## Information-based Learning Sections 4.4, 4.5

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- **Handling Continuous Descriptive Features**
- Predicting Continuous Targets
- **Noisy Data, Overfitting and Tree Pruning**
- **Model Ensembles** 
  - Bagging
  - Boosting
  - Gradient Boosting
- **Summary**

# Alternative Feature Selection Metrics

 One way of addressing this issue is to use information gain ratio which is computed by dividing the information gain of a feature by the amount of information used to determine the value of the feature:

$$GR(d, \mathcal{D}) = \frac{IG(d, \mathcal{D})}{-\sum_{l \in levels(d)} (P(d = l) \times log_2(P(d = l)))}$$
(1)

$$\begin{split} &H(\mathsf{STREAM}, \mathcal{D}) \\ &= -\sum_{I \in \left\{ true, 1 \atop false \right\}} P(\mathsf{STREAM} = I) \times log_2\left(P(\mathsf{STREAM} = I)\right) \\ &= -\left(\binom{4}{7} \times log_2\binom{4}{7}\right) + \binom{3}{7} \times log_2\binom{3}{7}\right) \right) \\ &= -\left(\binom{4}{7} \times log_2\binom{4}{7}\right) + \binom{3}{7} \times log_2\binom{3}{7}\right) \right) \\ &= -\sum_{I \in \left\{ \substack{flat, \\ noderale, \\ steep} \right\}} P(\mathsf{SLOPE} = I) \times log_2\left(P(\mathsf{SLOPE} = I)\right) \\ &= -\left(\binom{1}{7} \times log_2\binom{1}{7}\right) + \binom{1}{7} \times log_2\binom{1}{7}\right) + \binom{5}{7} \times log_2\binom{5}{7}\right) \right) \\ &= 1.1488 \ bits \\ &H(\mathsf{ELEVATION}, \mathcal{D}) \\ &= -\sum_{I \in \left\{ \substack{low, \\ medium, \\ high, \\ highest} \right\}} P(\mathsf{ELEVATION} = I) \times log_2\left(P(\mathsf{ELEVATION} = I)\right) \\ &= -\left(\binom{1}{7} \times log_2\binom{1}{7}\right) + \binom{2}{7} \times log_2\binom{2}{7}\right) + \binom{3}{7} \times log_2\binom{3}{7}\right) + \binom{1}{7} \times log_2\binom{1}{7}\right) \right) \\ &= 1.8424 \ bits \end{split}$$

Ensembles

Summary

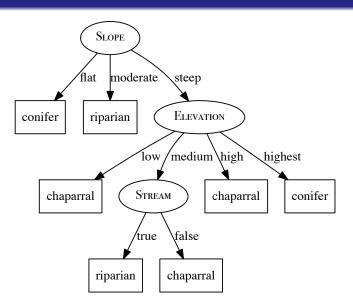


Figure 1: The vegetation classification decision tree generated using information gain ratio

 Another commonly used measure of impurity is the Gini index:

$$Gini(t, \mathcal{D}) = 1 - \sum_{l \in levels(t)} P(t = l)^2$$
 (2)

- The Gini index can be thought of as calculating how often you would misclassify an instance in the dataset if you classified it based on the distribution of classifications in the dataset.
- Information gain can be calculated using the Gini index by replacing the entropy measure with the Gini index.

### Gini (VEGETATION, $\mathcal{D}$ ) $= 1 - \sum P(VEGETATION = I)^2$ *l*∈ { chapparal, riparian, conifer } $= 1 - \left( \left( 3/_7 \right)^2 + \left( ^2/_7 \right)^2 + \left( ^2/_7 \right)^2 \right)$ = 0.6531

Split by				Partition		Info.
Feature	Level	Part.	Instances	Gini Index	Rem.	Gain
STREAM	true	$\mathcal{D}_1$	$\mathbf{d}_2, \mathbf{d}_3, \mathbf{d}_6, \mathbf{d}_7$	0.625	0.5476	0.1054
STREAM	false	$\mathcal{D}_{2}$	$\mathbf{d_1},\mathbf{d_4},\mathbf{d_5}$	0.4444	0.5476	0.1054
	flat	$\mathcal{D}_3$	<b>d</b> <sub>5</sub>	0		
SLOPE	moderate	$\mathcal{D}_4$	$\mathbf{d}_2$	0	0.4	0.2531
	steep	$\mathcal{D}_5$	$\boldsymbol{d}_1,\boldsymbol{d}_3,\boldsymbol{d}_4,\boldsymbol{d}_6,\boldsymbol{d}_7$	0.56		
	low	$\mathcal{D}_6$	$d_2$	0		
ELEVATION	medium	$\mathcal{D}_7$	$\mathbf{d_3},\mathbf{d_4}$	0.5	0.3333	0.3198
	high	$\mathcal{D}_8$	$\mathbf{d_1},\mathbf{d_5},\mathbf{d_7}$	0.4444	0.3333	0.3190
	highest	$\mathcal{D}_9$	<b>d</b> <sub>6</sub>	0		

Ensembles

- The easiest way to handle continuous valued descriptive features is to turn them into boolean features by defining a threshold and using this threshold to partition the instances based their value of the continuous descriptive feature.
- How do we set the threshold?

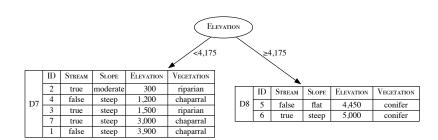
- The instances in the dataset are sorted according to the continuous feature values
- The adjacent instances in the ordering that have different classifications are then selected as possible threshold points.
- The optimal threshold is found by computing the information gain for each of these classification transition boundaries and selecting the boundary with the highest information gain as the threshold.

 This process can be repeated at each node as the tree grows.

ID	STREAM	SLOPE	ELEVATION	VEGETATION
1	false	steep	3 900	chapparal
2	true	moderate	300	riparian
3	true	steep	1 500	riparian
4	false	steep	1 200	chapparal
5	false	flat	4 450	conifer
6	true	steep	5 000	conifer
_ 7	true	steep	3 000	chapparal

ID	STREAM	SLOPE	ELEVATION	VEGETATION
2	true	moderate	300	riparian
4	false	steep	1 200	chapparal
3	true	steep	1 500	riparian
7	true	steep	3 000	chapparal
1	false	steep	3 900	chapparal
5	false	flat	4 450	conifer
6	true	steep	5 000	conifer

Split by			Partition		Info.
Threshold	Part.	Instances	Entropy	Rem.	Gain
>750	$\mathcal{D}_1$	<b>d</b> <sub>2</sub>	0.0	1.2507	0.3060
≥130	$\mathcal{D}_2$	$\bm{d}_4, \bm{d}_3, \bm{d}_7, \bm{d}_1, \bm{d}_5, \bm{d}_6$	1.4591	1.2307	0.3000
>1 350	$\mathcal{D}_3$	$\mathbf{d}_2,\mathbf{d}_4$	1.0	1.3728	0.1839
<u> </u>	$\mathcal{D}_4$	$\bm{d}_3, \bm{d}_7, \bm{d}_1, \bm{d}_5, \bm{d}_6$	1.5219	1.0720	0.1000
>2 250	$\mathcal{D}_5$	$\mathbf{d}_2,\mathbf{d}_4,\mathbf{d}_3$	0.9183	0.9650	0.5917
<u> </u>	$\mathcal{D}_{6}$	${f d}_7, {f d}_1, {f d}_5, {f d}_6$	1.0	0.3030	0.5517
>4 175	$\mathcal{D}_7$	$\boldsymbol{d}_2,\boldsymbol{d}_4,\boldsymbol{d}_3,\boldsymbol{d}_7,\boldsymbol{d}_1$	0.9710	0.6935	0.8631
≥ <del>+</del> 175	$\mathcal{D}_8$	$\mathbf{d}_5,\mathbf{d}_6$	0.0	0.0000	0.0001



**Figure 2:** The vegetation classification decision tree after the dataset has been split using ELEVATION  $\geq$  4 175.

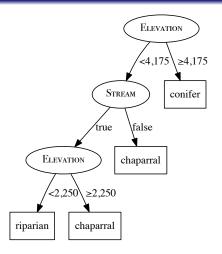


Figure 3: The decision tree that would be generated for the vegetation classification dataset listed in Table 3<sup>[17]</sup> using information gain.

### **Predicting Continuous Targets**

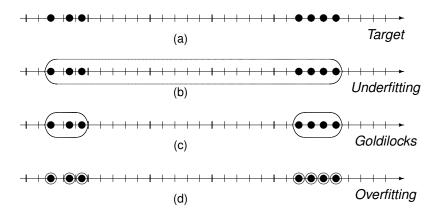
 We can do this by adapting the ID3 algorithm to use a measure of variance rather than a measure of classification impurity (entropy) when selecting the best attribute

Ensembles

$$var(t, \mathcal{D}) = \frac{\sum_{i=1}^{n} (t_i - \overline{t})^2}{n-1}$$
 (3)

 We select the feature to split on at a node by selecting the feature that minimizes the weighted variance across the resulting partitions:

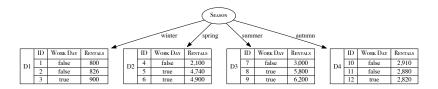
$$\mathbf{d}[best] = \arg\min_{d \in \mathbf{d}} \sum_{l \in levels(d)} \frac{|\mathcal{D}_{d=l}|}{|\mathcal{D}|} \times var(t, \mathcal{D}_{d=l})$$
 (4)



**Figure 4:** (a) A set of instances on a continuous number line; (b), (c), and (d) depict some of the potential groupings that could be applied to these instances.

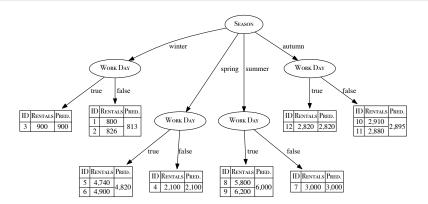
ID	SEASON	Work Day	RENTALS	ID	SEASON	Work Day	RENTALS
1	winter	false	800	7	summer	false	3 000
2	winter	false	826	8	summer	true	5800
3	winter	true	900	9	summer	true	6 200
4	spring	false	2100	10	autumn	false	2910
5	spring	true	4740	11	autumn	false	2880
6	spring	true	4900	12	autumn	true	2820

Split by				$ \mathcal{D}_{d=I} $		Weighted
Feature	Level	Part.	Instances	$\overline{ \mathcal{D} }$	var(t, D)	Variance
	winter	$\mathcal{D}_1$	$d_1, d_2, d_3$	0.25	2 692	
SEASON	spring	$\mathcal{D}_2$	$d_4, d_5, d_6$	0.25	$2472533\frac{1}{3}$	1 379 331 1
SEASON	summer	$\mathcal{D}_3$	$d_7, d_8, d_9$	0.25	3 040 000	13/93313
	autumn	$\mathcal{D}_4$	$\mathbf{d}_{10}, \mathbf{d}_{11}, \mathbf{d}_{12}$	0.25	2100	
WORK DAY	true	$\mathcal{D}_5$	$d_3, d_5, d_6, d_8, d_9, d_{12}$	0.50	$4026346\frac{1}{3}$	2551813 <sup>1</sup> / <sub>2</sub>
WORK DAY	false	$\mathcal{D}_6$	$\bm{d}_1, \bm{d}_2, \bm{d}_4, \bm{d}_7, \bm{d}_{10}, \bm{d}_{11}$	0.50	1 077 280	25516153



**Figure 5:** The decision tree resulting from splitting the data in Table  $5^{[25]}$  using the feature SEASON.

Summary



**Figure 6:** The final decision tree induced from the dataset in Table 5<sup>[25]</sup>. To illustrate how the tree generates predictions, this tree lists the instances that ended up at each leaf node and the prediction (PRED.) made by each leaf node.

The likelihood of over-fitting occurring increases as a tree gets deeper because the resulting classifications are based on smaller and smaller subsets as the dataset is partitioned after each feature test in the path.

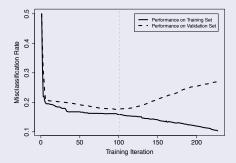
Pre-pruning: stop the recursive partitioning early.
 Pre-pruning is also known as forward pruning.

### **Common Pre-pruning Approaches**

- early stopping
- 2  $\chi^2$  pruning
  - Post-pruning: allow the algorithm to grow the tree as much as it likes and then prune the tree of the branches that cause over-fitting.

#### **Common Post-pruning Approach**

 Using the validation set evaluate the prediction accuracy achieved by both the fully grown tree and the pruned copy of the tree. If the pruned copy of the tree performs no worse than the fully grown tree the node is a candidate for pruning.



	Core-	STABLE-		
ID	ТЕМР	ТЕМР	GENDER	DECISION
1	high	true	male	gen
2	low	true	female	icu
3	high	false	female	icu
4	high	false	male	icu
5	low	false	female	icu
6	low	true	male	icu

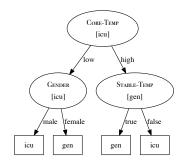
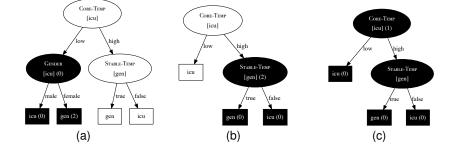


Figure 7: The decision tree for the post-operative patient routing task.



**Figure 8:** The iterations of reduced error pruning for the decision tree in Figure 7<sup>[34]</sup> using the validation set in Table 7<sup>[33]</sup>. The subtree that is being considered for pruning in each iteration is highlighted in black. The prediction returned by each non-leaf node is listed in square brackets. The error rate for each node is given in round brackets.

#### Advantages of pruning:

- Smaller trees are easier to interpret
- Increased generalization accuracy when there is noise in the training data (noise dampening).

## **Model Ensembles**

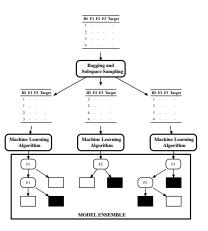
Summary

- Rather than creating a single model they generate a set of models and then make predictions by aggregating the outputs of these models.
- A prediction model that is composed of a set of models is called a model ensemble.
- In order for this approach to work the models that are in the ensemble must be different from each other.

- bagging.
- boosting

- When we use bagging (or bootstrap aggregating) each model in the ensemble is trained on a random sample of the dataset known as **bootstrap samples**.
- Each random sample is the same size as the dataset and sampling with replacement is used.
- Consequently, every bootstrap sample will be missing some of the instances from the dataset so each bootstrap sample will be different and this means that models trained on different bootstrap samples will also be different

- When bagging is used with decision trees each bootstrap sample only uses a randomly selected subset of the descriptive features in the dataset. This is known as subspace sampling.
- The combination of bagging, subspace sampling, and decision trees is known as a random forest model.



**Figure 9:** The process of creating a model ensemble using bagging and subspace sampling.

- Boosting works by iteratively creating models and adding them to the ensemble.
- The iteration stops when a predefined number of models have been added.
- When we use boosting each new model added to the ensemble is biased to pay more attention to instances that previous models miss-classified.
- This is done by incrementally adapting the dataset used to train the models. To do this we use a weighted dataset

## Weighted Dataset

- Each instance has an associated weight  $\mathbf{w}_i \geq 0$ ,
- Initially set to  $\frac{1}{n}$  where n is the number of instances in the dataset.
- After each model is added to the ensemble it is tested on the training data and the weights of the instances the model gets correct are decreased and the weights of the instances the model gets incorrect are increased.
- These weights are used as a distribution over which the dataset is sampled to created a replicated training set, where the replication of an instance is proportional to its weight.

Feature Selection

## During each training iteration the algorithm:

- f 0 Induces a model and calculates the total error,  $\epsilon$ , by summing the weights of the training instances for which the predictions made by the model are incorrect.
- Increases the weights for the instances misclassified using:

$$\mathbf{w}[i] \leftarrow \mathbf{w}[i] \times \left(\frac{1}{2 \times \epsilon}\right) \tag{5}$$

Decreases the weights for the instances correctly classified:

$$\mathbf{w}[i] \leftarrow \mathbf{w}[i] \times \left(\frac{1}{2 \times (1 - \epsilon)}\right) \tag{6}$$

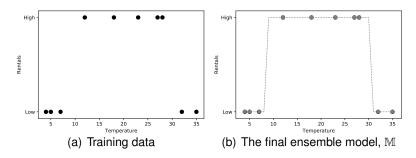
**Q** Calculate a **confidence factor**,  $\alpha$ , for the model such that  $\alpha$  increases as  $\epsilon$  decreases:

$$\alpha = \frac{1}{2} \times \log_{\theta} \left( \frac{1 - \epsilon}{\epsilon} \right) \tag{7}$$

- Once the set of models have been created the ensemble makes predictions using a weighted aggregate of the predictions made by the individual models.
- The weights used in this aggregation are simply the confidence factors associated with each model.

**Table 8:** A simple bicycle demand predictions dataset and the workings of the first three iterations of training an ensemble model using boosting to predict RENTALS given TEMP.

			lt	eration	0	lt	eration	1	Iteration 2		
ID	ТЕМР	RENTALS	Dist.	Freq.	$\mathbb{M}_0(d)$	Dist.	Freq.	$\mathbb{M}_1(\mathbf{d})$	Dist.	Freq.	$\mathbb{M}_2(\mathbf{d})$
1	4	Low	0.100	2	Low	0.062	0	High	0.167	2	Low
2	5	Low	0.100	1	Low	0.062	1	High	0.167	1	Low
3	7	Low	0.100	0	Low	0.062	1	High	0.167	3	Low
4	12	High	0.100	1	High	0.062	2	High	0.038	0	Low
5	18	High	0.100	1	High	0.062	0	High	0.038	0	Low
6	23	High	0.100	1	High	0.062	0	High	0.038	0	Low
7	27	High	0.100	1	High	0.062	1	High	0.038	0	Low
8	28	High	0.100	1	High	0.062	1	High	0.038	1	Low
9	32	Low	0.100	2	High	0.250	3	Low	0.154	1	Low
10	35	Low	0.100	0	High	0.250	1	Low	0.154	2	Low



**Figure 10:** (a) A plot of the bike rental dataset from Table 8<sup>[47]</sup>. (b) An illustration of the final ensemble model trained using the boosting algorithm. (c)–(e) A representation of the changing weights used to generate sample datasets for the first iterations of the boosting process.

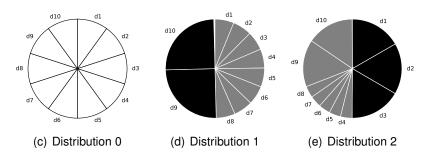


Figure 11: (a) A plot of the bike rental dataset from Table 8<sup>[47]</sup>. (b) An illustration of the final ensemble model trained using the boosting algorithm. (c)-(e) A representation of the changing weights used to generate sample datasets for the first iterations of the boosting process.

**w**[1] ← 0.100 × 
$$\left(\frac{1}{2 \times (1 - 0.200)}\right)$$
 ← 0.0625

$$\mathbf{w}\left[9\right] \leftarrow 0.100 \times \left(\frac{1}{2 \times 0.200}\right) \leftarrow 0.250$$

$$\mathbb{M}_0(\mathbf{d}) = \frac{1}{n} \sum_i t_i \tag{8}$$

$$\mathbb{M}_{1}(\mathbf{d}) = \mathbb{M}_{0}(\mathbf{d}) + \mathbb{M}_{\Delta 1}(\mathbf{d}) \tag{9}$$

$$\mathbb{M}_{i}(\mathbf{d}) = \mathbb{M}_{i-1}(\mathbf{d}) + \mathbb{M}_{\Delta i}(\mathbf{d}) \tag{10}$$

Ensembles

$$\begin{split} \mathbb{M}_{4}(\mathbf{d}) &= \mathbb{M}_{3}(\mathbf{d}) + \mathbb{M}_{\Delta 4}(\mathbf{d}) \\ &= (\mathbb{M}_{2}(\mathbf{d}) + \mathbb{M}_{\Delta 3}(\mathbf{d})) + \mathbb{M}_{\Delta 4}(\mathbf{d}) \\ &= ((\mathbb{M}_{1} + \mathbb{M}_{\Delta 2}(\mathbf{d})) + \mathbb{M}_{\Delta 3}(\mathbf{d})) + \mathbb{M}_{\Delta 4}(\mathbf{d}) \\ &= (((\mathbb{M}_{0}(\mathbf{d}) + \mathbb{M}_{\Delta 1}(\mathbf{d})) + \mathbb{M}_{\Delta 2}(\mathbf{d})) + \mathbb{M}_{\Delta 3}(\mathbf{d})) + \mathbb{M}_{\Delta 4}(\mathbf{d}) \\ &= \mathbb{M}_{0}(\mathbf{d}) + \mathbb{M}_{\Delta 1}(\mathbf{d}) + \mathbb{M}_{\Delta 2}(\mathbf{d}) + \mathbb{M}_{\Delta 3}(\mathbf{d}) + \mathbb{M}_{\Delta 4}(\mathbf{d}) \end{split}$$

$$(11)$$

**Table 9:** A simple bicycle demand predictions dataset and the workings of the first iterations of training a gradient boosting model.

ĪD	ТЕМР	RENTALS	$\mathbb{M}_0(\mathbf{d})$	$t-\mathbb{M}_0(\mathbf{d})$	$\mathbb{M}_{\Delta 1}(\mathbf{d})$	$\mathbb{M}_1(\mathbf{d})$	$t-\mathbb{M}_1(\mathbf{d})$	$\mathbb{M}_{\Delta 2}(\mathbf{d})$	$\mathbb{M}_2(\mathbf{d})$	$t - M_2(\mathbf{d})$	$\mathbb{M}_{\Delta 3}(\mathbf{d})$	$\mathbb{M}_3(\mathbf{d})$
1	4	602	1 287.1	-685.1	-460.9	826.2	-224.2	-167.2	659.0	-57.0	-34.1	624.9
2	5	750	1 287.1	-537.1	-460.9	826.2	-76.2	-167.2	659.0	91.0	-34.1	624.9
3	7	913	1 287.1	-374.1	-460.9	826.2	86.8	71.6	897.8	15.2	-34.1	863.7
4	12	1229	1 287.1	-58.1	-460.9	826.2	402.8	71.6	897.8	331.2	-34.1	863.7
5	18	1827	1 287.1	539.9	691.4	1 978.5	-151.5	71.6	2050.1	-223.1	-34.1	2016.1
6	23	2246	1 287.1	958.9	691.4	1 978.5	267.5	71.6	2050.1	195.9	136.4	2186.5
7	27	2127	1 287.1	839.9	691.4	1 978.5	148.5	71.6	2050.1	76.9	136.4	2186.5
8	28	1714	1 287.1	426.9	691.4	1 978.5	-264.5	71.6	2050.1	-336.1	-34.1	2016.1
9	32	838	1 287.1	-449.1	-460.9	826.2	11.8	71.6	897.8	-59.8	-34.1	863.7
10	35	625	1 287.1	-662.1	-460.9	826.2	-201.2	-167.2	659.0	-34.0	-34.1	624.9

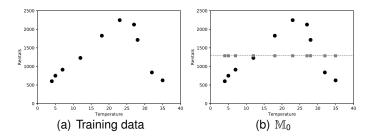
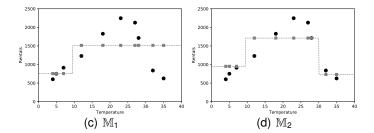
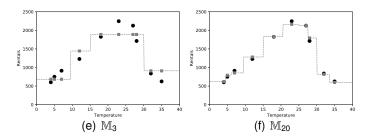


Figure 12: (a) A plot of the bike rental dataset from Table 9<sup>[53]</sup>. (b)–(e) Visualizations of the prediction models trained in the early iterations of the gradient boosting process. (f) The final ensemble model trained after 20 iterations of gradient boosting.



**Figure 13:** (a) A plot of the bike rental dataset from Table 9<sup>[53]</sup>. (b)–(e) Visualizations of the prediction models trained in the early iterations of the gradient boosting process. (f) The final ensemble model trained after 20 iterations of gradient boosting.



**Figure 14:** (a) A plot of the bike rental dataset from Table 9<sup>[53]</sup>. (b)–(e) Visualizations of the prediction models trained in the early iterations of the gradient boosting process. (f) The final ensemble model trained after 20 iterations of gradient boosting.

Gradient Boosting

$$\mathbb{M}_{i}(\mathbf{d}) = \mathbb{M}_{i-1}(\mathbf{d}) + \alpha \times \mathbb{M}_{\Delta i}(\mathbf{d})$$
 (12)

- Which approach should we use? Bagging is simpler to implement and parallelize than boosting and, so, may be better with respect to ease of use and training time.
- Empirical results indicate:
  - boosted decision tree ensembles were the best performing model of those tested for datasets containing up to 4,000 descriptive features.
  - random forest ensembles (based on bagging) performed better for datasets containing more that 4,000 features.

Ensembles

 The ID3 algorithm as a standard algorithm for inducing decision trees from a dataset.

Ensembles

- interpretable.
- handle both categorical and continuous descriptive features.
- has the ability to model the interactions between descriptive features (diminished if pre-pruning is employed)
- relatively, robust to the curse of dimensionality.
- relatively, robust to noise in the dataset if pruning is used.

- trees become large when dealing with continuous features.
- decision trees are very expressive and sensitive to the dataset, as a result they can overfit the data if there are a lot of features (curse of dimensionality)
- eager learner (concept drift).

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