

Scalable Learning of Probabilistic Circuits



Motivation

Given a selection of sushi...



...and people's preferences...

Alice: A sequence of five icons showing Alice's preference order: uramaki, maki, temaki, nigiri, and hand-rolled.

Bob: A sequence of five icons showing Bob's preference order: temaki, nigiri, maki, hand-rolled, and uramaki.

Carol: A sequence of five icons showing Carol's preference order: maki, nigiri, hand-rolled, uramaki, and temaki.

...how can we model this as a probability distribution...

$$p(1^{\text{st}} = \text{maki}, 3^{\text{rd}} = \text{nigiri})$$

$$p(2^{\text{nd}} = \text{temaki} | 1^{\text{st}} = \text{nigiri})$$

$$\arg \max p(1^{\text{st}} = ?, 2^{\text{nd}} = ?, 3^{\text{rd}} = ?, 4^{\text{th}} = \text{uramaki}, 5^{\text{th}} = \text{nigiri})$$

$$p((3^{\text{rd}} = \text{maki} \rightarrow 1^{\text{st}} = \text{nigiri}) \vee 2^{\text{nd}} = \text{temaki})$$

...and extract meaningful queries from it?

Motivation

Given a selection of sushi...



...and people's preferences...

Alice: A sequence of five icons showing Alice's preferences: uramaki, maki, gunkan, nigiri, and nigiri.

Bob: A sequence of five icons showing Bob's preferences: gunkan, nigiri, maki, hand-rolled, and nigiri.

Carol: A sequence of five icons showing Carol's preferences: maki, nigiri, nigiri, uramaki, and hand-rolled.

...how can we model this as a probability distribution...

Marginals

$$p(1^{\text{st}} = \text{maki}, 3^{\text{rd}} = \text{nigiri})$$

Conditionals

$$p(2^{\text{nd}} = \text{gunkan} | 1^{\text{st}} = \text{nigiri})$$

MPE

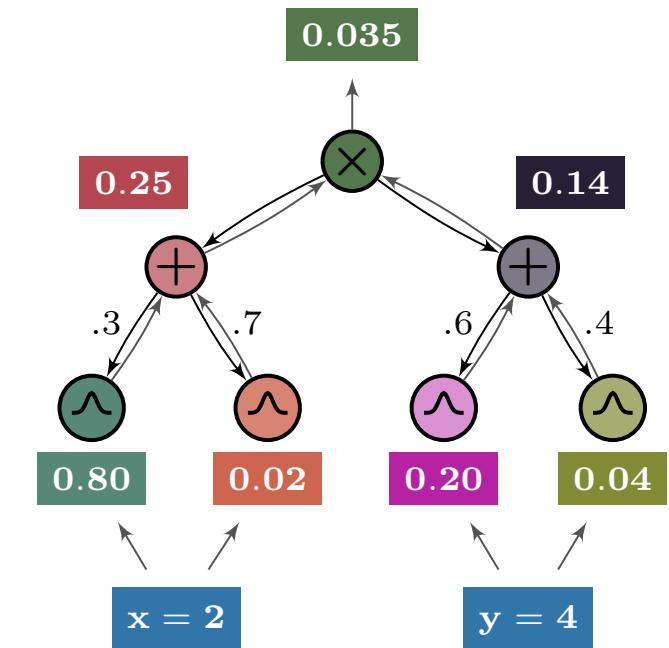
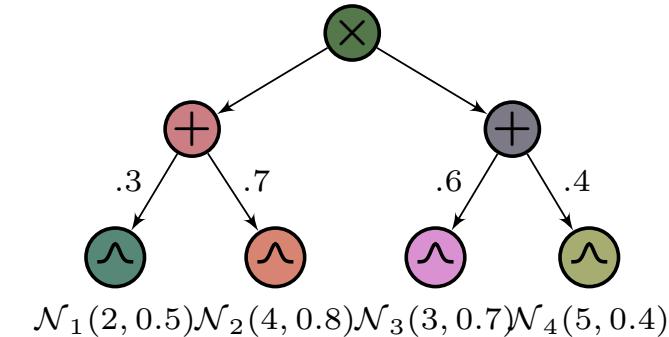
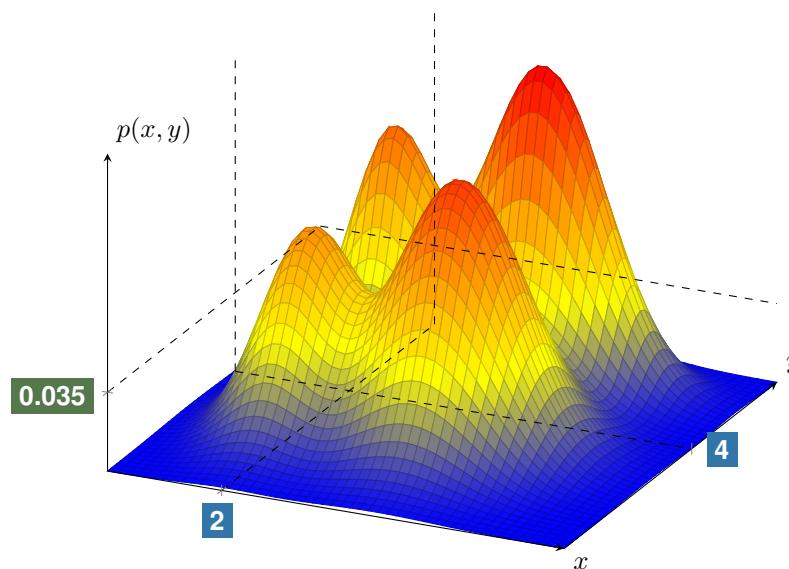
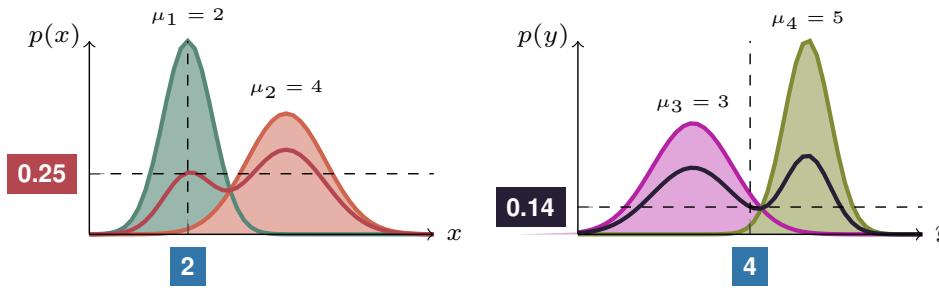
$$\arg \max p(1^{\text{st}} = ?, 2^{\text{nd}} = ?, 3^{\text{rd}} = ?, 4^{\text{th}} = \text{hand-rolled}, 5^{\text{th}} = \text{nigiri})$$

Logical events

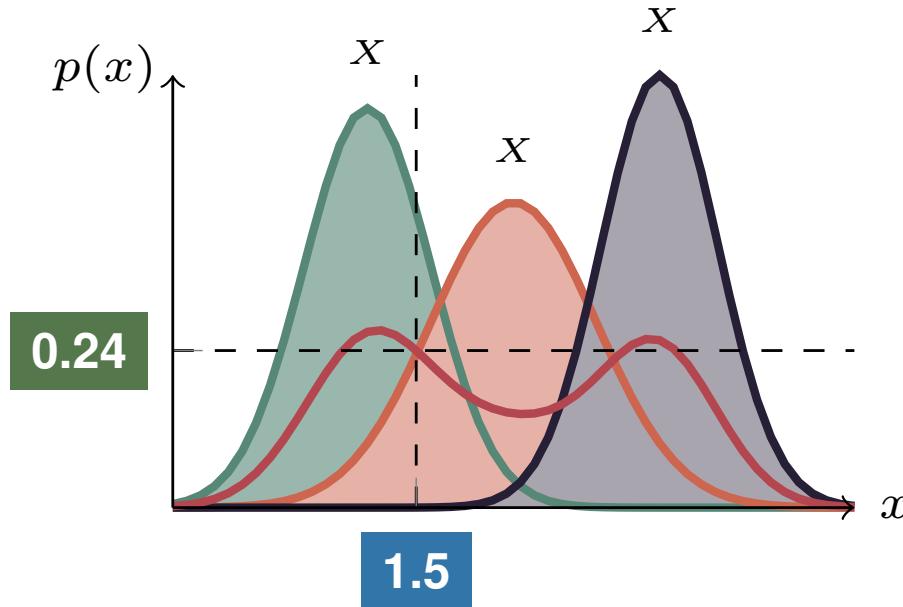
$$p((3^{\text{rd}} = \text{maki} \rightarrow 1^{\text{st}} = \text{nigiri}) \vee 2^{\text{nd}} = \text{gunkan})$$

...and extract meaningful queries from it?

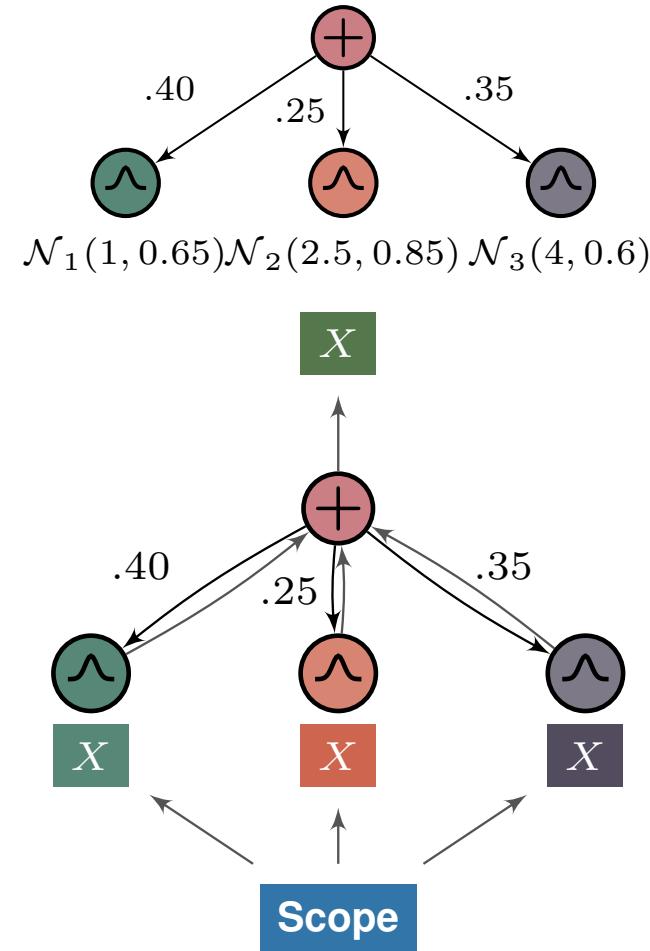
Probabilistic Circuits



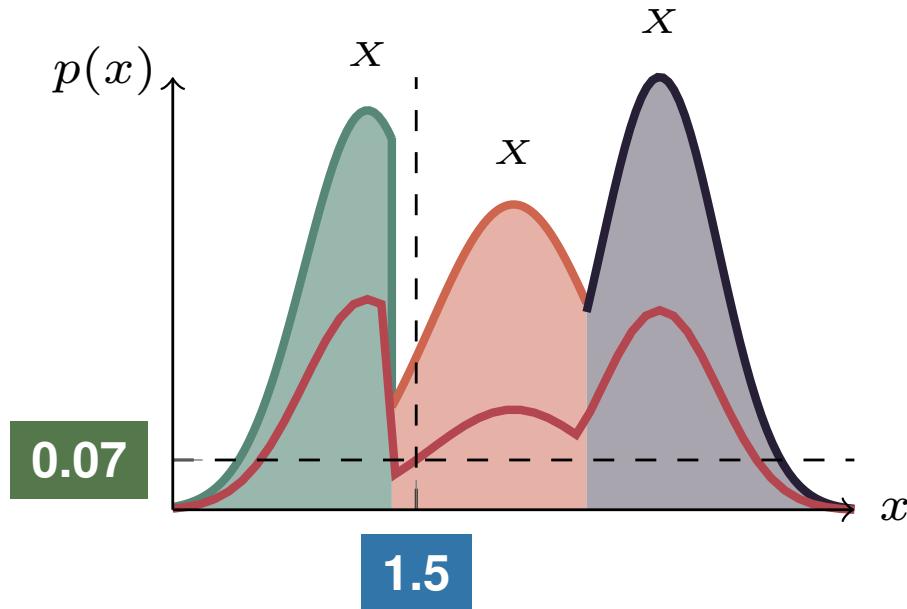
Probabilistic Circuits – Smoothness



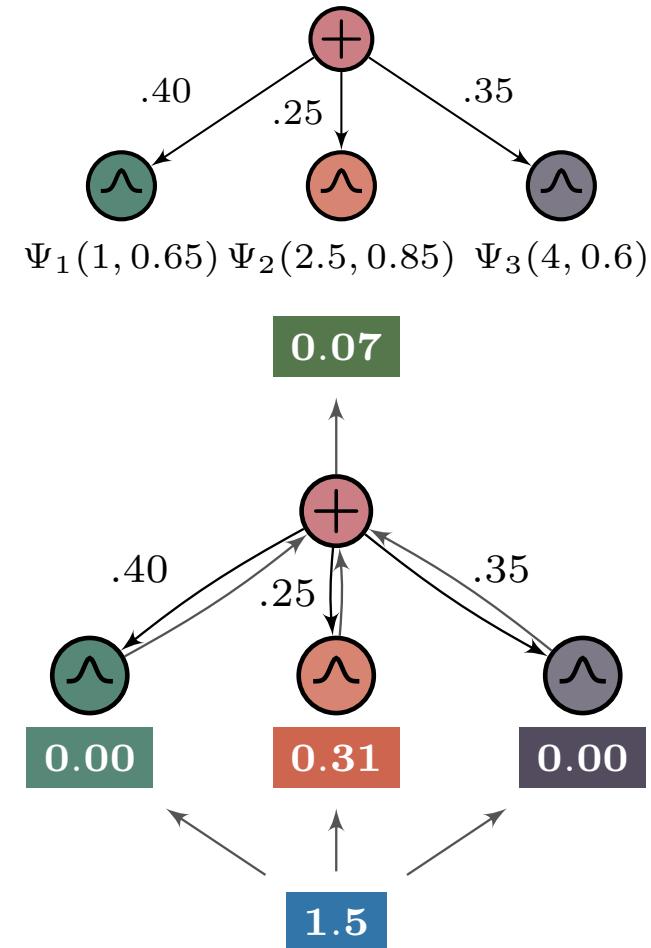
Definition 1 (Smoothness).
Every sum node child mentions the same variables.



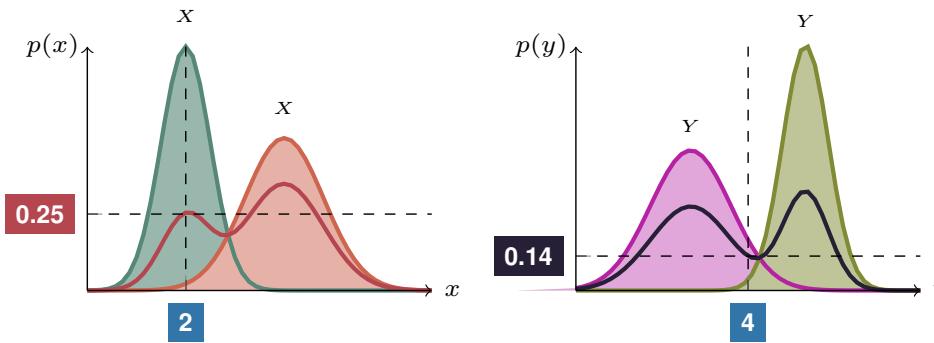
Probabilistic Circuits – Determinism



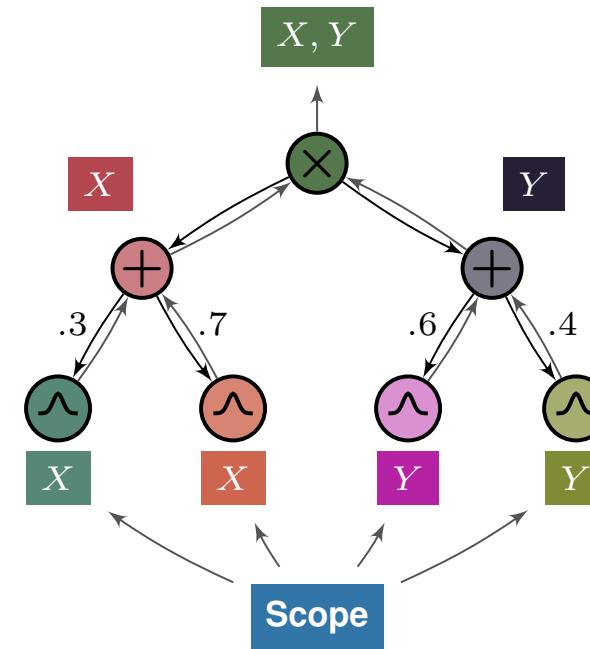
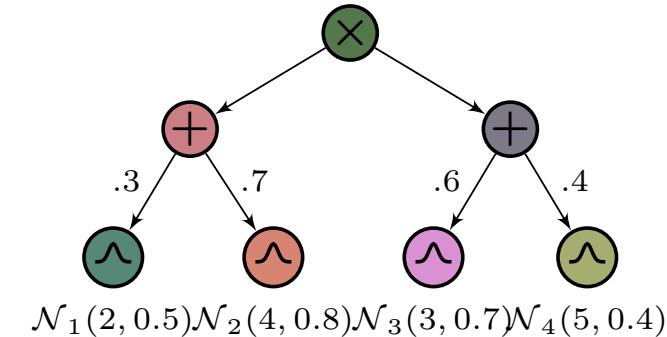
Definition 2 (Determinism).
At most one sum node child has a positive value.



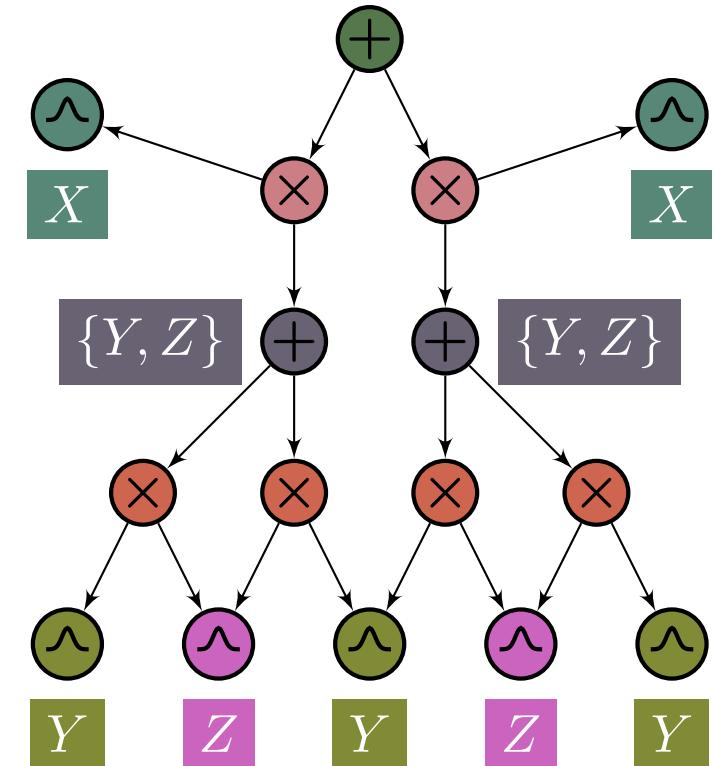
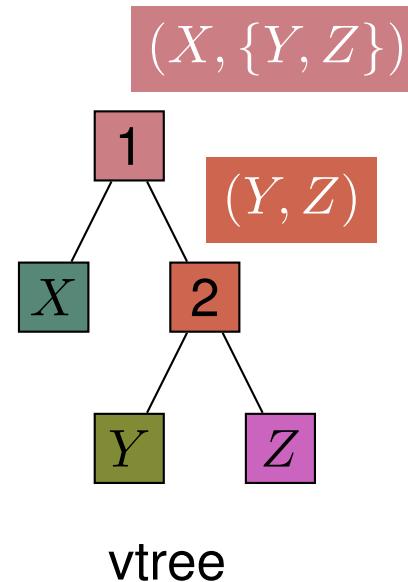
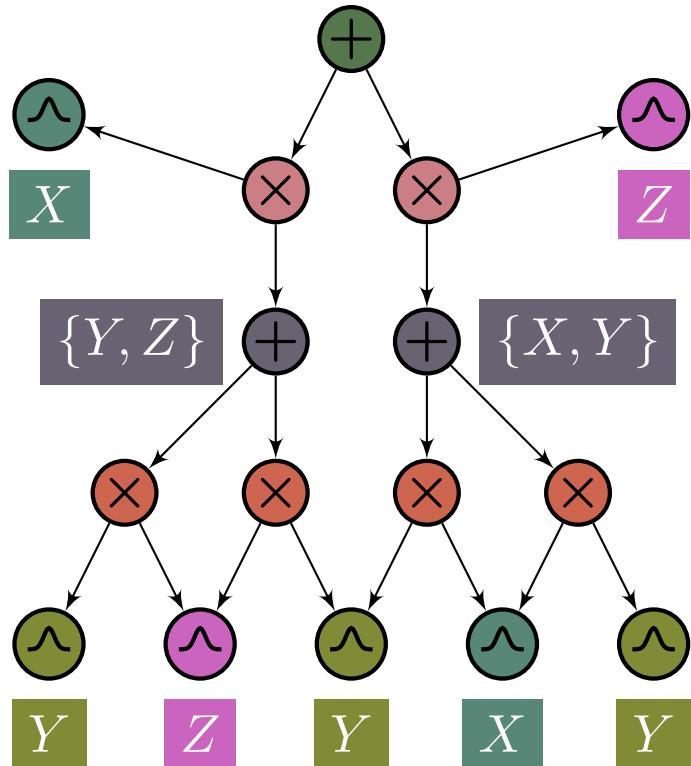
Probabilistic Circuits – Decomposability



Definition 3 (Decomposability).
Every product node child mentions different variables.



Probabilistic Circuits – Structured Decomposability



Definition 4 (Structured decomposability). *Every product node follows a vtree decomposition.*

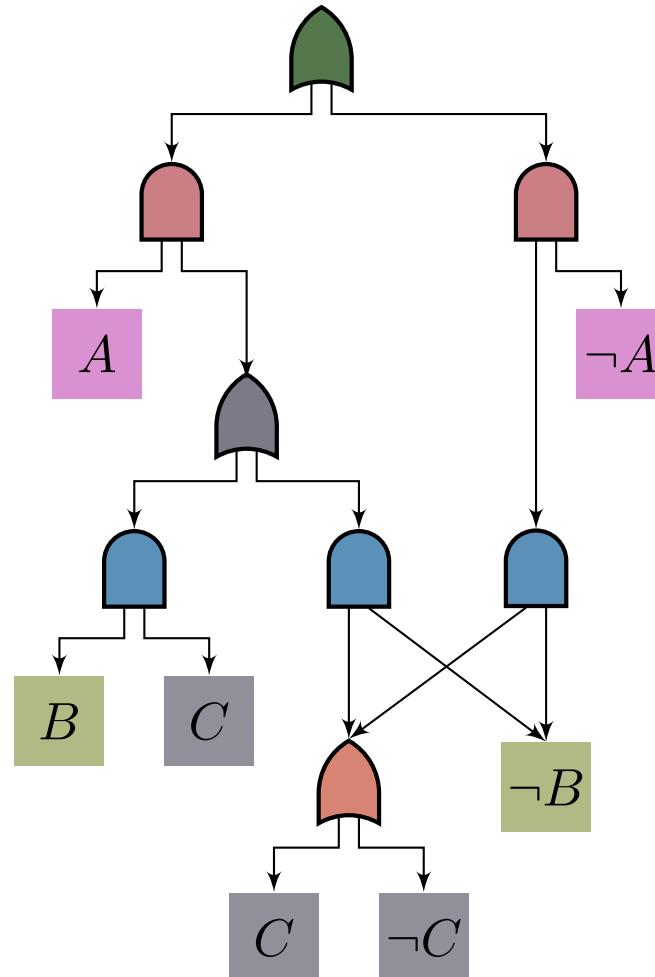
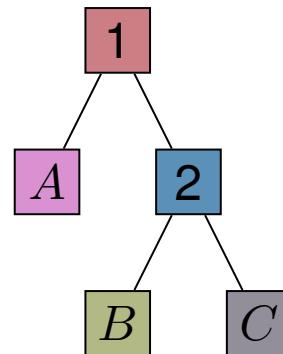
Probabilistic Circuits – Tractability

| Query | +Sm? | +Dec? | +Det? | +Str Dec? |
|-----------------------|------|-------|-------|-----------|
| Evidence | ✓ | ✓ | ✓ | ✓ |
| Marginals | ✗ | ✓ | ✓ | ✓ |
| Conditionals | ✗ | ✓ | ✓ | ✓ |
| MPE | ✗ | ✗ | ✓ | ✓ |
| Shannon Entropy* | ✗ | ✗ | ✓ | ✓ |
| Rényi Entropy* | ✗ | ✗ | ✓ | ✓ |
| Cross Entropy* | ✗ | ✗ | ✗ | ✓ |
| Kullback-Leibler Div* | ✗ | ✗ | ✗ | ✓ |
| Rényi's Alpha Div* | ✗ | ✗ | ✗ | ✓ |
| Cauchy-Schwarz Div* | ✗ | ✗ | ✗ | ✓ |
| Logical Events | ✗ | ✗ | ✗ | ✓ |
| Mutual Information* | ✗ | ✗ | ✗ | ✓ |

Probabilistic Circuits – Logic Circuits

| A | B | C | $\phi(\mathbf{x})$ |
|-----|-----|-----|--------------------|
| 0 | 0 | 0 | 1 |
| 1 | 0 | 0 | 1 |
| 0 | 1 | 0 | 0 |
| 1 | 1 | 0 | 0 |
| 0 | 0 | 1 | 1 |
| 1 | 0 | 1 | 1 |
| 0 | 1 | 1 | 0 |
| 1 | 1 | 1 | 1 |

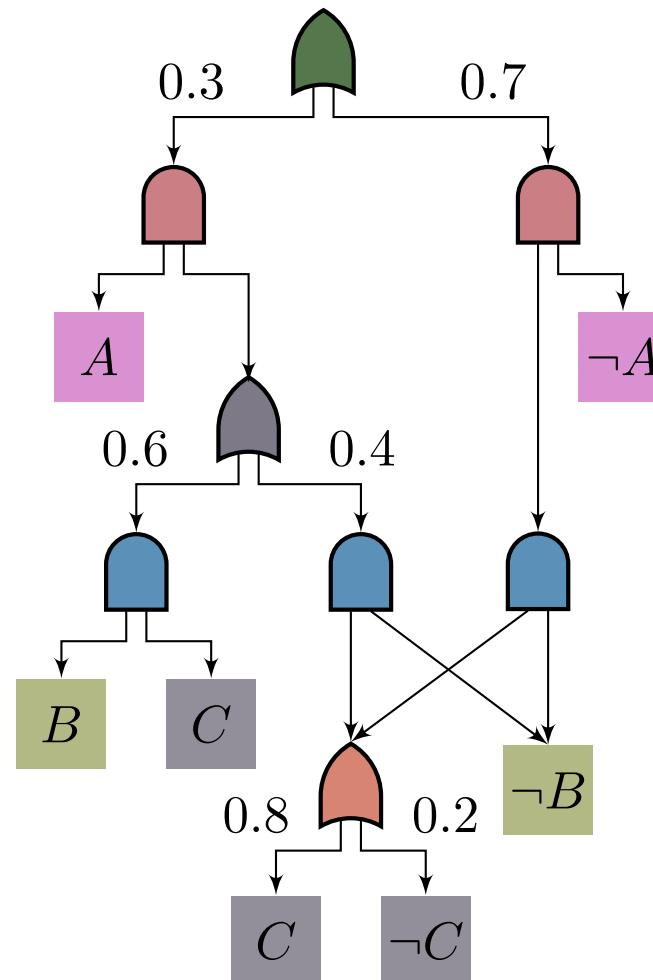
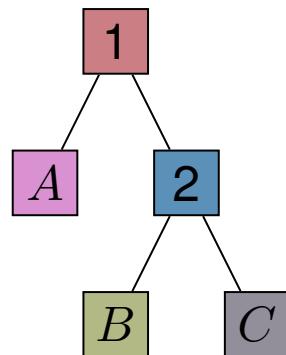
$$\phi(A, B, C) = (A \vee B) \wedge (\neg B \vee C)$$



Probabilistic Circuits – Support

| A | B | C | $\phi(\mathbf{x})$ | $p(\mathbf{x})$ |
|---|---|---|--------------------|-----------------|
| 0 | 0 | 0 | 1 | 0.140 |
| 1 | 0 | 0 | 1 | 0.024 |
| 0 | 1 | 0 | 0 | 0.000 |
| 1 | 1 | 0 | 0 | 0.000 |
| 0 | 0 | 1 | 1 | 0.560 |
| 1 | 0 | 1 | 1 | 0.096 |
| 0 | 1 | 1 | 0 | 0.000 |
| 1 | 1 | 1 | 1 | 0.180 |

$$\phi(A, B, C) = (A \vee B) \wedge (\neg B \vee C)$$



Learning Probabilistic Circuits

Divide-and-Conquer Approaches (DIV)

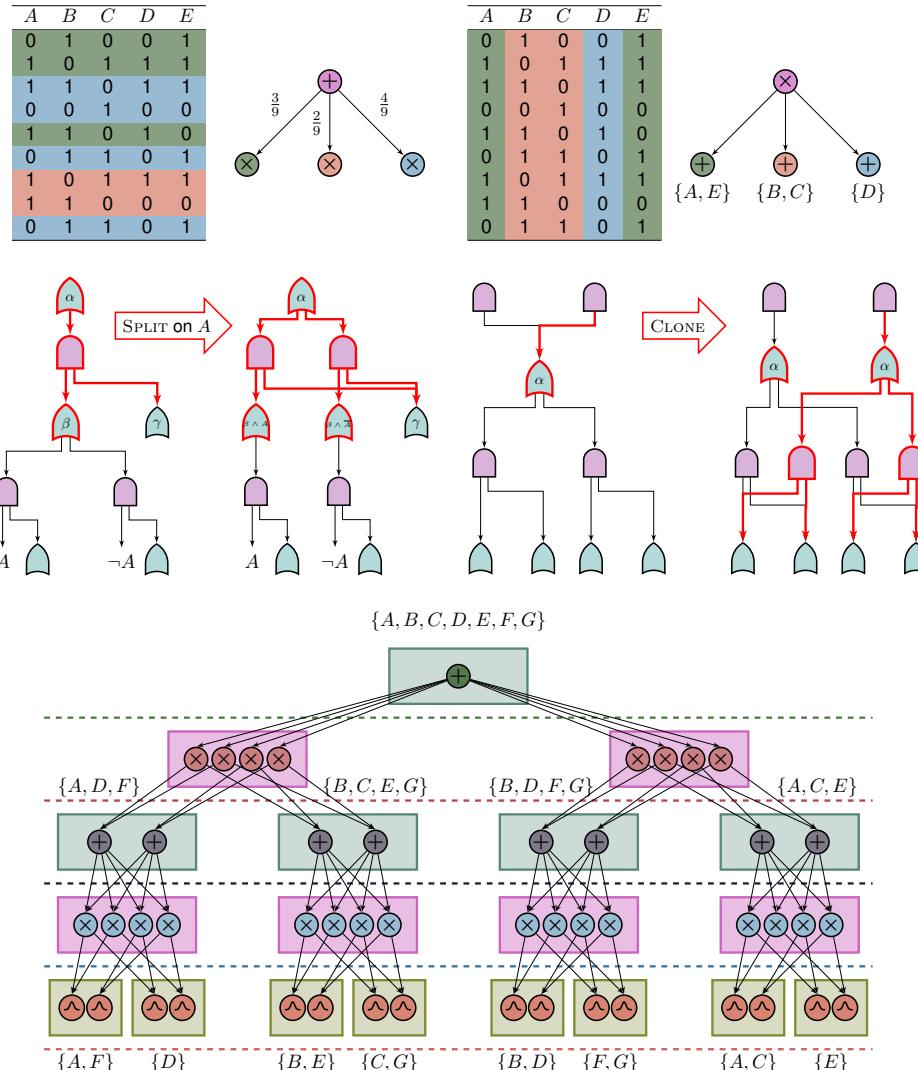
- Usually recursive;
- Splits data by similarity and stat dep;
- Stat dep usually costly;
- Usually tree-shaped.

Incremental Approaches (INCR)

- Requires an initial circuit;
- Grows from local transformations;
- Local transformations preserve properties;
- Searching for candidates to transform is costly.

Random Approaches (RAND)

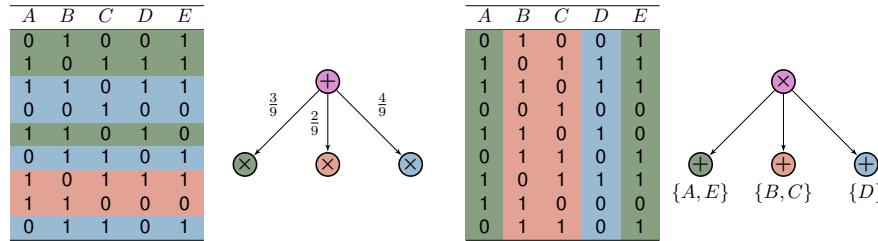
- Fast;
- Randomly generates circuits;
- Data blind and data guided approaches exist;
- Usually relies on many hyperparams;
- Worse performance.



Learning Probabilistic Circuits

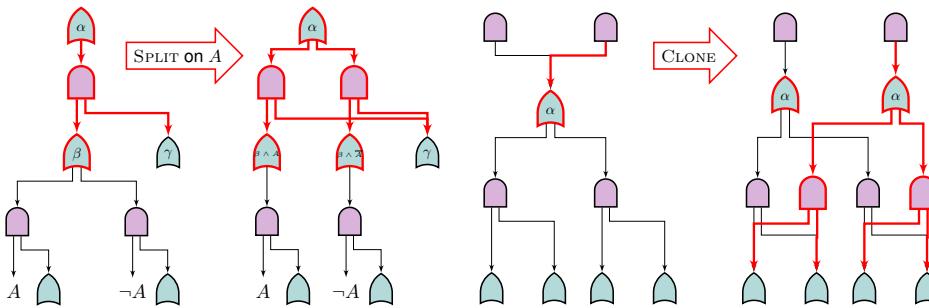
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- Stat dep usually costly;
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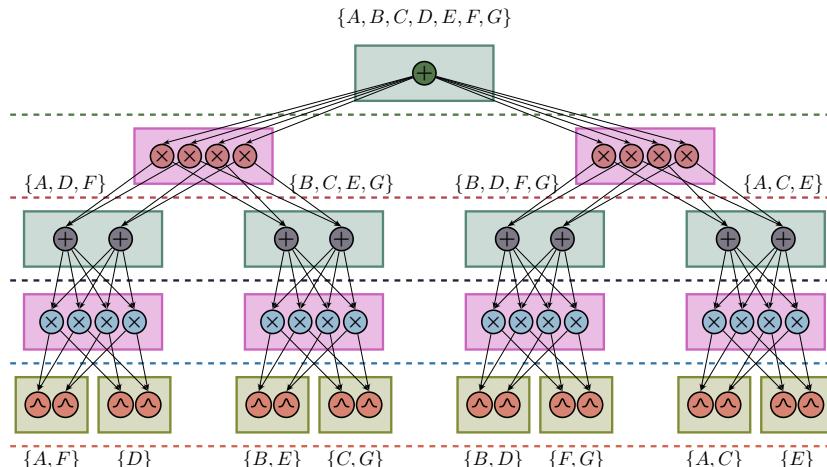
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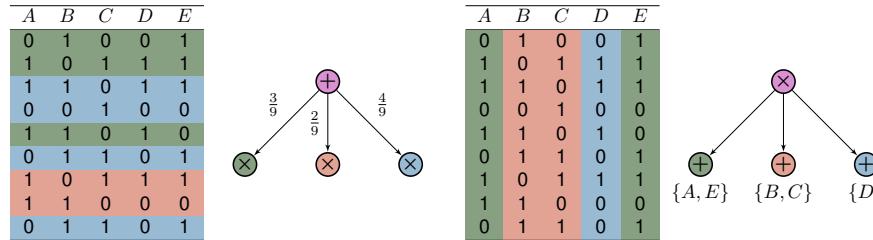
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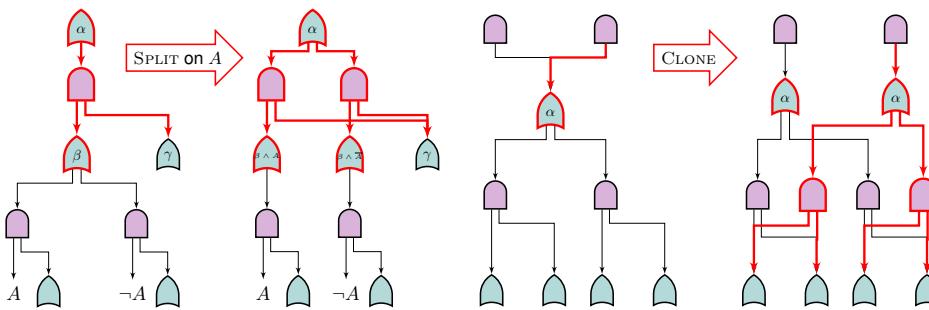
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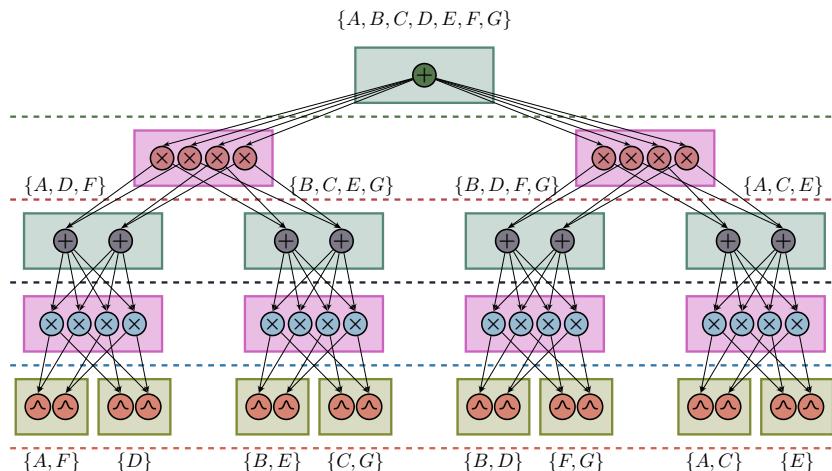
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Learning Probabilistic Circuits – Where are we right now?

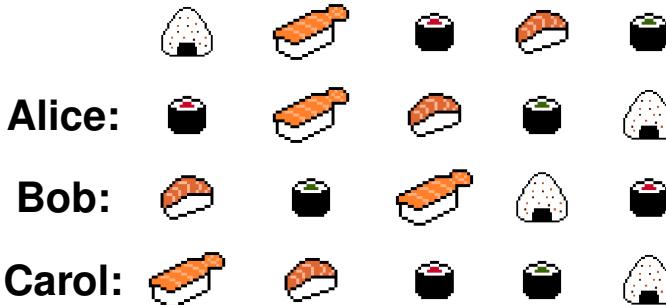
| Name | Class | Time Complexity | # hyperparams | Accepts logic? | Sm? | Dec? | Det? | Str Dec? | {0, 1}? | N? | R? | Reference |
|------------|-------|---|---------------|----------------|-----|------|------|----------|---------|----|----|---------------------------|
| LEARNSPN | DIV | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(nm^3) & , \text{if product} \end{cases}$ | ≥ 2 | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✓ | Gens and Domingos [2013] |
| ID-SPN | DIV | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(nm^3) & , \text{if product} \\ \mathcal{O}(ic(rn + m)) & , \text{if input} \end{cases}$ | $\geq 2 + 3$ | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✗ | Rooshenas and Lowd [2014] |
| PROMETHEUS | DIV | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(m(\log m)^2) & , \text{if product} \end{cases}$ | ≥ 1 | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✓ | Jaini et al. [2018a] |
| LEARNPSDD | INCR | $\begin{cases} \mathcal{O}(m^2) & , \text{top-down vtree} \\ \mathcal{O}(m^4) & , \text{bottom-up vtree} \\ \mathcal{O}(i \mathcal{C} ^2) & , \text{circuit structure} \end{cases}$ | 1 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Liang et al. [2017] |
| STRUDEL | INCR | $\begin{cases} \mathcal{O}(m^2n) & , \text{CLT + vtree} \\ \mathcal{O}(i(\mathcal{C} n + m^2)) & , \text{circuit structure} \end{cases}$ | 1 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Dang et al. [2020] |
| RAT-SPN | RAND | $\mathcal{O}(rd(s + l))$ | 4 | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✓ | Peharz et al. [2020] |
| XPC | RAND | $\mathcal{O}(i(t + kn) + ikm^2n)$ | 3 | ✗ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Mauro et al. [2021] |
| SAMPLEPSDD | RAND | $\begin{cases} \mathcal{O}(m) & , \text{random vtree} \\ \mathcal{O}(kc \log c + \log_2^2 k) & , \text{per call} \end{cases}$ | 1 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Geh and Mauá [2021] |
| LEARNRP | RAND | $\begin{cases} \mathcal{O}(m^2) & , \text{top-down vtree} \\ \mathcal{O}(m^4) & , \text{bottom-up vtree} \\ \mathcal{O}(knm) & , \text{per call} \end{cases}$ | 0 | ✗ | ✓ | ✓ | ✗ | ✓ | ✓ | ✓ | ✓ | To appear |

Learning Probabilistic Circuits – Where are we right now?

| Name | Class | Time Complexity | # hyperparams | Accepts logic? | Sm? | Dec? | Det? | Str Dec? | {0, 1}? | N? | R? | Reference |
|--------------|-------|---|---------------|----------------|-----|------|------|----------|---------|----|----|---------------------------|
| LEARNSPN | DIV | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(nm^3) & , \text{if product} \end{cases}$ | ≥ 2 | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✓ | Gens and Domingos [2013] |
| ID-SPN | DIV | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(nm^3) & , \text{if product} \\ \mathcal{O}(ic(rn + m)) & , \text{if input} \end{cases}$ | $\geq 2 + 3$ | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✗ | Rooshenas and Lowd [2014] |
| PROMETHEUS | DIV | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(m(\log m)^2) & , \text{if product} \end{cases}$ | ≥ 1 | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✓ | Jaini et al. [2018a] |
| LEARNPSDD | INCR | $\begin{cases} \mathcal{O}(m^2) & , \text{top-down vtree} \\ \mathcal{O}(m^4) & , \text{bottom-up vtree} \\ \mathcal{O}(i \mathcal{C} ^2) & , \text{circuit structure} \end{cases}$ | 1 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Liang et al. [2017] |
| STRUDEL | INCR | $\begin{cases} \mathcal{O}(m^2n) & , \text{CLT + vtree} \\ \mathcal{O}(i(\mathcal{C} n + m^2)) & , \text{circuit structure} \end{cases}$ | 1 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Dang et al. [2020] |
| RAT-SPN | RAND | $\mathcal{O}(rd(s + l))$ | 4 | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✓ | Peharz et al. [2020] |
| XPC | RAND | $\mathcal{O}(i(t + kn) + ikm^2n)$ | 3 | ✗ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Mauro et al. [2021] |
| ⇒ SAMPLEPSDD | RAND | $\begin{cases} \mathcal{O}(m) & , \text{random vtree} \\ \mathcal{O}(kc \log c + \log_2^2 k) & , \text{per call} \end{cases}$ | 1 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Geh and Mauá [2021] |
| LEARNRP | RAND | $\begin{cases} \mathcal{O}(m^2) & , \text{top-down vtree} \\ \mathcal{O}(m^4) & , \text{bottom-up vtree} \\ \mathcal{O}(knm) & , \text{per call} \end{cases}$ | 0 | ✗ | ✓ | ✓ | ✗ | ✓ | ✓ | ✓ | ✓ | To appear |

A Logical Perspective

Motivation



If we assume

n sushi types,

k sized rankings with $k \leq n$,

X_{ij} binary variables; i is sushi type, j is position in ranking;

then the total number of possible assignments of the $n \cdot k$ variables is 2^{nk} ...

...but many of these are zero probability assignments!

If we can embed total ranking constraints...

...we go down to $k!$ total assignments!

Takeaway: models which exploit domain knowledge are much more efficient!

Example:

$$n = 3, k = 3$$

| X_{11} | X_{12} | X_{13} | X_{21} | \dots | X_{33} | $p(\mathbf{x}) > 0$ |
|----------|----------|----------|----------|----------|----------|---------------------|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 1 | 0 | 0 | 0 | 0 | 0 |
| 1 | 1 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0 | 1 | 0 | 0 | 0 | 0 |
| \vdots |
| 0 | 1 | 1 | 1 | 1 | 1 | 0 |
| 1 | 1 | 1 | 1 | 1 | 1 | 0 |

Assignments: $2^{3 \cdot 3} = 512$

Positive assignments: $3! = 6$

Motivation

Existing approaches:

LEARNPSDD (Liang et al. [2017]):

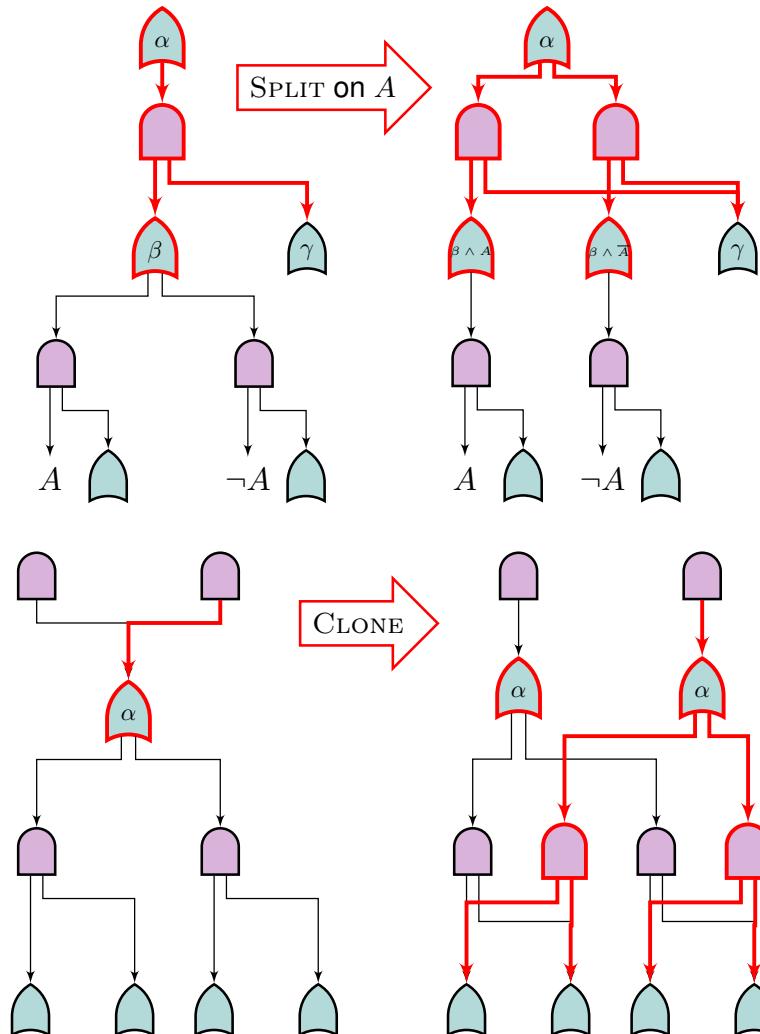
- ✗ Requires initial logic circuit encoding the support...
- ✗ Scales poorly to complex formulae and/or high dimension...
- ✗ Costly whole circuit evaluation at every iteration...
- ✓ Very good performance!

STRUDEL (Dang et al. [2020]):

- ✓ Constructs an initial structure (from a CLT)!
- ✗ But does not encode constraints...
- ✓ Scales to high dimension!
- ✗ As long as the circuit doesn't get too big...

SAMPLEPSDD (Geh and Mauá [2021]):

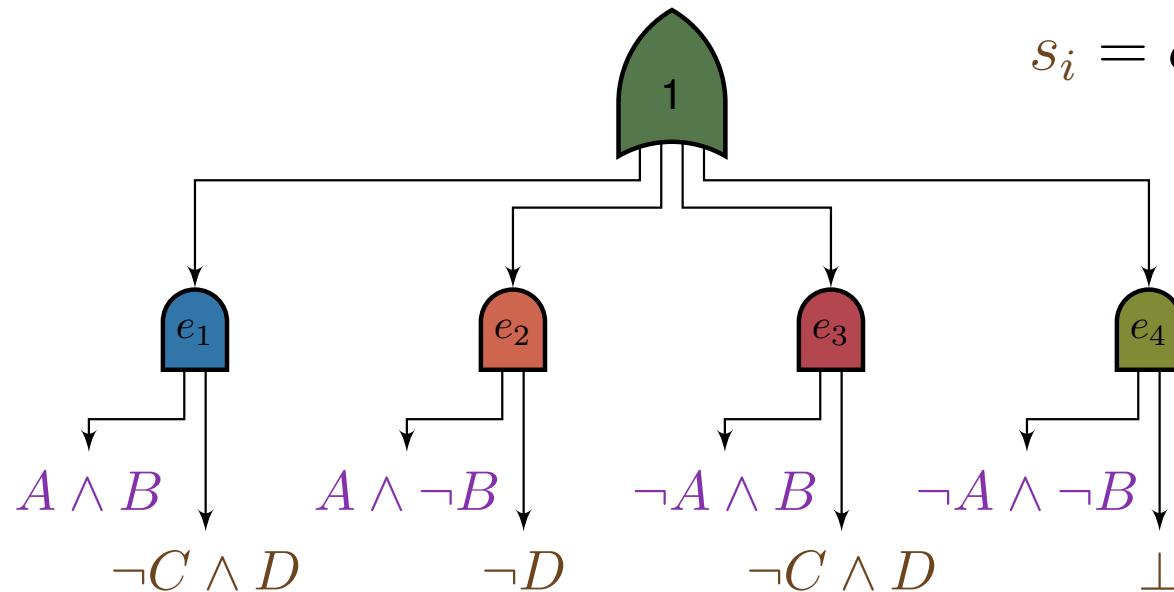
- ✓ Scales to high dimension and complex formulae!
- ✓ Constructs a structure consistent with constraints!
- ✗ But does so by relaxing the formula...
- ✗ Performance varies on set bounds and vtree structure...



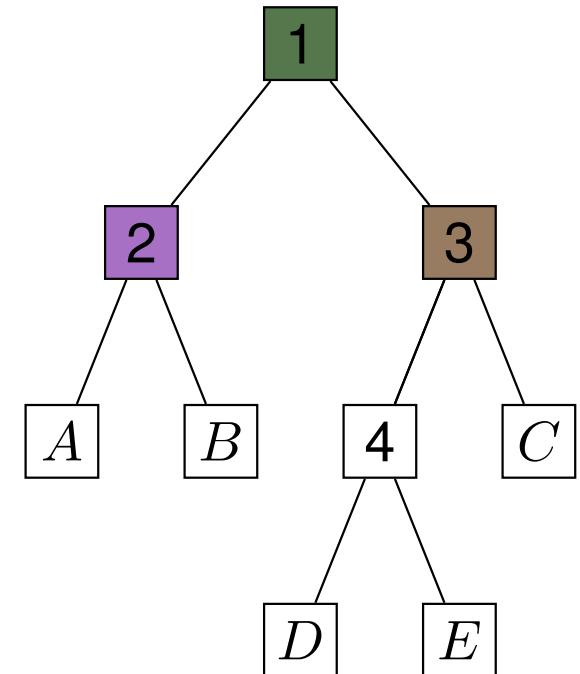
SAMPLEPSDD

Common assumption: p_i are conjunctions of literals .

$$\phi(A, B, C, D) = (A \wedge \neg B \wedge \neg D) \vee (B \wedge \neg C \wedge D)$$



$$s_i = \phi|_{p_i}$$

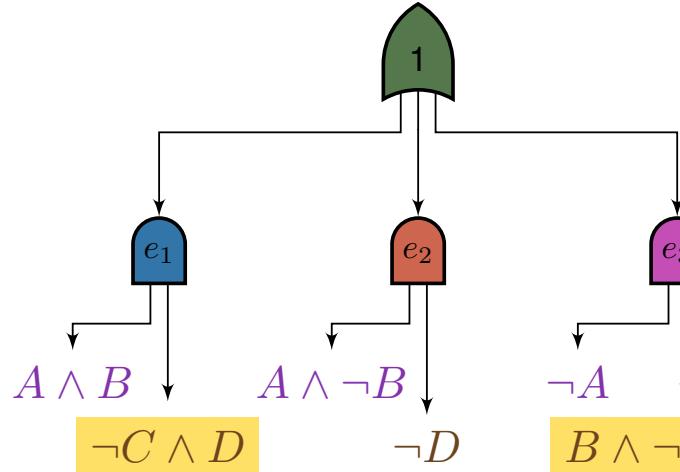


Problem: size of circuit is **exponential** in the size of p_i 's scope.

SAMPLEPSDD

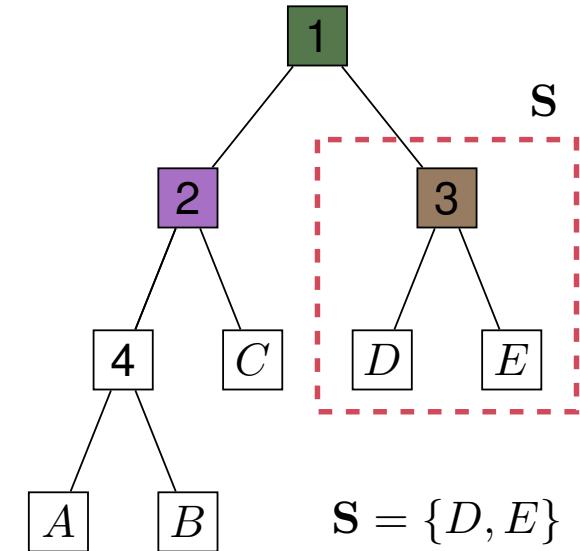
Solution: randomly sample a bounded number (k) of p_i

$$\phi(A, B, C, D) = (A \wedge \neg B \wedge \neg D) \vee (B \wedge \neg C \wedge D)$$



$$s_i = \phi|_{p_i}$$

$$\text{Sc}(s_3) \not\subseteq S$$



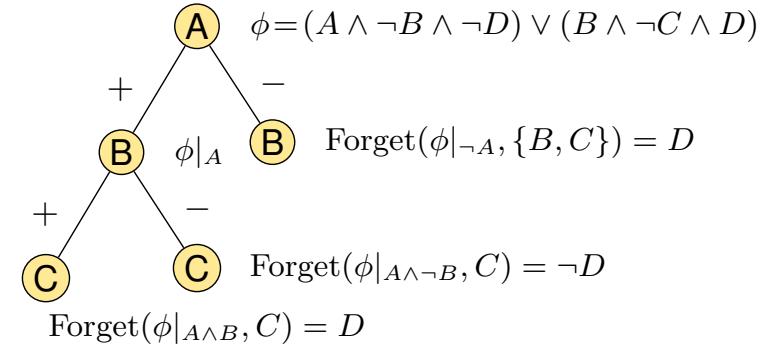
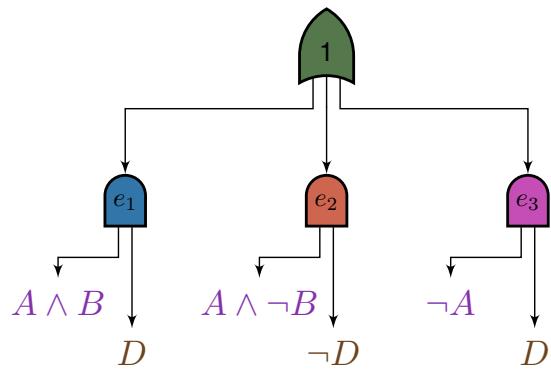
But: this violates structured decomposability:

$\neg C \wedge D$ contains C , and $C \notin S$

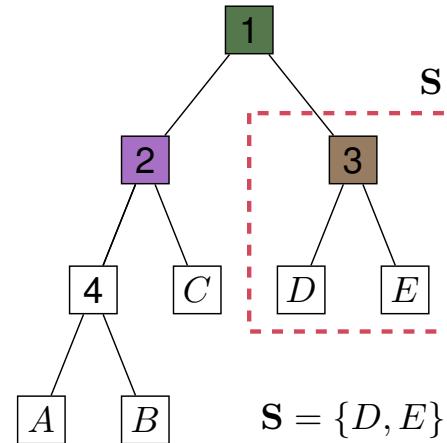
$\neg B \wedge \neg C \wedge D$ contains B and C , and $B, C \notin S$

SAMPLEPSDD

New solution: relax logical constraints ϕ

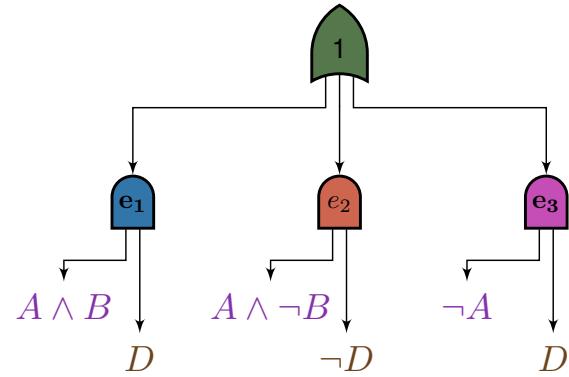


Now all s_i respect S

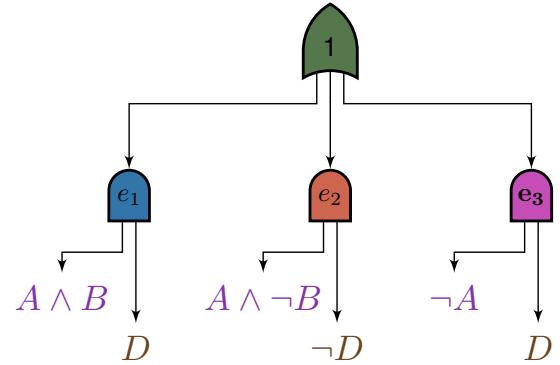
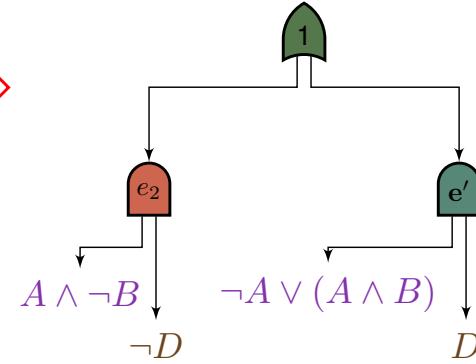


SAMPLEPSDD

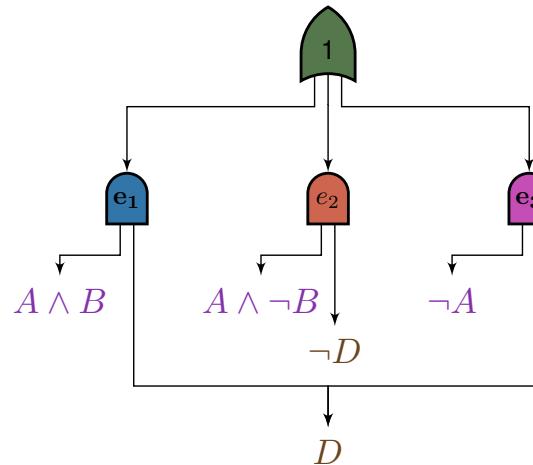
Apply **local transformations** for variety and size reduction



COMPRESS



MERGE



Experiments

Evaluation: we sample 30 PSDDs and use 5 ensemble strategies:

- **Likelihood weighting (LLW),**
- **Uniform weights,**
- ◆ **Expectation-Maximization (EM),**
- ▲ **Stacking,**
- ▼ **Bayesian Model Combination (BMC);**

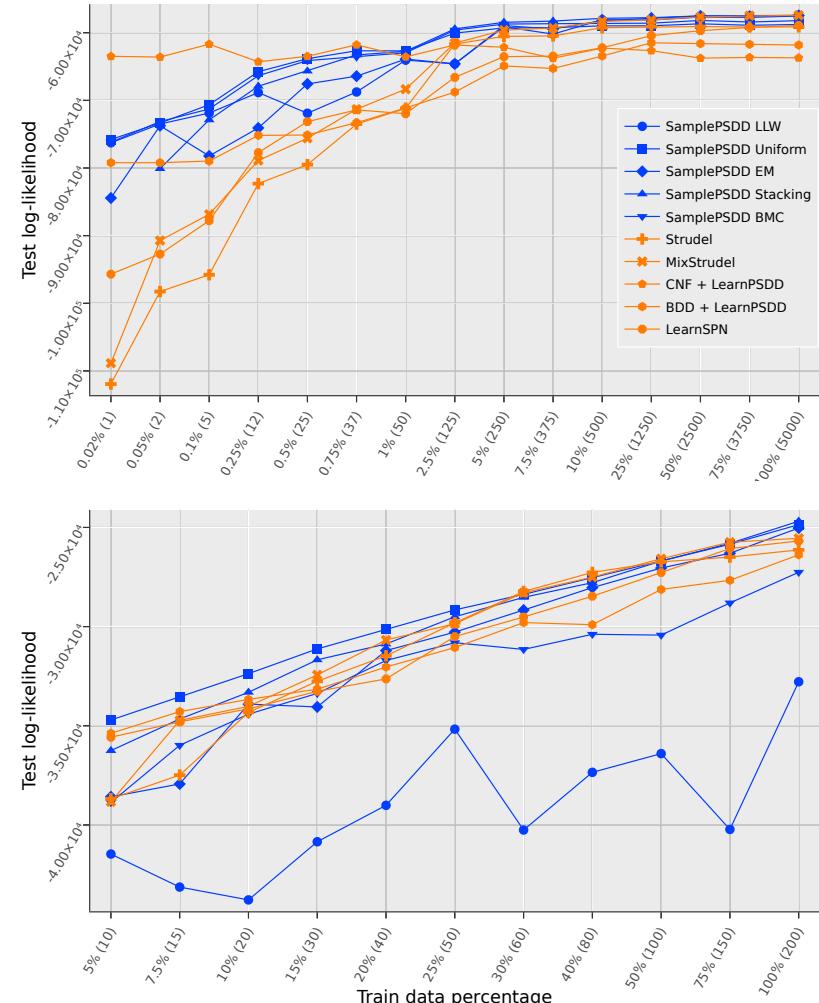
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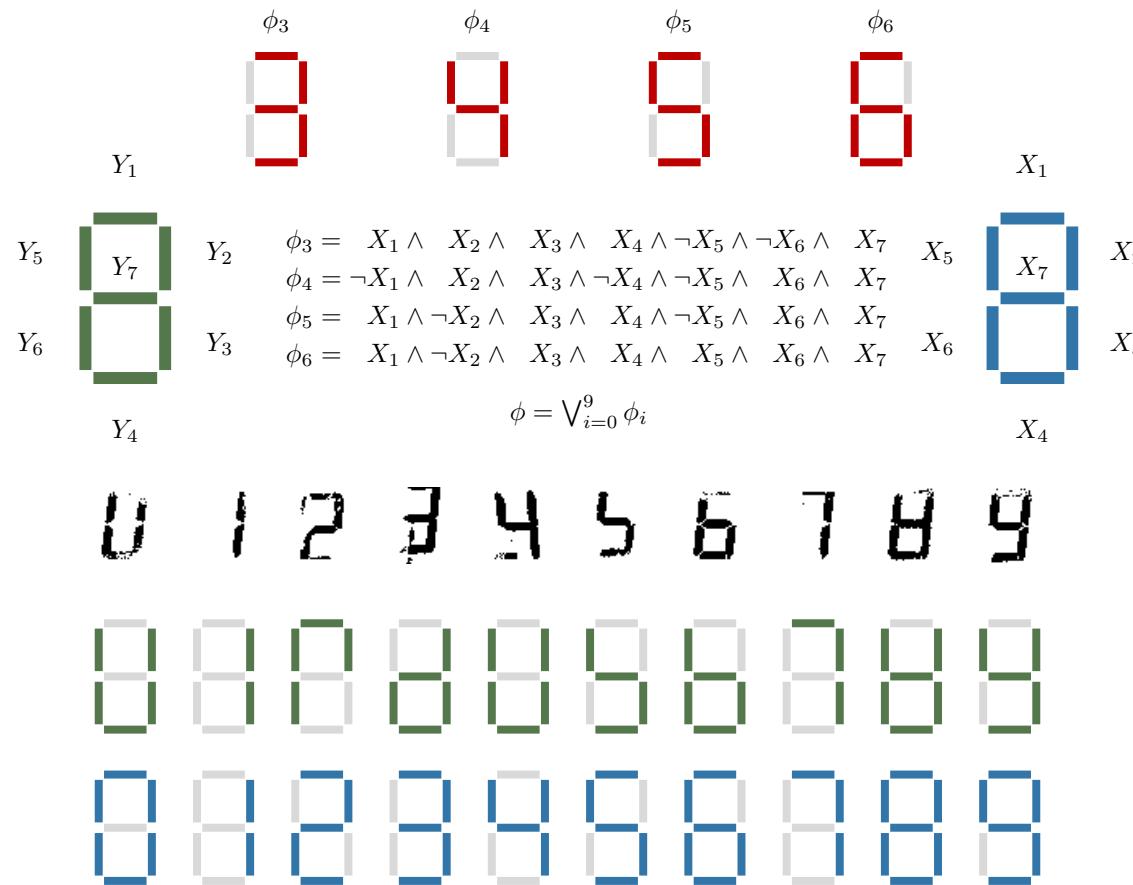
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|----------------|-------|--------|----------------|
| ⇒ LED | 14 | 5000 | 23 |
| ⇒ LED + IMAGES | 157 | 700 | 39899 |
| SUSHI RANKING | 100 | 3500 | 17413 |
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Mattei et al. [2020], Kamishima [2003], Shen et al. [2017],
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Experiments – LED



Experiments

Evaluation: we sample 30 PSDDs and use 5 ensemble strategies:

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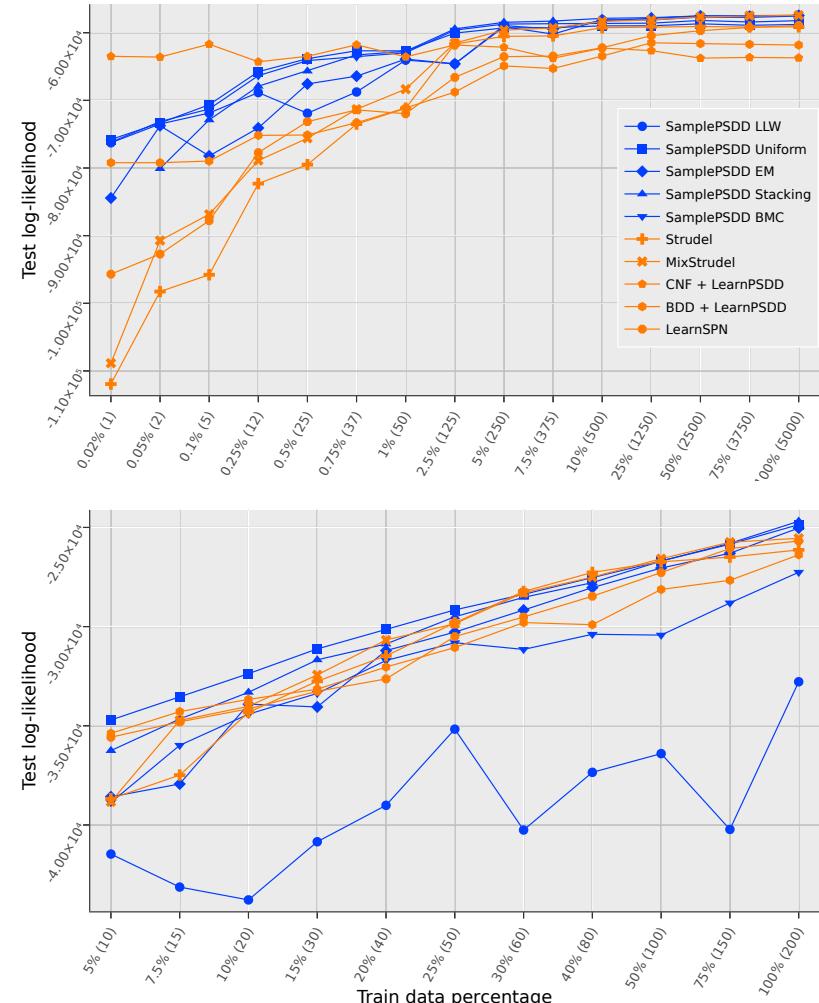
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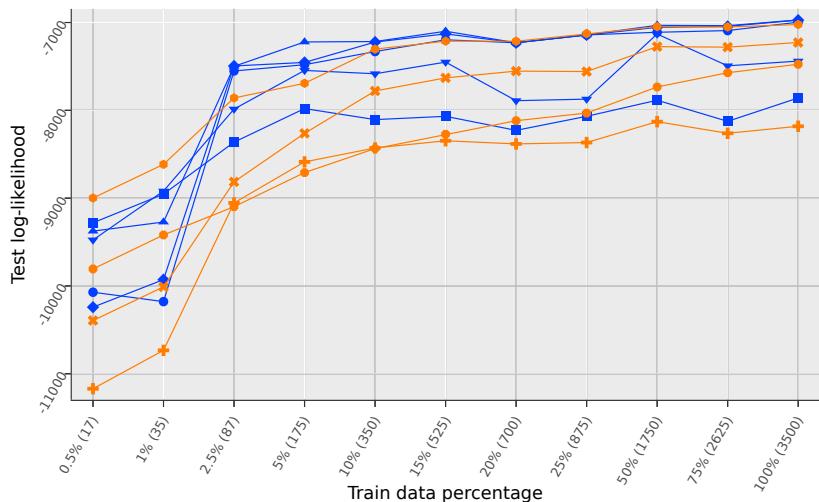
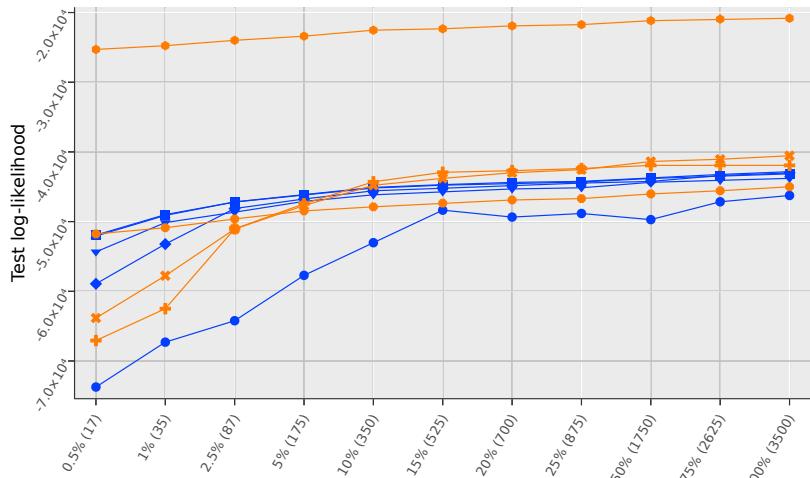
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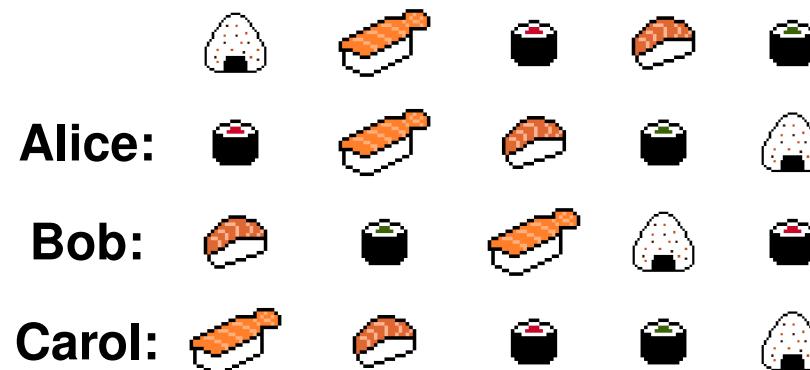
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Experiments – SUSHI RANKING



n sushi types and *k* rank positions

$$\begin{array}{ll} \alpha = & (X_{i1} \wedge \neg X_{i2} \wedge \cdots \wedge \neg X_{ik}) \\ & \vee (\neg X_{i1} \wedge X_{i2} \wedge \cdots \wedge \neg X_{ik}) \\ & \vdots \\ & \underbrace{\vee (\neg X_{i1} \wedge \neg X_{i2} \wedge \cdots \wedge X_{ik})}_{\text{Rank position}} \end{array} \quad \begin{array}{ll} \beta = & (X_{1j} \wedge \neg X_{2j} \wedge \cdots \wedge \neg X_{nj}) \\ & \vee (\neg X_{1j} \wedge X_{2j} \wedge \cdots \wedge \neg X_{nj}) \\ & \vdots \\ & \underbrace{\vee (\neg X_{1j} \wedge \neg X_{2j} \wedge \cdots \wedge X_{nj})}_{\text{Type uniqueness}} \end{array}$$

$$\phi = \alpha \wedge \beta$$

Experiments – SUSHI TOP 5



Alice: A row of five icons showing Alice's ranking of the sushi types.

Bob: A row of five icons showing Bob's ranking of the sushi types.

Carol: A row of five icons showing Carol's ranking of the sushi types.

n sushi types and *k* rank positions

Top *k* out of *n* sushi \equiv *n*-choose-*k* model

n-choose-*k* model \equiv cardinality Exactly(*k, n*)

$$\phi = \text{Exactly}(\textcolor{violet}{k}, \textcolor{brown}{n}) = \left(\sum_X X = \textcolor{violet}{k} \right)$$

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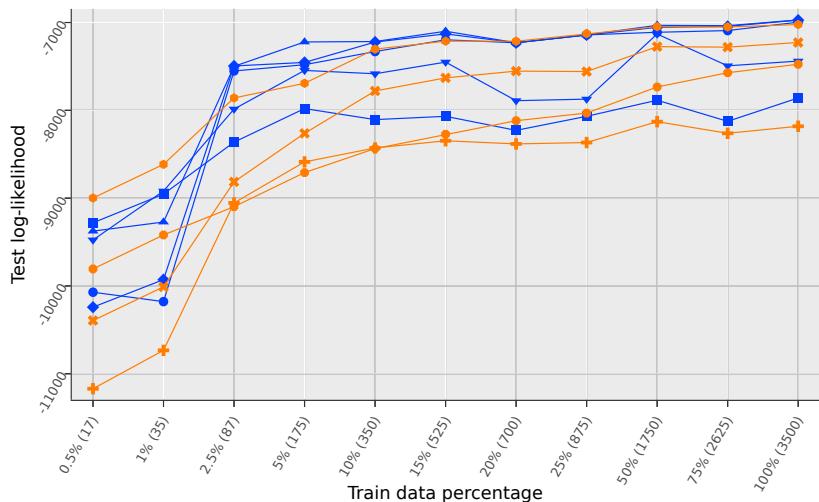
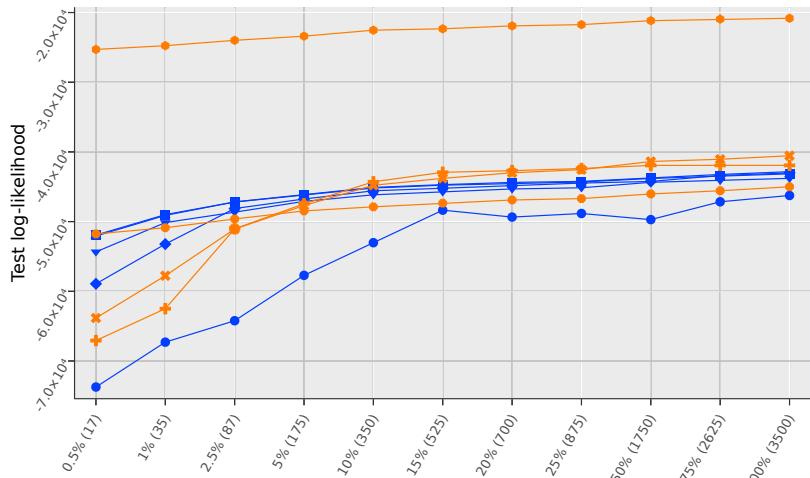
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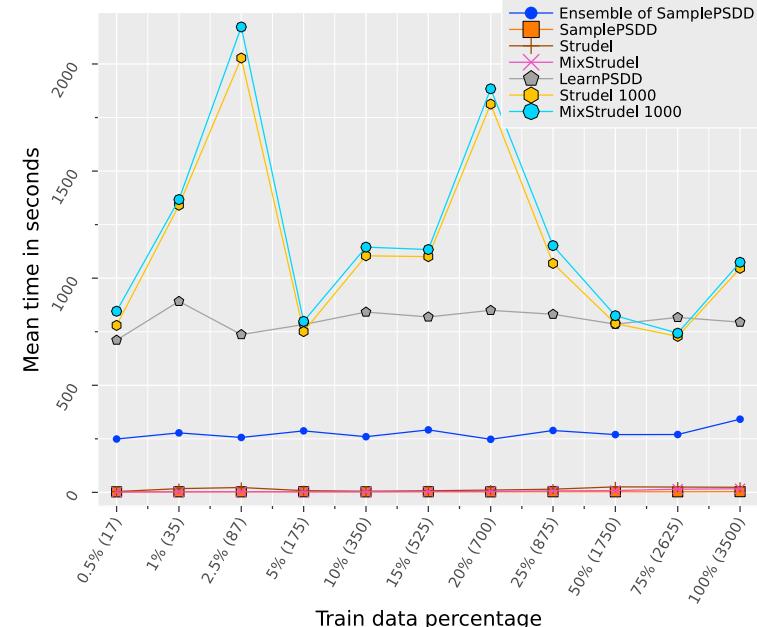
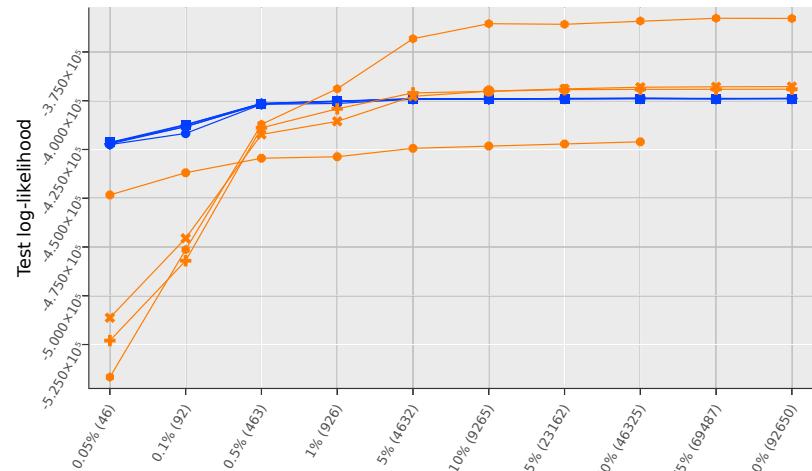
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Experiments – DOTA 2 GAMES

| | | | | | | | | | |
|----|----|----|----|----|----|----|----|----|----|
| 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
| 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
| 21 | 22 | 23 | 24 | 25 | 26 | 27 | 28 | 29 | 30 |

$X_1 \quad X_2 \quad X_3 \quad X_4 \quad X_5$

| | | | | |
|---|----|----|----|----|
| 4 | 11 | 17 | 23 | 28 |
|---|----|----|----|----|

$\alpha = \underbrace{\text{Exactly}(k, n)}_{\text{Intractable as CNF}}$

n characters, k for each team

$Y_5 \quad Y_4 \quad Y_3 \quad Y_2 \quad Y_1$

| | | | | |
|----|----|----|---|---|
| 25 | 20 | 13 | 8 | 5 |
|----|----|----|---|---|

$\beta = \underbrace{\text{Exactly}(k, n)}_{\text{Intractable as CNF}}$

$\gamma = \underbrace{X_i \neq Y_j, \forall X_i, Y_j}_{\text{Intractable as BDD}}$

$$\phi = \alpha \wedge \beta \wedge \gamma$$

Experiments

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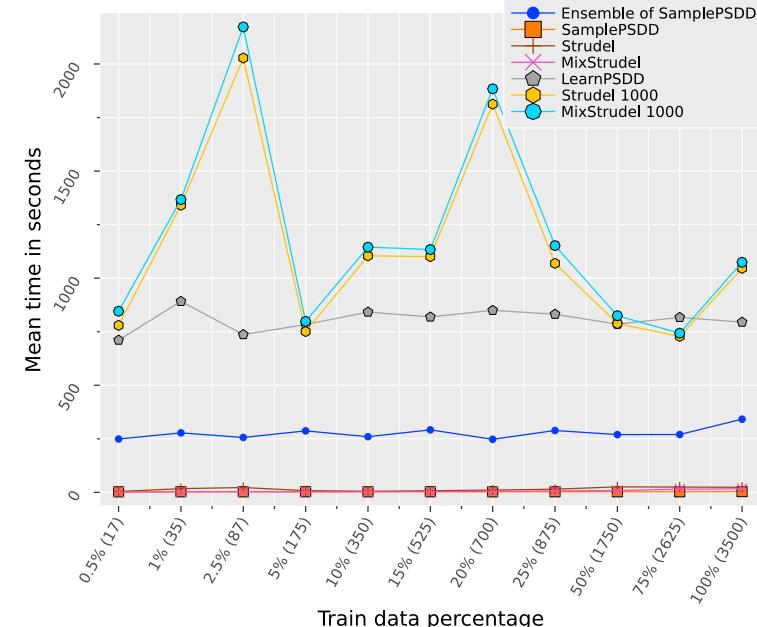
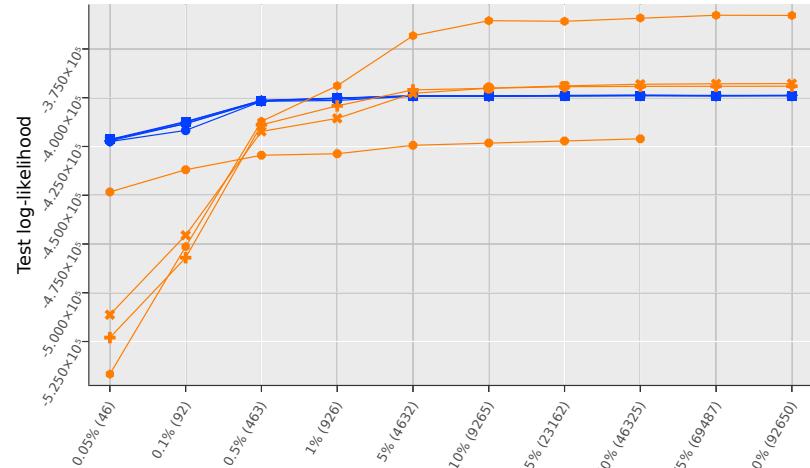
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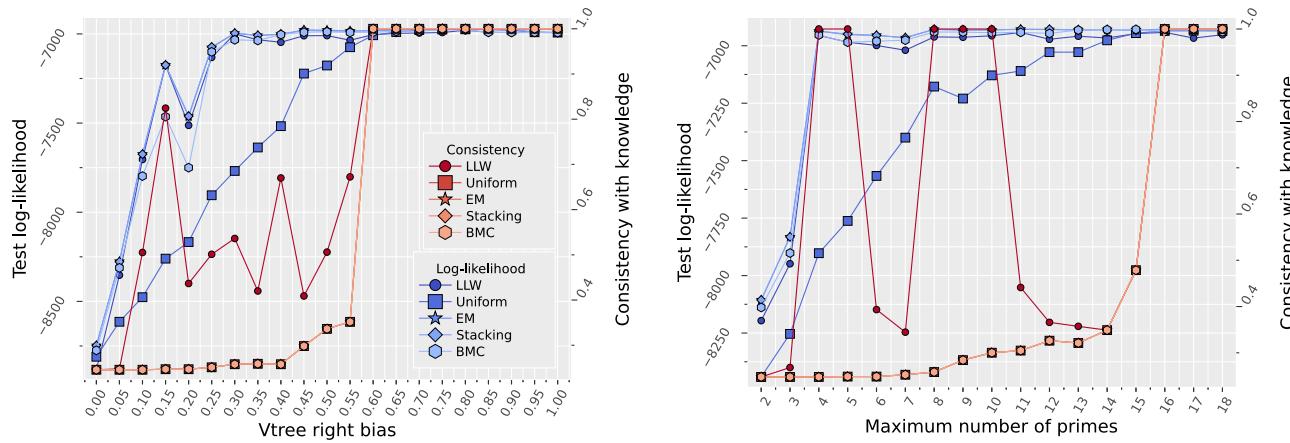
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SAMPLEPSDD – Experiments

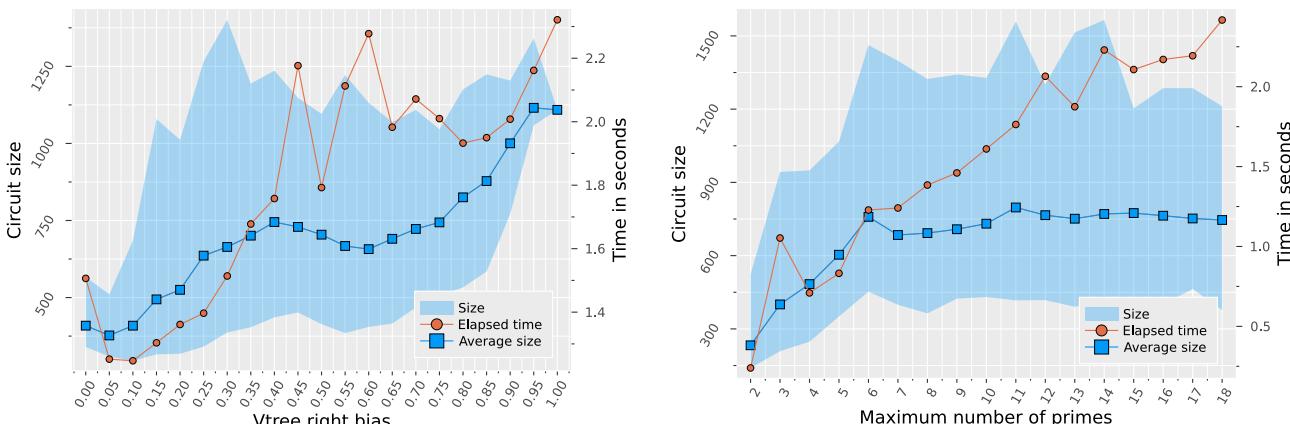
What is the impact of higher k 's and right-leaning vtrees

in log-likelihood and consistency?



Samples perform better with higher k 's and right-leaning vtrees ...

...but at a cost to complexity.



Learning Probabilistic Circuits – Where are we right now?

| Name | Class | Time Complexity | # hyperparams | Accepts logic? | Sm? | Dec? | Det? | Str Dec? | {0, 1}? | N? | R? | Reference |
|------------|-------|---|---------------|----------------|-----|------|------|----------|---------|----|----|---------------------------|
| LEARNSPN | DIV | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(nm^3) & , \text{if product} \end{cases}$ | ≥ 2 | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✓ | Gens and Domingos [2013] |
| | | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(nm^3) & , \text{if product} \\ \mathcal{O}(ic(rn + m)) & , \text{if input} \end{cases}$ | | | | | | | | | | |
| ID-SPN | DIV | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(nm^3) & , \text{if product} \\ \mathcal{O}(m(\log m)^2) & , \text{if product} \end{cases}$ | $\geq 2 + 3$ | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✗ | Rooshenas and Lowd [2014] |
| | | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(m(\log m)^2) & , \text{if product} \end{cases}$ | | | | | | | | | | |
| PROMETHEUS | DIV | $\begin{cases} \mathcal{O}(nkmc) & , \text{if sum} \\ \mathcal{O}(m(\log m)^2) & , \text{if product} \end{cases}$ | ≥ 1 | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✓ | Jaini et al. [2018a] |
| LEARNPSDD | INCR | $\begin{cases} \mathcal{O}(m^2) & , \text{top-down vtree} \\ \mathcal{O}(m^4) & , \text{bottom-up vtree} \\ \mathcal{O}(i \mathcal{C} ^2) & , \text{circuit structure} \end{cases}$ | 1 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Liang et al. [2017] |
| | | $\begin{cases} \mathcal{O}(m^2n) & , \text{CLT + vtree} \\ \mathcal{O}(i(\mathcal{C} n + m^2)) & , \text{circuit structure} \end{cases}$ | | | | | | | | | | |
| STRUDEL | INCR | | | | | | | | | | | Dang et al. [2020] |
| RAT-SPN | RAND | $\mathcal{O}(rd(s + l))$ | 4 | ✗ | ✓ | ✓ | ✗ | ✗ | ✓ | ✓ | ✓ | Peharz et al. [2020] |
| XPC | RAND | $\mathcal{O}(i(t + kn) + ikm^2n)$ | 3 | ✗ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Mauro et al. [2021] |
| SAMPLEPSDD | RAND | $\begin{cases} \mathcal{O}(m) & , \text{random vtree} \\ \mathcal{O}(kc \log c + \log_2^2 k) & , \text{per call} \end{cases}$ | 1 | ✓ | ✓ | ✓ | ✓ | ✓ | ✓ | ✗ | ✗ | Geh and Mauá [2021] |
| ⇒ LEARNRP | RAND | $\begin{cases} \mathcal{O}(m^2) & , \text{top-down vtree} \\ \mathcal{O}(m^4) & , \text{bottom-up vtree} \\ \mathcal{O}(knm) & , \text{per call} \end{cases}$ | 0 | ✗ | ✓ | ✓ | ✗ | ✓ | ✓ | ✓ | ✓ | To appear |

A Data Perspective

Motivation

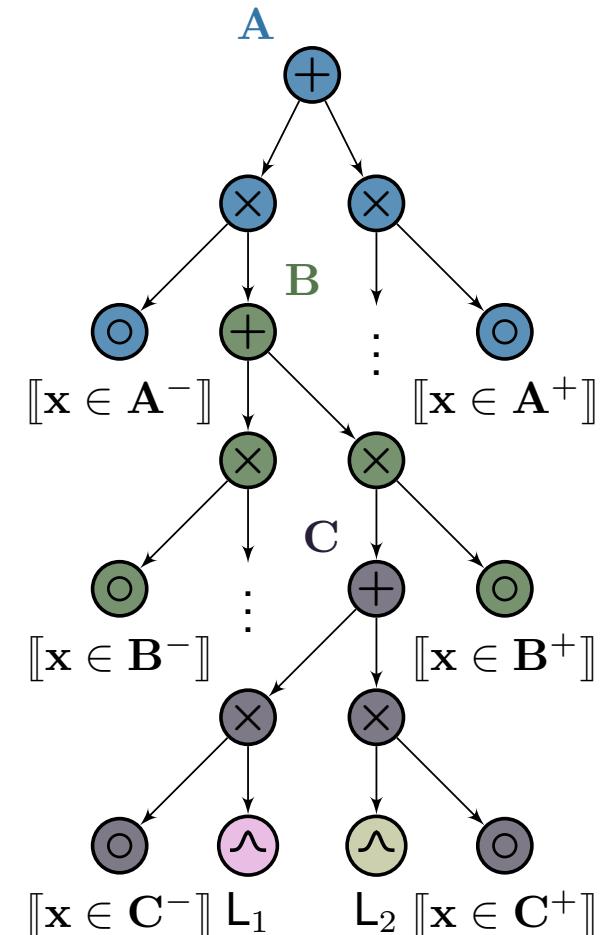
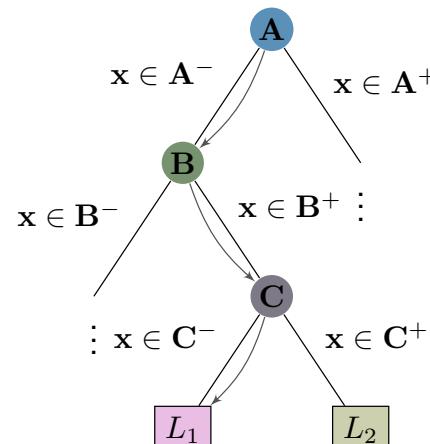
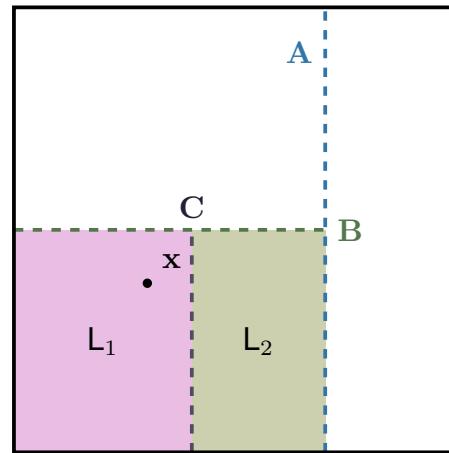
Density Estimation Trees...

- ...are fast;
- ...are interpretable;
- ...are (somewhat) explainable;
- ...have extensive literature coverage;
- ...are not so expressive;
- ...only accept marginalization queries;
- ...are not so accurate;

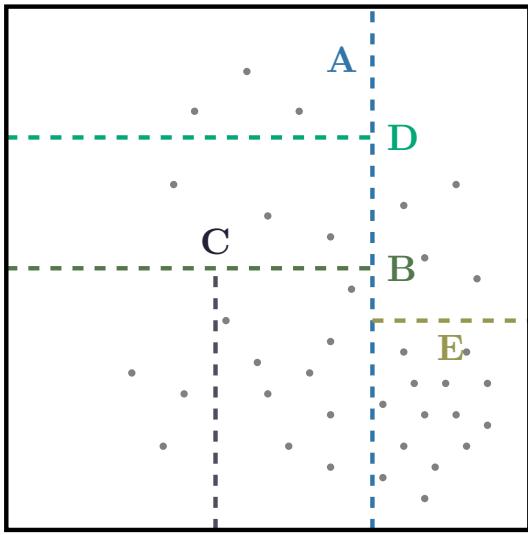
...but are subsumed by circuits!

Learn DETs \subseteq Learn PCs?

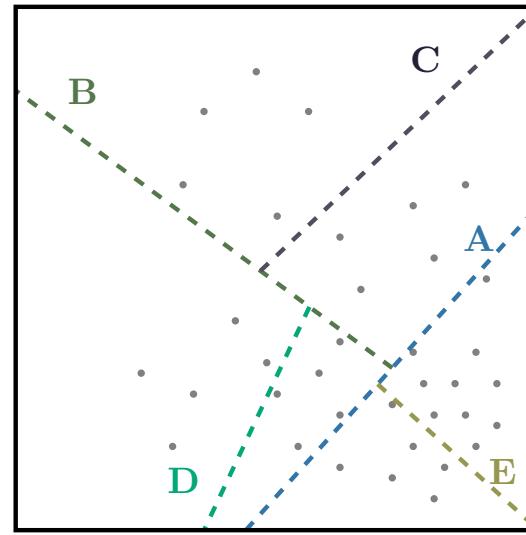
Can we take advantage of known learning procedures in DETs and transplant them to more general circuits?



Random Projections



Axis-aligned projections

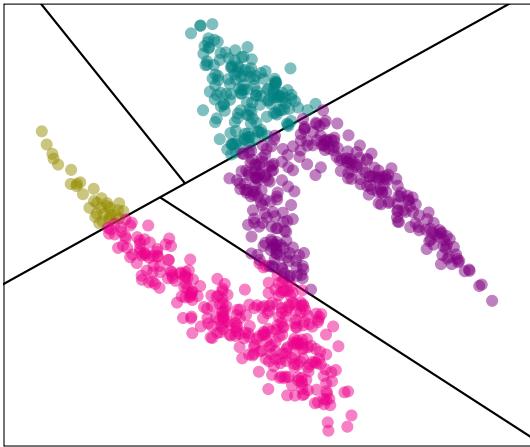


Random projections

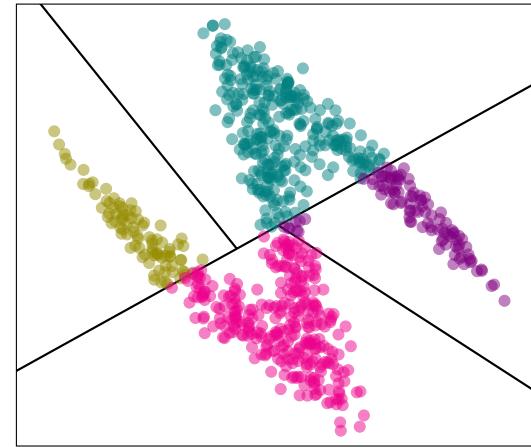
If the data has *intrinsic dimension* d , then with constant probability the part of the data at level d or higher of the tree has average diameter less than half of the data.

Random Projections

SPLITMAX

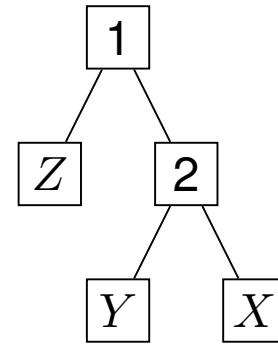
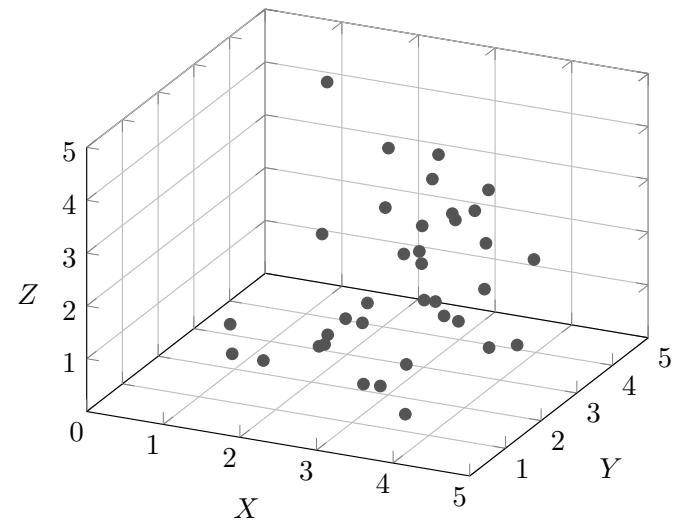


SPLITSID

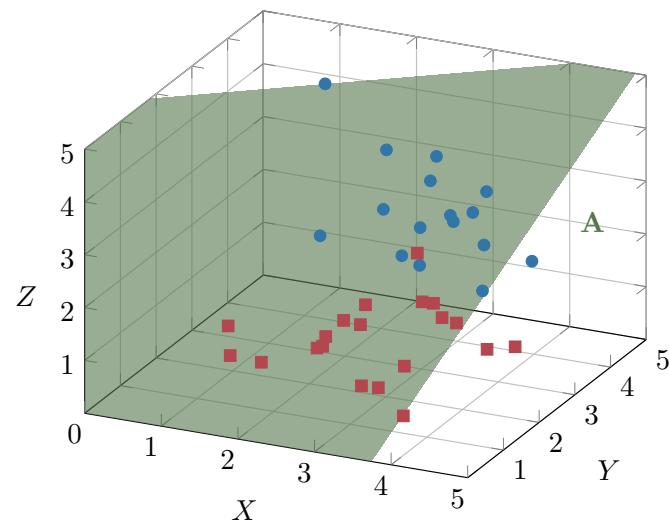


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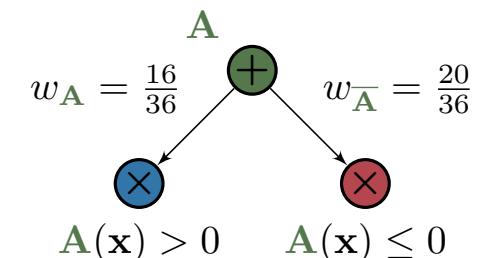
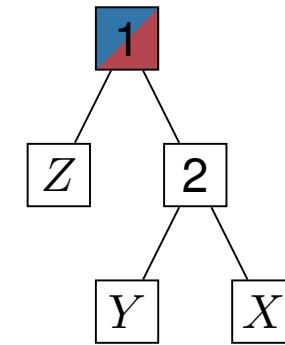
LearnRP



LearnRP

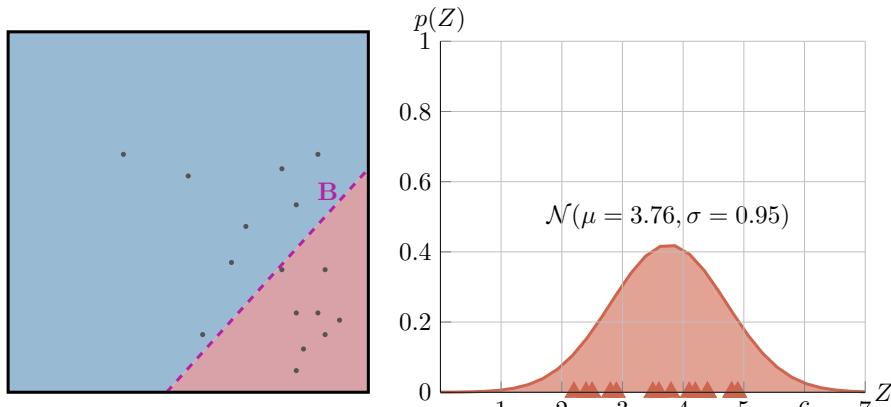
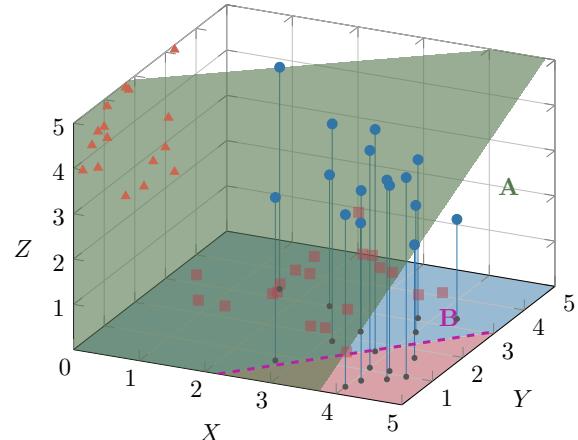


$$\mathbf{A}(x, y, z) = \begin{bmatrix} x & y & z \end{bmatrix} \cdot \underbrace{\begin{bmatrix} -0.31 \\ -0.40 \\ 0.85 \end{bmatrix}}_a + \underbrace{1}_\theta$$

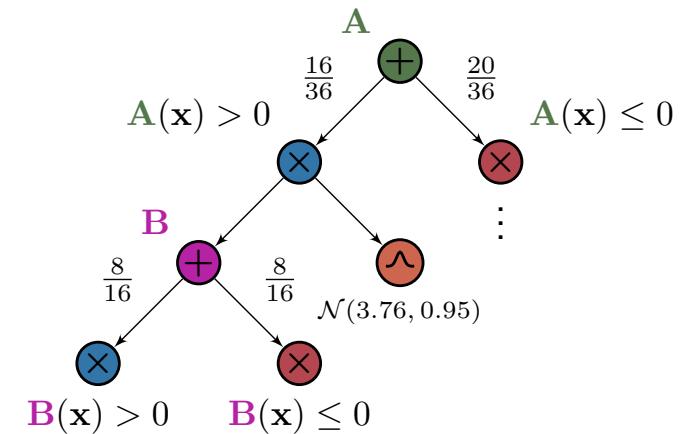
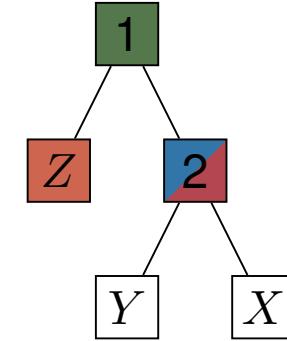


$w_{\mathbf{A}}$: probability of $\mathbf{A}(\mathbf{x}) > 0$

LearnRP



$$\mathbf{B}(x, y) = [x \ y] \cdot \underbrace{\begin{bmatrix} 1.10 \\ -1.00 \end{bmatrix}}_b - \underbrace{2.43}_\gamma$$



Parameter Optimization

Expectation-Maximization (EM)

- Full EM (dataset D)

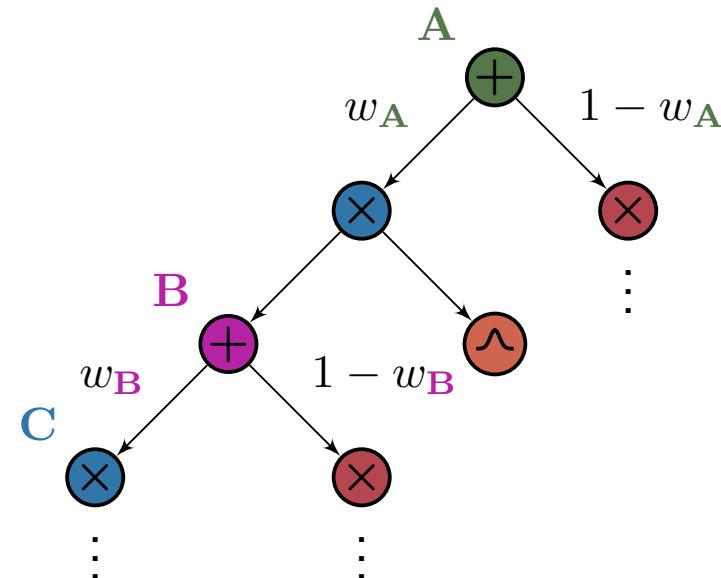
$$w_B \propto w_B \cdot \sum_{x \in D} \frac{1}{p_A(x)} \cdot \frac{\partial p_A(x)}{\partial p_B(x)} \cdot p_C(x)$$

- Minibatch EM (batch M ⊂ D)

$$w_B \propto w_B \cdot \sum_{x \in M} \frac{1}{p_A(x)} \cdot \frac{\partial p_A(x)}{\partial p_B(x)} \cdot p_C(x)$$

LEARNRP-100: LEARNRP + 100 itrs of minibatch

LEARNRP-F: LEARNRP-100 + 30 itrs of full



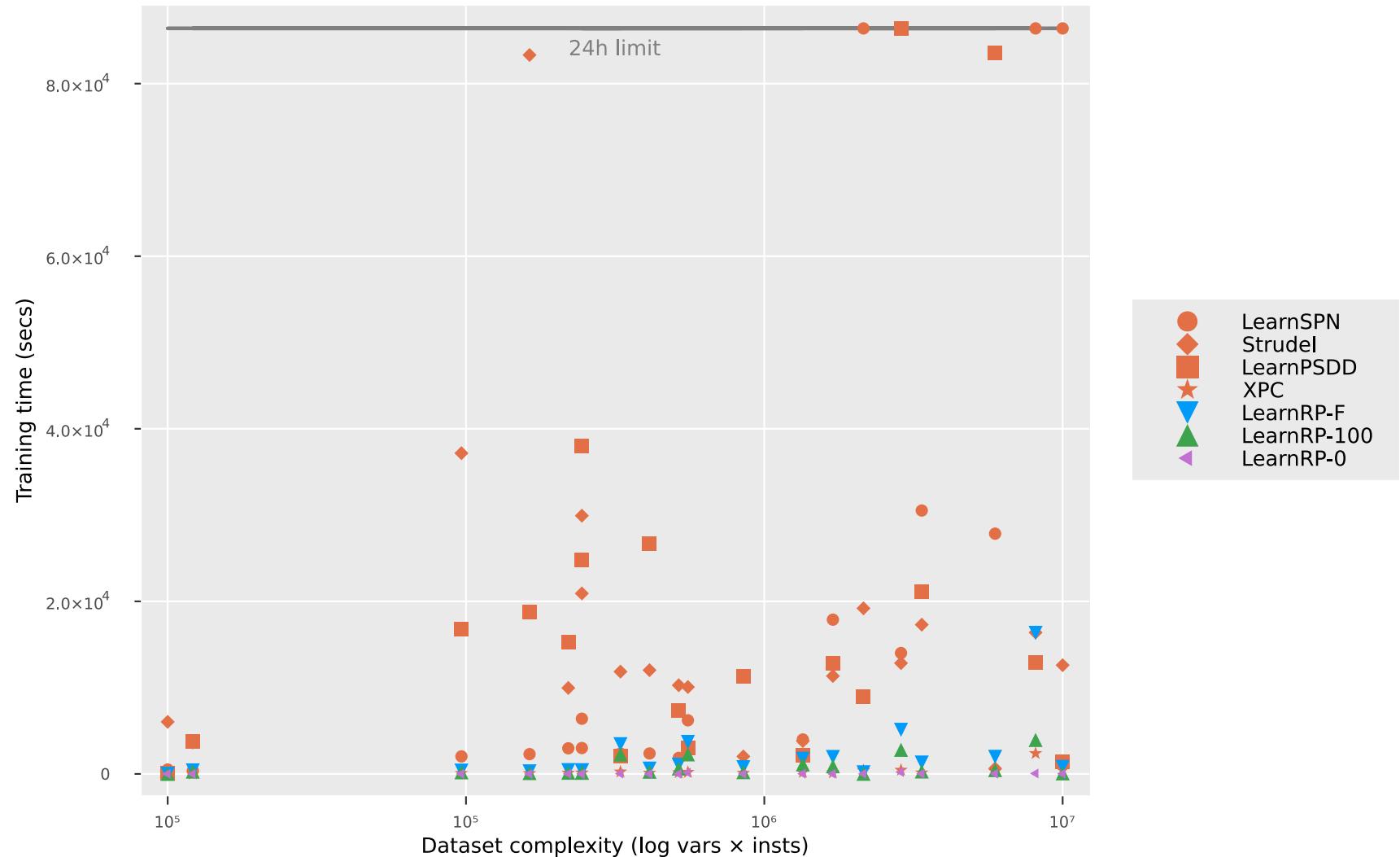
LEARNRP – Datasets

| Dataset | Vars | Train | Test | Domain | Dataset | Vars | Train | Test | Domain |
|----------------|-------------|--------------|-------------|---------------|----------------|-------------|--------------|-------------|---------------|
| ACCIDENTS | 111 | 12758 | 2551 | {0, 1} | NLTCS | 16 | 16181 | 3236 | {0, 1} |
| AD | 1556 | 2461 | 491 | {0, 1} | PLANTS | 69 | 17412 | 3482 | {0, 1} |
| AUDIO | 100 | 15000 | 3000 | {0, 1} | PUMSB-STAR | 163 | 12262 | 2452 | {0, 1} |
| BBC | 1058 | 1670 | 330 | {0, 1} | EACHMOVIE | 500 | 4524 | 591 | {0, 1} |
| NETFLIX | 100 | 15000 | 3000 | {0, 1} | RETAIL | 135 | 22041 | 4408 | {0, 1} |
| BOOK | 500 | 8700 | 1739 | {0, 1} | ABALONE | 8 | 3760 | 417 | ℝ |
| 20-NEWSGRP | 910 | 11293 | 3764 | {0, 1} | CA | 22 | 7373 | 819 | ℝ |
| REUTERS-52 | 889 | 6532 | 1540 | {0, 1} | QUAKE | 4 | 1961 | 217 | ℝ |
| WEBKB | 839 | 2803 | 838 | {0, 1} | SENSORLESS | 48 | 52659 | 5850 | ℝ |
| DNA | 180 | 1600 | 1186 | {0, 1} | BANKNOTE | 4 | 1235 | 137 | ℝ |
| JESTER | 100 | 9000 | 4116 | {0, 1} | FLOWSIZE | 3 | 1358674 | 150963 | ℝ |
| KDD | 65 | 180092 | 34955 | {0, 1} | KINEMATICS | 8 | 7373 | 819 | ℝ |
| KOSAREK | 190 | 33375 | 6675 | {0, 1} | IRIS | 4 | 90 | 10 | ℝ |
| MSNBC | 17 | 291326 | 58265 | {0, 1} | OLDFAITH | 2 | 245 | 27 | ℝ |
| MSWEB | 294 | 29441 | 5000 | {0, 1} | CHEMDIABET | 3 | 131 | 14 | ℝ |

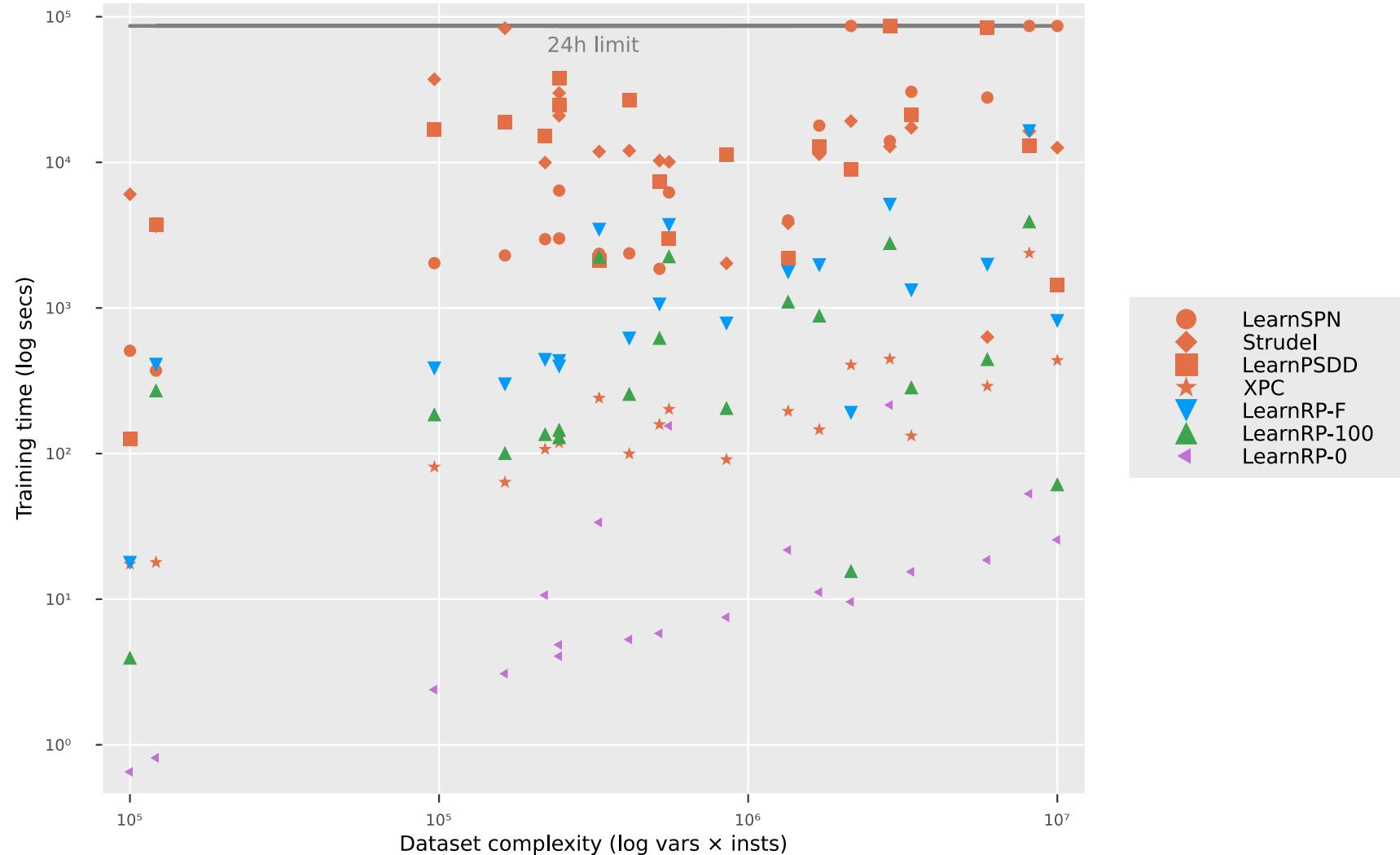
Experiments

| Dataset | LEARNSPN | STRUDEL | LEARNPSDD | XPC | PROMETHEUS | LEARNRP-F | LEARNRP-100 |
|--------------------|---------------|---------------|---------------|----------------|--------------------|----------------|----------------|
| ACCIDENTS | -30.03 | -28.73 | -30.16 | -31.02 | -27.91 | -28.66 | -28.81 |
| AD | -19.73 | <u>-16.38</u> | -31.78 | -15.50 | -23.96 | <u>-19.26</u> | -19.99 |
| AUDIO | -40.50 | -41.50 | <u>-39.94</u> | -40.91 | -39.80 | <u>-40.27</u> | -40.30 |
| BBC | -250.68 | -254.41 | -253.19 | -248.34 | <u>-248.50</u> | -254.15 | -251.57 |
| NETFLIX | <u>-57.02</u> | -58.69 | -55.71 | -57.58 | <u>-56.47</u> | <u>-57.02</u> | -57.03 |
| BOOK | -35.88 | -34.99 | -34.97 | -34.75 | <u>-34.40</u> | <u>-33.56</u> | -33.41 |
| 20-NEWSGRP | -155.92 | -154.47 | -155.97 | <u>-153.75</u> | -154.17 | <u>-152.63</u> | -152.34 |
| REUTERS-52 | <u>-85.06</u> | -86.22 | -89.61 | <u>-84.70</u> | -84.59 | -85.69 | -85.76 |
| WEBKB | -158.20 | -155.33 | -161.09 | <u>-153.67</u> | -155.21 | <u>-153.52</u> | -151.80 |
| DNA | -82.52 | -86.22 | -88.01 | -86.61 | -84.45 | <u>-83.57</u> | <u>-83.62</u> |
| JESTER | -75.98 | -55.03 | -51.29 | -53.43 | <u>-52.80</u> | -52.92 | <u>-52.86</u> |
| KDD | -2.18 | <u>-2.13</u> | -2.11 | -2.15 | <u>-2.12</u> | -2.14 | -2.14 |
| KOSAREK | -10.98 | -10.68 | -10.52 | -10.77 | <u>-10.59</u> | <u>-10.62</u> | -10.66 |
| MSNBC | <u>-6.11</u> | -6.04 | -6.04 | <u>-6.18</u> | -6.04 | -6.33 | -6.35 |
| MSWEB | -10.25 | -9.71 | <u>-9.89</u> | -9.93 | <u>-9.86</u> | -9.90 | -9.93 |
| NLTCS | -6.11 | -6.06 | -5.99 | <u>-6.05</u> | <u>-6.01</u> | -6.22 | -6.27 |
| PLANTS | <u>-12.97</u> | <u>-12.98</u> | -13.02 | -14.19 | -12.81 | -13.77 | -13.81 |
| PUMSB-STAR | <u>-24.78</u> | <u>-24.12</u> | -26.12 | -26.06 | -22.75 | -26.12 | -26.33 |
| EACHMOVIE | -52.48 | -53.67 | -58.01 | -54.82 | <u>-51.49</u> | <u>-51.41</u> | -50.95 |
| RETAIL | -11.04 | <u>-10.81</u> | -10.72 | -10.94 | -10.87 | <u>-10.84</u> | -10.86 |
| Avg. Rank | 4.83 ± 1.89 | 4.30 ± 1.92 | 4.03 ± 2.57 | 4.62 ± 1.88 | 2.50 ± 1.43 | 3.62 ± 1.47 | 4.10 ± 1.98 |
| Pos. (mean) | 7th | 5th | 3rd | 6th | 1st | 2nd | 4th |

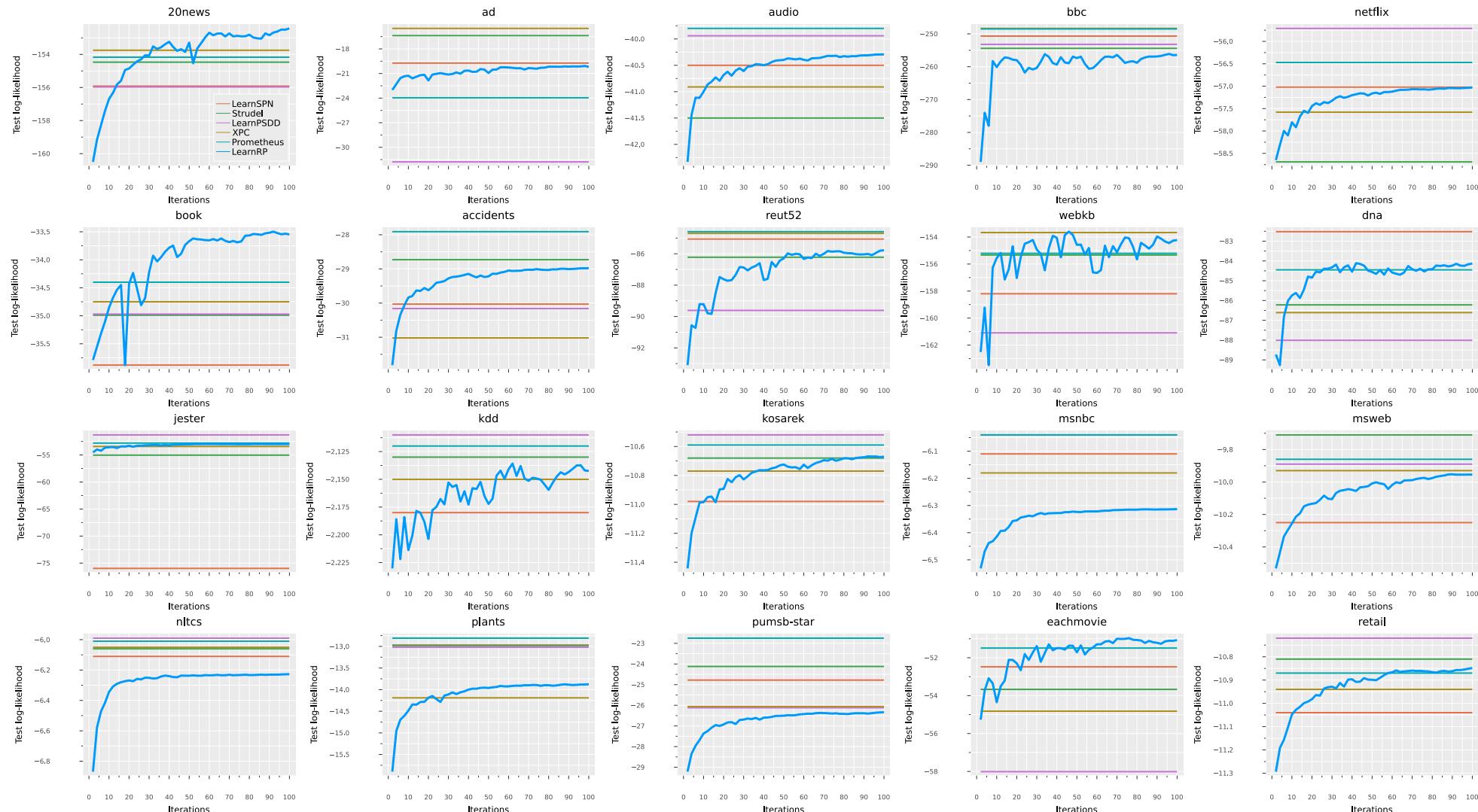
Experiments



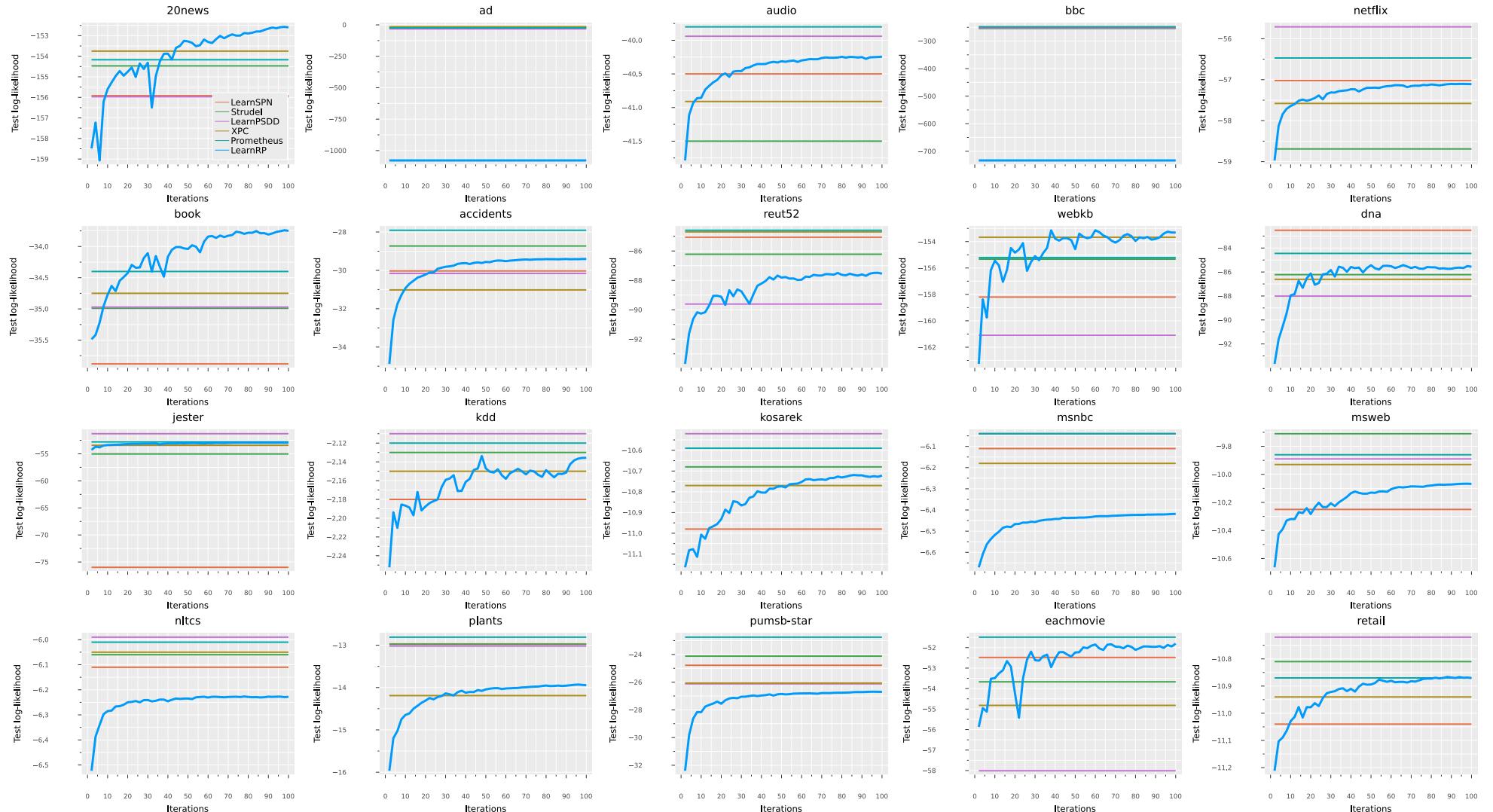
Experiments



LEARNRP – Learning Curves



LEARNRP – Random Initializations



Experiments

| Dataset | Vars | SRBMs | oSLRAU | GBMMs | iGMMs | GMMs | PROMETHEUS | iSPTs | LEARNRP | Size |
|----------------|-------------|--------------|---------------|--------------|--------------|--------------|-------------------|--------------|----------------|-------------|
| ABALONE | 8 | -2.28 | <u>-0.94</u> | -1.17 | — | -4.65 | -0.85 | — | -3.58 | 317 |
| BANKNOTE | 4 | -2.76 | -1.39 | -4.64 | — | -4.32 | <u>-1.96</u> | — | -4.27 | 79 |
| CA | 22 | -4.95 | <u>21.19</u> | 3.42 | — | -7.33 | 27.82 | — | 9.48 | 2675 |
| KINEMATICS | 8 | -5.55 | -11.13 | -11.20 | — | -11.15 | -11.12 | — | <u>-10.16</u> | 319 |
| QUAKE | 4 | -2.38 | -1.21 | -3.76 | — | -4.09 | <u>-1.50</u> | — | -1.63 | 79 |
| SENSORLESS | 48 | -26.91 | <u>60.72</u> | 8.56 | — | -34.14 | 62.03 | — | 17.52 | 12650 |
| CHEMDIABET | 3 | — | — | — | -3.02 | -18.49 | -2.59 | <u>-2.88</u> | -19.06 | 47 |
| FLOWSIZE | 3 | -0.79 | <u>15.32</u> | -5.72 | — | 2.27 | 18.03 | — | 2.83 | 49 |
| OLDFAITH | 2 | — | — | — | -1.73 | -4.18 | -1.48 | <u>-1.70</u> | -4.26 | 19 |
| IRIS | 4 | — | — | — | -3.94 | <u>-2.26</u> | -1.06 | -3.74 | -3.14 | 79 |

In conclusion

Contributions

Literature review

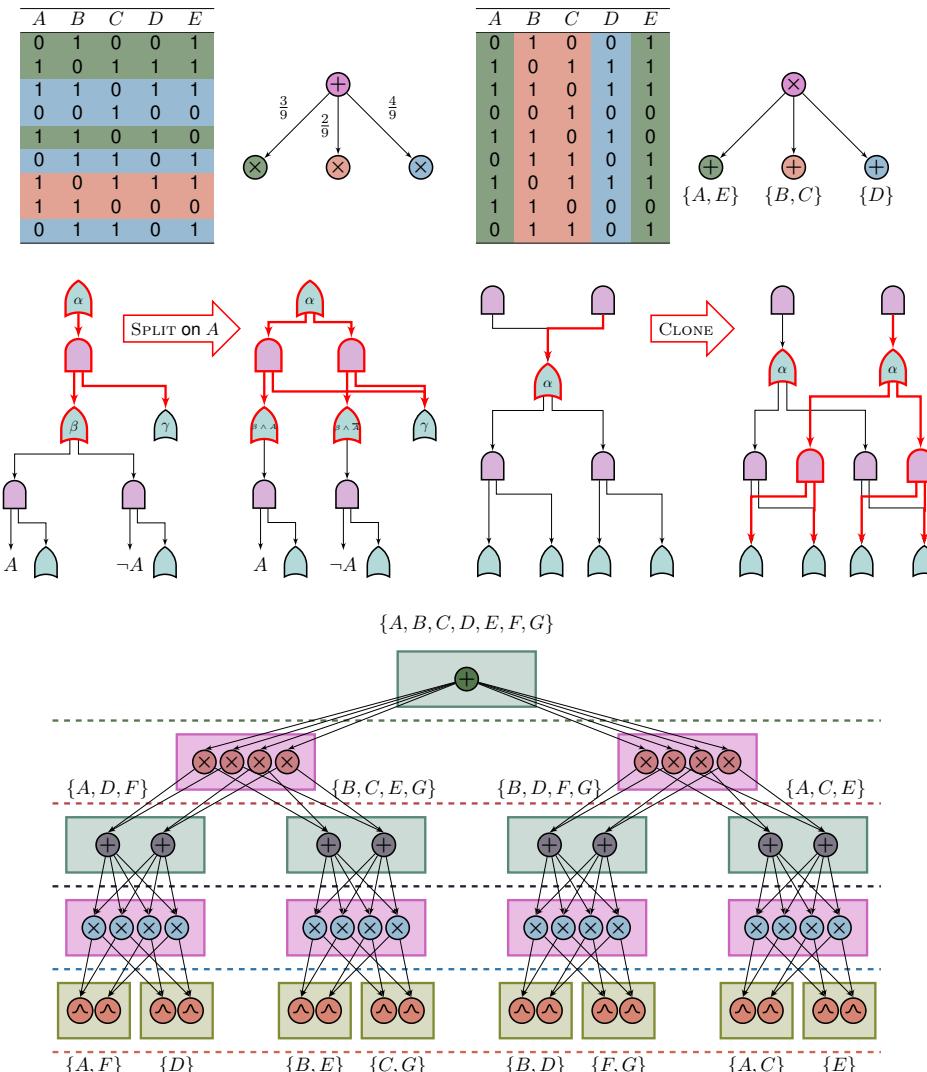
- Systematic review of literature;
- Taxonomy of popular algorithms;
- Complexity analysis;
- Pros and cons.

SAMPLEPSDD

- Consistent with a relaxation of a formula;
- Relaxation as a function of vtree and sampling;
- Compromise between tractability and consistency;
- Ensembles mitigate relaxation.

LEARNRP

- Simple strategy;
- Inspiration from known DET literature;
- Orders of magnitude faster;
- Competitive performance.



Contributions

Literature review

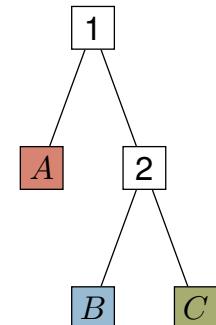
- Systematic review of literature;
- Taxonomy of popular algorithms;
- Complexity analysis;
- Pros and cons.

| A | B | C | $p(\mathbf{x})$ |
|-----|-----|-----|-----------------|
| 0 | 0 | 0 | 0.1 |
| 0 | 1 | 0 | 0.1 |
| 1 | 0 | 0 | 0.2 |
| 1 | 0 | 1 | 0.6 |

SAMPLEPSDD

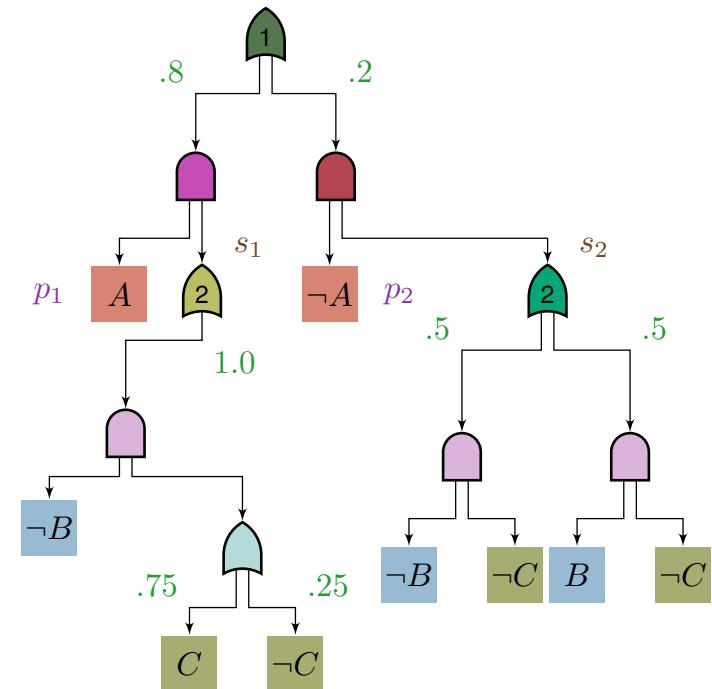
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$$\phi(A, B, C) = (A \rightarrow \neg B) \wedge (C \rightarrow A)$$



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Contributions

Literature review

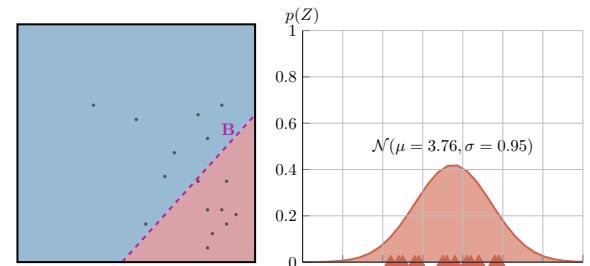
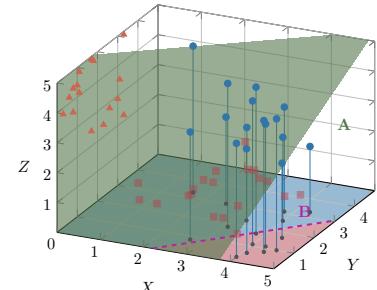
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$$\mathbf{B}(x, y) = [x \ y] \cdot \begin{bmatrix} 1.10 \\ -1.00 \end{bmatrix} - 2.43$$

