

A Framework for Incorporating General Domain Knowledge into Latent Dirichlet Allocation using First-Order Logic

David Andrzejewski¹ Xiaojin Zhu²
Mark Craven^{3,2} Benjamin Recht²

¹Center for Applied Scientific Computing
Lawrence Livermore National Laboratory (USA)

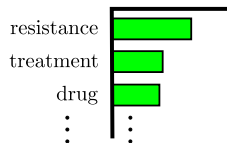
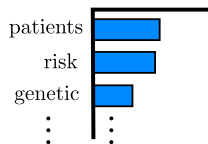
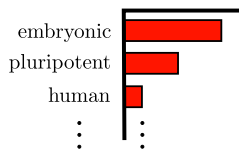
²Department of Computer Sciences
³Department of Biostatistics
and Medical Informatics
University of Wisconsin–Madison (USA)



Topic modeling with Latent Dirichlet Allocation (LDA)

Blei et al, JMLR 2003

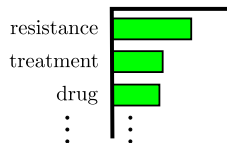
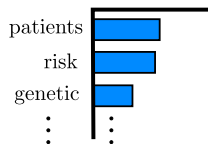
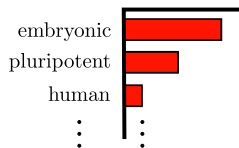
Topics ϕ



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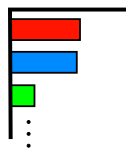
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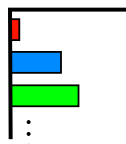


Document-topic weights θ

Human embryonic stem cell research may benefit patients with genetic risk factors...



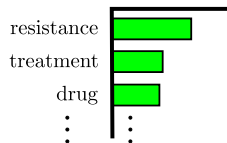
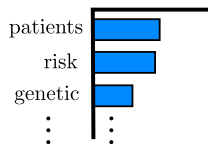
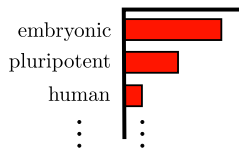
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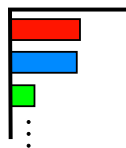
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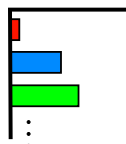


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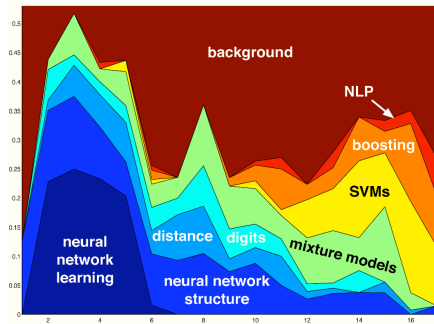
Observed $\mathbf{w}$
Latent $\mathbf{z}$

Patients | at | risk | for | drug-resistant



Topic modeling applications

- Research trends (Wang & McCallum, 2006)
- Info retrieval (UMass) (also KDD 2011!)
- Author/document profiling
 - Scientific impact/influence (Gerrish & Blei, 2009)
 - Match papers to reviewers (Mimno & McCallum, 2007)



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bayesian
View all topics sorted by [citations](#) | [topic diversity](#) | [H-Index](#)

Topic Terms

Words	Phrases
0.0607 bayesian	0.0576 monte carlo
0.0330 model	0.0079 monte carlo simulation
0.0226 inference	0.0055 monte carlo simulations

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Extend the model? Add domain knowledge

- “These words do (not) belong in the same topic”
- “I want a topic about X ”
- “This topic is incompatible with this document”
- “These topics are incompatible - should not co-occur”

First-Order Latent Dirichlet Allocation (Fold-all)

- Weighted knowledge base (KB) of first-order logic (FOL) rules (Markov Logic Networks, Richardson and Domingos 2006)
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Representing LDA with logical predicates

	Value	Logical Predicate	Description
LDA	$z_i = t$	$Z(i, t)$	Latent topic
	$w_i = v$	$W(i, v)$	Observed word
	$d_i = j$	$D(i, j)$	Observed document

Unified way to capture metadata / annotations

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Encoding domain knowledge in First-Order Logic

- CNF Knowledge Base $KB = \{(\lambda_1, \psi_1), \dots, (\lambda_L, \psi_L)\}$
 - Rule ψ_k
 - Weight $\lambda_k > 0$ (“strength” of rule)

Example KB

Rule	λ_k	$\forall$	ψ_k
Seed	5	i	$w(i, \text{embryo}) \Rightarrow z(i, 3)$
Doc label	500	i, j	$D(i, j) \wedge \text{HasLabel}(j, +) \Rightarrow \neg z(i, 3)$

Can specify “contradictory” domain knowledge!

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$$\lambda_k \quad \forall \quad \psi_k$$
$$5 \quad i, j, t \quad \mathbb{W}(i, \text{neural}) \wedge \mathbb{W}(j, \text{disorder}) \Rightarrow \neg \mathbb{Z}(i, t) \vee \neg \mathbb{Z}(j, t)$$

- $G(\psi_{CL})$ = set of ground formulas g for **EVERY** (i, j, t)
 $i \in \{1, 2, \dots, N\}$
 $j \in \{1, 2, \dots, N\}$
 $t \in \{1, 2, \dots, T\}$
- $1_g(\mathbf{z}) = \begin{cases} 1 & \text{if } g \text{ true under } \mathbf{z} \\ 0 & \text{else} \end{cases}$
- Each $g \in G(\psi_{CL}) \rightarrow \lambda 1_g(\mathbf{z})$ term (as in MLN)
- **Combinatorial explosion!**

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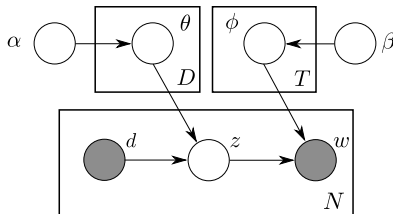
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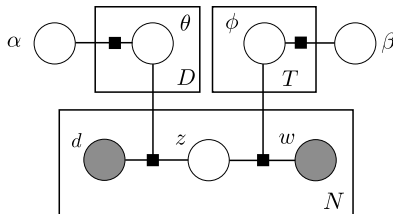
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LDA graphical model



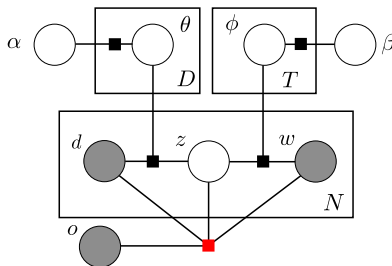
$$P \propto \left(\prod_t^T p(\phi_t | \beta) \right) \left(\prod_j^D p(\theta_j | \alpha) \right) \left(\prod_i^N \phi_{z_i}(w_i) \theta_{d_i}(z_i) \right)$$

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LDA graphical model $\rightarrow$ Fold-all



$$P \propto \left(\prod_t^T p(\phi_t | \beta) \right) \left(\prod_j^D p(\theta_j | \alpha) \right) \left(\prod_i^N \phi_{z_i}(w_i) \theta_{d_i}(z_i) \right) \\ \times \exp \left[\sum_k^L \sum_{g \in G(\psi_k)} \lambda_k \mathbb{1}_g(\mathbf{z}, \mathbf{w}, \mathbf{d}, \mathbf{o}) \right]$$

MAP inference - $Q(\mathbf{z}, \phi, \theta)$

Alternating Optimization with Mirror Descent

For each step

1 $(\phi, \theta) \leftarrow \underset{\phi, \theta}{\operatorname{argmax}} Q(\mathbf{z}, \phi, \theta)$

$\mathbf{z}$ fixed

2 $\mathbf{z} \leftarrow \underset{\mathbf{z}}{\operatorname{argmax}} Q(\mathbf{z}, \phi, \theta)$

(ϕ, θ) fixed

- $\mathbf{z} \setminus \mathbf{z}_{KB} \leftarrow \operatorname{argmax}$ with respect to (ϕ, θ)
- $\mathbf{z}_{KB} \leftarrow$ mirror descent

TRIVIAL
HARD

Scalable approach to optimize $\mathbf{z}_{KB}$

- 1 Relax discrete problem to continuous
- 2 Optimize relaxed problem with stochastic gradient descent
- 3 Round relaxed $\mathbf{z}$ to recover final assignment

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1 Relax discrete problem to continuous

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3 Round relaxed $\mathbf{z}$ to recover final assignment

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Alternating Optimization with Mirror Descent

For each step

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$\mathbf{z}$ fixed

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- $\mathbf{z} \setminus \mathbf{z}_{KB} \leftarrow \operatorname{argmax}$ with respect to (ϕ, θ)

TRIVIAL
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$$\operatorname{argmax}_{\mathbf{z}} \sum_i^N \sum_t^T z_{it} \log \phi_t(w_i) \theta_{d_i}(t) + \sum_k^L \sum_{g \in G(\psi_k)} \lambda_k \mathbb{1}_g(\mathbf{z})$$

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- $z_i = t$
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- Example datasets and *KBs* (see paper)
- *k*-fold cross-validation
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Synth	9.86	11.13	-2.18	-1.73	1.2×10^5
Comp	2.40	2.45	1.19	—	6.3×10^3
Con	2.51	2.56	1.09	—	2.9×10^3
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Biological concept expansion

Human Development Genes (HDG)

Given “seed” terms for each concept

Do discover other related terms

Concept	Provided terms
Neural	neur dendro(cyte), glia, synapse, neural crest
Embryo	human embryonic stem cell, inner cell mass, pluripotent
Blood	hematopoietic, blood, endothel(ium)
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Seed and n -gram rules

Neural $\rightarrow$ “synapse” $\rightarrow$ Topic 0

$$\bar{w}(i, \text{synapse}) \Rightarrow z(i, 0)$$

Embryo $\rightarrow$ “inner cell mass” $\rightarrow$ Topic 1

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Sentence rules

Sentence inclusion

- New *development* Topic 6
{differentiation, maturation, develops, formation, differentiates}
- Development Topic 6 allows each seed Topic t in sentence

$$\text{Sentence}(i, i_1, \dots, i_{S_k}) \wedge \neg z(i_1, 6) \wedge \dots \wedge \neg z(i_{S_k}, 6) \Rightarrow \neg z(i, 0)$$

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- New *disease* Topic 7
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Accuracy at Top 50 threshold

(means over 10 randomized runs)

	Fold-all <i>KBs</i>				LDA
	ALL	INCL	EXCL	SEED	
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Blood	0.46	0.47	0.40	0.39	0.13
Gast.	0.18	0.18	0.16	0.16	0.00
Cardiac	0.36	0.37	0.34	0.35	0.08
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Novel terms discovered for *neural*

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- Fold-all topic modeling with domain knowledge
 - user-specified constraints
 - side information
- Scalable inference
- Experimental results
 - Logic *KBs* generalize to unseen documents
 - Inference scales to realistic datasets and *KBs*
 - Topics reflect domain knowledge in interesting ways

Acknowledgements

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 - AFOSR FA9550-09-1-0313
 - NIH/NLM R01 LM07050
- HDG experiments: Ron Stewart (Thomson Lab, UW–Madison)

Source code

<https://github.com/davidandrzej/LogicLDA>

Find most probable $(\mathbf{z}, \phi, \theta)$

$$Q(\mathbf{z}, \phi, \theta) = \sum_t^T \log p(\phi_t | \beta) + \sum_j^D \log p(\theta_j | \alpha) \\ + \sum_i^N \log \phi_{z_i}(\mathbf{w}_i) \theta_{d_i}(z_i) + \sum_k^L \sum_{g \in G(\psi_k)} \lambda_k \mathbb{1}_g(\mathbf{z}, \mathbf{w}, \mathbf{d}, \mathbf{o})$$

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- LDA terms
- Logic terms

Find most probable $(\mathbf{z}, \phi, \theta)$

$$Q(\mathbf{z}, \phi, \theta) = \sum_t^T \log p(\phi_t | \beta) + \sum_j^D \log p(\theta_j | \alpha) \\ + \sum_i^N \log \phi_{z_i}(\mathbf{w}_i) \theta_{d_i}(z_i) + \sum_k^L \sum_{g \in G(\psi_k)} \lambda_k \mathbb{1}_g(\mathbf{z}, \mathbf{w}, \mathbf{d}, \mathbf{o})$$

- LDA terms
- Logic terms

Ignore trivial rule groundings

Shavlik & Natarajan, 2009

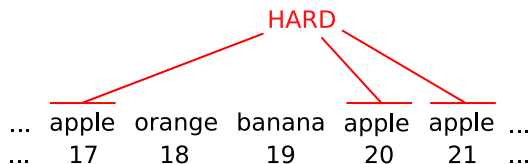
$$\frac{\lambda_k \quad \forall \quad \psi_k}{5 \quad i \quad w(i, \text{apple}) \Rightarrow z(i, 3)}$$

...	apple	orange	banana	apple	apple	...
...	17	18	19	20	21	...

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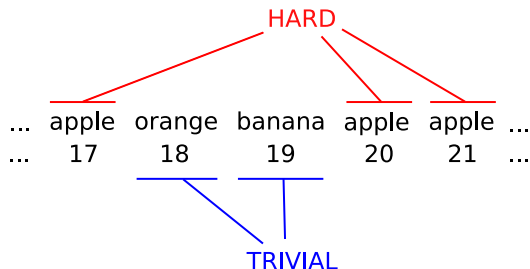
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Represent $\mathbb{1}$ as a polynomial

$g = z(i, 1) \vee \neg z(j, 2)$, and $t \in \{1, 2, 3\}$

1 Take complement $\neg g$

$$\neg z(i, 1) \wedge z(j, 2)$$

2 Remove negations $(\neg g)_+$

$$(z(i, 2) \vee z(i, 3)) \wedge z(j, 2)$$

3 Numeric $z_{it} \in \{0, 1\}$

$$(z_{i2} + z_{i3})z_{j2}$$

4 Polynomial $\mathbb{1}_g(\mathbf{z})$

$$1 - (z_{i2} + z_{i3})z_{j2}$$

5 Relax discrete z_{it}

$$z_{it} \in \{0, 1\} \rightarrow z_{it} \in [0, 1]$$

$$\mathbb{1}_g(\mathbf{z}) = 1 - \prod_{g_i \neq \emptyset} \left(\sum_{z(i,t) \in (\neg g_i)_+} z_{it} \right)$$

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|---|---------------------------------------|---|
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Standard LDA: *Neural* concept

Do standard LDA, then find topics containing seed terms in Top 50

brain system nervous neurons neuronal central development 's **neural**
human gene disease function cortex spinal disorders developing motor
cerebral **glial** peripheral cortical cord disorder astrocytes nerve
neurological regions suggest schizophrenia including syndrome
neurodegenerative mental involved retardation behavior cerebellum
migration behavioral abnormal cerebellar found precursor results
amyloid hippocampus sclerosis neurotrophic present

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Fold-all can encode existing LDA variants

Example: Hidden Topic Markov Model (HTMM) - Gruber et al, 2007

- Each sentence uses only *one* topic
- Topic transitions possible between sentences with probability ϵ

FOL encoding of HTMM

$$\frac{\lambda_k \quad \forall \quad \psi_k}{\infty \quad i, j, s, t \quad S(i, s) \wedge S(j, s) \wedge Z(i, t) \Rightarrow Z(j, t)}$$

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FOL encoding of HTMM

λ_k	$\forall$	ψ_k
∞	i, j, s, t	$S(i, s) \wedge S(j, s) \wedge Z(i, t) \Rightarrow Z(j, t)$
$-\log \epsilon$	i, s, t	$S(i, s) \wedge \neg S(i+1, s) \wedge Z(i, t) \Rightarrow Z(i+1, t)$