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 $\mathcal{D} = \{\mathbf{x}^i\}_{i=1}^m$ over r.v.s $\mathbf{X} = \{X_1, \ldots, X_n\}$

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)

Classical Probabilistic Graphical Models like ***Bayesian Networks*** (**BNs**) and ***Markov Networks*** (**MNs**) are highly expressive but exact inference is generally NP-hard [6].

Tractable Probabilistic Models (**TPMs**) on the other hand, are density estimators for which some kind of ***exact*** inference is ***tractable***, i.e. *polynomial* in the number of RVs or their domains. → Learning them may still be hard to scale.

2.1 Product of Bernoullis (PoBs)

The least expressive, assuming all RVs to be independent:

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

Learning a PoB has linear time complexity $O(nm)$.
Inference is linear as well, $O(n)$.

2.2 Chow-Liu Trees (CLTrees)

A *directed tree-structured model* [3] over $\mathbf{X}$ is a BN in which each node $X_i \in \mathbf{X}$ has at most one parent, Pa_{X_i}.

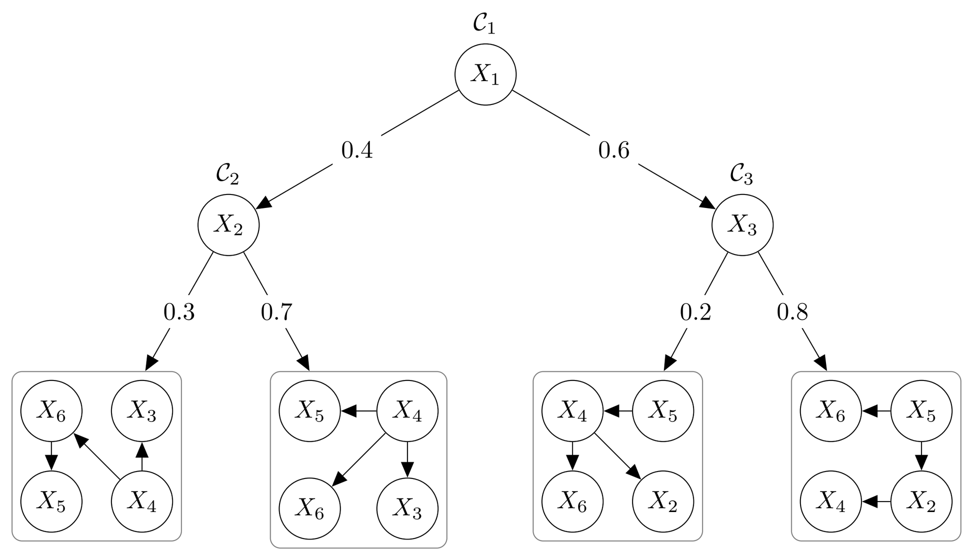
$$\mathrm{p}(\mathbf{x}) = \prod_{i=1}^{n} \mathrm{p}(x_i|\mathrm{Pa}_{x_i})$$

Learning a CLtree takes quadratic time $O(n^2(m + \log n))$.
Inference is still linear like PoBs, $O(n)$.

3. 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$(\mathcal{C}_1) = \mathbf{X}_{\setminus i}$



A CNet over binary RVs $\mathbf{X} = \{X_1, \ldots, X_6\}$. Or nodes are rounded, while leaf squared nodes represent CLtrees.

Therefore, the joint pdf modeled by a CNet $\mathcal{C}$ is:

$$\mathrm{p}(\mathbf{x}) = \mathrm{p}_l(\mathbf{x}_{|\mathrm{scope}(\mathcal{C})\setminus\mathrm{scope}(\mathcal{M}_l)})\mathrm{p}_{\mathcal{M}_l}(\mathbf{x}_{|\mathrm{scope}(\mathcal{M}_l)}) \tag{1}$$

4. Learning CNets

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

LearnCNet($\mathcal{D}$, $\mathbf{X}$, α, δ, σ)

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

different select implementations have different complexities:

entCNet [5] choosing X_i to lower approximate average joint entropy → $O(mn^2)$

dCSN [2] choosing X_i in a principled way improving likelihood → $O(n^3(m + \log n))$

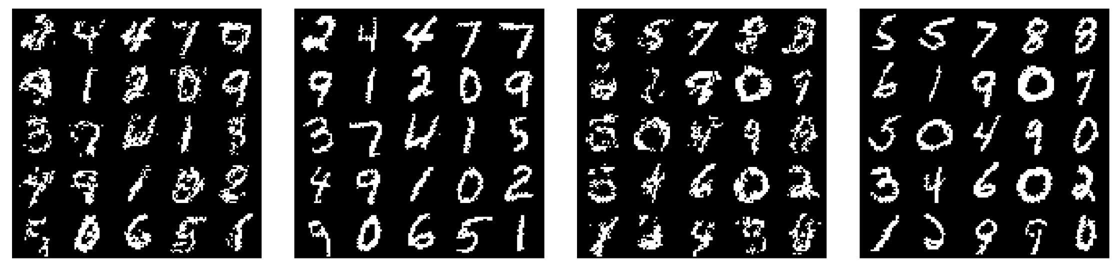
5. XCNets

XCNets (**Extremely Randomized CNets**) are CNets built by LearnCNet when select chooses one RV *completely at random*.
select time complexity → $O(1)$!

5.1 Mixture of Experts Interpretation

A single CNet can be seen as a peculiar *mixture of experts*: the OR tree plays as a *deterministic gating function* and leaf distributions as *local experts*. A path $p = p_{(1)}p_{(2)} \cdots p_{(k)}$ connects the root to a single leaf $\mathcal{M}_l$ after observing $x_1 x_2 \cdots x_k$, Equation 1.
$\mathrm{p}_l(\mathbf{x}_{|\mathrm{sc}(\mathcal{C})\setminus\mathrm{sc}(\mathcal{M}_l)})$ is decomposed by the chain rule across path p.
→ randomly shuffling $X_{p_{(0)}}, \ldots, X_{p_k}$ does not influence inference!

Therefore a single XCNet is only only slightly less accurate than a CNet and as good at generating samples.

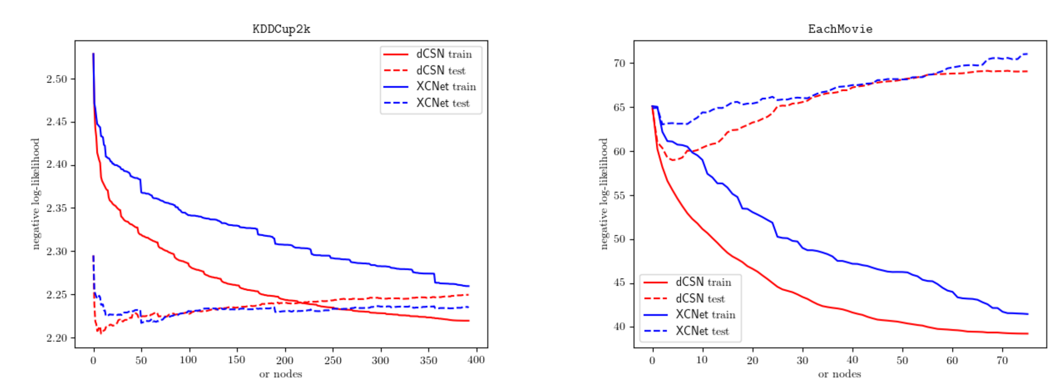


(a) (b) (c) (d)

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).

5.2 Regularizing learning

Single CNets learned with LearnCNet are prone to overfitting, randomization in XCNets alleviate this issue



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

5.3 Ensembles

of XCNets do not require to additionally diversify components and learning up to 500 components is still faster than learning 40 of other variants:

CNet$_{\mathrm{bag}}$ bagging entCSN [4]
CNet$_{\mathrm{boost}}$ boosting entCSN [4]
dCSN^k bagging dCSN [2, 1]

6. Experiments

6.1 Single model comparisons

single XCNets are comparable (same order of magnitude) to entCNet and dCSN.

dataset	entCNet	dCSN	XCNet	dCSN$_{\mathrm{PoB}}$	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 dCSN$_{\mathrm{PoB}}$ and XCNet$_{\mathrm{PoB}}$. For randomized models, mean and standard deviation over 10 runs are reported).

6.2 Ensemble model comparisons

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

dataset	CNet$^{40}_{\mathrm{bag}}$	CNet$^{40}_{\mathrm{boost}}$	dCSN^{40}	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).

6.3 Learning time comparison

...in a fraction of the time other competitor need

dataset	dCSN	XCNet	dCSN$_{\mathrm{PoB}}$	XCNet$_{\mathrm{PoB}}$	dCSN^{40}	XCNet$^{40}_{\mathrm{PoB}}$	XCNet^{40}	XCNet^{500}	ID-SPN
NLTCS	0	0.2	0.1	0.01	10	0.2	0.01	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, dCSN$_{\mathrm{PoB}}$, XCNet$_{\mathrm{PoB}}$, their ensembles and ID-SPN

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