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STAR AI

Polynomial semantics of probabilistic circuits

Oliver Broadrick, Honghua Zhang, Guy VdB – UAI 2024

The limits of tractable marginalization

Oliver Broadrick, Sanyam Agarwal, Markus Bläser, Guy VdB – ICML 2025

Marginal Inference

X_1	X_2	Pr
0	0	.1
0	1	.2
1	0	.3
1	1	.4

$$\begin{aligned}\Pr[X_1 = 1] &= \Pr[X_1 = 1, X_2 = 0] + \Pr[X_1 = 1, X_2 = 1] \\ &= 0.3 + 0.4 \\ &= 0.7\end{aligned}$$

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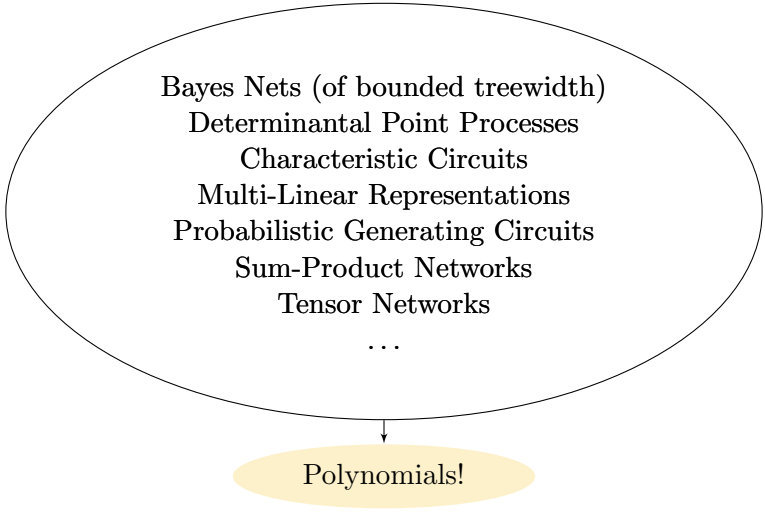
Goal: Find maximally expressive-efficient models that support marginal inference in time polynomial in the model size.

Approaches

Bayes Nets (of bounded treewidth)
Determinantal Point Processes
Characteristic Circuits
Multi-Linear Representations
Probabilistic Generating Circuits
Sum-Product Networks
Tensor Networks
...

Approaches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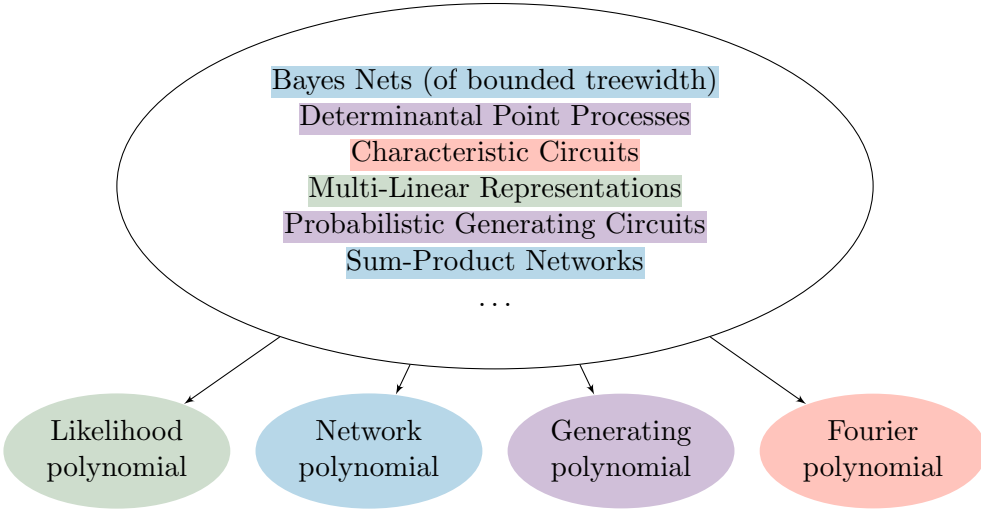
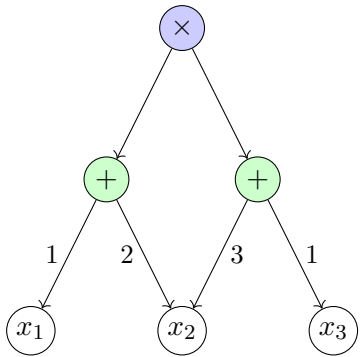
Polynomials!

How to encode distributions in polynomials?



Circuits represent polynomials succinctly



$$3x_1x_2 + x_1x_3 + 6x_2^2 + 2x_2x_3$$

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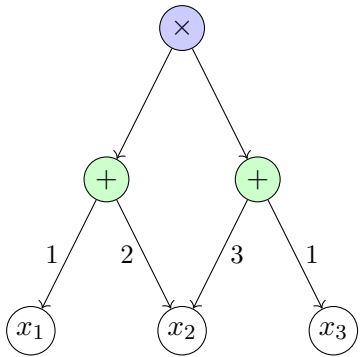

Circuits are *fully expressive*

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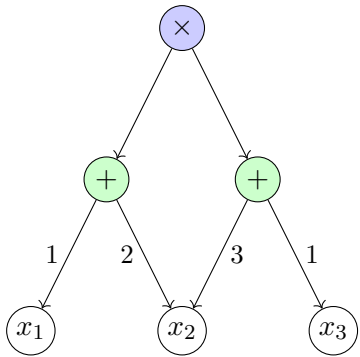
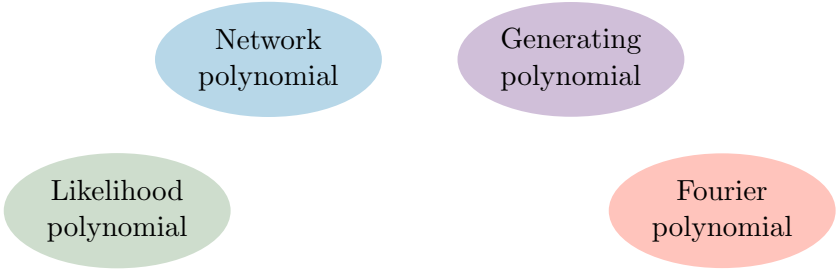


$$3x_1x_2 + x_1x_3 + 6x_2^2 + 2x_2x_3$$

Circuits are *fully expressive*

They can also be *expressive-efficient*

Polynomial Semantics



Polynomial Semantics

Darwiche [2003]

Network polynomial

Zhang et al. [2021]

Generating polynomial

Likelihood polynomial

Roth and Samdani [2009]

Fourier polynomial

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Polynomial Semantics

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Network polynomial

$$p(x_1, x_2, \bar{x}_1, \bar{x}_2) = .1\bar{x}_1\bar{x}_2 + .2\bar{x}_1 x_2 + .3x_1\bar{x}_2 + .4x_1 x_2$$

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0	0	.1
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$$\begin{aligned}
\Pr[X_1 = 1] &= p(1, 1, 0, 1) \\
&= .1(0)(1) + .2(0)(1) + .3(1)(1) + .4(1)(1) \\
&= 0 + 0 + .3 + .4 \\
&= .7
\end{aligned}$$

Network polynomial

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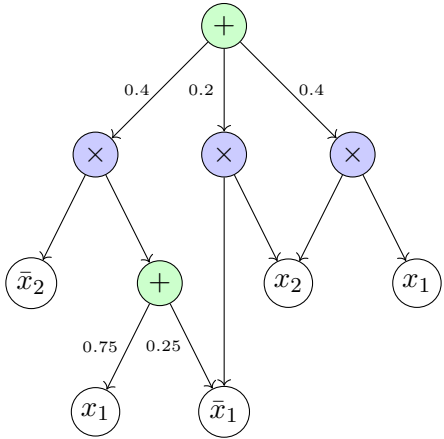

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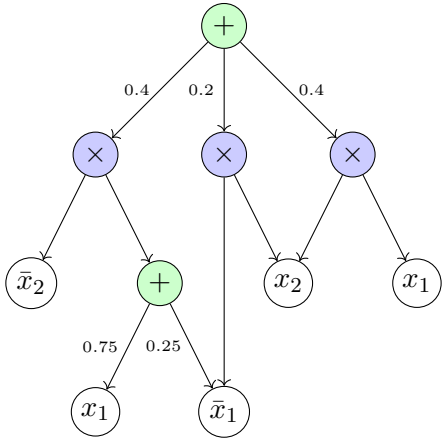

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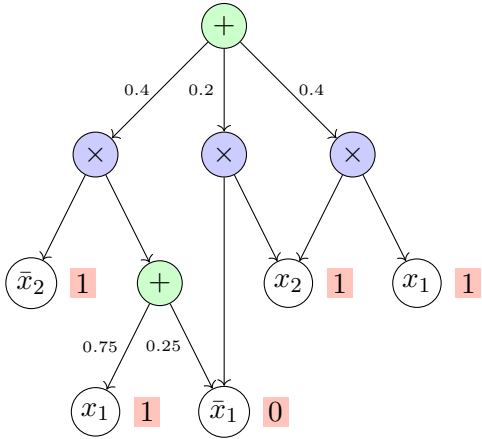

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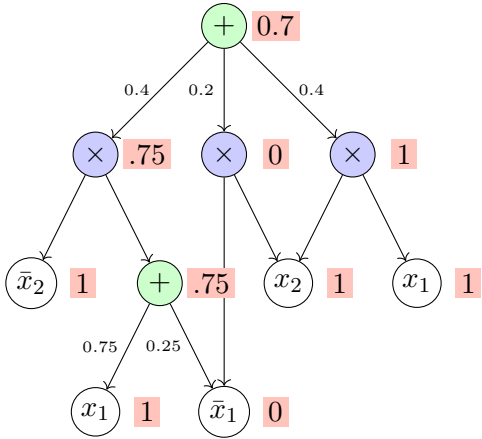

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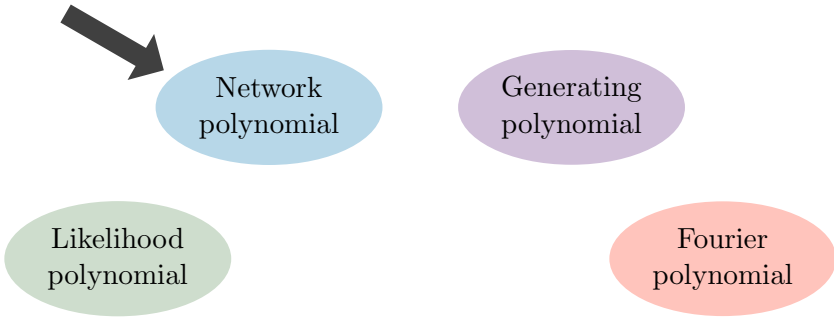
Progress Update



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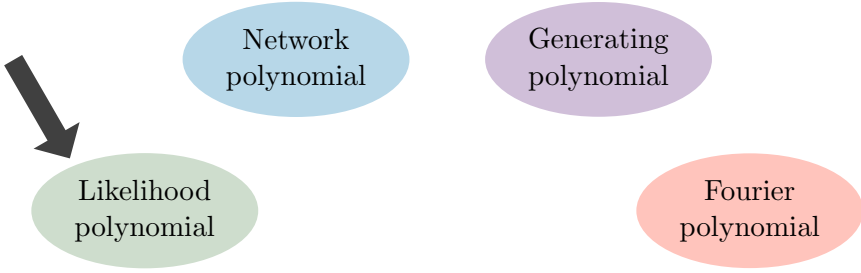

Likelihood polynomial

$p(x_1, x_2) = .2x_1 + .1x_2 + .1$

$\approx$ A neural net that for an input vector outputs its probability

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Marginal inference?

Relation to network polynomial?

(1) Transform network to likelihood:

$p(x, \bar{x}) = .1\bar{x}_1\bar{x}_2 + .2\bar{x}_1x_2 + .3x_1\bar{x}_2 + .4x_1x_2$

$\rightarrow$ Replace $\bar{x}_i$ with $1 - x_i$

Likelihood polynomial

(2) Transform likelihood to network:

$p(x_1, x_2) = .2x_1 + .1x_2 + .1$

Likelihood polynomial

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$p(x_1, x_2) = .2x_1 + .1x_2 + .1$

$$(x_1 + \bar{x}_1)(x_2 + \bar{x}_2)\left(.2\frac{x_1}{x_1 + \bar{x}_1} + .1\frac{x_2}{x_2 + \bar{x}_2} + .1\right)$$

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$$= .2x_1(x_2 + \bar{x}_2) + .1x_2(x_1 + \bar{x}_1) + .1(x_1 + \bar{x}_1)(x_2 + \bar{x}_2)$$

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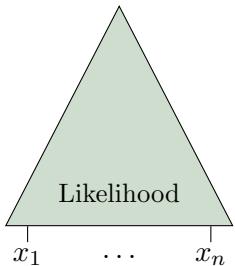
&= .2x_1(x_2 + \bar{x}_2) + .1x_2(x_1 + \bar{x}_1) + .1(x_1 + \bar{x}_1)(x_2 + \bar{x}_2) \\
&= p(x_1, x_2, \bar{x}_1, \bar{x}_2)
\end{aligned}
$$

Likelihood polynomial

Transform likelihood to network:



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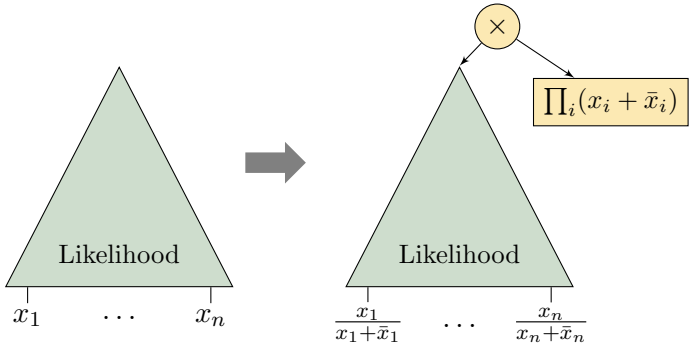

Removing Divisions

Theorem (Strassen [1973]). *You can remove divisions in polynomial time!*

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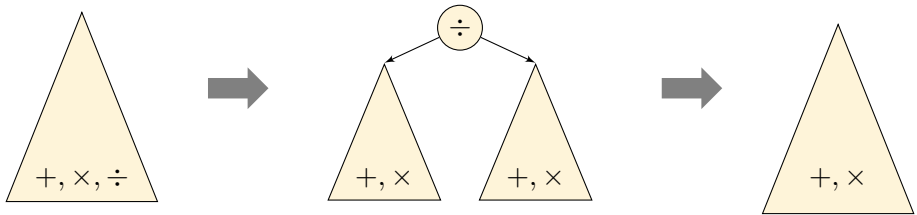

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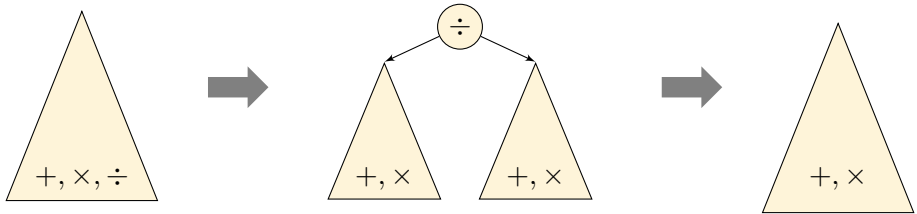

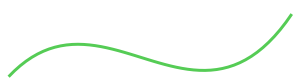

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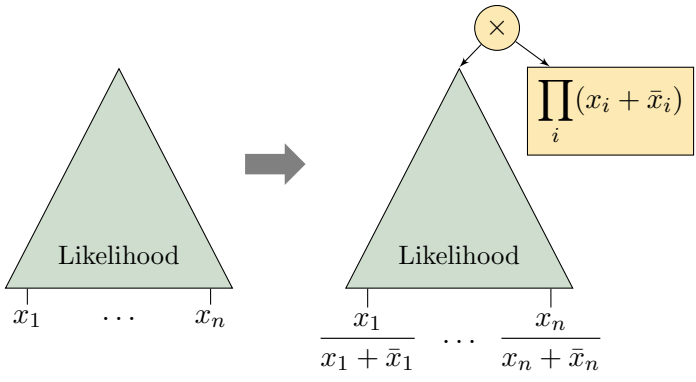

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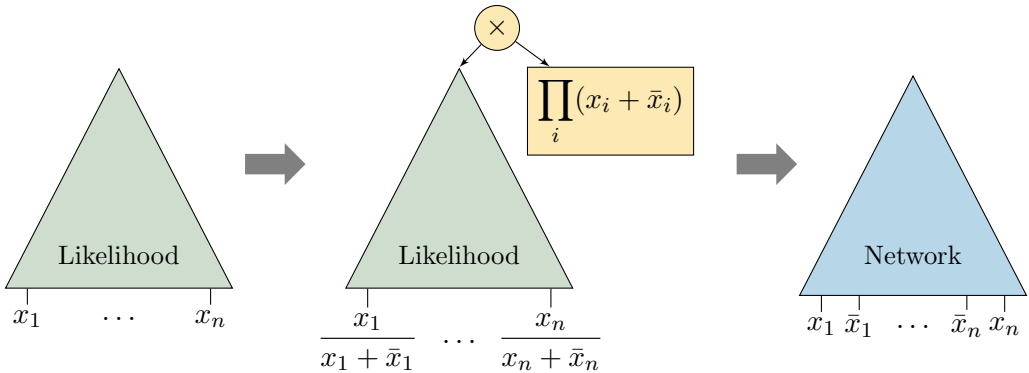
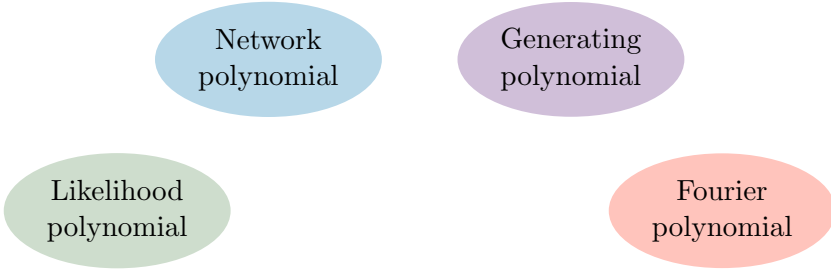


Progress Update



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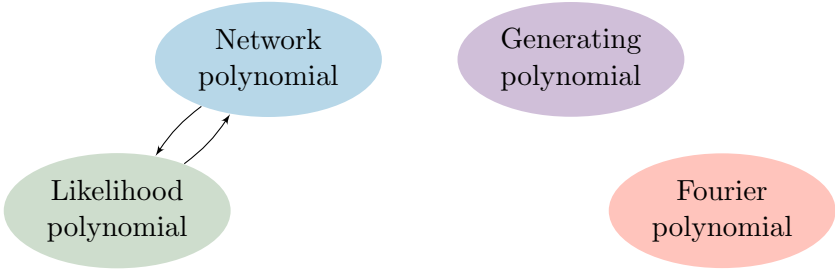

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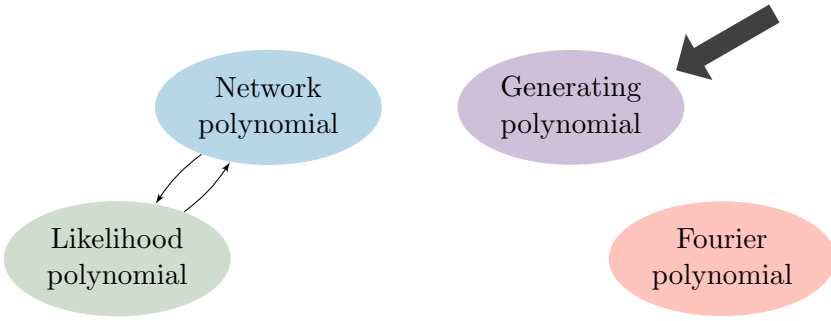
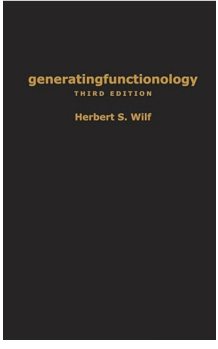


Generating polynomial



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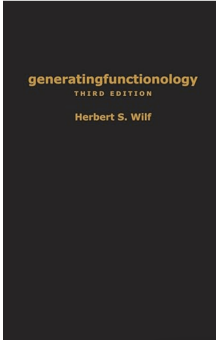
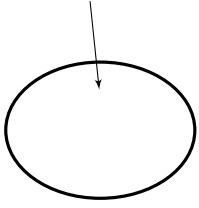


Monotone, decomposable circuits computing network polynomials (SPNs, PCs)



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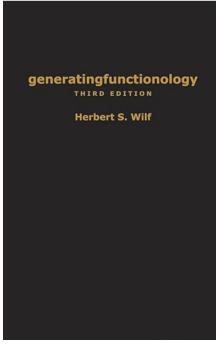

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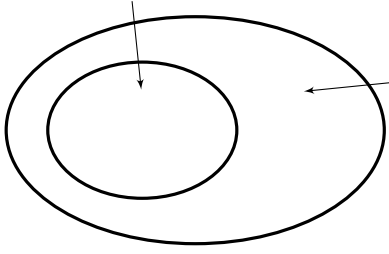
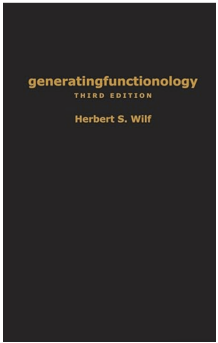
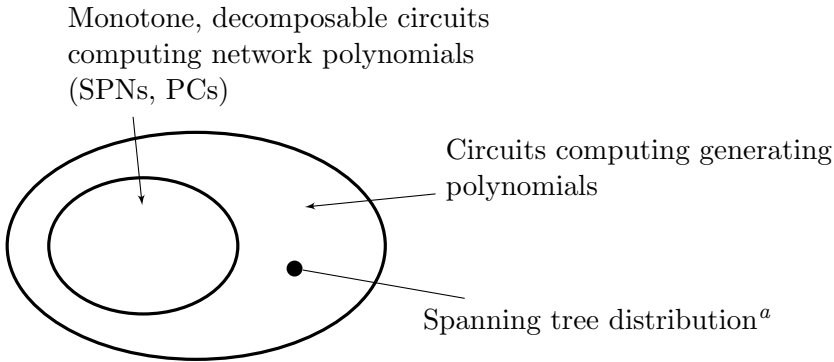


Circuits computing generating polynomials

Generating polynomial





[a]Martens and Medabalimi [2015], Zhang et al. [2021]

Generating polynomial

$$g(x) = .1 + .2x_2 + .3x_1 + .4x_1x_2$$

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Marginal inference: ✓ [Zhang et al., 2021]

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Relation to network polynomial?

(1) Transform network to generating:

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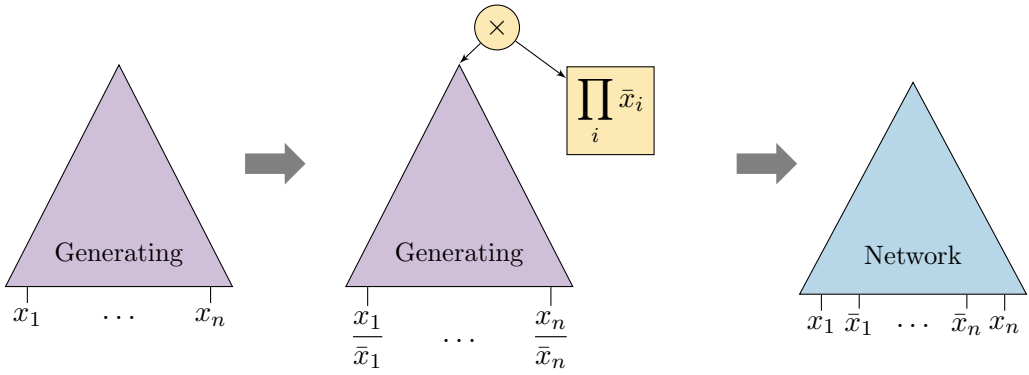
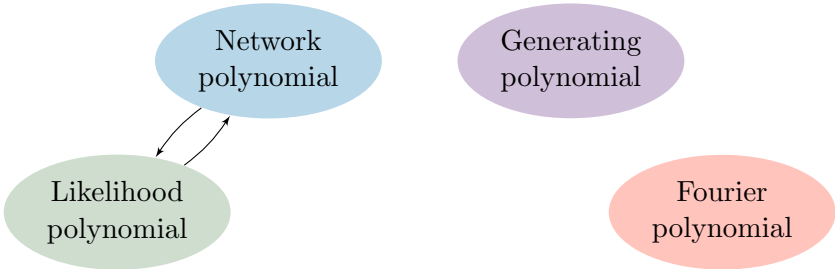
$\rightarrow$ Replace $\bar{x}_i$ with 1

Generating polynomial

(2) Transform generating to network:



Progress Update



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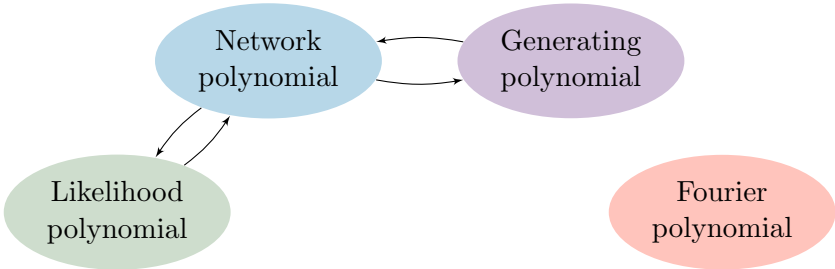

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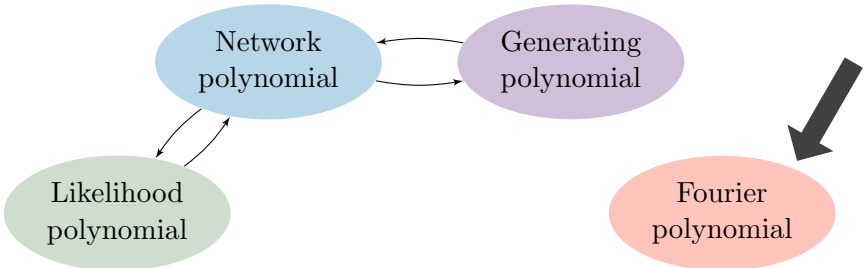
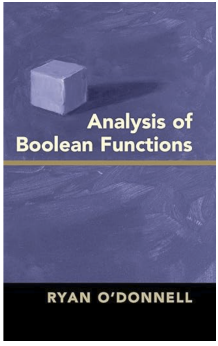


Fourier Polynomial



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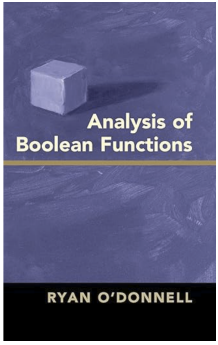
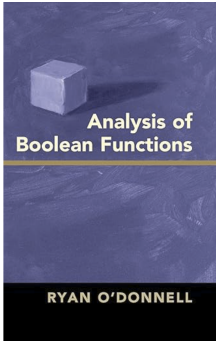


Fourier transform of the probability mass function

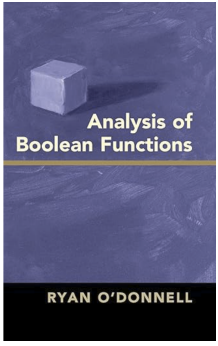
Fourier Polynomial



Fourier transform of the probability mass function

- Graphical model approximate inference
- Characteristic Circuits

Fourier Polynomial



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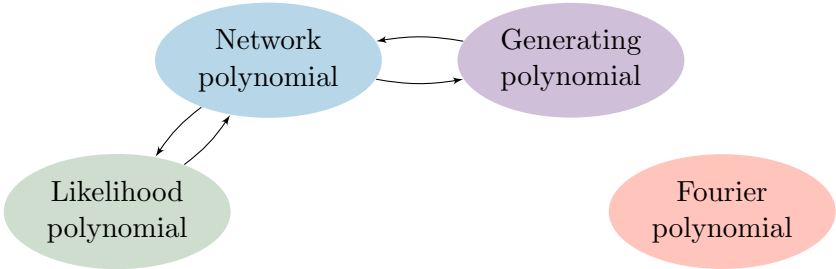
- Graphical model approximate inference
- Characteristic Circuits

Proposition. *Generating polynomials and Fourier polynomials compute* ***the same function*** *on respective domains* $\{-1,1\}^n$ *and* $\{0,1\}^n$.

Progress Update



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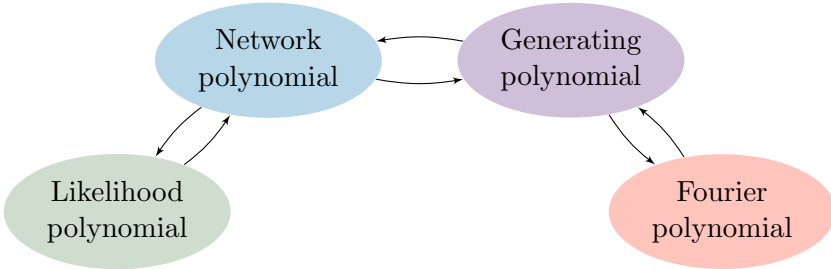
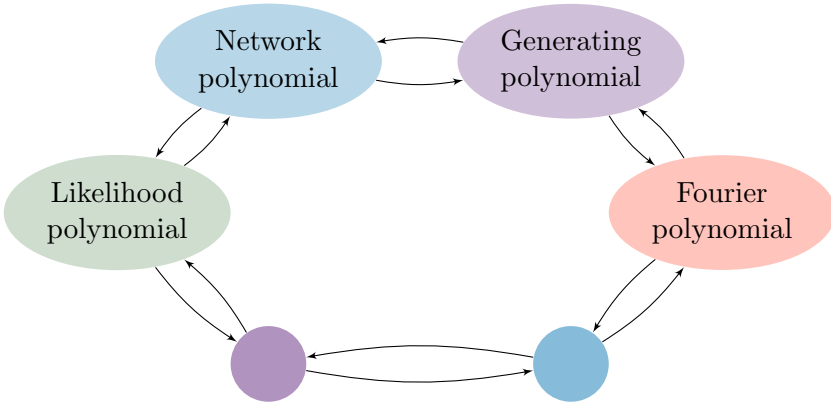


Some New Semantics



Non-binary variables?

X_1	X_2	Pr
0	1	.1
1	3	.3
3	2	.2
⋮	⋮	⋮

Non-binary variables?

Literature: just use a binary encoding

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Generating polynomial

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Generating polynomial

Theorem. *For $|K| \geq 4$, computing likelihoods on a circuit for $g(x)$ is #P-hard.*

Approach: Reduction from $0,1$-permanent.

Midway Conclusion

What we've done:

- Shown several distinct circuit models are equally expressive-efficient
- Unified existing (and one new) inference algorithms
- Inference is #P-hard in generating polynomials circuits for $k \geq 4$ categories

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- Unified existing (and one new) inference algorithms
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What's next?

- How can this theoretical progress be leveraged in practice?
- Are there more expressive-efficient tractable representations?

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Polynomial semantics of probabilistic circuits

Oliver Broadrick, Honghua Zhang, Guy VdB – UAI 2024

The limits of tractable marginalization

Oliver Broadrick, Sanyam Agarwal, Markus Bläser, Guy VdB – ICML 2025

Uniform Finally Multilinear Arithmetic Circuits (UFMAC)

$$f : \{0,1\}^n \to \mathbb{R}$$

$$p(x_1, \ldots, x_n) = \sum_{S \subseteq \{1,\ldots,n\}} f([S]) \prod_{i \in S} x_i \prod_{i \notin S} (1 - x_i)$$

X_1	X_2	f
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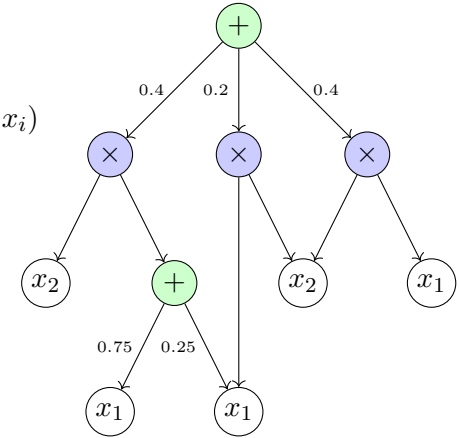

$$p(x_1, x_2) = .1(1 - x_1)(1 - x_2) + .2(1 - x_1)x_2 + .3x_1(1 - x_2) + .4x_1x_2$$

Functions Tractable for Marginalization

Let $f : \{0,1\}^n \to \{0,1\}$ be a function (family).

Define $\mathsf{PM}(f)$, the marginalization problem for f, which on input $m \in \{0,1,*\}^n$, asks for $\sum_{x \in M_m} f(x)$ where $M_m = \{x \in \{0,1\}^n : m_i \in \{0,1\} \implies x_i = m_i\}$.

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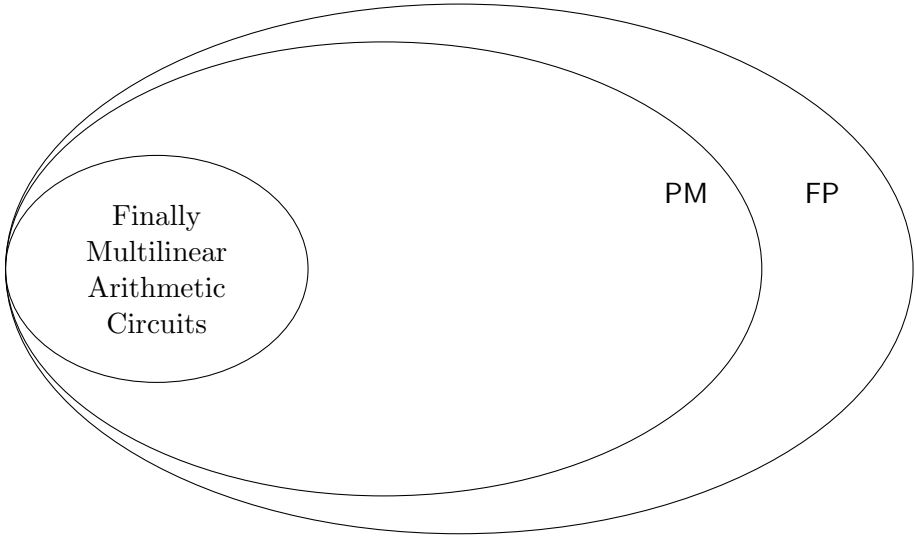
E.g., the earlier example was an instance of $\mathsf{PM}(\Pr)$ with input $m = 1*$.

X_1	X_2	Pr
0	0	.1
0	1	.2
1	0	.3
1	1	.4

$$\begin{aligned}\Pr[X_1 = 1] &= \Pr[X_1 = 1, X_2 = 0] + \Pr[X_1 = 1, X_2 = 1] \\ &= 0.3 + 0.4 \\ &= 0.7\end{aligned}$$


Finally
Multilinear
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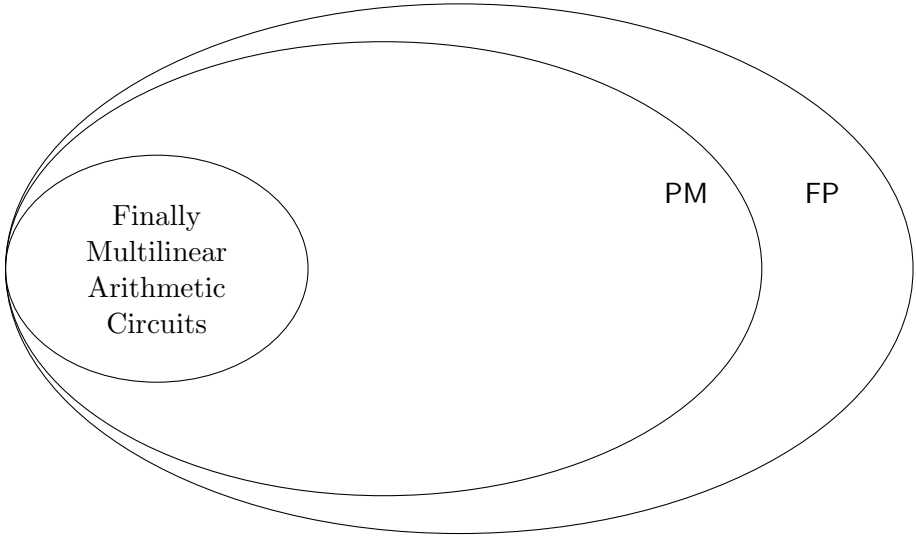
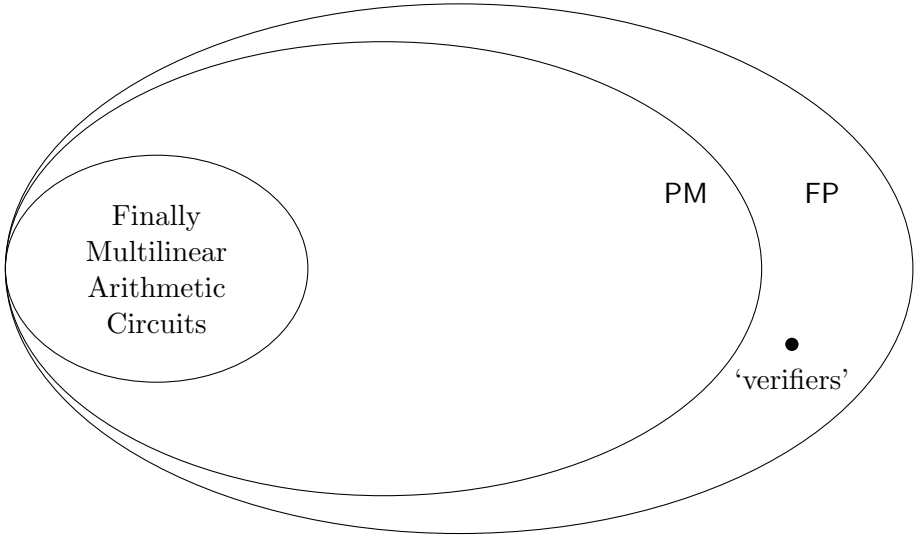
PM
FP



Main Question: Does every function family with tractable marginalization have uniform finally multilinear arithmetic circuits of polynomial size?



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Find stronger queries that are tractable for finally multilinear arithmetic circuits

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Evaluate circuit on any real point
(Virtual evidence marginalization)

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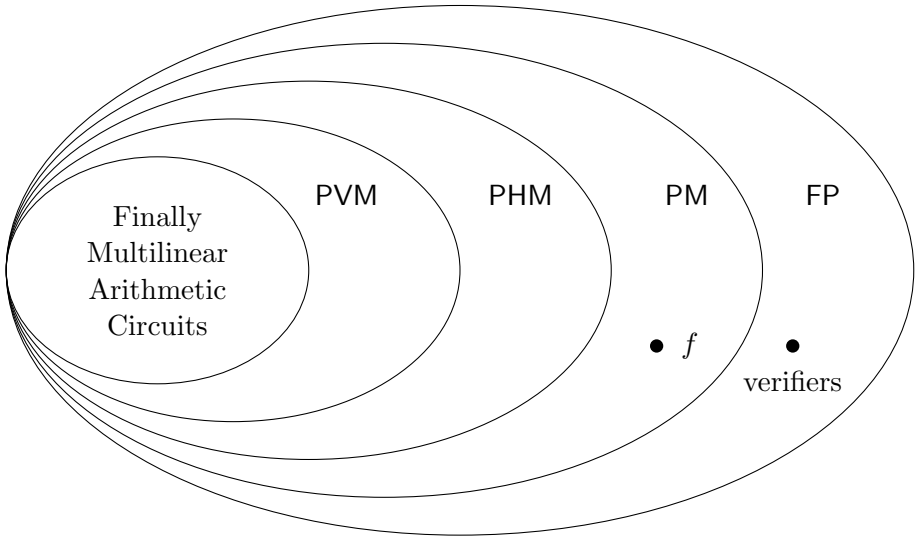
Sum over inputs of a given Hamming weight
(Hamming weight marginalization)

Our Approach



Hamming weight marginalization

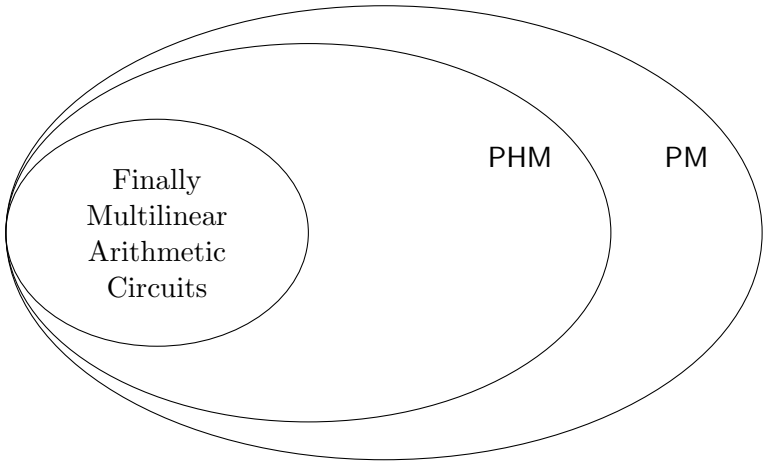
Let $f : \{0,1\}^n \to \{0,1\}$. Define $\mathsf{PHM}(f)$ which on input $m \in \{0,1,*\}^n$ and $k \in \{0,1,2,\ldots,n\}$, asks for

$$\sum_{x \in M_{m,k}} f(x)$$

where

$$M_{m,k} = \{x \in \{0,1\}^n : (m_i \in \{0,1\} \implies x_i = m_i) \wedge (|x| = k)\}.$$

Hamming weight marginalization



Hamming weight marginalization

x_1	x_2	x_3	x_4	Pr
0	0	0	0	.25
0	1	0	1	.05
1	0	0	0	.05
1	0	0	1	.05
1	0	1	0	.10
1	0	1	1	.50

Input:
$m = 10 * *$
$k = 2$

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Output:
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Use the *network polynomial*:

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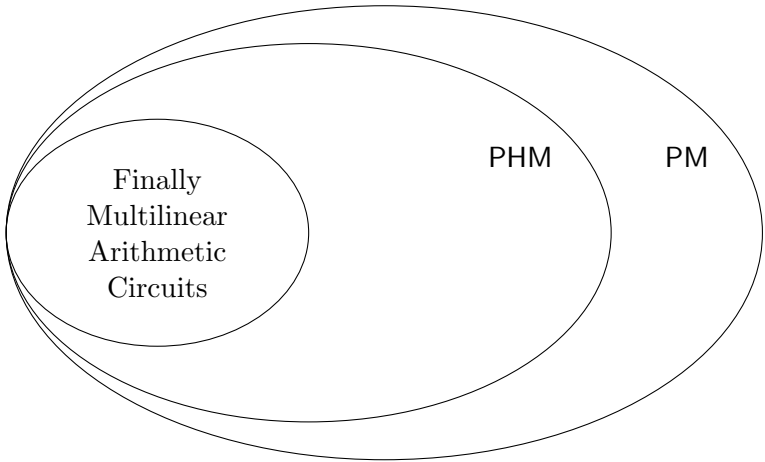
Substitute as follows:

x_1	$\bar{x}_1$	x_2	$\bar{x}_2$	x_3	$\bar{x}_3$	x_4	$\bar{x}_4$
1	0	0	1	t	1	t	1

$$=.25 \cdot 0 \cdot 1 \cdot 1 \cdot 1 \quad + .05 \cdot 0 \cdot 0 \cdot 1 \cdot t \quad +.05 \cdot 1 \cdot 1 \cdot 1 \cdot 1$$
$$+ .05 \cdot 1 \cdot 1 \cdot 1 \cdot t \quad + .10 \cdot 1 \cdot 1 \cdot t \cdot 1 \quad +.50 \cdot 1 \cdot 1 \cdot t \cdot t$$
$$=.05 + .05t + .1t + .50t^2$$
$$=.05 + .15t + .50t^2$$

Hamming weight marginalization



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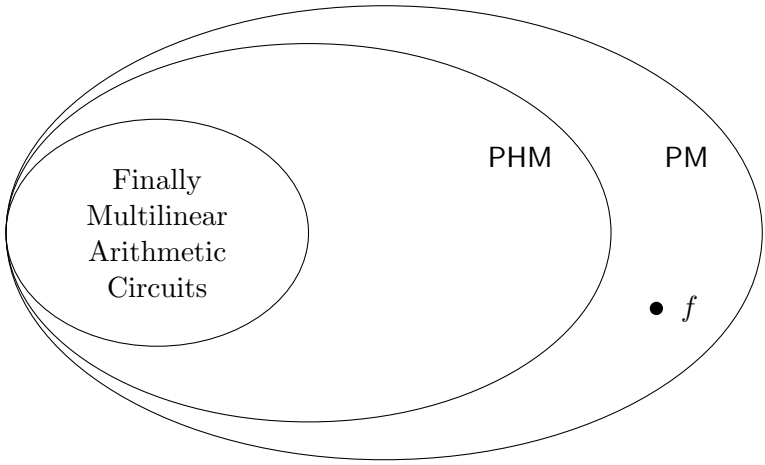

A separating example: constraint satisfaction problems

A constraint language Γ is a set of relations each of the form $R \subseteq \{0,1\}^k$ for some $k \geq 1$.

Example:
$\Gamma = \{\text{disjunctions of} \leq 3 \text{ literals}\}$

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Problems:

$\mathsf{CSP}(\Gamma)$
  In: a Γ-formula $\phi(x)$
  Q: Is there an x that satisfies ϕ?

$k - \mathsf{ONES}(\Gamma)$
  In: a Γ-formula $\phi(x)$, $k \in \{0, 1, \ldots, n\}$
  Q: Is there an x with k ones that satisfies ϕ?

Example:
$\Gamma = \{\text{disjunctions of} \leq 3 \text{ literals}\}$

$\phi = (x_1 \vee \neg x_2 \vee x_3) \wedge (x_2 \vee \neg x_4 \vee \neg x_5)$

$\mathsf{CSP}(\Gamma) = 3\mathsf{SAT}$

Dichotomy Theorems

A relation is (width-k) *affine* if it is logically equivalent to a system of linear equations over $\mathbb{F}_2$ (each mentioning at most k variables).

For example, $x_1 \oplus x_2 \oplus x_3 = 1$ and $x_3 \oplus x_4 = 0$ form a width-3 affine relation.

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Theorem (Creignou et al. [2010]). *If Γ contains only width-2 affine relations, then $\#k$-$\mathsf{ONES}(\Gamma)$ is in PTIME. Otherwise, $\#k$-$\mathsf{ONES}(\Gamma)$ is $\#\mathsf{P}$-complete.*

A separating function

$$f(x,y,z) = \bigwedge_{i,j,k\in[n]^3} y_{ijk} \oplus x_i \oplus x_j \oplus x_k \wedge \bigwedge_{i,j,k\in[n]^3} y_{ijk} \oplus z_{ijk}. \tag{1}$$

Theorem. $\mathsf{PM}(f)$ *is tractable, but* $\mathsf{PHM}(f)$ *is* $\#\mathsf{P}$*-hard.*

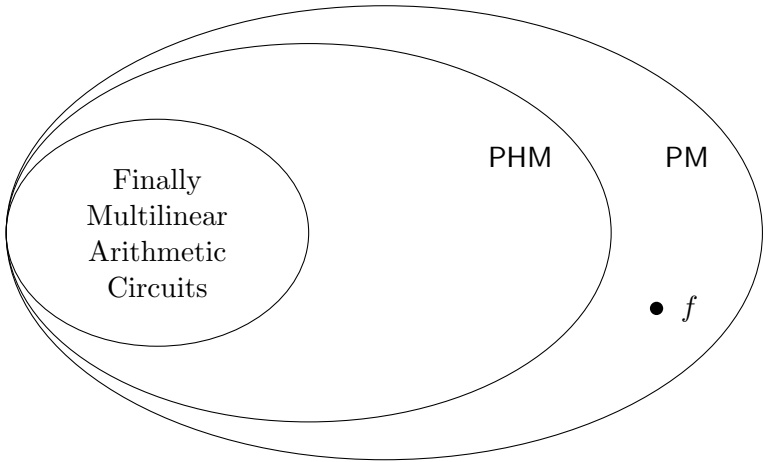
Proof summary: Tractability by Gaussian elimination. Hardness by reducing from $\#k\text{-}\mathsf{ONES}(\Gamma)$ with $\Gamma = \{a \oplus b \oplus c\} = \{\{(0,0,1),(0,1,0),(1,0,0),(1,1,1)\}\}$.

A separating function: hardness of PHM(f)

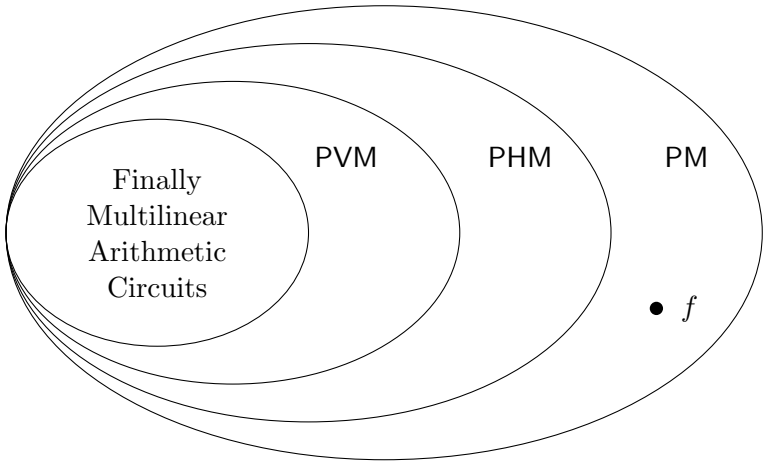
$$f(x,y,z) = \bigwedge_{i,j,k\in[n]^3} y_{ijk} \oplus x_i \oplus x_j \oplus x_k \wedge \bigwedge_{i,j,k\in[n]^3} y_{ijk} \oplus z_{ijk}.$$

Reduction: We get input a Γ-formula $\phi(x_1,\ldots,x_n)$ and an integer $k \in \{0,1,\ldots,n\}$. For any $x_i \oplus x_j \oplus x_k = 1$ in ϕ, set $y_{ijk} = 0$ and $z_{ijk} = 1$. Call the resulting 'evidence string' m. Then $\#k\text{-ONES}(\Gamma)(\phi,k) = \mathsf{PHM}(f)(m, k+n^3)$. Suppose $\phi(x) = 1$; we find the only y and z such that $f(x,y,z) = 1$, and we then observe that $|x,y,z| = |x| + n^3$. Every constraint of ϕ is satisfied, and so every width-4 constraint in f with $y_{ijk} = 0$ is satisfied. For constraints $x_i \oplus x_j \oplus x_k$ not in ϕ, the corresponding width-4 clause in f is satisfied by setting the free variable y_{ijk} to whichever value is necessary. The values z_{ijk} are then set to the opposite of the values of y_{ijk} which satisfies the remaining width-2 clauses of f. For every $i,j,k \in [n]^3$ we have $z_{ijk} \neq y_{ijk}$, and so $|y| + |z| = n^3$.

Update



Update



Virtual evidence marginalization

Let $f : \{0,1\}^n \to \{0,1\}$. Define $\mathsf{PVM}(f)$ which on input $x_1, \ldots, x_n \in \mathbb{Q}$ outputs $p(x_1, \ldots, x_n)$ where p is the multilinear polynomial computing f.

Hard evidence: observe that $X_i = 0$ or $X_i = 1$.
Virtual evidence instead 'scales' your belief in $X_i = 0$ and $X_i = 1$ by $\bar{\alpha}_i, \alpha_i \geq 0$.
Happens when having noisy measurements of data, many applications ...

Marginalizing with virtual evidence reduces to $\mathsf{PVM}(f)$:

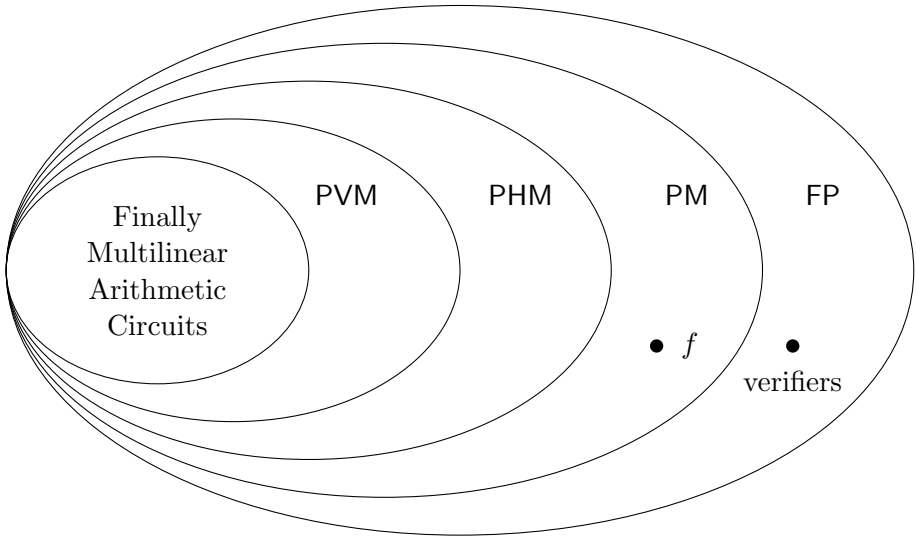
$$\left(\prod_{i=1}^{n}(\alpha_i x_i + \bar{\alpha}_i \bar{x}_i)\right) p\left(\frac{\alpha_1 x_1}{\alpha_1 x_1 + \bar{\alpha}_1 \bar{x}_1}, \ldots, \frac{\alpha_n x_n}{\alpha_n x_n + \bar{\alpha}_n \bar{x}_n}\right) \tag{2}$$

PVM $\subseteq$ PHM

Recall our algorithm for PHM: we substituted the inputs of p to obtain a univariate polynomial of degree at most n

It can therefore be recovered by black-box evaluation at $n + 1$ distinct points

Update


Finally
Multilinear
Arithmetic
Circuits
PVM
PHM
PM
FP
f
verifiers

Are circuits 'complete' for virtual evidence marginalization?

real-RAM: real (and discrete) inputs followed (discrete operations and) by sums, products, and *comparisons* (i.e., $>, =$)

Proposition. *If there is a polynomial time real-RAM for* $\mathsf{PVM}(f)$*, then there are (uniform) FMACs for* f*.*

Does a similar 'completeness' hold for Turing machines?
Possibly hard. [Koiran and Perifel, 2011]

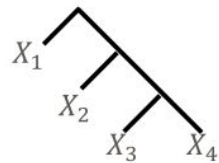
Conclusion

Ongoing/open questions:

- More expressive tractable probabilistic models?
- Are finally multilinear circuits 'complete' for virtual evidence marginalization?
- Are there more interesting (useful?) queries living between virtual evidence and marginalization?
- Are there non-parallelizable marginalization algorithms (or is marginalization inherently parallelizable?)?

When can we multiply circuits efficiently?

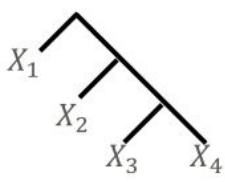
- Obviously when they
  - Are structured decomposable and
  - have the same vtree
    - E.g., two OBDDs with the same variable order
    - E.g., Hidden Markov model with DFA-turned-into-OBDD
- Otherwise easy to prove intractable
- *That's it?*

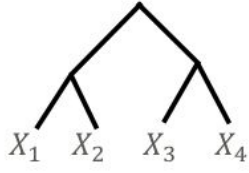


Honghua Zhang, Benjie Wang, Marcelo Arenas and Guy Van den Broeck. Restructuring Tractable Probabilistic Circuits, *AISTATS*, 2021.

When can we multiply circuits efficiently?

- We could "**restructure**" the circuits to give same vtree
  - Boring answer: modify constant-size sub-circuits
  - Otherwise … no global differences allowed?





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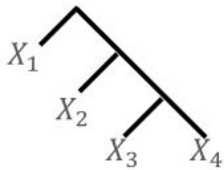
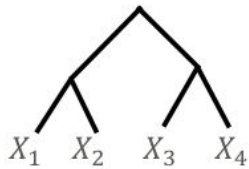
Contiguous Circuits

We say that a circuit is compatible with a total order $<$ on its variables if for every product node g, its children $g_1, \ldots, g_m$ (in some order) satisfy: [ABJM'17]

$$max(g_i) < min(g_{i+1}) \forall i = 1, \ldots, m-1$$

We say that a circuit is contiguous if it is compatible with some order.





Honghua Zhang, Benjie Wang, Marcelo Arenas and Guy Van den Broeck. Restructuring Tractable Probabilistic Circuits, *AISTATS*, 2021.

Multiplying Contiguous Circuits, Deep case

Thm: Let A and B be **contiguous structured** circuits.
If A has a **linear** vtree, then A and B can be multiplied in PTIME and the size of the product circuit is $O(|A|^2|B|)$.

Example: *A is a Hidden Markov Model,*
B is a (Prob./Unambiguous) Context-Free Grammar
Example: *A is an OBDD, B is an SDD, both contiguous*

Thm: Theorem still works if B is **unstructured** but contiguous.

You can efficiently multiply a structured and unstructured circuit!!!!

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Multiplying Contiguous Circuits, Shallow case

Thm: Let A and B be **contiguous structured** circuits.
Let d be the **depth** of the vtree for A,
then A and B can be multiplied in time $O(|A|^{12d}|B|)$.

Example: A is log-depth, then multiplication is quasi-polynomial.

Cor: Every structured circuit can be made **structured log-depth**.
Thus, contiguous multiplication is quasipolynomial for some order.

Everything else is an open problem…
(lower bounds, reachable vtrees, what if vtree is deep but non-linear)

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