PSDDs for Tractable Learning in Structured and Unstructured Spaces

Guy Van den Broeck



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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



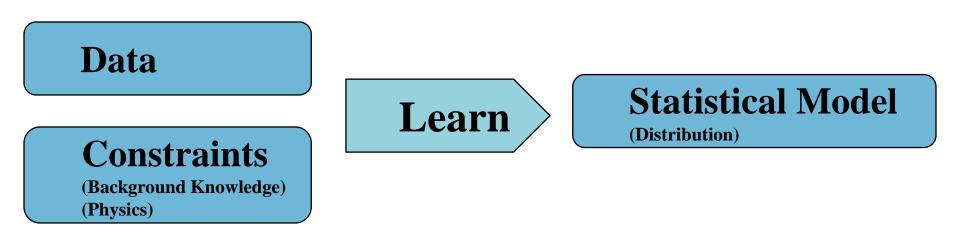
- Must take at least one of Probability or Logic.
- Probability is a prerequisite for AI.
- The prerequisites for KR is either AI or Logic.

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

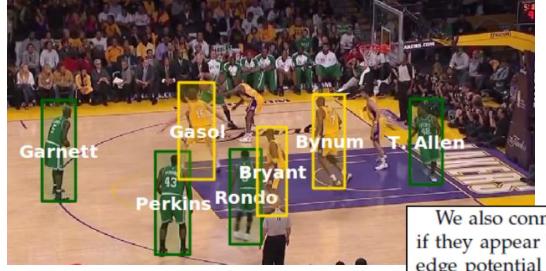
Learning with Constraints



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.]

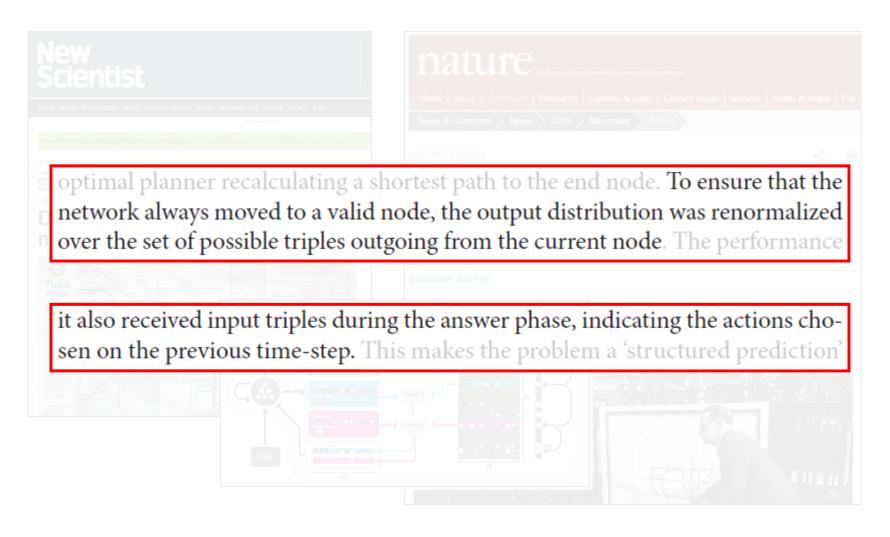
Example: Language

- 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_{ij} item *i* at position *j*(*n* items require *n*²
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> ₁₁	A ₁₂	<i>A</i> ₁₃	<i>A</i> ₁₄
item 2	A ₂₁	A ₂₂	A ₂₃	<i>A</i> ₂₄
item 3	<i>A</i> ₃₁	A ₃₂	A ₃₃	<i>A</i> ₃₄
item 4	<i>A</i> ₄₁	A ₄₂	A ₄₃	A_{44}

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

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

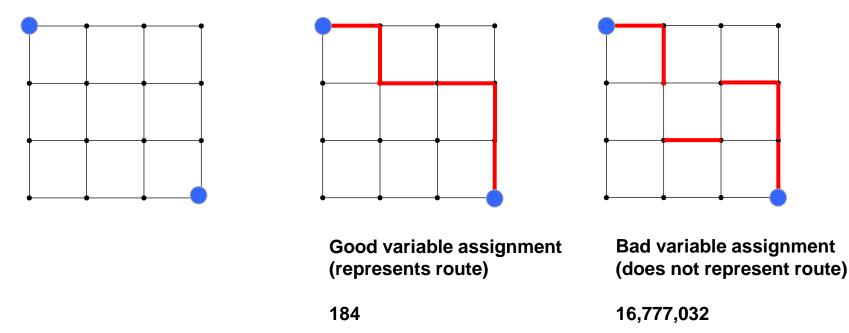
constraint: each position *j* assigned a unique item (*n* constraints)

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

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

Structured Space for Paths cf. Nature paper



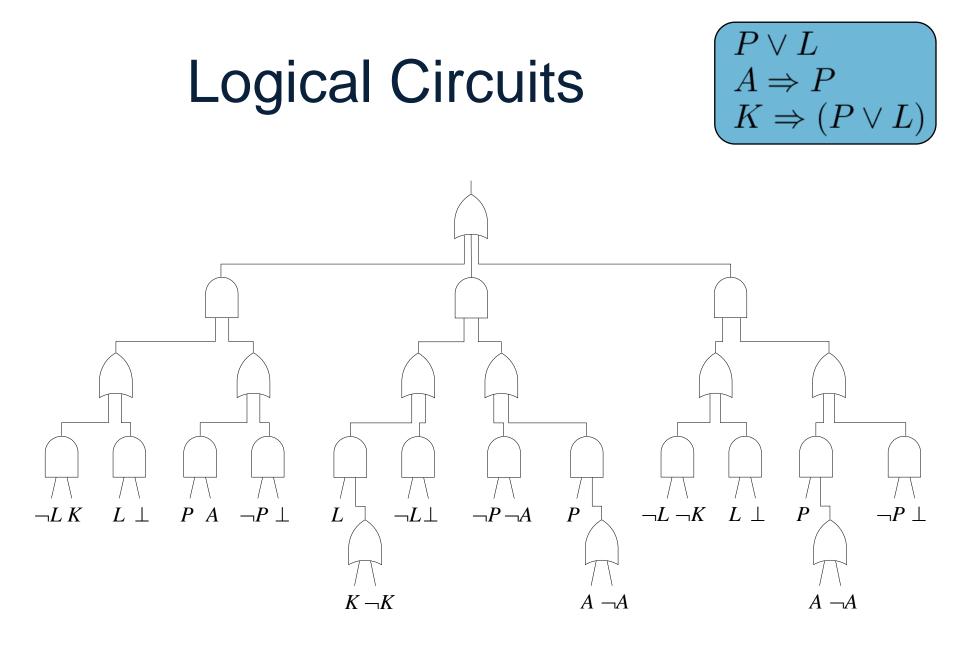


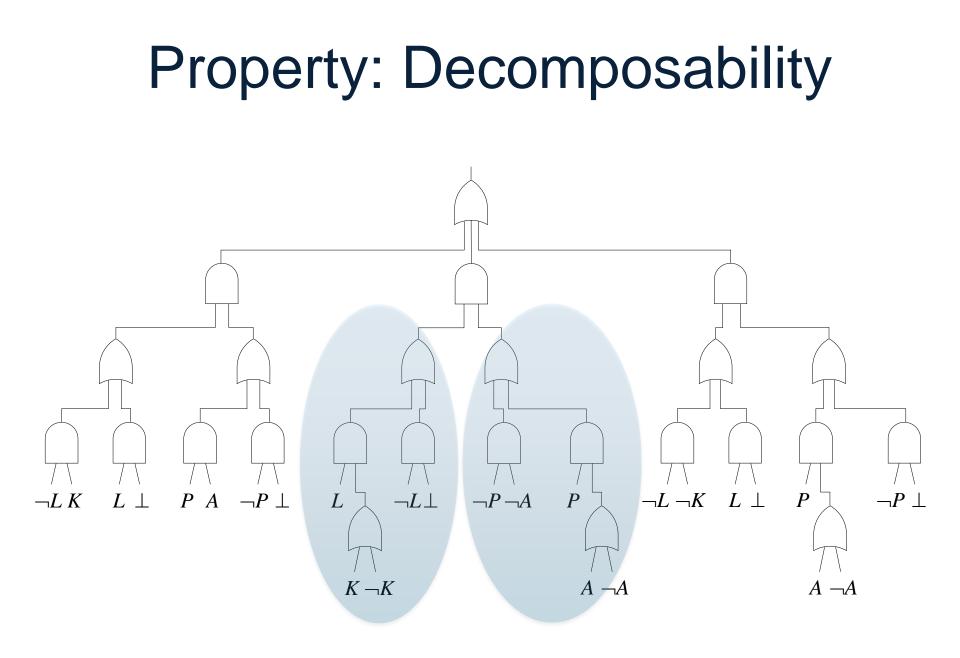
Space easily encoded in logical constraints ③ See [Choi, Tavabi, Darwiche, AAAI 2016]

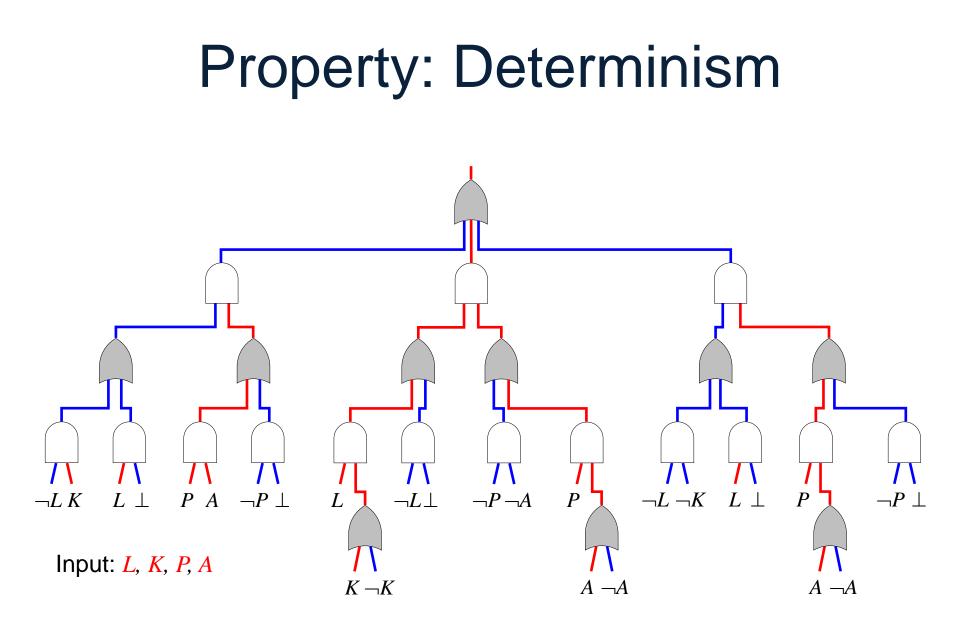
Unstructured probability space: $184+16,777,032 = 2^{24}$

"Deep Architecture"

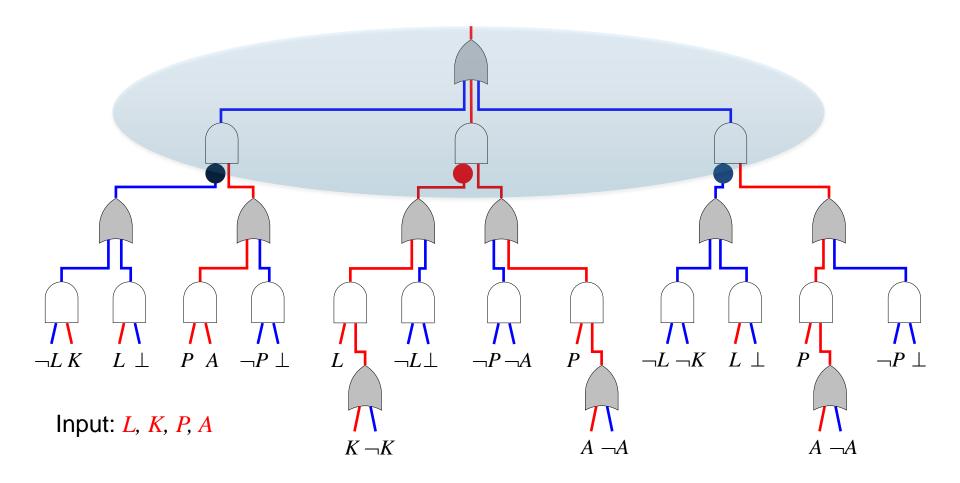
Logic + Probability







Sentential Decision Diagram (SDD)



Tractable for Logical Inference

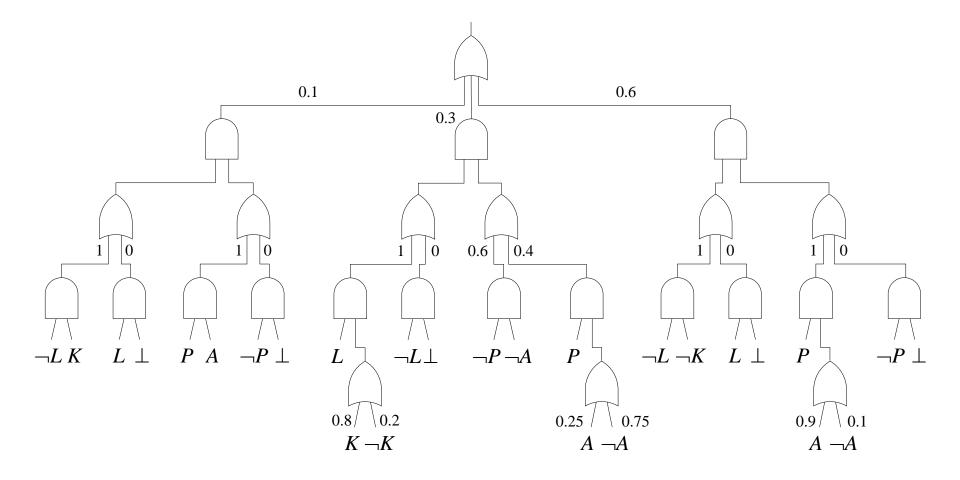
- Is structured space empty? (SAT)
- Count size of structured space (#SAT)
- Check equivalence of spaces
- Algorithms linear in circuit size (pass up, pass down, similar to backprop)

SCIENCE + TECHNOLOGY

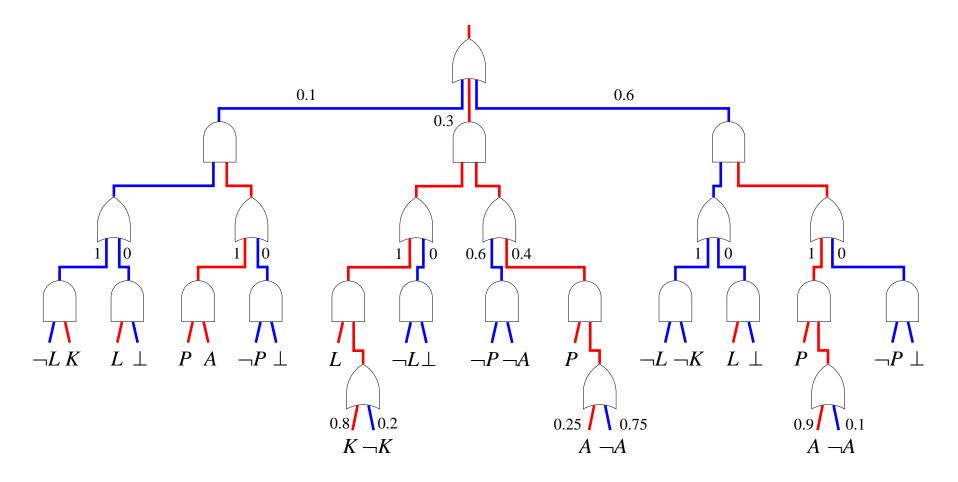
Artificial intelligence framework developed by UCLA professor now powers Toyota websites

Adnan Darwiche's invention helps consumers customize their vehicles online

PSDD: Probabilistic SDD

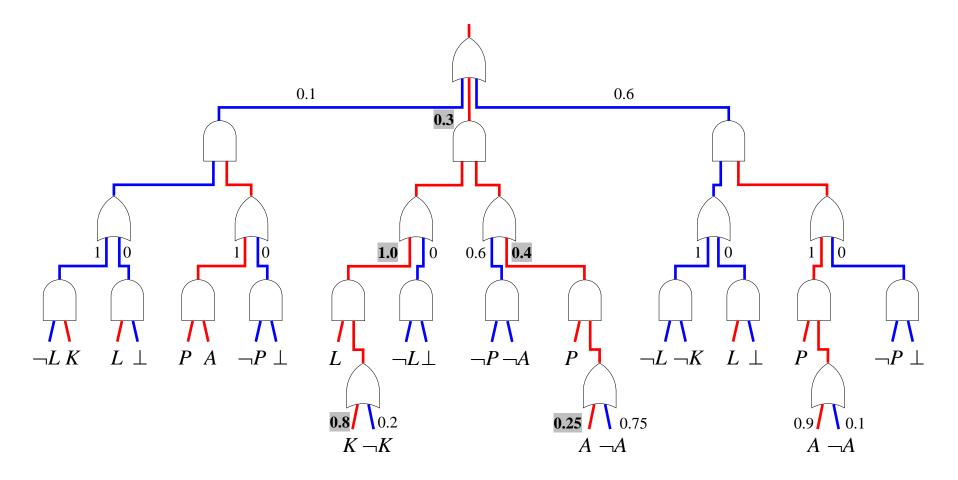


PSDD: Probabilistic SDD

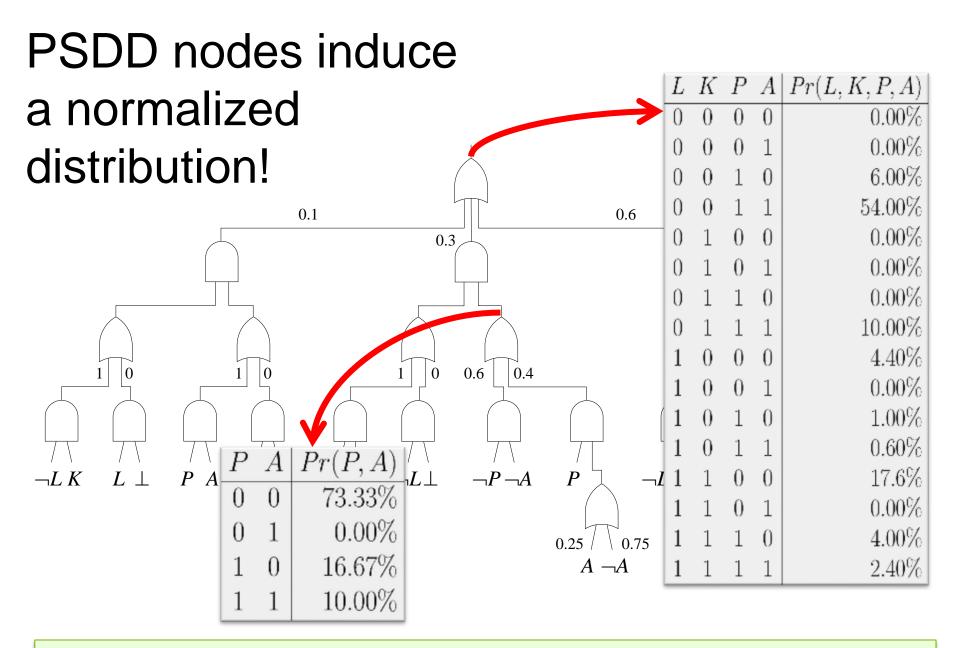


Input: *L*, *K*, *P*, *A*

PSDD: Probabilistic SDD



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



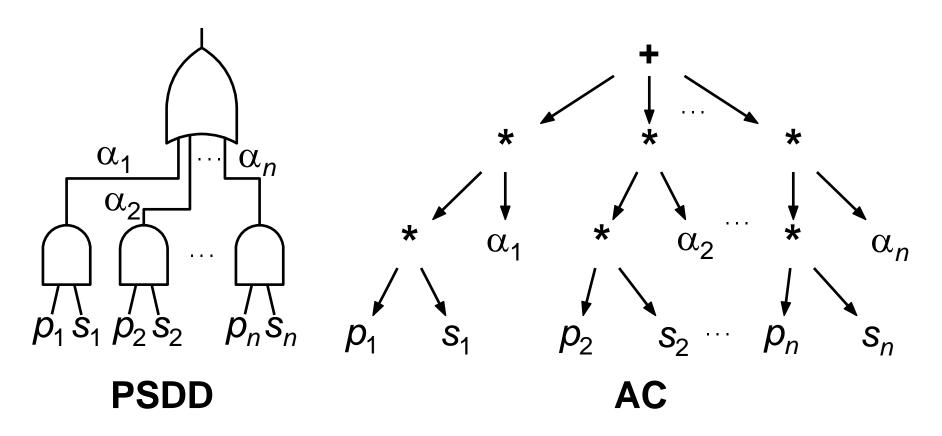
Can read probabilistic independences off the circuit structure

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]



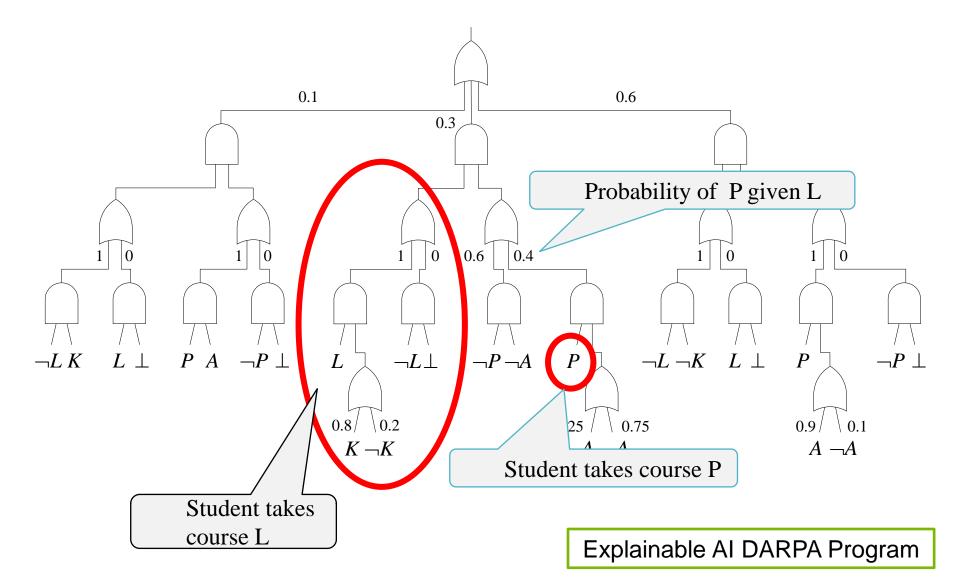
Known in the ML literature as SPNs UAI 2011, NIPS 2012 best paper awards

[ICML 2014] (SPNs equivalent to ACs)

Learning PSDDs

Logic + Probability + ML

Parameters are Interpretable



Learning Algorithms

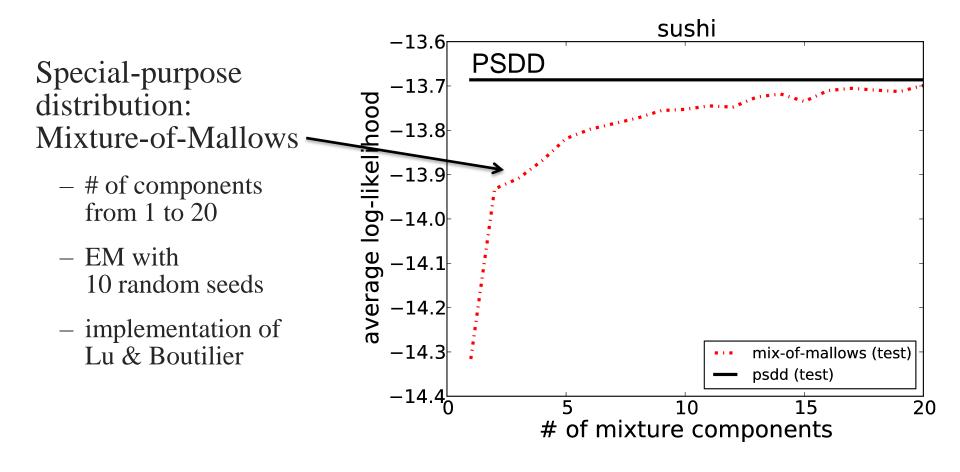
• Parameter learning:

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

Not a lot to say: very easy!

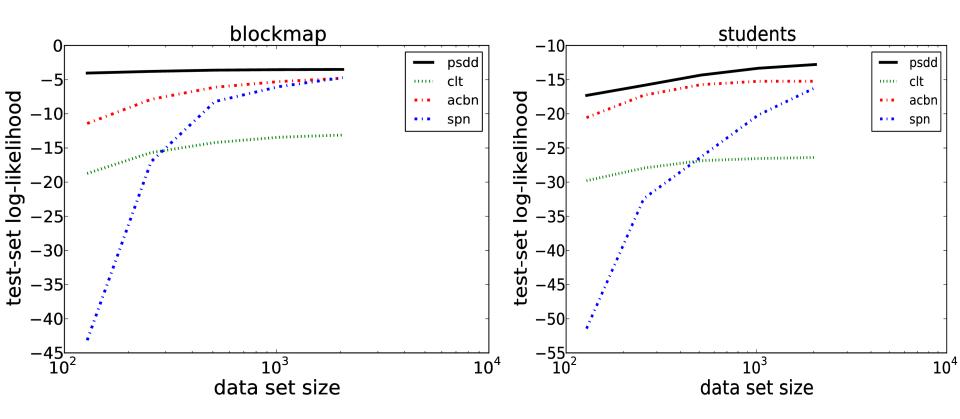
- Circuit learning (naïve): Compile constraints to SDD circuit
 - Use SAT solver technology
 - Circuit does not depend on data

Learning Preference Distributions



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

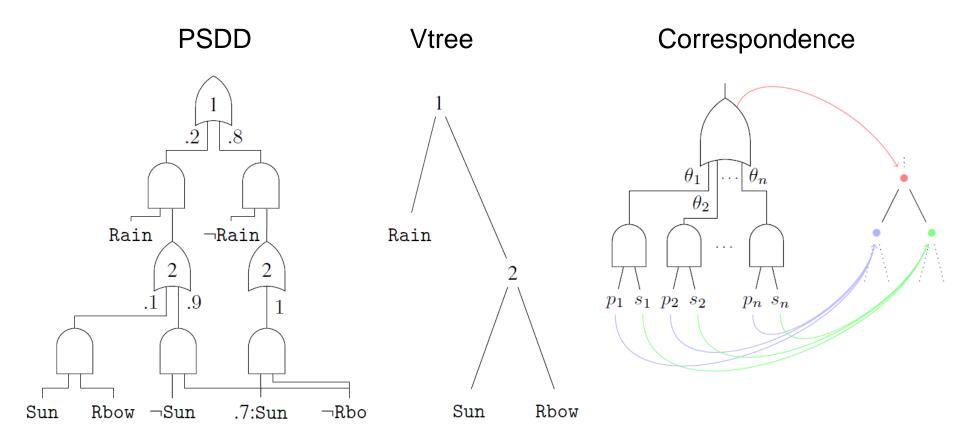
What happens if you **ignore** constraints?



Learn Circuit from Data

Even in unstructured spaces

Variable Trees (vtrees)

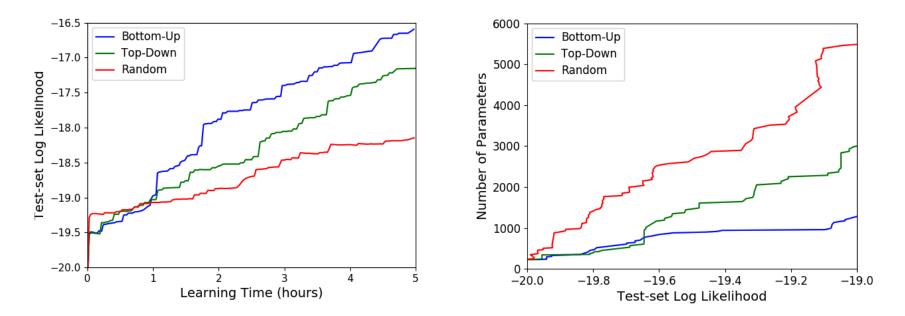


Learning Variable Trees

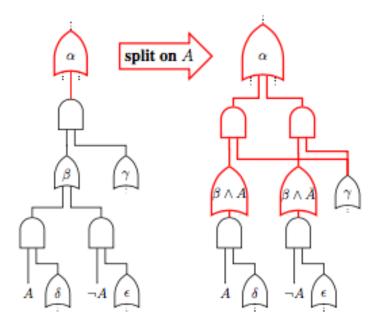
• How much do vars depend on each other?

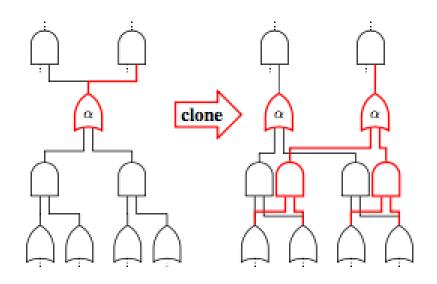
 $\mathrm{MI}(\mathbf{X},\mathbf{Y}) = \sum_{X \in \mathbf{X}} \sum_{Y \in \mathbf{Y}} \mathrm{Pr}(X,Y) \log \frac{\mathrm{Pr}(X,Y)}{\mathrm{Pr}(X) \, \mathrm{Pr}(Y)}$

Learn vtree by hierarchical clustering



Learning Primitives





Tractable Learning

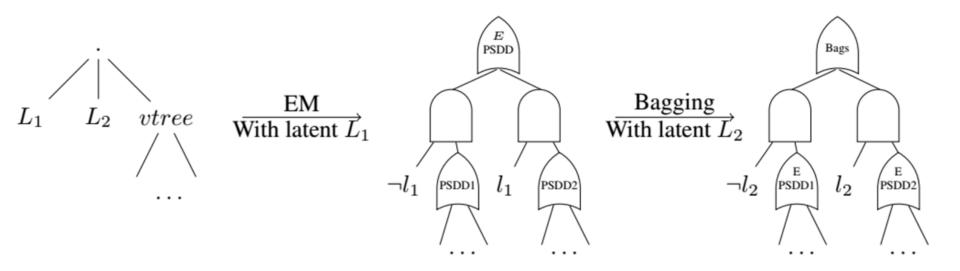
- Circuit size is measurement of tractability
- Trade off size and quality of model

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	x ₁	y ₂	Z ₁
2	x ₂	У ₁	Z ₂
3	x ₂	У ₁	Z ₂
4	x ₁	У ₁	Z ₁
5	x ₁	У ₂	Z ₂

a classical incomplete dataset

id	X	Y	Z
1	x ₁	У ₂	?
2	x ₂	У ₁	?
3	?	?	Z ₂
4	?	У ₁	Z ₁
5	x ₁	У ₂	Z ₂

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 st sushi	2 nd sushi	3 rd 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 st sushi	2 nd sushi	3 rd 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 st sushi	2 nd sushi	3 rd 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 st sushi	2 nd sushi	3 rd sushi	
1	(fatty tuna > sea urchin) and (tuna > sea eel)			
2	(fatty tuna is 1 st) 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

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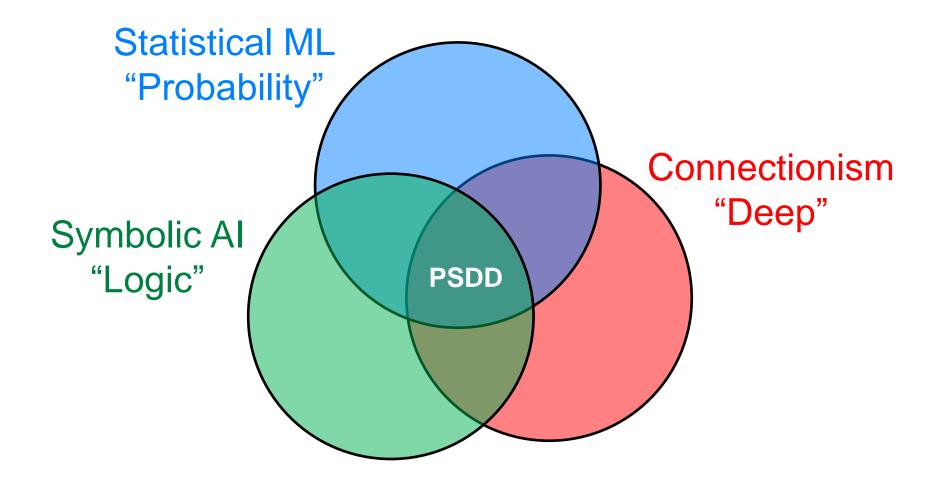
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Conclusions



Questions?



PSDD with 15,000 nodes