

Review of Feature selection approaches based on Grouping of features

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With the rapid development in technology, large amounts of high-dimensional data have been generated. This high dimensionality including redundancy and irrelevancy poses a great challenge in data analysis and decision making. Feature selection (FS) is an effective way to reduce dimensionality by eliminating redundant and irrelevant data. Most traditional FS approaches score and rank each feature individually; and then perform FS either by eliminating lower ranked features or by retaining highly-ranked features. In this review, we discuss an emerging approach to FS that is based on initially grouping features, then scoring groups of features rather than scoring individual features. Despite the presence of reviews on clustering and FS algorithms, to the best of our knowledge, this is the first review focusing on FS techniques based on grouping. The typical idea behind FS through grouping is to generate groups of similar features with dissimilarity between groups, then select representative features from each cluster. Approaches under supervised, unsupervised, semi supervised and integrative frameworks are explored. The comparison of experimental results indicates the effectiveness of sequential, optimization-based (fuzzy or evolutionary), hybrid and multi-method approaches. When it comes to biological data, involvement of external biological sources can improve analysis results. We hope this work's findings can guide effective design of new FS approaches using feature grouping.

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23 Abstract

24 With the rapid development in technology, large amounts of high-dimensional data have been
25 generated. This high dimensionality including redundancy and irrelevancy poses a great
26 challenge in data analysis and decision making. Feature selection (FS) is an effective way to
27 reduce dimensionality by eliminating redundant and irrelevant data. Most traditional FS
28 approaches score and rank each feature individually; and then perform FS either by eliminating
29 lower ranked features or by retaining highly-ranked features. In this review, we discuss an
30 emerging approach to FS that is based on initially grouping features, then scoring groups of
31 features rather than scoring individual features. Despite the presence of reviews on clustering and
32 FS algorithms, to the best of our knowledge, this is the first review focusing on FS techniques
33 based on grouping. The typical idea behind FS through grouping is to generate groups of similar
34 features with dissimilarity between groups, then select representative features from each cluster.
35 Approaches under supervised, unsupervised, semi supervised and integrative frameworks are
36 explored. The comparison of experimental results indicates the effectiveness of sequential,
37 optimization-based (i.e., fuzzy or evolutionary), hybrid and multi-method approaches. When it
38 comes to biological data, involvement of external biological sources can improve analysis
39 results. We hope this work's findings can guide effective design of new FS approaches using

40 feature grouping.

41

42

43 **Introduction**

44 In the current digital era, the data produced by many applications in fields such as image
45 processing, pattern recognition, machine learning and network communication grow
46 exponentially in both dimension and size. Due to this high-dimensionality, the search space is
47 widening and extraction of valuable knowledge from the data becomes a challenging task [1,2].
48 Also, utilizing all features in a dataset is unlikely to develop a predictive model with high
49 accuracy. Existence of irrelevant and redundant features may weaken the generalizability of the
50 model and decrease the overall precision of a classifier [3]. Hence, reducing the number of input
51 variables is highly desired as it lowers the computational cost of model construction and allows
52 improving model performance. As such, feature selection (FS) becomes an inevitable step for
53 domain experts and data analysts.

54

55 FS is the process of selecting the minimally sized feature subset from the original set that is
56 optimal for the target concept. It plays a crucial role in removing irrelevant and redundant
57 features while keeping relevant and non-redundant ones [4]. Irrelevant features do not alter the
58 target concept in any way and redundant features do not contribute to the target concept [5].
59 These features may contain a considerable amount of noise which can be misleading, resulting in
60 significant computational overhead and poor predictor performance. Contrary to other
61 dimensionality reduction techniques, FS preserves the data semantics as it does not distort the
62 original feature representation and hence provides straightforward data interpretation for data
63 scientists. Additionally, reduction in dimension by FS prevents overfitting that can lead to
64 undesired validation results.

65

66 Although various FS techniques have been developed, traditional approaches to FS neglect
67 structures of features during the selection process. Another issue is that retention and elimination
68 of features on an individual basis ignores dependence among them. Because of these reasons,
69 correlation between features may not be detected efficiently resulting in irrelevant or redundant
70 features in the final subset. Some studies grouped samples (i.e., observations) for improving
71 classification performance but these studies were not concerned with feature reduction at all
72 [6,7].

73

74 On the other hand, FS based on grouping is an effective technique for reducing feature
75 redundancy and enhancing classifier learning. By grouping the features, the search space is
76 reduced substantially. Moreover, it can reduce estimator variance [8], improve stability, and
77 reinforce generalization capability of the model. Although there are reviews of clustering
78 methods [9] and of FS techniques [2,10], to the best of our knowledge, this is the first paper
79 reviewing the literature on approaches to FS based on grouping. In this procedure, the process of
80 grouping features into clusters is generally performed as the initial step, aiming to have maximal
81 intra-class similarity (i.e., similarity in between the objects of the same cluster) and minimal
82 inter-class similarity (i.e., objects in a cluster are more similar to those in another one) between
83 features. These feature groups can be created by K-Means, fuzzy c-mean (FCM), hierarchical

84 clustering, graph theory and other methods [11-14]. After cluster formation, features within each
85 cluster are scored and selected using various techniques or metrics.

86

87 The remainder of this paper is organized as follows: We will give a concise overview of different
88 FS methods in Section 2. In Section 3, we will present different works carried out in FS using
89 feature grouping following the summary of traditional approaches. Then, in Section 4, we will
90 review different studies which benefited from Recursive Cluster Elimination based on Support
91 Vector Machine (SVM-RCE) [15-17]. Next, in Section 5, we will address FS techniques
92 involving both feature grouping and incorporating domain knowledge. We discuss the
93 advantages and disadvantages of the presented methods in Section 6. Lastly, in Section 7, we
94 conclude our review with further discussions and future directions.

95

96

97 **Rationale behind the review and intended audience**

98

99 Nowadays, the advancements in different technologies resulted in the generation of high
100 dimensional data in many different fields, which makes data analysis a challenging issue.
101 Existence of irrelevant and redundant features makes it hard to infer meaningful conclusions
102 from data, degrades model performance and leads to computational overhead. Especially in the
103 field of molecular biology, the advancements in high throughput technologies have induced the
104 emergence of a wealth of -omics data produced by different studies, such as genomics,
105 transcriptomics, epigenomics, proteomics, meta-genomics, meta-transcriptomics, meta-
106 proteomics, metabolomics, etc [18]. For instance, high-dimensional RNA-sequencing data can be
107 used for cancer subtype identification in order to ease cancer diagnosis and discover effective
108 treatments. However, only a subset of features (i.e., mRNAs) carries information associated with
109 the cancer subtype. Furthermore, this kind of biological data often involves redundant and
110 irrelevant features which can mislead the learning procedure in modeling and can cause
111 overfitting. As another example, in metagenomics studies the number of features (i.e., taxa) is
112 much higher than the number of samples. This phenomenon is known as the curse of
113 dimensionality. In this respect, some metagenomics studies focus on the FS process rather than
114 focusing on classification [19]. Hence, FS has become a real prerequisite in the biological
115 domain [20–23]. Due to these reasons, FS became an indispensable preprocessing step in
116 different fields dealing with high dimensional data. Traditional approaches evaluate features
117 without considering the correlation among them, and also this evaluation is performed on an
118 individual basis. Furthermore, these methods generally fail to scale on a large space.

119

120 On the other hand, FS based on feature grouping is a powerful approach due to the following
121 reasons: i) it enables the discovery of correlations among features, ii) search space is
122 significantly diminished, iii) it relieves computational burden. Although some grouping-based FS
123 methods are proposed in the literature, to the best of our knowledge, none of the existing papers
124 evaluate these existing approaches in detail as a review. For these reasons, compared to current
125 literature, we believe that this review will be more guiding and suggestive for those learning the

126 above-mentioned methods, for those working to derive such methods, and for those who want to
127 apply this approach into their data analysis.

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130

131 **Survey Methodology**

132

133 Our main focus in this review is to examine FS approaches via grouping. In this context, we
134 reviewed Web of Science, Scopus, and Google Scholar on January 10, 2022 using the following
135 query: "feature clustering" OR "feature grouping" OR "clustering based feature selection" OR
136 "grouping based feature selection" OR "cluster based feature selection" OR "group based feature
137 selection". We excluded those studies grouping samples (i.e., observations) or features as the
138 final outcome and those concerned with feature extraction. We particularly focused on grouping
139 of features as the preprocessing step followed by extraction of a reduced subset of features by a
140 certain procedure which is subsequently input into a classification or clustering process for
141 validation. Other articles for context were added while writing the review. Studies of this
142 paradigm under an unsupervised setting are on a limited scale compared to the supervised
143 setting, due to lack of labels in the former. Even though it's not known clearly, we think that
144 inclusion of this approach may have emerged in late 90s. Recently, interest in this concept has
145 grown rapidly in different forms as we point out in the following sections of this review. In fact,
146 selection of significant features by removing irrelevant or redundant ones is just one aspect;
147 ranking of these features in terms of being informative or having discriminative power, and
148 stability of them for different models are other issues that are taken into consideration. Here, we
149 examined different studies that are identified in literature mining, categorized them, and
150 presented readers a versatile work in which we aimed at providing a robust basis on the topic.

151

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153

154 **2. Basics of Feature Selection**

155

156 In this section, we present basic concepts in FS. According to their interaction with classification
157 model, FS techniques can be classified into filter, wrapper, and embedded techniques [24]. Later
158 in the literature, hybrid and ensemble techniques have emerged as variants of them. Hybrid
159 approach combines two different methods to utilize the advantages of both approaches, where
160 the common combination is filter and wrapper methods. Ensemble technique integrates an
161 ensemble of feature subsets and then yields the result from the ensemble. The overview of the
162 three main types of methods is shown in **Fig. 1**.

163

164 **2.1. Filter Method**

165

166 Filter type methods select features by assessing intrinsic properties of data based on statistical

167 measures instead of cross-validation performance. They are easily scalable to high-dimensional
 168 datasets, independent of the learning algorithm; they are simple and computationally fast; and
 169 they are resistant to overfitting. In this method, each feature is assigned a score determined by
 170 the selected statistical method. Afterwards, all features are ranked in descending order and those
 171 with low scores are removed using a threshold value. The remaining features comprise the
 172 feature subset and are then fed into the classification model. Consequently, FS is carried out once
 173 and then various classifiers can be employed. Disadvantages of this technique are i) features are
 174 selected irrespective of the classifier, and ii) feature dependencies are ignored. Some common
 175 statistical measures used in this technique are Information Gain (IG), Pearson's Correlation (PS),
 176 Chi Square (χ^2), Mutual Information (MI), and Symmetrical Uncertainty (SU).

177
 178
 179

180 **2.1.1. Information Gain**

181

182 Information gain (IG) [25] is an entropy-based FS method and used to measure how much
 183 information a feature carries about the target variable. *IG* of a feature X in a data group D with n
 184 class labels, $IG(X)$, is calculated using

185

$$186 \quad IG(X) = E(D) - \sum_{i=1}^n \frac{D_i}{D} E(D_i) \quad (1)$$

187

188 where $E(D)$ denotes the general entropy belonging to class labels, $\frac{D_i}{D}$ is the ratio of number of
 189 occurrences of each value on feature X , and $E(D_i)$ specifies the entropy of i th feature value
 190 calculated by splitting dataset D based on feature X . Entropy is a measurement of
 191 unpredictability or impurity of a data distribution and defined as

192

$$193 \quad E(D) = - \sum_{i=1}^n p(i) \log_2 p(i) \quad (2)$$

194

195 where $p(i)$ is the probability of class i in the data group D for n class labels. A feature is relevant
 196 to target variable if it has a high information gain. The way the features are selected is in a
 197 univariate way (i.e., features are selected independently), therefore, redundant features cannot be
 198 eliminated in this technique.

199

200

201

202 **2.1.2. Pearson's correlation**

203

204 Pearson's correlation is a measure of the dependency (or similarity) of two variables and used for
 205 finding the relationship between continuous features and the target feature [26,27]. It produces
 206 the correlation coefficient r ranging between -1 to 1, where 1 shows a strong correlation and -1
 207 means a total negative correlation. So, 0 value implies no correlation between the features. A
 208 positive correlation states that if one variable increases, so does the other variable, whereas a
 209 negative correlation implies that while one variable raises, another one decreases. This method
 210 can also be used to measure correlation between pairs of features. In this way redundant features

211 can be identified. Pearson's correlation coefficient r can be found for feature X with values x
 212 and classes Y with values y where X, Y are random variables by the following equation:

213
 214
 215

$$216 \quad r = \frac{\sum(x - \bar{x})(y - \bar{y})}{\sqrt{\sum(x - \bar{x})^2 \sum(y - \bar{y})^2}} \quad (3)$$

217
 218

219 where \bar{x} and \bar{y} are means of x and y , respectively. Note that Pearson's correlation is mainly
 220 covariance of two variables divided by product of their standard deviations.

221
 222
 223

224 2.1.3. Chi Square

225

226 Chi square (χ^2) [28] is a statistical method to test the independence of two events. It's a
 227 measurement of the degree of association between two categorical values. It measures the
 228 deviation from the expected frequency assuming the feature event is independent of the class
 229 label. This assumption is tested for a given feature with n class and m different feature values by
 230 the formula

231

$$232 \quad \chi^2 = \sum_{i=1}^m \sum_{j=1}^n \frac{(O_{ij} - E_{ij})^2}{E_{ij}} \quad (4)$$

233

234 where O_{ij} is the observed (i.e., actual) value and E_{ij} refers to the expected value suggested by the
 235 null hypothesis. E_{ij} is calculated as

236

$$237 \quad E_{ij} = \frac{(O_{*j} O_{i*})}{o} \quad (5)$$

238

239 where O_{*j} means the number of samples in class m , and O_{i*} indicates the number of samples
 240 with the i^{th} feature value for the feature under study. Higher value of χ^2 shows rejection to the
 241 null hypothesis, namely, higher dependency between the feature and the class label.

242

243

244

245 2.1.4. Mutual Information

246

247 Mutual information (MI) [29] is another statistical method used to assess the mutual dependence
 248 between the two variables. MI quantifies the amount of information that one random variable
 249 includes in the other random variable. MI between two continuous random variables X and Y
 250 with their joint probability functions $p(x,y)$, and their marginal probability density functions
 251 $p(x)$ and $p(y)$, respectively is given by

252

253

254

$$I(X;Y) = \iint p(x,y) \log \frac{p(x,y)}{p(x)p(y)} dx dy \quad (6)$$

255

256

257 For discrete random variables, the double integral is substituted by a summation as

258

259

$$I(X;Y) = \sum_{x \in X} \sum_{y \in Y} p(x,y) \log \frac{p(x,y)}{p(x)p(y)} \quad (7)$$

260

261 We can also define the conditional mutual information (CMI) of two random variables X and Y
 262 given a third variable Z as

263

264

$$I(X;Y | Z) = \iiint p(x,y,z) \log \frac{p(x,y|z)}{p(x|z)p(y|z)} dx dy dz \quad (8)$$

266

267

268 It can be interpreted as the amount of information X includes in Y which is not shared by Z .

269

270

271 2.1.5. Symmetrical Uncertainty

272

273 This is one of the techniques that are used to measure redundancy between two random variables
 274 [30]. It is obtained by normalizing MI to the entropies of two variables and limiting it to the
 275 range of $[0,1]$. It's able to circumvent inherent bias of MI toward features with a wide range of
 276 different values. Symmetrical Uncertainty (SU) is defined as

277

278

$$SU(X,Y) = \frac{2MI(X,Y)}{H(X) + H(Y)} \quad (9)$$

279

280 where $H(X)$ and $H(Y)$ are entropy of variable X and Y , respectively. A value 1 between a pair of
 281 features indicates that knowledge of feature value can fully predict the values of other and 0
 282 value shows that X and Y are not correlated.

283

284 Based on SU, C-Relevance between a feature and a target variable C , and F-Correlation between
 285 feature pair can be defined as follows [31]:

286

287 C-Relevance: SU between feature $F_i \in F$ and target variable C , denoted by $SU_{i,c}$.

288

289 F-Correlation: SU between any feature pair F_i and $F_j (i \neq j)$, denoted by $SU_{i,j}$.

290

291

292

293

294 **2.2. Wrapper Method**

295

296 In this methodology, a search strategy for possible subsets of features is defined, and the learning
297 algorithm is trained using these subsets in an iterative manner. Unlike filter methods, wrapper
298 methods are in interaction with the classifier, however, the evaluation of feature subsets is
299 obtained using a specific classification model which makes this method specific to a learning
300 model. Several possible combinations of features are evaluated in the model by wrapping the
301 search algorithm around it [32]. This method provides suboptimal feature subsets for training the
302 model since evaluating all possible subsets is computationally not practical, and generally gives
303 better predictive accuracy than filter methods but is computationally intensive due to searching
304 overhead and learner dependence.

305

306 The search for generating subsets can be performed with schemes such as Forward Selection,
307 Backward Elimination, Stepwise Selection or a heuristic search [33]. Forward selection is a
308 repetitive technique where no feature is considered at the onset. Initially, the feature with the best
309 performance is added. Then another most significant feature giving the best performance
310 together with the previously added feature is selected. This process proceeds until the inclusion
311 of a new feature does not improve the classifier performance. In backward elimination, the
312 algorithm starts with all the features available and discards the most insignificant feature from
313 the model recursively. This elimination process is repeated until removal of features does not
314 enhance the performance of the model. For stepwise selection, this technique is a combination of
315 both forward selection and backward elimination. It starts with an empty set and the most
316 significant feature is added at each iteration. While adding a new feature, previously selected
317 features are removed if any of them has become insignificant. Heuristic search is concerned with
318 optimization and aims at optimizing the objective function in evaluation of different subsets [34].

319

320 Support Vector Machines with Recursive Feature Elimination (SVM-RFE) [35] is a popular
321 example of wrapper methods. The idea is mainly to train the classifier by the given data and
322 assign a rank by SVM for each feature as its weight. Then, features with the smallest weights
323 are removed by a specific rate determined by the user. This procedure is repeated until reaching a
324 predefined number of features.

325

326

327

328 **2.3. Embedded Method**

329

330 This method includes advantages of filter and wrapper methods and performs FS and model
331 construction at the same time. Just like wrapper techniques, they are specific to a learning model
332 but they have less computational complexity than wrapper methods [36]. One technique of this
333 type of FS is regularization that adds a penalty to the coefficients to overcome overfitting in the
334 model. As an example, Lasso [37] is an embedded method that uses L_1 norm of the coefficient of
335 a linear classifier \mathbf{w} and penalty term (φ) is defined as

336

337

338

$$\varphi(\mathbf{w}) = \sum_{i=1}^k |w_i|$$

(10)

339 and

$$340 \quad \hat{\mathbf{w}} = \min_{\mathbf{w}} c(\mathbf{w}, X) + \alpha \varphi \quad (11)$$

341

342 where $c(\cdot)$ is the objective function for classification, φ is a regularization term, k is the number
343 of features, α is the regularization parameter controlling the trade-off between the objective
344 function and the penalty. These coefficients may even be reduced to 0 for features that do not
345 contribute to the model. Features with non-zero coefficients are retained and those with low or
346 zero coefficient are excluded [38]. Another technique to integrate FS in model creation is
347 decision trees. These tree-based methods are non-parametric models that consider features as
348 nodes. Tree-based strategies used by random forests accumulate various numbers of decision
349 trees and rank the nodes (i.e., features) by decrease in the impurity (e.g., Gini impurity) over all
350 the trees, e.g., Classification And Regression Tree (CART) [39].

351

352

353

354

355 **3. Feature Selection Approaches**

356

357 Broadly speaking, FS algorithms conducted in many studies can be categorized into the
358 following two classes: i) traditional FS, ii) FS based on grouping. Traditional approaches
359 generally consider all features contingent on “singularity” during the selection process. To put it
360 another way, they comprise inclusion or elimination of features based on some statistical
361 measures or classifying capacity at a singular level. On the other hand, grouping-based methods
362 detect relevant features by grouping them into clusters; and then remove redundant ones which
363 lead to reduced search space.

364

365

366 **3.1. Traditional Feature Selection**

367

368 Different FS methods exist in abundance in the literature, including filters based on distinct
369 criteria such as dependency, information, distance and consistency [40], and wrapper and
370 embedded methods employing different induction algorithms. Due to their simplicity, filter
371 methods are often preferable in the context of high dimensional data; the absence of necessity for
372 a search route and the interaction with a classifier makes them computationally efficient and
373 practically feasible in applications. A comparative study on various filtering methods including
374 mixture model, regression modeling and t-test was presented in [41] where the authors outlined
375 similar and dissimilar aspects of these methods. The authors noted that all the three methods
376 employ two-sample t-test or its variation; but these methods vary in different significance levels
377 and the number of detected features. Lazar et al. [42] also reviewed filter type FS algorithms
378 used in gene expression data analysis and presented them as a top-bottom strategy in a
379 taxonomy.

380

381 Wrapper methods carry the computational burden since they require navigation in the search
382 domain and and since they interact with the predictor. However, they provide better accuracy
383 than filter approaches due to their interaction with the learning algorithm. Talavera L. et al. [43]
384 compared filter and wrapper approaches in clustering. They confirm the superiority of wrappers

385 along with some of their problems and they suggest filter techniques as an alternative approach
386 due to their computational efficiency. A recent study [44] overviewed existing wrapper
387 techniques and evaluated the pros and cons of them. Embedded methods, like wrapper
388 techniques, possess computational complexity when it comes to high-dimensional data. They are
389 more efficient than wrappers and have less complexity. Applications of this approach in the
390 bioinformatics domain have been reviewed in [45].

391

392 Hybrid methods combine two methods such as filter and wrapper to take advantage of both
393 methods in order to increase efficiency and performance. Ensemble methods integrate different
394 methods for FS, classification or both. In this approach, multiple feature selectors, induction
395 algorithms, different subsets may be included according to the design scheme. A detailed
396 discussion on hybrid methods and a good review on ensemble FS techniques can be found in
397 [46] and [47], respectively. In some studies, FS methods are divided into these five categories
398 [48].

399

400 Traditional FS approaches have several shortcomings. For instance, filter methods evaluate the
401 significance of each feature individually without considering the relationships and interactions
402 between the features. Wrapper methods can provide the optimal feature subset but their
403 complexity makes them imperfect, they are not preferable especially in combinatorial techniques
404 such as in ensemble methods. In addition, they are not applicable to data with small number of
405 samples due to overfitting. Embedded methods, like wrappers, are specific to the model hence
406 may give a different feature subset for the same dataset. The main drawback behind such
407 methods is their inability to remove redundant features and retain informative features efficiently
408 [49,50].

409

410

411

412 **3.2. Feature Selection Through Feature Grouping**

413

414 In this section, we will categorize FS approaches based on feature grouping under supervised,
415 unsupervised and semi-supervised context. Supervised FS utilizes data labels to measure
416 importance and relevance of features. Unsupervised FS, on the other hand, assesses feature
417 relevance by exploiting natural structure of the data without using the class label. Semi-
418 supervised FS benefits from both labeled and unlabeled data. **Fig. 2** illustrates a taxonomy of
419 grouping-based FS approaches covered in this study. A typical scenario in FS approaches based
420 on grouping is that the features are first partitioned into clusters and then (a) representative
421 feature(s) is (are) selected from each cluster according to a specific metric or technique as shown
422 in **Fig. 3**.

423

424

425

426 **3.2.1. Grouping-based Feature Selection under Supervised Setting**

427

428 In the literature, there are many studies that conducted FS through feature grouping. The
429 grouping of features is performed by various techniques including K-means [51], hierarchical
430 clustering [52,53], affinity propagation [54], graph theories [55], information theory metrics [56],

431 kernel density estimation [57], logistic regression [58] and regularization methods [59]. With the
432 availability of class labels in datasets, this prevalence is increasing day by day, offering new
433 approaches and gaining new insights into the field.

434
435 Several studies performed K-means or hierarchical clustering for grouping features and then they
436 chose genes from each cluster. Sahu et al. [60] proposed an ensemble approach where K-means
437 is applied first for feature grouping and then three different filter-based ranking techniques (t-
438 test, signal-to-noise ratio (SNR) and significance analysis of microarrays (SAM)) are
439 implemented for each cluster independently; and the feature in the front rank from each cluster is
440 selected to form three distinct feature subsets. Afterwards, features in subsets are subject to
441 additional elimination by checking the inclusion of each feature in other subsets. In other words,
442 a feature is discarded if it is not available in other subsets. They obtain good accuracy for
443 different combinations in general but this study ignores correlations between genes. Another
444 study [61] applied information compression index to group features by hierarchical clustering
445 and then sorted features within each cluster by Fisher criterion measuring the classification
446 capacity of each feature in a cluster. Subsequently, the feature in the front rank is selected for
447 each cluster to form the feature subset.

448
449 Regarding selection of features from groups, in addition to ranking, selection can also be
450 performed sequentially. For instance, Zhu and Yang [62] group features into clusters by a
451 modified affinity propagation algorithm, and then they apply sequential FS for each cluster.
452 Later on, they gather selected features in clusters to acquire the reduced subset. Their
453 experimental results show improvement in execution time and the accuracies are comparable
454 with sequential FS. Alimoussa et al. [63] proposed a sequential FS method based on feature
455 grouping mainly consisting of three steps. They first remove irrelevant features using Pearson
456 correlation. Then, the same correlation metric is employed for grouping of features into clusters
457 by considering intercorrelated features directly or indirectly via other features. Finally, a feature
458 from each cluster is selected sequentially and features belonging to the same cluster are removed
459 in each round. Their proposed method gives better accuracy and reduction in size compared to
460 filter and wrapper methods. However, despite their approach being fully filter-based, execution
461 time of the proposed method is moderate due to the grouping procedure. In their other work for
462 color texture classification [64], they incorporate a classifier into their previous work in order to
463 measure accuracy when a feature is added at each step of their procedure, thereby determining
464 the dimensionality of the feature subset. They show that combining several descriptor
465 configurations performs better compared to a predefined configuration.

466
467 Au et al. [65] proposed an effective algorithm called k-modes Attribute Clustering Algorithm
468 (ACA) for gene expression data analysis. This algorithm uses an information measure to quantify
469 correlation between features, and performs K-mode algorithm, similar to K-means, to cluster
470 features. They defined mode of each cluster as the attribute (i.e., feature) with the highest sum of
471 relevancy with others in each feature group. These modes constituted the final reduced subset.
472 Their measure was also utilized to get good clustering configurations automatically. Chitsaz et
473 al. [66] presented a fuzzy variant of this study which relies on the basic underlying idea in fuzzy
474 clustering approaches, that each feature may belong to more than one group. Rather than
475 considering association of each feature with a sole cluster, association with all features among
476 the overall clusters is considered by assigning different grades of membership to features. Their
477 extended work [67] integrates chi-square test to assess the dependency of each feature on the

478 class labels during the FS process. In their method, objective function is computed by the
 479 following formula

$$480 \quad J = \sum_{r=1}^k \sum_{i=1}^p u_{ri}^m R(A_i; \eta_r) \quad (12)$$

482 where k and p designate number of clusters and features, respectively and u_{ri} is membership
 483 degree of i^{th} feature in r^{th} cluster and m is a weighting exponent with η_r being the mode of r^{th}
 484 cluster which is essentially center of that cluster. R function denotes interdependence measure
 485 between feature A_i and mode η_r . Their experimental results achieve improvement in the accuracy
 486 of the classifier with significant reduction in selected feature size compared to the basic version.
 487

488
 489 Graph-based approaches are also common in studies involving FS through grouping. Song et al.
 490 [31] proposed an algorithm, called Fast clustering-bAsed feature Selection algoriThm (FAST),
 491 and benefited from minimum spanning trees (MST) to create feature clusters. They adopted SU
 492 to determine relevance between any pair of features or between the feature and the target class.
 493 Finally, the feature with the highest correlation with the class label is selected from each cluster.
 494 Another study [68] under supervised framework similarly used MST for grouping and variation
 495 of information for relevance measure. Desired number of features and the pruning rate should be
 496 given as inputs in their algorithm. A recent study by Zheng et al. [69] builds the graph by
 497 interaction gain, makes use of MST to produce feature groups and probabilistic consistency
 498 measure for quality metric including two different techniques for FS: in the first one, they apply
 499 the conventional way of selecting representatives from each feature groups; and in the second
 500 they use harmony search as a metaheuristic search. The metaheuristic approach dominates their
 501 first proposed algorithm together with other search mechanisms. Quite recently, the study
 502 proposed by Wan et al [70] employs graph theory for feature grouping and selection in a fuzzy
 503 space. They initially construct the fuzzy space using neighborhood adaptive β -precision fuzzy
 504 rough set (NA- β -PFRS) and then constitute feature groups using MST and acquire the final
 505 subset considering feature-to feature and feature-to class relevance in the space. They achieve
 506 slightly better results in accuracy with reduced number of features in comparison with other FS
 507 approaches and they also show robustness of their model.
 508

509 Speaking of metaheuristic, García-Torres et al. [71] employed Markov blanket for clustering
 510 features and then these predominant groups are involved in Variable Neighborhood Search
 511 (VNS) metaheuristic. Their algorithm yields competitive results in classifier performance and
 512 exhibits effective results in terms of number of features and running time. Another optimization-
 513 based approach in [72] adopted a Scatter Search (SS) strategy based on feature grouping where
 514 Greedy Predominant Groups Generator (GreedyPGG) [71] is used to group features. In their
 515 metaheuristic approach, each solution generated by the search is enhanced with sequential
 516 forward selection for selection of the reduced set of features. Their experimental work shows
 517 comparable classification results with SS but a significant reduction in feature subset size. Song
 518 et al. [73] presents a three-step hybrid study for high dimensional data. Their work initially
 519 removes irrelevant features with SU by a predetermined threshold ρ_0 which is defined as
 520

$$521 \quad \rho_0 = \min (0.1 * SU_{max}, SU_{[D/\log D]-th}) \quad (13)$$

522

523 where SU_{max} is the maximal relevance value between a feature and class labels among all D
524 features. Secondly, it constitutes feature groups using a SU-based clustering approach in which
525 cluster centers are chosen at first and initial number of clusters is not required. As the third step,
526 representative features are selected from clusters based on particle swarm optimization (PSO)
527 with global search capability. Their proposed methodology yields comparative results with
528 respect to accuracy and running time. García-Torres et al. extended their previous SS work in
529 [74], integrating an additional stopping criterion into their algorithm along with hyperparameter
530 tuning. Their experimental results present the effectiveness of the additional stopping condition
531 with respect to the computing time, and also exhibit similar classifier performance with highly
532 reduced size of feature subset among other evolutionary and popular approaches.

533
534 Although many studies focused their attention on discriminative power and redundancy removal
535 of features, most of them neglect the stability of the selected features. Yu et al. addressed this
536 issue in their two studies [57,75]. In [57], rather than relying on typical clustering algorithms,
537 they applied kernel density estimation accompanied by an iterative mean shift procedure to find
538 feature clusters. Subsequently, these feature clusters were evaluated according to relevance using
539 F-statistic and a representative feature is selected within each cluster. The same authors extended
540 this study in [75], where consensus feature groups were identified in an ensemble learning
541 manner and features were extracted in the same way as their first study. The experiments
542 conducted in both studies showed the stability of the selected features.

543
544 All the works mentioned until now are considered as global FS, i.e., finding a reduced subset of
545 global features for the entire population. However, there are cases where these approaches are
546 not applicable. For instance, take an image recognition task, where feature importance may alter
547 since a set of relevant features may be important for identifying a specific object but insignificant
548 for another object at a different position. This gap paved the way for a different technique, called
549 Instance-wise FS that associates each feature's relationship to its labels by assigning a different
550 selector for each instance. Interested readers to grouping and selection of features in this
551 approach can refer to [76,77]. A summary of above-mentioned approaches under the supervised
552 framework is outlined in **Table I**.

553
554 FS approaches based on grouping are not necessarily in the manner of grouping features into
555 clusters and choosing representatives. Distinctly, selection of the features may happen with
556 different cluster configurations. Moshlei et al. [79] initially implement K-means for clustering all
557 samples for a given dataset and a sample from each cluster is chosen at random to acquire the
558 samples with the greatest differences for the preliminary dataset. Subsequently, variances of all
559 features on the determined samples are calculated and a predefined number of features with the
560 highest variances are selected, thereby forming the primary dataset. Thereafter, remaining
561 features are added gradually to this dataset and K-means clustering with a predefined number of
562 clusters is applied iteratively in each step. Features causing changes in the structure of clusters
563 are observed in a repetitive manner and considered as significant. Other features that don't lead
564 to any alteration in clusters are eliminated.

565
566 Another work by Yousef et al. [15] introduced "*recursive cluster elimination*" term into the
567 community and their approach was later adopted in many studies. Since this approach was
568 widely employed by different studies, in Section 4 we elaborate this method in detail by

569 reviewing its application areas and modified usages.

570

571

572

573 **3.2.2. Grouping-based Feature Selection under Unsupervised Setting**

574

575 As with the traditional methods in FS, many of feature grouping-based FS approaches belong to
576 the supervised learning paradigm. Unsupervised FS is more challenging than supervised FS
577 because of no prior knowledge about class labels and unknown number of clusters. Unsupervised
578 FS methods typically involve i) maximization of clustering performance by some index or ii)
579 selection of features based on dependency. Since this paper is about FS, first one is out of scope
580 for this study. Many statistical dependency/distance measures are available in the literature
581 including correlation coefficient, least square regression error, Euclidean distance, entropy, and
582 variance. Selected features in unsupervised FS methods can be evaluated in terms of both
583 classification performance and clustering performance. **Table II** summarizes works on
584 unsupervised FS based on grouping.

585

586 Mitra et al. [80] proposed an unsupervised FS algorithm using feature similarity. A new
587 similarity measure called *maximum information compression index* is introduced in their study.
588 Also, they demonstrated use of representation entropy for measuring redundancy and
589 information loss quantitatively. Features are partitioned into clusters using K-Nearest Neighbors
590 (KNN) principle along with a similarity measure. Entropy metric is chosen as the FS criterion
591 and applied to select a single feature from each cluster to constitute the reduced subset. To
592 evaluate the effectiveness of selected features, the proposed method is compared with KNN,
593 Naive Bayes and class separability including Relief-F for classification capability, and with
594 entropy and fuzzy feature evaluation index for clustering performance. Their algorithm is rapid
595 since no search is required and hence their study is one of the state of the art work in the
596 literature.

597

598 Another example is the study of Li et al. [81], which uses the same similarity measure in [80]
599 and employs a distance function to obtain clusters of features. A representative feature, having
600 the shortest distance to others within a cluster, is selected from each cluster. Their approach is
601 based on hierarchical clustering which enables them to choose feature subsets with different
602 sizes by choosing from top clusters in the hierarchy. Their algorithm works for both
603 unsupervised and supervised learning tasks. Moreover, they run clustering just one time in their
604 algorithm. The authors presented their experimental results for both clustering and classification.

605

606 As stated previously, FS methods developed under unsupervised framework do not utilize class
607 labels. As an example, Covões T.F. et al. [82] presents a comparative study of their approach
608 with the algorithm proposed by Mitra et al [80]. Again, maximal information compression index
609 is utilized to find clusters of features. Hereafter, they employed the simplified silhouette criterion
610 to find optimum clusters, allowing to find the number of clusters as well. The computation for
611 simplified silhouette depends only on obtained partitions, and it is not dependent on any
612 clustering algorithm. Hence, this silhouette is, not only determines the number of clusters
613 automatically, but also it is capable of evaluating partitions acquired by any clustering
614 algorithms. They employed the k-medoids algorithm along with the silhouette method in order to
615 achieve optimum clusters. Then the corresponding medoid for each cluster is selected as the

616 representative feature. The prerequisite for number of clusters known a priori in this algorithm
617 has been overcome by the simplified silhouette since one can implement this algorithm for
618 different values of number of clusters, and then select the best clustering according to the
619 maximum value obtained in the silhouette.

620

621 Another study under unsupervised framework is suggested in [83], where maximal information
622 coefficient and affinity propagation (MICAP) are exploited for selection of features. Features are
623 chosen as the centroid of each cluster in the final step. Although they present competitive results
624 in classification with typical classifiers, no comparison is made for clustering.

625

626 FS methods developed under supervised framework can be an inspiration to unsupervised
627 studies. For instance, Zhou et al. [84] developed an attribute clustering algorithm along with an
628 FS method in an unsupervised manner. They test their algorithm considering different FS
629 methods with different classifiers and achieve slightly improved mean accuracies. The
630 unsupervised FS algorithm proposed by Zhu et al. [85] groups features according to their SU
631 similarities. In their clustering approach, cluster centers are firstly determined and the features
632 are assigned to these centers subsequently. Then, the feature with the highest SU on average is
633 selected from each cluster as a representative based on the following formula

634

635

$$636 \quad AR(f, C) = \frac{\sum_{i=1}^{|C|} SU(f, f_i)}{|C|} \quad (14)$$

637

638 where $AR(f, C)$ is the average redundancy for a feature f in cluster C and $f_i \in C$. Their
639 experiments showed that compared to other methods, the proposed algorithm performs more
640 efficiently in terms of running time and in terms of the size of the reduced subset of features.
641 Also, clustering performance of their algorithm surpasses the compared techniques for various
642 clustering performance measurements. Apart from this, a recent hybrid work which is a
643 combination of grouping and binary ant system (BAS) can be found in [86].

644

645 More recently, Yuan et al. formulated this phenomenon as an optimization problem [87], where
646 their optimization benefits from feature grouping and orthogonal constraints. Clustering
647 performance of their algorithm shows better performance in general compared to other
648 unsupervised FS methods.

649

650

651 **3.2.3. Grouping-based Feature Selection under Semi-supervised Setting**

652

653 There are cases when a significant amount of data is unlabeled and only few samples are labeled.
654 In such a case, the learning problem is denominated as semi-supervised. Quinzán et al. [88]
655 conducted a grouping-based FS study under this setting. In their study, the distance measure
656 between each pair of features is computed by both conditional entropy and conditional mutual
657 information. Next, hierarchical clustering is applied to attain feature clusters and the feature with
658 the highest MI is selected as the representative inside each cluster. They test the performance of
659 their algorithm for a different number of labeled samples with other algorithms and their results

660 exhibit satisfactory performance when there is not enough labeled data. Semi-supervised FS
661 techniques are common in the literature and reviewed in many studies [89–91].

662

663

664

665

666 **4. Feature Grouping with Recursive Cluster Elimination**

667

668 In the original framework [15], the first step in SVM-RCE is to group genes (i.e., features) into
669 clusters using K-means in which correlated gene clusters are identified. As the second step, SVM
670 is used to score and rank these clusters and finally clusters with low scores are eliminated.

671 Remaining genes in clusters are combined and then clustering along with SVM is applied

672 iteratively until a predefined number of clusters are left. In each iteration, surviving genes are

673 used for classification to measure the accuracy at each level. Interests in this method have grown

674 rapidly over time and many studies conducted their research via integrating this approach. The

675 schematic diagram of this approach is illustrated in **Fig. 4**.

676

677 Weis et al. [92] presented a SVM-RCE-like approach where they included assessment of clusters

678 collaboratively rather than evaluating clusters individually. The study of Deshpande et al. [93]

679 utilized SVM-RCE with small modifications for brain state classification.

680

681 Another study by Luo [94] aimed to reduce the computational complexity of SVM-RCE. They

682 apply infinite norm of weight coefficient vector from the SVM model to score each cluster

683 instead of scoring clusters by cross-validation. Their results show considerable reduction in

684 computation time while exhibiting comparative performance as SVM-RCE.

685

686 In the study associated with military service members, in addition to the statistical significance

687 test, SVM-RCE is used to classify individuals between posttraumatic stress disorder (PTSD),

688 postconcussion syndrome (PCS) + PTSD, and controls [95]. In their study, the features refer to

689 the connectivity paths acquired from 125 brain regions. In their experimental works using SVM-

690 RCE, they conclude that higher classification rate (by 4%) is achieved through imaging-based

691 grouping than conventional grouping. Furthermore, imaging measures dominate non-imaging

692 measures by 9% for both conventional and imaging-based groupings.

693

694 Jin et al. [96] conducted a similar study and adopted a modified version of SVM-RCE in their

695 study of brain connectivity. In their study, the diagnostic label of a novel subject is tested

696 whether it belongs to subjects with PTSD or healthy group. The connectivity features are

697 measured from mean resting-state time series taken from 190 regions across the entire brain.

698 They employ SVM-RCE in their experimental work to suggest that dynamic functional and

699 effective connectivity gives higher classification results compared to their static counterparts.

700

701 Interestingly, Zhao et al. [97] applied SVM-RCE tool to the detection of expression profiles

702 identifying microRNAs related to venous metastasis in hepatocellular carcinoma.

703

704 Chaitra et al. [98] conducted a study to identify biomarkers of autism spectrum disorder (ASD)

705 using imaging datasets. They utilized SVM-RCE to assess the classification performance for

706 three distinct feature sets consisting of connectivity features alone, complex network (i.e., graph)
707 measures alone, and a feature set including both. Their accuracy results are not competitive;
708 however, the emphasis is on assessing different feature sets, especially on the combined feature
709 set.

710
711

712 **5. Grouping Features with Biological Domain Knowledge**

713

714 Aforementioned FS approaches typically apply statistical analysis and run computational
715 algorithms to create the feature groups. Hence, these approaches are fully data-driven and they
716 generate the groups of features without using any domain knowledge. However, in some fields,
717 the automatic transformation of data into information via exploiting the background knowledge
718 in the domain is very beneficial. Background knowledge refers to the domain knowledge
719 obtained from the literature, domain experts or from available knowledge repositories [99]. In
720 such fields, the integration of domain knowledge into the feature selection process might
721 improve performance, and also might reveal novel knowledge. For example, in the field of
722 bioinformatics and computational biology, the integration of biological domain knowledge is
723 used to improve the process of feature selection (i.e. gene selection in gene expression data
724 analysis, in other words biomarker discovery) [100,101].

725

726 This section deals with how feature groups are created and how FS is realized using biological
727 external sources. The main idea behind the integration of biological knowledge to FS is to apply
728 a biological function to create groups of features (i.e., groups of genes) and then employ a
729 learning algorithm to score these generated groups. Finally, the genes in the top scoring groups
730 form the reduced subset of features. We would like to note that this section is especially designed
731 for researchers working in the field of molecular biology, genetics, bioinformatics; and we
732 believe that this section is especially informative for those with a biological background. Still,
733 scientists working in different fields can get inspiration from the studies presented in this section
734 and apply similar domain knowledge-based feature grouping in their problems. For example, in
735 the field of text mining, a related tool named TextNetTopics [102] uses Latent Dirichlet
736 Allocation (LDA) to detect topics of words, which serve as groups of features.

737

738 As one of the pioneers in this field, Bellazzi and Zupan discussed the shift of gene expression
739 data analysis approaches from purely data-centric approaches to integrative approaches which
740 aim at complementing statistical analysis with knowledge acquired from diverse available
741 resources [99]. The authors reported that with the growing number of knowledge bases, the field
742 has shifted from purely data-oriented methods to methods that aim to include additional
743 knowledge in the data analysis process [99]. The authors presented the modifications of
744 clustering algorithms for embedding background knowledge. More specifically, the authors
745 provide a survey of approaches that adapt distance-based, model-based and template-based
746 clustering methods so that they take the additional background knowledge into account.

747

748 Yet as another review article in this field, recently Perscheid published a survey on prior
749 knowledge-based approaches for biomarker detection through the analysis of gene expression
750 datasets [100]. In that article, she evaluated the main characteristics of different integrative gene
751 selection approaches; and she presented an overview of external knowledge bases that are

752 utilized in these approaches [100]. It is reported that Gene Ontology (GO) [103] and Kyoto
753 Encyclopedia of Genes and Genomes (KEGG) [104] resources are predominantly used as
754 external knowledge bases for integrative gene selection. The author classified existing integrative
755 gene selection approaches into three distinct categories (i.e., modifying approaches, combining
756 approaches, module extraction approaches). The same review article presented a qualitative
757 comparison of existing approaches and discussed the current challenges for applying integrative
758 gene selection in practice via pointing out directions for future research. An interested reader can
759 refer to [100] for further details.

760

761 As one of the biological knowledge-based feature grouping approaches, Support Vector
762 Machines with Recursive Network Elimination (SVM-RNE) [105], was proposed as an
763 extension of SVM-RCE, which is presented in the previous section. In [105], genes are grouped
764 into clusters using Gene eXpression Network Analysis (GXNA) [106] and clusters with low
765 scores are eliminated in each iteration. The algorithm terminates when some predefined
766 constraints on the number of groups are met.

767

768 As another biological knowledge-based integrative approach, Qi and Tang attempt to incorporate
769 GO annotations into the gene selection process, where they start by finding a discriminative
770 score for each gene (i.e., feature) via applying IG, and eliminating those with a score of zero
771 [107]. The next step is to annotate these genes with GO terms. After that, the score of each term
772 is calculated as the mean of discriminative scores of associated genes involved in the respective
773 term. The GO term with the highest score is determined and the most discriminative associated
774 gene is selected and extracted. The steps including calculation of scores for GO terms and
775 selection of the next most informative gene is repeated until the final subset is formed. Their
776 comparative results with only using IG shows the effectiveness of GO integration in the gene
777 selection process [107]. Some other approaches for biological data integration include Bayesian
778 methods, tree-based and network-based techniques [108].

779

780 Incorporating biological knowledge in the clustering algorithm is reported as a very challenging
781 task [100]. Along this line, the GOstats package [109] allows one to define semantic similarity
782 between the genes via incorporating the GO. As another example of domain knowledge-based
783 gene selection, in SoFoCles [110], genes are initially ranked by typical filter methods such as IG,
784 Relief-F or χ^2 , and then a reduced subset of genes is created using a predefined threshold. Next,
785 for each gene in the reduced subset, semantically similar genes from GO are determined. Finally,
786 top semantically similar genes are selected to enrich the reduced subset. Experimental works
787 conducted using SoFoCles reveal enhancement in classification results by integrating biological
788 knowledge into gene selection.

789

790 An additional study by Mitra et al. [111] adopted the Clustering Large Applications based on
791 RAN-domized Search (CLARANS) technique to gene (i.e., feature) clustering via utilizing GO
792 analysis. In [111], the final reduced feature subset is composed of the genes which were medoids
793 of biologically enriched clusters. Their experimental results showed that the incorporation of
794 biological knowledge enhanced classifier performance and reduced computational complexity.
795 The same authors subsequently made use of a fuzzy technique, Fuzzy Clustering Large
796 Applications based on RAN-domized Search (FCLARANS), to obtain clusters and they selected
797 representative genes from clusters based on the fold change [112].

798

799 The study suggested by Fang et al.[113] utilizes both KEGG and GO terms with IG. In [113], IG
800 is applied on the initial dataset as filtering and then GO and KEGG annotations are explored for
801 the remaining genes. As the next step, association mining is applied to this annotation
802 information and the interestingness of the frequent itemsets is determined by averaging the
803 original discriminative scores of the involved genes. The final gene set is attained via the
804 selection of the highest ranked genes from the top n frequent itemsets. They assessed their
805 method using GO, KEGG, and both against IG and study of [107]. Despite the lower rate of
806 improvement in the overall accuracy, they are able to achieve the increase in accuracy with a
807 significant reduction in the number of genes.

808

809 Yet as another domain knowledge-based gene selection approach, Raghu et al. [114] utilize the
810 KEGG [104], DisGeNET [115] and other genetic meta information in their integrated approach.
811 In their framework, two metrics, i.e., gene importance and gene distance, are computed.
812 Importance score for each gene is calculated using DisGeNET, which is a public platform
813 containing gene collections associated with diseases. Distance between genes is computed based
814 on their chromosomal locations and associations to the same diseases. Both scores are then
815 employed to compose gene sets with maximum relevance and diversity. Compared to variance-
816 based techniques, their method performs better in the predictive modeling task on a small scale.

817

818 Another related study developed maTE tool [116], where gene groups are created based on the
819 miRNA-target gene information, and then each group is ordered by cross-validation. The average
820 accuracy after a specific number of iterations determines the rank of each cluster. Genes on the
821 top m groups are selected as the reduced subset [116].

822

823 As another example, the Grouping-Scoring-Modeling (G-S-M) method benefits from the
824 biological knowledge for its grouping step, followed by the ranking and classification steps
825 [101]. Following the G-S-M approach, CogNet framework [117] initially implements pathfindR
826 [118] to group the genes. The genes in each group are actually the genes of an enriched KEGG
827 pathway, identified as a result of the active subnetwork search and functional enrichment steps of
828 pathFindR. Then, a new dataset involving genes for the specific pathway is created for each
829 group (i.e., pathway). These datasets are scored through Monte Carlo cross-validation (MCCV)
830 and the pathways are ranked according to the assigned scores. Ultimately, genes found in top
831 chosen pathways are taken as selected features and they are used for classification. Another
832 study, developed the miRcorrNet tool [119], which finds gene groups on the basis of their
833 correlation to miRNA expression. Afterwards, these groups are subject to a ranking function for
834 classification. The results showed Area Under Curve (AUC) scores above 95%, proving that
835 miRcorrNet is capable of prioritizing pan-cancer-regulating high-confidence miRNAs. The G-S-
836 M approach has been used by other bioinformatics tools. An example of such tools are:
837 miRModuleNet [120], which detects groups via calculating the correlations between the mRNA
838 and miRNA expression profiles; Integrating of Gene Ontology [121] that uses Gene Ontology
839 information for grouping; PriPath [122] that uses KEGG pathways for grouping; GediNet [123]
840 that uses disease gene associations as groups; 3Mint [124] that employs mRNA expression,
841 miRNA expression and methylation profiles for grouping; and miRdisNET [125] that uses
842 miRNA target gene information while creating the groups.

843

844 Very recently Zhang et al. [126] proposed a method called Distance Correlation Gain-Network
845 (DCG-Net); where they quantify distance correlation gain between features to construct the
846 biological network. In their algorithm, a greedy search method is applied to detect network
847 modules. The edge with the highest weight is selected, then this edge is extended with respect to
848 correlation metric to obtain the module in the network. This is done iteratively to extract modules
849 and the module with the highest distance correlation is selected for analysis. Their experimental
850 results showed effective results in terms of FS and classification accuracy.

851

852 Perscheid et al. [127] comparatively evaluated traditional gene selection methods with
853 knowledge-based methods. Their approach produces gene rankings by integrating knowledge
854 bases and each of these rankings are evaluated with a predefined number of selected genes.
855 Finally, the ranking with the best performance is selected. Moreover, they proposed a framework
856 allowing external knowledge utilization, gene selection and evaluation in an automatic fashion.
857 Although the framework seems to be knowledge base dependent, their experimental results
858 demonstrate that incorporating biological knowledge into the gene selection process improves
859 classification performance, decreases computational running time, and enhances the stability of
860 selected genes.

861

862

863

864 **6. Discussion**

865

866 As stated previously, FS based on feature grouping is a powerful technique with important
867 advantages. Next, one may wonder which FS technique is the best in this context. Surely, it's
868 hard to answer this question because the concept of FS is not dependent only on one parameter.
869 The intrinsic structure and size of the dataset, the learning model and the selected parameters are
870 known as effective factors in the field. In this section we make a cross-comparison and share our
871 deductions among the approaches we have examined in the literature.

872

873 We mentioned before that a typical approach in grouping-based FS is to select representative
874 features from groups. However, selection of multiple representatives from groups may enhance
875 the classifier performance as shown in [128]. In [128], the least correlated feature with other
876 features in the same cluster is selected in addition to the selection of the representative. Hence,
877 higher accuracy values are achieved.

878

879 The superiority of feature grouping is apparent in sequential-based FS because once a feature is
880 selected, features of the same cluster can be discarded at each iteration, thereby diminishing
881 search complexity in total. We particularly want to emphasize here that sequential-based FS
882 approaches generally employ wrapper models which cause huge running time. We motivate
883 researchers for filter-based sequential FS techniques since such an approach benefits both from
884 the strength of feature grouping and from the high speed of filter models as presented in [63,64].
885 Dominance of this approach over deep learning algorithms can be seen in [64]. As a result,
886 sequential approaches are effective in the field since they consider interactivity between features
887 and are also used during subset search in evolutionary approaches [71,74].

888

889 Fuzzy approaches for FS based on grouping are effective because features can belong to more

890 than one cluster rather than typical assignment of a feature to a specific cluster, which can
891 improve the subset quality and accuracy. We should also say that feature-class relevance is an
892 important metric in supervised setting for fuzzy or other approaches and importance of its
893 utilization is specified in [67]. On the other hand, evolutionary algorithms such as genetic
894 algorithms can be implemented as subset search algorithms during the selection process [129].
895 These approaches outperform the conventional way of selecting representatives due to inclusion
896 of inter-feature collaboration as shown in [69]. The main challenge for these algorithms is their
897 high computational cost. A comparison of fuzzy and evolutionary approaches is available in
898 [78], where both methods obtain similar accuracies but the proposed fuzzy technique dominates
899 others in terms of running time and subset quality.

900
901 Incorporating different techniques can increase the strength of an approach rather than sticking to
902 a specific one alone. For instance, the study of [70] combines the advantages of fuzziness, graph
903 theory and conditional mutual information, and acquires better results in general than graph-
904 based or fuzzy approaches.

905
906 As implied in Section 5, integrative gene selection is an important matter when biological data is
907 considered since statistical methods lack the ability to identify the underlying biological
908 processes. Effectiveness of integrating domain knowledge from external sources is reviewed in
909 [100] and [127].

910
911 FS methods based on deep learning (DL) are common in the literature [130-132] but these
912 methods adopt feature extraction, i.e., transformation of the original feature space into a reduced
913 size of new features which leads to loss of original semantics of features. In short, they provide
914 competitive class accuracies but are far from interpretability [133].

915
916 Despite the plenitude of FS techniques, there's still room for further progress in this field. The
917 current studies are mostly based on pairwise interactions; whereas interactions of multiple
918 features should be explored. In addition, running time is still a barrier, and especially for
919 complex algorithms smart steps should be taken on it.

920
921

922 **7. Conclusions**

923
924 The advances in high-throughput technologies have generated large high-dimensional data sets
925 in many applications. The inevitable presence of redundant and noisy features increases
926 computational complexity and degrades classifier capability. Hence, FS has become a required
927 pre-processing step in itself as a primary concern for a long time. Here we present works done in
928 the literature regarding FS techniques through feature grouping. Feature grouping is a powerful
929 and efficient concept; it reduces search space and complexity, is resistant to the variations of
930 samples, gives lower levels internal redundancy and provides better generalization capability to
931 the classifier. The form of feature grouping and selection of features out of groups are
932 determined by different metrics or techniques as reviewed in this paper.

933
934 In FS based on feature grouping, the aim is to first keep similar features together within clusters
935 while maximizing diversity between clusters followed by selection of features out of clusters.

936 We can conclude that sequential and optimization-based (i.e., fuzzy and evolutionary) FS
937 approaches are noteworthy in this context since they take feature interactivity into consideration
938 during the selection phase. Hybrid approaches or utilizing a combination of different techniques
939 are also effective because each method brings its advantage. In case of biological data,
940 integrating external knowledge can yield better results in the overall analysis. In fact, availability
941 of independent and relevant features, correlation between features, and feature correlation to the
942 decision are important items to be taken into consideration. The models with the ability to take
943 these factors into consideration are likely to be effective in FS.

944

945 In this study, our goal is to inform interested readers about the recent trends in FS by feature
946 grouping. Despite the wealth of many techniques in this field, there is still need for enhancement
947 and novelty in the area. We believe approaches mentioned here may provide new insights into
948 designing new schemes for FS in terms of better efficiency, effectiveness, stability,
949 generalization and discrimination.

950

951

952

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Table 1 (on next page)

Applications of FS by Grouping under Supervised Context

1

Table I. Applications of FS by Grouping under Supervised Context

Grouping Method		FS Method (metric)	FS Strategy	Validation	Types of Data	Study
K-means		correlation	selection of features from front rank	classification accuracy	text and microarray	[51]
		SNR, SAM, t-test	checking existence of a feature in other subsets	leave one out cross validation (LOOCV)	microarray	[60]
Hierarchical		Fisher	selection of features from front rank	classification accuracy	miscellaneous	[61]
		average similarity	choosing representative in each group	cross validation	miscellaneous	[53]
Sequential	Correlation-based	trace criterion	features are added sequentially only when trace is maximum.	cross validation	color texture	[64]
	Modified Affinity Propagation	sequential feature selection	applying sequential search in each group and merging selected features	cross validation	miscellaneous	[62]

	ACA	interdependence mesure	selection of mode of each cluster	classification accuracy	synthetic & gene expression	[65]
Fuzzy	Correlation	fuzzy-rough subset evaluation	selection of representative features among groups in the fuzzy environment	classification accuracy	miscellaneous	[78]
	Fuzzy ACA	fuzzy multiple interdependence redundancy		classification accuracy	miscellaneous	[67]
		fuzzy multiple interdependence redundancy		classification accuracy	microarray	[66]
Graph-based		neighborhood adaptive fuzzy mutual information	using feature-to- feature & feature-to-class relevance	cross validation	publicly available datasets	[70]
		probabilistic consistency	i) choosing representative in each group ii) metaheuristic search	cross validation	miscellaneous	[69]

		variation of information	choosing representative in each group	silhouette index & classification accuracy	miscellaneous	[68]
		SU	choosing representative in each group	classification accuracy	miscellaneous	[31]
Evolutionary	GreedyPGG	SS	using SS to find subset of features	cross validation	gene expression & text-mining	[74]
	SU-based	PSO	adopting PSO to determine final subset	cross validation	miscellaneous	[73]
	GreedyPGG	SS	using SS to find subset of features	cross validation	biomedical datasets	[72]
	GreedyPGG	VNS	utilizing VNS to decide reduced subset	cross validation	microarray & text-mining	[71]

Table 2 (on next page)

Applications of FS by Grouping under Unsupervised Context

1

Table II. Applications of FS by Grouping under Unsupervised Context

Grouping Method	FS Method (metric)	FS Strategy	Validation	Types of Data	Study
K-means	generalized incoherent regression model	grouping and selection of optimal features based on orthogonal constraints	unsupervised clustering accuracy (ACC) & normalized mutual information (NMI)	face image & biological datasets	[87]
Louvain community detection	BAS	features in each group are sorted by modified BAS and best features are selected iteratively	classification error rate (CER)	real-world datasets	[86]
SU-based	SU	feature with the highest SU on average is chosen as representative in each cluster	scatter separability criterion, random adjust index, normalized mutual information, F-score	miscellaneous	[85]
K-mode	mode	selection of mode of each cluster	classification accuracy	miscellaneous	[84]

Affinity Propagation	MICAP	centroid of each cluster is selected for final subset	classification accuracy	miscellaneous	[83]
k-medoids	Simplified Silhouette Filter (SSF)	medoid of each cluster is chosen as the representative feature	classification accuracy	miscellaneous	[82]
hierarchical	FS through Feature Clustering (FSFC)	feature with the shortest distance to others is selected in each cluster	Minkowski Score	public gene datasets	[81]
kNN	entropy	a single feature from each cluster is chosen applying entropy	entropy, fuzzy feature evaluation index, classification accuracy	real life public domain	[80]

Figure 1

Three basic types of FS methods.

'(A) Filter. (B) Wrapper. (C) Embedded.'

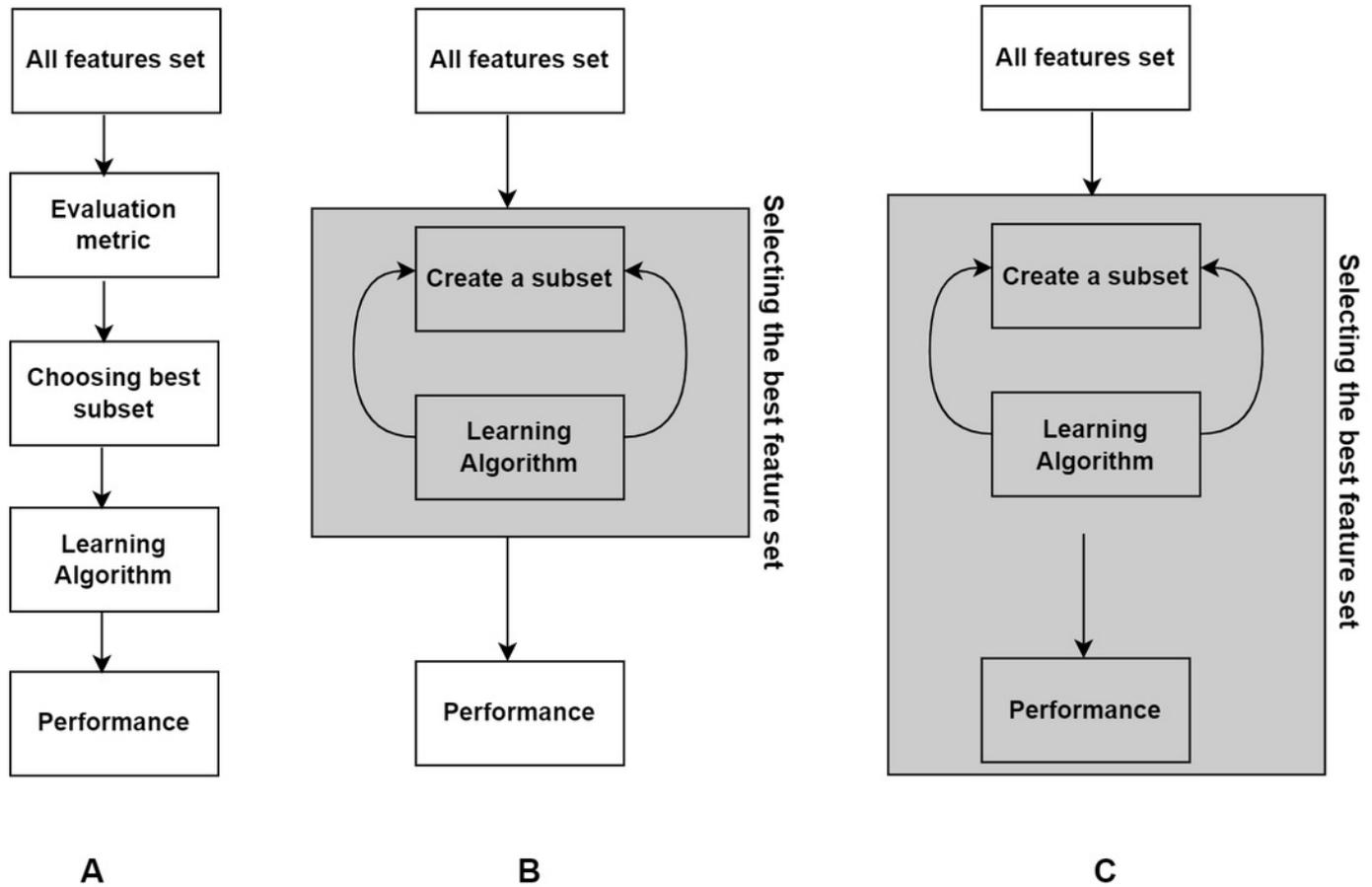


Figure 2

The representation of feature selection approaches based on grouping.

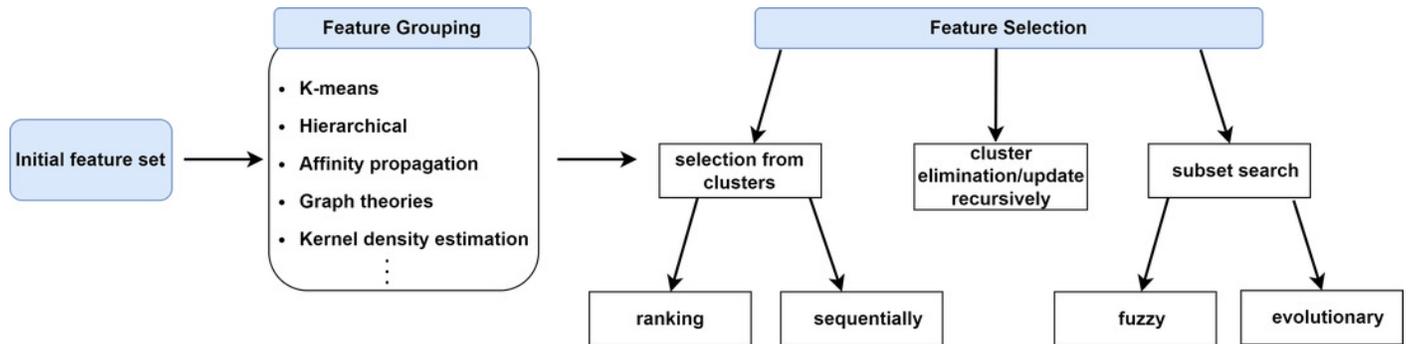


Figure 3

Typical approach for representative feature selection based on grouping.

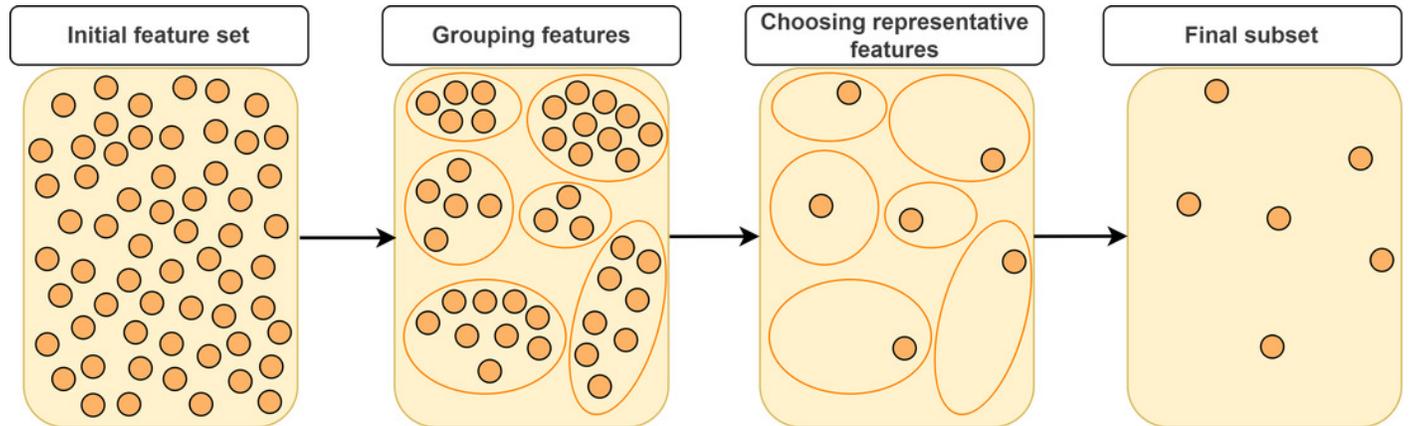


Figure 4

The workflow of the SVM-RCE algorithm.

The Grouping step for grouping genes into clusters, the Scoring step for assigning score for each cluster and selecting significant clusters, the Modeling step for training the model with top-ranked clusters.

