Polynomial semantics of probabilistic circuits

Oliver Broadrick, Honghua Zhang, Guy Van den Broeck – UAI 2024

The limits of tractable marginalization

Oliver Broadrick, Sanyam Agarwal, Markus Bläser, Guy Van den Broeck – wip

Probabilistic Models

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

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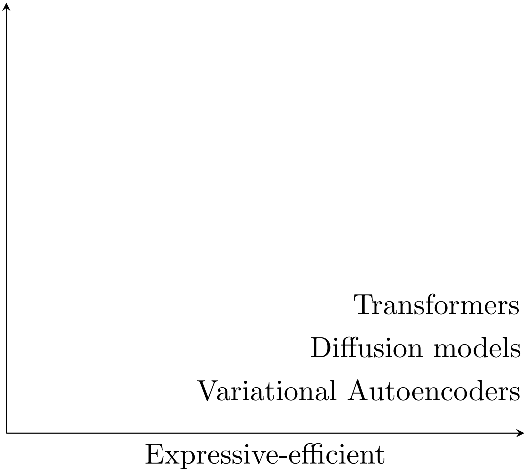

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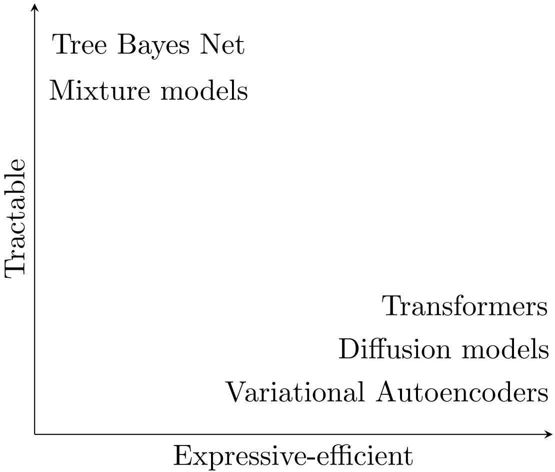

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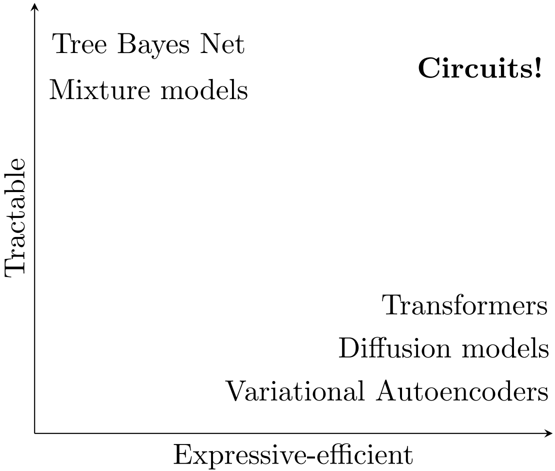

Marginal Inference

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

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

Tractable Marginalization is Useful

Logical control of language models (see Honghua Zhang)

Efficient causal reasoning (see Benjie Wang)

Data compression and control for diffusion models (see Anji Liu)

Probabilistic program inference (see Poorva Garg)

Neurosymbolic learning (see Kareem Ahmed)

Probabilistic logic programming (see Renato Geh)

etc. etc. etc.

Approaches

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

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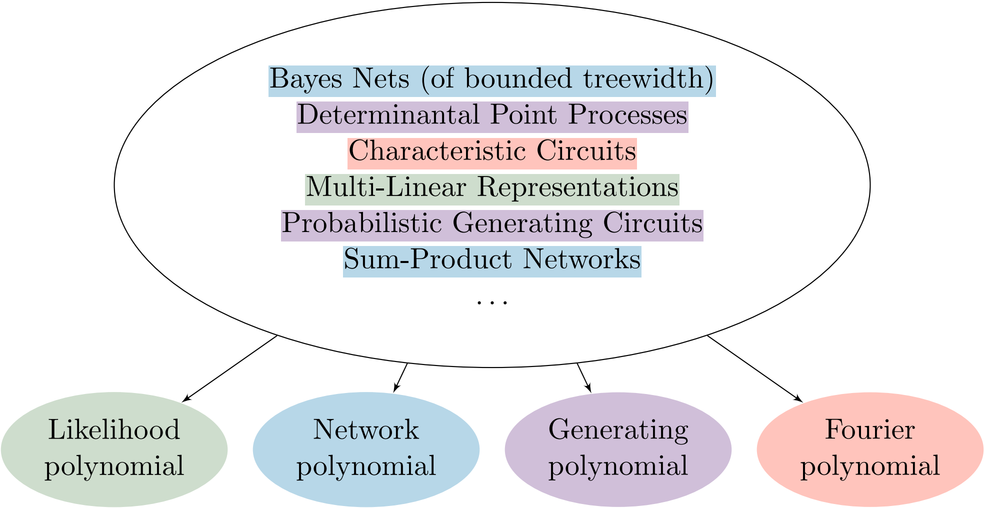
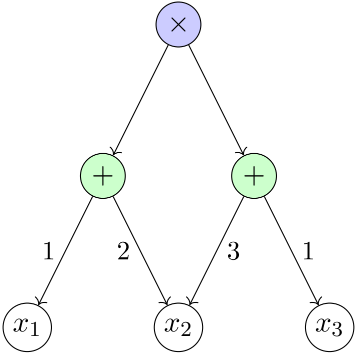
$\downarrow$

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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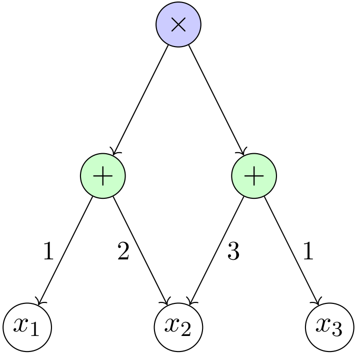

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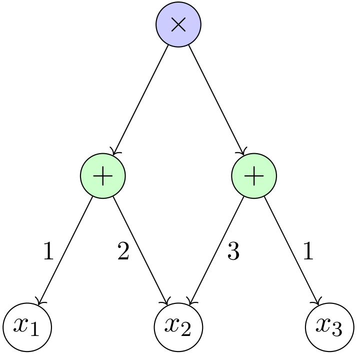
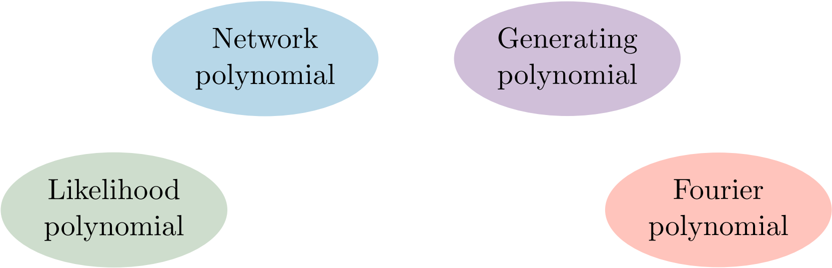


$$3x_1x_2 + x_1x_3 + 6x_2^2 + 2x_2x_3$$

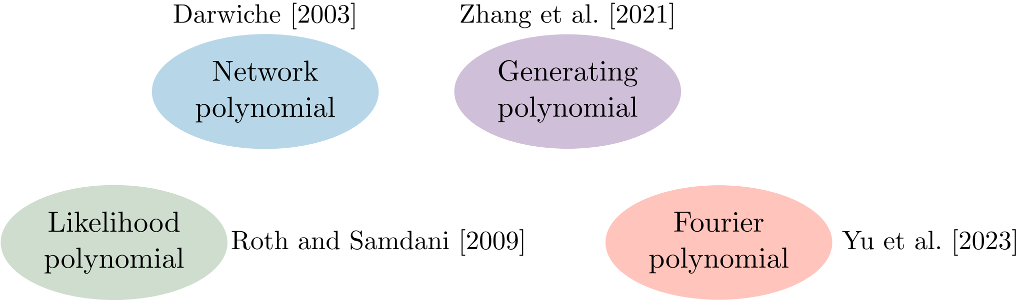
Circuits are *fully expressive*

They can also be *expressive-efficient*

Polynomial Semantics



Polynomial Semantics



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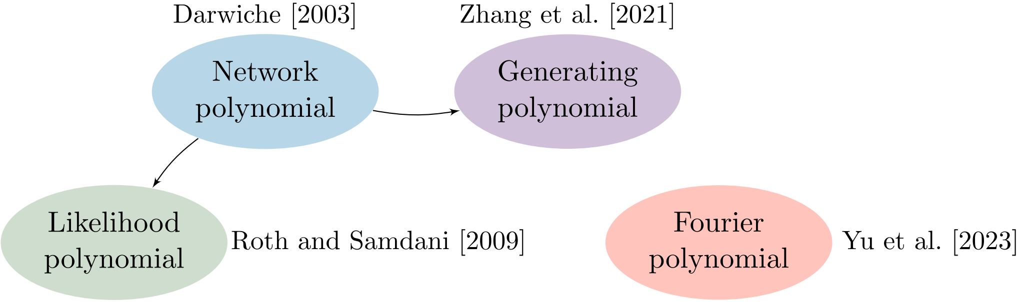

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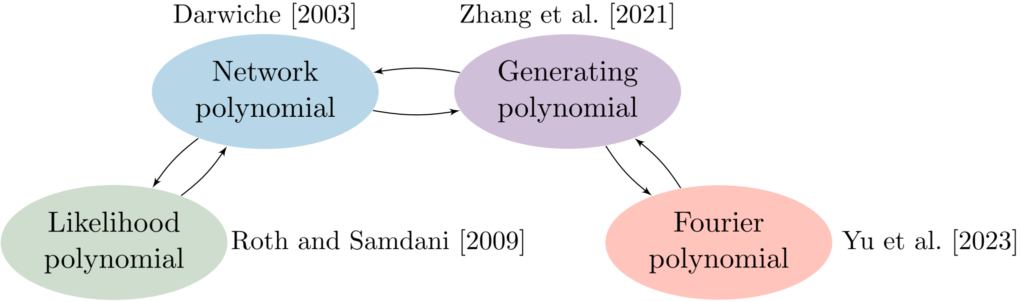

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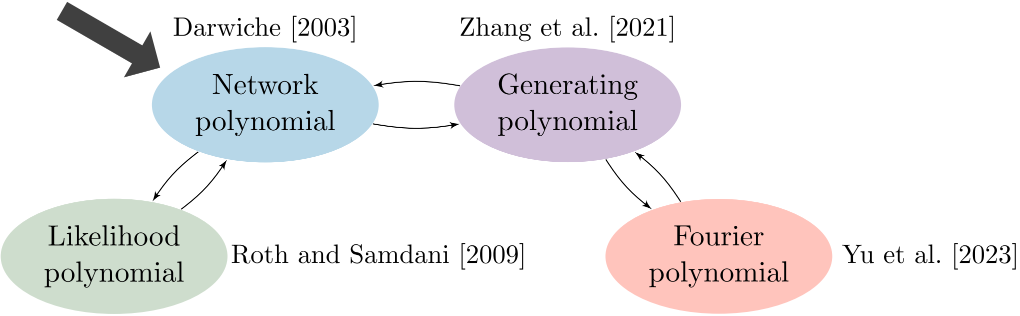

Network polynomial

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

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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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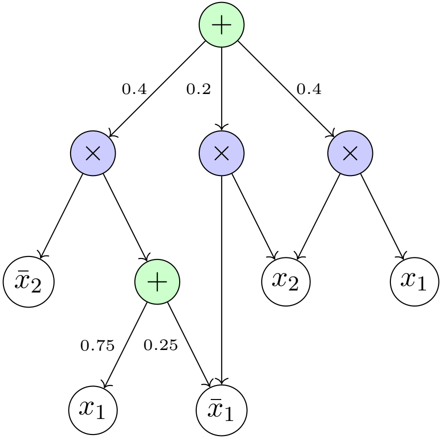

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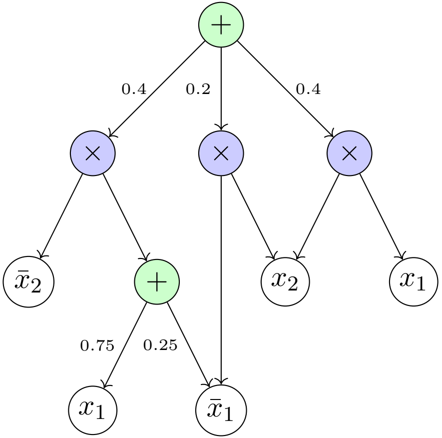

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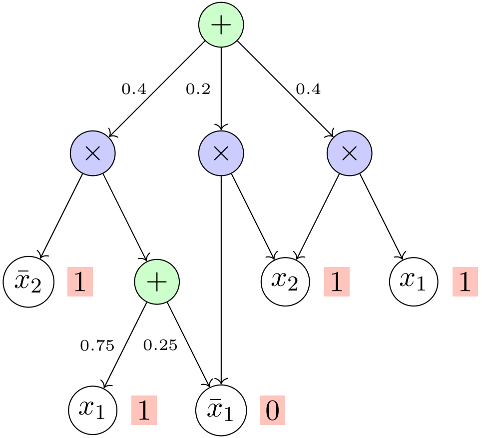

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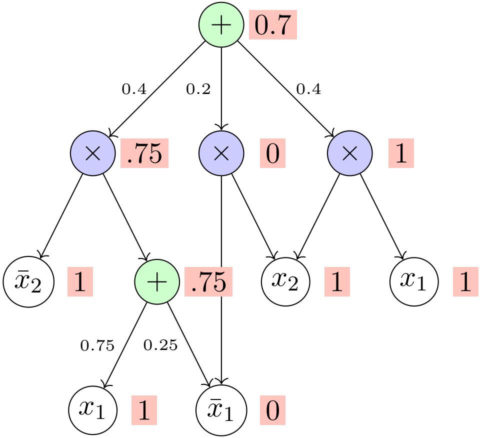

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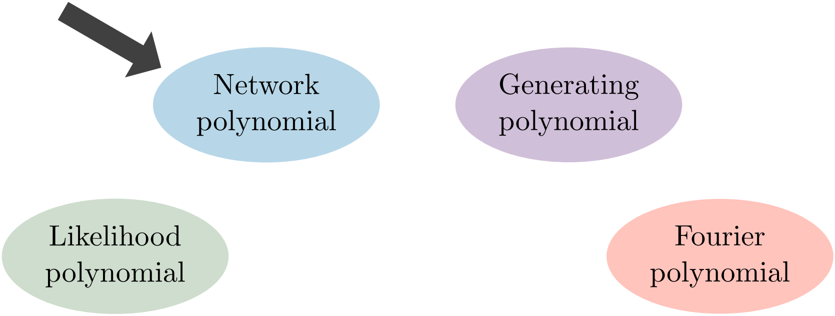
Progress Update



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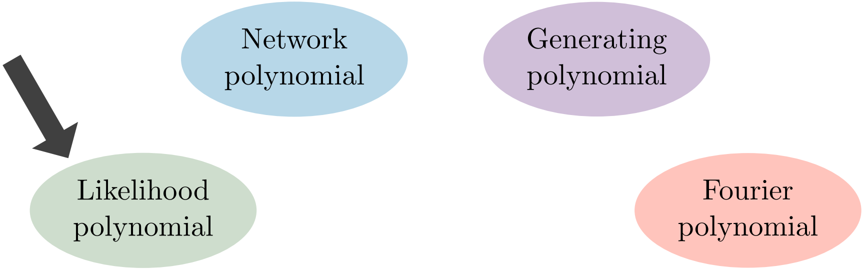

Likelihood polynomial

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

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

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Relation to network polynomial?

(1) Transform network to likelihood:

$$p(x, \bar{x}) = .1\bar{x}_1\bar{x}_2 + .2\bar{x}_1 x_2 + .3x_1\bar{x}_2 + .4x_1x_2$$

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

Likelihood polynomial

(2) Transform likelihood to network:

$$p(x_1, x_2) = \boxed{.2x_1} + .1x_2 + .1$$

Likelihood polynomial

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$p(x_1, x_2) = \boxed{.2x_1} + .1x_2 + .1$

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

Likelihood polynomial

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

Likelihood polynomial

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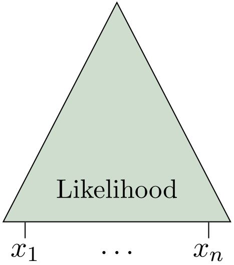
&= \boxed{.2x_1(x_2 + \bar{x}_2)} + .1x_2(x_1 + \bar{x}_1) + .1(x_1 + \bar{x}_1)(x_2 + \bar{x}_2) \\
&= p(x_1, x_2, \bar{x}_1, \bar{x}_2)
\end{aligned}$$

Likelihood polynomial

Transform likelihood to network:



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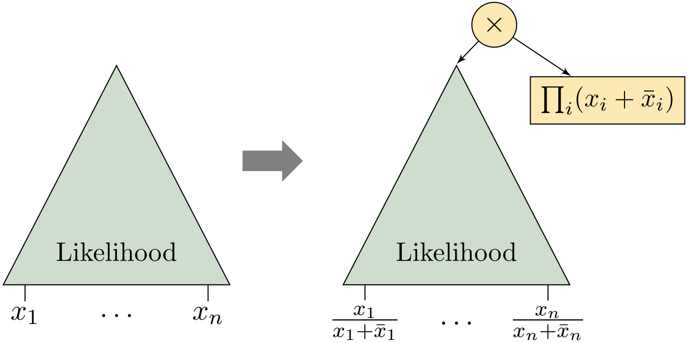

Removing Divisions

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

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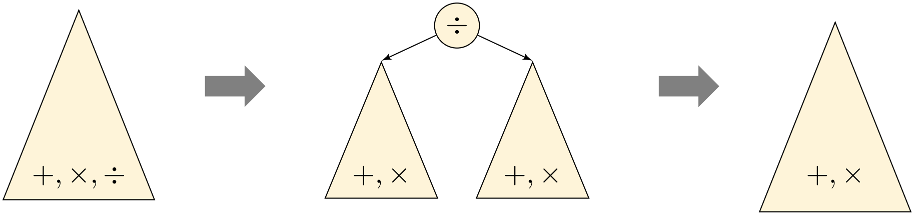

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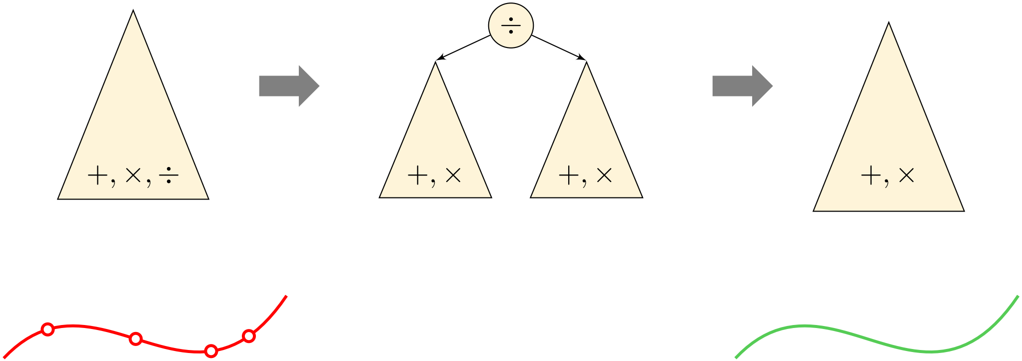

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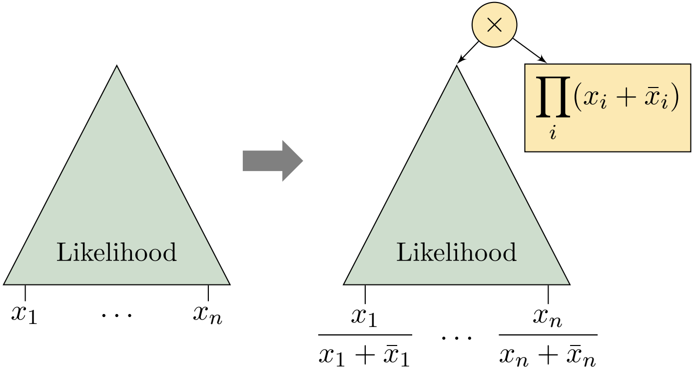

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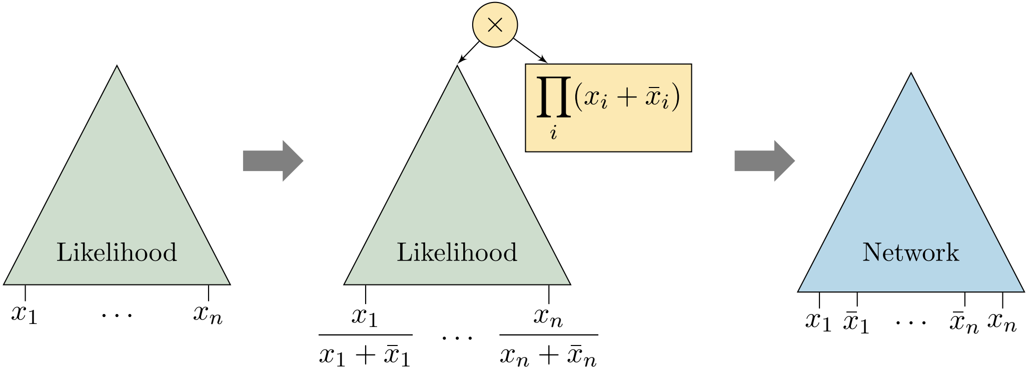
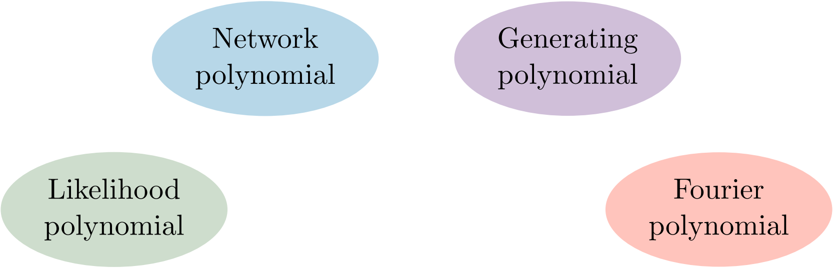


Progress Update



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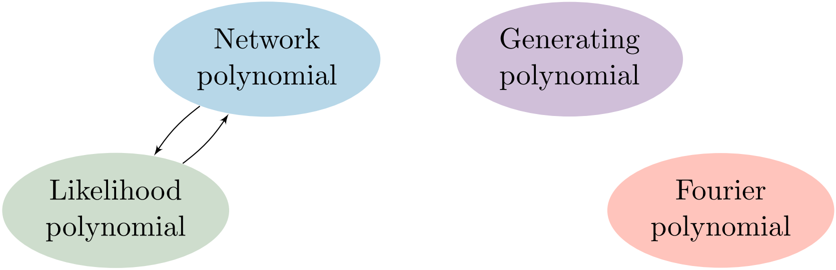

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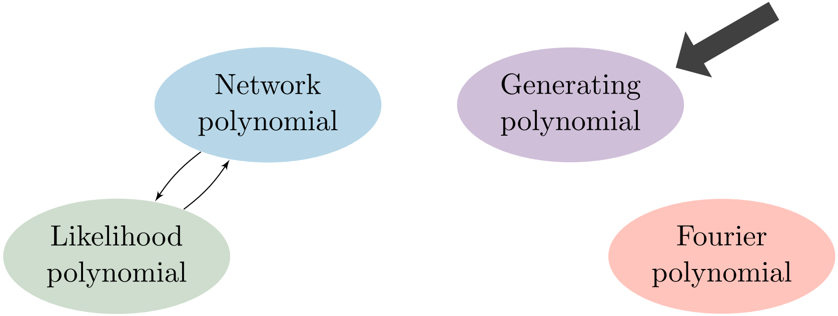
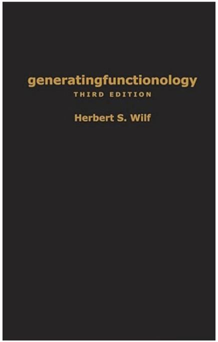


Generating polynomial



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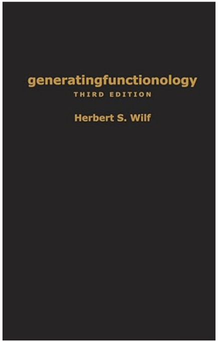
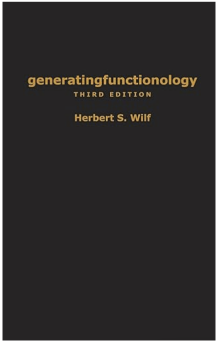


Monotone, decomposable circuits computing network polynomials (SPNs, PCs)

Generating polynomial



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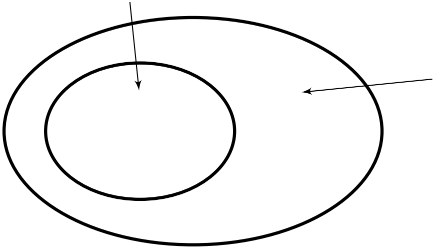

Circuits computing generating polynomials

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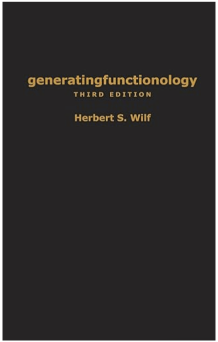

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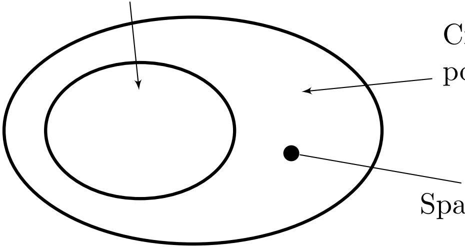

Circuits computing generating polynomials

Spanning tree distribution[a]

[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?

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

Relation to network polynomial?

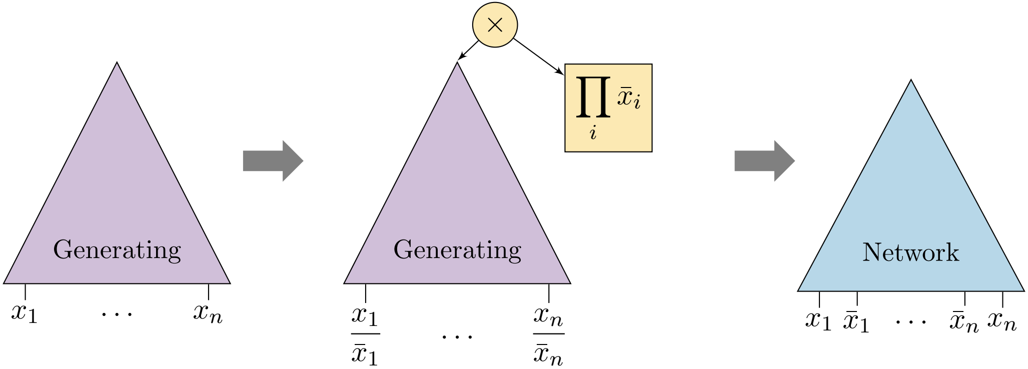
(1) Transform network to generating:

$p(x_1, x_2, \bar{x}_1, \bar{x}_2) = .1\bar{x}_1\bar{x}_2 + .2\bar{x}_1x_2 + .3x_1\bar{x}_2 + .4x_1x_2$

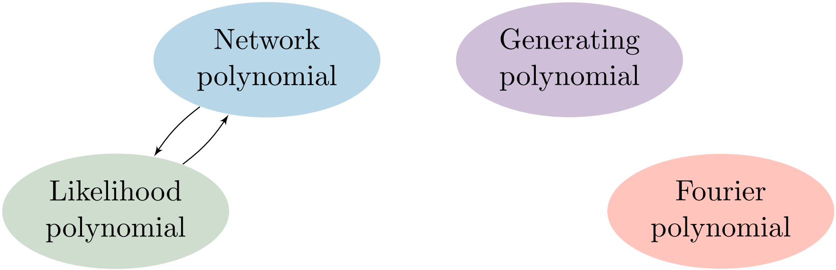
$\rightarrow$ Replace $\bar{x}_i$ with 1

Generating polynomial

(2) Transform generating to network:



Progress Update



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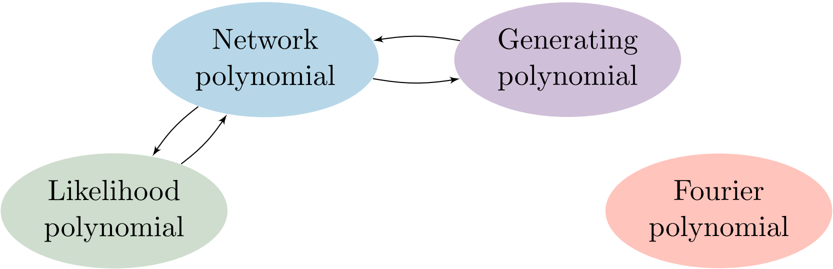

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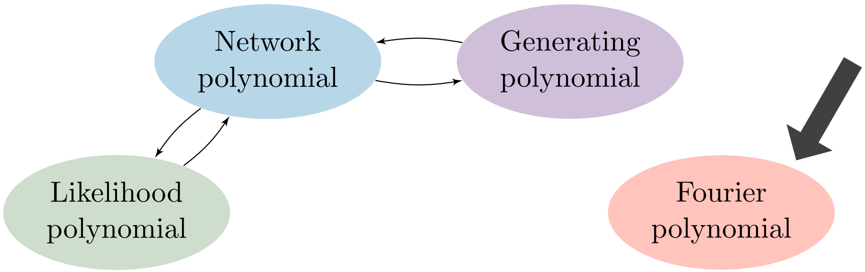
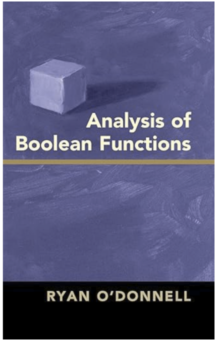


Fourier Polynomial



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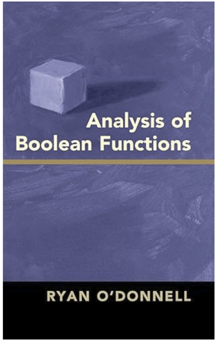
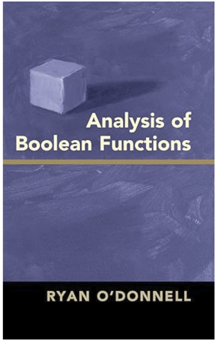


Fourier transform of the probability mass function

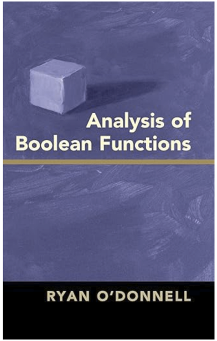
Fourier Polynomial



Fourier transform of the probability mass function

- Graphical model approximate inference
- Characteristic Circuits

Fourier Polynomial

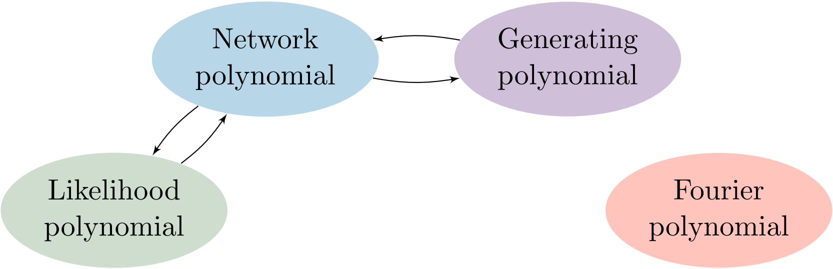


Fourier transform of the probability mass function

- 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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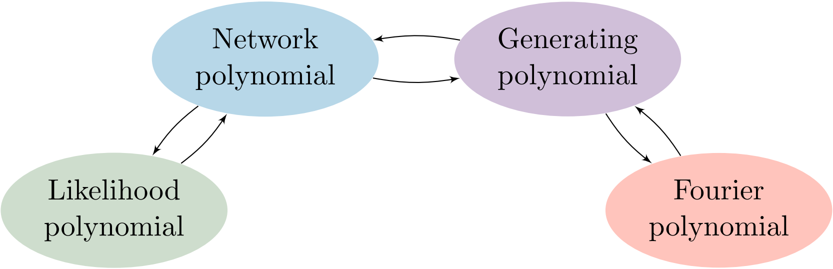
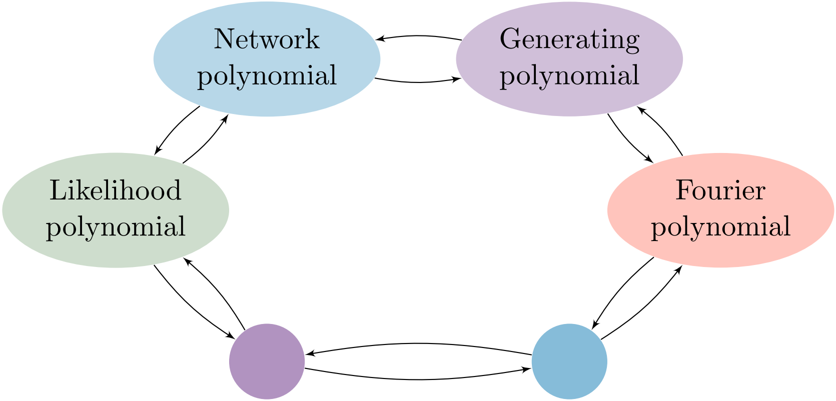


Some New Semantics



Non-binary variables?

X_1	X_2	Pr
0	1	.1
1	3	.3
3	2	.2
$\vdots$	$\vdots$	$\vdots$

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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What's next?

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

Polynomial semantics of probabilistic circuits

Oliver Broadrick, Honghua Zhang, Guy Van den Broeck – UAI 2024

The limits of tractable marginalization

Oliver Broadrick, Sanyam Agarwal, Markus Bläser, Guy Van den Broeck – wip

Finally Multilinear Arithmetic Circuits

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

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

X_1	X_2	f
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1	0	.3
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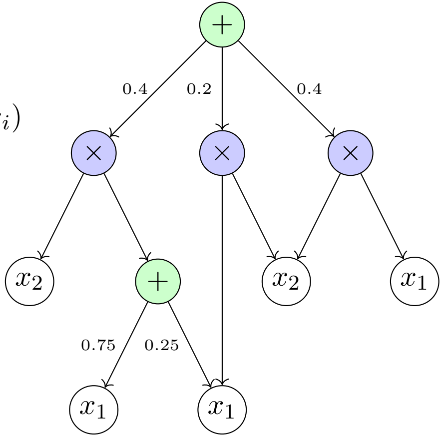

$$p(x_1, x_2) = .1(1 - x_1)(1 - x_2) + .2(1 - x_1)x_2 + .3x_1(1 - x_2) + .4x_1x_2$$

Functions Tractable for Marginalization

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

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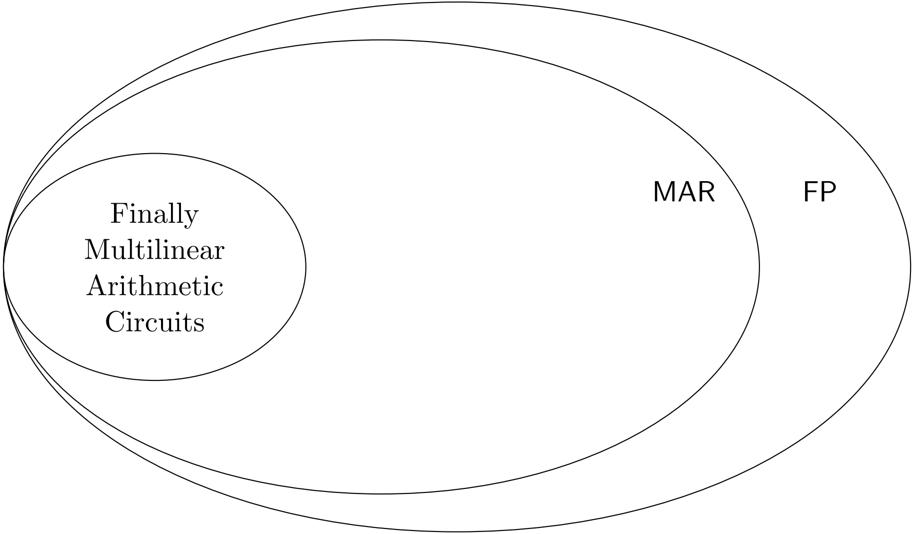
E.g., the earlier example was an instance of $\mathsf{MAR}(\mathrm{Pr})$ with input $m = 1*$.

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
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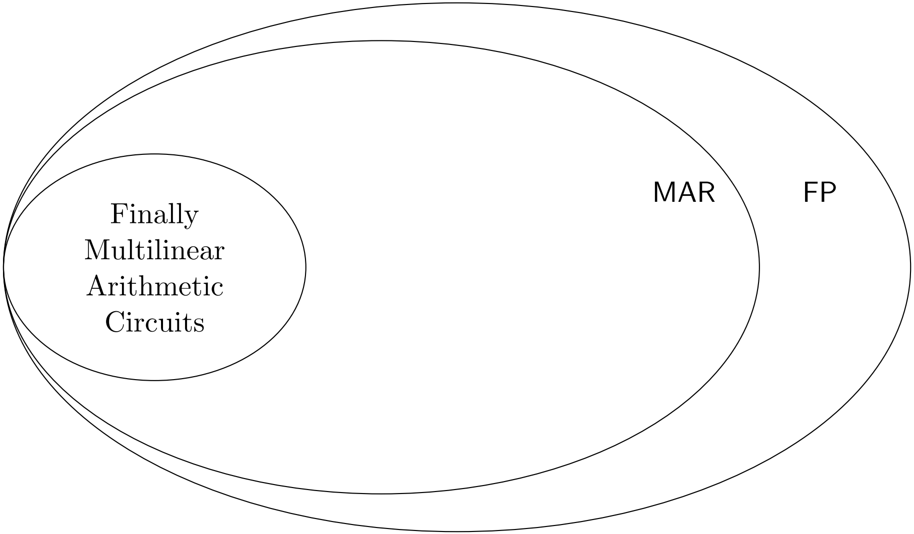
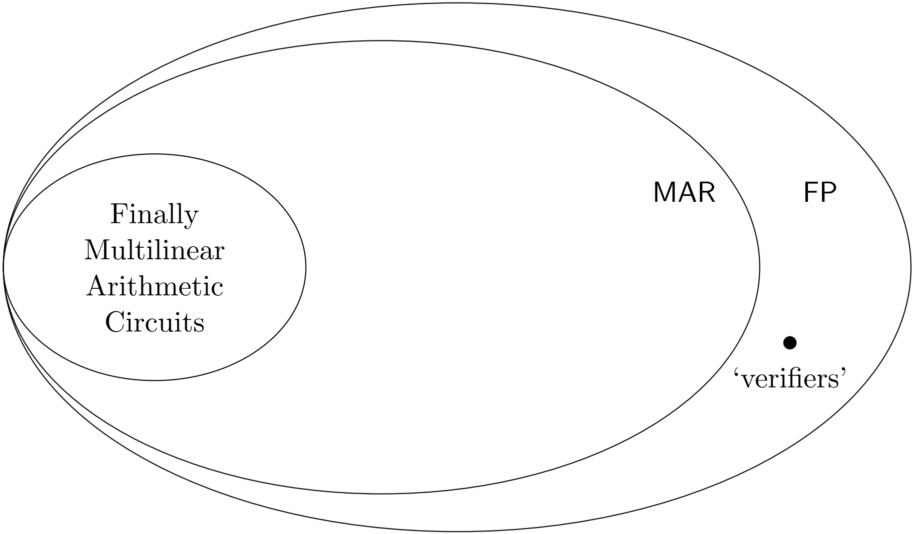


Main Question: Does every function family with tractable marginalization have uniform finally multilinear arithmetic circuits of polynomial size?



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Find stronger queries that are tractable for finally multilinear arithmetic circuits

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(Virtual evidence marginalization)

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

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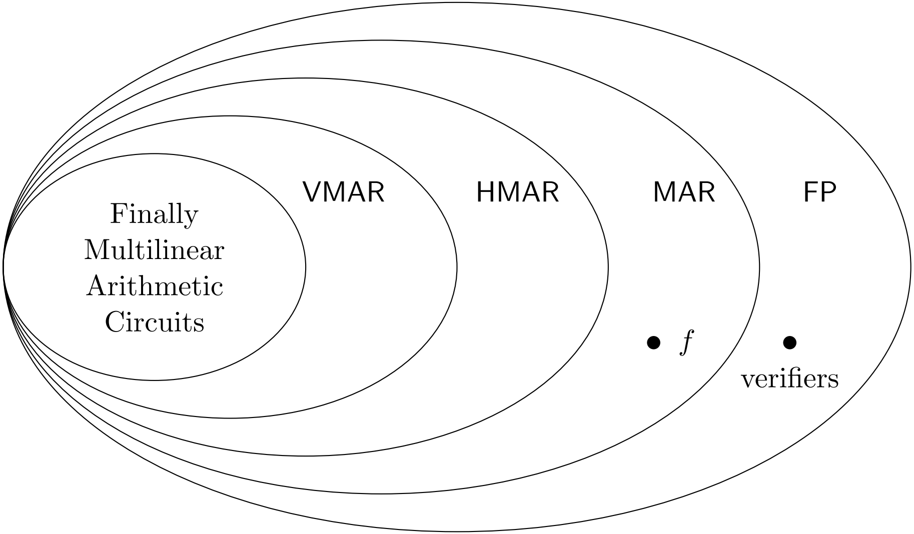


Hamming weight marginalization

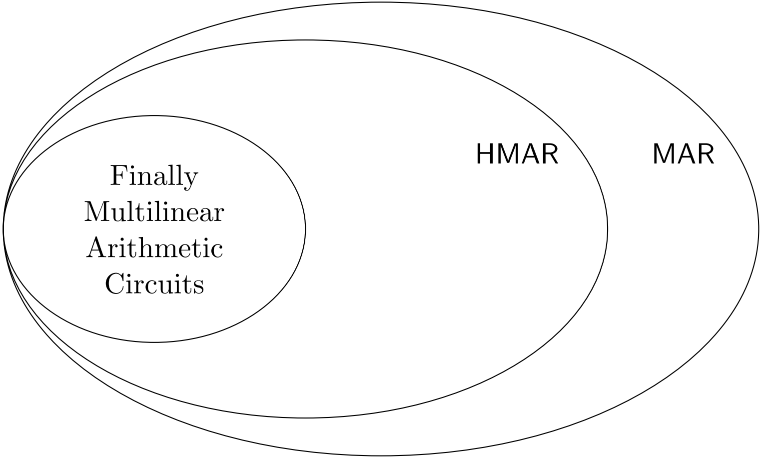
Let $f : \{0,1\}^n \to \{0,1\}$. Define $\mathsf{HMAR}(f)$ which on input $m \in \{0,1,*\}^n$ and $k \in \{0,1,2,\ldots,n\}$, asks for

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

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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$$+ .05x_1\bar{x}_2\bar{x}_3 x_4 + .10x_1\bar{x}_2 x_3\bar{x}_4 + .50x_1\bar{x}_2 x_3 x_4$$

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

$$= .25 \cdot 0 \cdot 1 \cdot 1 \cdot 1 + .05 \cdot 0 \cdot 0 \cdot 1 \cdot t + .05 \cdot 1 \cdot 1 \cdot 1 \cdot 1$$
$$+ .05 \cdot 1 \cdot 1 \cdot 1 \cdot t + .10 \cdot 1 \cdot 1 \cdot t \cdot 1 + .50 \cdot 1 \cdot 1 \cdot t \cdot t$$
$$= .05 + .05t + .1t + .50t^2$$
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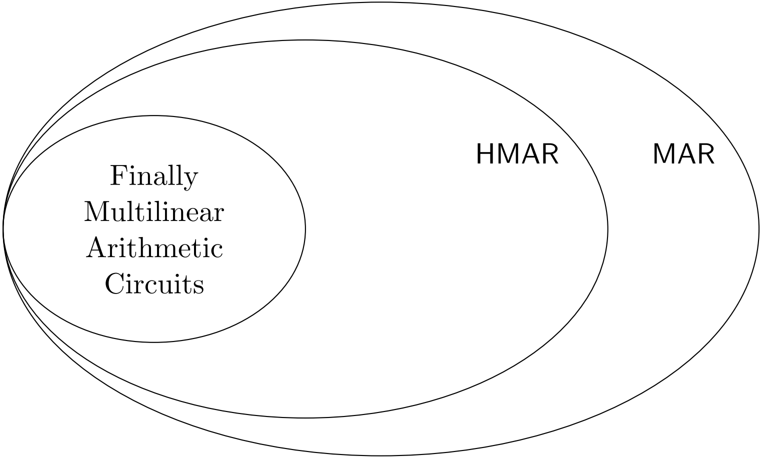
Hamming weight marginalization



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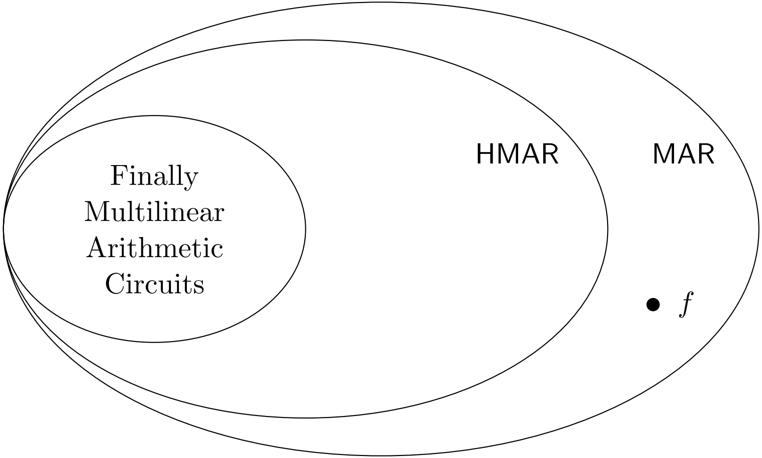

A separating example: constraint satisfaction problems

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

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

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

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

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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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. $\mathsf{MAR}(f)$ *is tractable, but* $\mathsf{HMAR}(f)$ *is* $\#\mathsf{P}$*-hard.*

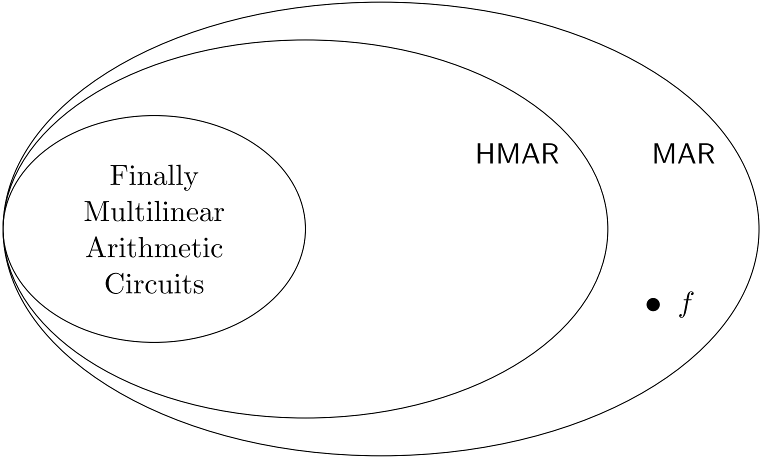
Proof summary: Tractability by Gaussian elimination. Hardness by reducing from $\#k\text{-}\mathsf{ONES}(\Gamma)$ with $\Gamma = \{a \oplus b \oplus c\} = \{\{(0,0,1),(0,1,0),(1,0,0),(1,1,1)\}\}$.

A separating function: hardness of $\mathsf{HMAR}(f)$

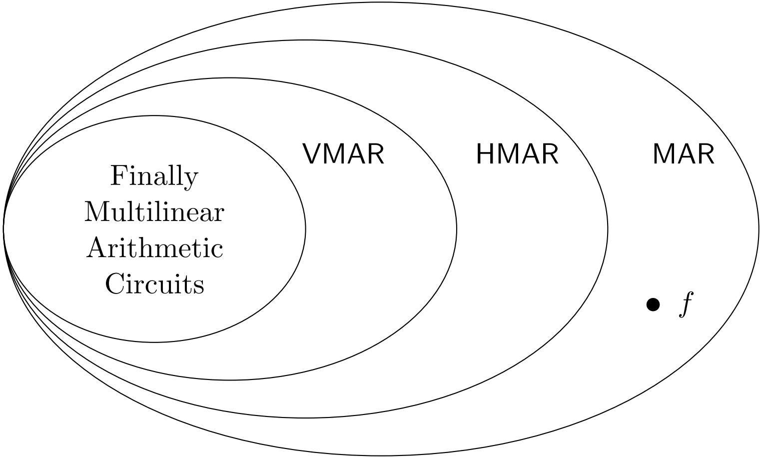
$$f(x,y,z) = \bigwedge_{i,j,k \in [n]^3} y_{ijk} \oplus x_i \oplus x_j \oplus x_k \wedge \bigwedge_{i,j,k \in [n]^3} y_{ijk} \oplus z_{ijk}.$$

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 $\#k\text{-}\mathsf{ONES}(\Gamma)(\phi, k) = \mathsf{HMAR}(f)(m, k + n^3)$. 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 $\mathsf{VMAR}(f)$ 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 $\mathsf{VMAR}(f)$:

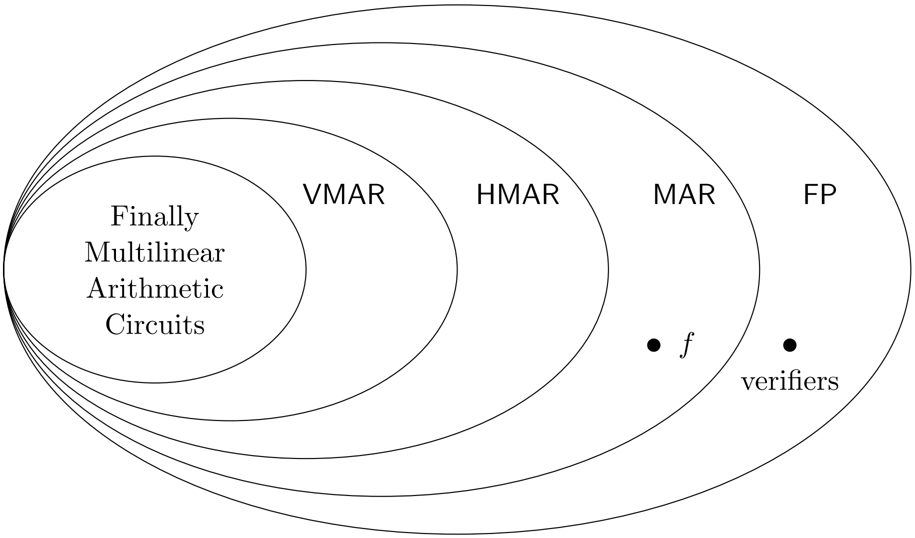
$$\left(\prod_{i=1}^{n} (\alpha_i x_i + \bar{\alpha}_i \bar{x}_i)\right) p\left(\frac{\alpha_1 x_1}{\alpha_1 x_1 + \bar{\alpha}_1 \bar{x}_1}, \ldots, \frac{\alpha_n x_n}{\alpha_n x_n + \bar{\alpha}_n \bar{x}_n}\right) \tag{2}$$

VMAR $\subseteq$ HMAR

Recall our algorithm for HMAR: 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


VMAR
HMAR
MAR
FP
Finally Multilinear Arithmetic Circuits
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* $\mathsf{VMAR}(f)$, *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?)?

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