### PSDDs for Tractable Learning in Structured and Unstructured Spaces

#### Guy Van den Broeck



UBC Jun 7, 2017

### References

#### **Probabilistic Sentential Decision Diagrams**

Doga Kisa, Guy Van den Broeck, Arthur Choi and Adnan Darwiche KR, 2014

#### Learning with Massive Logical Constraints

Doga Kisa, Guy Van den Broeck, Arthur Choi and Adnan Darwiche ICML 2014 workshop

#### **Tractable Learning for Structured Probability Spaces**

Arthur Choi, Guy Van den Broeck and Adnan Darwiche IJCAI, 2015

#### **Tractable Learning for Complex Probability Queries**

Jessa Bekker, Jesse Davis, Arthur Choi, Adnan Darwiche, Guy Van den Broeck. NIPS, 2015

#### Learning the Structure of PSDDs

Jessa Bekker, Yitao Liang and Guy Van den Broeck Under review, 2017

#### Towards Compact Interpretable Models: Learning and Shrinking PSDDs

Yitao Liang and Guy Van den Broeck Under review, 2017

# Structured vs. unstructured probability spaces?

### Running Example

#### Courses:

- Logic (L)
- Knowledge Representation (K)
- Probability (P)
- Artificial Intelligence (A)

#### Constraints

- Must take at least one of Probability or Logic.
- Probability is a prerequisite for AI.
- The prerequisites for KR is either AI or Logic.

#### Data

	$\mathbf{L}$	Κ	Р	A	Students
-	0	0	1	0	6
	0	0	1	1	54
	0	1	1	1	10
	1	0	0	0	5
	1	0	1	0	1
	1	0	1	1	0
	1	1	0	0	17
	1	1	1	0	4
	1	1	1	1	3

### **Probability Space**

#### unstructured

L	К	Р	А
0	0	0	0
0	0	0	1
0	0	1	0
0	0	1	1
0	1	0	0
0	1	0	1
0	1	1	0
0	1	1	1
1	0	0	0
1	0	0	1
1	0	1	0
1	0	1	1
1	1	0	0
1	1	0	1
1	1	1	0
1	1	1	1

### **Structured Probability Space**

#### unstructured

L	К	Р	А
0	0	0	0
0	0	0	1
0	0	1	0
0	0	1	1
0	1	0	0
0	1	0	1
0	1	1	0
0	1	1	1
1	0	0	0
1	0	0	1
1	0	1	0
1	0	1	1
1	1	0	0
1	1	0	1
1	1	1	0
1	1	1	1



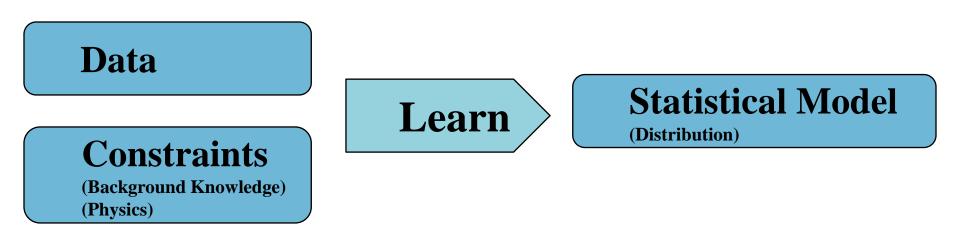
- Must take at least one of Probability or Logic.
- Probability is a prerequisite for AI.
- The prerequisites for KR is either AI or Logic.

#### 7 out of 16 instantiations are impossible

#### structured

L	К	Р	А
0	0	0	0
0	0	0	1
0	0	1	0
0	0	1	1
0	1		0
0	1	0	1
0	1	1	0
0	1	1	1
1	0	0	0
1	0	0	1
1	0	1	0
1	0	1	1
1	1	0	0
1	1	0	1
1	1	1	0
1	1	1	1

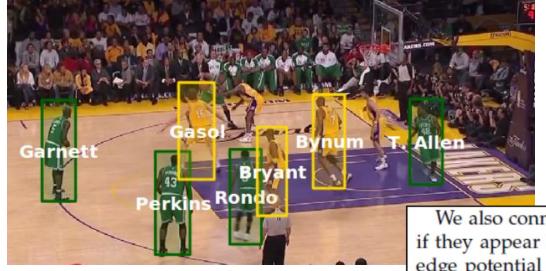
### Learning with Constraints



## Learn a statistical model that assigns **zero probability**

to instantiations that violate the constraints.

### Example: Video



We also connect all pairs of identity nodes  $y_{t,i}$  and  $y_{t,j}$  if they appear in the same time *t*. We then introduce an edge potential that enforces mutual exclusion:

$$\psi_{\text{mutex}}(y_{t,i}, y_{t,j}) = \begin{cases} 1 & \text{if } y_{t,i} \neq y_{t,j} \\ 0 & \text{otherwise} \end{cases}$$
(5)

This potential specifies the constraint that a player can be appear only *once* in a frame. For example, if the *i*-th detection  $y_{t,i}$  has been assign to Bryant,  $y_{t,j}$  cannot have the same identity because Bryant is impossible to appear twice in a frame.

[Lu, W. L., Ting, J. A., Little, J. J., & Murphy, K. P. (2013). Learning to track and identify players from broadcast sports videos.]

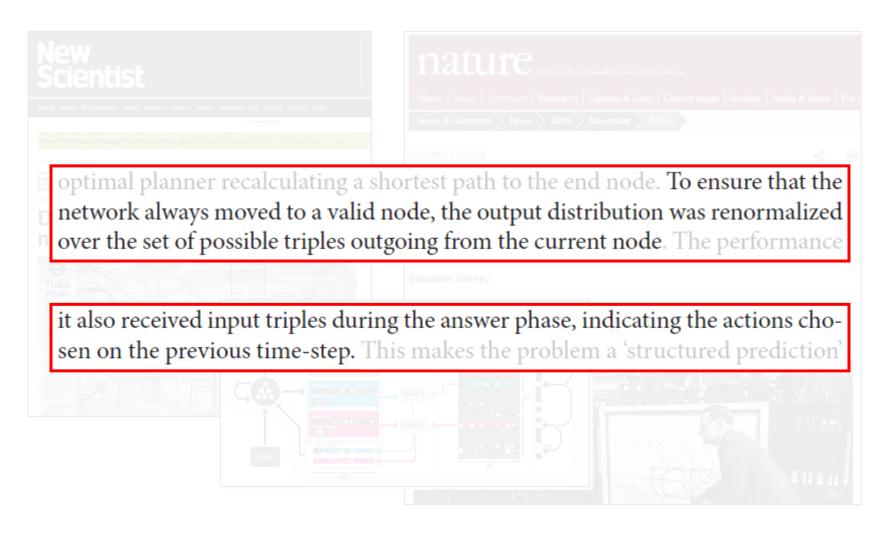
### Example: Language

- Non-local dependencies:
   At least one verb in each sentence
- Sentence compression If a modifier is kept, its subject is also kept
- Information extraction
- Semantic role labeling
- ... and many more!

	Citations				
Start	The citation must start with author				
	or editor.				
AppearsOnce	Each field must be a consecutive list				
	of words, and can appear at most				
	once in a citation.				
Punctuation	State transitions must occur on				
	punctuation marks.				
BookJournal	The words proc, journal, proceed-				
	ings, ACM				
	are JOURNAL or BOOKTITLE.				
TechReport	The words <i>tech</i> , <i>technical</i> are				
	TECH_REPORT.				
Title	Quotations can appear only in titles.				
Location	The words CA, Australia, NY are				
	LOCATION.				

[Chang, M., Ratinov, L., & Roth, D. (2008). Constraints as prior knowledge],..., [Chang, M. W., Ratinov, L., & Roth, D. (2012). Structured learning with constrained conditional models.], [https://en.wikipedia.org/wiki/Constrained\_conditional\_model]

### **Example: Deep Learning**



[Graves, A., Wayne, G., Reynolds, M., Harley, T., Danihelka, I., Grabska-Barwińska, A., et al.. (2016). Hybrid computing using a neural network with dynamic external memory. *Nature*, *538*(7626), 471-476.]

### What are people doing now?

E2

Κ

E1

- Ignore constraints
- Handcraft into models —
- Use specialized distributions
- Find non-structured encoding
- Try to learn constraints
- Hack your way around

Accuracy ?

- Specialized skill ?
- Intractable inference ?
  - Intractable learning ?
    - Waste parameters ?

Risk predicting out of space ?

#### you are on your own ⊗

### **Structured Probability Spaces**

#### • Everywhere in ML!

- Configuration problems, inventory, video, text, deep learning
- Planning and diagnosis (physics)
- Causal models: cooking scenarios (interpreting videos)
- Combinatorial objects: parse trees, rankings, directed acyclic graphs, trees, simple paths, game traces, etc.
- Some representations: constrained conditional models, mixed networks, probabilistic logics.

## No statistical ML boxes out there that take constraints as input! 🛞

<u>Goal</u>: Constraints as important as data! General purpose!

### Specification Language: Logic

### **Structured Probability Space**

#### unstructured

L	К	Р	А
0	0	0	0
0	0	0	1
0	0	1	0
0	0	1	1
0	1	0	0
0	1	0	1
0	1	1	0
0	1	1	1
1	0	0	0
1	0	0	1
1	0	1	0
1	0	1	1
1	1	0	0
1	1	0	1
1	1	1	0
1	1	1	1



- Must take at least one of Probability or Logic.
- Probability is a prerequisite for AI.
- The prerequisites for KR is either AI or Logic.

#### 7 out of 16 instantiations are impossible

#### structured

L	К	Р	А
0	0	0	0
0	0	0	1
0	0	1	0
0	0	1	1
0	1		0
0	1	0	1
0	1	1	0
0	1	1	1
1	0	0	0
1	0	0	1
1	0	1	0
1	0	1	1
1	1	0	0
1	1	0	1
1	1	1	0
1	1	1	1

### **Boolean Constraints**

un	stru	ctu	red	
L	K	Р	А	
0	0	0	0	
0	0	0	1	
0	0	1	0	$P \lor L$
0	0	1	1	$A \Rightarrow P$
0	1	0	0	
0	1	0	1	$K \Rightarrow (P \lor L)$
0	1	1	0	
0	1	1	1	
1	0	0	0	
1	0	0	1	
1	0	1	0	7 out of 16 instantiations
1	0	1	1	/ out of to instantiations
1	1	0	0	are impossible
1	1	0	1	L.
1	1	1	0	
1	1	1	1	

#### structured

L	K	Р	А
	0		0
0	0	0	1
0	0	1	0
0	0	1	1
0	1	0	1
0	1	1	1
1	0	0	0
1	0	0	1
1	0	1	0
1	0	1	1
1	1	0	0
1	1	0	1
1	1	1	0
1	1	1	1

### **Combinatorial Objects: Rankings**

rank	sushi	rank	sushi
1	fatty tuna	1	shrimp
2	sea urchin	2	sea urchin
3	salmon roe	3	salmon roe
4	shrimp	4	fatty tuna
5	tuna	5	tuna
6	squid	6	squid
7	tuna roll	7	tuna roll
8	see eel	8	see eel
9	egg	9	egg
10	cucumber roll	10	cucumber roll

**10 items**: 3,628,800 rankings

**20 items**: 2,432,902,008,176,640,000 rankings

### **Combinatorial Objects: Rankings**

rank	sushi	rank	sushi
1	fatty tuna	1	shrimp
2	sea urchin	2	sea urchin
3	salmon roe	3	salmon roe
4	shrimp	4	fatty tuna
5	tuna	5	tuna
6	squid	6	squid
7	tuna roll	7	tuna roll
8	see eel	8	see eel
9	egg	9	egg
10	cucumber roll	10	cucumber roll

A<sub>ij</sub> item *i* at position *j*(*n* items require *n*<sup>2</sup>
Boolean variables)

An item may be assigned to more than one position

A position may contain more than one item

### **Encoding Rankings in Logic**

#### $A_{ij}$ : item *i* at position *j*

	pos 1	pos 2	pos 3	pos 4
item 1	<i>A</i> <sub>11</sub>	A <sub>12</sub>	<i>A</i> <sub>13</sub>	<i>A</i> <sub>14</sub>
item 2	A <sub>21</sub>	A <sub>22</sub>	A <sub>23</sub>	<i>A</i> <sub>24</sub>
item 3	<i>A</i> <sub>31</sub>	A <sub>32</sub>	A <sub>33</sub>	<i>A</i> <sub>34</sub>
item 4	<i>A</i> <sub>41</sub>	A <sub>42</sub>	A <sub>43</sub>	$A_{44}$

constraint: each item *i* assigned to a unique position (*n* constraints)

$$\bigvee_{j} A_{ij} \wedge \left(\bigwedge_{k \neq j} \neg A_{ik}\right)$$

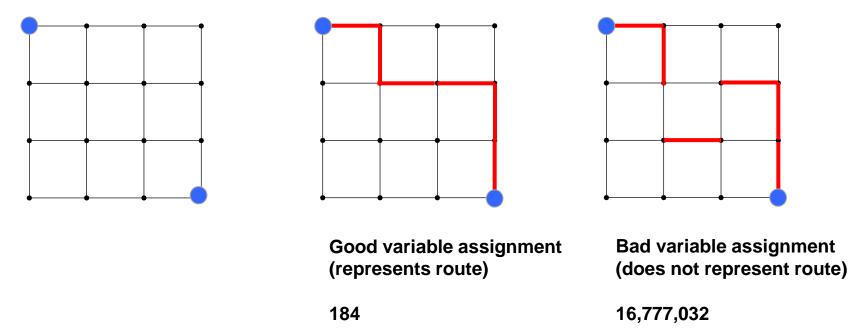
constraint: each position *j* assigned a unique item (*n* constraints)

$$\bigvee_i A_{ij} \wedge \left(\bigwedge_{k \neq i} \neg A_{kj}\right)$$

total constraints 2n<u>unstructured</u> space  $2^{n^2}$ structured space n!

### Structured Space for Paths cf. Nature paper



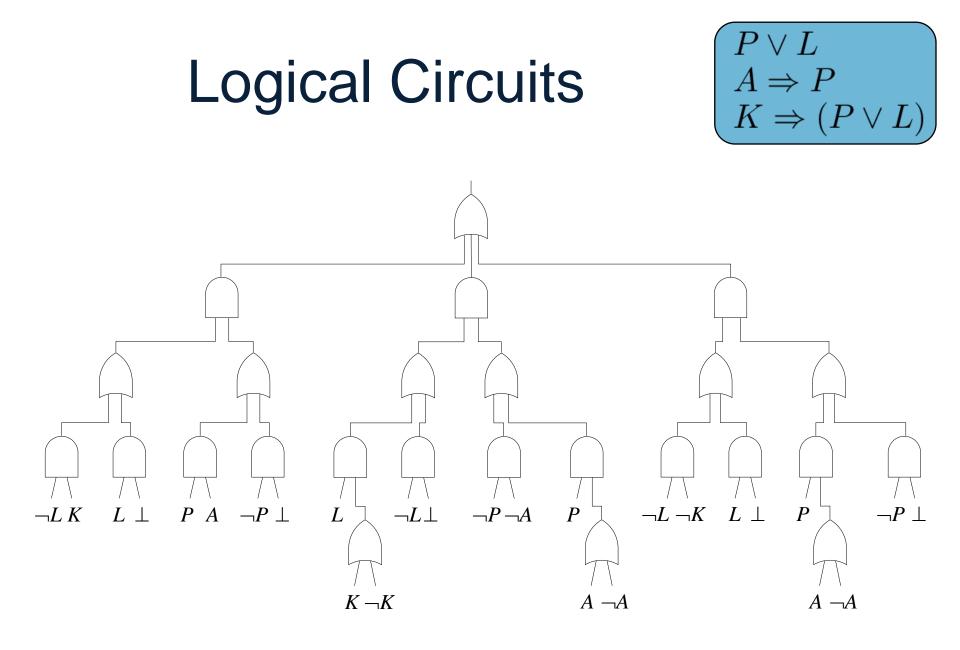


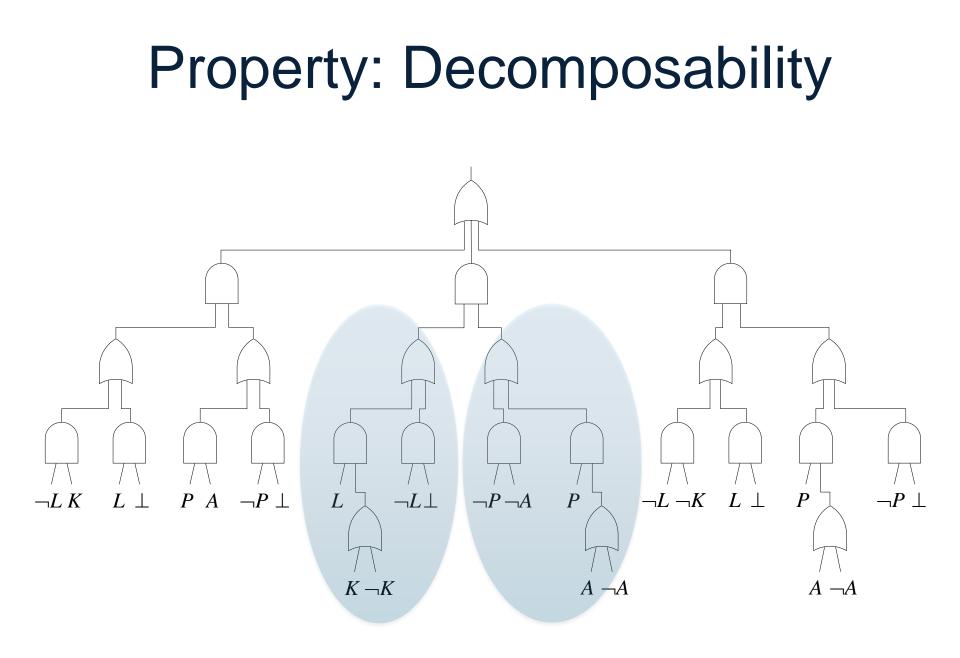
Space easily encoded in logical constraints ③ See [Choi, Tavabi, Darwiche, AAAI 2016]

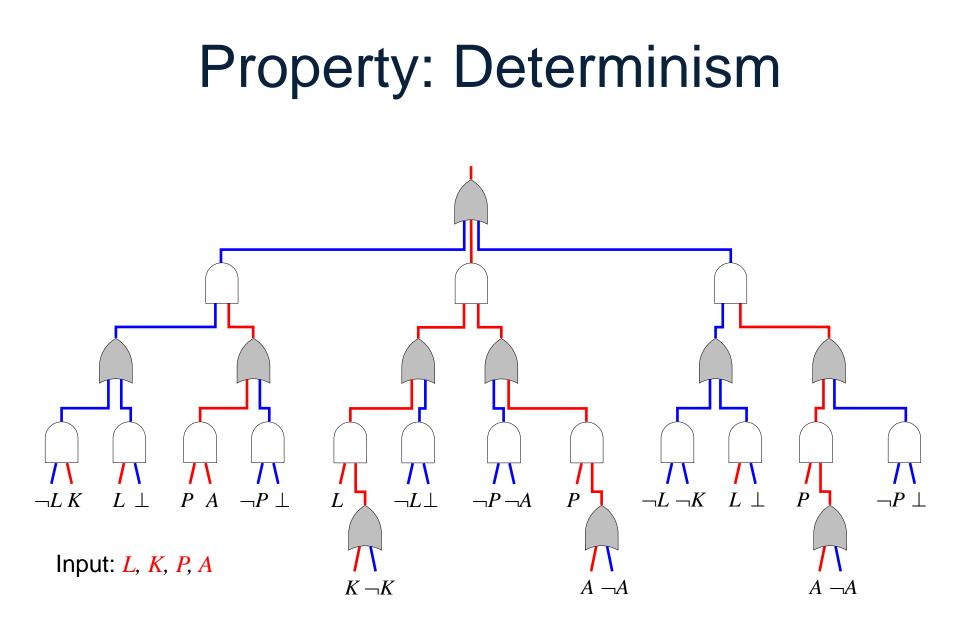
Unstructured probability space:  $184+16,777,032 = 2^{24}$ 

### "Deep Architecture"

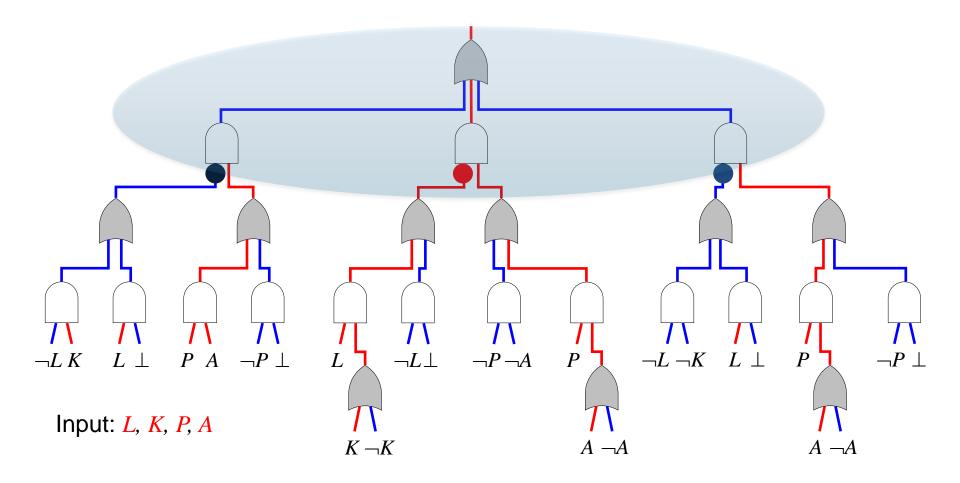
### Logic + Probability







### Sentential Decision Diagram (SDD)



### **Tractable for Logical Inference**

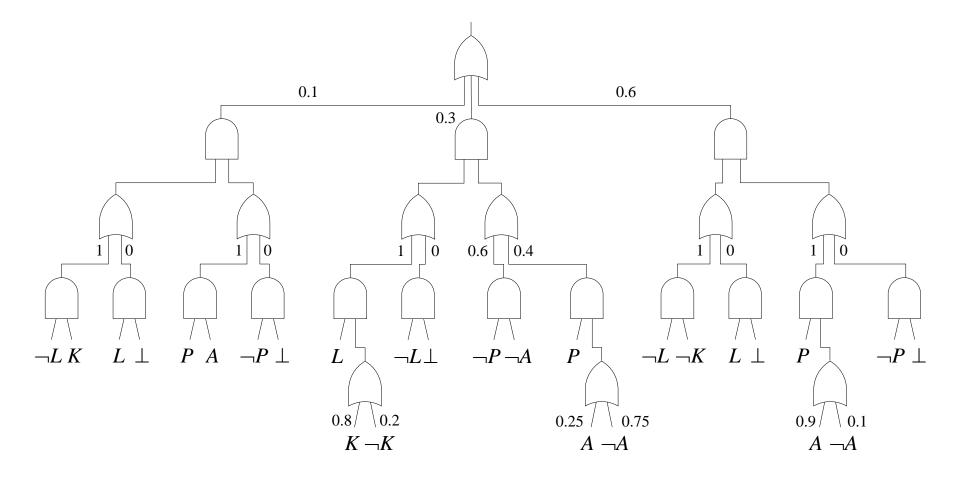
- Is structured space empty? (SAT)
- Count size of structured space (#SAT)
- Check equivalence of spaces
- Algorithms linear in circuit size (pass up, pass down, similar to backprop)

#### SCIENCE + TECHNOLOGY

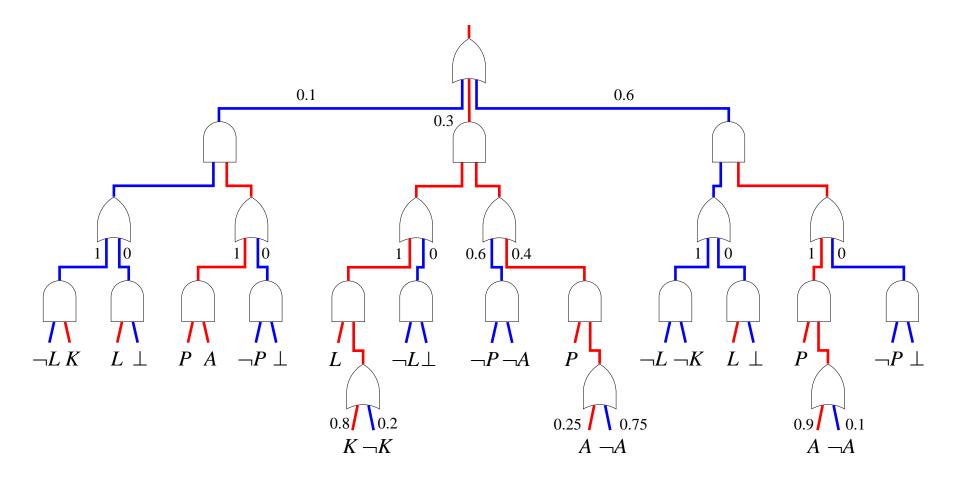
Artificial intelligence framework developed by UCLA professor now powers Toyota websites

Adnan Darwiche's invention helps consumers customize their vehicles online

### **PSDD:** Probabilistic SDD

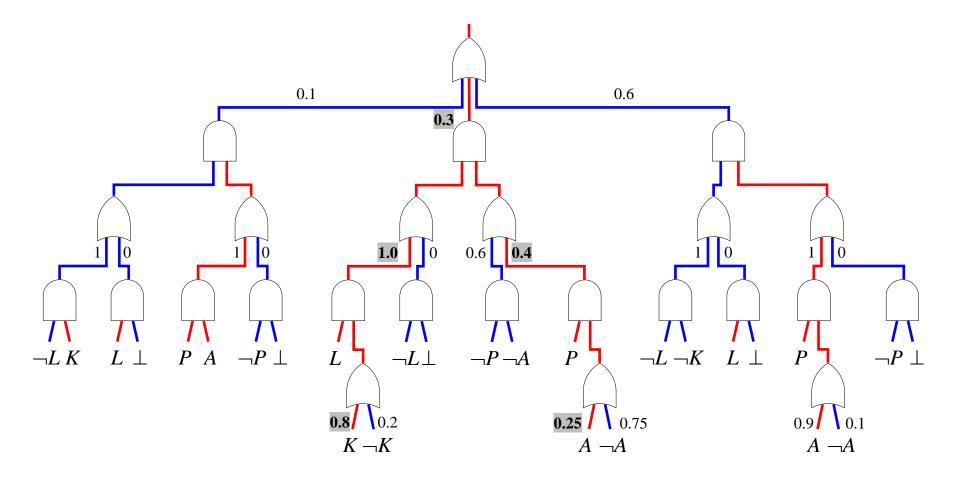


### **PSDD:** Probabilistic SDD

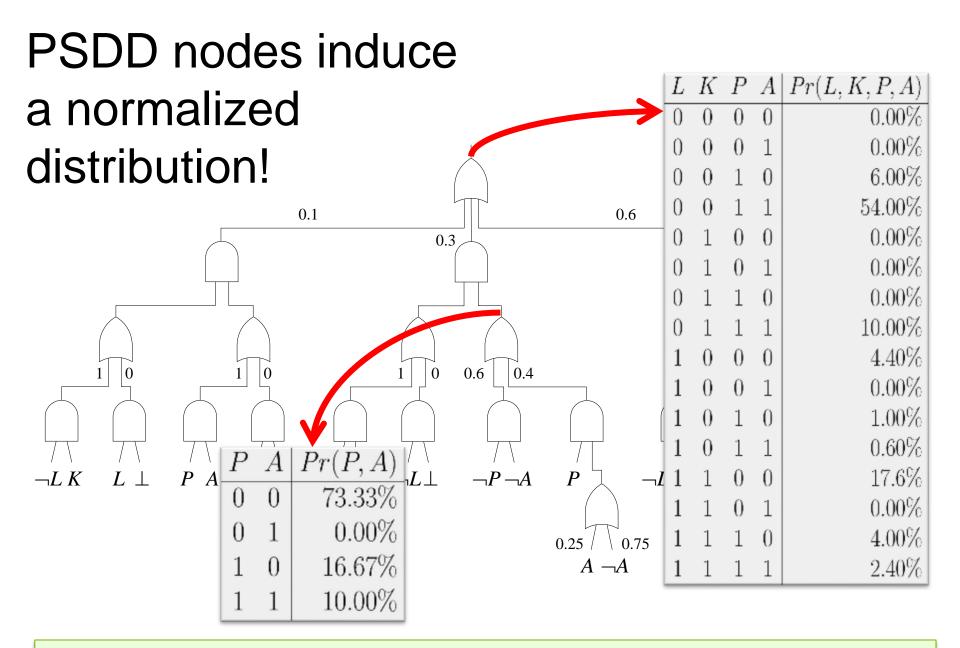


#### Input: *L*, *K*, *P*, *A*

### **PSDD: Probabilistic SDD**



Input: *L*, *K*, *P*, *A*  $P(L, K, P, A) = 0.3 \ge 1.0 \ge 0.4 \ge 0.25 = 0.024$ 



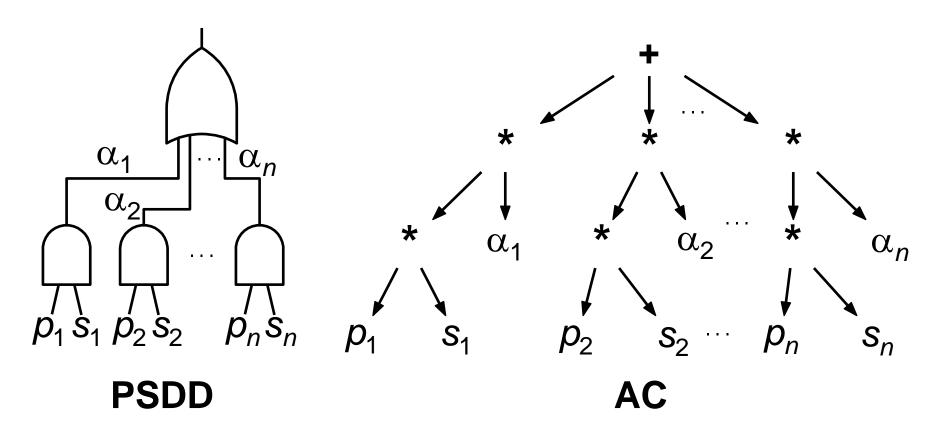
Can read probabilistic independences off the circuit structure

### Tractable for Probabilistic Inference

- **MAP inference**: Find most-likely assignment (otherwise NP-complete)
- Computing conditional probabilities Pr(x|y) (otherwise PP-complete)
- **Sample** from Pr(x|y)
- Algorithms linear in circuit size (pass up, pass down, similar to backprop)

### **PSDDs are Arithmetic Circuits**

[Darwiche, JACM 2003]



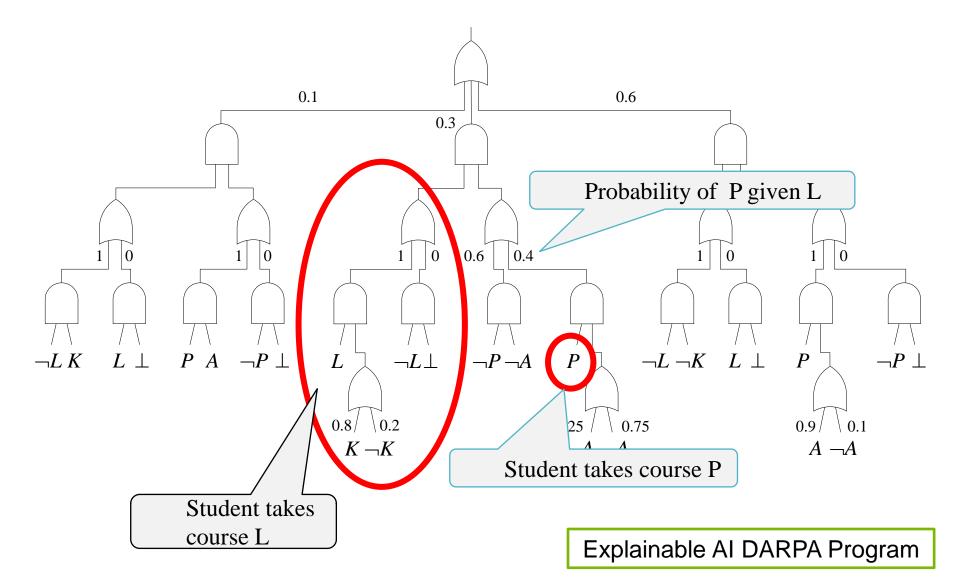
Known in the ML literature as SPNs UAI 2011, NIPS 2012 best paper awards

[ICML 2014] (SPNs equivalent to ACs)

### Learning PSDDs

### Logic + Probability + ML

### Parameters are Interpretable



### Learning Algorithms

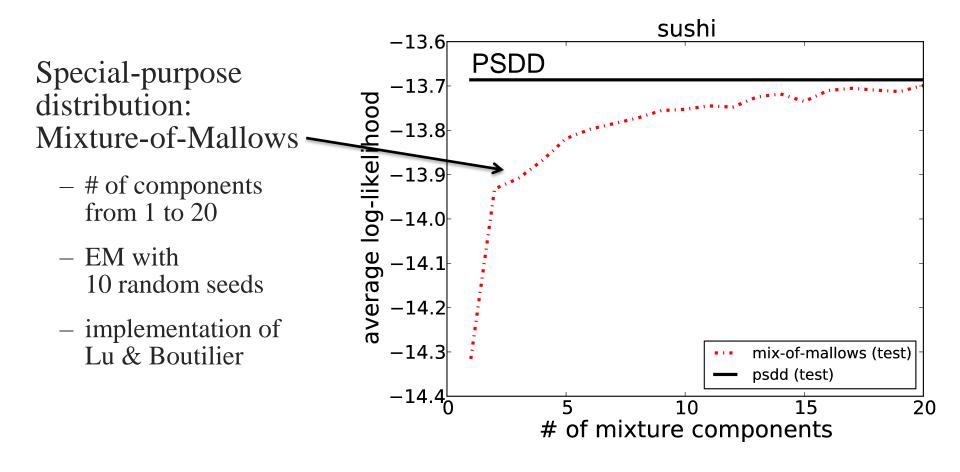
• Parameter learning:

Closed form max likelihood from complete data One pass over data to estimate Pr(x|y)

Not a lot to say: very easy!

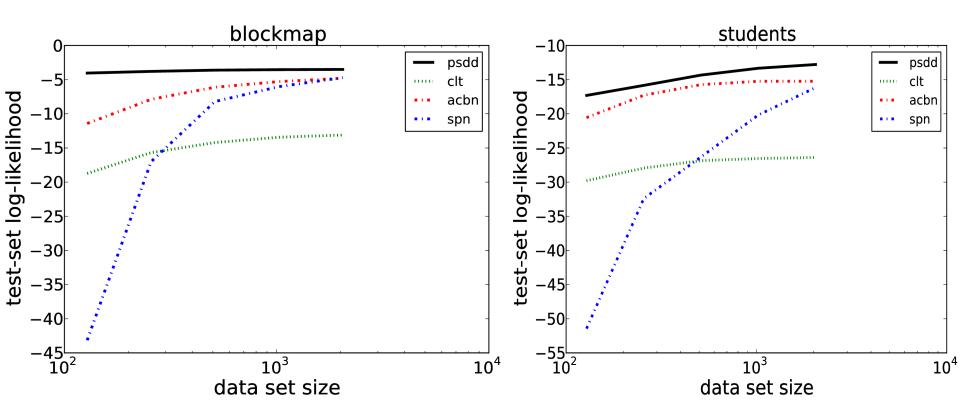
- Circuit learning (naïve): Compile constraints to SDD circuit
  - Use SAT solver technology
  - Circuit does not depend on data

### Learning Preference Distributions



This is the naive approach, circuit does not depend on data!

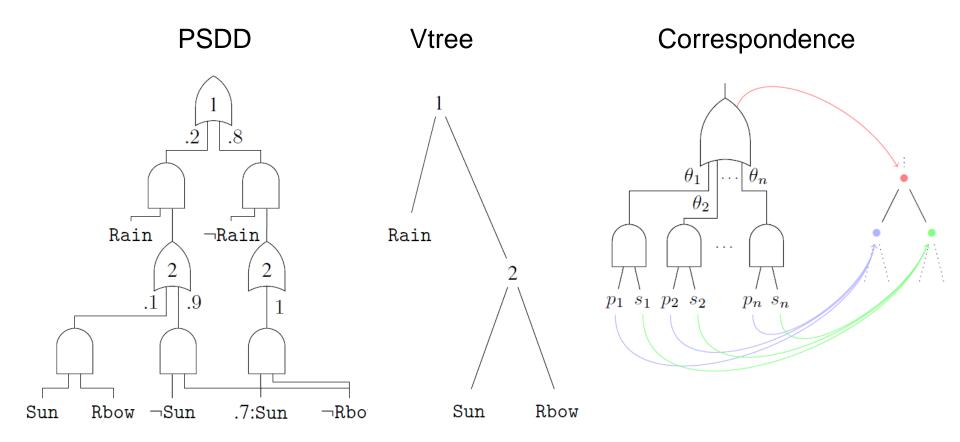
# What happens if you **ignore** constraints?



# Learn Circuit from Data

Even in unstructured spaces

# Variable Trees (vtrees)

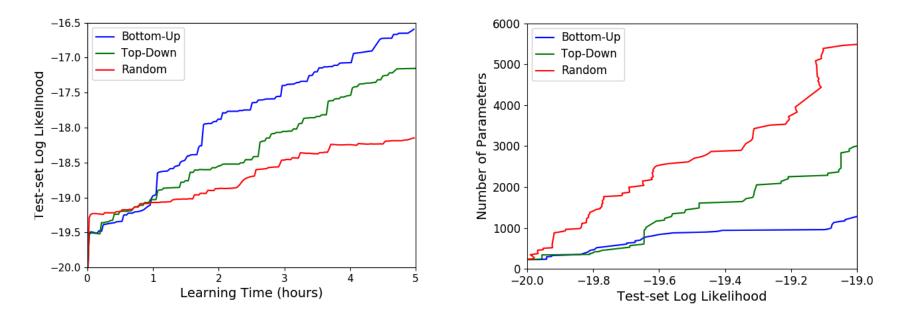


# Learning Variable Trees

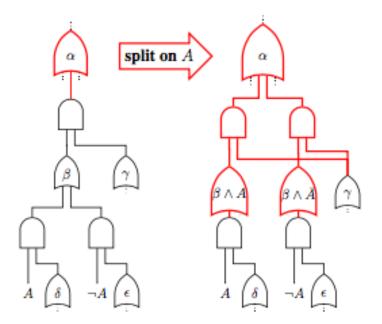
• How much do vars depend on each other?

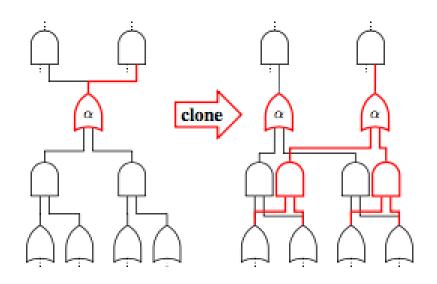
 $\mathrm{MI}(\mathbf{X},\mathbf{Y}) = \sum_{X \in \mathbf{X}} \sum_{Y \in \mathbf{Y}} \mathrm{Pr}(X,Y) \log \frac{\mathrm{Pr}(X,Y)}{\mathrm{Pr}(X) \, \mathrm{Pr}(Y)}$ 

Learn vtree by hierarchical clustering



# Learning Primitives





# **Tractable Learning**

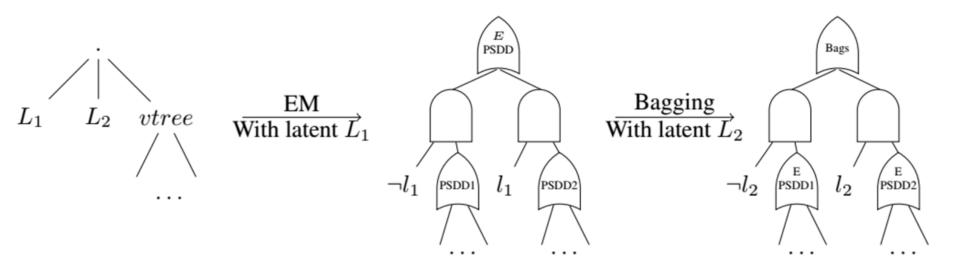
- Circuit size is measurement of tractability
- Trade off size and quality of model

score = 
$$\frac{\ln \mathcal{L}(r' \mid \mathcal{D}) - \ln \mathcal{L}(r \mid \mathcal{D})}{\operatorname{size}(r') - \operatorname{size}(r)}$$

- Perform greedy local search
   Split and Clone
- Re-learn parameters in between

## Ensembles

- Performance boost
  - Add a few latent variables (L1,L2)
  - Perform expectation maximization
  - Perform bagging



## **Experimental Results**

Dataset	Var	LearnPSDD Ensemble	Best-to-Date
NLTCS	16	$-5.99^{\dagger}$	-6.00
MSNBC	17	$-6.04^{\dagger}$	$-6.04^{\dagger}$
KDD	64	$-2.11^{\dagger}$	-2.12
Plants	69	-13.02	$-11.99^{\dagger}$
Audio	100	-39.94	$-39.49^{\dagger}$
Jester	100	-51.29	$-41.11^{\dagger}$
Netflix	100	$-55.71^{\dagger}$	-55.84
Accidents	111	-30.16	$-24.87^{\dagger}$
Retail	135	$-10.72^{\dagger}$	-10.78
Pumsb-Star	163	-26.12	$-22.40^{\dagger}$
DNA	180	-88.01	$-80.03^{\dagger}$
Kosarek	190	$-10.52^{\dagger}$	-10.54
MSWeb	294	-9.89	$-9.22^{\dagger}$
Book	500	-34.97	$-30.18^{\dagger}$
EachMovie	500	-58.01	$-51.14^{\dagger}$
WebKB	839	-161.09	$-150.10^{\dagger}$
Reuters-52	889	-89.61	$-80.66^{\dagger}$
20NewsGrp.	910	-155.97	$-150.88^{\dagger}$
BBC	1058	-253.19	$-233.26^{\dagger}$
AD	1556	-31.78	$-14.36^{\dagger}$

Surpasses the state of the art (SPNs, Cutset networks, ACs) on 6/20 datasets.

# **Complex queries**

and

# Learning from constraints

# **Incomplete Data**

### a classical complete dataset

id	X	Y	Z
1	<b>x</b> <sub>1</sub>	y <sub>2</sub>	Z <sub>1</sub>
2	<b>x</b> <sub>2</sub>	У <sub>1</sub>	Z <sub>2</sub>
3	<b>x</b> <sub>2</sub>	У <sub>1</sub>	Z <sub>2</sub>
4	<b>x</b> <sub>1</sub>	У <sub>1</sub>	Z <sub>1</sub>
5	<b>x</b> <sub>1</sub>	У <sub>2</sub>	Z <sub>2</sub>

a classical incomplete dataset

id	X	Y	Z
1	x <sub>1</sub>	У <sub>2</sub>	?
2	<b>x</b> <sub>2</sub>	У <sub>1</sub>	?
3	?	?	<b>Z</b> <sub>2</sub>
4	?	У <sub>1</sub>	Z <sub>1</sub>
5	<b>x</b> <sub>1</sub>	У <sub>2</sub>	<b>Z</b> <sub>2</sub>

closed-form (maximum-likelihood estimates are unique) EM algorithm (on PSDDs)

### a new type of incomplete dataset

id	X Y Z	
1	$X \equiv Z$	
2	$x_2$ and $(y_2 \text{ or } z_2)$	
3	$x_2 \Rightarrow y_1$	
4	$X \oplus Y \oplus Z \equiv 1$	
5	$x_1$ and $y_2$ and $z_2$	2

### Missed in the ML literature

## **Structured Datasets**

#### a classical **complete** dataset (e.g., total rankings)

id	1 <sup>st</sup> sushi	2 <sup>nd</sup> sushi	3 <sup>rd</sup> sushi	
1	fatty tuna	sea urchin	salmon roe	
2	fatty tuna	tuna	shrimp	
3	tuna	tuna roll	sea eel	
4	fatty tuna	salmon roe	tuna	
5	egg	squid	shrimp	

#### a classical **incomplete** dataset (e.g., top-*k* rankings)

id	1 <sup>st</sup> sushi	2 <sup>nd</sup> sushi	3 <sup>rd</sup> sushi	
1	fatty tuna	sea urchin	?	
2	fatty tuna	?	?	
3	tuna	tuna roll	?	
4	fatty tuna	salmon roe	?	
5	egg	?	?	

## **Structured Datasets**

#### a classical **complete** dataset (e.g., total rankings)

id	1 <sup>st</sup> sushi	2 <sup>nd</sup> sushi	3 <sup>rd</sup> sushi	
1	fatty tuna	sea urchin	salmon roe	
2	fatty tuna	tuna	shrimp	
3	tuna	tuna roll	sea eel	
4	fatty tuna	salmon roe	tuna	
5	egg	squid	shrimp	

#### a new type of **incomplete** dataset (e.g., **partial** rankings)

id	1 <sup>st</sup> sushi	2 <sup>nd</sup> sushi	3 <sup>rd</sup> sushi	
1	(fatty tuna > sea urchin) and (tuna > sea eel)			
2	(fatty tuna is 1 <sup>st</sup> ) and (salmon roe > egg)			
3	tuna > squid			
4	egg is last			
5	egg > squid > shrimp			

(represents constraints on possible *total rankings*)

### Learning from Incomplete Data

- Movielens Dataset:
  - 3,900 movies, 6,040 users, 1m ratings
  - take ratings from 64 most rated movies
  - ratings 1-5 converted to pairwise prefs.
- PSDD for partial rankings
  - 4 tiers
  - 18,711 parameters

#### movies by expected tier

rank	movie
1	The Godfather
2	The Usual Suspects
3	Casablanca
4	The Shawshank Redemption
5	Schindler's List
6	One Flew Over the Cuckoo's Nest
7	The Godfather: Part II
8	Monty Python and the Holy Grail
9	Raiders of the Lost Ark
10	Star Wars IV: A New Hope

### **PSDD** Sizes

items	tier size		Size	
n	k	SDD	Structured Space	Unstructured Space
8	2	443	840	$1.84\cdot10^{19}$
27	3	$4,\!114$	$1.18\cdot 10^9$	$2.82 \cdot 10^{219}$
64	4	$23,\!497$	$3.56\cdot10^{18}$	$1.04\cdot 10^{1233}$
125	5	$94,\!616$	$3.45\cdot10^{31}$	$3.92\cdot 10^{4703}$
216	6	$297,\!295$	$1.57\cdot 10^{48}$	$7.16\cdot 10^{14044}$
343	7	$781,\!918$	$4.57\cdot 10^{68}$	$7.55 \cdot 10^{35415}$

# **Structured Queries**

rank	movie
1	Star Wars V: The Empire Strikes Back
2	Star Wars IV: A New Hope
3	The Godfather
4	The Shawshank Redemption
5	The Usual Suspects

- no other Star Wars movie in top-5
- at least one comedy in top-5

rank	movie
1	Star Wars V: The Empire Strikes Back
2	American Beauty
3	The Godfather
4	The Usual Suspects
5	The Shawshank Redemption

### diversified recommendations via *logical constraints*

# Conclusions

- Structured spaces are everywhere ③
- PSDDs build on logical circuits
  - 1. Tractability
  - 2. Semantics
  - 3. Natural encoding of structured spaces
- Learning is effective
  - From constraints encoding structured space
     State of the art preference distribution learning
  - 2. From standard unstructured datasets using search State of the art on standard tractable learning datasets
- Novel settings for inference and learning Structured spaces / learning from constraints / complex queries

## References

### **Probabilistic Sentential Decision Diagrams**

Doga Kisa, Guy Van den Broeck, Arthur Choi and Adnan Darwiche KR, 2014

### Learning with Massive Logical Constraints

Doga Kisa, Guy Van den Broeck, Arthur Choi and Adnan Darwiche ICML 2014 workshop

### **Tractable Learning for Structured Probability Spaces**

Arthur Choi, Guy Van den Broeck and Adnan Darwiche IJCAI, 2015

### **Tractable Learning for Complex Probability Queries**

Jessa Bekker, Jesse Davis, Arthur Choi, Adnan Darwiche, Guy Van den Broeck. NIPS, 2015

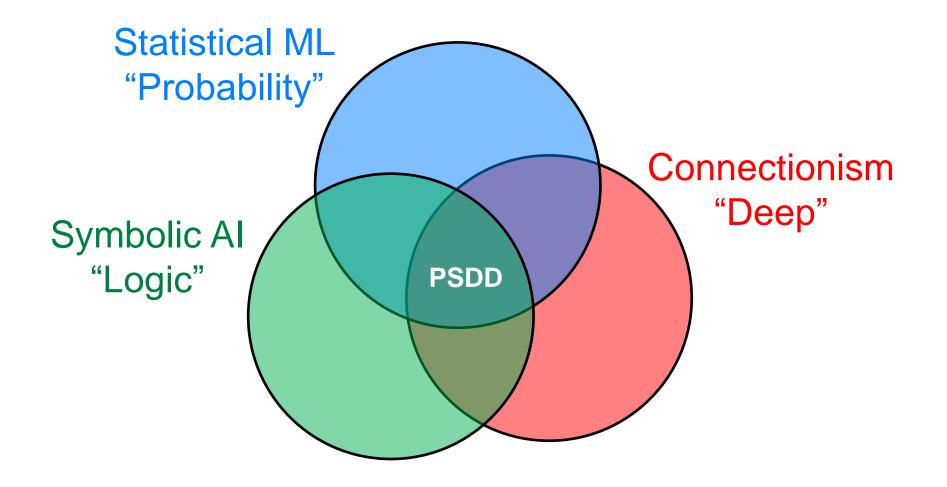
### Learning the Structure of PSDDs

Jessa Bekker, Yitao Liang and Guy Van den Broeck Under review, 2017

## Towards Compact Interpretable Models: Learning and Shrinking PSDDs

Yitao Liang and Guy Van den Broeck Under review, 2017

### Conclusions



### Questions?



PSDD with 15,000 nodes