# Cautious learning: Three-way out approach 

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Uncertainty in Computer Science

## Cautious learning

- Not enough evidence to take a decision
- a generalization of supervised learning in which the Machine Learning (ML) models are allowed to express set-valued predictions



## Three-way strategy

Define algorithms that can abstain

- a general method based on cost of abstention vs cost of error
- ad hoc methods: TW-decision tree, TW-random forest based on orthopartition

Result: three-way algorithms offer a trade-off among accuracy and coverage (the points that are classified)

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- Labels $\mathrm{L}=\{1,2,3,4,5\}$
- Probabilities for object $x$ classification:

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A(x)=\langle 0.2,0.3,0.15,0.1,0.25\rangle
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- Since $A(x)_{2}=0.3$ is the biggest, then the label of $x$ is 2 . However, 0.2 and 0.25 can be considered close to 0.3
- The classification of $x$ is ambiguous: $\{1,2,5\}$


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STRATEGY 2: balance the cost of errors and abstention

1. set a cost of error and abstention
2. define the risk of a decision (using probabilities $A(x)$ )
3. the decision is the less risky set of labels

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Some more details:

- $\epsilon$ cost of prediction error

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- $\alpha: \mathcal{P}(X) \mapsto \mathfrak{R}$ cost of partial abstention
$\alpha(Z)$ the cost of abstaining among the alternatives in Z
- The risk of decision $Z$

$$
R(Z)=\alpha(Z) \cdot \sum_{y_{i} \in Z} A(x)_{i}+\epsilon \sum_{y_{j} \notin Z} A(x)_{j}
$$

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- Compute the risk for all sets containing label ' 2 '
- $R(\{1,2\})=\frac{1}{4}(0.2+0.3)+1(0.15+0.1+0.25)=0.625$


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- $R(\{2\})=0 \cdot 0.3+1 \cdot 0.7$
- The less risky is $Z=\{2,5\}$


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More details on Decision Trees

## Decision Tree

| Temperature | Outlook | Humidity | Windy | Do Sport? |
| :---: | :---: | :---: | :---: | :---: |
| hot | sunny | high | false | no |
| hot | sunny | high | true | no |
| hot | sunny | high | false | yes |
| cool | rain | normal | false | yes |
| cool | overcast | normal | true | yes |
| mild | sunny | high | false | no |
| cool | sunny | normal | false | yes |
| mild | rain | normal | false | yes |
| mild | sunny | normal | true | yes |
| mild | overcast | high | true | yes |
| hot | overcast | normal | false | yes |
| mild | rain | high | true | no |
| cool | rain | normal | true | no |
| mild | rain | normal | false | yes |

## Decision Tree (ID3)



## The idea

A classification can be

```
YES/NO/UNDECIDED
```

Two steps

1. Define an orthopartition from each attribute
2. Select as split attribute the one with greatest mutual information wrt the decision

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When to abstain from a decision? When it is less costly!

- Two parameters $\alpha<\epsilon$ to weight errors
- $\alpha$ the cost of an abstention
- $\epsilon$ : the cost of a classification error
- Compute total error for each attribute $a$ and each value $i$
- If total classification error $\geq$ total abstention error $\rightarrow$ better to abstain


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- The elements in $D_{i}^{a}$ are in majority classified as yes or no?

We associate to $D_{i}^{a}$ the classification
$C_{i}^{a}=\operatorname{argmax}_{j \in\{y e s, n o\}}\left\{\left|\left\{x \in D_{i}^{a} \mid C(x)=j\right\}\right|\right\}$

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- and compute the error/abstention costs
- Expected classification error cost

$$
E\left(D_{i}^{a} \mid C_{i}^{a}\right)=\epsilon * \min _{j \in\{y e s, n o\}}\left\{\left|\left\{x \in D_{i}^{a} \mid C(x)=j\right\}\right|\right\}
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- Expected abstention error cost

$$
E\left(D_{i}^{a} \mid \perp\right)=\alpha\left|D_{i}^{a}\right|
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- If $E\left(D_{i}^{a} \mid C_{i}^{a}\right)<E\left(D_{i}^{a} \mid \perp\right)$ we assign to the objects in $D_{i}^{a}$ the decision $C_{i}^{a}$ otherwise, the decision is $\perp$


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- If $E\left(D_{i}^{a} \mid C_{i}^{a}\right)<E\left(D_{i}^{a} \mid \perp\right)$ we assign to the objects in $D_{i}^{a}$ the decision $C_{i}^{a}$ otherwise, the decision is $\perp$
- Union over all values $i \rightarrow$ define an orthopair $O_{a}=\left(P_{a}, N_{a}\right)$

$$
P_{a}=\bigcup\left\{D_{i}^{a} \mid C_{i}^{a}=y e s\right\} \text { and } N_{a}=\bigcup\left\{D_{i}^{a} \mid C_{i}^{a}=n o\right\}
$$

- Define the orthopartition $\mathcal{O}_{a}=\left\{O_{a}, \neg O_{a}\right\}$


## The algorithm

Input: Dataset $D$, error $\operatorname{cost} \epsilon$, abstention cost $\alpha$
Output: Three-way Decision Tree built on $D$
1 Feature $a \rightarrow$ orthopartition $\mathcal{O}_{a}$ using $\epsilon, \alpha$;
2 Orthopartition $\mathcal{O}_{a} \rightarrow$ mutual information $m\left(D, \mathcal{O}_{a}\right)$;
3 split attribute $=$ the feature $a_{\text {max }}$ which gives the greatest mutual information value;
4 Recur on the subsets of $D$ determined by $a_{\max }$;

## Example



## Some comments

- Not discussed here
- Extension of the method to more than two-valued (yes/no) decisions


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- Extension of the method to more than two-valued (yes/no) decisions
- In case of indecision the algorithm returns a subset of decisions: the correct one is always included in this subset
- problem: accuracy depends on arbitrary error weights $\epsilon$ and $\alpha$


## TWO experiments

- Compared KNN,Logistic Regression, Random Forest, Naive Bayes, SVM and their 3-way variants


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- 6 UCl datasets +1 real-world medical dataset

| Dataset | \# instances | \# attributes | \# classes |
| :---: | :---: | :---: | :---: |
| Iris | 150 | 4 | 3 |
| Wine | 178 | 13 | 3 |
| Digits | 1797 | 64 | 10 |
| Breast cancer | 569 | 30 | 2 |
| Olivetti faces | 400 | 4096 | 40 |
| Yeast | 1484 | 8 | 10 |
| SF12 | 462 | 10 | 2 |

## TWO experiments

The three-way versions (Strategies $1 / 2$ ) are better than the standard version
Yeast dataset


## TWO experiments

The best algorithms are the ones derived from random forest

| Alg. | TWRF | DIFID-TWRF | $\epsilon$-TWRF | $L_{\epsilon}$-TWLC | TWLR | TWSVM | TWKNN | RF | KNN $/ \epsilon$-TWLR/ $\epsilon$-TWSVM |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Rank | 2.14 | 2.28 | 2.71 | 3.71 | 4.00 | 4.14 | 4.42 | 4.86 | 5.86 |

Table: Average ranks of the top 10 performing algorithms.

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Table: Average ranks of the top 10 performing algorithms.

- No significant differences among strategy 1, strategy 2 and ad-hoc algorithms
- Strategy 1: comparable performance but with less parameters to set and increased computational efficiency


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- The capability of directly using and conveniently communicating the ambiguity encountered by the algorithm in recommending a class could be critical to deliver reliable Machine Learning-based Decision Support Systems


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- The capability of directly using and conveniently communicating the ambiguity encountered by the algorithm in recommending a class could be critical to deliver reliable Machine Learning-based Decision Support Systems
- Abstention in ML output is a way to trade (decision) accuracy with efficiency: unresolved advice implies that decision-makers have to look for and consider more evidence, even beyond the available data

