MeLiF+: Optimization of Filter Ensemble Algorithm with Parallel Computing

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Abstract. Search of algorithms ensemble – that is, best algorithms combination is common used approach in machine learning. MeLiF algorithm uses this technique for filter feature selection. In our research we proposed parallel version of this algorithm and showed that it is not only improves algorithm performance significantly, but also improves feature selection quality.

Keywords: feature selection, variable selection, attribute selection, ensemble learning, feature filters, metrics aggregation, MeLiF, parallel computing

1 Introduction

In modern world, machine learning became one of the most promising and studied science areas, mainly, because of its universal application to any data-related problem. One example of such an area is bioinformatics [3; 4; 6; 10], which produces giant amount of data about gene expression of different organisms. This data could potentially allow to determine which DNA pieces are responsible for some visual change of individual, or for reactions to particular environment change. The main problem of such data is its huge number of features and relatively low amount of objects. Because of high-dimensional space, it is very hard to build a model which generalizes such data well. Furthermore, a lot of features in such datasets have nothing in common with results, so, they should be treated as noise.

$$A^* = 4$$

It seems to be logical in this case to select somehow the most relevant features and to learn a classifier on these only. This idea is implemented in such area of machine learning as feature selection. There are three main methods of feature selection: filter selection based on statistical measures of every single feature or features subsets, wrapper selection based on subspace search with classifier result as an optimization measure, and embedded selection that uses classifiers inner properties [12].

The main peculiarity of filter methods is their speed. This leads to the fact that they are frequently used for preprocessing, and resulting subsets of features further passed to other wrapper or embedded method. This is especially important for bioinformatics, where number of features in datasets is sometimes dozens and hundreds of thousands.

These days, many machine learning algorithms use ensembling [1; 4; 8]. MeLiF algorithm [13] tries to apply this method to feature selection. It builds a linear combination of basic filters, that selects the most relevant features. MeLiF has a structural characteristic that it can be easily modified to work in concurrent or distributed manner. At this research, we implemented parallel version of MeLiF called MeLiF+ and achieved significant speed improvement without losing in selection quality.

The remainder of the paper is organized as follows: MeLiF algorithm is described in Section 2, parallelization scheme is proposed in Section 3, experiment setup and used quality measures are outlined in Section 4, and finally experiment results are contained in Section 5.

2 MeLiF

Algorithm treats some linear combinations of basic filters as starting points. It has been observed during experiments that the best option is this following choice of starting points: $(1, 0, \dots, 0)$, $(0, 1, \dots, 0)$, $\dots$, $(0, 0, \dots, 1)$ – only one basic filter matters at the beginning, and $(1, 1, \dots, 1)$ – all basic filters are equal at the beginning. Algorithm iterates over the starting points and tries to shift each coordinate value to small constants $+\delta$ and $-\delta$ – value of grid spacing for each point. If some of applied changes succeed, i.e. quality measure for a point after a shift is greater than the maximum value: the algorithm chooses that point and starts searching from its first coordinate. If, all coordinates were shifted to $+\delta$ and $-\delta$ and no quality improvement observed, algorithm stops.

Algorithm 1 MeLiF algorithm

Input: points, delta, evaluate

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1:  $q^* \leftarrow 0$ 
2:  $p^* \leftarrow 0$ 
3: for each  $p \in \text{points}$  do
4:    $q \leftarrow \text{evaluate}(p)$ 
5:   if  $q > q^*$  then
6:      $p^* \leftarrow p$ 
7:      $q^* \leftarrow q$ 
8:  $\text{smthChanged} = \text{true}$ 
9: while  $\text{smthChanged}$  do
10:  for each  $\text{dim} \in p.\text{size}$  do
11:     $p^+ \leftarrow p$ 
12:     $p^+[\text{dim}] \leftarrow p^+[\text{dim}] + \text{delta}$ 
13:     $q^+ \leftarrow \text{evaluate}(p^+)$ 
14:    if  $q^+ > q^*$  then
```

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15:       $q^* \leftarrow q^+$ 
16:       $p^* \leftarrow p^+$ 
17:       $smthChanged = \mathbf{true}$ 
18:      break
19:       $p^- \leftarrow p$ 
20:       $p^-[dim] \leftarrow p^-[dim] - \delta$ 
21:       $q^- \leftarrow evaluate(p^-)$ 
22:      if  $q^- > q^*$  then
23:           $q^* \leftarrow q^-$ 
24:           $p^* \leftarrow p^-$ 
25:           $smthChanged = \mathbf{true}$ 
26:          break
27: return( $p^*, q^*$ )

```

Then, for each point obtained during coordinate descent, the algorithm measures value of resulting linear combination of basic filters for each feature in dataset. After that, results are sorted, and the algorithm selects N best features. Then, the algorithm runs some classifier only with that feature subset. The obtained result is saved for comparing with other points and caching. It helps to reduce working time due to visited points usage.

3 MeLiF+

We proposed the following improvements to the MeLiF method: each starting point is processed in a distinct thread with global maximum maintained through synchronization point. Moreover, *evaluate* submethod is run concurrently for $+\delta$ and $-\delta$, and selects the best point after retrieving both results. We showed that it not only improves the algorithm performance on multicore system, but also usually improves feature selection quality.

This fact has the following explanation: the original MeLiF algorithm is greedy, so it assumes that if each point it steps in is a local optimum then resulting point will be the global optimum, adding an ability to lookup for two deltas simultaneously allows algorithm to select better local optimum. Also, as starting points are processed in parallel, one thread can find a local optimum. This causes other threads to stop their work even if further descent leads to the better result. This can cause different selection result, better or worse (both cases are presented in Section 5), but experiments show that average MeLiF+ results are better.

4 Experiments

We used SVM [5] from WEKA [14] library, with polynomial kernel and soft margin parameter $C = 1$ as classifier. To improve stability, we used 5-fold cross-validation. The number of selected features was constant: $N = 100$. In order to compare our method with the old one, we used F_1 score [11] of SVM classifier.

As we wanted to know how much our method differs from the original one in terms of space search strategy, we calculated z -score for each dataset.

We ran our experiments on a machine with following characteristics: 32-core CPU AMD Opteron 6272 @ 2.1 GHz, 128 GB RAM. We used $N = 50$ threads, $N = 2 \cdot p \cdot f$ threads, where p is the number of starting points, f is the number of folders used for cross-validation.

As basic filters, we used Spearman Rank Correlation (SPC), Symmetric Uncertainty (SU), Fit Criterion (FC) and Value Difference Metric (VDM) [2; 9]. For each dataset, we executed MeLiF and MeLiF+ and stored their working time and points with the best classification result.

We used 50 datasets of different sizes: 33 datasets have been taken from Gene Expression Omnibus, 5 from Kent Ridge Bio-Medical Dataset, 5 from RSCTC'2010 Discovery Challenge, 4 from Broad institute Cancer Program Data Sets, 3 from Feature Selection Datasets at Arizona State University. Some datasets were multi-labeled, therefore we splitted them into several derivative binary datasets with commonly used one-versus-all technique. Then we excluded datasets that contained too few instances of one of the classes. After that, we used standard feature scaling and discretized all features to 11 different values from -5 to 5.

5 Results

Table below contains experiment results. All the datasets are sorted by their total size which is basically a multiplication of their features and objects number. In F_1 score comparison of MeLiF and MeLiF+ better results for each dataset are highlighted in grey, equal results are not highlighted. Runtime is presented in seconds. At the last column, z -score is provided.

Table 1: MeLiF in comparison with swarm algorithms

Dataset	Size	F_1 score		Time		z -score
		MeLiF	MeLiF+	MeLiF	MeLiF+	
SRBCT30	191k	0.900	0.891	13	2	0.23
SRBCT31	191k	1.000	1.000	17	3	0
GDS2960	417k	0.971	0.980	33	7	-10.98
CNS	427k	0.742	0.791	33	6	-1.06
Leuk3c0	513k	0.986	0.986	34	5	0
Leuk3c1	513k	0.933	0.933	33	5	0
GDS2961	566k	0.845	0.845	49	13	0
GDS2962	566k	0.784	0.887	45	11	-11.15
DLBCK	962k	0.799	0.734	65	13	4.67
GDS2901	1337k	1.000	1.000	88	17	0
Prostate	1713k	0.925	0.903	93	34	7.27
GDS4109	1760k	0.936	0.936	142	38	0
GDS5083	2131k	0.862	0.862	195	60	0

d2t0	2339k	0.765	0.765	172	71	0
d2t1	2339k	0.779	0.844	180	60	-9.73
breast	2346k	0.769	0.812	161	24	-11.71
GDS4261	2367k	1.000	1.000	130	16	0
GDS3257	2384k	0.980	1.000	131	17	-33.65
GDS4901	2515k	0.899	0.946	220	60	-7.6
GDS3553	2543k	1.000	1.000	142	18	0
GDS3116	2584k	0.826	0.826	142	23	0
GDS4336	2598k	0.865	0.865	200	66	0
GDS5047	2925k	0.989	0.989	185	41	0
GDS3995	3200k	1.000	1.000	181	24	0
GDS496840	3296k	0.890	0.890	226	40	0
GDS496841	3296k	0.953	0.936	224	40	4.04
GDS2947	3499k	1.000	1.000	217	28	0
GDS43181	3591k	0.913	0.913	275	64	0
arizona5	3738k	0.730	0.754	219	67	-7.47
Ovarian	3833k	1.000	1.000	192	23	0
GDS4103	4264k	0.918	0.918	265	71	0
GDS2771	4265k	0.760	0.760	299	81	0
GDS503730	4428k	0.738	0.826	243	140	-16.77
GDS503732	4428k	0.782	0.782	293	69	0
GDS3929	4488k	0.821	0.821	376	74	0
GDS483731	4811k	0.920	0.920	413	130	0
GDS483733	4811k	0.951	0.951	316	48	0
d5t	4860k	0.869	0.869	370	70	0
GDS3622	4961k	1.000	1.000	266	33	0
GDS2819	5412k	0.991	1.000	436	149	-4.05
d6t	5428k	0.792	0.792	381	69	0
GDS4130	5685k	1.000	1.000	315	39	0
d4t	6178k	0.719	0.719	513	124	0
GDS4129	6561k	1.000	1.000	354	43	0
GDS4222	7107k	0.965	0.971	454	84	-7.42
GDS4431	7973k	0.802	0.802	537	100	0
arizona1	8847k	0.823	0.823	558	85	0
GDS4600	9294k	0.979	0.968	472	124	23.27
GDS3244	9787k	1.000	1.000	505	65	0

As it can be seen from the table above, MeLiF+ is always at least 3 times faster than the MeLiF, and this difference gets up to 6 times for some datasets. Although MeLiF and MeLiF+ have almost the same results in F_1 score, there is some difference in their work on 15 datasets as provided via z -score. But only in 5 cases MeLiF+ had worse results than original the MeLiF algorithm. But on 36 datasets, they performed equally and at 11 datasets new algorithm outperformed the original one.

6 Conclusion

The proposed parallelization scheme made algorithm in average to work 5.5 times faster without affecting selection quality. Unfortunately, in this research we did not achieved linear speed improvement because of the fixed maximum of parallel processed points. In our future work, we are planning to use threads pool which is limited by the testing system and achieve linear speed growth with using exploration and exploitation [7] strategy to spread the search points in the search space. Also this should lead to high increase in optimized measure.

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