measure
  - Not effective for browsing

$(|V| \gg D)$



How to Model Semantic?

- Q: What is it about?
- A: Mainly MT, with syntax, some learning

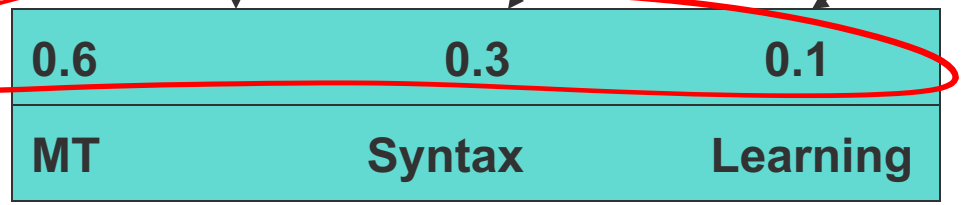


A Hierarchical Phrase-Based Model for Statistical Machine Translation

We present a statistical phrase-based Translation model that uses *hierarchical phrases*—phrases that contain sub-phrases. The model is formally a synchronous context-free grammar but is learned from a bitext without any syntactic information. Thus it can be seen as a shift to the *formal* machinery of syntax based translation systems without any *linguistic* commitment. In our experiments using BLEU as a metric, the hierarchical Phrase based model achieves a relative Improvement of 7.5% over Pharaoh, a state-of-the-art phrase-based system.

Why this is Useful?

- Q: What is it about?
- A: Mainly MT, with syntax, some learning



Mixing Proportion

A Hierarchical Phrase-Based Model for Statistical Machine Translation

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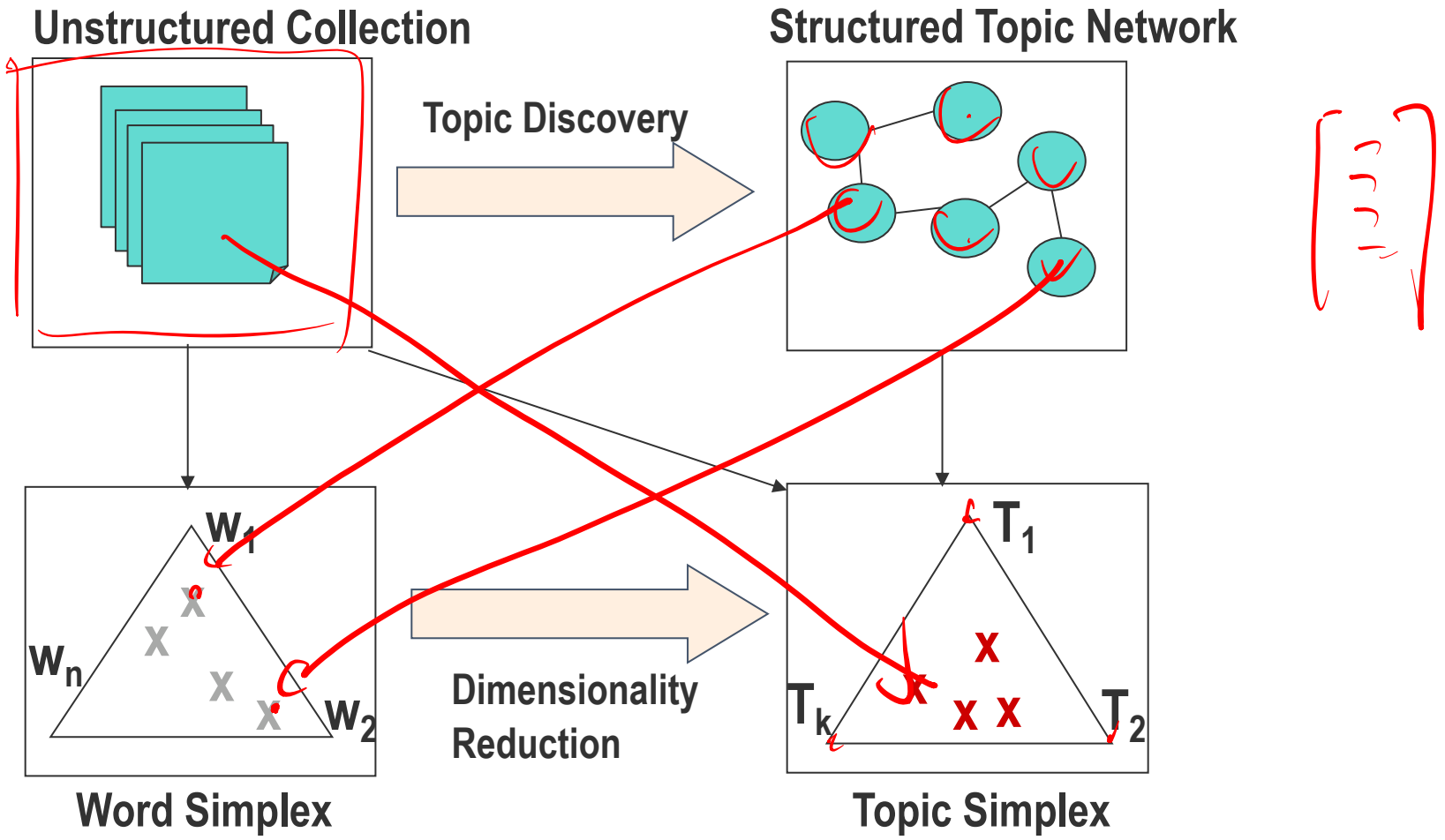
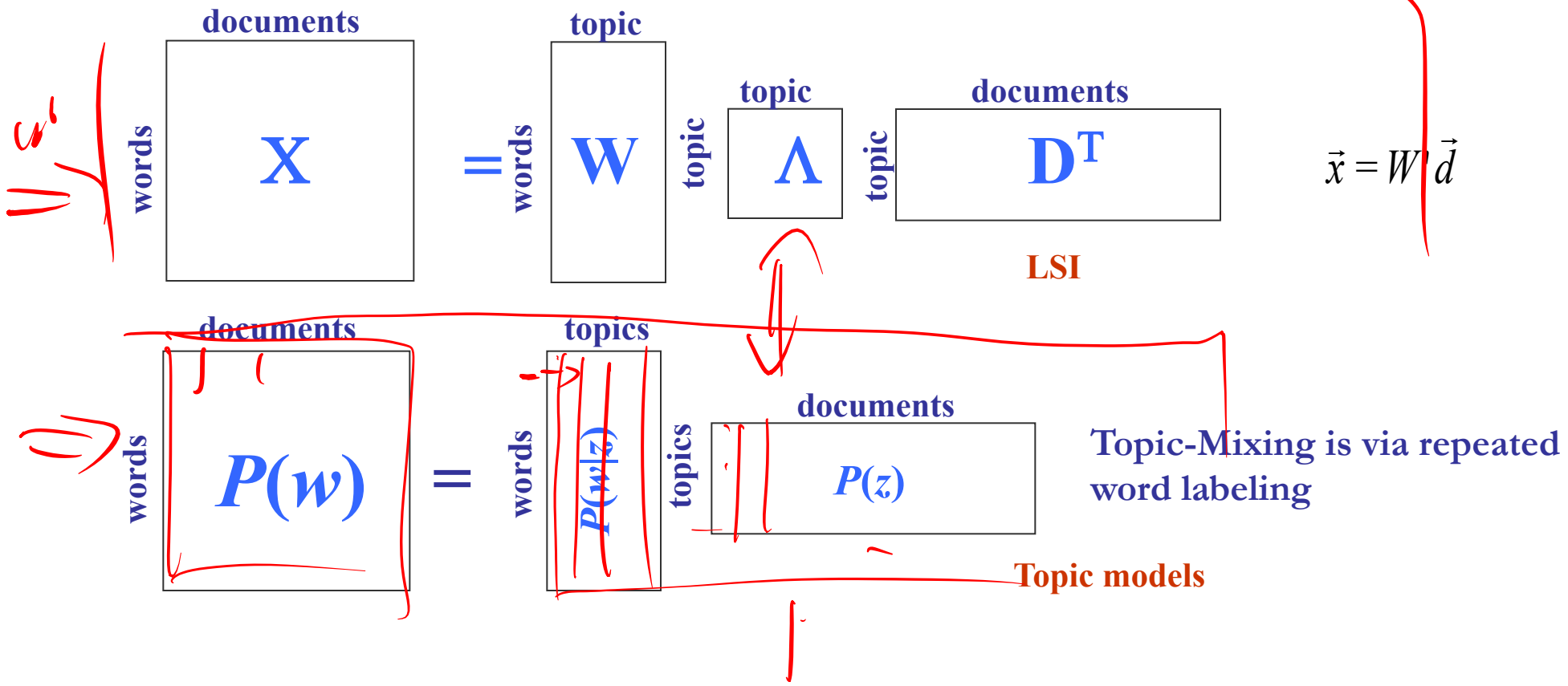
- **Q: give me similar document?**
  - Structured way of browsing the collection
- **Other tasks**
  - Dimensionality reduction
    - TF-IDF vs. topic mixing proportion
    - Classification, clustering, and more …

Topic Models: The Big Picture



LSI versus Topic Model (probabilistic LSI)

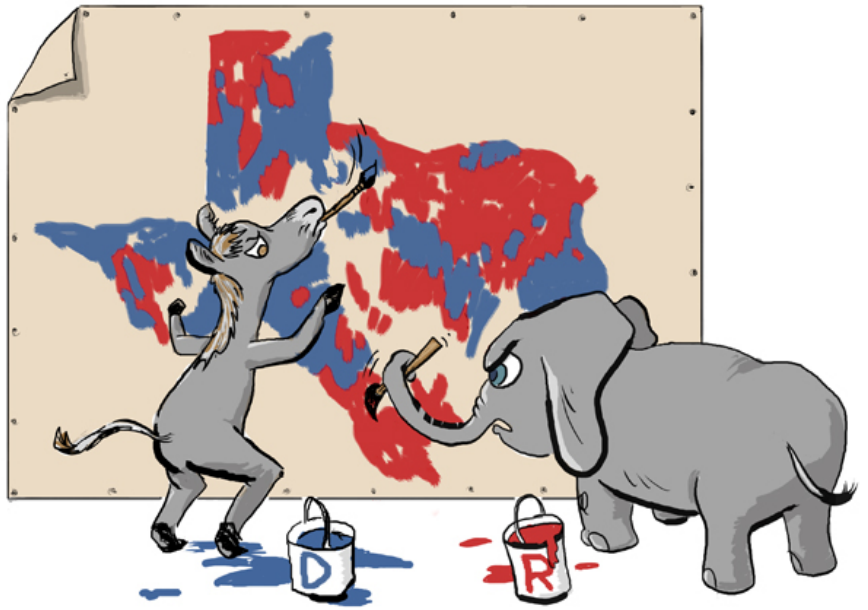


Words in Contexts

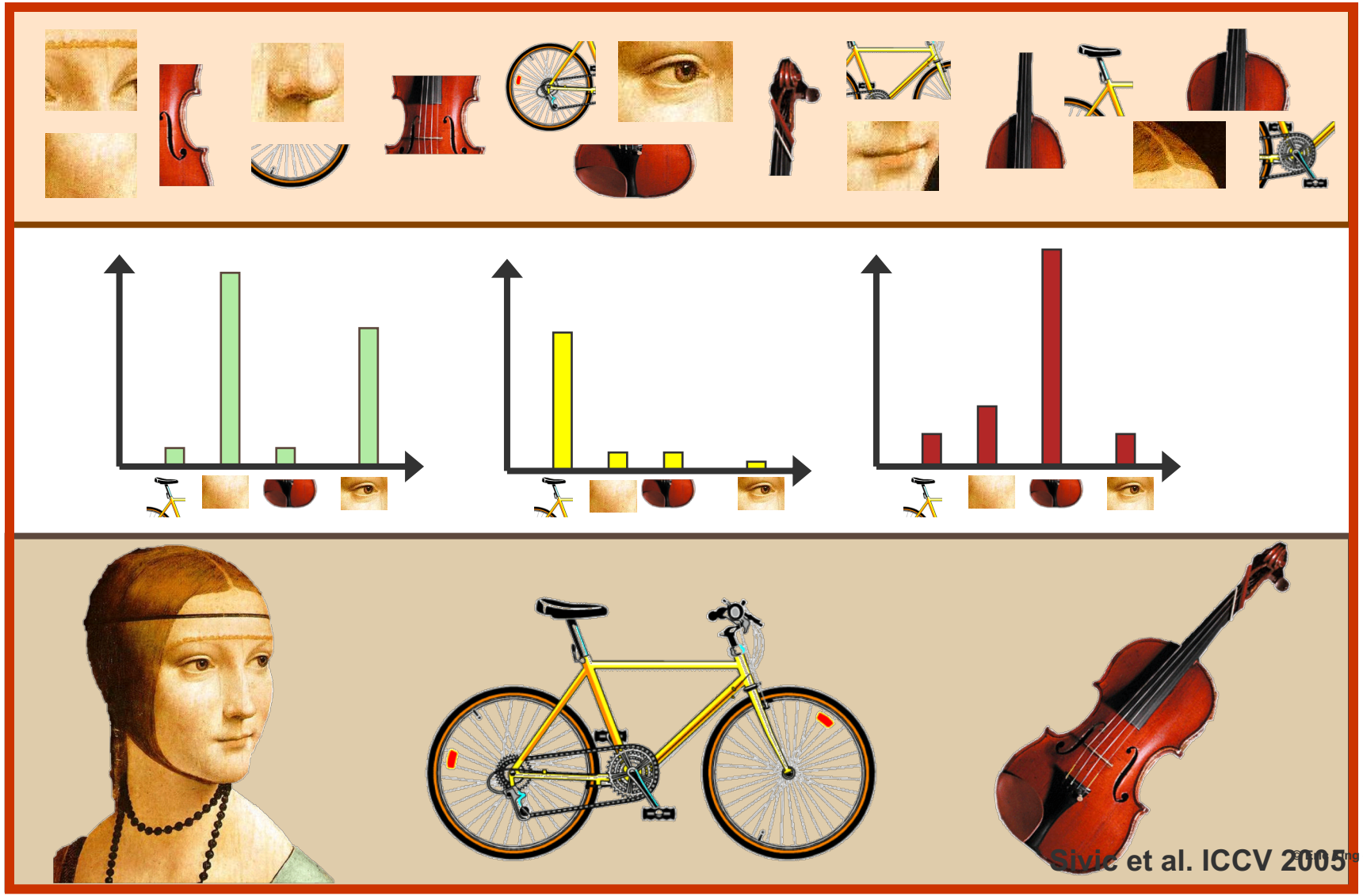
- “It was a nice shot.”

Words in Contexts (con'd)

- The opposition Labor **Party** fared even worse, with a predicted 35 seats, seven less than last **election**.



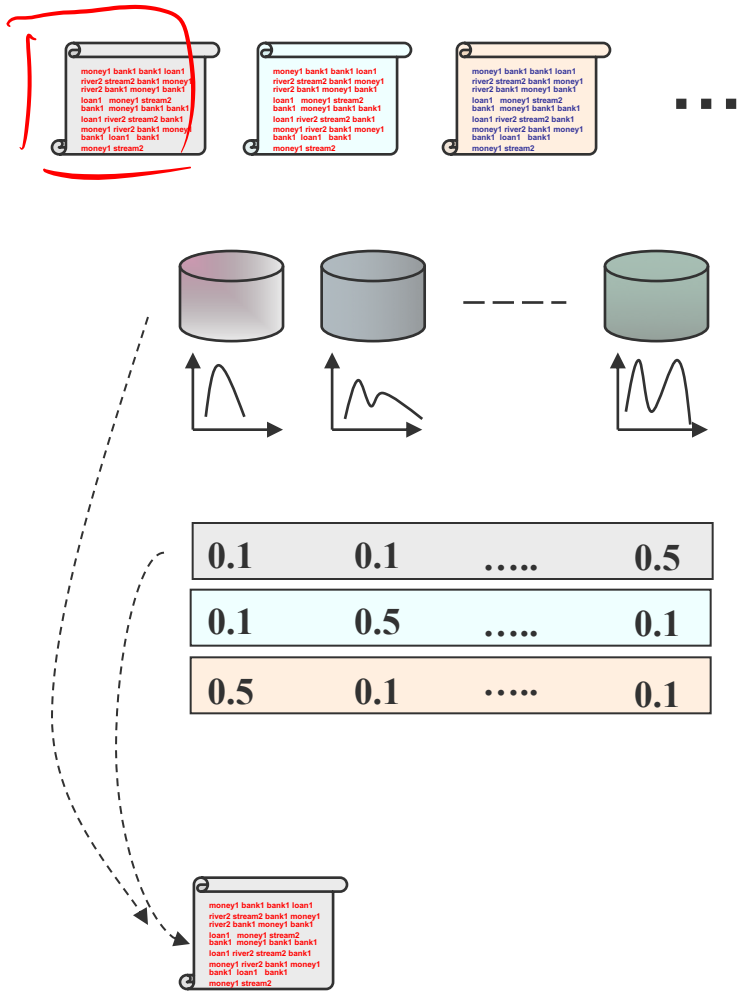
"Words" in Contexts (con'd)



Sivic et al. ICCV 2005

Admixture Models

- Objects are bags of elements
- Mixtures are distributions over elements
- Objects have mixing vector θ
  - Represents each mixtures' contributions
- Object is generated as follows:
  - Pick a mixture component from θ
  - Pick an element from that component



Topic Models

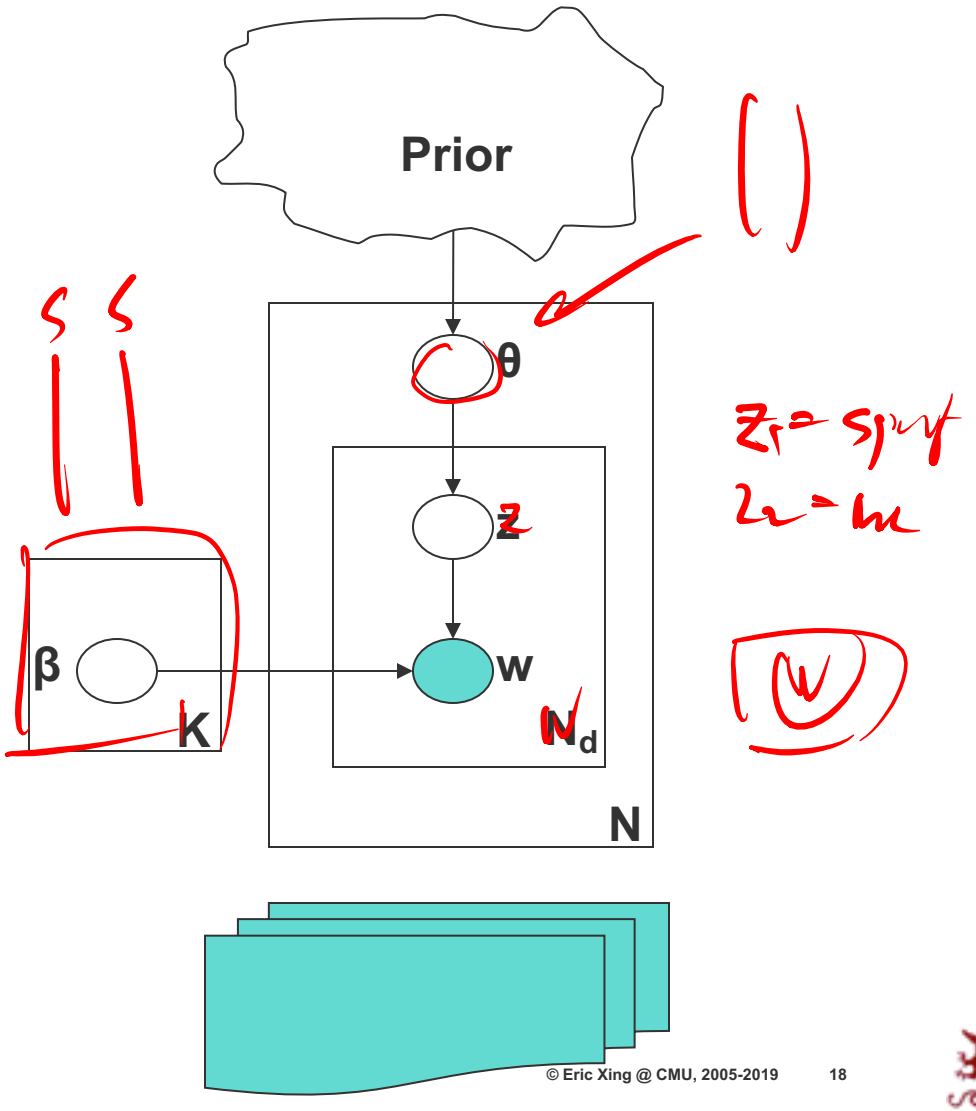
Generating a document

– *Draw* θ from the prior

For each word n

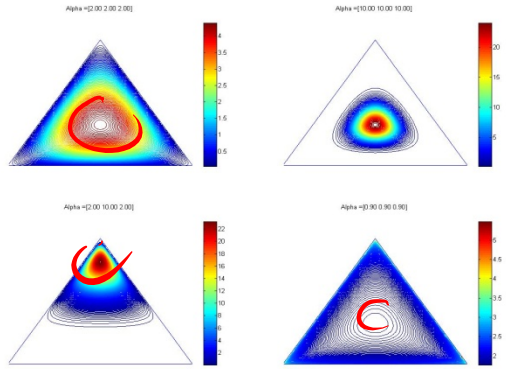
- Draw z_n from $multinomial(\theta)$
- Draw $w_n \mid z_n, \{\beta_{1:k}\}$ from $multinomial(\beta_{z_n})$

Which prior to use?

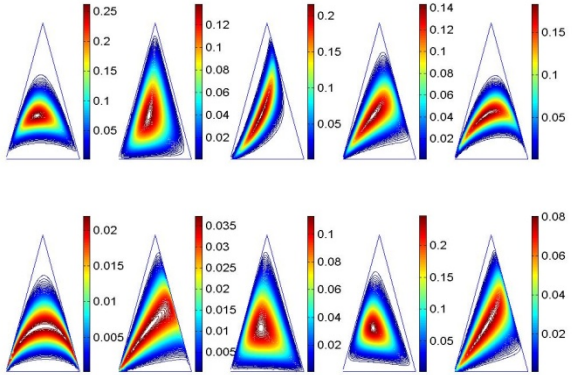


Choices of Priors

- Dirichlet (LDA) (Blei et al. 2003)
  - Conjugate prior means efficient inference
  - Can only capture variations in each topic's intensity independently



- Logistic Normal (CTM=LoNTAM) (Blei & Lafferty 2005, Ahmed & Xing 2006)
  - Capture the intuition that some topics are highly correlated and can rise up in intensity together
  - Not a conjugate prior implies hard inference



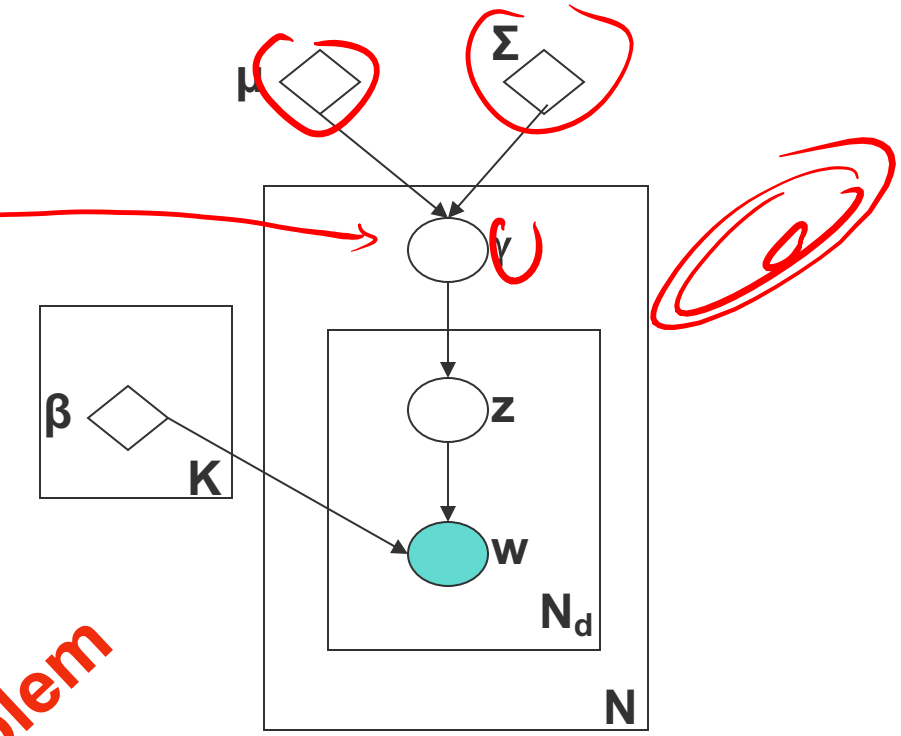
Generative Semantic of LoNTAM

Generating a document

– *Draw* θ from the prior

For each word n

- Draw z_n from $multinomial(\theta)$
- Draw $w_n \mid z_n, \{\beta_{1:k}\}$ from $multinomial(\beta_{z_n})$



$$\theta \sim LN_K(\mu, \Sigma)$$

$$\gamma \sim N_{K-1}(\mu, \Sigma) \qquad \gamma_K = 0$$

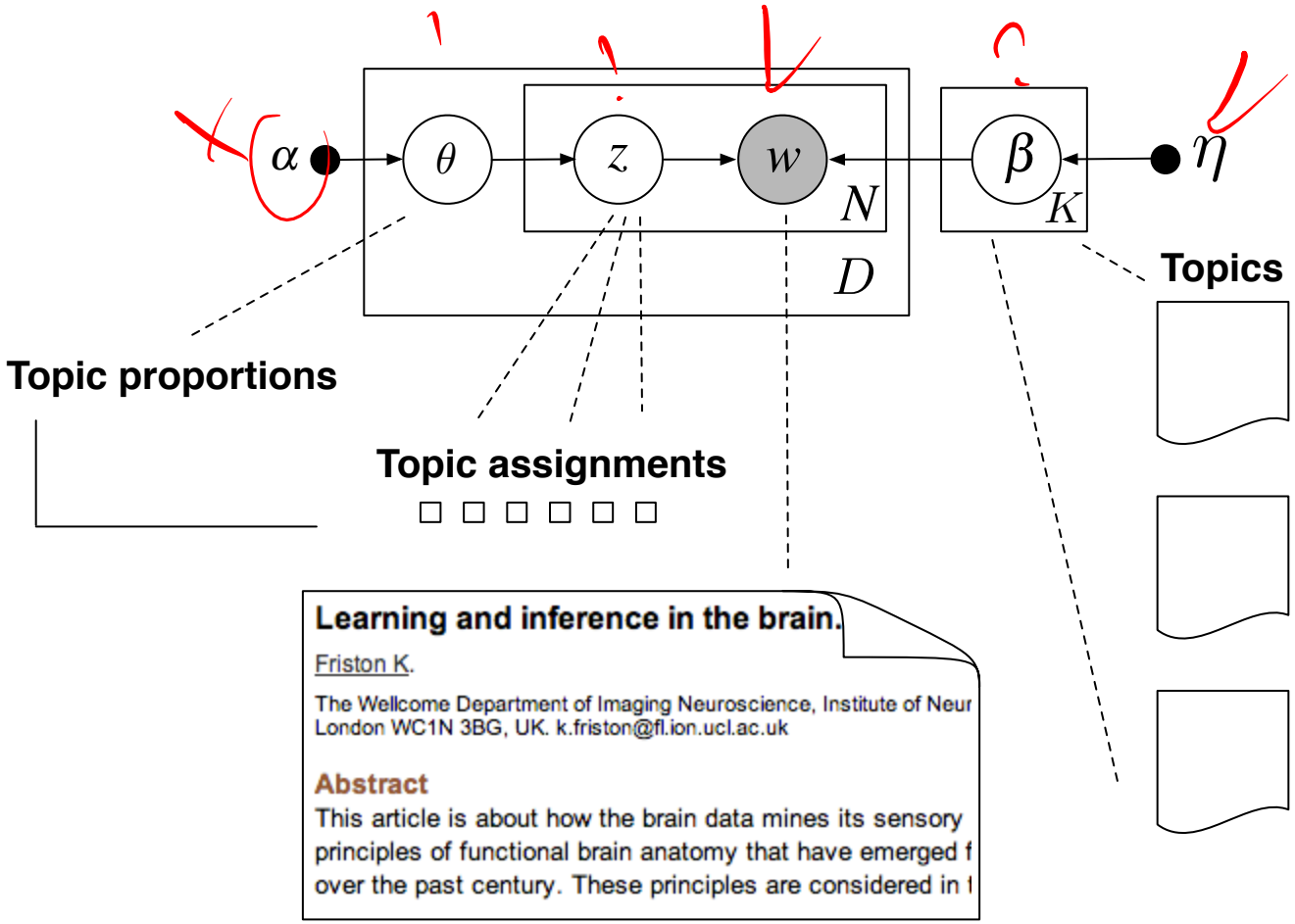
$$\theta_i = \exp\left\{\gamma_i - \log\left(1 + \sum_{i=1}^{K-1} e^{\gamma_i}\right)\right\}$$

$$C(\gamma) = \log\left(1 + \sum_{i=1}^{K-1} e^{\gamma_i}\right)$$

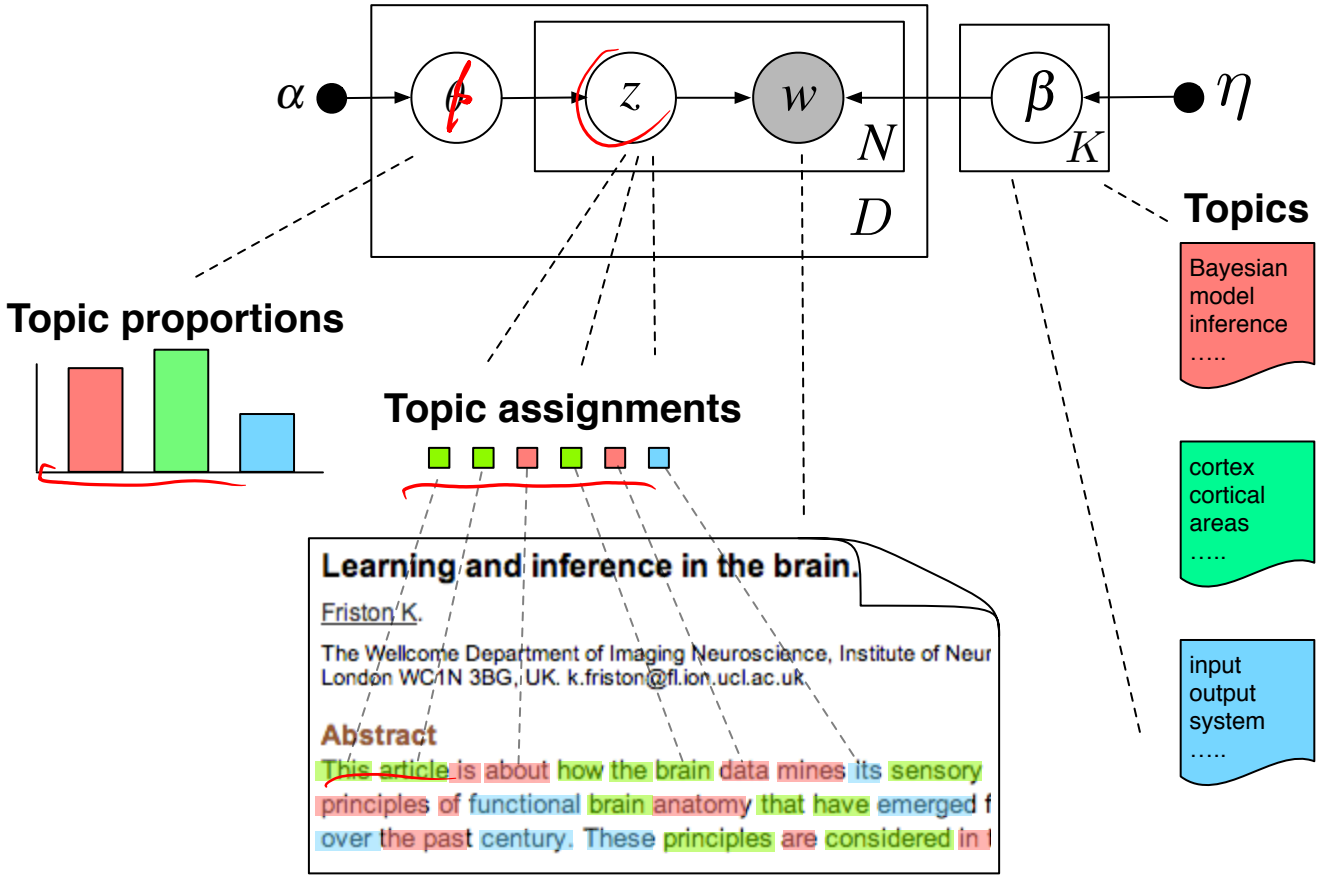
Problem

- Log Partition Function
- Normalization Constant

Posterior inference

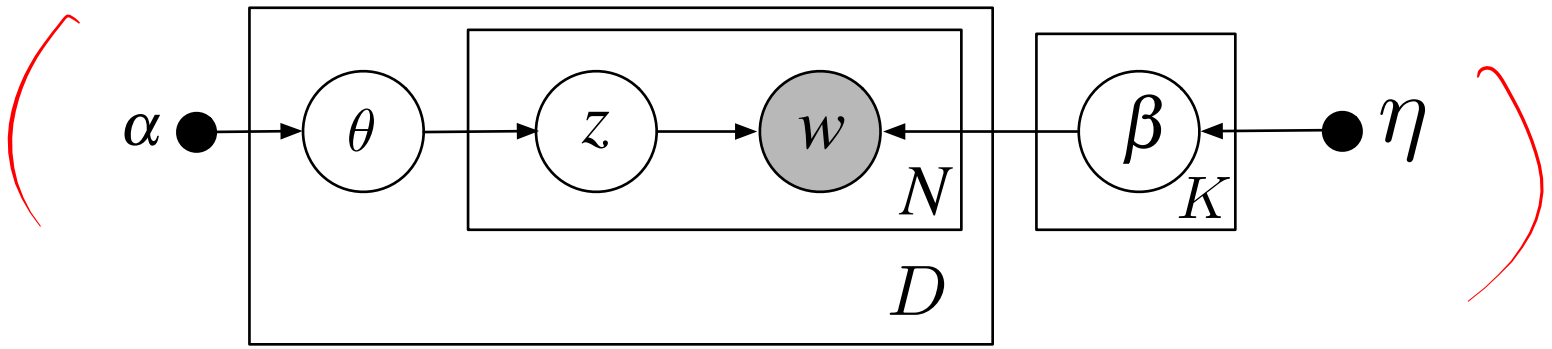


Posterior inference results



Joint likelihood of all variables

$$p(\beta, \theta, \boldsymbol{z}, \boldsymbol{w}) = \prod_{k=1}^{K} p(\beta_k|\eta) \prod_{d=1}^{D} p(\theta_d|\alpha) \prod_{n=1}^{N} p(z_{dn}|\theta_d)\, p(w_{dn}|z_{dn}, \beta)$$



We are interested in computing the posterior, and the data likelihood!

Inference and Learning are both intractable

- A possible query:

$$p(\theta_n \mid D) = ?$$

$$p(z_{n,m} \mid D) = ?$$

  - Close form solution?

$$p(\theta_n \mid D) = \frac{p(\theta_n, D)}{p(D)}$$

$$= \frac{\sum_{\{z_{n,m}\}} \int \left(\prod_n \left(\prod_m p(w_{n,m} \mid \beta_{z_n}) p(z_{n,m} \mid \theta_n) \right) p(\theta_n \mid \alpha) \right) p(\beta \mid \eta) d\theta_{-i} d\beta}{p(D)}$$

$$p(D) = \sum_{\{z_{n,m}\}} \int \cdots \int \left(\prod_n \left(\prod_m p(x_{n,m} \mid \beta_{z_n}) p(z_{n,m} \mid \theta_n) \right) p(\theta_n \mid \alpha) \right) p(\beta \mid \eta) d\theta_1 \cdots d\theta_N d\beta$$

  - Sum in the denominator over T^n terms, and integrate over n k-dimensional topic vectors
- Learning: What to learn? What is the objective function?

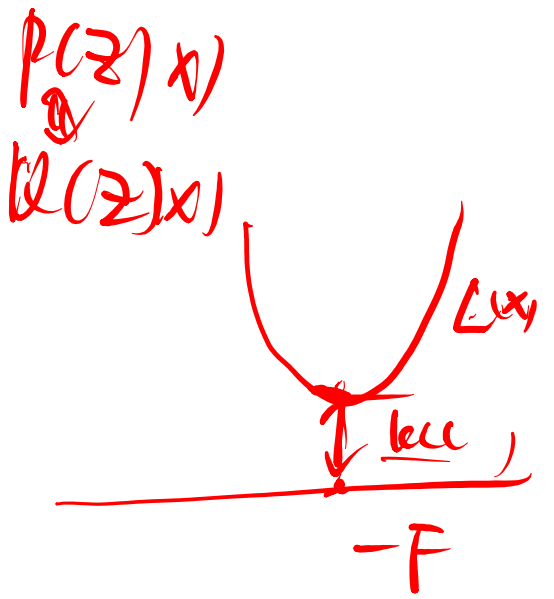
Approximate Inference

- Variational Inference
  - Mean field approximation (Blei et al.)
  - Expectation propagation (Minka et al.)
  - Variational 2nd-order Taylor approximation (Xing)
- Markov Chain Monte Carlo
  - Gibbs sampling (Griffiths et al)

Variational Inference

- Consider a generative model $p_\theta(\boldsymbol{x}|\boldsymbol{z})$, and prior $p(\boldsymbol{z})$
  - Joint distribution: $p_\theta(\boldsymbol{x}, \boldsymbol{z}) = p_\theta(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})$
- Assume variational distribution $q_\phi(\boldsymbol{z}|\boldsymbol{x})$
- Objective: Maximize lower bound for log likelihood

$$\begin{aligned}
&\log p(\boldsymbol{x}) \\
&= KL\left(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x})\right) + \int_{\boldsymbol{z}} q_\phi(\boldsymbol{z}|\boldsymbol{x}) \log \frac{p_\theta(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \\
&\geq \int_{\boldsymbol{z}} q_\phi(\boldsymbol{z}|\boldsymbol{x}) \log \frac{p_\theta(\boldsymbol{x}, \boldsymbol{z})}{q_\phi(\boldsymbol{z}|\boldsymbol{x})} \\
&:= \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x})
\end{aligned}$$



  - Equivalently, minimize free energy

$$F(\boldsymbol{\theta}, \phi; \boldsymbol{x}) = -\log p(\boldsymbol{x}) + KL(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}))$$

Variational Inference

Maximize the variational lower bound:

$$\mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x}) = \mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)] + KL\left(q_\phi(z|x)||p(z)\right)$$
$$= \log p(\boldsymbol{x}) - KL(q_\phi(\boldsymbol{z}|\boldsymbol{x}) \,||\, p_{\boldsymbol{\theta}}(\boldsymbol{z}|\boldsymbol{x}))$$

- E-step: maximize $\mathcal{L}$ w.r.t. $\boldsymbol{\phi}$, with $\boldsymbol{\theta}$ fixed

$$\max_\phi \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x})$$

  - If closed form solutions exist:

$$q_\phi^*(z|x) \propto \exp[\log p_\theta(x, z)]$$

- M-step: maximize $\mathcal{L}$ w.r.t. $\boldsymbol{\theta}$, with $\boldsymbol{\phi}$ fixed

$$\max_\theta \mathcal{L}(\boldsymbol{\theta}, \boldsymbol{\phi}; \boldsymbol{x})$$

Mean-field assumption (in topic models)

- True posterior

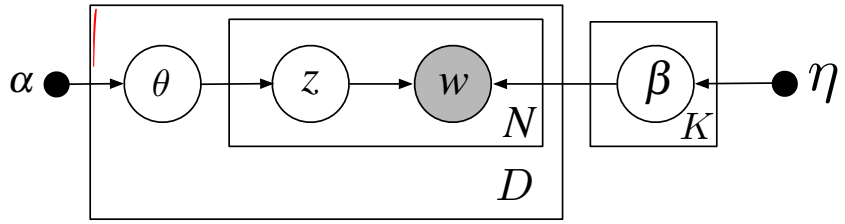
$$p(\beta, \theta, \boldsymbol{z}|\boldsymbol{w}) = \frac{p(\beta, \theta, \boldsymbol{z}, \boldsymbol{w})}{p(\boldsymbol{w})}$$

- Break the dependency using the fully factorized distribution

$$q(\beta, \theta, \boldsymbol{z}) = \prod_k q(\beta_k) \prod_d q(\theta_d) \prod_n q(z_{dn})$$

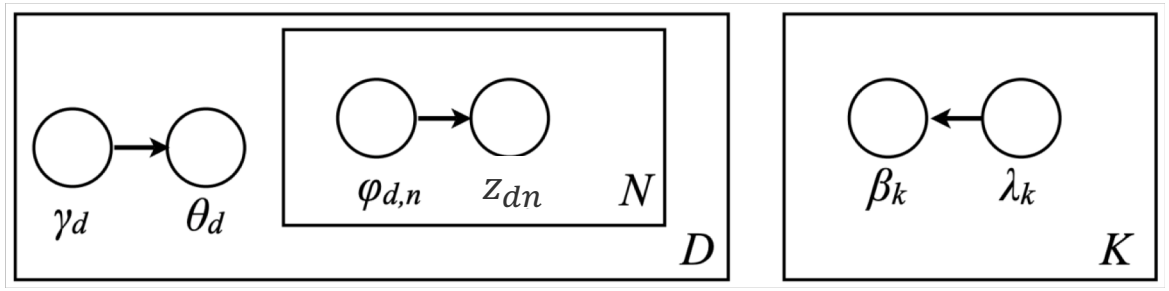
- Mean-field family usually does NOT include the true posterior.

Mean Field Approximation



- Parametric form for each marginal factor in $q(\beta, z, \theta \mid \lambda, \phi, \gamma)$:

$$q(\beta_k \mid \lambda_k) = \text{Dirichlet}(\beta_k \mid \lambda_k)$$
$$q(\theta_d \mid \gamma_d) = \text{Dirichlet}(\theta_d \mid \gamma_d)$$
$$q(z_{dn} \mid \phi_{dn}) = \text{Multinomial}(z_{dn} \mid \phi_{dn})$$



- Learning parameters of the variational distribution (E-step):

$$\gamma^\star, \lambda^\star, \phi^\star = \arg\min_{\gamma,\lambda,\phi} \text{KL}(q(\beta, \theta, \mathbf{z} \mid \gamma, \phi) \parallel p(\beta, \theta, \mathbf{z} \mid \mathbf{w}, \alpha, \eta))$$

- For LDA, we can compute the optimal MF approximation in closed form.

Update each marginal

- Update:

$$q(\theta_d) \propto \exp\left\{\mathbb{E}_{\prod_n q(z_{dn})}\left[\log p(\theta_d|\alpha) + \sum_n \log p(z_{dn}|\theta_d)\right]\right\}$$

- Where in LDA:

$$p(\theta_d|\alpha) \propto \exp\left\{\sum_{k=1}^{K}(\alpha_k - 1)\log\theta_{dk}\right\} \text{ --Dirichlet}$$

$$p(z_{dn}|\theta_d) = \exp\left\{\sum_{k=1}^{K} 1[z_{dn} = k]\log\theta_{dk}\right\} \text{ --Multinomial}$$

- And we obtain:

$$q(\theta_d) \propto \exp\left\{\sum_{k=1}^{K}\left(\sum_{n=1}^{N} q(z_{dn} = k) + \alpha_k - 1\right)\log\theta_{dk}\right\}$$

This is also a Dirichlet — the same as its prior!

Update each marginal

- Similarly to $q(\theta_d \mid \gamma_d)$, we obtain optimal parameters $\phi^{\star}_{dn}$ for $q(z_{dn} \mid \phi_{dn})$:

$$q(z_dn = k \mid \phi_{dn}) = \phi_{dn}(k) = \beta_k(w_{dn}) \exp\left\{\Psi(\gamma_d(k)) - \Psi(\sum_{j=1}^{K} \gamma_d(j))\right\}$$

- And optimal parameters $\lambda^{\star}_k$ for $q(\beta_k \mid \lambda_k)$:

$$\lambda_k(j) = \eta(j) + \sum_{d=1}^{D}\sum_{n=1}^{N_d} \phi^{\star}_{dn}(k) 1[w_{dn} = j]$$

- Iterating these equations to convergence yields the MF approximation to the posterior distribution.

Coordinate ascent algorithm for LDA

1: Initialize variational topics $q(\beta_k)$, $k = 1, ..., K$.
2: **repeat**
3: **for** each document $d \in \{1, 2, ..., D\}$ **do**
4: Initialize variational topic assigments $q(z_{dn})$, $n = 1, ..., N$
5: **repeat**
6: Update variational topic proportions $q(\theta_d)$
7: Update variational topic assigments $q(z_{dn})$, $n = 1, ..., N$
8: **until** Change of $q(\theta_d)$ is small enough
9: **end for**
10: Update variational topics $q(\beta_k)$, $k = 1, ..., K$.
11: **until** Lower bound $L(q)$ converges

Conclusion

- GM-based topic models are cool
  - Flexible
  - Modular
  - Interactive
- There are many ways of implementing topic models
  - unsupervised
  - supervised
- Efficient Inference/learning algorithms
  - GMF, with Laplace approx. for non-conjugate dist.
  - MCMC
- Many applications
  - …
  - Word-sense disambiguation
  - Image understanding
  - Network inference

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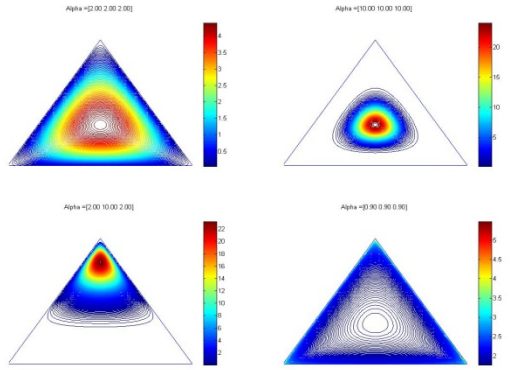
Supplementary

Supplementary: More on strategies in VI

- Alternative approximation scheme
- How to evaluate: empirical (ground truth unknown) vs. simulation (ground truth known)
- Comparison (of what)
- Building blocks

Recall Choices of Priors

- Dirichlet (LDA) (Blei et al. 2003)
  - Conjugate prior means efficient inference
  - Can only capture variations in each topic's intensity independently



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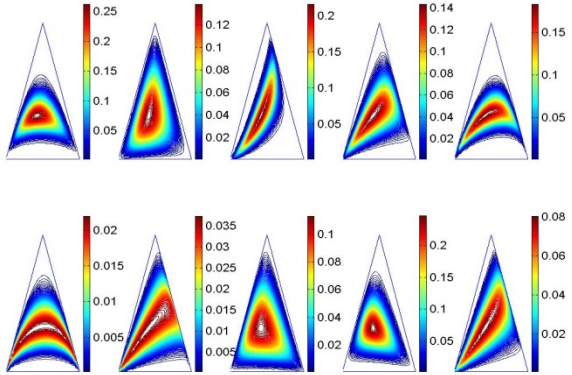
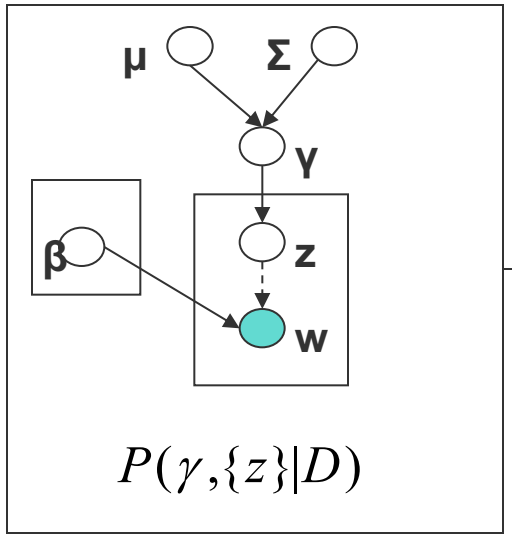
  - Capture the intuition that some topics are highly correlated and can rise up in intensity together
  - Not a conjugate prior implies hard inference



Choice of q() does matter



$$P(\gamma,\{z\}|D)$$

Σ* is full matrix

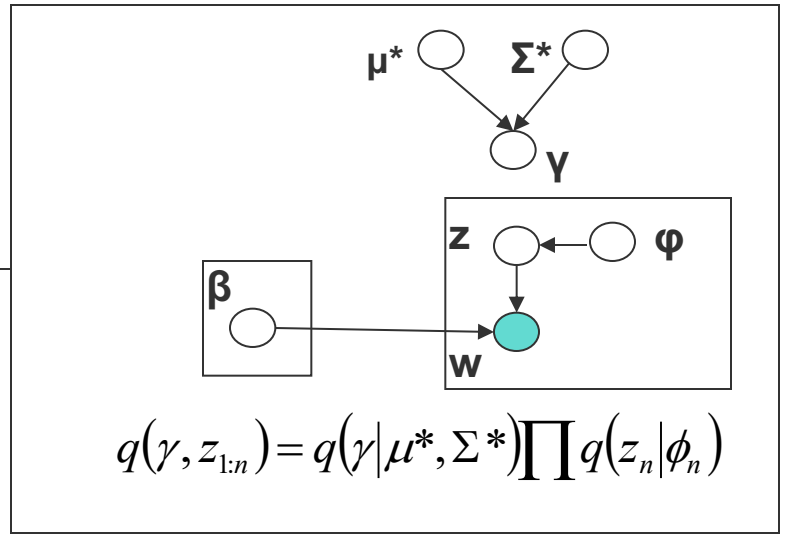
Multivariate Quadratic Approx.

Closed Form Solution for μ*, Σ*

Ahmed&Xing

Log Partition Function

$$\log\left(1+\sum_{i=1}^{K-1}e^{\gamma_i}\right)$$



$$q(\gamma,z_{1:n})=q(\gamma|\mu^*,\Sigma^*)\prod q(z_n|\phi_n)$$

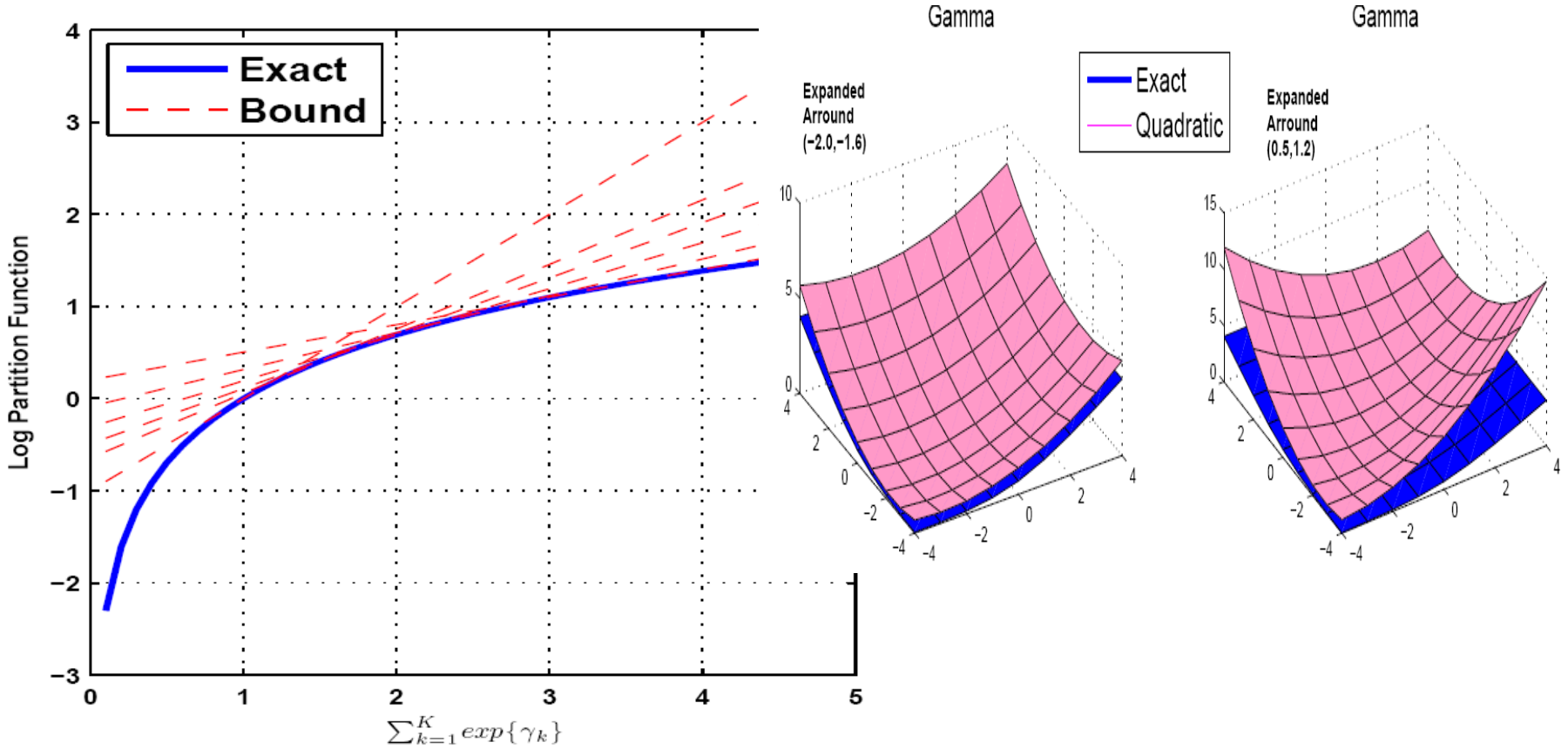
Σ* is assumed to be diagonal

Tangent Approx.

Numerical Optimization to fit μ*, Diag(Σ*)

Blei&Lafferty

Tangent Approximation



How to evaluate?

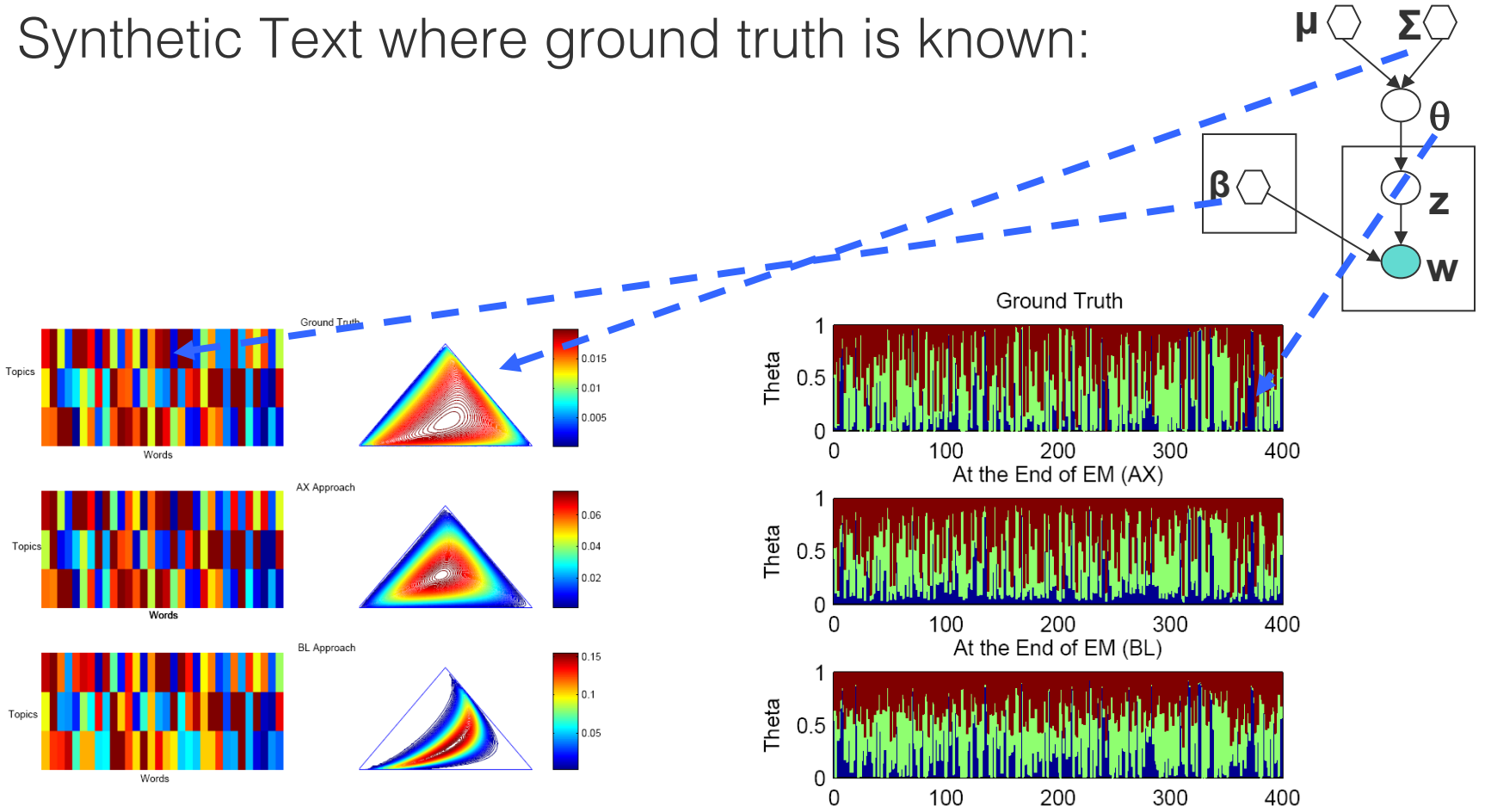
- Empirical Visualization: e.g., topic discovery on New York Times

The 5 most frequent topics from the HDP on the *New York Times*.

game	life	film	book	wine
season	know	movie	life	street
team	school	show	books	hotel
coach	street	life	novel	house
play	man	television	story	room
points	family	films	man	night
games	says	director	author	place
giants	house	man	house	restaurant
second	children	story	war	park
players	night	says	children	garden

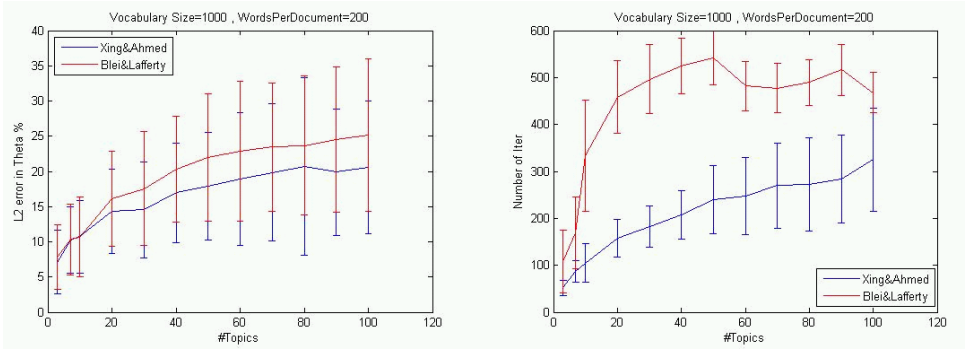
How to evaluate?

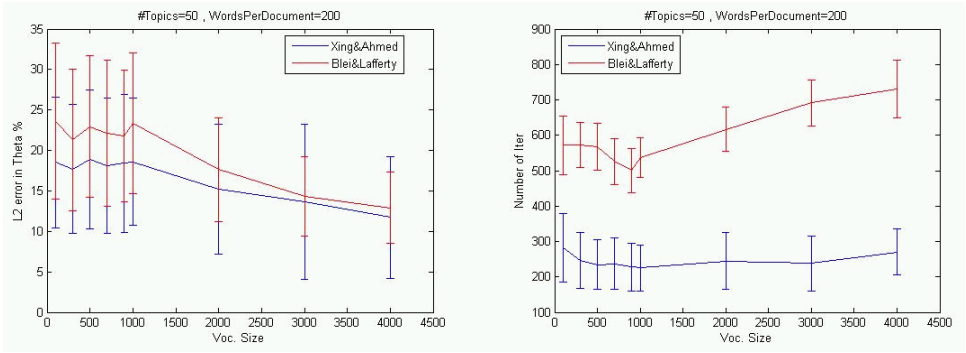
- Test on Synthetic Text where ground truth is known:

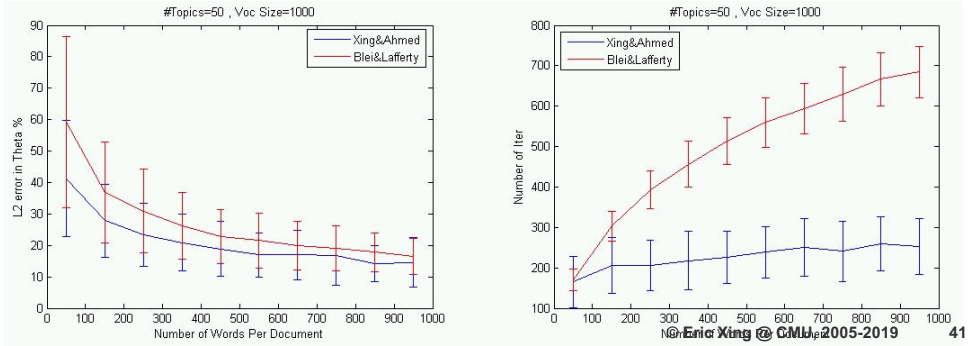


Comparison: accuracy and speed

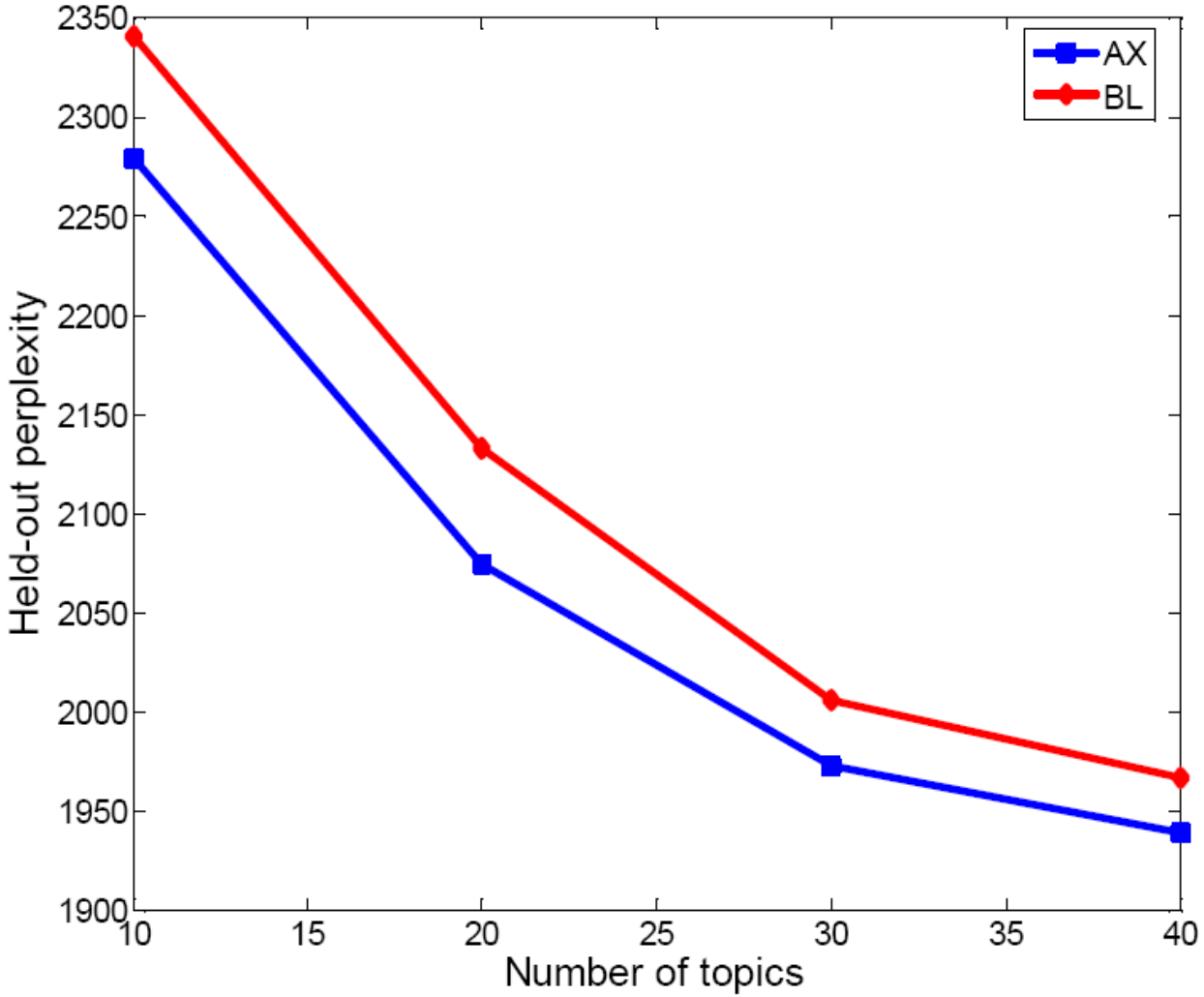
- L2 error in topic vector est. and # of iterations
  - Varying Num. of Topics
  - Varying Voc. Size
  - Varying Num. Words Per Document







Comparison: perplexity



Classification Result on PNAS collection

- PNAS abstracts from 1997-2002
  - 2500 documents
  - Average of 170 words per document
- Fitted 40-topics model using both approaches
- Use low dimensional representation to predict the abstract category
  - Use SVM classifier
  - 85% for training and 15% for testing

Classification Accuracy

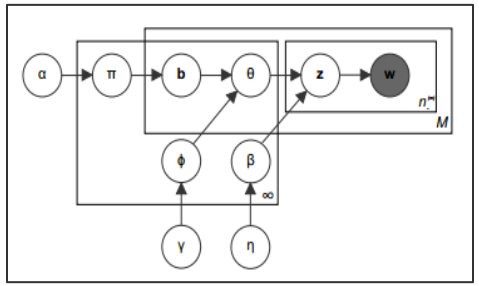
Category	Doc	BL	AX
Genetics	21	61.9	61.9
Biochemistry	86	65.1	77.9
Immunology	24	70.8	66.6
Biophysics	15	53.3	66.6
Total	146	64.3	72.6

-Notable Difference
-Examine the low dimensional representations below

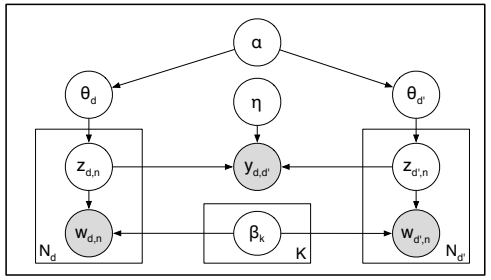
What makes topic models useful --- The Zoo of Topic Models!

- It is a building block of many models.

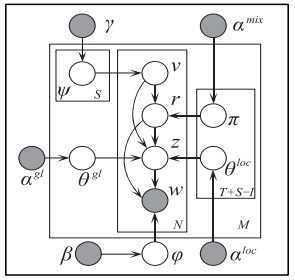
Williamson et al. 2010



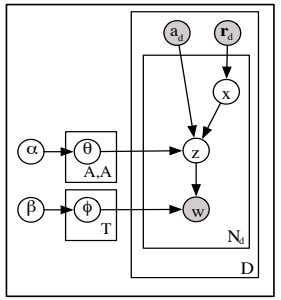
Chang & Blei, 2009



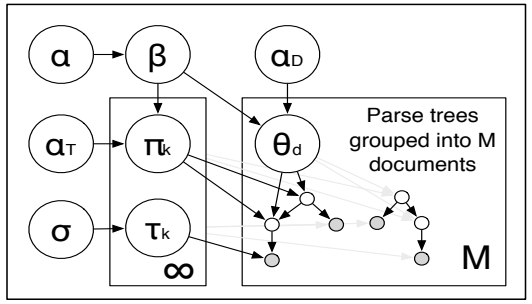
Titov & McDonald, 2008



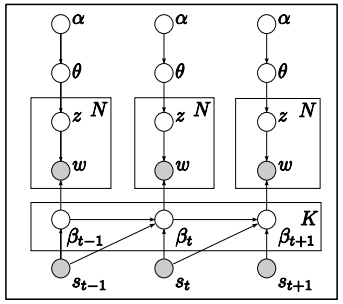
McCallum et al. 2007



Boyd-Graber & Blei, 2008



Wang & Blei, 2008



PETUUM

More on Mean Field Approximation

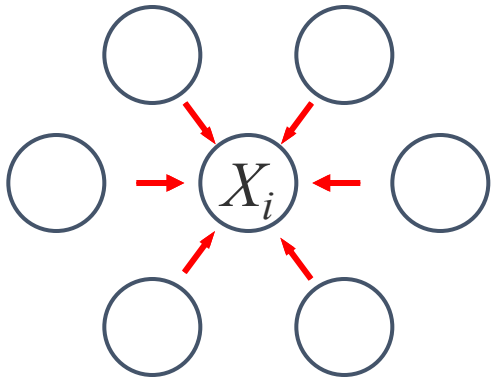
The naive mean field approximation

- Approximate $p(\mathbf{X})$ by fully factorized $q(\mathbf{X})=\mathrm{P}_i q_i(X_i)$
- For Boltzmann distribution $p(X)=\exp\{\sum_{i<j} q_{ij}X_iX_j+q_{io}X_i\}/Z$:

mean field equation:

$$q_i(X_i) = \exp\left\{\theta_{i0}X_i + \sum_{j\in\mathcal{N}_i}\theta_{ij}X_i\langle X_j\rangle_{q_j} + A_i\right\}$$

$$= p(X_i \mid \{\langle X_j\rangle_{q_j} : j\in\mathcal{N}_i\})$$



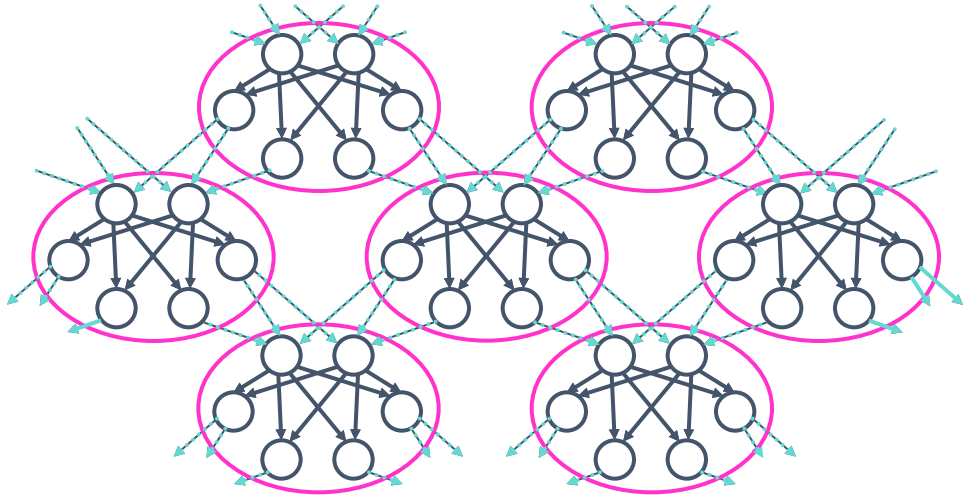
- $\langle X_j\rangle_{q_j}$ resembles a "message" sent from node j to i
- $\{\langle X_j\rangle_{q_j} : j\in\mathcal{N}_i\}$ forms the "mean field" applied to X_i from its neighborhood

Cluster-based approx. to the Gibbs free energy

(Wiegerinck 2001,
Xing *et al* 03,04)

Exact: $G[p(X)]$ *(intractable)*

Clusters: $G[\{q_c(X_c)\}]$



Mean field approx. to Gibbs free energy

- Given a disjoint clustering, $\{C_1, \ldots, C_I\}$, of all variables
- Let

$$q(\mathbf{X}) = \prod_i q_i(\mathbf{X}_{C_i}),$$

- Mean-field free energy

$$G_{\text{MF}} = \sum_i \sum_{\mathbf{x}_{C_i}} \prod_i q_i(\mathbf{x}_{C_i}) E(\mathbf{x}_{C_i}) + \sum_i \sum_{\mathbf{x}_{C_i}} q_i(\mathbf{x}_{C_i}) \ln q_i(\mathbf{x}_{C_i})$$

e.g., $$G_{\text{MF}} = \sum_{i<j} \sum_{x_i x_j} q(x_i) q(x_j) \phi(x_i x_j) + \sum_i \sum_{x_i} q(x_i) \phi(x_i) + \sum_i \sum_{x_i} q(x_i) \ln q(x_i)$$ (naïve mean field)

  - Will never equal to the exact Gibbs free energy no matter what clustering is used, but it does always define a lower bound of the likelihood
- Optimize each $q_i(x_c)$'s.
  - Variational calculus …
  - Do inference in each $q_i(x_c)$ using any tractable algorithm

The Generalized Mean Field theorem

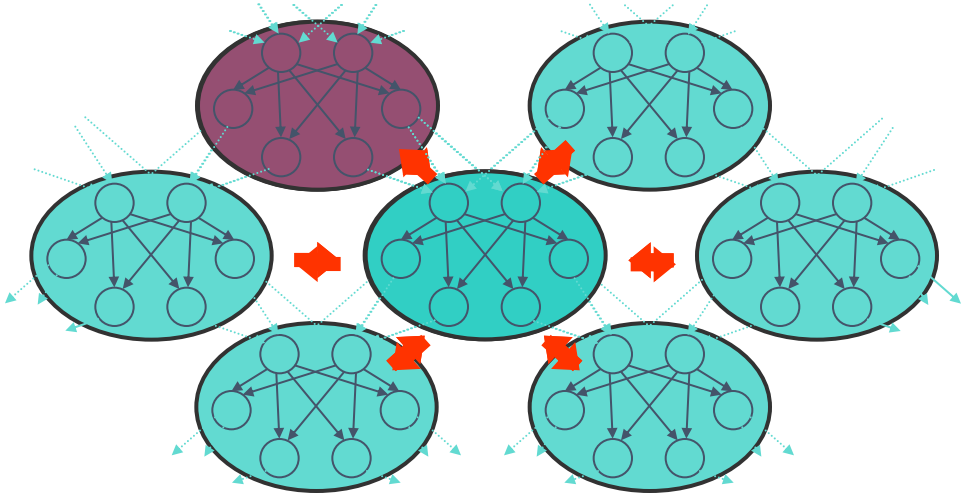
Theorem: The optimum GMF approximation to the cluster marginal is isomorphic to the cluster posterior of the original distribution given internal evidence and its generalized mean fields:

$$q_i^*(\mathbf{X}_{H,C_i}) = p(\mathbf{X}_{H,C_i} \mid \mathbf{x}_{E,C_i}, \left\langle \mathbf{X}_{H,MB_i} \right\rangle_{q_{j\neq i}})$$

GMF algorithm: Iterate over each q_i

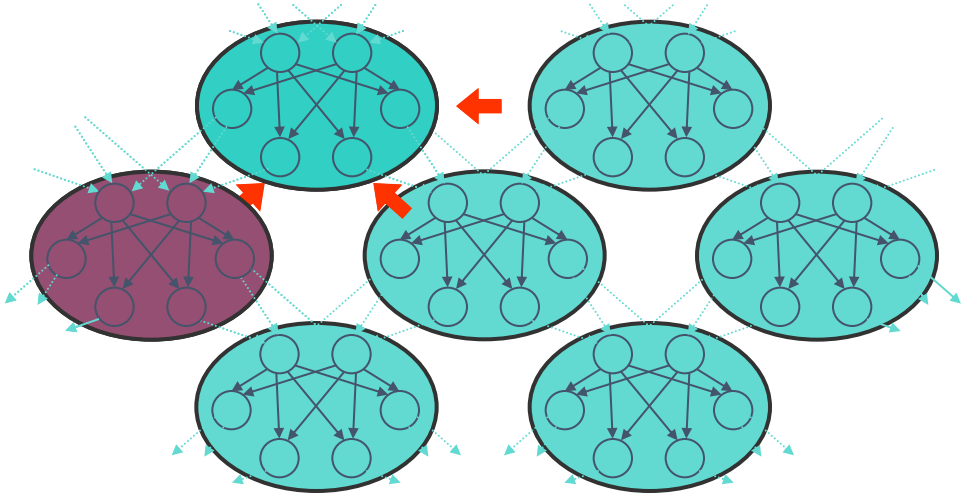
A generalized mean field algorithm

[xing *et al*. UAI 2003]



A generalized mean field algorithm

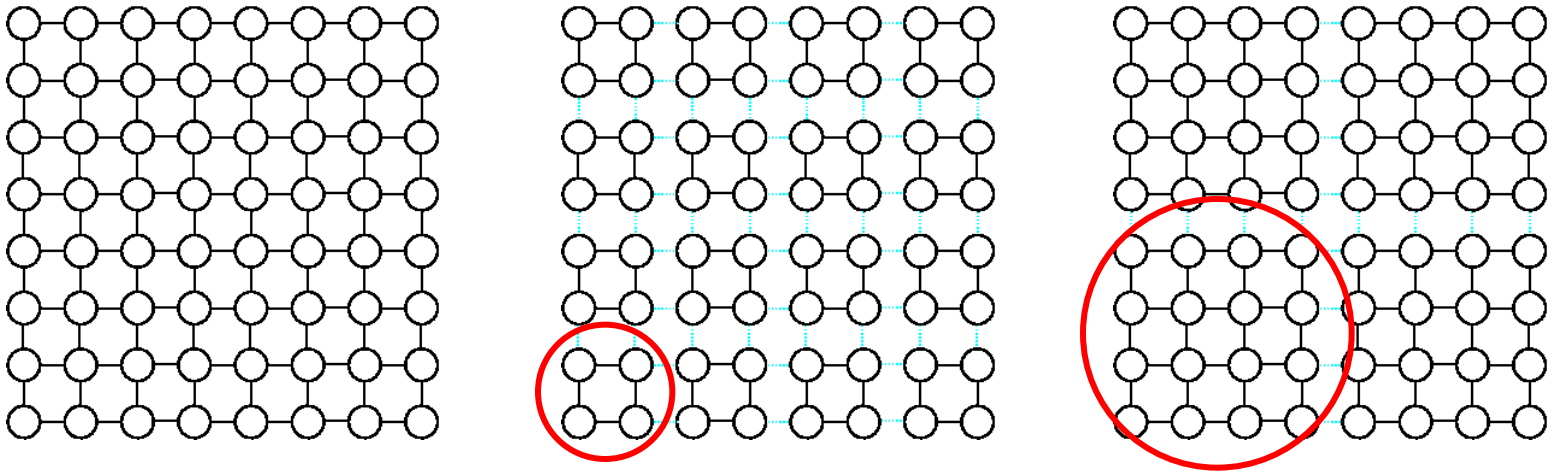
[Xing et al. UAI 2003]



Convergence theorem

Theorem: The GMF algorithm is guaranteed to converge to a local optimum, and provides a lower bound for the likelihood of evidence (or partition function) the model.

Example 1: Generalized MF approximations to Ising models

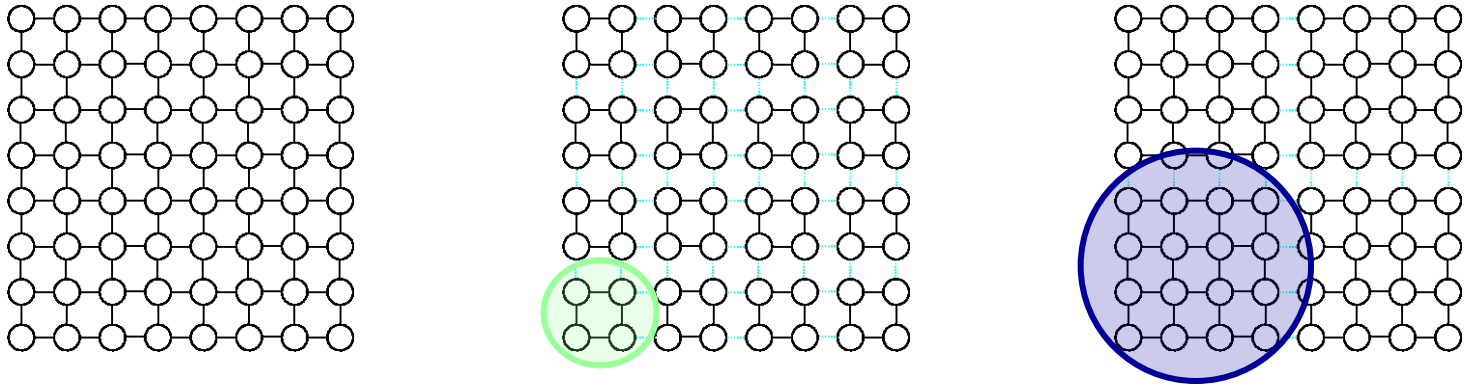


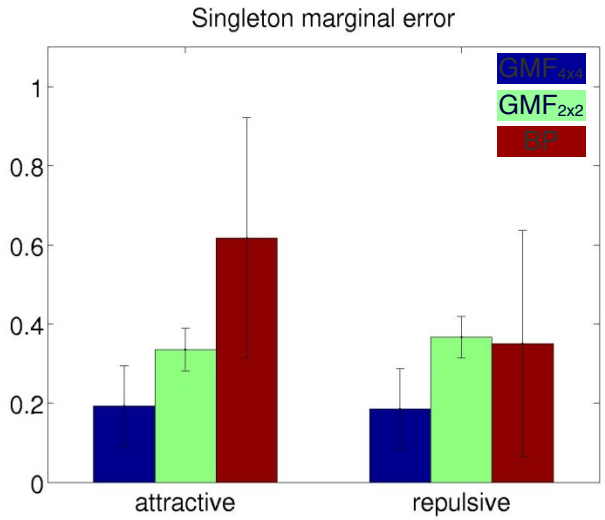
Cluster marginal of a square block C_k:

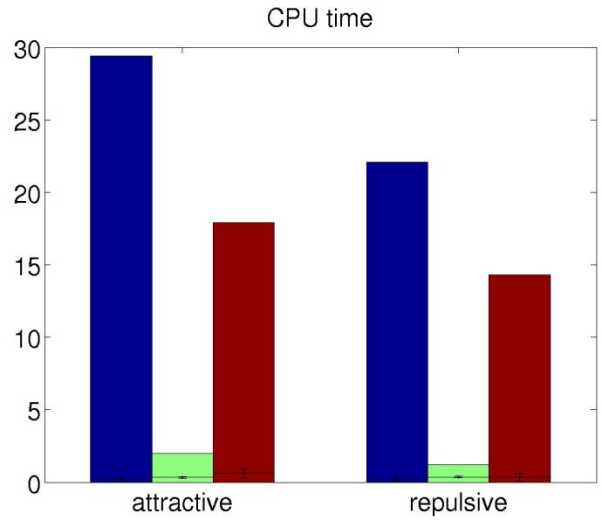
$$q(X_{C_k}) \propto \exp\left\{ \sum_{i,j \in C_k} \theta_{ij} X_i X_j + \sum_{i \in C_k} \theta_{i0} X_i + \sum_{\substack{i \in C_k,\, j \in MB_k, \\ k' \in MBC_k}} \theta_{ij} X_i \left\langle X_j \right\rangle_{q(X_{C_{k'}})} \right\}$$

Virtually a reparameterized Ising model of small size.

GMF approximation to Ising models

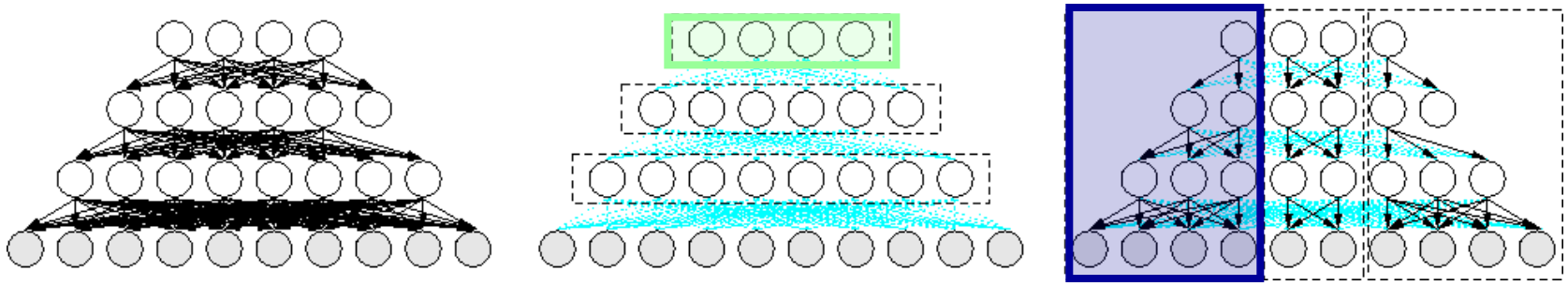


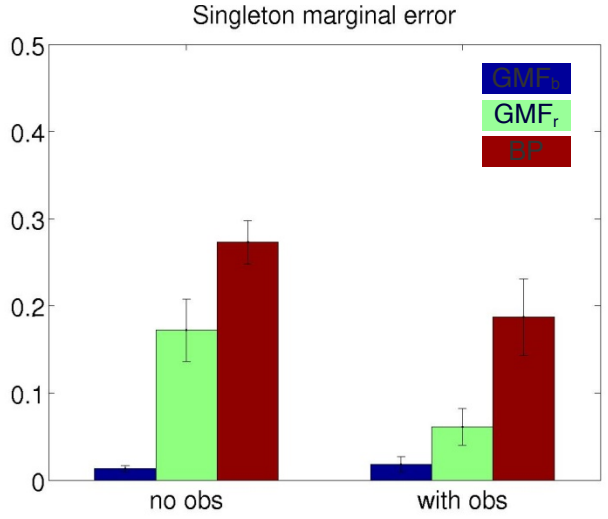


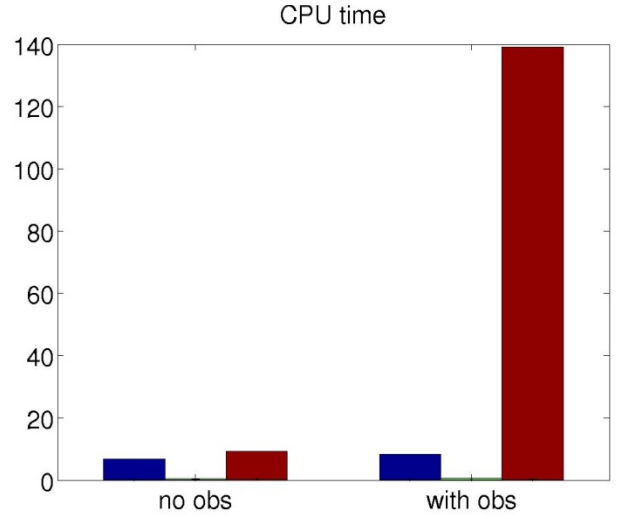


Attractive coupling: positively weighted
Repulsive coupling: negatively weighted

Example 2: Sigmoid belief network







Example 3: Factorial HMM