Feature Selection

Feature Selection

1. Overview
2. Perspectives
3. Aspects
4. Most Representative Methods

Feature Selection

1. Overview
2. Perspectives
3. Aspects
4. Most Representative Methods

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.

Feature Selection

1. Overview
2. Perspectives
3. Aspects
4. Most Representative Methods

Perspectives

1. searching for the best subset of features.

2. criteria for evaluating different subsets.

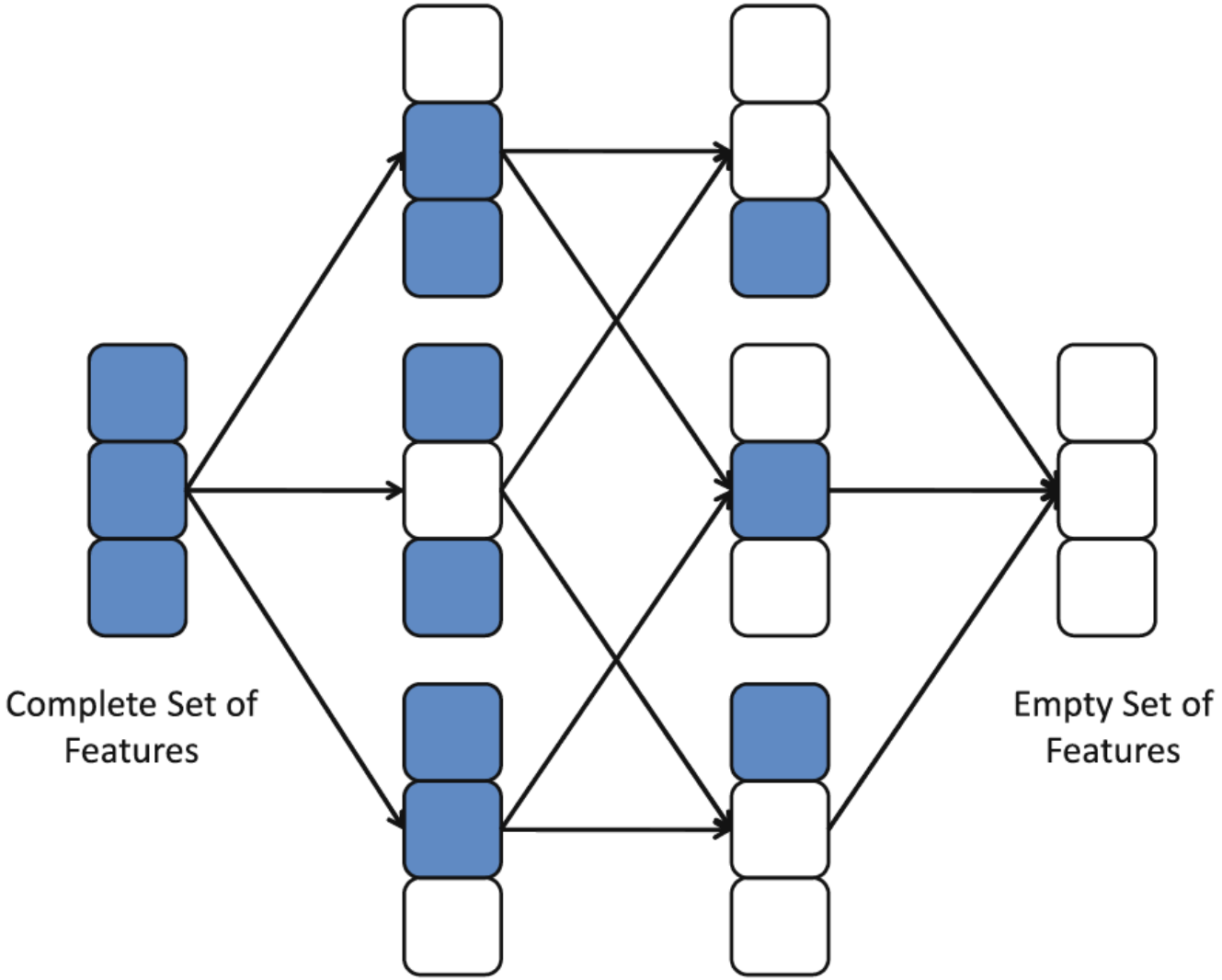
3. principle for selecting, adding, removing or changing new features during the search.

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.
- The selection can be represented as a binary array, with each element corresponding to the value 1, if the feature is currently selected by the algorithm and 0, if it does not occur.
- 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: $S = \{\}$ ▷ 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):** Begins the search in both directions, performing SFG and SBG 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 a features is a random decision. RGtries to avoid the stagnation into a local optima by not following a fixed way 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

– Information Measures.

- Information serves to measure the uncertainty of the receiver when she/he receives a message.
- Shannon's Entropy:

$$-\sum_{i} P(c_i) \log_2 P(c_i).$$

- Information gain:

$$IG(A) = I(D) - \sum_{j=1}^{p} \frac{|D_j|}{|D|} I(D_j^A)$$

Perspectives: Selection Criteria

– Distance Measures.

- Measures of separability, discrimination or divergence measures . The most typical is derived from 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	$D_{cb} = \sum_{i=1}^{m} \lvert x_i - y_i \rvert$
Cebyshev distance	$D_{ch} = \max_i \lvert x_i - y_i \rvert$
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	$D_{ca} = \sum_{i=1}^{m} \frac{\lvert x_i - y_i \rvert}{x_i + y_i}$
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, in such way that knowing the value of one of them, we can derive the value for the other.
- *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|FullSet) = P(C|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

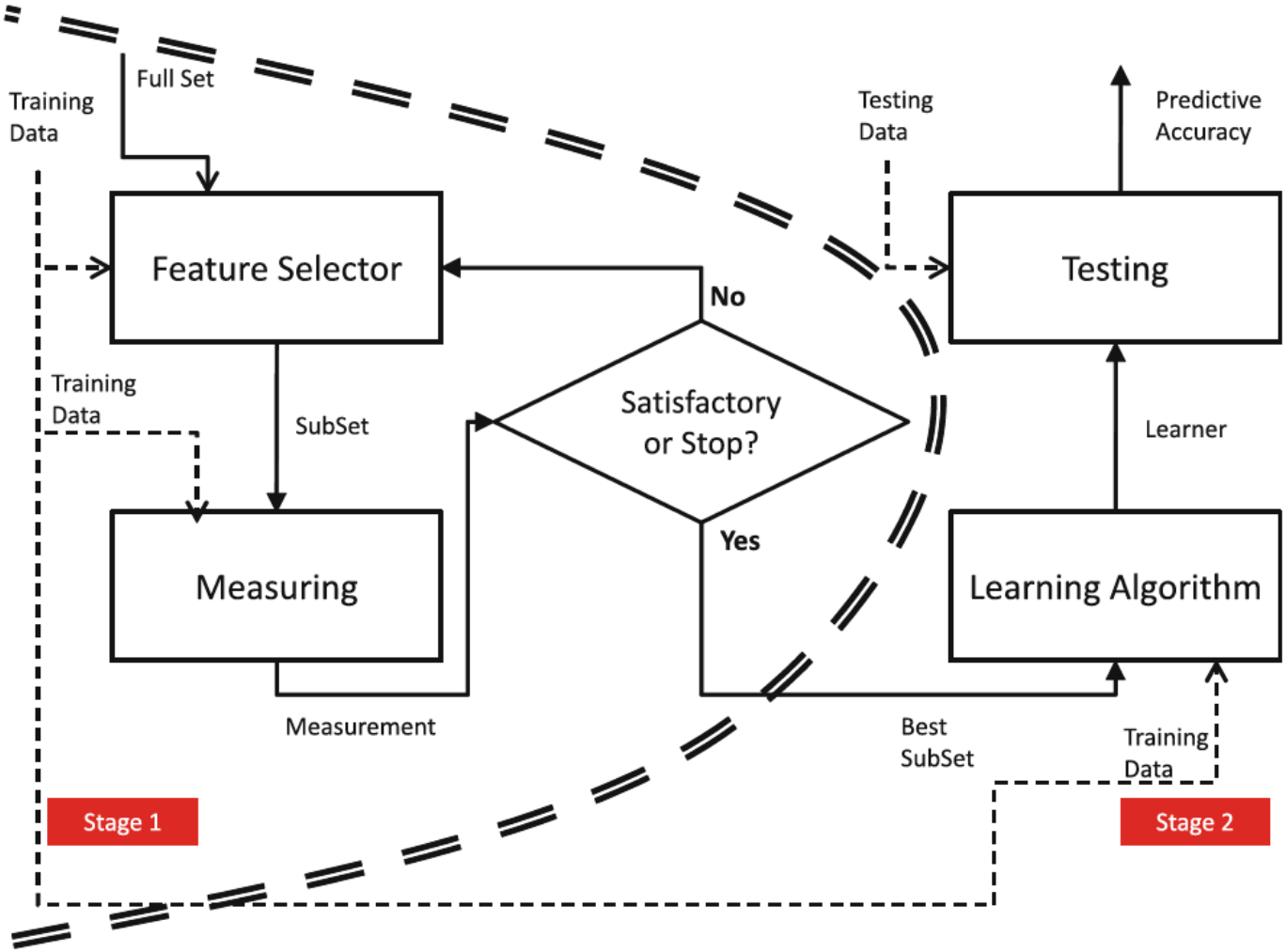
– Accuracy Measures.

- 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	$\frac{tp+fp}{tp+tn+fp+fn}$
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	$\frac{\frac{tpr}{1-tpr}}{\frac{fpr}{1-fpr}} = \frac{tp \times tn}{fp \times fn}$
Probability ratio	$\frac{tpr}{fpr}$

Perspectives

- Filters:

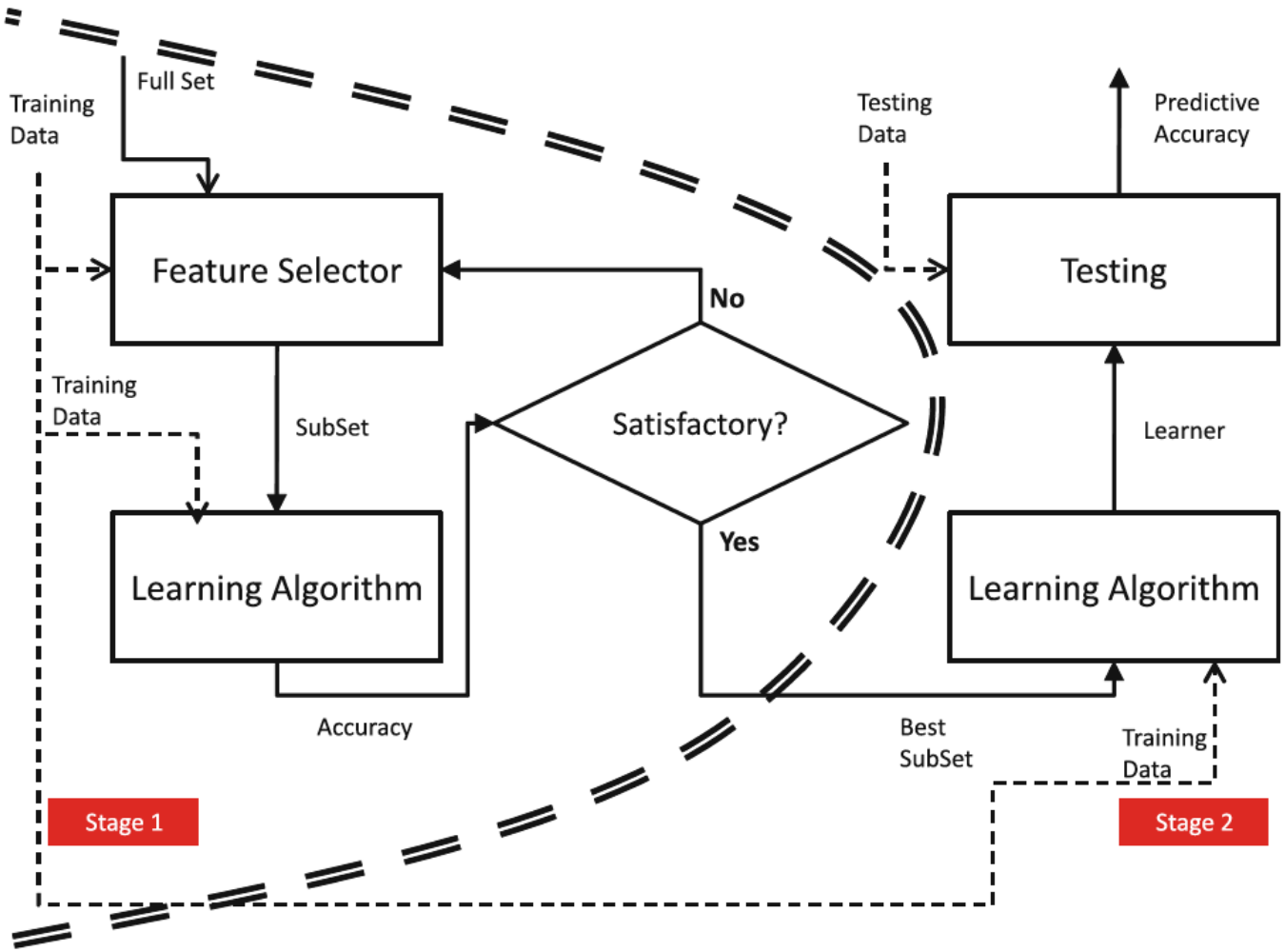


Perspectives

- 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 DM techniques.
  - it can handle larger sized data, due to the simplicity and low time complexity of the evaluation measures.

Perspectives

- Wrappers:



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.
  - 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.

Feature Selection

1. Overview
2. Perspectives
3. Aspects
4. Most Representative Methods

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, $i \in \{1, \ldots, M\}$ **do**
    v_i = 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 that is often not known by the practitioner.
  - There must be a second category of techniques focused 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: $L = \{\}$, stop = *false* ▷ S holds the minimum set
  repeat
    S_k = 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 stop = *true*
  return S - the minimum subset of features
end function

Aspects: Evaluation

- Goals:
  - **Inferability:** For predictive tasks, considered as an improvement of the prediction of unseen examples with respect to the direct usage of the raw training data.
  - **Interpretability:** Given the incomprehension of raw data by humans, DM is also used for generating more understandable structure representation that can explain the behavior of the data.
  - **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 resulted 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 with many input features and the removal of any of them will seriously effect the learning performance.
- A backward removal strategy is very slow when working with large-scale data sets. This is because in the firsts stages of the algorithm, it has to make decisions funded 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 which is required to find a subset.

- Decision tree inducers can be considered as anytime algorithms for FS, due to the fact that they gradually improve the performance and can be stopped at any time, providing sub-optimal feature subsets.

Feature Selection

1. Overview
2. Perspectives
3. Aspects
4. Most Representative Methods

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 CALU(S,D) = 0 then                    ▷ 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 $\mathrm{I}(C, f_i)$
end for
Find f_{max} that maximizes $\mathrm{I}(C, f)$
$F = F - \{f_{max}\}$
$S = S \bigcup f_{max}$
repeat
    for all couples of features ($f_i \in F, s_j \in S$) **do**
        Compute $\mathrm{I}(f_i, s_j)$
    end for
    Find f_{max} that maximizes $\mathrm{I}(C, f) - \beta \sum_{s \in S} \mathrm{I}(f_i, s_j)$
    $F = F - \{f_{max}\}$
    $S = S \bigcup f_{max}$
until $|S| = k$
return S

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, γ - an allowed inconsistency rate)
  initialize: list $L = \{\}$ ▷ L stores equally good sets
  $C_{best} = M$
  for $maxTries$ iterations **do**
    S = RANDOMSET(seed)
    $C = \#(S)$ ▷ # - the cardinality of S
    if $C < C_{best}$ *and* CALU(S,D) $< \gamma$ **then**
      $S_{best} = S$
      $C_{best} = C$
      $L = \{S\}$ ▷ L is reinitialized
    else if $C = C_{best}$ *and* CALU(S,D) $< \gamma$ **then**
      L = 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} = ESTIMATE(D,F,LA)
  for $maxTries$ iterations **do**
    S = RANDOMSET(seed)
    A = 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 = 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 (multipe classes).

Algorithm 11 Relief algorithm.

function RELIEF(**x** - features, m - number of instances sampled, τ - relevance threshold)
  initialize: $\mathbf{w} = 0$
  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**
      $\mathbf{w}(j) = \mathbf{w}(j) - dist(j, I, H)^2/m + dist(j, I, J)^2/m$ ▷ *dist* is a distance function
    end for
  end for
  return w greater than τ
end function