Credal ensembling in multi-class classification

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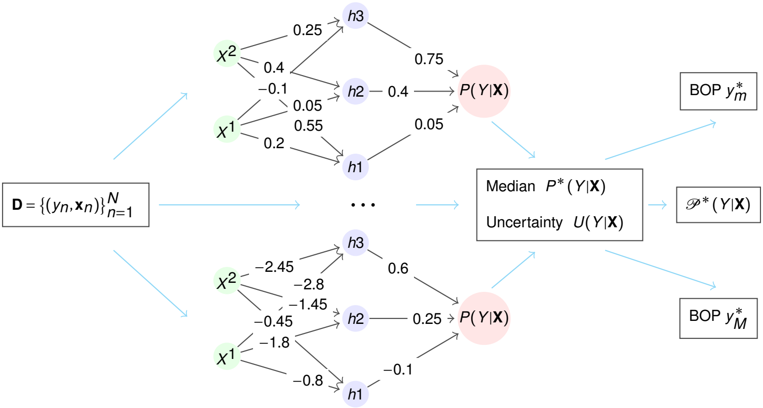
Outline

- Credal ensembling
  - A median classifier: Learning and inference
  - A credal classifier: Learning and inference
- Applications in machine learning
- Points of discussions
- Conlusion

A formal framework [2, 3]

Basic setup:

- Features $(X^1, \ldots, X^P)$ and a class variables Y
- An finite output space $\mathscr{Y} = \{y^1, \ldots, y^C\}$



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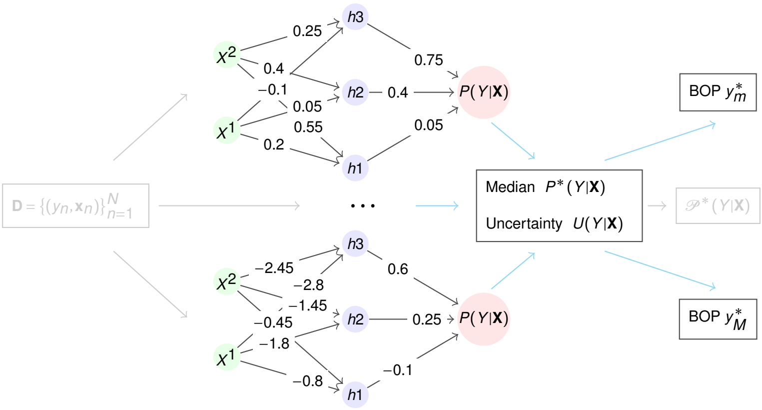
A median classifier and its predictions [2, 3]



Compute a median classifier

Basic setting:

- An ensemble $\mathbf{H} := \{\mathbf{h}^m | m \in [M] := \{1, \dots, M\}\}$ is made available
- A specified statistical distance d between distributions

A median classifier minimizes the average expected distance:

$$\mathbf{h}_d \in \operatorname*{argmin}_{\mathbf{h} \in \mathcal{H}} \mathbf{E}\left[\sum_{m=1}^{M} d(\mathbf{h}, \mathbf{h}^m)\right] = \operatorname*{argmin}_{\mathbf{h} \in \mathcal{H}} \int_{\mathbf{x} \in \mathcal{X}} \left[\sum_{m=1}^{M} d(\mathbf{h}(\mathbf{x}), \mathbf{h}^m(\mathbf{x}))\right] d\mathbf{x}.$$

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If no constraint on $\mathscr{H}$, $\mathbf{h}_d$ can be defined in an instance-wise manner:

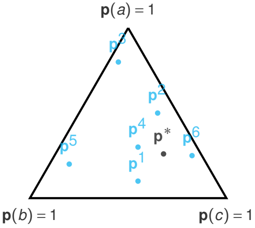
$$\mathbf{h}_d(\mathbf{x}) \in \operatorname*{argmin}_{\mathbf{h}(\mathbf{x}) \in \Delta^K} \sum_{m=1}^{M} d(\mathbf{h}(\mathbf{x}), \mathbf{h}^m(\mathbf{x})). \tag{1}$$

Compute a median classifier (cont.)

For each **x**, dropping **x** and denoting $\mathbf{p} = \mathbf{h}$ give

$$\mathbf{p}_d \in \operatorname*{argmin}_{\mathbf{p} \in \Delta^K} \sum_{m=1}^{M} d(\mathbf{p}, \mathbf{p}^m). \tag{2}$$

Examples of d are squared Euclidean distance (sE), L_1 distance, and KL divergence.



Ensemble **H** and $\mathbf{p}_{\text{sE}}$

Compute a median classifier (cont.)

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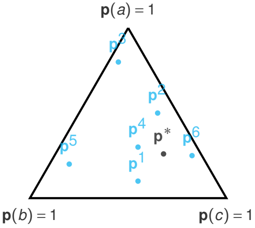

Ensemble $\mathbf{H}$ and $\mathbf{p}_{\mathrm{sE}}$

For any convex distance d:

- The convex optimization problem (2) can be solved using any solver.
- Close-form solution $\mathbf{p}_{\mathrm{sE}}$ = averaging the distributions class-wise.

Bayesian-optimal predictions

Basic set (instance-wise manner):

- The median distribution $\mathbf{p}_d$ is given.
- A the higher the better utility $u : \mathscr{Y} \times \mathscr{Y} \longmapsto \mathbb{R}_+$

A **Bayesian-optimal prediction (BOP) of** u is

$$y_d^u \in \operatorname*{argmax}_{y' \in \mathscr{Y}} \mathbf{E}\left[u(y', y)\right] = \operatorname*{argmax}_{y' \in \mathscr{Y}} \sum_{y \in \mathscr{Y}} u(y', y)\mathbf{p}_d(y). \tag{3}$$

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Commonly used utilities, such as $0/1$ and cost-sensitive accuracies:

- Find a BOP (3) takes from $O(K)$ to $O(K^2)$
- A BOP $y_d^{0/1}$ (3) of $0/1$ accuracy = a most probable class

Bayesian-optimal set-valued predictions

Basic set (instance-wise manner):

- The median distribution $\mathbf{p}_d$ is given.
- A the higher the better utility $U : \mathscr{Y} \times 2^{\mathscr{Y}} \longmapsto \mathbb{R}_+$

A **Bayesian-optimal prediction (BOP) of** U is

$$Y_d^U \in \operatorname*{argmax}_{Y' \subset \mathscr{Y}} \mathbf{E}\left[U(Y', y)\right] = \operatorname*{argmax}_{Y' \subset \mathscr{Y}} \sum_{y \in \mathscr{Y}} U(Y', y)\mathbf{p}_d(y). \tag{4}$$

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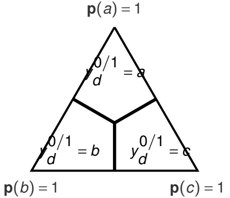
Commonly used utilities, such as utility-discounted accuracies:

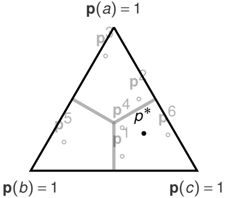
$$U(Y', y) = \frac{1}{g(|Y'|)} \llbracket y \in Y' \rrbracket, \tag{5}$$

- Find a BOP Y_d^U (4) takes $O(K \log(K))$.
- A BOP Y_d^U (4) consists of the most probable classes on $\mathbf{p}_d$.

Probabilistic uncertainty scores

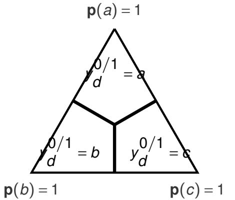


Regions $\Delta^{\text{st}}_{\mathbf{x}}$ for different $y_d^{0/1}$

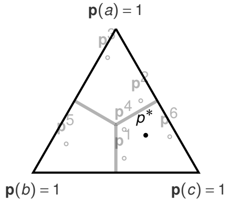


Ensemble $\mathbf{H}$ and $\mathbf{p}_{\text{sE}}$

Probabilistic uncertainty scores



Regions $\Delta_{\mathbf{x}}^{st}$ for different $y_d^{0/1}$



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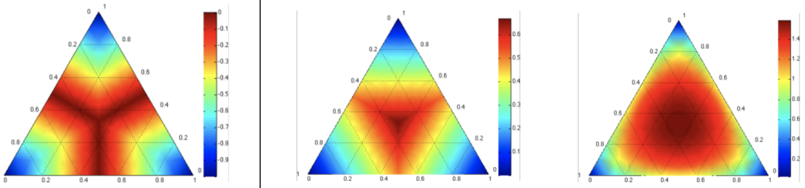

(a) Smallest margin (↑) (b) Least confidence (↓) (c) Entropy (↓)

Heatmaps illustrating the **behavior of probabilistic uncertainty scores**

Probabilistic uncertainty scores (Cont.)

Smallest margin (↑) is defined as

$$S_{\mathrm{SM}}\left(\mathbf{p}_d\right) = \mathbf{p}_d\left(y^{\mathrm{st}}\right) - \mathbf{p}_d\left(y^{\mathrm{nd}}\right). \tag{6}$$

Example: A classification problem with $\mathscr{Y} = \{a, b, c\}$:

	$\mathbf{H}^1$	$\mathbf{H}^2$
	50→(0.6, 0.4, 0.0) 50→(0.0, 0.4, 0.6)	100→(0.3, 0.4, 0.3)
$\mathbf{p}_{\mathrm{sE}}$	(0.3, 0.4, 0.3)	
S_{SM} (↑)	0.1	
	Should we consider $\mathbf{H}^1$ and $\mathbf{H}^2$ the same?	

Probabilistic uncertainty scores (Cont.)

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	$\mathbf{H}^3$	$\mathbf{H}^4$
	80→(1.0, 0.0, 0.0) 20→ (0.0, 1.0, 0.0)	100→(0.8, 0.2, 0.0)
$\mathbf{p}_{\text{sE}}$	(0.8, 0.2, 0.0)	
S_{SM} (↑)	0.6	
	Should we consider $\mathbf{H}^3$ and $\mathbf{H}^4$ the same?	

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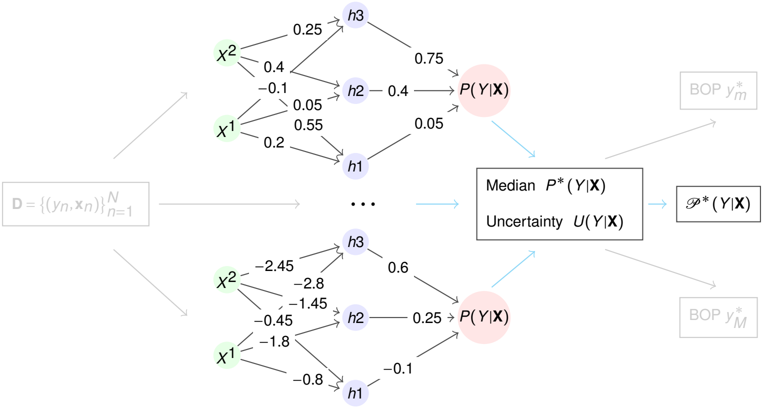
A credal classifier and its predictions [2]



For any query instance, once $\mathscr{P}^*(\mathscr{Y}|\mathbf{x})$ is estimated:

- IP decision rules can be called to make set-valued predictions
- uncertainty scores defined for credal sets can be computed.

Estimate a credal classifier

Each credal classifier $\mathbf{CH}_{\alpha}^{d}$ is defined in a point-wise manner:

$$\mathbf{CH}_{\alpha}^{d} := \left\{ \mathbf{p} := \sum_{m=1}^{M_{\alpha}} \gamma_m \mathbf{p}^{(m)} | \gamma_m \geq 0, m \in [M_{\alpha}], \sum_{m=1}^{M_{\alpha}} \gamma_m = 1 \right\}, \tag{7}$$

where $\mathbf{p}^{(m)}$ is the m-th closet point to $\mathbf{p}_d$ **according to the distance** d.

Estimate a credal classifier

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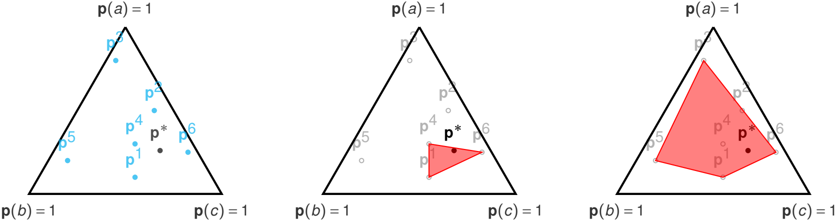

Ensemble **H** and $\mathbf{p}^*_{sE}$ — Credal set $\mathbf{CH}^{sE}_{0.5}$ — Credal set $\mathbf{CH}^{sE}_{0}$

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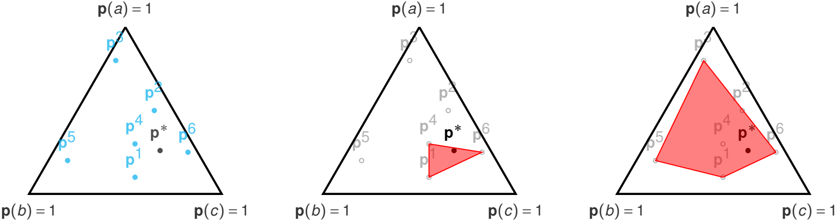
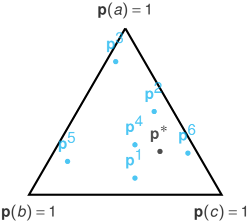


Ensemble $\mathbf{H}$ and $\mathbf{p}_{sE}^{*}$ — Credal set $\mathbf{CH}_{0.5}^{sE}$ — Credal set $\mathbf{CH}_{0}^{sE}$

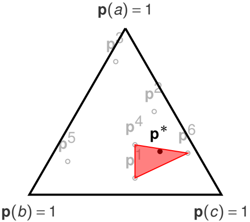
The hyperparameter α^* $\leftarrow$ nested cross validation or a validation set.

Optimal set-valued predictions under IP decision rules

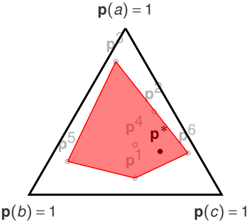
Basic set (instance-wise manner): The credal set $\mathbf{CH}^{d}_{\alpha^*}$ is given.



Ensemble **H** and $\mathbf{p}_{sE}$



Credal set $\mathbf{CH}^{sE}_{0.5}$



Credal set $\mathbf{CH}^{sE}_{0}$

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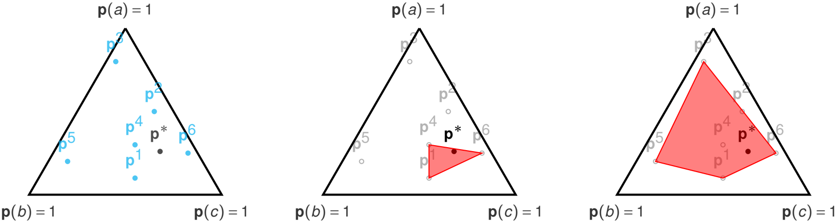

Ensemble $\mathbf{H}$ and $\mathbf{p}_{\mathrm{sE}}$ | Credal set $\mathbf{CH}^{\mathrm{sE}}_{0.5}$ | Credal set $\mathbf{CH}^{\mathrm{sE}}_{0}$

- Any IP decision rule $R_{\mathrm{IP}} : 2^{\Delta^K} \longmapsto 2^{\mathscr{Y}}$ can be applied.
- Any related algorithmic solutions can be leveraged.

Optimal set-valued predictions under IP decision rules (Cont.)

Basic set (instance-wise manner):

- The credal set $\mathbf{CH}_{\alpha^*}^{d}$ is given.
- A the higher the better utility $u : \mathscr{Y} \times \mathscr{Y} \longmapsto \mathbb{R}_+$

E-admissibility under u:

- A class y is E-admissible if there exist $\mathbf{p} \in \mathbf{CH}_{\alpha^*}^{d}$ so that $y = y^u$.
- This can be checked by solving a linear program.

Optimal set-valued predictions under IP decision rules (Cont.)

Basic set (instance-wise manner):

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E-admissibility under u:

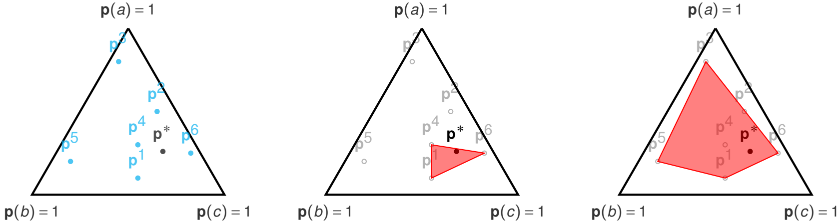
- A class y is E-admissible if there exist $\mathbf{p} \in \mathbf{CH}^d_{\alpha^*}$ so that $y = y^u$.
- This can be checked by solving a linear program.

Maximality under u:

- A class y is maximal if there doesn't exist $y' \neq y$ such that y' dominates y on at least one $\mathbf{p} \in \mathbf{CH}^d_{\alpha^*}$ (w.r.t. u).
- This can be checked by solving $K-1$ linear programs.
- We can also enumerate all the distributions $\mathbf{p}^m$, $m \in [M]$.

Credal set-based uncertainty scores

Basic set (instance-wise manner): The credal set $\mathbf{CH}^{d}_{\alpha^*}$ is given.



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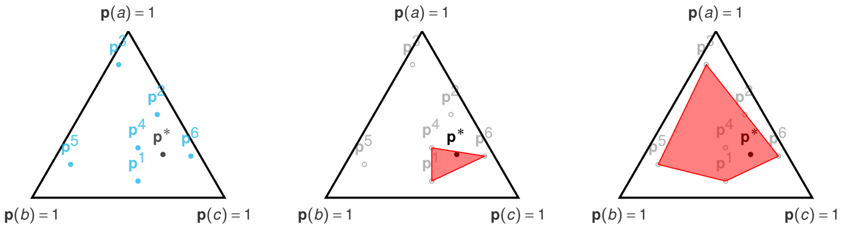


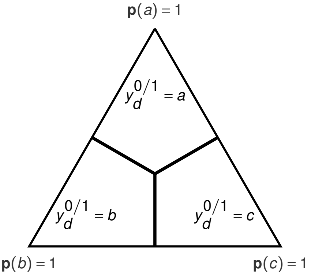
Ensemble $\mathbf{H}$ and $\mathbf{p}_{\mathrm{sE}}$ Credal set $\mathbf{CH}^{\mathrm{sE}}_{0.5}$ Credal set $\mathbf{CH}^{\mathrm{sE}}_{0}$

- Any credal set-based uncertainty score can be used.
- Any related algorithmic solutions can be leveraged.

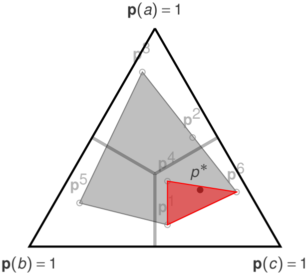
Credal set-based uncertainty scores (Cont.)

Decision-related uncertainty scores:

- How certain the ensemble **H** is about y_d^u?
- How consensus of the ensemble members is about y_d^u?



Regions $\Delta_{\mathbf{x}}^{st}$ for different $y_d^{0/1}$



Credal set $\mathbf{CH}_0^{sE}(\mathbf{x})$ with $\mathbf{p}_{sE}$

Decision-related uncertainty scores

Basic setting (instance-wise manner):

- The median distribution $\mathbf{p}_d$ is given.
- The predictions $\{\mathbf{p}^m | m \in [M]\}$ are given.
- A probabilistic uncertainty score $S : \Delta^K \longmapsto \mathbb{R}$ is given.

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A **decision-related uncertainty** version of S is (its empirical expectation over the decision region of the 1st class, normalized by the upper score)

$$\mathrm{RS}(\mathbf{p}_d^u) := \frac{1}{M+1} \left(\sum_{m=1}^{M} [\![\mathbf{p}^m \in \mathbf{CH}^d_{y_d^u}]\!] S(\mathbf{p}^m) + S(\mathbf{p}_d) \right), \tag{8}$$

where $[\![\mathbf{p}^m \in \mathbf{CH}^d_{y_d^u}]\!] = 1$ implies y_d^u is a best solution on $\mathbf{p}^m$ under u.

Decision-related uncertainty scores (Cont.)

Smallest margin (↑) is defined as

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$\mathbf{p}_{\mathrm{sE}}$	(0.3, 0.4, 0.3)	
S_{SM} (↑)	0.1	
$\mathrm{RS}_{\mathrm{SM}}$ (↑)	0.0	0.1

Decision-related uncertainty scores (Cont.)

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$\mathbf{p}_{\mathrm{sE}}$	(0.8, 0.2, 0.0)	
S_{SM} (↑)	0.6	
$\mathrm{RS}_{\mathrm{SM}}$ (↑)	0.798	0.6

Should we put weights on the impact of ensemble members?

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  - Classification with rejection
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Experimental setting

Basic setting:

- Use random forests of cardinality 100 as the ensembles
- Follow a 10-cross validation protocal.
- Use hyperparameter $\alpha^* \leftarrow$ nested 10 fold cross validation

Assess the impact of $\mathbf{p}_{\mathrm{sE}}$, $\mathbf{p}_{\mathrm{L1}}$ and $\mathbf{p}_{\mathrm{KL}}$ on

- the clean version of the data sets
- noisy version (randomly flip the class of 25% of training instances)

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- the clean version of the data sets
- noisy version (randomly flip the class of 25% of training instances)

Once credal set $\mathrm{CH}^{d}_{\alpha^*}$ is computed, it is used to

- find the set-valued prediction under the E-admissibility rule.

Results on clean data sets: U_{65} scores (in %) [3]

Data set: (N,P,K)	NDC	SQE-E	L1-E	KL-E	CRF	$\mathbf{CH_0}$
eco.: (336,7,8)	85.51	86.07	85.81	**87.07**	84.46	43.60
der.: (358,34,6)	97.18	97.05	97.22	**98.59**	96.19	51.74
lib.: (360, 90, 15)	76.58	73.35	75.24	**79.41**	73.45	14.60
vow.: (990, 10, 11)	86.63	86.35	87.65	**92.35**	82.68	17.75
win.: (1599, 11, 6)	**68.66**	68.32	68.39	68.63	67.35	36.53
seg.: (2300, 19, 7)	97.17	97.12	96.99	**97.64**	96.73	71.00

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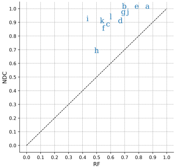
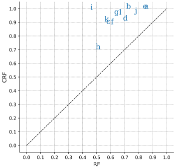
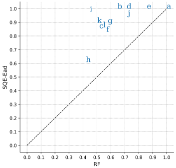
lib.: (360, 90, 15)	76.58	73.35	75.24	**79.41**	73.45	14.60
vow.: (990, 10, 11)	86.63	86.35	87.65	**92.35**	82.68	17.75
win.: (1599, 11, 6)	**68.66**	68.32	68.39	68.63	67.35	36.53
seg.: (2300, 19, 7)	97.17	97.12	96.99	**97.64**	96.73	71.00



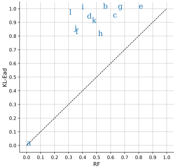
(a) NDC vs RF



(b) CRF vs RF



(e) SQE-Ead vs RF



(f) KL-Ead vs RF

Correctness of cautious predictors (vertical) vs accuracy of RF (horizontal)

Outline

- Credal ensembling
- Applications in machine learning
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  - Classification with rejection
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Experimental setting [3]

Basic setting:

- Randomly flip the class of 25% of training instances
- Using random forests of cardinality 100 as the ensembles
- The median $\mathbf{p}_{\mathrm{sE}}$ is employed
- Assess smallest margin S_{SM} ($\uparrow$) and $\mathbf{RS}_{\mathrm{SM}}$ ($\uparrow$)

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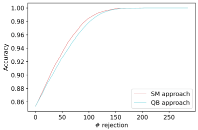
Budget based rejection protocal requires

- a sufficiently large number of test instances,
- a predefined number (or proportion) of rejections.

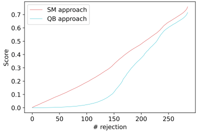
Threshold-based rejection protocal

- requires a predefined threshold on uncertainty score (↑),
- rejects instances whose scores are lower than the threshold.

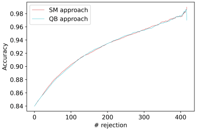
Results on noisy data sets [3]



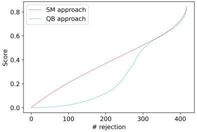
(a) derma. + SM



(b) derma. + SM



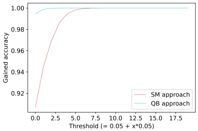
(c) forest + SM



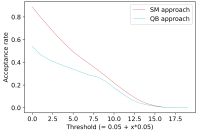
(d) forest + SM

Test accuracy and chosen score as the functions of the number of rejections

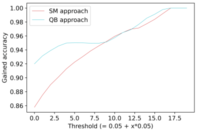
20×5 cross-validation with (train, test) = (20%, 80%)



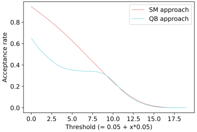
(a) derma. + SM



(b) derma. + SM



(c) forest + SM



(d) forest + SM

Test accuracy and acceptance rate as the functions of the threshold

20×5 cross-validation with (train, test) = (20%, 80%)

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Budget based sampling protocal

- requires a predefined number (or proportion) of queries,
- stops when the predefined number is reached.

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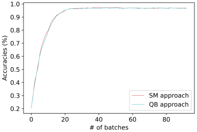
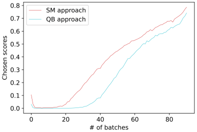


(a) derma. + SM



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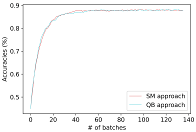
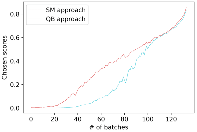


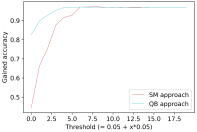
(c) forest + SM



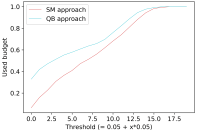
(d) forest + SM

Test accuracy and chosen score as the functions of the number of queries

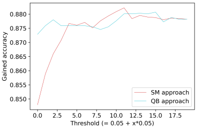
10×5 cross-validation with (train, pool, test) = (3%, 77%, 20%)



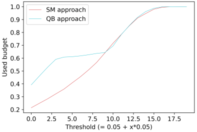
(a) derma. + SM



(b) derma. + SM



(e) forest + SM



(f) forest + SM

Test accuracy and used budget as the functions of the threshold

10×5 cross-validation with (train, pool, test) = (3%, 77%, 20%)

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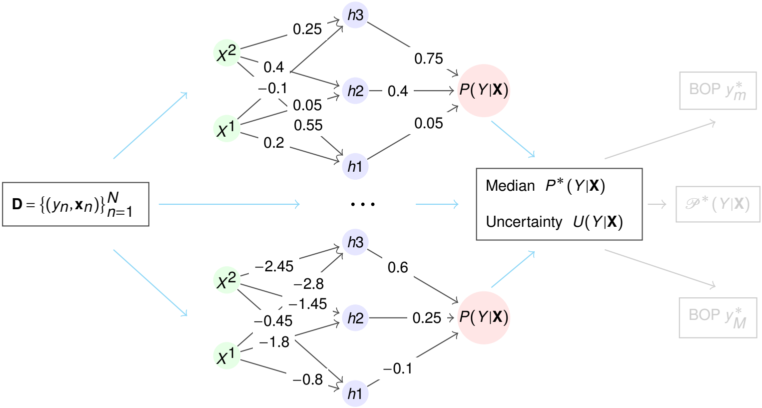
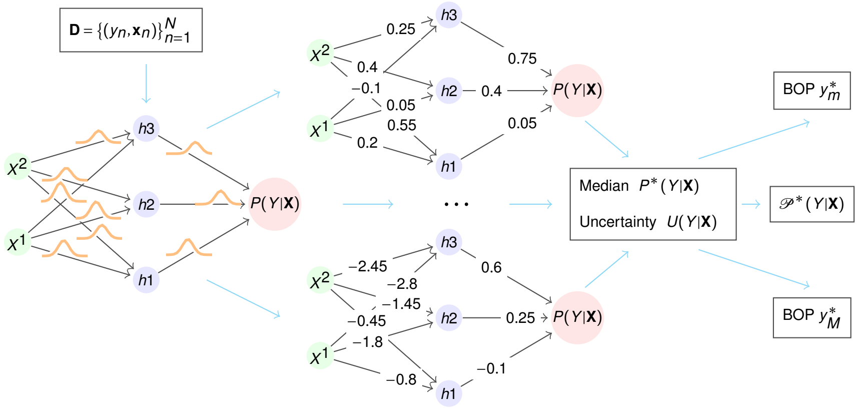
Conventional deep ensembles



Compared to the use of a single network:

- Much longer training time + Much larger storage memory
- Longer inference time

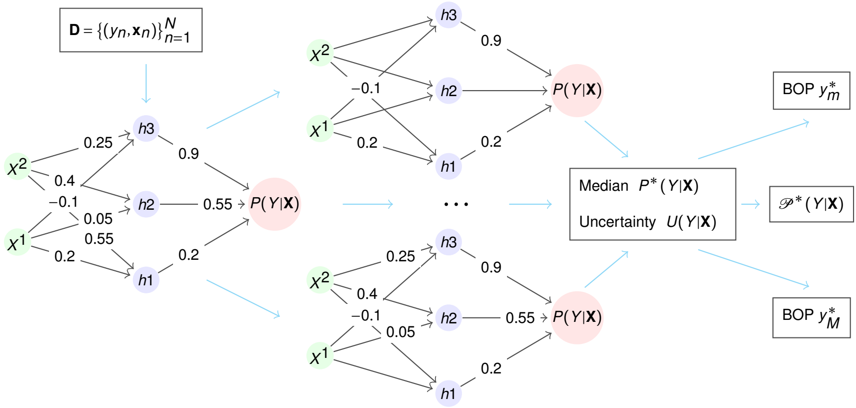
A BNN as an ensemble [5]



Compared to the use of a single network:

- A bit longer training time + A bit larger storage memory
- Longer inference time

A CNN with dropout predictions as an ensemble [4]



Compared to the use of a single network:

- Similar training time + Similar storage memory
- Longer inference time

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Experimental setting

Basic setting:

- Use BNNs with 100 Monte Carlo runs as the ensembles
- Use the clean version of the data sets

Assess the impact of $\mathbf{p}_{\mathrm{sE}}$, $\mathbf{p}_{\mathrm{L1}}$ and $\mathbf{p}_{\mathrm{KL}}$ on

	Image	train/test	# classes
CIFAR-10	32x32 color	50,000/10,000	10
Fashion-MNIST	grayscale	60,000/10,000	10

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Once $\mathbf{p}_d$ is computed, it is used to

- find precise prediction optimizing the $u_{0,1}$,
- find set-valued predictions optimizing the u_{65} and u_{80} [1].

Results [5]	CIFAR-10			Fashion MNIST		
	sE	L1	KL	sE	L1	KL
$u_{0/1}$ (↑)	90.04	90.10	**90.14**	93.07	**93.11**	93.08
u65_set_size (↓)	2.03	**2.02**	2.03	**2.02**	**2.02**	**2.02**
u80_set_size (↓)	2.04	**2.02**	2.03	**2.02**	**2.02**	**2.02**
c_pr_u65_c_si (↑)	94.91	95.91	**97.53**	97.53	97.19	**98.43**
c_pr_u65_c_se (↓)	5.08	4.08	**2.46**	2.46	2.80	**1.56**
w_pr_u65_c_se (↑)	**32.12**	26.86	17.64	24.96	**25.39**	15.75
w_pr_u65_w_se (↓)	15.26	11.81	**7.50**	5.05	5.95	**4.62**
w_pr_u65_w_si (↓)	**52.61**	61.31	74.84	69.98	**68.65**	79.62
c_pr_u80_c_si (↑)	86.89	93.22	**94.28**	94.34	94.03	**95.47**
c_pr_u80_c_se (↓)	13.10	6.77	**5.71**	5.65	5.96	**4.52**
w_pr_u80_c_se (↑)	**53.21**	37.07	34.38	43.86	**44.26**	37.28
w_pr_u80_w_se (↓)	23.89	19.19	**16.32**	10.82	10.44	**8.67**
w_pr_u80_w_si (↓)	**22.89**	43.73	49.29	45.31	**45.28**	54.04

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Conclusion

The **credal ensembling** framework for multi-class classification

- is simple and easy to use (in a few complex applications),
- is a direct generalization of the voting ensemble framework,
- might help to enlarge the set of credal classifiers,
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It might **facilitate applications of IP decision rules**

- in a few complex application domains,
- which can be directly compared with probabilistic frameworks.

References I

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[4] K.-D. Tran, X.-T. Hoang, D.-M. Nguyen, V.-L. Nguyen, S. Destercke, and V.-N. Huynh.
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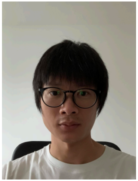
Thanks to the fruitful collaborations with



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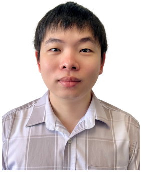

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