



Computational Probabilistic Models

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What is the right abstraction for distributions?

Probabilistic graphical models is how we do probabilistic AI!

Graphical models of variable-level (in)dependence are a broken abstraction.





What is the right abstraction for distributions?

Probabilistic graphical models is how we do probabilistic AI!

Graphical models of variable-level (in)dependence are a broken abstraction.

3.14 Smokes(x) \land Friends(x,y) \Rightarrow Smokes(y)



What is the right abstraction for distributions?

Probabilistic graphical models is how we do probabilistic AI!

Graphical models of variable-level (in)dependence are a broken abstraction.

```
Bean Machine

\mu_k \sim \text{Normal}(\alpha, \beta)
\sigma_k \sim \text{Gamma}(\nu, \rho)
\theta_k \sim \text{Dirichlet}(\kappa)
x_i \sim \begin{cases} \text{Categorical}(init) & \text{if } i = 0 \\ \text{Categorical}(\theta_{x_{i-1}}) & \text{if } i > 0 \end{cases}
y_i \sim \text{Normal}(\mu_{x_i}, \sigma_{x_i})
```



Computational Abstractions

Let us think of probability as something that is computed.

Abstraction = Structure of Computation

Two levels of abstraction:

Probabilistic Programs

Probabilistic Circuits

"High-level code"

"Machine code"

Probabilistic Circuits





Intractable and tractable models



a unifying framework for tractable models

Tractable Probabilistic Models



"Every talk needs a joke and a literature overview slide, not necessarily distinct" - after Ron Graham

Probabilistic circuits



Likelihood
$$p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$$



Likelihood $p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$



Likelihood
$$p(X_1 = -1.85, X_2 = 0.5, X_3 = -1.3, X_4 = 0.2)$$



Tractable marginals

A sum node is *smooth* if its children depend on the same set of variables.

A product node is *decomposable* if its children depend on disjoint sets of variables.



smooth circuit



decomposable circuit

Smoothness + decomposability = tractable MAR

If $m{p}(\mathbf{x}) = \sum_i w_i m{p}_i(\mathbf{x})$, (smoothness):

$$\int \mathbf{p}(\mathbf{x}) d\mathbf{x} = \int \sum_{i} w_{i} \mathbf{p}_{i}(\mathbf{x}) d\mathbf{x} =$$
$$= \sum_{i} w_{i} \int \mathbf{p}_{i}(\mathbf{x}) d\mathbf{x}$$

 \Rightarrow integrals are "pushed down" to children



Smoothness + decomposability = tractable MAR

If $p(\mathbf{x}, \mathbf{y}, \mathbf{z}) = p(\mathbf{x})p(\mathbf{y})p(\mathbf{z})$, (decomposability):

$$\int \int \int \mathbf{p}(\mathbf{x}, \mathbf{y}, \mathbf{z}) d\mathbf{x} d\mathbf{y} d\mathbf{z} =$$
$$= \int \int \int \int \mathbf{p}(\mathbf{x}) \mathbf{p}(\mathbf{y}) \mathbf{p}(\mathbf{z}) d\mathbf{x} d\mathbf{y} d\mathbf{z} =$$
$$= \int \mathbf{p}(\mathbf{x}) d\mathbf{x} \int \mathbf{p}(\mathbf{y}) d\mathbf{y} \int \mathbf{p}(\mathbf{z}) d\mathbf{z}$$



 \Rightarrow integrals decompose into easier ones

Smoothness + decomposability = tractable MAR

Forward pass evaluation for MAR

inear in circuit size!

E.g. to compute $p(x_2, x_4)$: leafs over X_1 and X_3 output $\mathbf{Z}_i = \int p(x_i) dx_i$ for normalized leaf distributions: 1.0

leafs over X_2 and X_4 output **EVI**

feedforward evaluation (bottom-up)



Learning Expressive Probabilistic Circuits

Hidden Chow-Liu Trees



Learning Expressive Probabilistic Circuits

Hidden Chow-Liu Trees







Lossless Data Compression



A Typical Streaming Code – Arithmetic Coding

We want to compress a set of variables (e.g., pixels, letters) $\{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_k\}$



Lossless Neural Compression with Probabilistic Circuits



Probabilistic Circuits

- Expressive \rightarrow SoTA likelihood on MNIST.
- Fast

- \rightarrow Time complexity of en/decoding is O(|p| log(D)), where D is the # variables and |p| is the size of the PC.

```
Arithmetic Coding:
  p(X_1 < x_1)
  p(X_1 \leq x_1)
  p(X_2 < x_2 | x_1)
  p(X_2 \leq x_2 | x_1)
  p(X_3 < x_3 | x_1, x_2)
  p(X_3 \leq x_3 | x_1, x_2)
```

Lossless Neural Compression with Probabilistic Circuits

SoTA compression rates

Dataset	HCLT (ours)	IDF	BitSwap	BB-ANS	JPEG2000	WebP	McBits
MNIST	1.24 (1.20)	1.96 (1.90)	1.31 (1.27)	1.42 (1.39)	3.37	2.09	(1.98)
FashionMNIST	3.37 (3.34)	3.50 (3.47)	3.35 (3.28)	3.69 (3.66)	3.93	4.62	(3.72)
EMNIST (Letter)	1.84 (1.80)	2.02 (1.95)	1.90 (1.84)	2.29 (2.26)	3.62	3.31	(3.12)
EMNIST (ByClass)	1.89 (1.85)	2.04 (1.98)	1.91 (1.87)	2.24 (2.23)	3.61	3.34	(3.14)

Compress and decompress 5-40x faster than NN methods with similar bitrates

Method	# parameters	Theoretical bpd	Codeword bpd	Comp. time (s)	Decomp. time (s)
PC (HCLT, $M = 16$)	3.3M	1.26	1.30	9	44
PC (HCLT, $M = 24$)	5.1M	1.22	1.26	15	86
PC (HCLT, $M = 32$)	7.0M	1.20	1.24	26	142
IDF	24.1M	1.90	1.96	288	592
BitSwap	2.8M	1.27	1.31	578	326

Lossless Neural Compression with Probabilistic Circuits

Can be effectively combined with Flow models to achieve better generative performance

Model	CIFAR10	ImageNet32	ImageNet64
RealNVP	3.49	4.28	3.98
Glow	3.35	4.09	3.81
IDF	3.32	4.15	3.90
IDF++	3.24	4.10	3.81
PC+IDF	3.28	3.99	3.71



Expressive models without compromises

Prediction with Missing Features



Test with missing features

Expected Predictions

Consider **all possible complete inputs** and **reason** about the *expected* behavior of the classifier

$$\mathbb{E}_{\mathbf{X}^m \sim p(\mathbf{x}^m | \mathbf{x}^o)} \begin{bmatrix} f(\mathbf{x}^m \mathbf{x}^o) \end{bmatrix} \qquad \begin{array}{l} \mathbf{x}^o = \text{observed features} \\ \mathbf{x}^m = \text{missing features} \end{array}$$

Experiment:

• f(x) = logistic regres.

p(x) =
 naive Bayes



[Khosravi et al. IJCAI19, NeurIPS20, Artemiss20]

Probabilistic Circuits for Missing Data



[Khosravi et al. IJCAI19, NeurIPS20, Artemiss20]

Tractable Computation of Expected Kernels

- How to compute the expected kernel given two distributions **p**, **q**?

$$\mathbb{E}_{\mathbf{x}\sim\mathbf{p},\mathbf{x}'\sim\mathbf{q}}[\mathbf{k}(\mathbf{x},\mathbf{x}')]$$

- Circuit representation for kernel functions, e.g., $\mathbf{k}(\mathbf{x}, \mathbf{x}') = \exp\left(-\sum_{i=1}^{4} |X_i - X'_i|^2\right)$

$$\exp(-|X_{1} - X_{1}'|^{2}) \bigwedge^{1} \bigoplus^{1} \bigoplus^{$$

Tractable Computation of Expected Kernels: Applications

- Reasoning about support vector regression (SVR) with missing features

$$\mathbb{E}_{\mathbf{x}_{m} \sim \mathbf{p}(\mathbf{X}_{m} | \mathbf{x}_{o})} \left[\sum_{i=1}^{m} w_{i} \mathbf{k}(\mathbf{x}_{i}, \mathbf{x}) + b \right]$$

missing
features SVR model

- Collapsed Black-box Importance Sampling: minimize kernelized Stein discrepancy

Model-Based Algorithmic Fairness: FairPC

Learn classifier given

- features S and X
- training labels/decisions D

Group fairness by demographic parity:

Fair decision D_f should be independent of the sensitive attribute S

Discover the **latent fair decision** D_f by learning a PC.



[Choi et al. AAAI21]

Probabilistic Sufficient Explanations

<u>Goal</u>: explain an instance of classification (a specific prediction)

Explanation is a subset of features, s.t.

 The explanation is "probabilistically sufficient"

> Under the feature distribution, given the explanation, the classifier is likely to make the observed prediction.

2. It is minimal and "simple"



Queries as pipelines: KLD

 $\mathbb{KLD}(p \parallel q) = \int p(\mathbf{x}) \times \log((p(\mathbf{x})/q(\mathbf{x}))d\mathbf{X})$



Queries as pipelines: Cross Entropy

 $H(p,q) = \int p(\boldsymbol{x}) \times \log(q(\boldsymbol{x})) d\boldsymbol{X}$



Determinism

A sum node is *deterministic* if only one of its children outputs non-zero for any input



 \Rightarrow allows **tractable MAP** inference $argmax_{x} p(x)$

deterministic circuit

Darwiche and Marquis, "A Knowledge Compilation Map", 2002

Operation			Tractability
		Input conditions	Output conditions
Log	$\log(p)$	Sm, Dec, Det	Sm, Dec
	$\Delta $		
	smooth,		smooth,
	decomposable,		decomposable
	deterministic		

Tractable circuit operations

Operation			II	
		Input properties	Output properties	Hardness
SUM	$\theta_1 p + \theta_2 q$	(+Cmp)	(+SD)	NP-hard for Det output
PRODUCT	$p\cdot q$	Cmp (+Det, +SD)	Dec (+Det, +SD)	#P-hard w/o Cmp
POWER	$p^n, n \in \mathbb{N}$	SD (+Det)	SD (+Det)	#P-hard w/o SD
	$p^{\alpha}, \alpha \in \mathbb{R}$	Sm, Dec, Det (+SD)	Sm, Dec, Det (+SD)	#P-hard w/o Det
QUOTIENT	p/q	Cmp; q Det (+ p Det,+SD)	Dec (+Det,+SD)	#P-hard w/o Det
LOG	$\log(p)$	Sm, Dec, Det	Sm, Dec	#P-hard w/o Det
Exp	$\exp(p)$	linear	SD	#P-hard

Inference by tractable operations

systematically derive tractable inference algorithm of complex queries

	Query	Tract. Conditions	Hardness
CROSS ENTROPY	$-\int p(oldsymbol{x})\log q(oldsymbol{x})\mathrm{d}\mathbf{X}$	Cmp, q Det	#P-hard w/o Det
SHANNON ENTROPY	$-\sum p(oldsymbol{x})\log p(oldsymbol{x})$	Sm, Dec, Det	coNP-hard w/o Det
Ρέννι Εντροργ	$(1-lpha)^{-1}\log\int p^lpha(oldsymbol{x})d\mathbf{X}, lpha\in\mathbb{N}$	SD	#P-hard w/o SD
KENTT ENTROPT	$(1-lpha)^{-1}\log\int p^lpha(oldsymbol{x})d\mathbf{X}, lpha\in\mathbb{R}_+$	Sm, Dec, Det	#P-hard w/o Det
MUTUAL INFORMATION	$\int p(oldsymbol{x},oldsymbol{y}) \log(\hat{p}(oldsymbol{x},oldsymbol{y})/(p(oldsymbol{x})p(oldsymbol{y})))$	Sm, SD, Det*	coNP-hard w/o SD
KULLBACK-LEIBLER DIV.	$\int p(oldsymbol{x}) \log(p(oldsymbol{x})/q(oldsymbol{x})) d \mathbf{X}$	Cmp, Det	#P-hard w/o Det
RÉNVI'S AIDHA DIV	$(1-lpha)^{-1}\log\int p^{lpha}(oldsymbol{x})q^{1-lpha}(oldsymbol{x})\;d\mathbf{X},lpha\in\mathbb{N}$	Cmp, q Det	#P-hard w/o Det
RENTI 5 ALFIIA DIV.	$(1-lpha)^{-1}\log \int p^{lpha}(\boldsymbol{x})q^{1-lpha}(\boldsymbol{x}) d\mathbf{X}, lpha \in \mathbb{R}$	Cmp, Det	#P-hard w/o Det
Itakura-Saito Div.	$\int [p(oldsymbol{x})/q(oldsymbol{x}) - \log(p(oldsymbol{x})/q(oldsymbol{x})) - 1] d \mathbf{X}$	Cmp, Det	#P-hard w/o Det
CAUCHY-SCHWARZ DIV.	$-\lograc{\int p(oldsymbol{x})q(oldsymbol{x})d\mathbf{X}}{\sqrt{\int p^2(oldsymbol{x})d\mathbf{X}\int q^2(oldsymbol{x})d\mathbf{X}}}$	Cmp	#P-hard w/o Cmp
SQUARED LOSS	$\int (p(oldsymbol{x}) - q(oldsymbol{x}))^2 d \mathbf{X}$	Cmp	#P-hard w/o Cmp

Even harder queries

Marginal MAP

Given a set of query variables $Q \subset X$ and evidence e, find: $argmax_q p(q|e)$

 \Rightarrow i.e. MAP of a marginal distribution on **Q**

NP^{PP}-complete for PGMs

NP-hard even for PCs tractable for marginals, MAP & entropy

Pruning circuits



Any parts of circuit not relevant for MMAP state can be pruned away

e.g.
$$p(X_1 = 1, X_2 = 0)$$

We can find such edges in *linear time*

Iterative MMAP solver

Prune edges

	runtime (# solved) 🛛 🧹			
Dataset	search	pruning		
NLTCS	0.01 (10)	0.63 (10)		
MSNBC	0.03 (10)	0.73 (10)		
KDD	0.04 (10)	0.68 (10)		
Plants	2.95 (10)	2.72 (10)		
Audio	2041.33 (6)	13.70 (10)		
Jester	2913.04 (2)	14.74 (10)		
Netflix	- (0)	47.18 (10)		
Accidents	109.56 (10)	15.86 (10)		
Retail	0.06 (10)	0.81 (10)		
Pumsb-star	2208.27 (7)	20.88 (10)		
DNA	- (0)	505.75 (9)		
Kosarek	48.74 (10)	3.41 (10)		
MSWeb	1543.49 (10)	1.28 (10)		
Book	- (0)	46.50 (10)		
EachMovie	- (0)	1216.89 (8)		
WebKB	- (0)	575.68 (10)		
Reuters-52	- (0)	120.58 (10)		
20 NewsGrp.	- (0)	504.52 (9)		
BBC	– (0)	2757.18 (3)		
Ad	– (0)	1254.37 (8)		



tractability is a spectrum





Learn more about probabilistic circuits?



Tutorial (3h)

Inference

Learning

Theory

Representations

Probabilistic Circuits

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September 14th, 2020 - Ghent, Belgium - ECML-PKDD 2020

▶ ▶| ➡) 0:00 / 3:02:44

•••

https://youtu.be/2RAG5-L9R70

Overview Paper (80p)

Probabilistic Circuits: A Unifying Framework for Tractable Probabilistic Model	\mathbf{s}^*
YooJung Choi	
Antonio Vergari	
Guy Van den Broeck Computer Science Department University of California Los Angeles, CA, USA	
1 Introduction 2 Probabilistic Inference: Models, Queries, and Tractability 2.1 Probabilistic Models 2.2 Probabilistic Queries 2.3 Tractable Probabilistic Inference 2.4 Properties of Tractable Probabilistic Models	3 4 5 6 8 9

http://starai.cs.ucla.edu/papers/ProbCirc20.pdf

Probabilistic Programs



Motivation from the AI side: Making modern AI systems is **too hard**





System Builders

Model Builders

AI System Builder

Need to integrate uncertainty over the whole system



20% chance of obstacle! 94% chance of obstacle! 99% certain about current location

Inside the Self-Driving Tesla Fatal Accident

By ANJALI SINGHVI and KARL RUSSELL UPDATED July 12, 2016

The accident may have happened in part because the crash-avoidance system is designed to engage only when radar and computer vision systems agree that there is an obstacle, according to an industry executive with direct

Al Model Builder



"When you have the flu you have a cough 70% of the time"



"Routers fail on average every 5 years"

"What is the probability that a patient with a fever has the flu?" "What is the probability that my packet will reach the target server?" [SGTVV SIGCOMM'20]

Probabilistic Programs

```
let x = flip 0.5 in
let y = flip 0.7 in
let z = x || y in
let w = if z then
    my func(x,y)
else
     . . .
in
observe(z)
```

means "flip a coin, and output true with probability 1/2"

Standard (functional) programming constructs: let, if, ...

means

"reject this execution if z is not true"

Why Probabilistic Programming?



Venture, Church, IBAL, WebPPL, Infer.NET, Tensorflow Probability, ProbLog, PRISM, LPADs, CPLogic, CLP(BN), ICL, PHA, Primula, Storm, Gen, PRISM, PSI, Bean Machine, etc. ... and many many more

- Programming languages are humanity's biggest knowledge representation achievement!
- Programs should be AI models

Focus on Discrete Models

- Real programs have inherently discrete structure (e.g. if-statements)
- Discrete structure is inherent in many domains (graphs, text, ranking, etc.)
- 3. Many existing PPLs assume smooth and differentiable densities and do not handle discreteness well.

Web**PPL**



Does not support if-statements!

coroutines. Whenever a discrete variable is encountered in a program's execution, the program is suspended and resumed multiple times with all possible values in the support of that distribution. Listing 10, which implements a simple finite [AADB+'19]

Discrete probabilistic programming is the important unsolved open problem!

Dice language for discrete probabilistic programs

http://dicelang.cs.ucla.edu/

[Holtzen et al. OOPSLA20]



Network Verification in Dice



fun n1(init: bool) {
 let l1succeed = flip 0.99 in
 let l2succeed = flip 0.91 in
 init && l1succeed && l2succeed

fun n2(init: bool) {
 let routeChoice = flip 0.5 in
 if routeChoice then
 init && flip 0.88 && flip 0.93
 else

init && flip 0.19 && flip 0.33

ECMP equal-cost path protocol: choose randomly which router to forward to Main routine, combines the networks

n2(n2(n1(true)))

Network Verification i



This doesn't show all the language features of dice:

- Integers
- Tuples

. . .

- **Bounded recursion**
- **Bayesian conditioning**

fun n2(init: bool) { let routeChoice = flip 0.5 in if routeChoice then init && flip 0.88 && flip 0.93 else

init && flip 0.19 && flip 0.33

ECMP equal-cost path protocol: choose randomly which router to forward to

let 1

let 12

init &

Main routine, combines the networks

n2(n2(n1(true)))

Probabilistic Program Inference



0.99 x 0.91 x 0.5 x 0.88 x 0.93 x 0.5 x 0.88 x 0.93

- + 0.99 x 0.91 x 0.5 x 0.19 x 0.33 x 0.5 x 0.88 x 0.93
- + ...

Probabilistic Program Inference

Path enumeration: find all of them!





Key to Fast Inference: Factorization (product nodes)



how about on the program?

Symbolic Compilation in Dice

- Construct Boolean formula
- Satisfying assignments ≈ paths
- Variables are flips
- Associate weights with flips
- Compile factorized circuit

1 let x = flip₁ 0.1 in 2 let y = if x then flip₂ 0.2 else 3 flip₃ 0.3 in 4 let z = if y then flip₄ 0.4 else 5 flip₅ 0.5 in z

$$\underbrace{\begin{array}{c}0.1\\x=T\end{array}}_{x=T} \cdot \underbrace{0.2}_{y=T} \cdot \underbrace{0.4}_{z=T} + \underbrace{0.1}_{x=T} \cdot \underbrace{0.8}_{y=F} \cdot \underbrace{0.5}_{z=T} + \underbrace{0.9}_{x=F} \cdot \underbrace{0.3}_{y=T} \cdot \underbrace{0.4}_{z=T} + \underbrace{0.9}_{x=F} \cdot \underbrace{0.7}_{y=F} \cdot \underbrace{0.5}_{z=T} \\ \underbrace{\begin{array}{c}471\\(f_1)\\(48)(f_2)\\(48)(f_2)\\(4)(f_4)\\(4)(f_4)\\(5)(5)\\(1)(T)\\($$

Symbolic Compilation in Dice to **Probabilistic Circuits**



Experimental Evaluation

• Example from text analysis: breaking a Caesar cipher



More program paths than atoms in the universe

 Competitive with specialized Bayesian network solvers

 $10^0 \ 10^1 \ 10^2 \ 10^3 \ 10^4$

Characters

Time (ms)

 10^{5} 10^{4} 10^{3}

 10^{2}

$\operatorname{Benchmark}$	Psi (ms)	DP (ms)	Dice (ms)	# Parameters	# Paths	BDD Size
Cancer	772	46	13	10	1.1×10^{3}	28 /
Survey	2477	152	13	21	1.3×10^{4}	73 /
Alarm	X	X	25	509	1.0×10^{36}	1.3×10^{3}
Insurance	X	X	212	984	1.2×10^{40}	1.0×10^{5}
Hepar2	X	×	54	48	$2.9 imes 10^{69}$	1.3×10^{3}
Hailfinder	X	×	618	2656	$2.0 imes 10^{76}$	6.5×10^4
Pigs	X	×	72	5618	$7.3 imes 10^{491}$	2/35
Water	X	X	2590	$1.0 imes10^4$	$3.2{ imes}10^{54}$	5.1×10^{4}
Munin	X	X	1866	8.1×10^5	2.1×10^{162}	1.1×10^4

Better Inference. How?

Exploit modularity - program structure

1. <u>AI modularity</u>:

Discover contextual independencies and factorize

2. <u>PL modularity</u>:

Compile procedure summaries and reuse at each call site

Reason about programs! Compiler optimizations:

- 3. Flip hoisting optimization
- 4. Determinism, optimize integer representation, etc.

Flip Hoisting

1	let $x = flip 0.1$ in	1 let $x = flip 0.1$ in let $z = flip 0.2$	in
2	let $z = flip 0.2$ in	<pre>2 let tmp = flip 0.3 in</pre>	
3	<pre>let y = if x && z then flip 0.3</pre>	3 let y = if x && z then tmp	
4	else if x && !z then flip 0.4	4 else if x && !z then flip 0.4	
5	else flip 0.3	5 else tmp	
6	in y	6 in y	

- Fewer flips = smaller compiled circuits = faster
- But, be careful with soundness:

If you build it they will come

As soon as *dice* was put online people started using it in surprising ways we had not foreseen



Quantum Simulation



Probabilistic Model Checking



If you build it they will come

In both cases, *dice* outperforms existing specialized methods on important examples!



Probabilistic Model Checking



Quantum Simulation



Competitive with well-known simulators like Google qsim and qtorch [FSC+ PloS one '18] !

Computational Abstractions

Let us think of probability as something that is computed.

Abstraction = Structure of Computation

Two levels of abstraction:

Probabilistic Programs

Probabilistic Circuits

"High-level code"

"Machine code"

Thanks

This was the work of many wonderful students/postdoc/collaborators!

References: http://starai.cs.ucla.edu/publications/