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Fast and Accurate Denstiy Estimation with Extremely Randomized Cutset Networks

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Outline

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 random variables (RVs) $\mathbf{X} = \{X_1, \ldots, X_n\}$

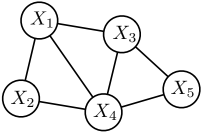
Given such an estimator, one uses it to *answers probabilistic queries* about configurations on $\mathbf{X}$, i.e. to do ***inference***. E.g., classification can be performed by Most Probable Explanaition (MPE) inference: $y^* = \mathrm{argmax}_{y \sim Y}\, p(y|\mathbf{X})$.

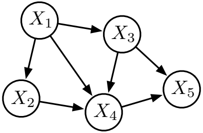
The main challenge in density estimation is balancing:

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

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*** with them [Roth 1996].



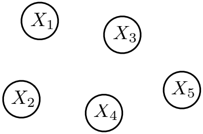


Tractable Probabilistic Models (**TPMs**) on the other hand, are density estimators for which some kind of ***exact* inference is *tractable***, i.e. *polynomial* in the number of RVs, i.e., n, or their domains.

$\rightarrow$ learning may still be hard to scale on high-dimensional data

Product of Bernoullis (PoBs)

A not so much expressive TPM, assuming all RVs to be independent:



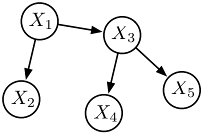
$$\mathsf{p}(\mathbf{x}) = \prod_{i=1}^{n} \mathsf{p}(x_i)$$

Learning a PoB has linear time complexity $O(nm)$.

Complete evidence inference is linear $O(n)$.

Chow-Liu Trees (CLTrees)

A *directed tree-structured model* [Meilă and Jordan 2000] over $\mathbf{X}$ is a BN in which each node $X_i \in \mathbf{X}$ has at most one parent, Pa_{X_i}.

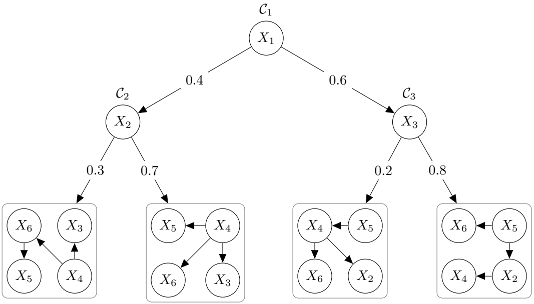


$$\mathsf{p}(\mathbf{x}) = \prod_{i=1}^{n} \mathsf{p}(x_i | \mathrm{Pa}_{x_i})$$

Complete evidence inference is still linear for CLtrees: $O(n)$.

But learning now takes quadratic time $O(n^2(m + \log n))$.

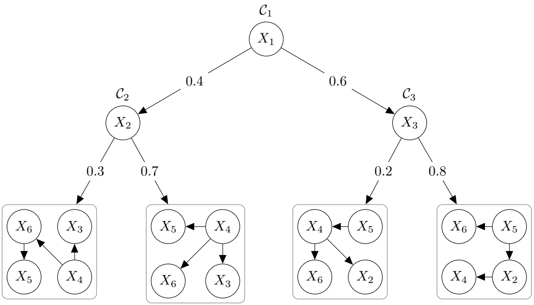
Cutset Networks (CNets)



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

1. a TPM $\mathcal{M}$, with $\text{scope}(\mathcal{M}) = \mathbf{X}$
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 $\text{scope}(\mathcal{C}_0) = \text{scope}(\mathcal{C}_1) = \mathbf{X}_{\setminus i}$

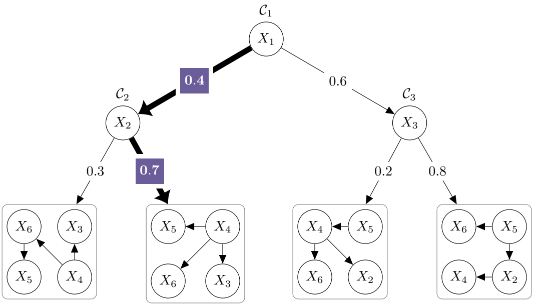
CNets I



A CNet $\mathcal{C}$ defines the following joint distribution:

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

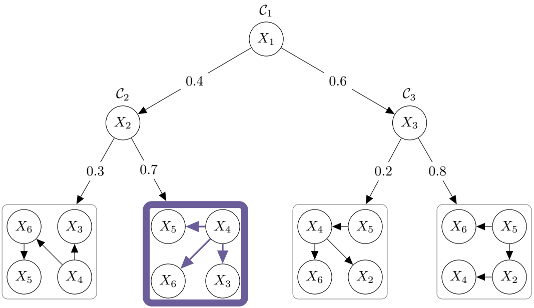
CNets II



A CNet $\mathcal{C}$ acts as a ***deterministic mixture of experts*** in which the OR tree acts as the **gating function**

$$\mathsf{p}(\mathbf{x}) = \boxed{\mathsf{p}_l(\mathbf{x}_{|\mathsf{scope}(\mathcal{C})\setminus\mathsf{scope}(\mathcal{M}_l)})}\,\mathsf{p}_{\mathcal{M}_l}(\mathbf{x}_{|\mathsf{scope}(\mathcal{M}_l)})$$

CNets III



and in which leaf models $\mathcal{M}_l$ play the role of **local experts**

$$\mathsf{p}(\mathbf{x}) = \mathsf{p}_l(\mathbf{x}_{|\mathsf{scope}(\mathcal{C})\setminus\mathsf{scope}(\mathcal{M}_l)})\,\boxed{\mathsf{p}_{\mathcal{M}_l}(\mathbf{x}_{|\mathsf{scope}(\mathcal{M}_l)})}$$

complete evidence inference is still linear $\boxed{O(n)}$!

Learning CNets I

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 $\mathsf{p}_{\mathcal{C}}(\mathbf{X})$ learned from $\mathcal{D}$
if $|\mathcal{D}| > \delta$ **and** $|\mathbf{X}| > \sigma$ **then**
  $X_i \leftarrow \mathsf{select}(\mathcal{D}, \mathbf{X}, \alpha)$
  $\mathcal{D}_0 \leftarrow \{\xi \in \mathcal{D} : \xi[X_i] = 0\}$, $\mathcal{D}_1 \leftarrow \{\xi \in \mathcal{D} : \xi[X_i] = 1\}$
  $w_0 \leftarrow |\mathcal{D}_0|/|\mathcal{D}|$, $w_1 \leftarrow |\mathcal{D}_1|/|\mathcal{D}|$
  $\mathcal{C} \leftarrow w_0 \cdot \mathsf{LearnCNet}(\mathcal{D}_0, \mathbf{X}_{\setminus i}, \alpha, \delta, \sigma) + w_1 \cdot \mathsf{LearnCNet}(\mathcal{D}_1, \mathbf{X}_{\setminus i}, \alpha, \delta, \sigma)$
else
  $\mathcal{C} \leftarrow$ $\mathsf{learnLeafDistribution}(\mathcal{D}, \mathbf{X}, \alpha)$ ▷ Grow a leaf TPM
return $\mathcal{C}$

in which for the base case, if no conditioning is possible, *a leaf distribution is estimated*

Learning CNets II

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 $\mathsf{p}_{\mathcal{C}}(\mathbf{X})$ learned from $\mathcal{D}$
if $|\mathcal{D}| > \delta$ **and** $|\mathbf{X}| > \sigma$ **then**
    $X_i \leftarrow \mathsf{select}(\mathcal{D}, \mathbf{X}, \alpha)$ ▷ select the RV to condition on
    $\mathcal{D}_0 \leftarrow \{\xi \in \mathcal{D} : \xi[X_i] = 0\}, \mathcal{D}_1 \leftarrow \{\xi \in \mathcal{D} : \xi[X_i] = 1\}$
    $w_0 \leftarrow |\mathcal{D}_0|/|\mathcal{D}|, w_1 \leftarrow |\mathcal{D}_1|/|\mathcal{D}|$
    $\mathcal{C} \leftarrow w_0 \cdot \mathsf{LearnCNet}(\mathcal{D}_0, \mathbf{X}_{\setminus i}, \alpha, \delta, \sigma) + w_1 \cdot \mathsf{LearnCNet}(\mathcal{D}_1, \mathbf{X}_{\setminus i}, \alpha, \delta, \sigma)$
else
    $\mathcal{C} \leftarrow \mathsf{learnLeafDistribution}(\mathcal{D}, \mathbf{X}, \alpha)$
return $\mathcal{C}$

or selecting a RV to condition on is performed, splitting the dataset and recursing

Learning CNets III

Different implementations of select lead to different time complexities:

entCNet choosing X_i to lower approximate average joint entropy [Rahman, Kothalkar, and Gogate 2014]

$\rightarrow \boxed{O(mn^2)}$

dCSN choosing X_i in a principled way improving likelihood [Di Mauro, Vergari, and Esposito 2015]

$\rightarrow \boxed{O(n^3(m + \log n))}$

Quadratic and cubic times for *each* RV selection do not scale on high dimensional data

We aim at drastically reducing it!

XCNets I

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

select time complexity $\longrightarrow$ $O(1)$!

Advantages of a **single** XCNet over a classically learned CNet:

- extremely fast to learn
- only slightly less accurate as density estimators
- almost as good at generating samples
- less prone to overfitting

When plugged into **ensembles** they outperform state-of-the-art density estimators in a fraction of the time!

XCNets II

Why a single XCNet is *not much worse* than a CNet?

Because of the mixture of experts interpretations, a path $p = p_{(1)} p_{(2)} \cdots p_{(k)}$ connects the root to a single leaf $\mathcal{M}_l$ after observing $x_1 x_2 \cdots x_k$, $\mathsf{p}_l\left(\mathbf{x}_{|\mathsf{sc}(\mathcal{C})\setminus\mathsf{sc}(\mathcal{M}_l)}\right)$ is decomposed by the chain rule across path p .

$\rightarrow$ shuffling $X_{p_{(0)}}, \ldots, X_{p_k}$ does not influence inference!

Focus on learning ***accurate local experts*** (leaves) than the gating function!

Sampling is less affected:

CNet

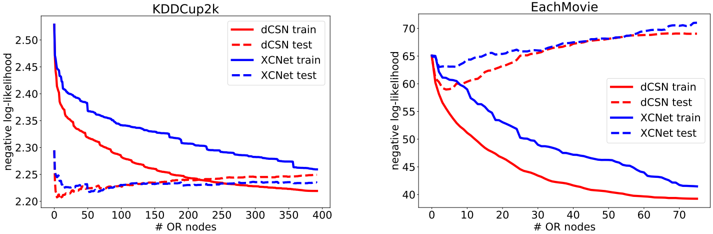
Train

XCNet

Train

XCNets III

Single CNets learned with LearnCNet are prone to overfitting.
Randomizing the gating function in XCNets alleviate this issue.



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

Moreover, it helps differentiating the local leaf experts

Ensembles of XCNets

Ensembles of XCNets do not require to additionally diversify each components (no bootstrapping required).

Learning up to **500 components** of XCNets is still **faster than learning 40** of other variants:

CNet$_{\text{bag}}$	bagging entCSN [Rahman and Gogate 2016]
CNet$_{\text{boost}}$	boosting entCSN [Rahman and Gogate 2016]
dCSN^k	bagging dCSN [Di Mauro, Vergari, and Basile 2015; Di Mauro, Vergari, and Esposito 2015]

Experiments

We validate the following research questions:

(Q1) how does a single XCNet compare to the optimal one learned by dCSN?

(Q2) how accurate are ensembles of XCNets compared state-of-the-art density estimators?

(Q3) how much time do actually XCNets save in practice?

We employ the **20 standard benchmark datasets** for density estimation *[Haaren and Davis 2012; Vergari, Mauro, and Esposito 2015]*

We compare to single and ensembles of CNets plus other state-of-the-art TPMs like Sum-Product Networks (ID-SPN) and Markov Networks learned with ACs (ACMN) and even untractable Bayesian Networks (BN).

(Q1) Single Model Comparison

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

(Q2) Ensemble Model Comparison

new ***state-of-the-art*** scores on 11/20 datasets…

dataset	$\text{CNet}^{40}_{\text{bag}}$	$\text{CNet}^{40}_{\text{boost}}$	dCSN^{40}	$\text{XCNet}^{40}_{\text{PoB}}$	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

(Q3) Learning Times

...in a ***fraction of the time*** required by other competitors

dataset	dCSN	XCNet	dCSN_{PoB}	$\text{XCNet}_{\text{PoB}}$	dCSN^{40}	$\text{XCNet}^{40}_{\text{PoB}}$	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_{PoB}, $\text{XCNet}_{\text{PoB}}$, their ensembles and ID-SPN

Conclusions

Due to their simplicity to implement, ***fast learning times***, and ***accurate inference performances***, XCNets set the **new baseline to compare against** for density estimation with TPMs (and not!).

Future works

Exploiting the mixture of experts interpretation to devise more expressive gating functions to still perform exact and fast inference

Code

`https://github.com/nicoladimauro/cnet`

Paper

`http://www.di.uniba.it/~ndm/pubs/ndm17ecml.pdf`

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Discuss