Two Perspectives to Learning with Circuits



Motivation

Given a selection of sushi...











...and people's preferences...































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







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







$$p((\mathbf{3}^{\mathsf{rd}} = \bigcirc) \to \mathbf{1}^{\mathsf{st}} = \bigcirc) \lor \mathbf{2}^{\mathsf{nd}} = \bigcirc)$$

...and extract meaningful queries from it?

Motivation

Given a selection of sushi...











...and people's preferences...





























Marginals

Conditionals

MPE

Logical events

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

 $p(1^{st} = \bigcirc, 3^{rd} = \bigcirc)$

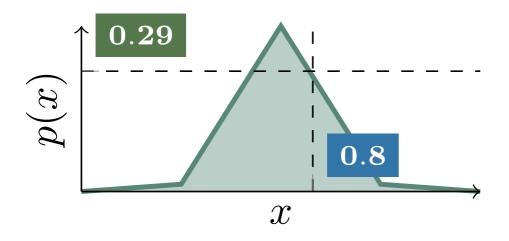
$$p(2^{nd} = P(1^{st} = P(1^{st}$$

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

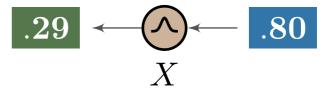
$$p((\mathbf{3}^{\mathsf{rd}} = \bigcirc) \to \mathbf{1}^{\mathsf{st}} = \bigcirc) \lor \mathbf{2}^{\mathsf{nd}} = \bigcirc)$$

...and extract meaningful queries from it?

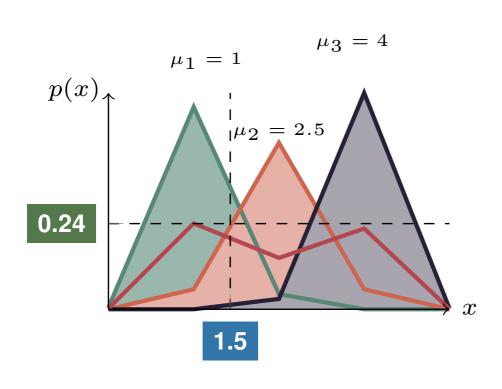
Probabilistic Circuits – Inputs

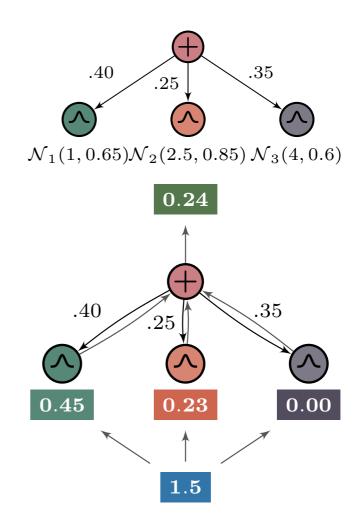


$$p(x) \longleftarrow x$$

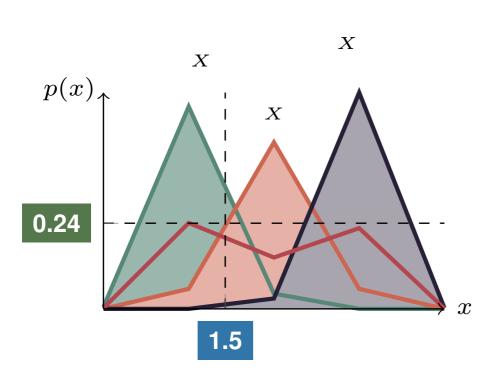


Probabilistic Circuits – Sums

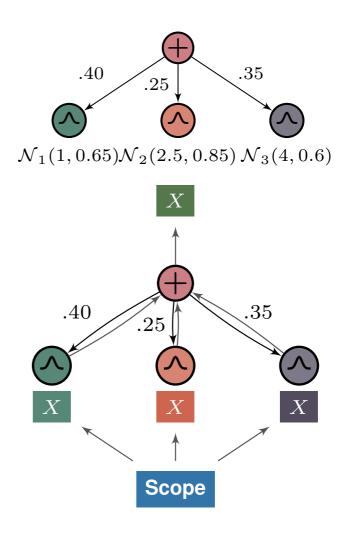




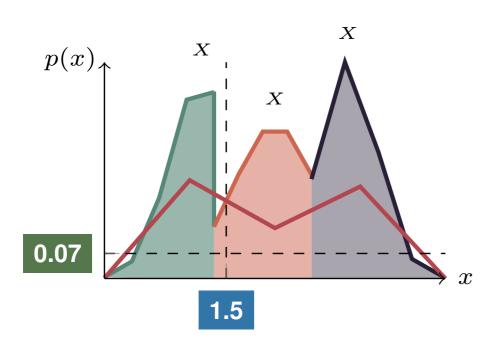
Probabilistic Circuits – Smoothness



Definition 1 (Smoothness). *Every sum node child mentions the <u>same</u> variables.*

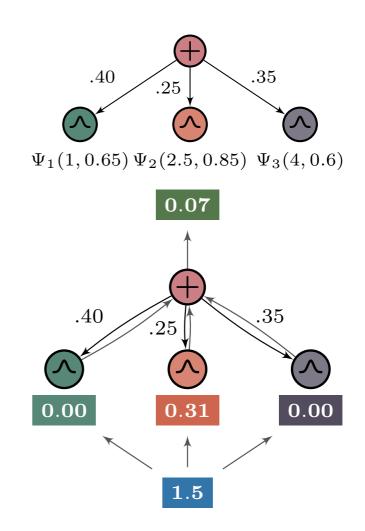


Probabilistic Circuits – Determinism

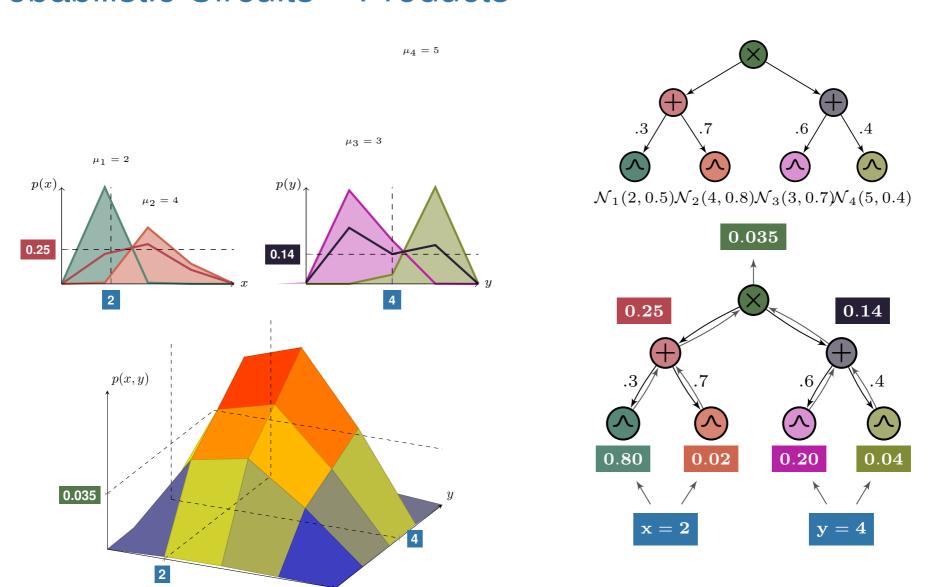


Definition 2 (Determinism).

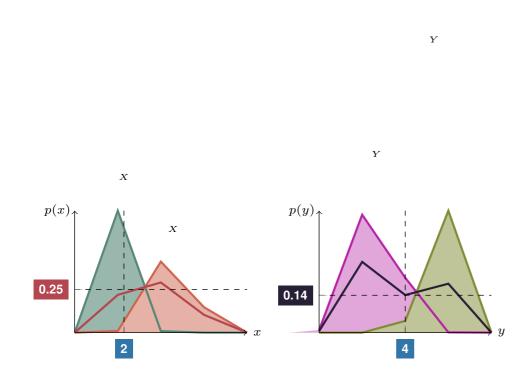
At most one sum node child has a positive value.



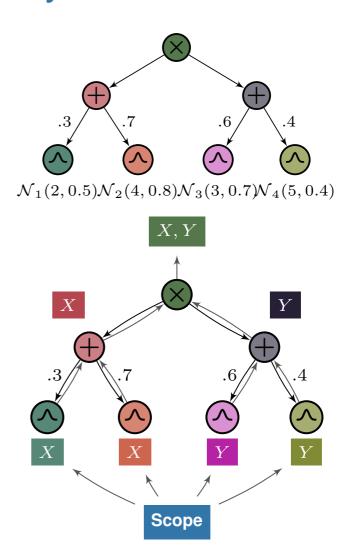
Probabilistic Circuits – Products



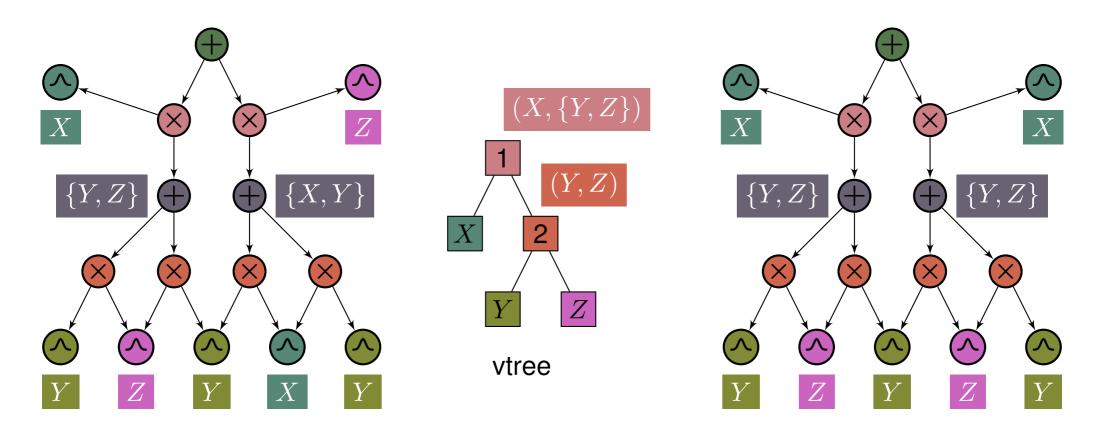
Probabilistic Circuits – Decomposability



Definition 3 (Decomposability). *Every product node child mentions <u>different</u> variables.*



Probabilistic Circuits – Structured Decomposability



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

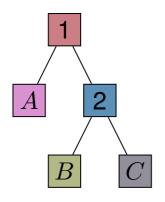
Probabilistic Circuits – Tractability

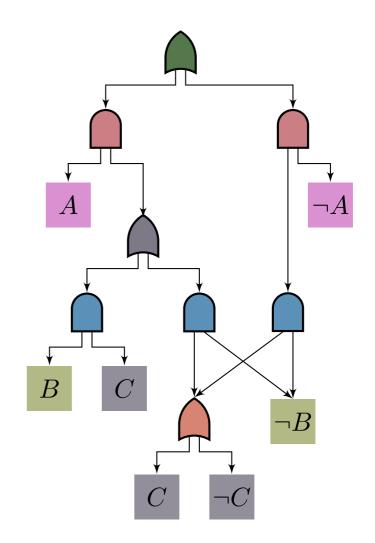
Query	+Sm?	+Dec?	+Det?	+Str Dec?
Evidence	√	√	√	√
Marginals	X	√	\checkmark	√
Conditionals	X	/	\checkmark	√
MPE	X	X	\checkmark	√
Shannon Entropy	X	X	\checkmark	√
Rényi Entropy	X	X	/	√
Cross Entropy	X	X	X	√
Kullback-Leibler Div	X	X	X	√
Rényi's Alpha Div	X	X	X	√
Cauchy-Schwarz Div	X	X	X	√
Logical Events	X	X	X	√
Mutual Information	X	X	X	√

Probabilistic Circuits – Logic Circuits

$\overline{\Delta}$	B	\overline{C}	$\phi(\mathbf{x})$
			$\varphi(\mathbf{A})$
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

$$\phi(A, B, C) = (A \lor B) \land (\neg B \lor C)$$

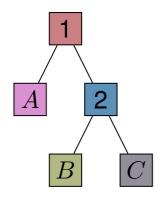


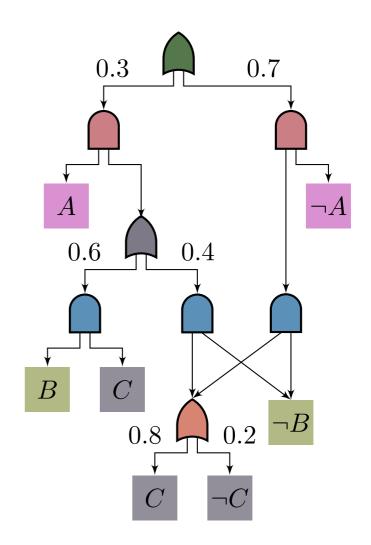


Probabilistic Circuits – Support

\overline{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 – Where are we right now?

Name	Class	Time Complexity	# hyperparams	Accepts logic?	Sm?	Dec?	Det?	Str Dec?	$\{0,1\}$?	№?	ℝ?	Reference
LEARNSPN	DIV	$egin{cases} \mathcal{O}\left(nkmc ight) & ext{, if sum} \ \mathcal{O}\left(nm^3 ight) & ext{, if product} \end{cases}$	≥ 2	×	1	√	Х	X	1	√	/	Gens and Domingos [2013]
ID-SPN	DIV	$ \begin{cases} \mathcal{O}\left(nkmc\right) & \text{, if sum} \\ \mathcal{O}\left(nm^3\right) & \text{, if product} \\ \mathcal{O}\left(ic(rn+m)\right) & \text{, if input} \end{cases} $	$\geq 2+3$	х	1	1	X	Х	✓	✓	X	Rooshenas and Lowd [2014]
PROMETHEUS	DIV	$\begin{cases} \mathcal{O}\left(nkmc\right) & \text{, if sum} \\ \mathcal{O}\left(m(\log m)^2\right) & \text{, if product} \end{cases}$	≥ 1	X	1	✓	X	×	✓	✓	✓	Jaini et al. [2018]
LEARNPSDD	INCR	$ \begin{cases} \mathcal{O}\left(m^2\right) & \text{, top-down vtree} \\ \mathcal{O}\left(m^4\right) & \text{, bottom-up vtree} \\ \mathcal{O}\left(i \mathcal{C} ^2\right) & \text{, circuit structure} \end{cases} $	1	✓	1	1	✓	✓	1	Х	Х	Liang et al. [2017]
STRUDEL	INCR	$ \begin{cases} \mathcal{O}\left(m^2n\right) & \text{, CLT + vtree} \\ \mathcal{O}\left(i\left(\mathcal{C} n+m^2\right)\right) & \text{, circuit structure} \end{cases} $	1	✓	1	✓	✓	✓	✓	X	X	Dang et al. [2020]
RAT-SPN	RAND	$\mathcal{O}\left(rd(s+l)\right)$	4	×	1	✓	X	×	✓	✓	✓	Peharz et al. [2020]
XPC	RAND	$\mathcal{O}\left(i(t+kn)+ikm^2n\right)$	3	×	1	✓	✓	✓	✓	X	X	Mauro et al. [2021]
SAMPLEPSDD	RAND	$\begin{cases} \mathcal{O}\left(m\right) & \text{, random vtree} \\ \mathcal{O}\left(kc\log c + \log_2^2 k\right) & \text{, per call} \end{cases}$	1	✓	1	1	✓	√	1	Х	X	Geh and Mauá [2021]
LEARNRP	RAND	$\begin{cases} \mathcal{O}\left(m^2\right) & \text{, top-down vtree} \\ \mathcal{O}\left(m^4\right) & \text{, bottom-up vtree} \\ \mathcal{O}\left(knm\right) & \text{, per call} \end{cases}$	0	×	1	✓	X	✓	✓	✓	1	To appear

A Logical Perspective

Motivation



















Bob: 🥮











Carol:









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 <u>k!</u> 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}	• • •	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
:	:	:	÷	÷	:	:
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]):

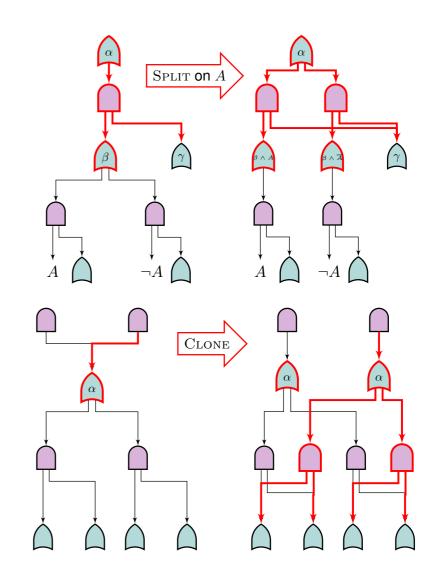
- Requires initial logic circuit encoding the support...
- Scales poorly to complex formulae and/or high dimension...
- Costly whole circuit evaluation at every iteration...
- ✓ Very good performance!

STRUDEL (Dang et al. [2020]):

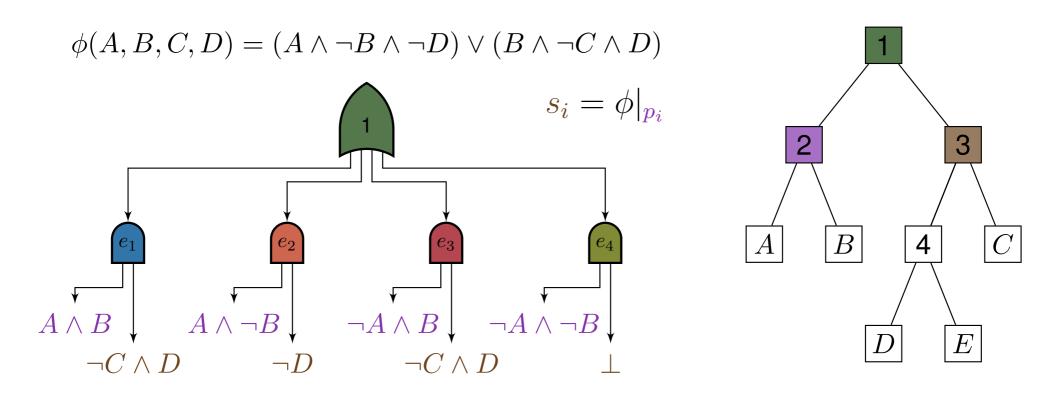
- ✓ Constructs an initial structure (from a CLT)!
- But does not encode constraints...
- Scales to high dimension!
- As long as the circuit doesn't get too big...

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...

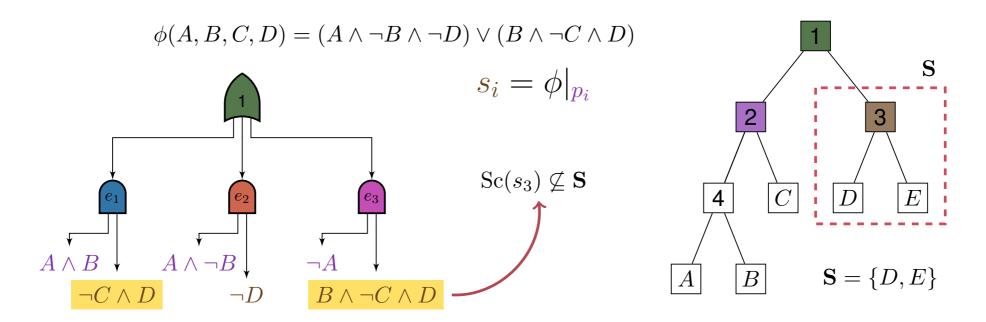


Common assumption: p_i are conjunctions of literals.



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

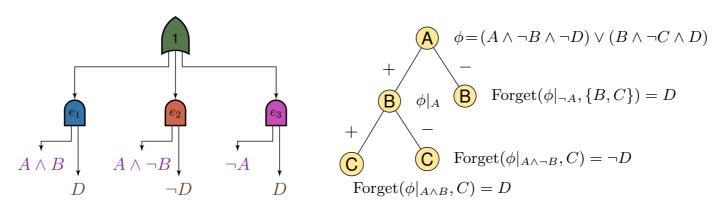
Solution: randomly sample a bounded number (k) of p_i



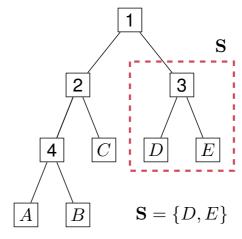
But: this violates structured decomposability:

 $\neg C \land D$ contains C, and $C \notin \mathbf{S}$ $\neg B \land \neg C \land D$ contains B and C, and $B, C \notin \mathbf{S}$

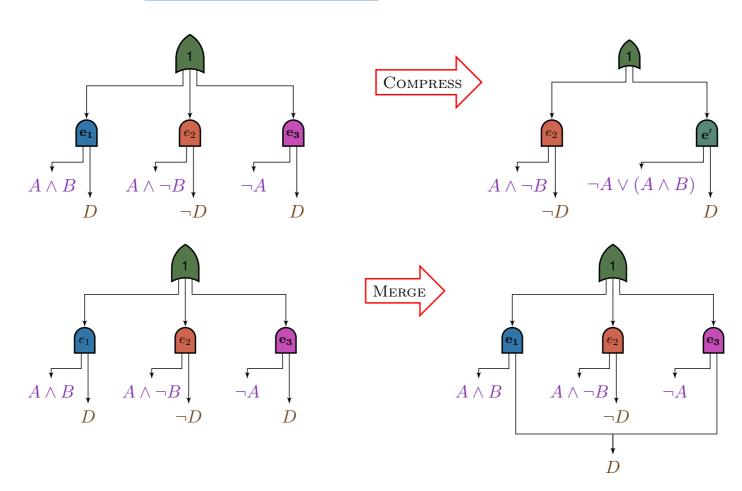
New solution: relax logical constraints ϕ



Now all s_i respect S



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



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

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

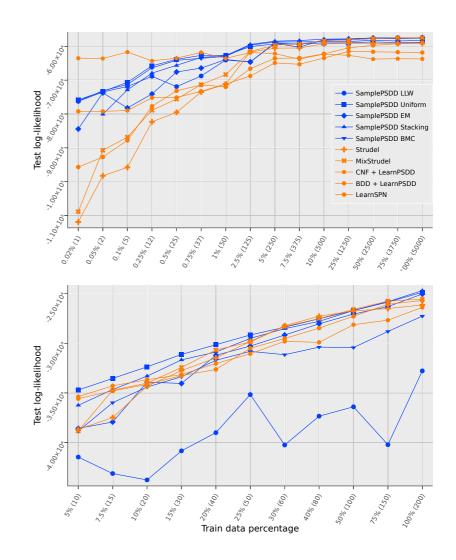
comparing against STRUDEL, LEARNPSDD and LEARNSPN.

Datasets: we evaluate with 5 data + knowledge as logic constraints:

	Dataset	#vars	#train	ϕ 's size
\Rightarrow	LED	14	5000	23
\Rightarrow	LED + IMAGES	157	700	39899
	Sushi Ranking	100	3500	17413
	Sushi Top 5	10	3500	37
	Dota 2 Games	227	92650	1308

Our approach fares **better** with **fewer** data , yet remains **competitive** under **lots of data** .

Mattei et al. [2020], Kamishima [2003], Shen et al. [2017], Choi et al. [2015], Gens and Domingos [2013], Dang et al. [2020]



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

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

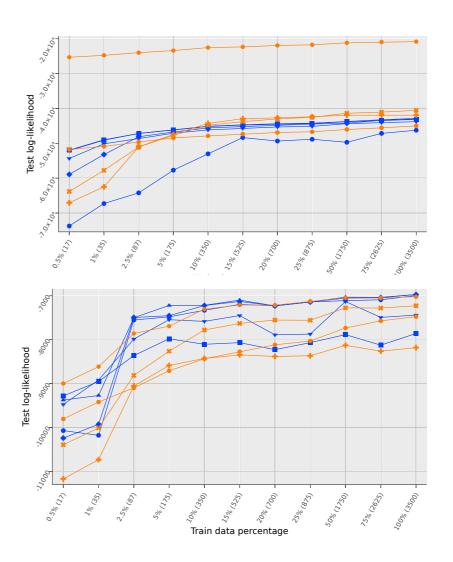
comparing against STRUDEL, LEARNPSDD and LEARNSPN.

Datasets: we evaluate with 5 data + knowledge as logic constraints:

	Dataset	#vars	#train	ϕ 's size
	LED	14	5000	23
	LED + IMAGES	157	700	39899
\Rightarrow	Sushi Ranking	100	3500	17413
\Rightarrow	Sushi Top 5	10	3500	37
	Dota 2 Games	227	92650	1308

Our approach fares **better** with **fewer** data , yet remains **competitive** under **lots of data** .

Mattei et al. [2020], Kamishima [2003], Shen et al. [2017], Choi et al. [2015], Gens and Domingos [2013], Dang et al. [2020]



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

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

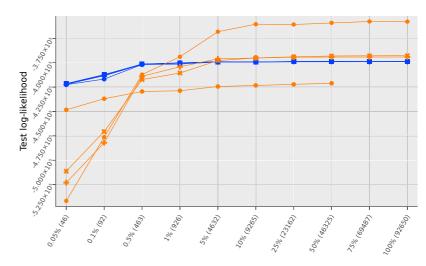
comparing against STRUDEL, LEARNPSDD and LEARNSPN.

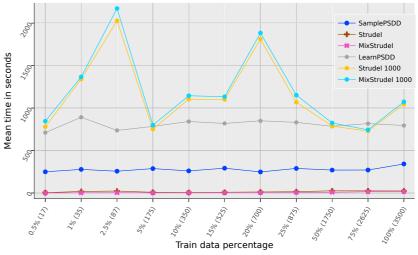
Datasets: we evaluate with 5 data + knowledge as logic constraints:

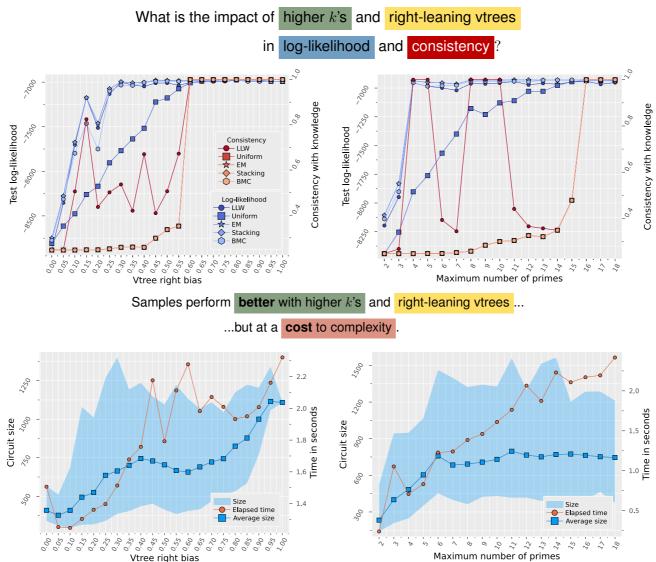
Dataset	#vars	#train	ϕ 's size
LED	14	5000	23
LED + IMAGES	157	700	39899
Sushi Ranking	100	3500	17413
Sushi Top 5	10	3500	37
Dota 2 Games	227	92650	1308

Our approach fares **better** with **fewer** data , yet remains **competitive** under **lots of data** .

Mattei et al. [2020], Kamishima [2003], Shen et al. [2017], Choi et al. [2015], Gens and Domingos [2013], Dang et al. [2020]







What do we gain from this?

Available queries:

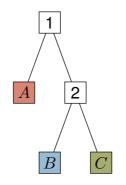
- ✓ Probability of Evidence;
- ✓ Marginal Probability;
- ✓ Conditional Probability;
- ✓ Most Probable Explanation;
- ✓ Shannon Entropy;
- Cross Entropy;
- ☑ Kullback-Leibler Divergence;
- ☑ Rényi's Alpha Divergence;
- ☑ Cauchy-Schwarz Divergence;
- ✓ Probability of Logical Events;
- Mutual Information.

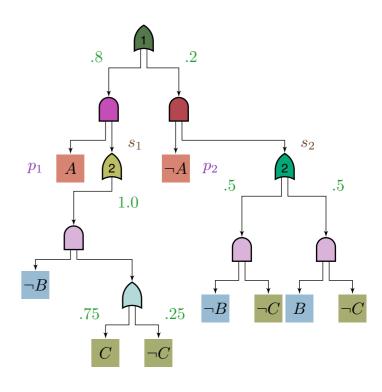
Support:

- ☑ Defineable as a logic formula;
- Consistent with a relaxation;
- ☑ Ensembles mitigate relaxation.

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

$$\phi(A, B, C) = (A \to \neg B) \land (C \to A)$$





A Data Perspective

Motivation

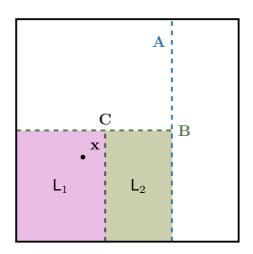
Density Estimation Trees...

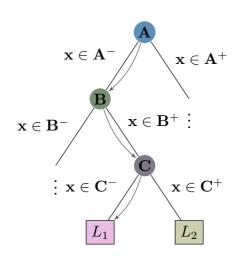
- ✓ ...are fast;
- ✓ ...are interpretable;
- ✓ ...have extensive literature coverage;
- ...are not so expressive;
- ...only accept marginalization queries;
- ...are not so accurate;

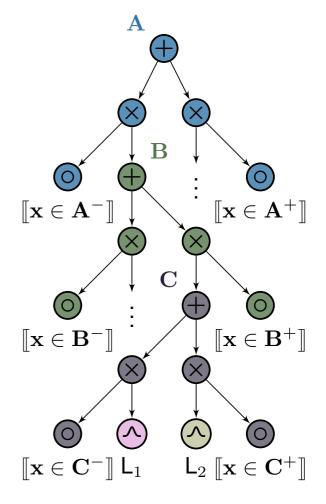
...but are subsumed by circuits!

Learn DETs ⊂ Learn PCs?

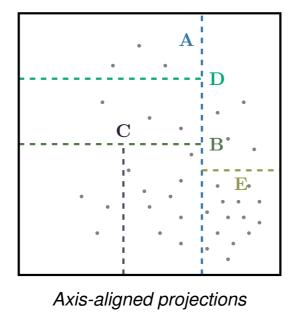
Can we take advantage of known learning procedures in DETs and transplant them to more general circuits?

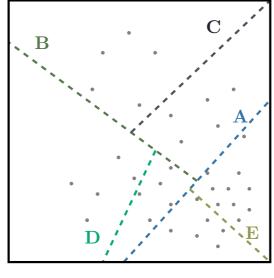






Random Projections

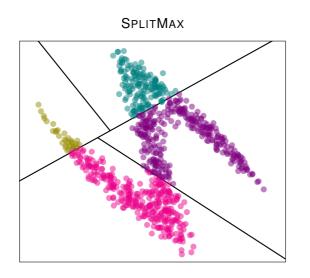


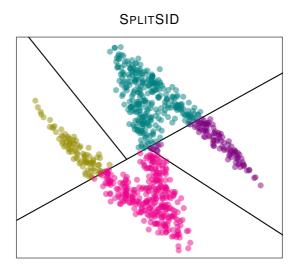


Random projections

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.

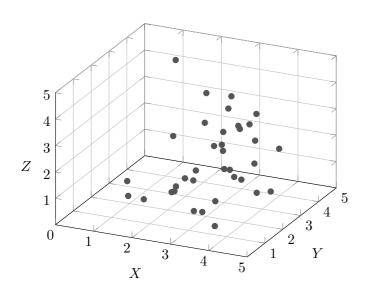
Random Projections

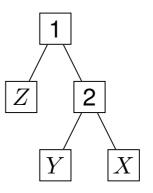




If the data has *intrinsic dimension* d, then with constant probability the part of the data at level d or higher of the tree has average diameter less than half of the data.

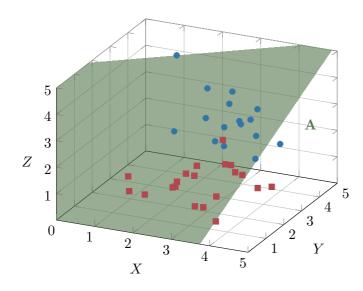
LearnRP



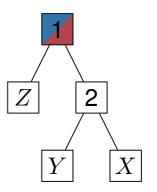


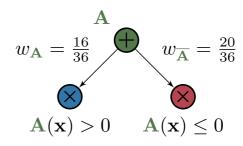


LearnRP



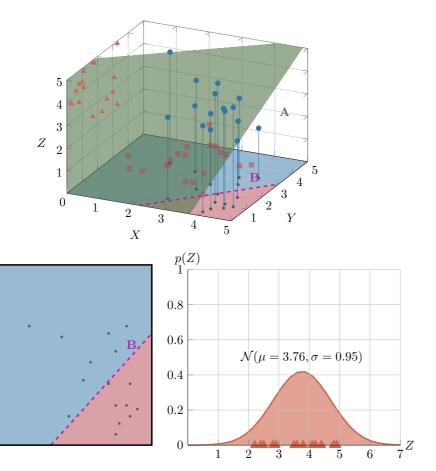
$$\mathbf{A}(x, y, z) = \begin{bmatrix} x & y & z \end{bmatrix} \cdot \begin{bmatrix} -0.31 \\ -0.40 \\ 0.85 \end{bmatrix} + 1$$



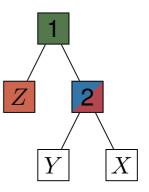


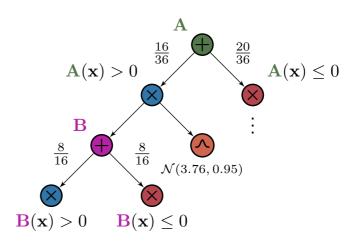
 $w_{\mathbf{A}}$: probability of $\mathbf{A}(\mathbf{x}) > 0$

LearnRP



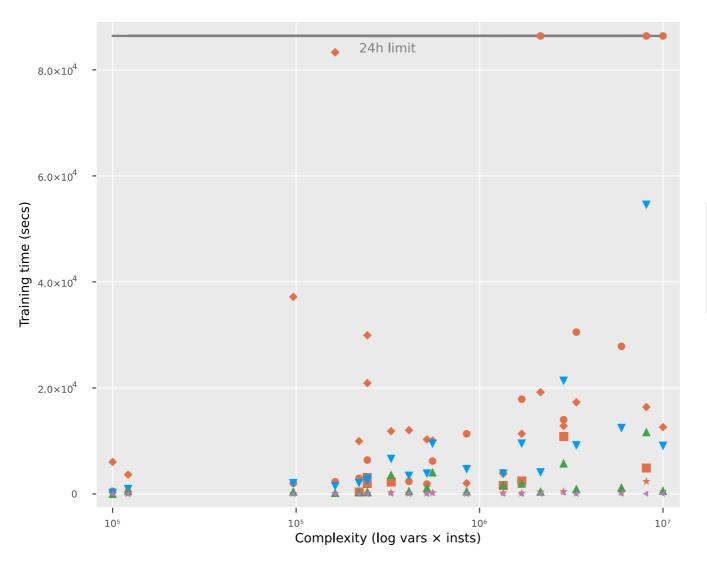
$$\mathbf{B}(x,y) = \begin{bmatrix} x & y \end{bmatrix} \cdot \begin{bmatrix} 1.10 \\ -1.00 \end{bmatrix} - 2.43$$

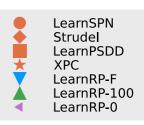


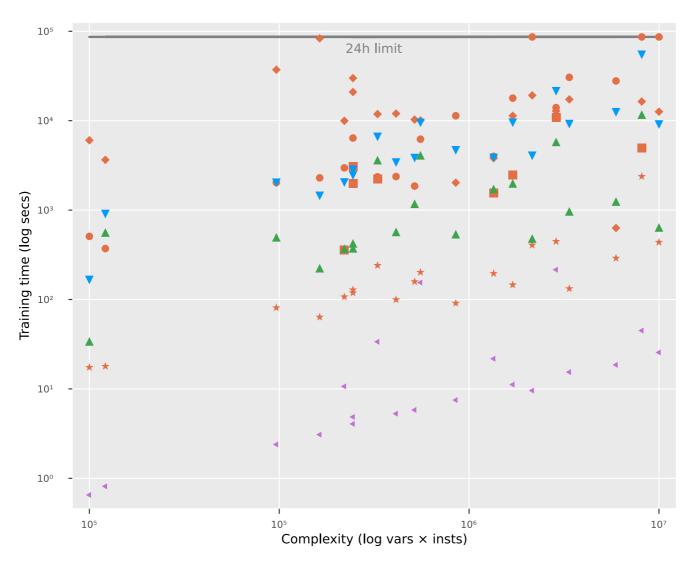


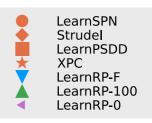
Dataset	Vars	Train	Test	Domain	Dataset	Vars	Train	Test	Domain
ACCIDENTS	111	12758	2551	$\{0,1\}$	NLTCS	16	16181	3236	$\overline{\{0,1\}}$
AD	1556	2461	491	$\{0,1\}$	PLANTS	69	17412	3482	$\{0, 1\}$
AUDIO	100	15000	3000	$\{0, 1\}$	PUMSB-STAR	163	12262	2452	$\{0, 1\}$
BBC	1058	1670	330	$\{0,1\}$	EACHMOVIE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

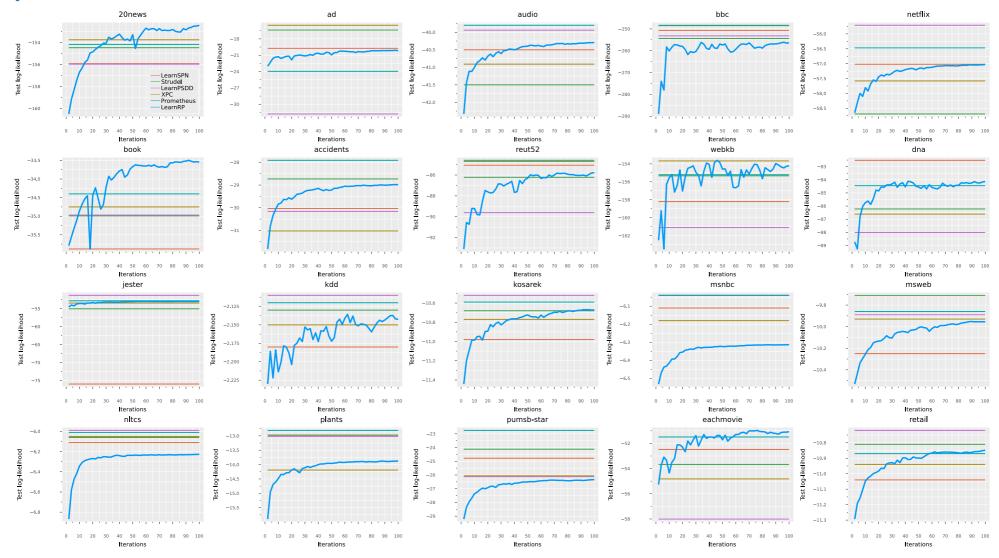
Dataset	LEARNSPN	STRUDEL	LEARNPSDD	XPC	PROMETHEUS	LEARNRP-F	LEARNRP-100	LEARNRP-30	LEARNRP-20	LEARNRP-10
ACCIDENTS	-30.03	-28.73	-30.16	-31.02	-27.91	-28.65	-28.87	-29.38	-29.58	-29.99
AD	-19.73	-16.38	-31.78	-15.50	-23.96	-19.20	-20.32	-21.42	-21.44	-21.94
AUDIO	-40.50	-41.50	<u>-39.94</u>	-40.91	-39.80	-40.18	-40.23	-40.46	-40.63	-40.94
BBC	-250.68	-254.41	-253.19	-248.34	<u>-248.50</u>	-254.97	-255.55	-262.35	-257.67	-262.39
NETFLIX	-57.02	-58.69	-55.71	-57.58	<u>-56.47</u>	-57.07	-57.05	-57.29	-57.48	-57.66
BOOK	-35.88	-34.99	-34.97	-34.75	-34.40	<u>-33.57</u>	-33.52	-34.34	-34.24	-34.73
20-NEWSGRP	-155.92	-154.47	-155.97	-153.75	-154.17	<u>-152.78</u>	-152.76	-154.32	-155.03	-156.26
REUTERS-52	-85.06	-86.22	-89.61	<u>-84.70</u>	-84.59	-85.73	-85.47	-87.41	-87.05	-89.26
WEBKB	-158.20	-155.33	-161.09	<u>-153.67</u>	-155.21	-154.43	-152.60	-154.83	-154.33	-158.01
DNA	-82.52	-86.22	-88.01	-86.61	-84.45	<u>-83.03</u>	-83.85	-84.77	-84.98	-85.40
JESTER	-75.98	-55.03	-51.29	-53.43	<u>-52.80</u>	-52.92	-52.89	-53.23	-53.22	-53.54
KDD	-2.18	-2.13	-2.11	-2.15	<u>-2.12</u>	-2.13	-2.14	-2.17	-2.16	-2.20
KOSAREK	-10.98	-10.68	-10.52	-10.77	<u>-10.59</u>	-10.65	-10.67	-10.79	-10.86	-11.00
MSNBC	<u>-6.11</u>	-6.04	-6.04	-6.18	-6.04	-6.31	-6.36	-6.40	-6.41	-6.44
MSWEB	-10.25	-9.71	-9.89	-9.93	-9.86	<u>-9.85</u>	-9.97	-10.06	-10.21	-10.27
NLTCS	-6.11	-6.06	-5.99	-6.05	<u>-6.01</u>	-6.35	-6.23	-6.25	-6.27	-6.32
PLANTS	<u>-12.97</u>	-12.98	-13.02	-14.19	-12.81	-13.68	-14.00	-14.26	-14.40	-14.70
PUMSB-STAR	-24.78	<u>-24.12</u>	-26.12	-26.06	-22.75	-25.88	-26.19	-26.36	-26.54	-27.17
EACHMOVIE	-52.48	-53.67	-58.01	-54.82	-51.49	<u>-51.37</u>	-51.06	-51.55	-52.86	-52.21
RETAIL	-11.04	<u>-10.81</u>	-10.72	-10.94	-10.87	-10.85	-10.86	-10.93	-10.97	-11.04
A Dank	6.08 ± 3.03	$\textbf{5.28} \pm \textbf{2.97}$	5.20 ± 3.86	5.55 ± 2.76	$\textbf{2.90} \pm \textbf{2.07}$	3.83 ± 1.98	$ 4.15 \pm 2.03 $	6.35 ± 1.50	6.95 ± 1.70	8.72 ± 1.50
Avg. Rank	4.80 ± 1.91	$\textbf{4.22} \pm \textbf{1.81}$	$ 4.05\pm2.56 $	4.60 ± 1.93	$\textbf{2.55} \pm \textbf{1.43}$	3.62 ± 1.56	$\textbf{4.15} \pm \textbf{2.03}$			
Dog (magn)	7th	5th	4th	6th	1st	<u>2nd</u>	3rd	8th	9th	10th
Pos. (mean)	7th	5th	3rd	6th	1st	<u>2nd</u>	4th			

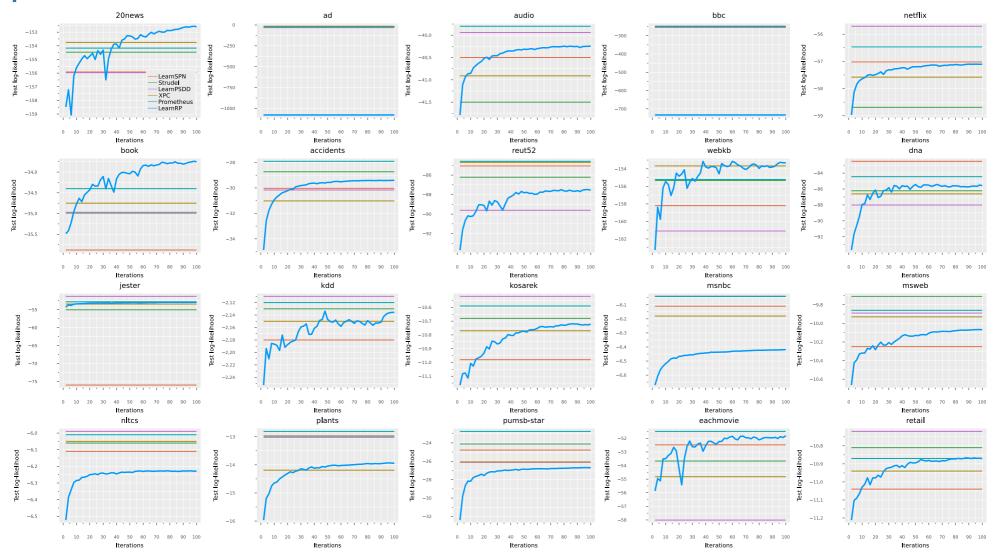












Dataset	Vars	SRBMs	oSLRAU	GBMMs	iGMMs	GMMs	PROMETHEUS	iSPTs	LEARNRP	Size
ABALONE	8	-2.28	-0.94	-1.17	_	-0.59	-0.85	_	-6.13	317
CA	22	-4.95	<u>21.19</u>	3.42	_	-1.08	27.82		-5.84	2765
QUAKE	4	-2.38	<u>-1.21</u>	-3.76		-0.58	-1.50		-3.76	79
SENSORLESS	48	-26.91	60.72	8.56	_	-1.39	62.03		-38.46	12589
BANKNOTE	4	-2.76	<u>-1.39</u>	-4.64	_	-1.05	-1.96		-6.06	79
FLOWSIZE	3	-0.79	<u>15.32</u>	5.72		-36.50	18.03		2.20	49
KINEMATICS	8	-5.55	-11.13	-11.20	_	<u>-6.11</u>	-11.12		-11.02	319
IRIS	4				-3.94	0.20	<u>-1.06</u>	-3.74	-3.47	79
OLDFAITH	2				-1.73	-2.09	-1.48	<u>-1.70</u>	-4.33	19
CHEMDIABET	3	_			-3.02	-0.58	<u>-2.59</u>	-2.88	-18.68	48