

Feature Selection

Feature Selection

1. Overview
2. Perspectives
3. Aspects
4. Most Representative Methods
5. Related and Advanced Topics
6. Experimental Comparative Analyses

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Overview

- Why we need FS:
 1. to improve performance (in terms of speed, predictive power, simplicity of the model).
 2. to visualize the data for model selection.
 3. To reduce dimensionality and remove noise.
- *Feature Selection* is a process that chooses an optimal subset of features according to a certain criterion.

Overview

- Reasons for performing FS may include:
 - removing irrelevant data.
 - increasing predictive accuracy of learned models.
 - reducing the cost of the data.
 - improving learning efficiency, such as reducing storage requirements and computational cost.
 - reducing the complexity of the resulting model description, improving the understanding of the data and the model.

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Perspectives

1. searching for the best subset of features.
2. criteria for evaluating different subsets.
3. principle for selecting, adding, removing or changing new features during the search.

Perspectives:

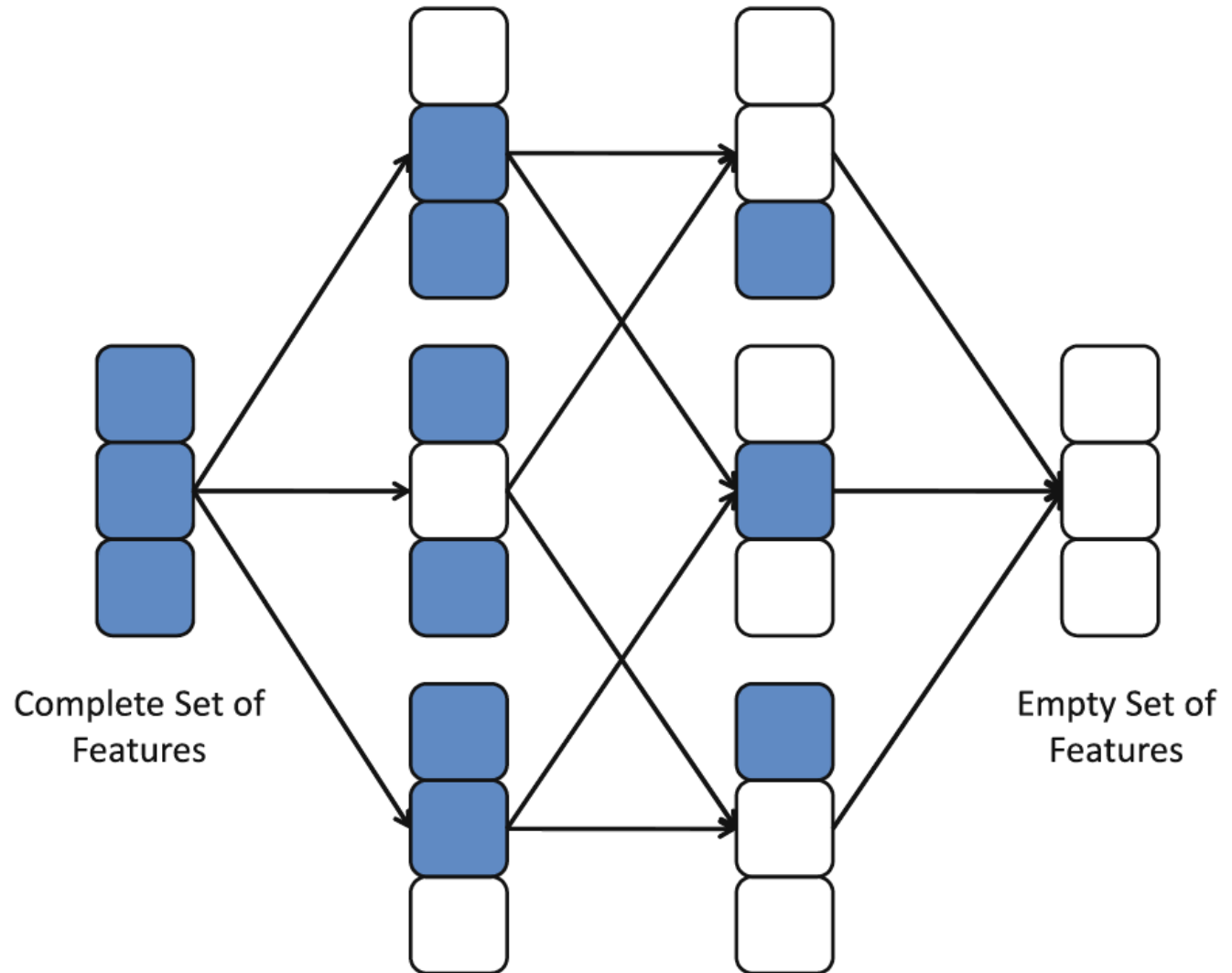
Search of a Subset of Features

- FS can be considered as a search problem, where each state of the search space corresponds to a concrete subset of features selected.
- There should be a total of 2^M subsets where M is the number of features of a data set.

Perspectives:

Search of a Subset of Features

Search
Space:



Perspectives:

Search of a Subset of Features

- Search Directions:
 - **Sequential Forward Generation (SFG):** It starts with an empty set of features S . As the search starts, features are added into S according to some criterion that distinguish the best feature from the others. S grows until it reaches a full set of original features. The stopping criteria can be a threshold for the number of relevant features m or simply the generation of all possible subsets in brute force mode.
 - **Sequential Backward Generation (SBG):** It starts with a full set of features and, iteratively, they are removed one at a time. Here, the criterion must point out the worst or least important feature. By the end, the subset is only composed of a unique feature, which is considered to be the most informative of the whole set. As in the previous case, different stopping criteria can be used.

Perspectives:

Search of a Subset of Features

- Search Directions:

Algorithm 1 Sequential forward feature set generation - SFG.

function SFG(F - full set, U - measure)

initialize: $S = \{\}$

$\triangleright S$ stores the selected features

repeat

$f = \text{FINDNEXT}(F)$

$S = S \cup \{f\}$

$F = F - \{f\}$

until S satisfies U or $F = \{\}$

return S

end function

Perspectives:

Search of a Subset of Features

- Search Directions:

Algorithm 2 Sequential backward feature set generation - SBG.

function SBG(F - full set, U - measure)

initialize: $S = \{\}$

 ▷ S holds the removed features

repeat

$f = \text{GETNEXT}(F)$

$F = F - \{f\}$

$S = S \cup \{f\}$

until S does not satisfy U or $F = \{\}$

return $F \cup \{f\}$

end function

Perspectives:

Search of a Subset of Features

- Search Directions:
 - **Bidirectional Generation (BG):** The search begins in both directions, and SFG and SBG are performed concurrently. They stop in two cases: (1) when one search finds the best subset comprised of m features before it reaches the exact middle, or (2) both searches achieve the middle of the search space. It takes advantage of both SFG and SBG.
 - **Random Generation (RG):** It starts the search in a random direction. The choice of adding or removing features is a random decision. RG tries to avoid stagnation in a local optima by not following a fixed method for subset generation. Unlike SFG or SBG, the size of the subset of features cannot be stipulated.

Perspectives:

Search of a Subset of Features

- Search Directions:

Algorithm 3 Bidirectional feature set generation - BG.

function BG(F_f , F_b - full set, U - measure)

initialize: $S_f = \{\}$

 ▷ S_f holds the selected features

initialize: $S_b = \{\}$

 ▷ S_b holds the removed features

repeat

$f_f = \text{FINDNEXT}(F_f)$

$f_b = \text{GETNEXT}(F_b)$

$S_f = S_f \cup \{f_f\}$

$F_b = F_b - \{f_b\}$

$F_f = F_f - \{f_f\}$

$S_b = S_b \cup \{f_b\}$

until (a) S_f satisfies U or $F_f = \{\}$ or (b) S_b does not satisfy U or $F_b = \{\}$

return S_f if (a) or $F_b \cup \{f_b\}$ if (b)

end function

Perspectives:

Search of a Subset of Features

- Search Directions:

Algorithm 4 Random feature set generation - RG.

function RG(F - full set, U - measure)

initialize: $S = S_{best} = \{\}$

▷ S - subset set

initialize: $C_{best} = \#(F)$

▷ $\#$ - cardinality of a set

repeat

$S = \text{RANDGEN}(F)$

$C = \#(S)$

if $C \leq C_{best}$ *and* S satisfies U **then**

$S_{best} = S$

$C_{best} = C$

end if

until some stopping criterion is satisfied

return S_{best}

▷ Best set found so far

end function

Perspectives:

Search of a Subset of Features

- **Search Strategies:**
 - **Exhaustive Search:** It corresponds to explore all possible subsets to find the optimal ones. As we said before, the space complexity is $O(2^M)$. If we establish a threshold m of minimum features to be selected and the direction of search, the search space is, independent of the forward or backward generation. Only exhaustive search can guarantee the optimality. Nevertheless, they are also impractical in real data sets with a high M .
 - **Heuristic Search:** It employs heuristics to carry out the search. Thus, it prevents brute force search, but it will surely find a non-optimal subset of features. It draws a path connecting the beginning and the end of the previous Figure, such in a way of a depth-first search. The maximum length of this path is M and the number of subsets generated is $O(M)$. The choice of the heuristic is crucial to find a closer optimal subset of features in a faster operation.

Perspectives:

Search of a Subset of Features

- Search Strategies:
 - **Nondeterministic Search:** Complementary combination of the previous two. It is also known as random search strategy and can generate best subsets constantly and keep improving the quality of selected features as time goes by. In each step, the next subset is obtained at random.
 - it is unnecessary to wait until the search ends.
 - we do not know when the optimal set is obtained, although we know which one is better than the previous one and which one is the best at the moment.

Perspectives: Selection Criteria

– Distance Measures.

- Measures of separability, discrimination, or divergence are used. The most typical is derived from the distance between the class conditional density functions.

	Mathematical form
Euclidean distance	$D_e = \left\{ \sum_{i=1}^m (x_i - y_i)^2 \right\}^{\frac{1}{2}}$
City-block distance	$D_{cb} = \sum_{i=1}^m x_i - y_i $
Cebyshev distance	$D_{ch} = \max_i x_i - y_i $
Minkowski distance of order m	$D_M = \left\{ \sum_{i=1}^m (x_i - y_i)^m \right\}^{\frac{1}{m}}$
Quadratic distance Q , positive definite	$D_q = \sum_{i=1}^m \sum_{j=1}^m (x_i - y_i) Q_{ij} (x_j - y_j)$
Canberra distance	$D_{ca} = \sum_{i=1}^m \frac{ x_i - y_i }{x_i + y_i}$
Angular separation	$D_{as} = \frac{\sum_{i=1}^m x_i \cdot y_i}{\left[\sum_{i=1}^m x_i^2 \sum_{i=1}^m y_i^2 \right]^{\frac{1}{2}}}$

Perspectives: Selection Criteria

– Dependence Measures.

- Known as measures of association or correlation.
- Its main goal is to quantify how strongly two variables are correlated or present some association with each other so that we can derive the value for the other by knowing the value of one of them.
- *Pearson correlation coefficient*:

$$\rho(X, Y) = \frac{\sum_i (x_i - \bar{x})(y_i - \bar{y})}{\left[\sum_i (x_i - \bar{x})^2 \sum_i (y_i - \bar{y})^2 \right]^{\frac{1}{2}}}$$

Perspectives: Selection Criteria

– Consistency Measures.

- They attempt to find a minimum number of features that separate classes as the full set of features can.
- They aim to achieve $P(C | \text{FullSet}) = P(C | \text{SubSet})$.
- An inconsistency is defined as the case of two examples with the same inputs (same feature values) but with different output feature values (classes in classification).

Perspectives: Selection Criteria

– Accuracy Measures.

- This form of evaluation relies on the classifier or learner. Among various possible subsets of features, the subset which yields the best predictive accuracy is chosen

	Mathematical form
Accuracy	$\frac{tp+fn}{tp+tn+fp+fn}$
Error rate	1 – Accuracy
Chi-squared	$\frac{n(fp \times fn - tp \times tn)^2}{(tp+fp)(tp+fn)(fp+tn)(tn+fn)}$
Information gain	$e(tp+fn, fp+tn) - \frac{(tp+fp)e(tp,fp)+(tn+fn)e(fn,tn)}{tp+fp+tn+fn}$ where $e(x, y) = -\frac{x}{x+y} \log_2 \frac{x}{x+y} - \frac{y}{x+y} \log_2 \frac{y}{x+y}$
Odds ratio	$\frac{tpr}{1-tpr} \bigg/ \frac{fpr}{1-fpr} = \frac{tp \times tn}{fp \times fn}$
Probability ratio	$\frac{tpr}{fpr}$

- Filters:



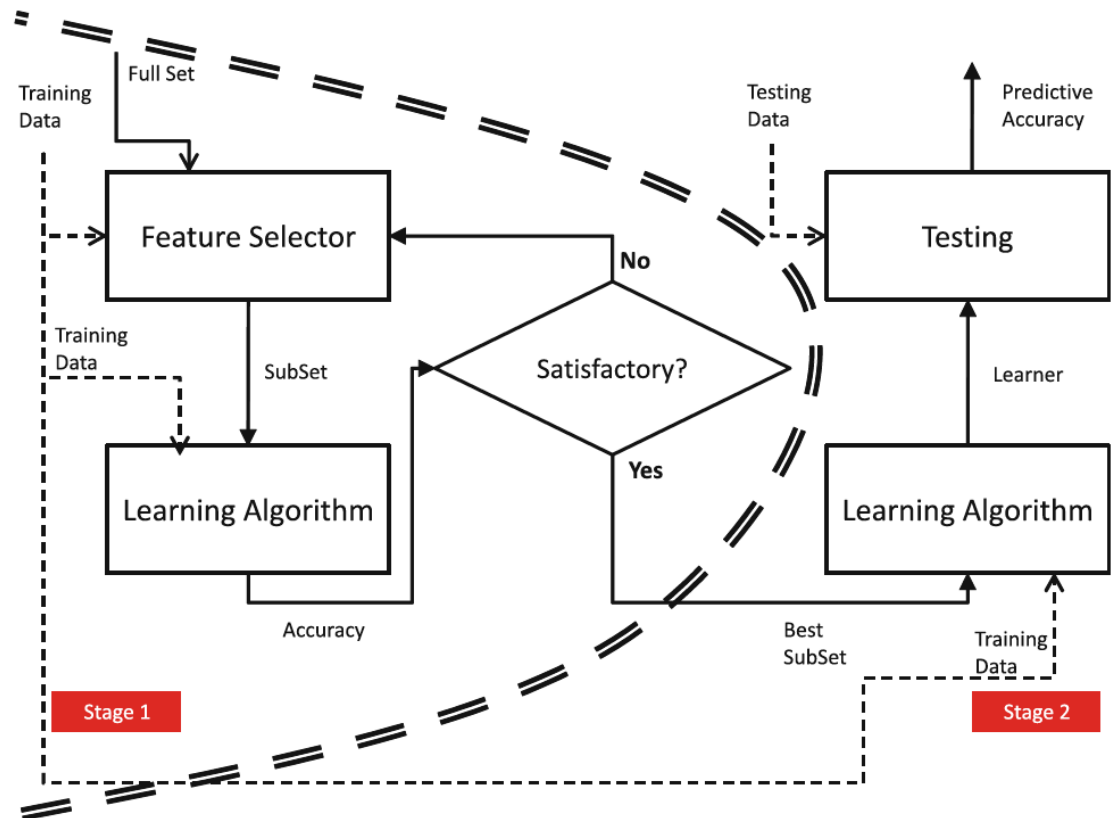
Perspectives

- Filters:

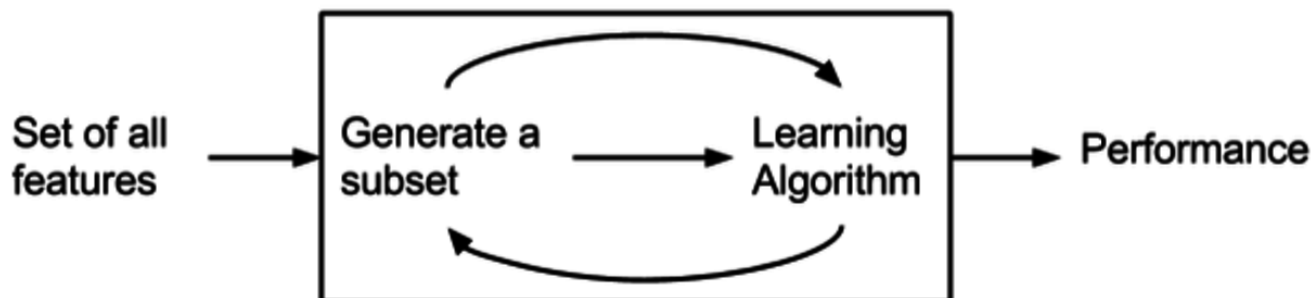
- measuring uncertainty, distances, dependence or consistency is usually cheaper than measuring the accuracy of a learning process. Thus, filter methods are usually faster.
- it does not rely on a particular learning bias, in such a way that the selected features can be used to learn different models from different ML techniques.
- it can handle larger sized data, due to the simplicity and low time complexity of the evaluation measures.

Perspectives

- Wrappers:



Selecting the best subset

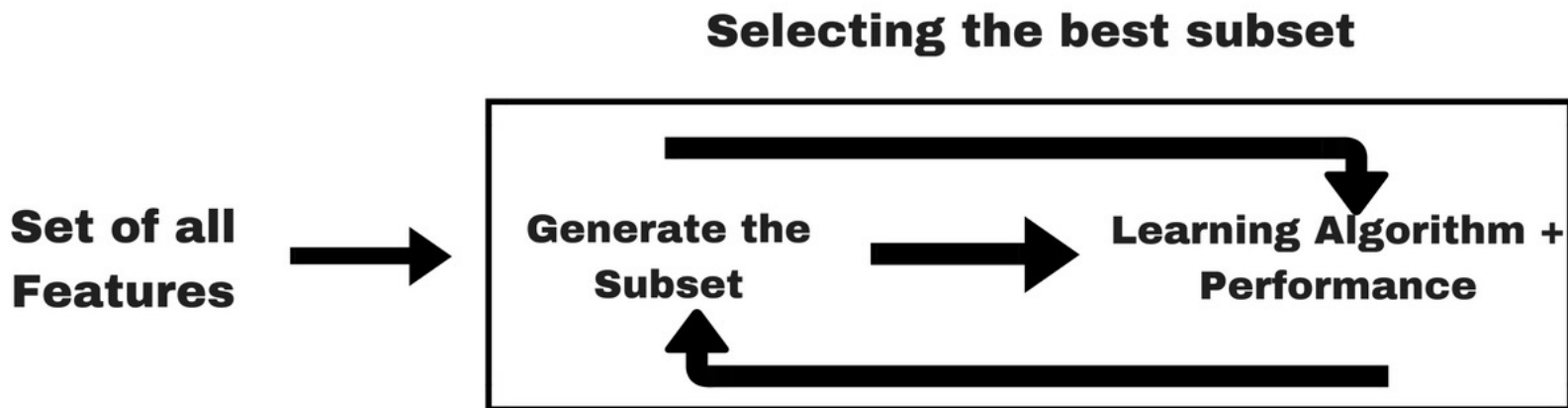


Perspectives

- Wrappers:
 - can achieve the purpose of improving the particular learner's predictive performance.
 - usage of internal statistical validation to control the overfitting, ensembles of learners and hybridizations with heuristic learning like Bayesian classifiers or Decision Tree induction.
 - filter models cannot allow a learning algorithm to fully exploit its bias, whereas wrapper methods do.

Perspectives

- **Embedded FS:**
- similar to the wrapper approach in the sense that the features are specifically selected for a certain learning algorithm, but in this approach, the features are selected during the learning process.



Perspectives

- Embedded FS:
 - they could take advantage of the available data by not requiring to split the training data into a training and validation set; they could achieve a faster solution by avoiding the re-training of a predictor for each feature subset explored.

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2. Perspectives
- 3. Aspects**
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Aspects:

Output of Feature Selection

- Feature Ranking Techniques:
 - we expect as the output a ranked list of features which are ordered according to evaluation measures.
 - they return the relevance of the features.
 - For performing actual FS, the simplest way is to choose the first m features for the task at hand, whenever we know the most appropriate m value.

Aspects:

Output of Feature Selection

- Feature Ranking Techniques:

Algorithm 5 A univariate feature ranking algorithm.

function RANKING ALGORITHM(x - features, U - measure)

initialize: list $L = \{\}$

 ▷ L stores ordered features

for each feature $x_i, i \in \{1, \dots, M\}$ **do**

$v_i = \text{COMPUTE}(x_i, U)$

 position x_i into L according to v_i

end for

return L in decreasing order of feature relevance.

end function

Aspects:

Output of Feature Selection

- Minimum Subset Techniques:
 - The number of relevant features is a parameter often unknown by the practitioner.
 - A second category of techniques must focus on obtaining the minimum possible subset without ordering the features.
 - Whatever is relevant within the subset is otherwise irrelevant.

Aspects:

Output of Feature Selection

- Minimum Subset Techniques:

Algorithm 6 A minimum subset algorithm.

function MIN- SET ALGORITHM(x - features, U - measure)

initialize: $L = \{\}$, $\text{stop} = \text{false}$

▷ S holds the minimum set

repeat

$S_k = \text{SUBSETGENERATE}(x)$

▷ **stop** can be set here

if LEGITIMACY(S_k , U) is *true* and $\#(S_k) < \#(S)$ **then**

$S = S_k$

▷ S is replaced by S_k

end if

until $\text{stop} = \text{true}$

return S - the minimum subset of features

end function

Aspects: Evaluation

- **Goals:**
 - **Inferability:** For predictive tasks, it is considered an improvement in the prediction of unseen examples with respect to the direct usage of the raw training data.
 - **Interpretability:** Given humans' incomprehension of raw data, ML is also used to generate more understandable structure representations that can explain the data's behavior.
 - **Data Reduction:** It is better and simpler to handle data with lower dimensions in terms of efficiency and interpretability.

Aspects: Evaluation

- We can derive three assessment measures from these three goals:
 - Accuracy
 - Complexity
 - Number of Features Selected
 - Speed of the FS method
 - Generality of the features selected

Aspects: Drawbacks

- The resulting subsets of many models of FS are strongly dependent on the training set size.
- It is not true that a large dimensionality input can always be reduced to a small subset of features because the objective feature is actually related to many input features, and the removal of any of them will seriously affect the learning performance.
- A backward removal strategy is very slow when working with large-scale data sets. This is because, in the first stages of the algorithm, it has to make decisions based on huge quantities of data.
- In some cases, the FS outcome will still be left with a relatively large number of relevant features which even inhibit the use of complex learning methods.

Aspects:

Using Decision Trees for FS

- Decision trees can be used to implement a trade-off between the performance of the selected features and the computation time required to find a subset.
- Decision tree inducers can be considered anytime algorithms for FS because they gradually improve performance and can be stopped at any time, providing sub-optimal feature subsets.

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3. Aspects
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Most Representative Methods

- Three major components to categorize combinations:
 - **Search Direction**
 - **Search Strategy**
 - **Evaluation Measure**

Search direction	Evaluation measure	Search strategy		
		Exhaustive	Heuristic	Nondeterministic
Forward	Probability	C1	C7	–
	Consistency	C2	C8	–
	Accuracy	C3	C9	–
Backward	Probability	C4	C10	–
	Consistency	C5	C11	–
	Accuracy	C6	C12	–
Random	Probability	–	C13	C16
	Consistency	–	C14	C17
	Accuracy	–	C15	C18

Most Representative Methods

Exhaustive Methods

- Cover the whole search space.
- Six Combinations (C1-C6).
 - Focus method: C2.
 - Automatic Branch and Bound (ABB): C5.
 - Best First Search (BFS): C1.
 - Beam Search: C3.
 - Branch and Bound (BB): C4.

Most Representative Methods

Exhaustive Methods

Algorithm 7 Focus algorithm.

```
function FOCUS( $F$  - all features in data  $D$ ,  $U$  - inconsistency rate as evaluation measure)
  initialize:  $S = \{\}$ 
  for  $i = 1$  to  $M$  do
    for each subset  $S$  of size  $i$  do
      if  $\text{CALU}(S, D) = 0$  then                                      $\triangleright \text{CalU}(S, D)$  returns inconsistency
        return  $S$  - a minimum subset that satisfies  $U$ 
      end if
    end for
  end for
end function
```

Most Representative Methods

Heuristic Methods

- They do not have any expectations of finding an optimal subset with a rapid solution.
- Nine Combinations (C7-C15).
 - Use a DM algorithm for FS: C12.
 - Wrapper Sequential Forward Selection: C9.
 - SetCover: C8.
 - Heuristic search algorithm and in each sub-search space: C13-C15.
 - **MIFS: C10.**

Most Representative Methods

Heuristic Methods

Algorithm 8 MIFS algorithm.

function MIFS(F - all features in data, S - set of selected features, k - desired size of S , β - regulator parameter)
 initialize: $S = \{\}$
 for each feature f_i in F **do**
 Compute $I(C, f_i)$
 end for
 Find f_{max} that maximizes $I(C, f)$
 $F = F - \{f_{max}\}$
 $S = S \cup f_{max}$
 repeat
 for all couples of features ($f_i \in F, s_j \in S$) **do**
 Compute $I(f_i, s_j)$
 end for
 Find f_{max} that maximizes $I(C, f) - \beta \sum_{s \in S} I(f_i, s_j)$
 $F = F - \{f_{max}\}$
 $S = S \cup f_{max}$
 until $|S| = k$
 return S
end function

Most Representative Methods

Nondeterministic Methods

- They add or remove features to and from a subset without a sequential order.
- Three Combinations (C16-C18).
 - Simulated Annealing / Genetic Algorithms are the most common techniques.
 - **LVF: C17.**
 - **LVW: C18.**

Most Representative Methods

Nondeterministic Methods

Algorithm 9 LVF algorithm.

```
function LVF( $D$  - a data set with  $M$  features,  $U$  - the inconsistency rate,  $maxTries$  - stopping
criterion,  $\gamma$  - an allowed inconsistency rate)
  initialize: list  $L = \{\}$  ▷  $L$  stores equally good sets
   $C_{best} = M$ 
  for  $maxTries$  iterations do
     $S = \text{RANDOMSET}(\text{seed})$ 
     $C = \#(S)$  ▷  $\#$  - the cardinality of  $S$ 
    if  $C < C_{best}$  and  $\text{CALU}(S, D) < \gamma$  then
       $S_{best} = S$ 
       $C_{best} = C$ 
       $L = \{S\}$  ▷  $L$  is reinitialized
    else if  $C = C_{best}$  and  $\text{CALU}(S, D) < \gamma$  then
       $L = \text{APPEND}(S, L)$ 
    end if
  end for
  return  $L$  ▷ all equivalently good subsets found by LVF
end function
```

Most Representative Methods

Nondeterministic Methods

Algorithm 10 LVW algorithm.

```
function LVW( $D$  - a data set with  $M$  features,  $LA$  - a learning algorithm,  $maxTries$  - stopping  
criterion,  $F$  - a full set of features)  
  initialize: list  $L = \{\}$  ▷  $L$  stores sets with equal accuracy  
   $A_{best} = \text{ESTIMATE}(D, F, LA)$   
  for  $maxTries$  iterations do  
     $S = \text{RANDOMSET}(\text{seed})$   
     $A = \text{ESTIMATE}(D, S, LA)$  ▷ # - the cardinality of  $S$   
    if  $A > A_{best}$  then  
       $S_{best} = S$   
       $A_{best} = A$   
       $L = \{S\}$  ▷  $L$  is reinitialized  
    else if  $A = A_{best}$  then  
       $L = \text{APPEND}(S, L)$   
    end if  
  end for  
  return  $L$  ▷ all equivalently good subsets found by LVW  
end function
```

Most Representative Methods

Feature Weighting Methods

- Provide weights to features, also can be used for FS.
- Relief (binary) and ReliefF (multiple classes).

Algorithm 11 Relief algorithm.

```
function RELIEF( $x$  - features,  $m$  - number of instances sampled,  $\tau$  - relevance threshold)
  initialize:  $w = 0$ 
  for  $i = 1$  to  $m$  do
    randomly select an instance  $I$ 
    find nearest-hit  $H$  and nearest-miss  $J$ 
    for  $j = 1$  to  $M$  do
       $w(j) = w(j) - dist(j, I, H)^2/m + dist(j, I, J)^2/m$   $\triangleright dist$  is a distance function
    end for
  end for
  return  $w$  greater than  $\tau$ 
end function
```

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1. Overview
2. Perspectives
3. Aspects
4. Most Representative Methods
- 5. Related and Advanced Topics**
6. Experimental Comparative Analyses

Related and Advanced Topics

Leading and Recent FS Techniques

- The related literature is huge, quite chaotic and difficult to understand or categorize the differences among the hundreds of algorithms published.
- Focus attention on the main ideas that lead to updates and improvements.

Related and Advanced Topics

Leading and Recent FS Techniques

- Modifications of classical FS:
 - MIFS-U, MIFS based on Parzen window, mRMR, NMIFS.
 - Several Relief modifications: Iterative-RELIEF.
- Separability and Similarity:
 - Kernel class separability.
 - Common subspace measure and Fisher subspace measure combination.
 - The redundancy-constrained FS (RCFS).
 - Many more...

Related and Advanced Topics

Leading and Recent FS Techniques

- Use of meta-heuristics:
 - Genetic algorithms.
 - Tabu search.
 - Hybridizations between genetic algorithms and local searches.
- Rough Sets theory:
 - evaluation criteria based onn reducts and approximations.
 - Fuzzy Rough FS (FRFS).

Related and Advanced Topics

Leading and Recent FS Techniques

- Fusion of filters and wrappers:
 - Evaluation criteria merging dependency, coefficients of correlations and error estimation by KNN.
 - GAMIFS: genetic algorithm to form an hybrid filter/wrapper.
- Extremely high-dimensional data:
 - Reduction of the FS task to a quadratic optimization problem: QPFS.
 - Big Data solutions.

Related and Advanced Topics

Feature Extraction

- Find new features that are calculated as a function of the original features.
- Dimensionality Reduction is done by mapping a multidimensional space into a space of fewer dimensions.
- It is another name given to Space Transformations.

Related and Advanced Topics

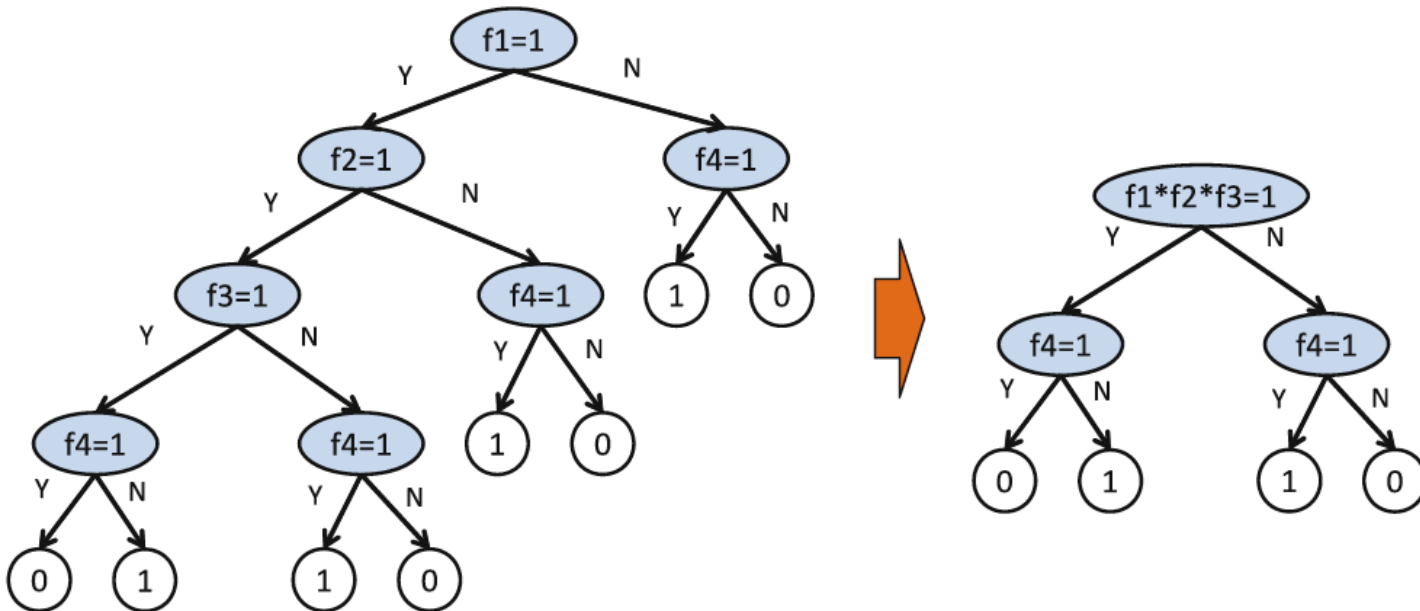
Feature Construction

- Attach to the algorithms some mechanism to compound new features from the original ones endeavouring to improve accuracy and the decrease in model complexity.
- They have been extensively applied on separate-and-conquer predictive learning approaches.

Related and Advanced Topics

Feature Construction

- Constructive operators:
 - Product, inequality, maximum, minimum, average, addition, subtraction, division, count, ...



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3. Aspects
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Experimental Comparative Analyses

- Summary of some major studies:
 - With 1-NN, the main conclusions point to the use of the bidirectional approaches for small and medium scale data sets.
 - Regarding evaluation measures, the inconsistency criterion was emphasized in several aspects.
 - Evaluation measure + stopping criterion: information theory based functions obtain better accuracy results; no cutting criterion can be generally recommended.
 - On synthetic data, ReliefF turned out to be the best option independent of the particulars of the data.