School of Computer Science
Carnegie Mellon

Probabilistic Graphical Models

Mean Fiend Approximation
&
Topic Models

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Reading: See class website

Variational Principle

- Exact variational formulation

$$A(\theta) = \sup_{\mu \in \mathcal{M}} \{\theta^T \mu - A^*(\mu)\}$$

  - $\mathcal{M}$: the marginal polytope, difficult to characterize
  - A^*: the negative entropy function, no explicit form

- Mean field method: non-convex inner bound and exact form of entropy

- Bethe approximation and loopy belief propagation: polyhedral outer bound and non-convex Bethe approximation

Mean Field Approximation

Mean Field Methods

- For a given tractable subgraph F, a subset of canonical parameters is

$$\mathcal{M}(F;\phi) := \{\tau \in \mathbb{R}^d \mid \tau = \mathbb{E}_\theta[\phi(X)] \text{ for some } \theta \in \Omega(F)\}$$

- Inner approximation

$$\mathcal{M}(F;\phi)^o \subseteq \mathcal{M}(G;\phi)^o$$

- Mean field solves the relaxed problem

$$\max_{\tau \in \mathcal{M}_F(G)} \{\langle \tau, \theta \rangle - A_F^*(\tau)\}$$

- $A_F^* = A^*\big|_{\mathcal{M}_F(G)}$ is the exact dual function restricted to $\mathcal{M}_F(G)$

Tractable Subgraphs

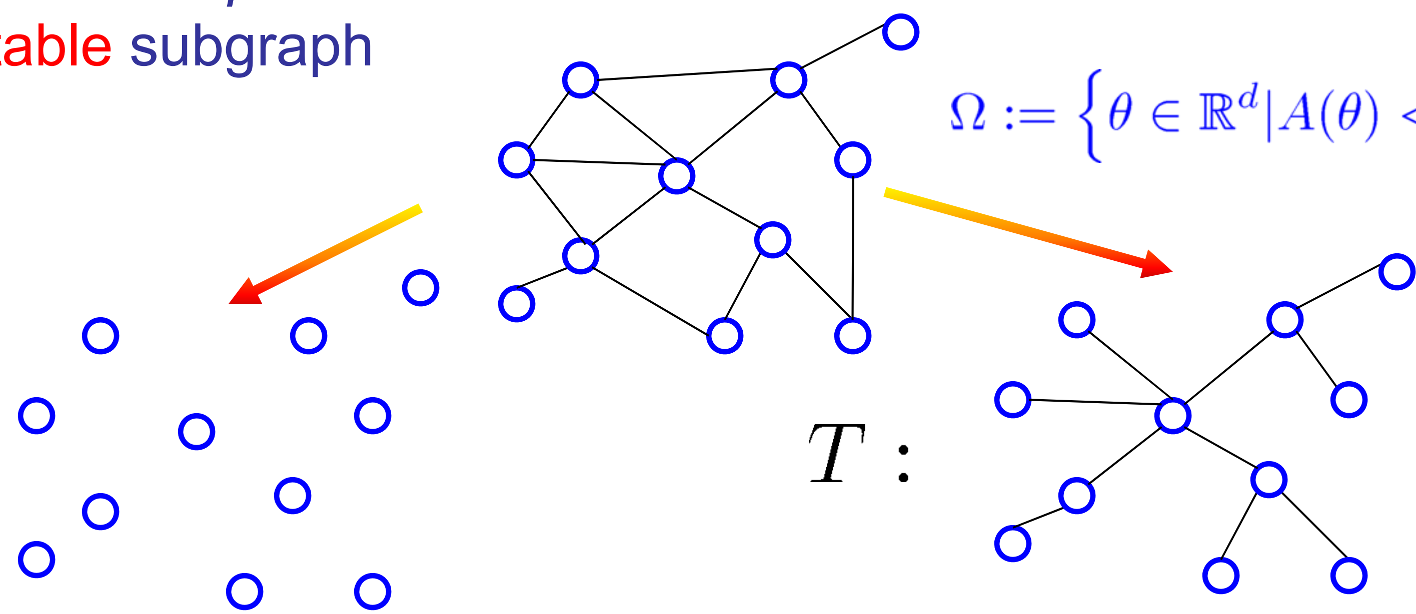
- For an exponential family with sufficient statistics ϕ defined on graph G, the set of realizable mean parameter set

$$\mathcal{M}(G;\phi) := \{\mu \in \mathbb{R}^d \mid \exists p \text{ s.t. } \mathbb{E}_p[\phi(X)] = \mu\}$$

- Idea: restrict *p* to a subset of distributions associated with a tractable subgraph

$$\Omega := \left\{\theta \in \mathbb{R}^d | A(\theta) < +\infty\right\}$$

$F_0 :$



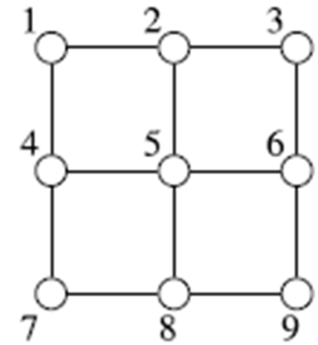
$T :$

$$\Omega(F_0) := \left\{\theta \in \Omega \mid \theta_{(s,t)} = 0 \; \forall \, (s,t) \in E\right\}. \quad \Omega(T) := \left\{\theta \in \Omega \mid \theta_{(s,t)} = 0 \;\; \forall \, (s,t) \notin E(T)\right\}.$$

Example: Naïve Mean Field for Ising Model

- Ising model in {0,1} representation

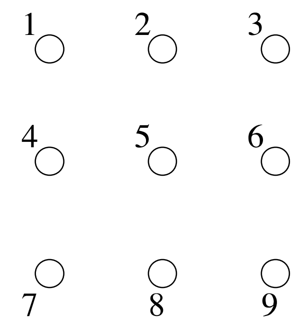
$$p(x) \propto \exp\left\{ \sum_{s \in V} x_s \theta_s + \sum_{(s,t) \in E} x_s x_t \theta_{st} \right\}$$



- Mean parameters

$\mu_s = E_p[X_s] = P[X_s = 1]$ for all $s \in V$, and

$\mu_{st} = E_p[X_s X_t] = P[(X_s, X_t) = (1,1)]$ for all $(s,t) \in E$.



- For fully disconnected graph F,

$$\mathcal{M}_F(G) := \{\tau \in \mathbb{R}^{|V|+|E|} \mid 0 \leq \tau_s \leq 1, \forall s \in V, \tau_{st} = \tau_s \tau_t, \forall (s,t) \in E\}$$

- The dual decomposes into sum, one for each node

$$A_F^*(\tau) = \sum_{s \in V} [\tau_s \log \tau_s + (1 - \tau_s) \log(1 - \tau_s)]$$

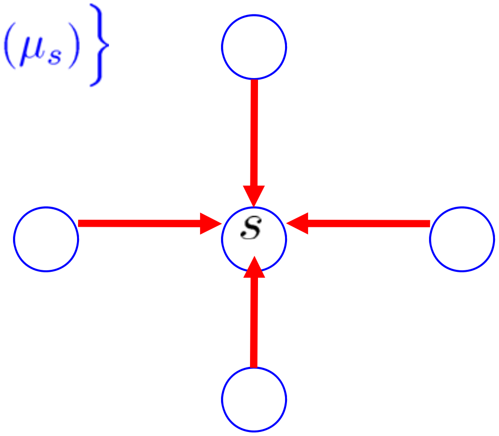
Naïve Mean Field for Ising Model

- Optimization Problem

$$\max_{\mu \in [0,1]^m} \left\{ \sum_{s \in V} \theta_s \mu_s + \sum_{(s,t) \in E} \theta_{st} \mu_s \mu_t + \sum_{s \in V} H_s(\mu_s) \right\}$$

- Update Rule

$$\mu_s \leftarrow \sigma\left(\theta_s + \sum_{t \in N(s)} \theta_{st} \mu_t\right)$$



- $\mu_t = p(X_t = 1) = \mathbb{E}_p[X_t]$ resembles "message" sent from node t to s
- $\{\mathbb{E}_p[X_t], t \in N(s)\}$ forms the "mean field" applied to s from its neighborhood
- Also yields lower bound on log partition function

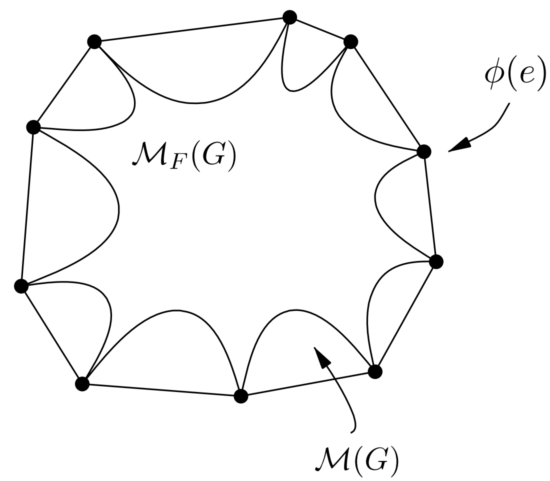
$$KL(Q \| P) = -H_Q(X) - \sum_{f_a \in F} E_Q \log f_a(X_a) + \log Z$$

Geometry of Mean Field

- Mean field optimization is always non-convex for any exponential family in which the state space $\mathcal{X}^m$ is finite

- Recall the marginal polytope is a convex hull

$$\mathcal{M}(G) = \mathrm{conv}\{\phi(e); e \in \mathcal{X}^m\}$$



- $\mathcal{M}_F(G)$ contains all the extreme points
  - If it is a strict subset, then it must be non-convex

- Example: two-node Ising model

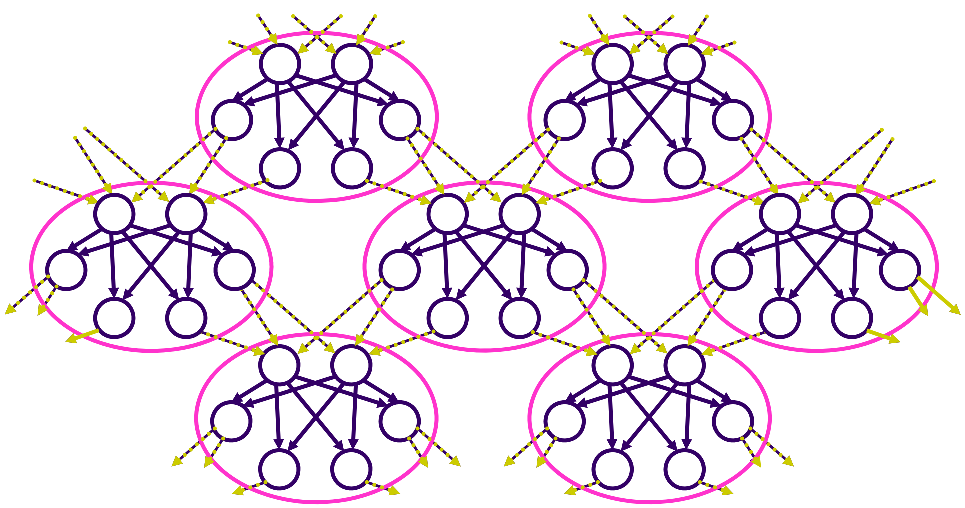
$$\mathcal{M}_F(G) = \{0 \leq \tau_1 \leq 1, 0 \leq \tau_2 \leq 1, \tau_{12} = \tau_1 \tau_2\}$$

  - It has a parabolic cross section along $\tau_1 = \tau_2$, hence non-convex

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$_1$, … , C$_I$}, of all variables
- Let
$$q(\mathbf{X}) = \prod_i q_i(\mathbf{X}_{C_i}),$$
- Mean-field free energy
$$G_{\mathrm{MF}} = \sum_i \sum_{\mathbf{x}_{C_i}} \prod_i q_i\left(\mathbf{x}_{C_i}\right) E(\mathbf{x}_{C_i}) + \sum_i \sum_{\mathbf{x}_{C_i}} q_i\left(\mathbf{x}_{C_i}\right) \ln q_i\left(\mathbf{x}_{C_i}\right)$$
e.g., $$G_{\mathrm{MF}} = \sum_{i<j} \sum_{x_i x_j} q(x_i) q(x_j) \phi(x_i x_j) + \sum_i \sum_{x_i} q(x_i) \phi(x_i) + \sum_i \sum_{x_i} q(x_i) \ln q(x_i)$$ (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

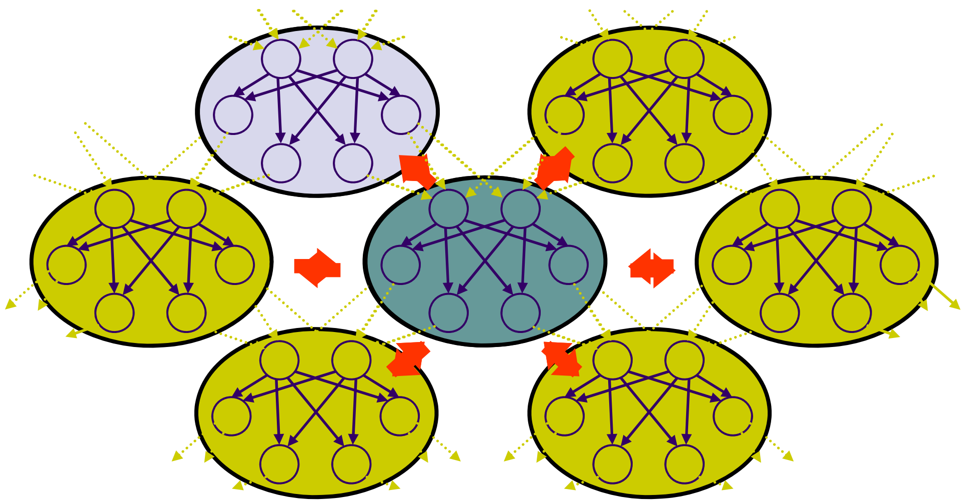
The Generalized Mean Field theorem

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:

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

GMF algorithm: Iterate over each q_i

A generalized mean field algorithm [xing *et al*. UAI 2003]



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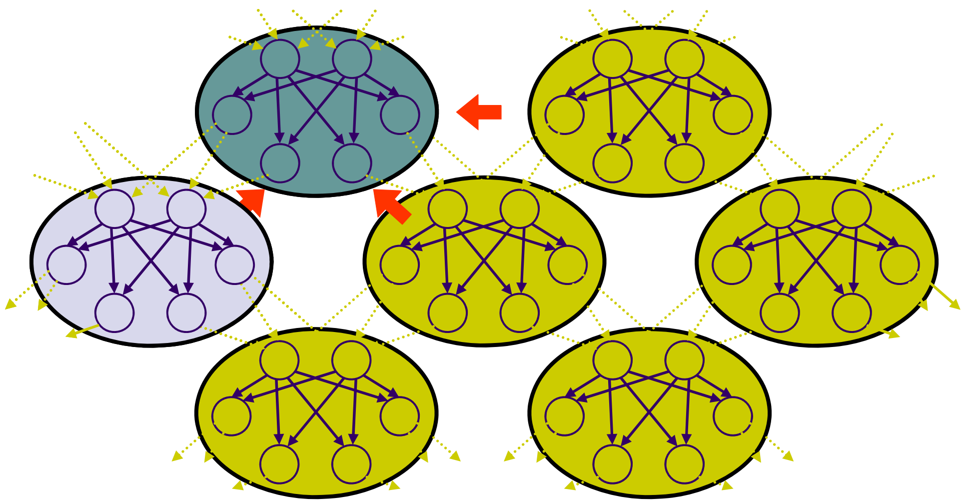


Convergence theorem

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.

The naive mean field approximation

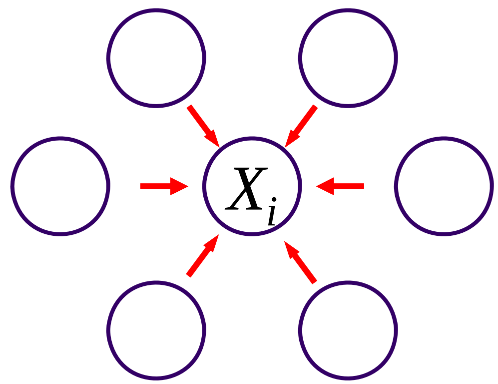
- Approximate $p(\mathbf{X})$ by fully factorized $q(\mathbf{X})=\prod_i q_i(X_i)$

- For Boltzmann distribution $p(X)=\exp\{\sum_{i<j} q_{ij}X_iX_j+q_{io}X_i\}/Z$:

mean field equation:

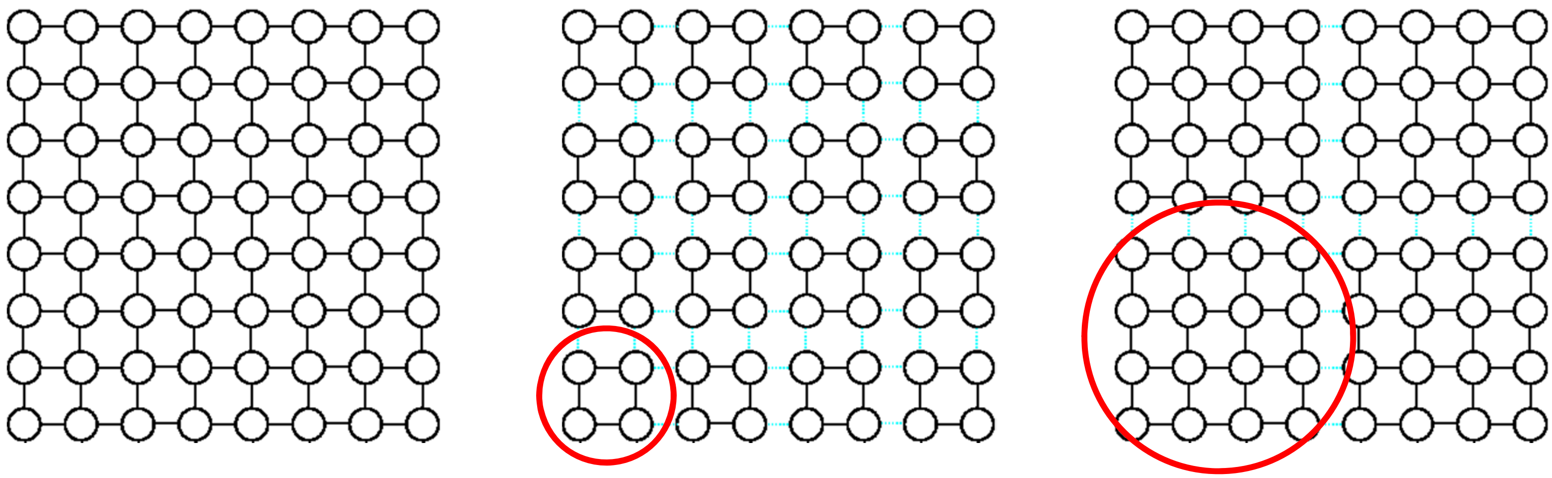
$$q_i(X_i) = \exp\left\{\theta_{i0}X_i + \sum_{j\in\mathcal{N}_i}\theta_{ij}X_i\langle X_j\rangle_{q_j} + A_i\right\}$$

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



- $\langle X_j\rangle_{q_j}$ 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

Example 1: Generalized MF approximations to Ising models

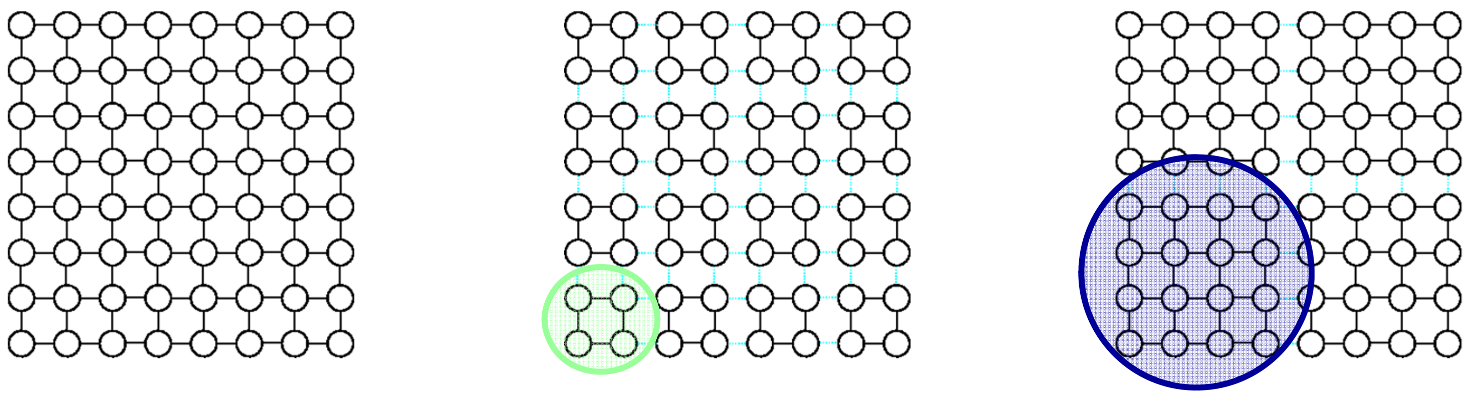


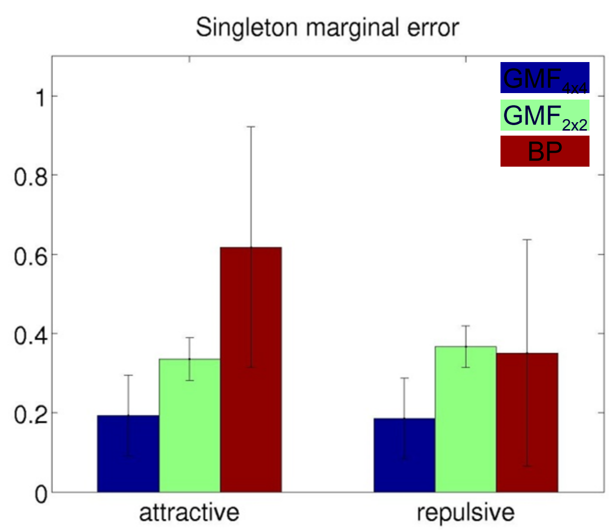
Cluster marginal of a square block C_k:

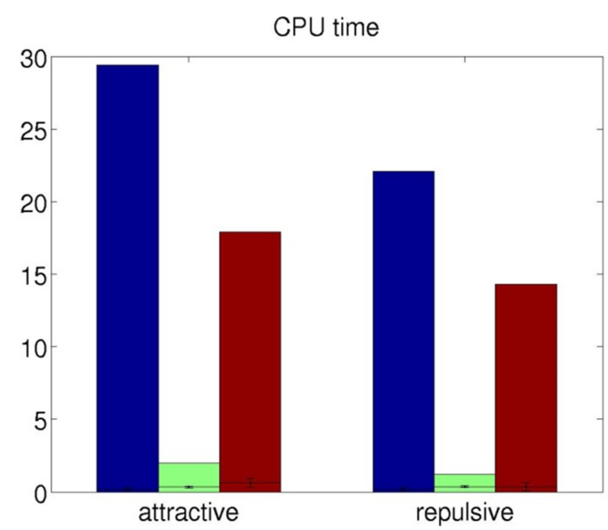
$$q(X_{C_k}) \propto \exp\left\{ \sum_{i,j \in C_k} \theta_{ij} X_i X_j + \sum_{i \in C_k} \theta_{i0} X_i + \sum_{\substack{i \in C_k,\, j \in MB_k, \\ k' \in MBC_k}} \theta_{ij} X_i \left\langle X_j \right\rangle_{q(X_{C_{k'}})} \right\}$$

Virtually a reparameterized Ising model of small size.

GMF approximation to Ising models



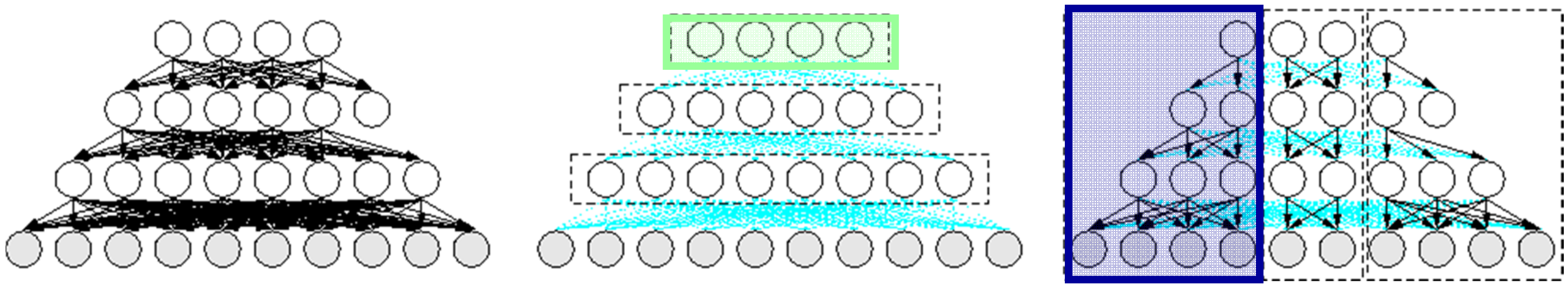


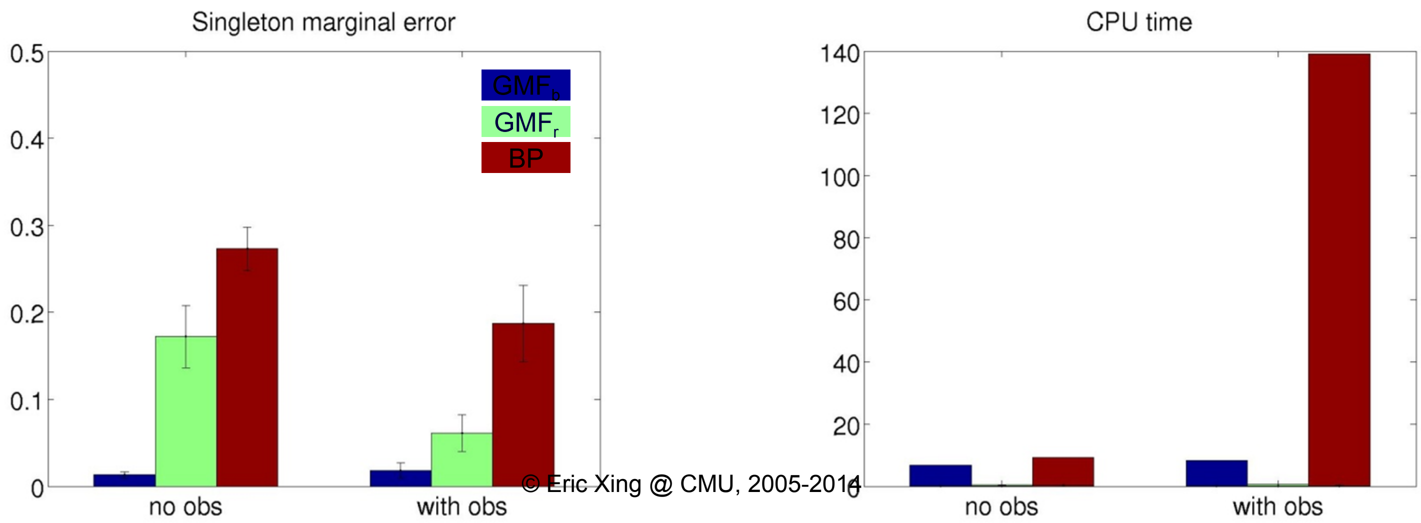


Attractive coupling: positively weighted

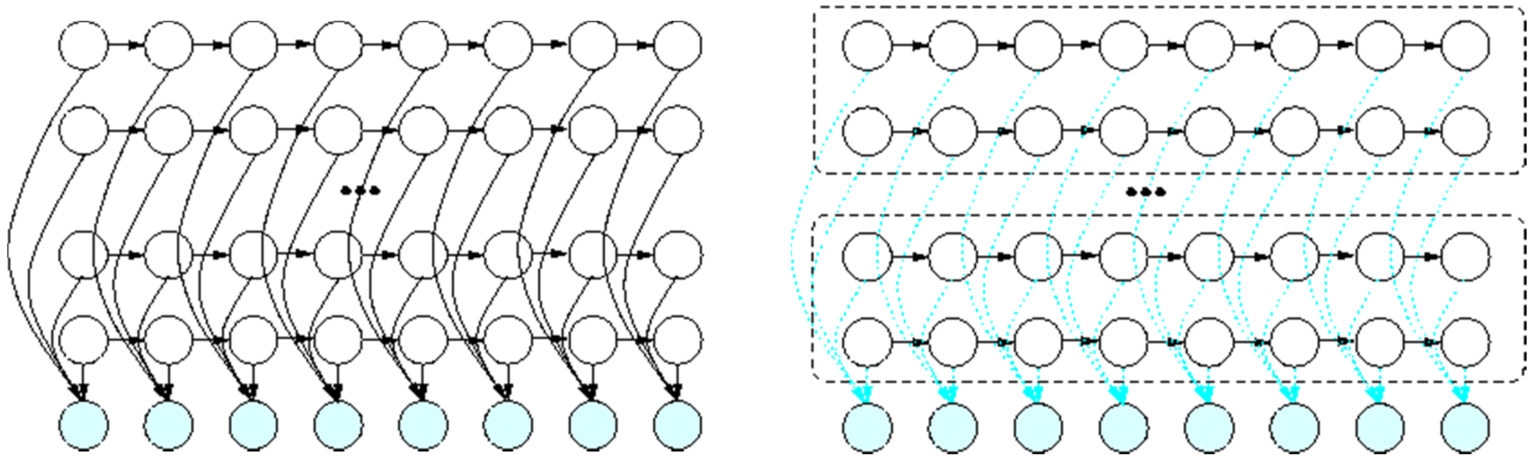
Repulsive coupling: negatively weighted

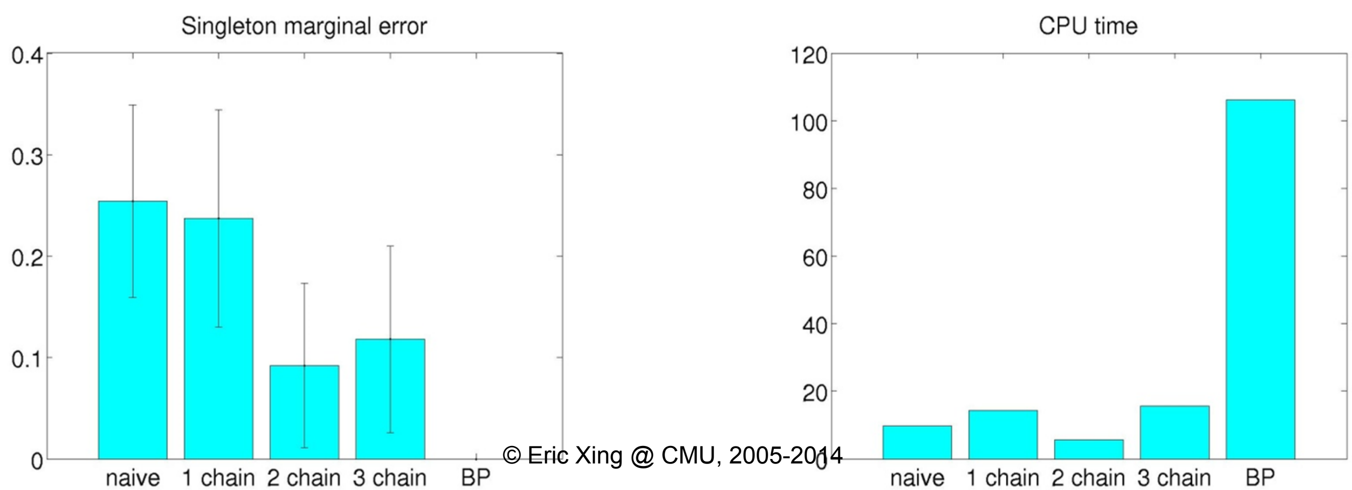
Example 2: Sigmoid belief network



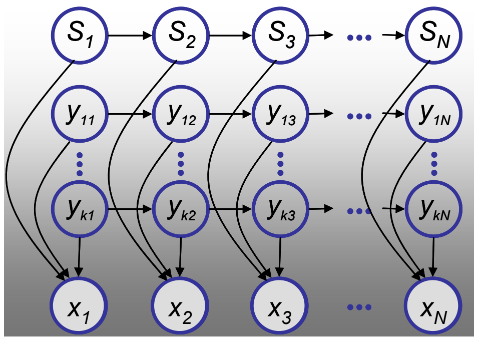


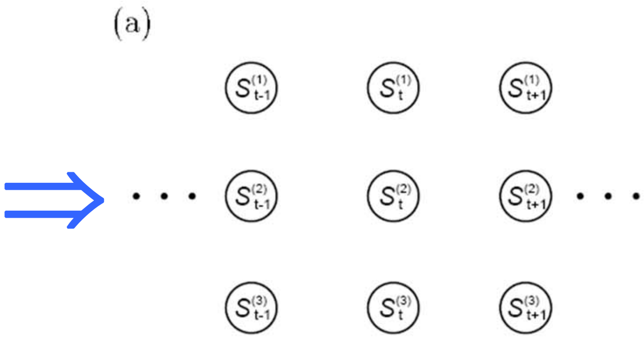
Example 3: Factorial HMM

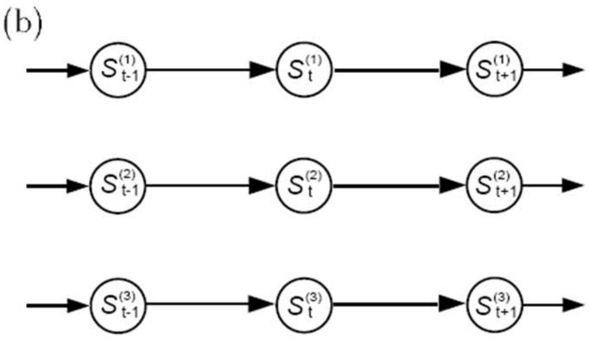




Automatic Variational Inference







fHMM **Mean field approx.** **Structured variational approx.**

- Currently for each new model we have to
  - derive the variational update equations
  - write application-specific code to find the solution

- Each can be time consuming and error prone

- Can we build a general-purpose inference engine which automates these procedures?

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 …

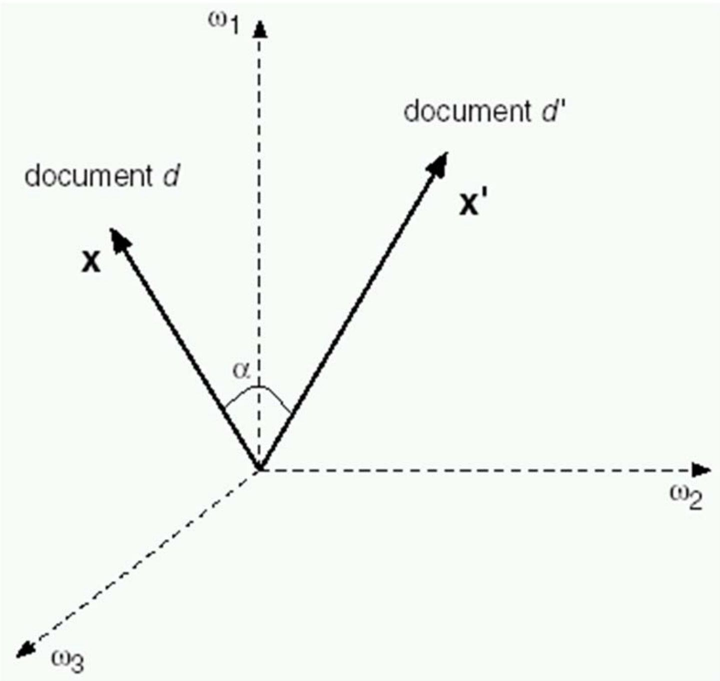
How to get started?

- **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

⇒

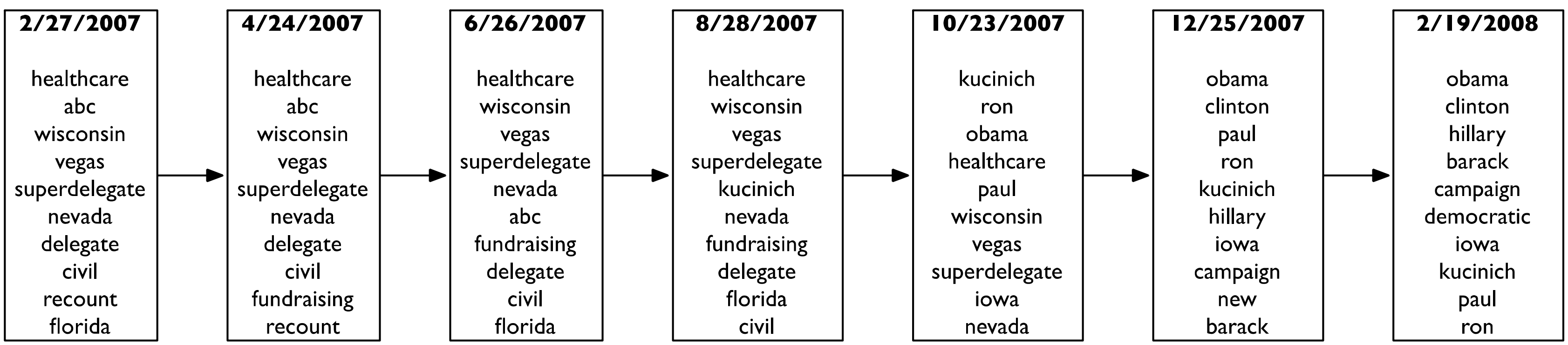


- Compare similarity
- Classify contents
- Cluster/group/categorizing
- Distill semantics and perspectives
- ..

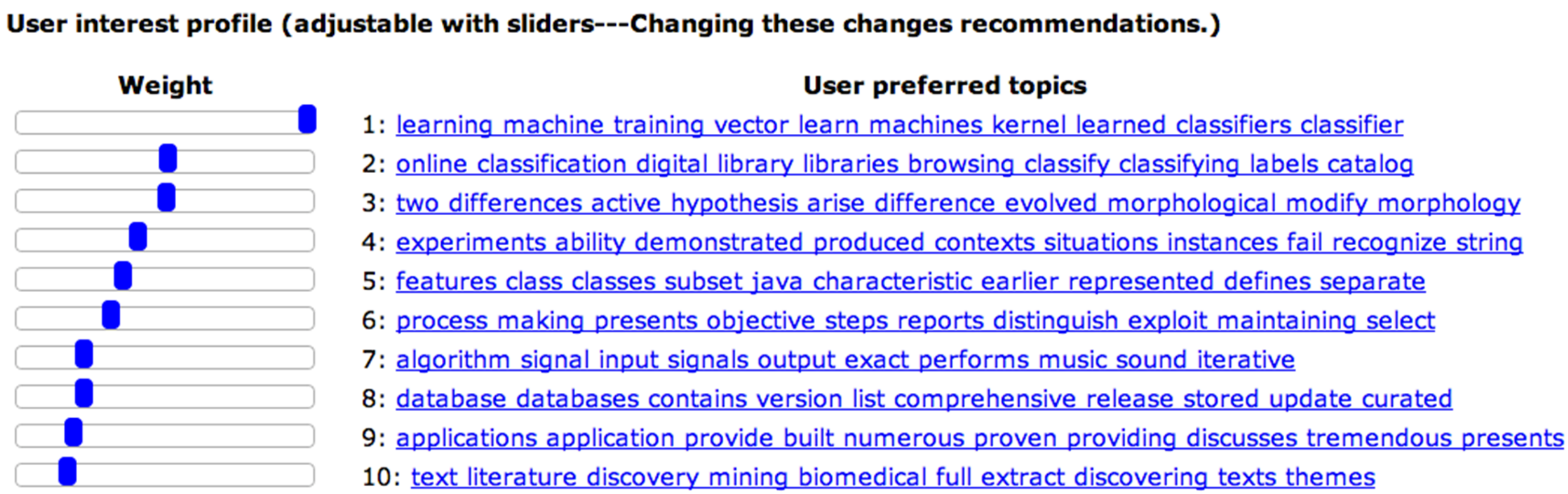
Summarizing the data using topics

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



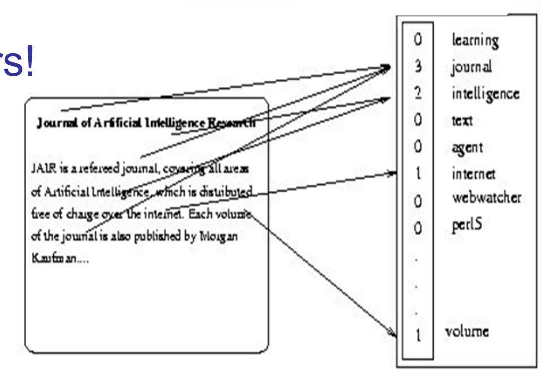
http://cogito-demos.ml.cmu.edu/cgi-bin/recommendation.cgi

Representation:

- Data: **Bag of Words Representation**

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 ?

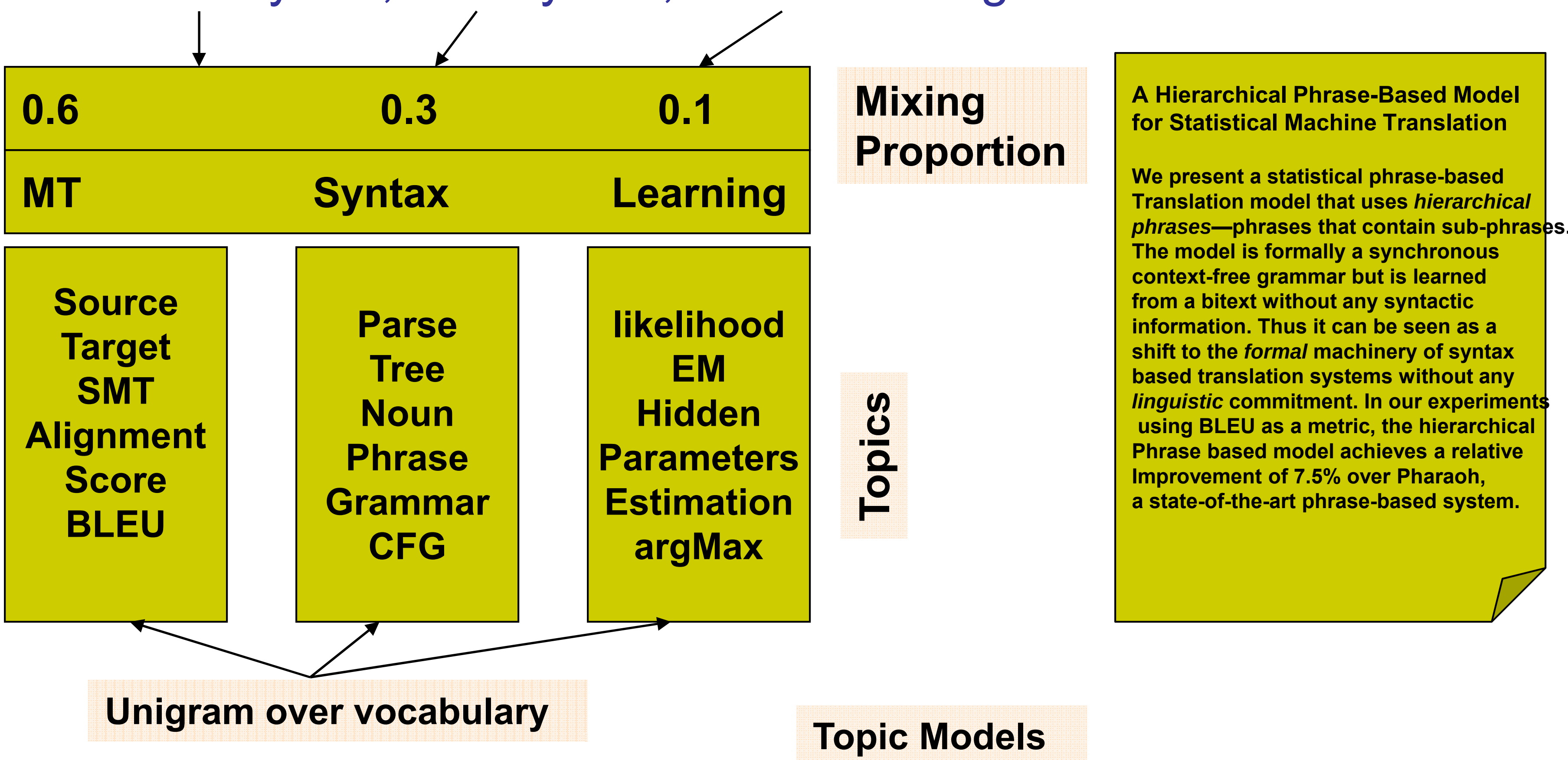
- Each document is a vector in the word space
- Ignore the order of words in a document. Only count matters!



- A high-dimensional and sparse representation ($|V| \gg D$)
  - Not efficient text processing tasks, e.g., search, document classification, or similarity measure
  - Not effective for browsing

How to Model Semantic?

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



Why this is Useful?

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

0.6	0.3	0.1
MT	Syntax	Learning

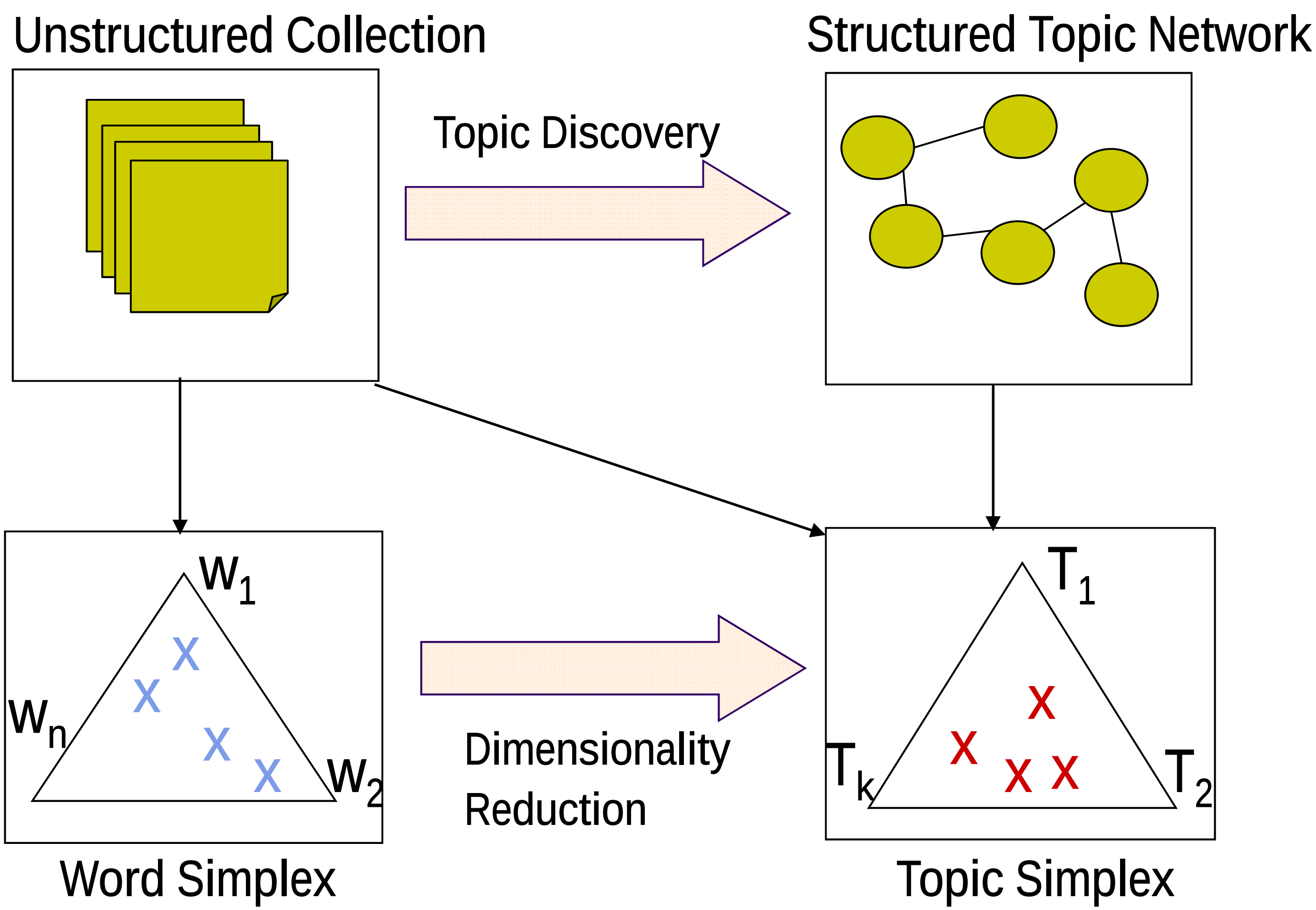
Mixing Proportion

A Hierarchical Phrase-Based Model for Statistical Machine Translation

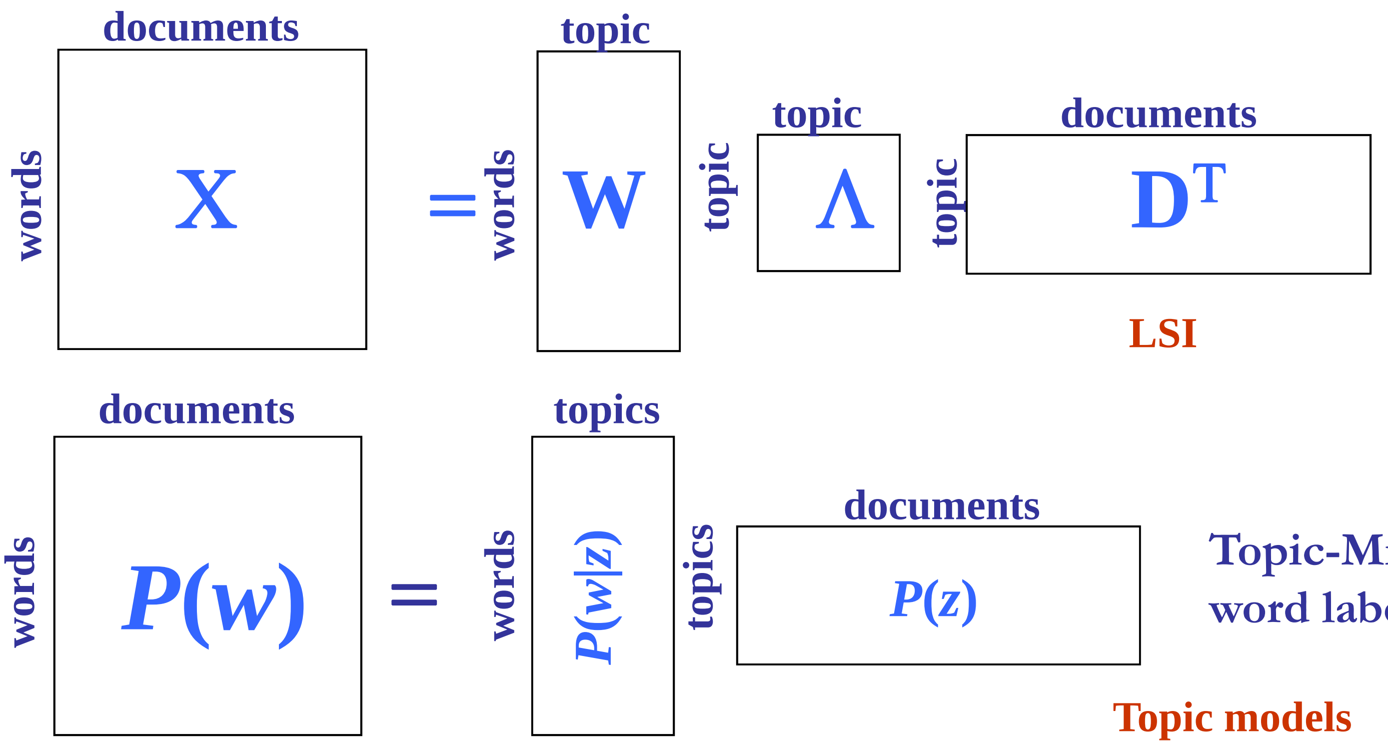
We present a statistical phrase-based Translation model that uses *hierarchical phrases*—phrases that contain sub-phrases. The model is formally a synchronous context-free grammar but is learned from a bitext without any syntactic information. Thus it can be seen as a shift to the *formal* machinery 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.

- **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)



$$\vec{x} = W'\vec{d}$$

Topic-Mixing is via repeated word labeling

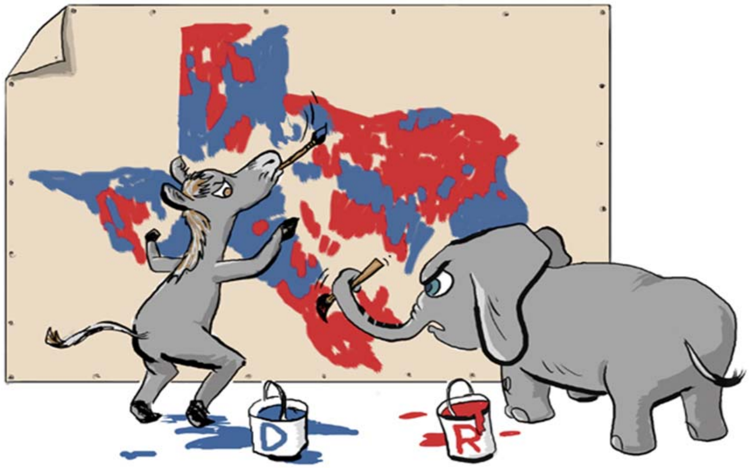
Words in Contexts

- “ It was a nice **shot**. ”

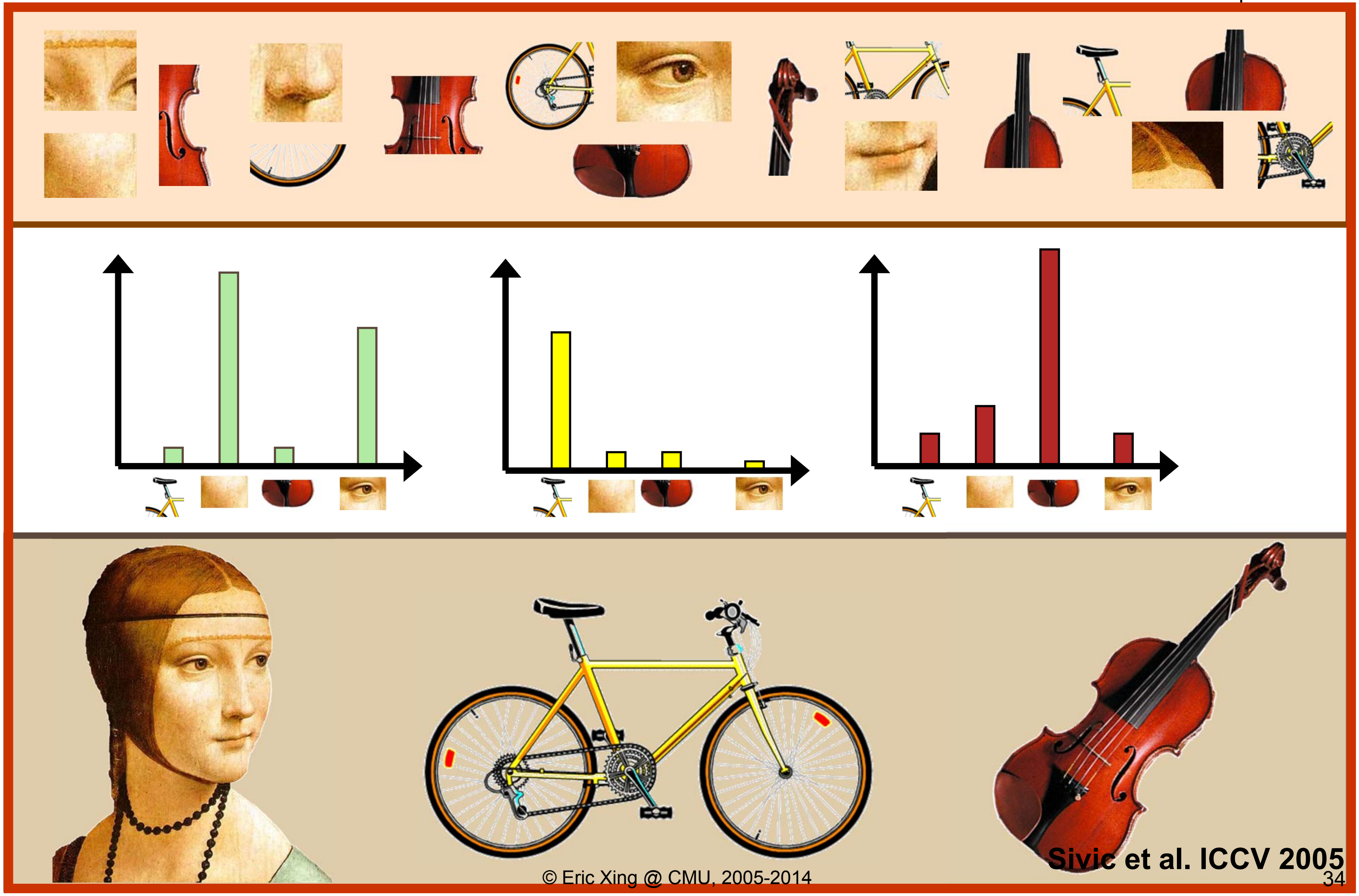


Words in Contexts (con'd)

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



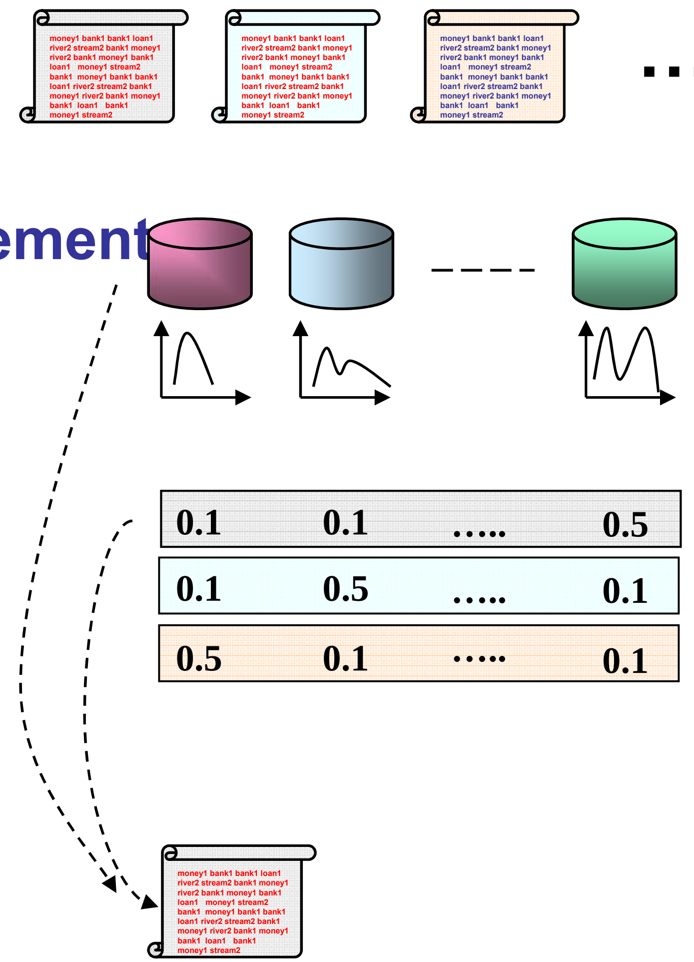
"Words" in Contexts (con'd)



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



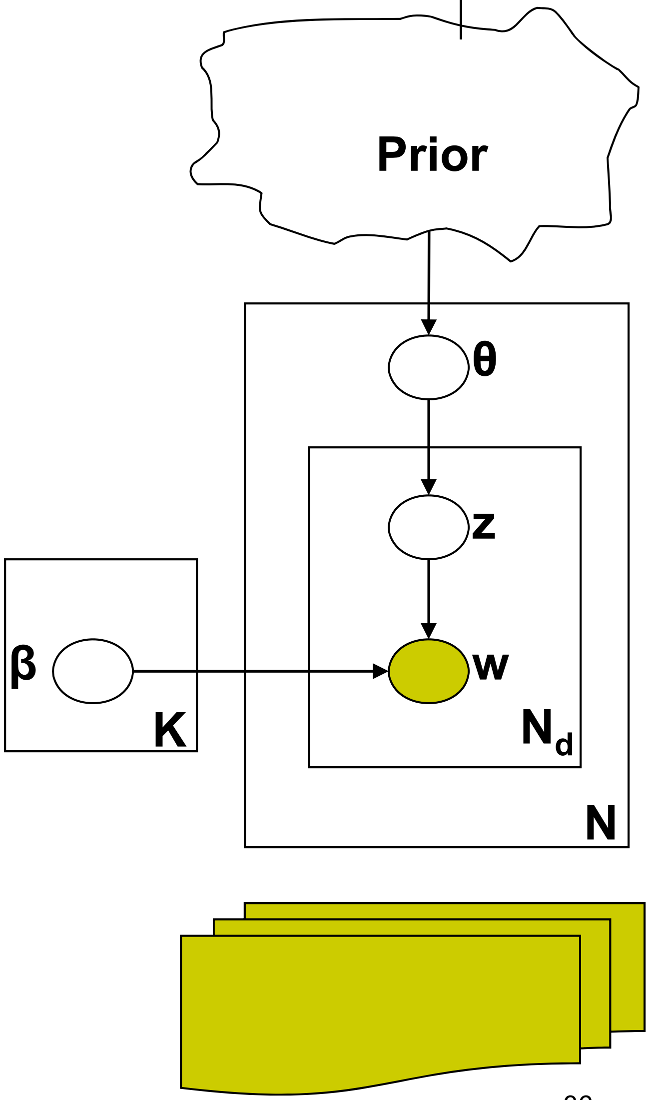
Topic Models

Generating a document

– *Draw* θ from the prior

For each word n

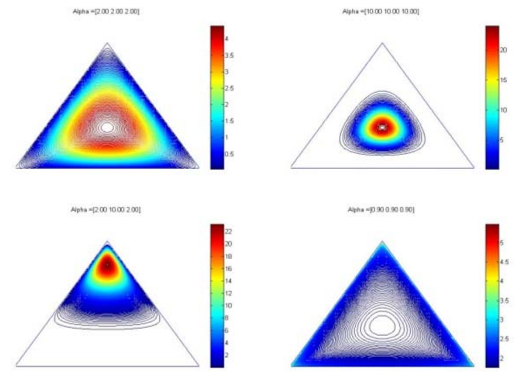
- Draw z_n from $multinomial(\theta)$
- Draw $w_n \mid z_n, \{\beta_{1:k}\}$ from $multinomial(\beta_{z_n})$



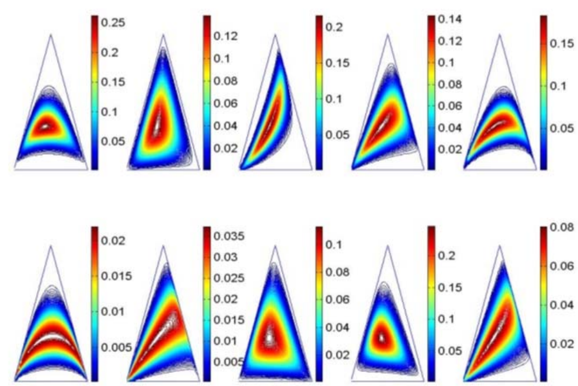
Which prior to use?

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



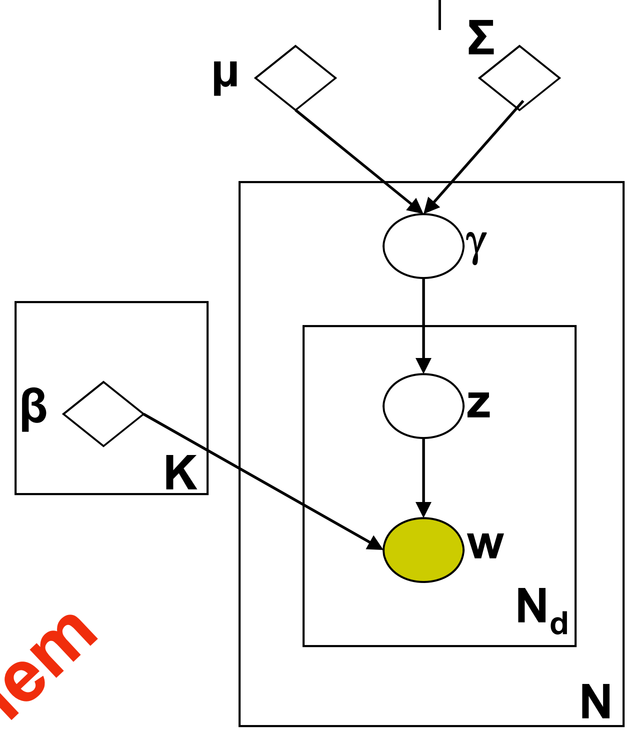
Generative Semantic of LoNTAM

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 $multinomial(\beta_{z_n})$



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

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

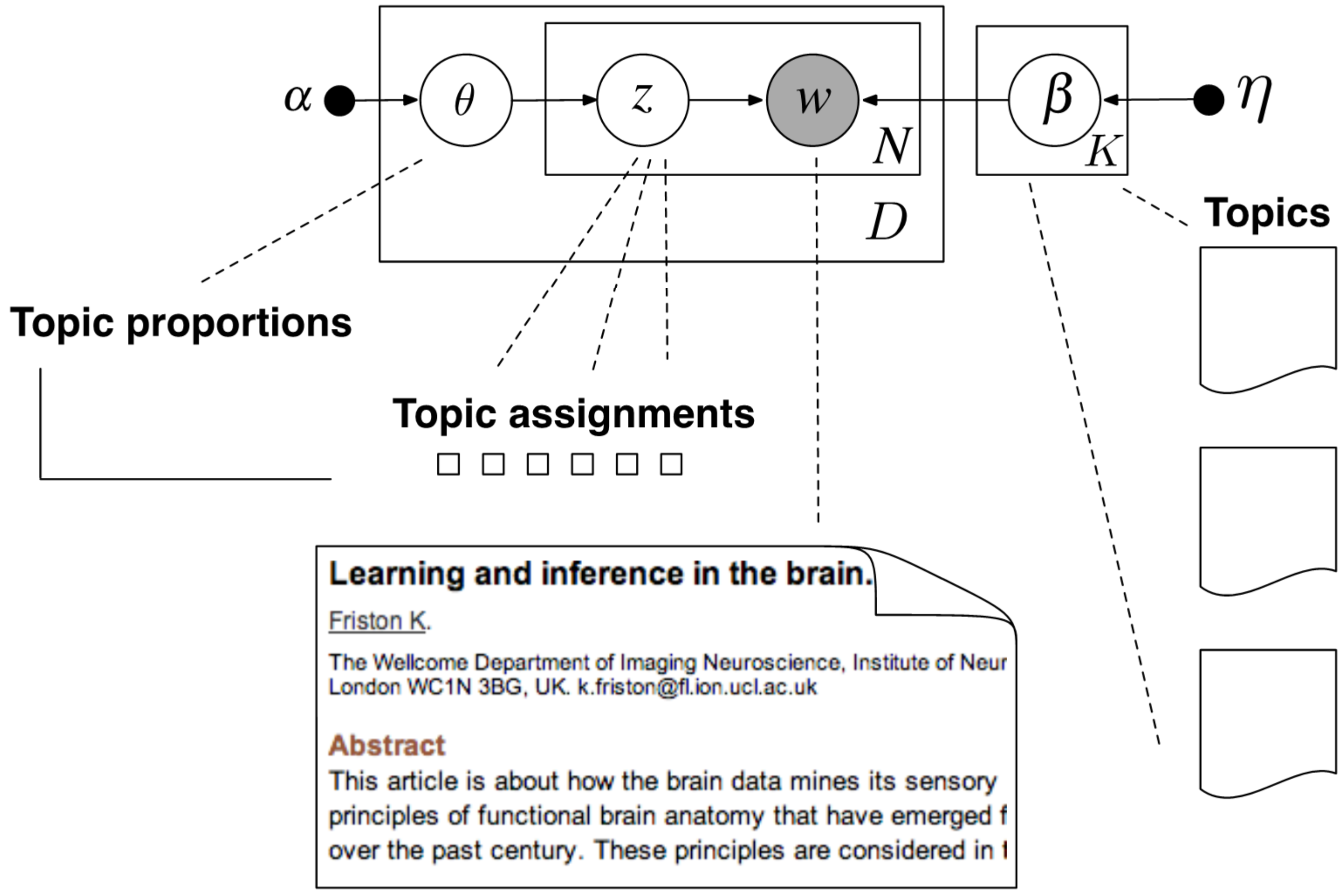
$$\theta_i = \exp\left\{\gamma_i - \log\left(1 + \sum_{i=1}^{K-1} e^{\gamma_i}\right)\right\}$$

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

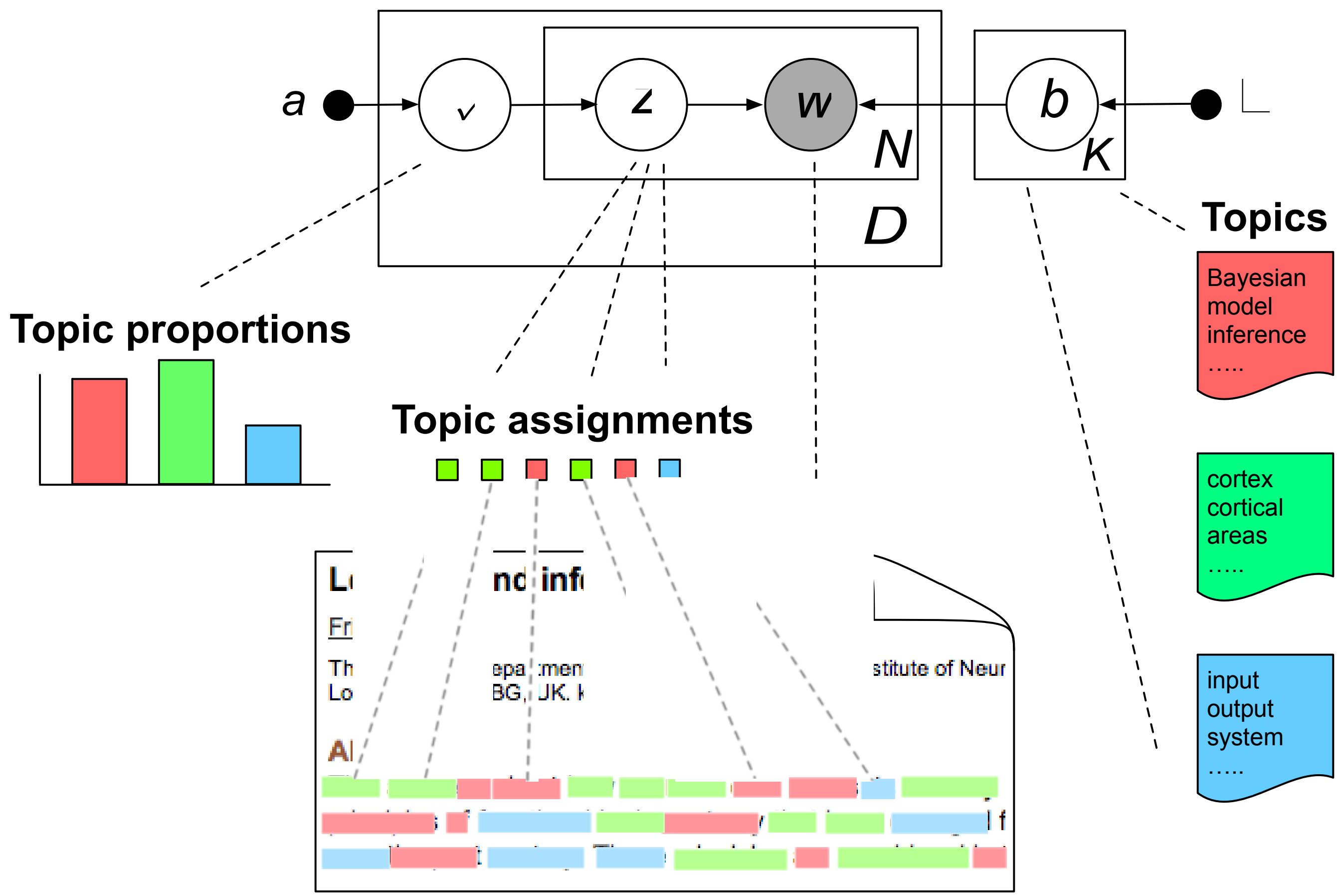
Problem

- **Log Partition Function**
- **Normalization Constant**

Posterior inference

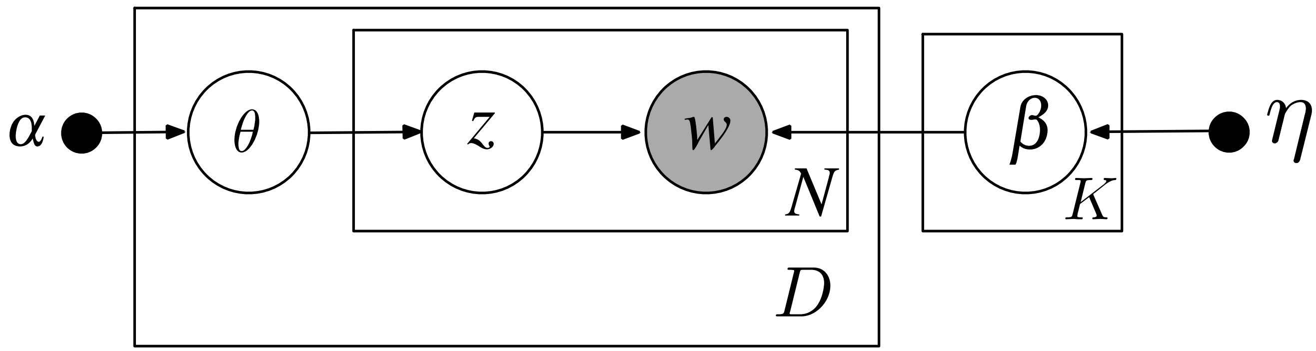


Posterior inference results



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 2^{nd}-order Taylor approximation (Xing)
- Markov Chain Monte Carlo
  - Gibbs sampling (Griffiths et al)

Mean-field assumption

- 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.

Update each marginals

- Update

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

- In LDA,

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

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

- We obtain

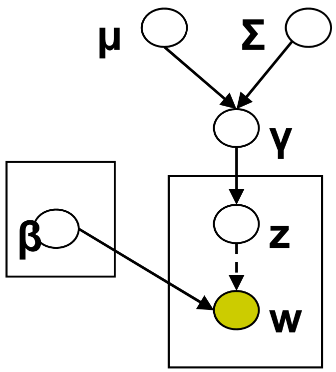
$$q(\theta_d) \propto \exp\left\{\sum_{k=1}^{K}\left(\sum_{n=1}^{N} q(z_{dn} = k) + \alpha_k - 1\right)\log\theta_{dk}\right\}$$

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

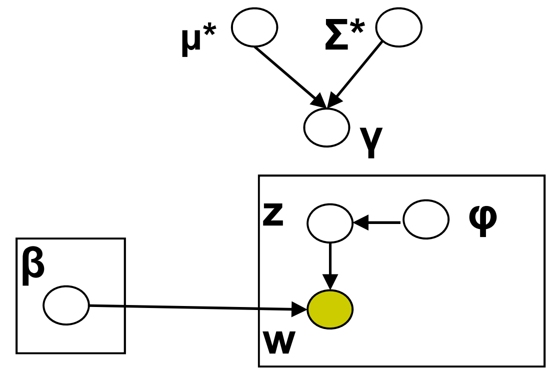
Coordinate ascent algorithm for LDA

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

Choice of q() does matter



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



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

Log Partition Function

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

Σ* is full matrix

Multivariate Quadratic Approx.

Closed Form Solution for μ*, Σ*

Ahmed&Xing

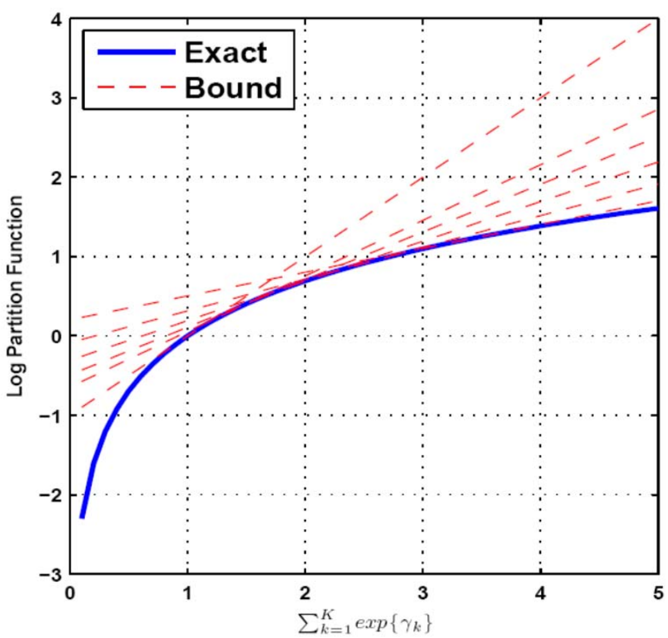
Σ* is assumed to be diagonal

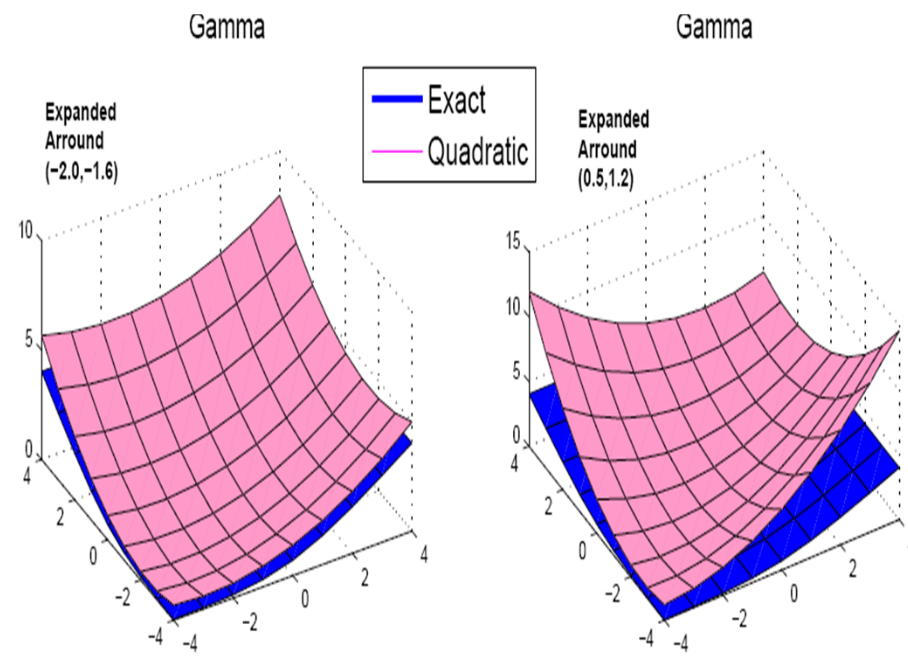
Tangent Approx.

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

Blei&Lafferty

Tangent Approximation





How to evaluate?

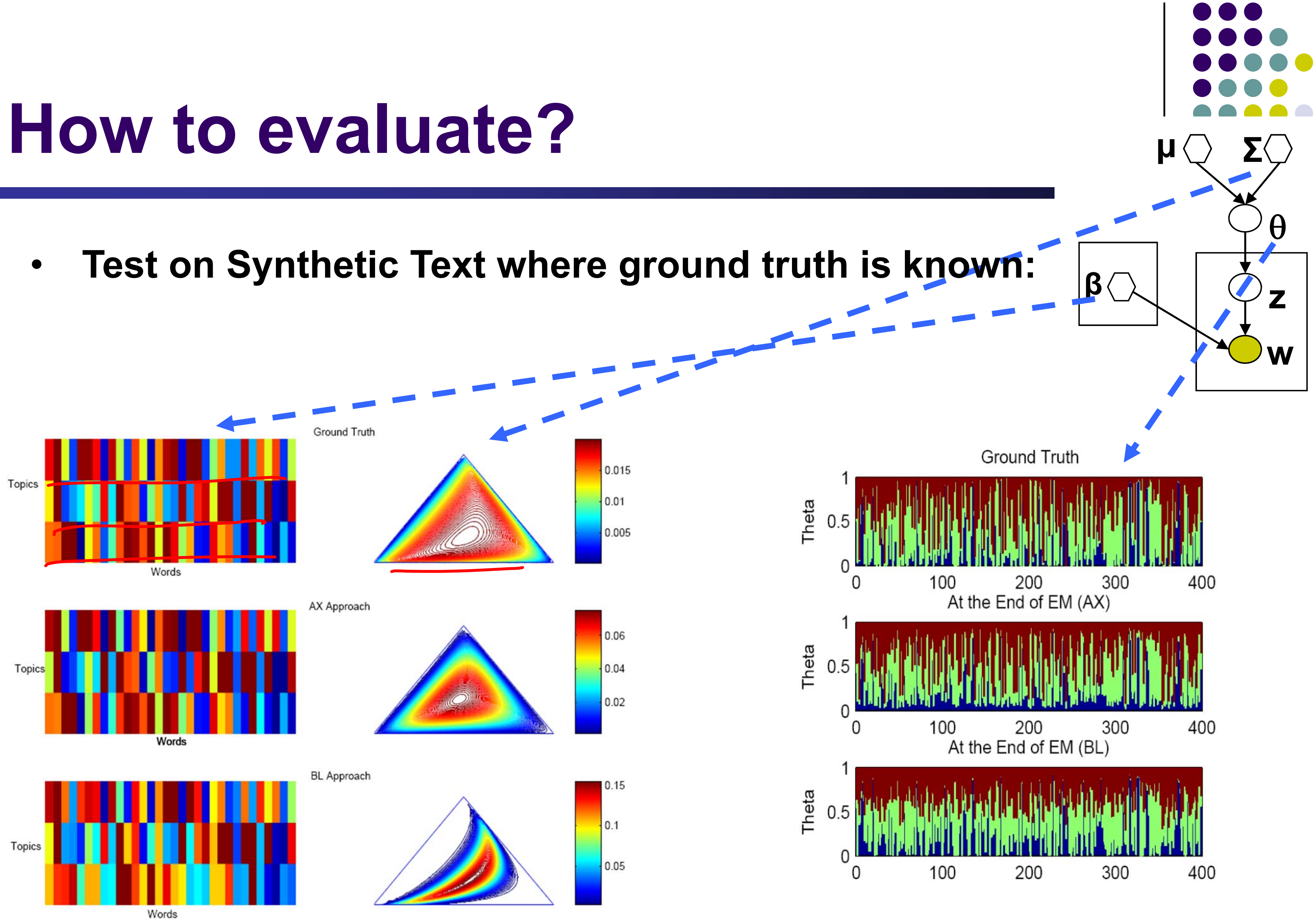
- Empirical Visualization: e.g., topic discovery on New York Times

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?

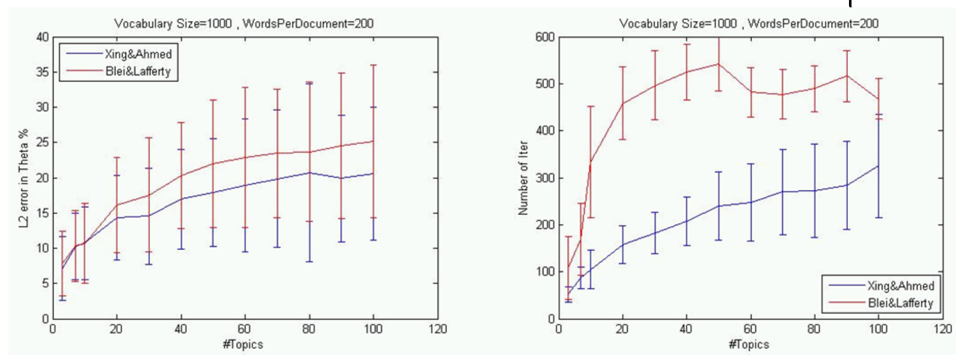
- **Test on Synthetic Text where ground truth is known:**



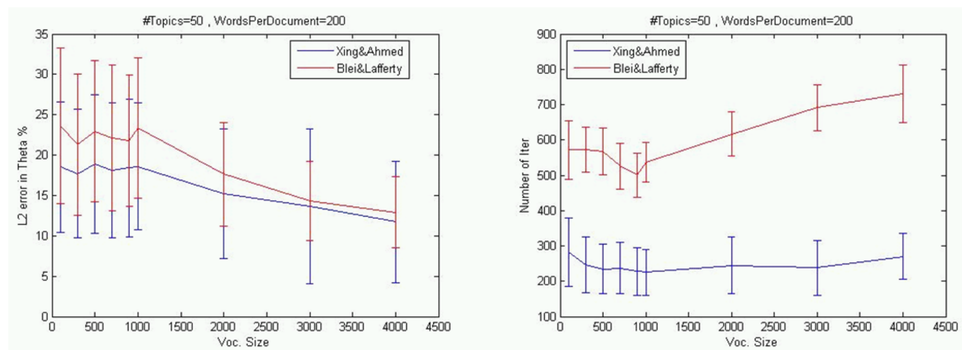
Comparison: accuracy and speed

L2 error in topic vector est. and # of iterations

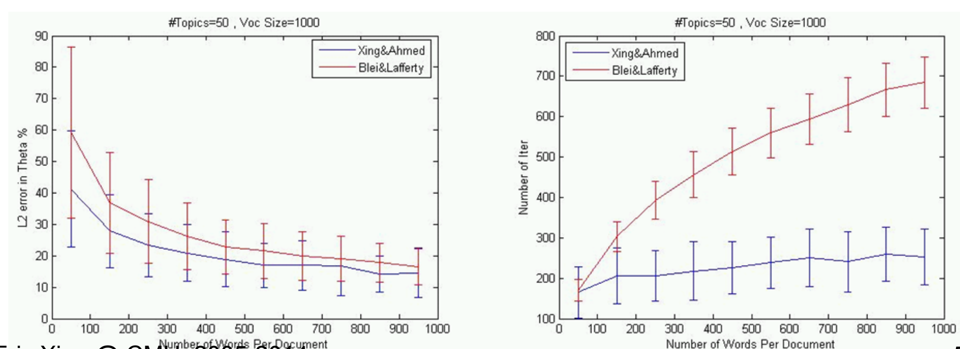
- Varying Num. of Topics



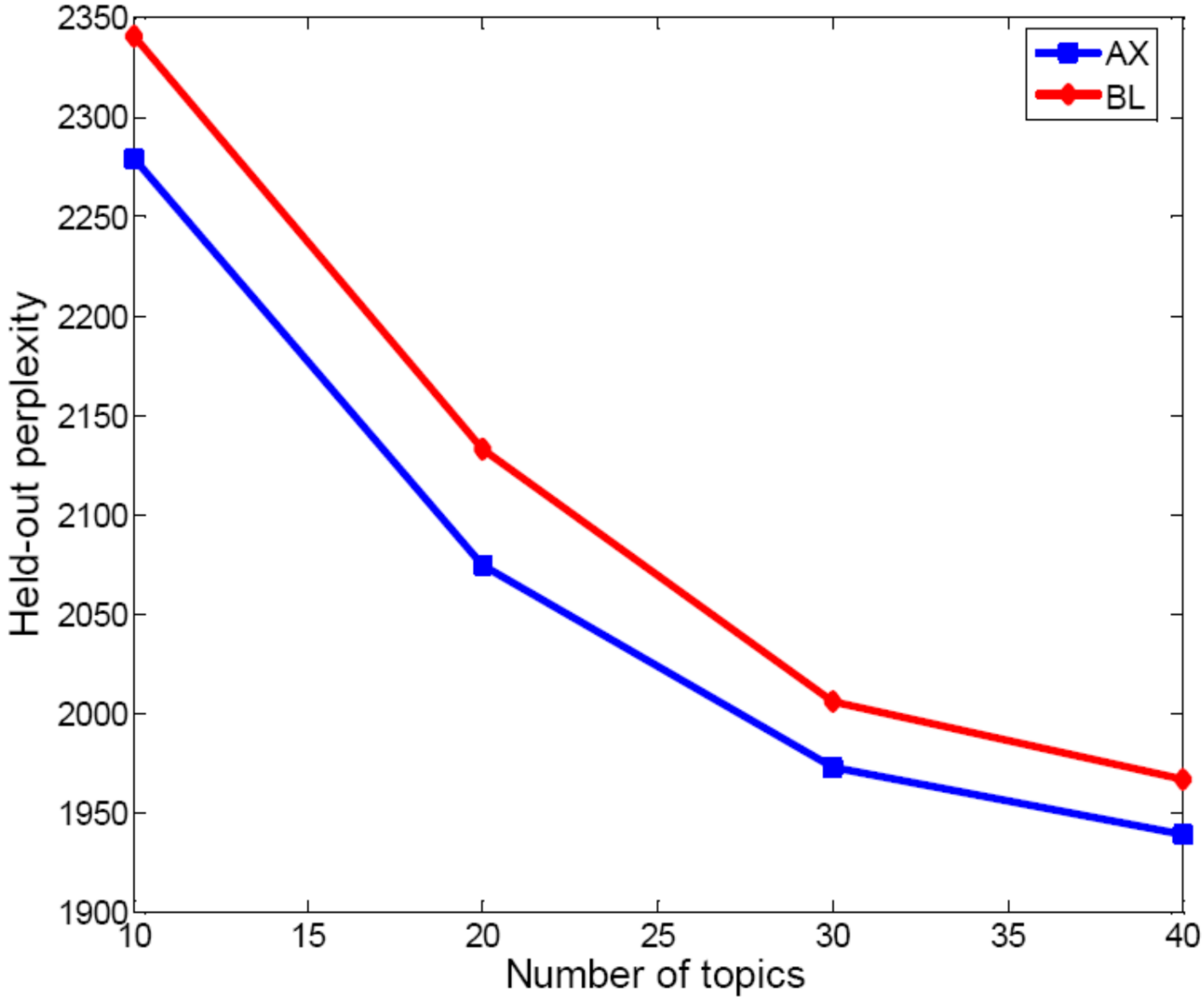
- Varying Voc. Size



- 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

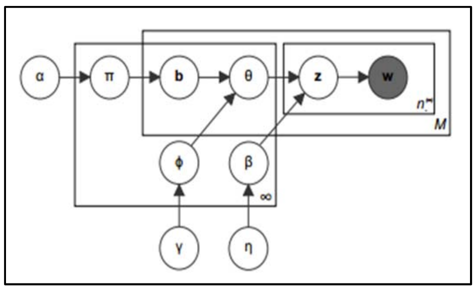
Category	Doc	BL	AX
Genetics	21	61.9	61.9
Biochemistry	86	65.1	77.9
Immunology	24	70.8	66.6
Biophysics	15	53.3	66.6
Total	146	64.3	72.6

- Notable Difference
- Examine the low dimensional representations below

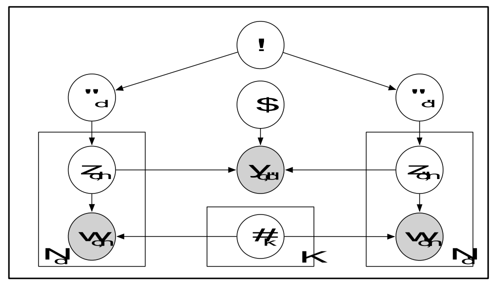
What makes topic models useful --- The Zoo of Topic Models!

- It is a building block of many models.

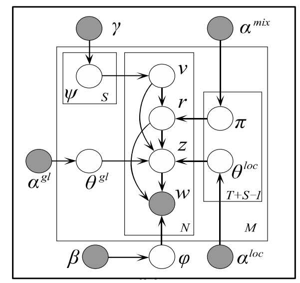
Williamson et al. 2010

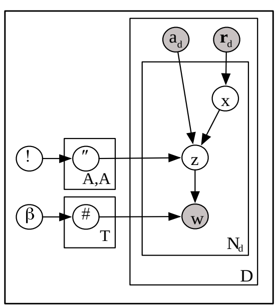


Chang & Blei, 2009

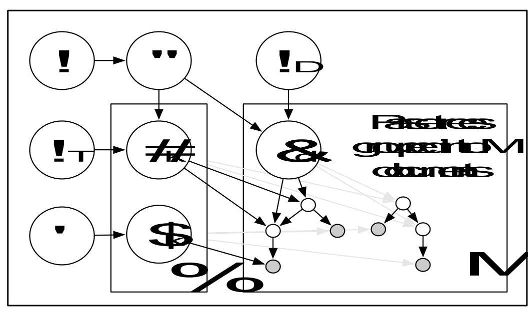


Titov & McDonald, 2008

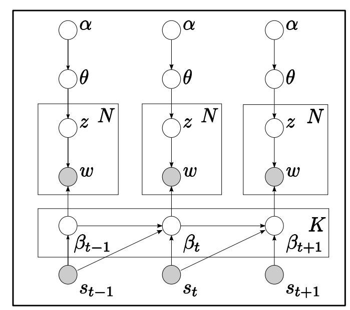




McCallum et al. 2007



Boyd-Graber & Blei, 2008



Wang & Blei, 2008

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

Summary on VI

- Variational methods in general turn inference into an optimization problem via exponential families and convex duality

- The exact variational principle is intractable to solve; there are two distinct components for approximations:
  - Either inner or outer bound to the marginal polytope
  - Various approximation to the entropy function

- Mean field: non-convex inner bound and exact form of entropy
- BP: polyhedral outer bound and non-convex Bethe approximation
- Kikuchi and variants: tighter polyhedral outer bounds and better entropy approximations (Yedidia et. al. 2002)