Fast and Accurate Density Estimation with Extremely Randomized Cutset Networks

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1. Density estimation

Density estimation is the unsupervised task of learning an estimator for the joint probability distribution $p(\mathbf{X})$ from a set of i.i.d. samples $\{\mathbf{x}^i\}_{i=1}^m$ over r.v.s $\mathbf{X}$

Given such an estimator, one uses it to answers probabilistic queries about configurations on $\mathbf{X}$, i.e. to do ***inference***.

The main challenge in density estimation is balancing:

- the ***representation expressiveness*** of a model
- the ***cost of learning*** it
- and the ***cost of performing inference*** on it.

2. Tractable Probabilistic Models (TPMs)

Tractable Probabilistic Models (**TPMs**) are density estimators for which some kind of ***exact*** inference is ***tractable***, i.e. polynomial in the number of r.v.s or their domains.

2.1 Product of Bernoullis (PoBs)

$$\mathsf{p}(\mathbf{x}) = \prod_{i=1}^{n} \mathsf{p}(x_i)$$

Learning a PoB from $\mathcal{D}$ over RVs $\mathbf{X}$ has linear time complexity $O(nm)$.

2.2 Chow-Liu Trees (CLTrees)

A *directed tree-structured model* [2] over $\mathbf{X}$ is a BN in which each node $X_i \in \mathbf{X}$ has at most one parent, Pa_{X_i}.

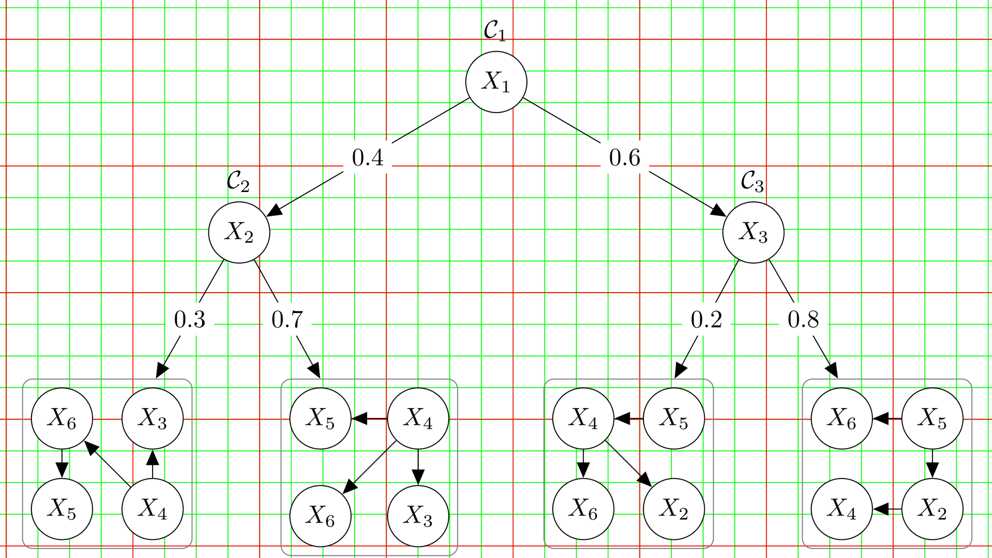
$$\mathsf{p}(\mathbf{x}) = \prod_{i=1}^{n} \mathsf{p}(x_i|\mathrm{Pa}_{x_i})$$

Learning a CLtree from $\mathcal{D}$ over RVs $\mathbf{X}$ has quadratic time complexity $O(n^2(m + \log n))$

2. Cutset Networks (CNets)

A Cutset Network (CNet) $\mathcal{C}$ is TPM represented via a weighted probabilistic model tree over $\mathbf{X}$ and recursively defined as:

1. a TPM $\mathcal{M}$, with scope$(\mathcal{M}) = \mathbf{X}$
2. a weighted disjunction (OR node) of two CNets $\mathcal{C}_0$ and $\mathcal{C}_1$ conditioned on RV $X_i \in \mathbf{X}$, with weights w_i^0 and w_i^1 s.t. $w_i^0 + w_i^1 = 1$, where scope$(\mathcal{C}_0)$ = scope$(\mathcal{C}_1) = \mathbf{X}_{\setminus i}$



Example of a CNet over binary RVs. Inner (rounded) nodes on variables X_i are OR nodes, while leaf (squared) nodes represent CLtrees.

2. Learning CNets

All top-down greedy CNet learners [3, 1] can be unified in single template, LearnCNet:

LearnCNet$(\mathcal{D}, \mathbf{X}, \alpha, \delta, \sigma)$

- **Input:** a dataset $\mathcal{D}$ over RVs $\mathbf{X}$; α: Laplace smoothing; δ min number samples; σ min number features
- **Output:** a CNet $\mathcal{C}$ encoding $\mathsf{p}_{\mathcal{C}}(\mathbf{X})$ learned from $\mathcal{D}$
- **if** $|\mathcal{D}| > \delta$ **and** $|\mathbf{X}| > \sigma$ **then**
  - X_i, success $\leftarrow$ select$(\mathcal{D}, \mathbf{X}, \alpha)$
  - **if** success **then**
    - $\mathcal{D}_0 \leftarrow \{\xi \in \mathcal{D} : \xi[X_i] = 0\}, \mathcal{D}_1 \leftarrow \{\xi \in \mathcal{D} : \xi[X_i] = 1\}$
    - $w_0 \leftarrow |\mathcal{D}_0|/|\mathcal{D}|, w_1 \leftarrow |\mathcal{D}_1|/|\mathcal{D}|$
    - $\mathcal{C} \leftarrow w_0 \cdot \mathrm{LearnCNet}(\mathcal{D}_0, \mathbf{X}_{\setminus i}, \alpha, \delta, \sigma) +$
      $w_1 \cdot \mathrm{LearnCNet}(\mathcal{D}_1, \mathbf{X}_{\setminus i}, \alpha, \delta, \sigma)$
- **else**
  - $\mathcal{C} \leftarrow$ learnDistribution$(\mathcal{D}, \mathbf{X}, \alpha)$
- **return** $\mathcal{C}$

select chooses one RV X_i to condition on. Its cost determines the complexity of the variants of LearnCNet:

entCNet [3] choosing X_i to lower approximate average joint entropy

$$O(mn^2)$$

dCSN [1] choosing X_i to improve model likelihood

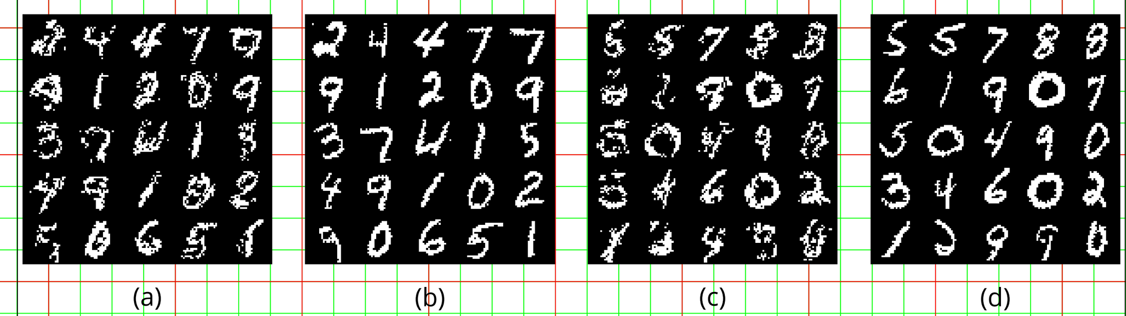
$$O(n^3(m + \log n))$$

3. XCNets

XCNets (**Extremely Randomized CNets**) are CNets built by LearnCNet when select chooses one RV *completely at random*.

$\rightarrow$ time complexity $O(1)$!

XCNets are comparable or only slightly less accurate as density estimators that CNets learned by $dCSN$ (see Exp 4.1) and as good as sample generators.



Samples obtained from a CNet (a), resp. XCNet (c), learned on a binarized version of MNIST, and their nearest neighbor in training set (b), resp. (d).

7. Mixture of Experts

A CNet can be seen as *mixture of experts* in which the OR tree plays as a *deterministic gating function* and leaf distributions act as the *local experts*.

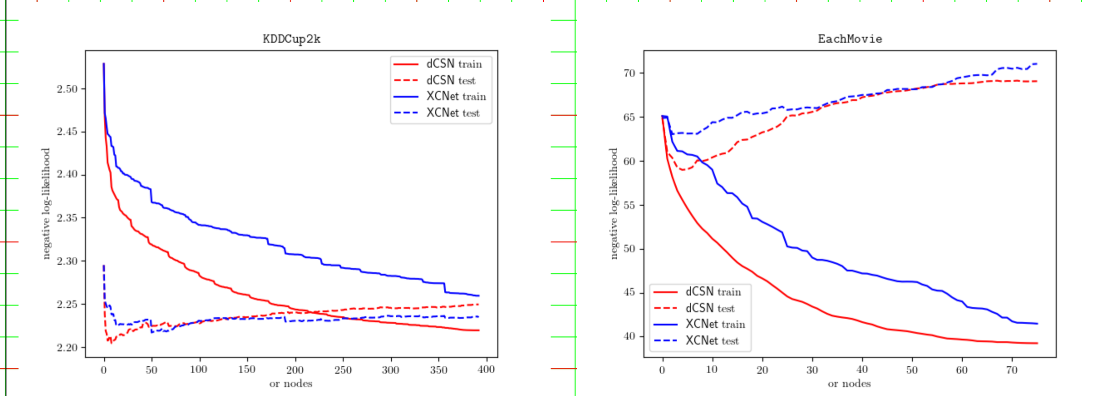
$$\mathsf{p}(\mathbf{x}) = \mathsf{p}_l(\mathbf{x}_{|\mathsf{sc}(\mathcal{C})\setminus \mathsf{sc}(\mathcal{M}_l)})\mathsf{p}_{\mathcal{M}_l}(\mathbf{x}_{|\mathsf{sc}(\mathcal{M}_l)}), \qquad (1)$$

$\mathsf{p}_l(\mathbf{x}_{|\mathsf{sc}(\mathcal{C})\setminus \mathsf{sc}(\mathcal{M}_l)})$ is decomposed by the chain rule across a path p going from the root to leaf model $\mathcal{M}_l$.

$\rightarrow$the order of appearance of $X_{\mathsf{p}(0)}, \ldots, X_{|\mathsf{p}|-1}$ does not change the factorization!

8. Regularization

As a single CNet can be seen as an ensemble, randomizing the gating function acts as regularization and lessens the overfitting issues with LearnCNet



Learning curves of CNets and XCNets (negative log-likelihoods) on KddCup2k and EachMovie The latter overfits much later that the former.

4. Experiments

4.1 Single model comparisons single XCNets are comparable (same order of magnitude) to entCNet and dCSN.

dataset	entCNet	dCSN	XCNet	$\mathrm{dCSN}_{\mathrm{PoB}}$	$\mathrm{XCNet}_{\mathrm{PoB}}$
NLTCS	-6.06	**-6.03**	6.06±0.01	-6.09	-6.17±0.05
MSNBC	**-6.05**	**-6.05**	-6.09±0.02	-6.05	-6.18±0.03
KDDCup2k	-	**-2.18**	-2.19±0.01	-2.19	-2.21±0.01
Plants	**-13.25**	**-13.25**	-13.43±0.07	-14.89	-15.66±0.22
Audio	**-42.05**	-42.10	-42.66±0.14	-42.95	-44.02±0.22
Jester	-55.56	**-55.40**	-56.10±0.19	-56.23	-57.39±0.15
Netflix	**-58.71**	**-58.71**	-59.21±0.06	-60.20	-61.40±0.25
Accidents	-30.69	**-29.84**	-31.58±0.24	-36.24	-40.22±0.46
Retail	**-10.94**	-11.24	-11.44±0.09	-11.06	-11.19±0.04
Pumsb-star	-24.42	**-23.91**	-25.55±0.34	-32.11	-39.91±2.48
DNA	-87.59	**-87.31**	-87.67±0.00	-98.83	-99.84±0.05
Kosarek	**-11.04**	-11.20	-11.70±0.13	-11.38	-11.80±0.07
MSWeb	**-10.07**	-10.10	-10.47±0.10	-10.19	-10.43±0.07
Book	**-37.35**	-38.93	-42.36±0.28	-38.21	-39.47±0.33
EachMovie	-58.37	**-58.06**	-60.71±0.89	-59.70	-62.58±0.38
WebKB	-162.17	**-161.92**	-167.45±1.59	-168.7	-174.78±0.81
Reuters-52	**-88.55**	-88.65	-99.52±1.93	-90.51	-100.25±0.57
20NewsG	-	**-161.72**	-172.6±1.40	-162.25	-167.39±0.74
BBC	-263.08	**-261.79**	**-261.79**±0.00	-264.56	-274.83±1.15
Ad	-16.92	**-16.34**	-18.70±1.44	-36.44	-36.94±1.41

Table 1. Average test log-likelihoods for entCNet, dCSN, XCNet and their PoB variants $\mathrm{dCSN}_{\mathrm{PoB}}$ and $\mathrm{XCNet}_{\mathrm{PoB}}$. For randomized models, mean and standard deviation over 10 runs are reported).

4.2 Ensemble model comparisons ensembles of XCNets set new state-of-the-art log-likelihoods for the 20 standard benchmark datasets for density estimation.

dataset	$\mathrm{CNet}^{40}_{\mathrm{bag}}$	$\mathrm{CNet}^{40}_{\mathrm{boost}}$	dCSN^{40}	$\mathrm{XCNet}^{40}_{\mathrm{PoB}}$	XCNet^{40}	XCNet^{500}	ID-SPN	ACMN	WM
NLTCS	**-6.00**	-6.01	**-6.00**	-6.01	**-6.00**	**-5.99**	-6.02	-6.00	-6.02
MSNBC	-6.08	-6.15	**-6.05**	-6.11	-6.06	-6.06	**-6.04**	**-6.04**	**-6.04**
KDDCup2k	-2.14	-2.15	-2.15	**-2.13**	**-2.13**	**-2.13**	**-2.13**	-2.17	-2.16
Plants	-12.32	-12.67	-12.59	-13.09	**-11.99**	**-11.84**	-12.54	-12.80	-12.65
Audio	-40.09	-39.84	-40.19	-40.30	**-39.77**	**-39.39**	-39.79	-40.32	-40.50
Jester	-52.88	-52.82	-52.99	-53.64	**-52.65**	**-52.21**	-52.86	-53.31	-53.85
Netflix	-56.55	-56.44	-56.69	-57.64	**-56.38**	**-55.93**	-56.36	-57.22	-57.03
Accidents	-29.88	-29.45	**-29.27**	-36.92	-29.31	-29.10	-26.98	-27.11	**-26.32**
Retail	-10.84	**-10.81**	-11.17	-10.88	-10.93	-10.91	-10.85	-10.88	-10.87
Pumsb-star	-23.98	-23.46	-23.78	-32.91	**-23.44**	-23.31	-22.41	-23.55	**-21.72**
DNA	**-81.07**	-85.67	-85.95	-98.28	-84.96	-84.17	-81.21	**-80.03**	-80.65
Kosarek	-10.74	**-10.60**	-10.97	-10.91	-10.72	-10.66	**-10.60**	-10.84	-10.83
MSWeb	-9.77	-9.74	-9.93	-9.83	**-9.66**	**-9.62**	-9.73	-9.77	-9.70
Book	-35.55	**-34.46**	-37.38	-34.77	-36.35	-35.45	**-34.14**	-35.56	-36.41
EachMovie	-53.00	**-51.53**	-54.14	-51.66	-51.72	**-50.34**	-51.51	-55.80	-54.37
WebKB	-153.12	**-152.53**	-155.47	-155.83	-153.01	**-149.20**	-151.84	-159.13	-157.43
Reuters-52	-83.71	**-83.69**	-86.19	-85.16	-84.05	**-81.87**	-83.35	-90.23	-87.55
20NewsG	-156.09	-153.12	-156.46	**-152.21**	-153.89	**-151.02**	-151.47	-161.13	-158.95
BBC	**-237.42**	-247.01	-248.84	-251.31	-238.47	**-229.21**	-248.93	-257.10	-257.86
Ad	-15.28	-14.36	-15.55	-26.25	**-14.20**	**-14.00**	-19.05	-16.53	-18.35

Table 2. Comparing CNet and XCNet ensemble average test log likelihoods to state-of-the-art density estimators as Sum-Product Networks (ID-SPN), Markov Networks (ACMN) and Bayesian Networks (WM).

4.3 Learning time comparison ...in a fraction of the time other competitor need

dataset	dCSN	XCNet	$\mathrm{dCSN}_{\mathrm{PoB}}$	$\mathrm{XCNet}_{\mathrm{PoB}}$	dCSN^{40}	$\mathrm{XCNet}^{40}_{\mathrm{PoB}}$	XCNet^{40}	XCNet^{500}	ID-SPN
NLTCS	0	0.2	0.1	0.01	10	0.2	0	3	310
MSNBC	12	0.3	0.7	0.01	499	13.1	13	155	46266
KDDCup2k	112	0.5	12.0	0.32	4126	21.2	16	247	32067
Plants	15	0.3	45.5	0.22	325	1.0	6	77	18833
Audio	58	0.3	74.8	0.48	980	0.8	6	136	21009
Jester	50	0.2	95.6	0.26	989	0.3	4	83	10412
Netflix	75	0.2	2.8	0.02	1546	0.4	9	118	30294
Accidents	54	0.2	153.7	0.04	996	0.7	11	138	15472
Retail	263	0.8	5.8	0.01	3780	3.2	13	164	4041
Pumsb-star	118	0.6	26.2	0.02	2260	0.8	23	290	20952
DNA	30	0.1	4.4	0.01	224	0.06	3	40	3040
Kosarek	588	2.4	41.2	0.01	10033	10.8	43	524	17799
MSWeb	1215	7.2	7.4	0.01	17123	13.2	129	1592	19682
Book	9235	9.7	113.0	0.04	155634	1.9	316	3476	61248
EachMovie	1297	7.1	4.7	0.01	16962	1.1	127	2601	118782
WebKB	4997	11.0	238.0	0.03	18875	0.9	190	2237	45451
Reuters-52	9947	39.3	24.3	0.05	65498	2.7	414	8423	70863
20NewsG	16866	51.3	40.7	0.01	153908	4.4	506	9883	163256
BBC	21381	8.4	7.3	0.02	69572	0.4	256	4251	61471
Ad	5212	116.5	134.0	0.08	75694	4.2	2403	30538	87522

Table 3. Times (in seconds) taken to learn the best models on each dataset for dCSN, XCNet, $\mathrm{dCSN}_{\mathrm{PoB}}$, $\mathrm{XCNet}_{\mathrm{PoB}}$, their ensembles and ID-SPN

References

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[2] Marina Meilă and Michael I. Jordan. "Learning with mixtures of trees". In: *Journal of Machine Learning Research* 1 (2000), pp. 1–48.

[3] Tahrima Rahman, Prasanna Kothalkar, and Vibhav Gogate. "Cutset Networks: A Simple, Tractable, and Scalable Approach for Improving the Accuracy of Chow-Liu Trees". In: *Machine Learning and Knowledge Discovery in Databases*. Vol. 8725. LNCS. Springer, 2014, pp. 630–645.

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Paper - `http://www.di.uniba.it/~ndm/pubs/ndm17ecml.pdf` · **Code** - `https://github.com/nicoladimauro/cnet`