Towards a Framework for Designing Full Model Selection and Optimization Systems

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Motivations

End-users of ML/DM now have to face the new problem of how to choose a combination of data processing tools and algorithms.

This problem is usually termed the Full Model Selection problem.

Full Model Selection (FMS)

The FMS problem consists of the following[1]:

Given a pool of preprocessing methods, feature selection and learning algorithms, select the combination of these that obtains the lowest classification error for a given data set.

FMS tasks also include the selection of hyperparameters for the considered methods, resulting in a vast search space.

[1] Escalante et al., Particle Swarm Model Selection. JMLR (2009)

Data Mining Operators

We attempt to define a search space that consists of all data mining actions (operators) that are available to a given data set for a user-specified goal, such as:

- a set of outlier filters
- a set of feature generation, transformation and selection methods
- a set of learning algorithms
- ...

In this sense, we call the subject of interest "the space of data mining operators (DMO)", or simply "the DMO space".

The DMO Space

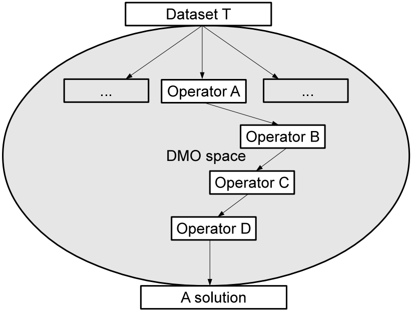


Figure: An illustration of the DMO space

Due to the resources at hand, usually we do not search in an infinite DMO space, and, moreover, we can make the DMO space a finite space by defining the DMOs that are to be included.

Related Work - The PSMS System

- The PSMS system (Escalante et al., JMLR, 2009) is an application of Particle Swarm Optimization (PSO) to the problem of FMS for binary classification problems.
- In total, 3 feature transformation objects, 13 feature selection objects and 10 classifier objects are used in the PSMS system.
- A full PSMS model is defined as a 16-dimensional particle position.

Related Work - The PSMS System

From the system architecture point of view, PSMS assumes a full model has three components: feature transformation, feature selection, and learning algorithm.

In the DMO framework, we can define the following DMO template for the search space covered by the PSMS system:

$$solution \Longleftarrow \quad DMO_{chain-search}(DMO_{random-topology-search}(DMO_{[feature-transformation]}, DMO_{[feature-selection]}), DMO_{[algorithm]})$$

The GPS Search Strategy

We propose a search strategy, which combines both a genetic algorithm (GA) and particle swarm optimization (PSO).

- GA is used for searching the optimal template structure of a DMO solution (structure space)
- PSO is used for searching the optimal parameter set for a particular solution instance (parameter space)

The algorithm is named GPS (**G**A-**P**SO FM**S**). It can be seen as a realization and an application of the DMO framework.

The GPS Search Strategy

We assume a FMS solution consists of five DMOs:
$DMO_{[data-cleansing]}$, $DMO_{[data-sampling]}$, $DMO_{[feature-transformation]}$, $DMO_{[feature-selection]}$, and $DMO_{[algorithm]}$.

A DMO template for the FMS problem covered by GPS is defined as:

$$
\begin{aligned}
& solution \Longleftarrow \\
& \quad DMO_{chain-search}(\\
& \quad\quad DMO_{random-topology-search}(\\
& \quad\quad DMO_{[data-cleansing]}, DMO_{[data-sampling]}, \\
& \quad\quad DMO_{[feature-transformation]}, DMO_{[feature-selection]}), \\
& \quad DMO_{[algorithm]})
\end{aligned}
$$

The GPS Search Strategy

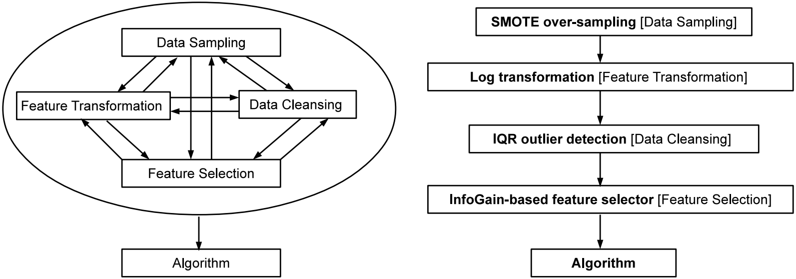


Figure: Left: a graphical representation of the DMO template used by GPS; Right: a DMO solution instance

The GPS Algorithm

Algorithm 1 Pseudocode of the GPS strategy for searching a FMS solution

procedure GPS(T,P,M,W,G)

Input:

T (number of generations for GA), P (population size for GA), M (number of evolutions for PSO), W (swarm size for PSO), G (goal metric)

Get P random template instances based on template (3).

Populate template instances with objects in the DMO pools (Table 2)

for $i \leftarrow 1$ to T **do**

Use a standard PSO procedure **PSO**(M,W,G,I) to search for the optimal parameters for each template instance I (optimising the goal metric G), and assign an evaluation score to each template instance I. This procedure is similar to the PSMS system [3].

Do *crossover* // single point crossover among the top 20% template instances.

Do *mutation* // randomly choose 30% template instances from the population, and randomly change one DMO in each template instance.

Replace the worst N template instances with the N new template instances generated in above two steps, here we use $N = (20\% + 30\%) \times P$.

$solution_{best} \leftarrow population_{best}$

end for

return $solution_{best}$

end procedure

Generate initial solution structures and instances

Optimize a solution instance

Generate new solution structures and instances

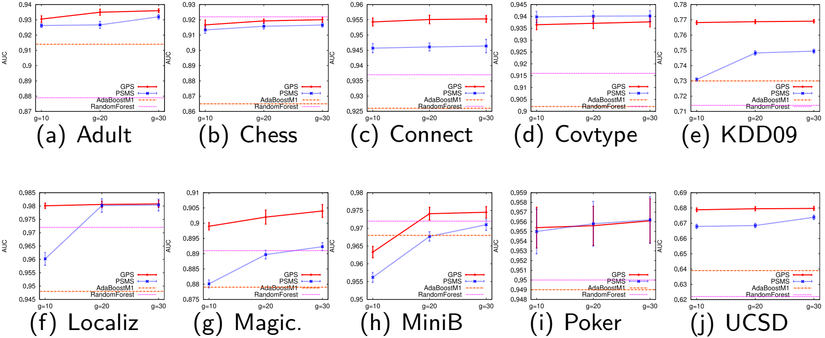
Experiments

1. Comparing GPS to PSMS and other algorithms
2. Speeding up the GPS system

Experiments: Datasets

Original data sets			Final binary data sets
Data set with release year	#Insts	Atts:Classes	Class distribution (#Insts)
Adult 96	48,842	14:2	23% vs 77% (10,000)
Chess 94	28,056	6:18	48% vs 52% (8,747)
Connect-4 95	67,557	42:3	26% vs 74% (10,000)
Covtype 98	581,012	54:7	43% vs 57% (10,000)
KDD09 Customer Churn 09	50,000	190:2	8% vs 92% (10,000)
Localization Person Activity 10	164,860	8:11	37% vs 63% (10,000)
MAGIC Gamma Telescope 07	19,020	11:2	35% vs 65% (10,000)
MiniBooNE Particle 10	130,065	50:2	28% vs 72% (10,000)
Poker Hand 07	1,025,010	11:10	45% vs 55% (10,000)
UCSD FICO Contest 10	130,475	334:2	9% vs 91% (10,000)

Experiment 1: Comparing GPS to PSMS



(a) Adult (b) Chess (c) Connect (d) Covtype (e) KDD09

(f) Localiz (g) Magic. (h) MiniB (i) Poker (j) UCSD

- GPS wins in 83% (25 out of 30) evaluation setups (benefit of combining GA and PSO for the FMS problem)
- The best performance of both GPS and PSMS outperform AdaBoost. and RF on 9 datasets (advantage of a full model over the single algorithm model)
- GPS outperforms the baseline algorithms with big margin on imbalanced datasets

Experiment 2: Speeding Up the GPS System

Some observations

- The training complexity of the GPS algorithm depends on the base learners found and evaluated during the search.
- The main cost for GPS is the cost for estimating a base learner's performance (e.g., cross-validation).

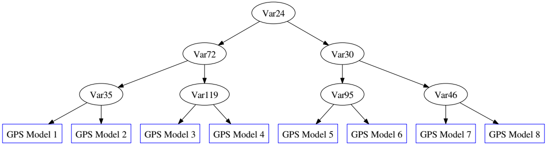
Users may have to wait for several hours, or even days on relatively large data sets. Therefore, in this work we also present a strategy for speeding up the GPS algorithm.

Experiment 2: Speeding Up the GPS System

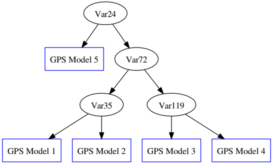
Full Model Trees (FMT):

Instead of training the GPS algorithm on the full training data, we build GPS models at the leaves of a tree structure.

Experiment 2: Speeding Up the GPS System



(k) FMT-perfect



(l) FMT-random

We compare GPS to Full Model Tree with two different tree structures, namely, the perfect binary tree and the random binary tree.

Experiment 2: Speeding Up the GPS System

Theoretically (theorem 1 and 2, pp. 9-10), the two Full Model Tree variants are faster than GPS-0 in the case that the (empirical) training complexity of GPS-0 is worse than linear.

Experiment 2: Speeding Up the GPS System

Table: Performance and runtime of the GPS and the Full Model Tree algorithms; A "$\ominus$" indicates that in terms of AUC, the GPS algorithm is significantly better than the respective algorithm; A "$\Diamond$" indicates that in terms of runtime, the GPS algorithm is significantly slower than the respective algorithm

Dataset	**GPS**	**FMT-perf.**	**FMT-rand.**	**GPS**	**FMT-perf.**	**FMT-rand.**
	AUC			Runtime (mins)		
Adult	0.94	0.93	0.93 $\ominus$	45 $\pm$ 6	37 $\pm$ 4 $\Diamond$	48 $\pm$ 11
Connect-4.	0.95	0.95	0.95 $\ominus$	91 $\pm$ 5	77 $\pm$ 9 $\Diamond$	74 $\pm$ 14 $\Diamond$
KDD Cup.	0.77	0.77	0.76 $\ominus$	178 $\pm$ 9	157 $\pm$ 11 $\Diamond$	189 $\pm$ 8
Mini.B.E.	0.98	0.98 $\ominus$	0.97 $\ominus$	124 $\pm$ 7	123 $\pm$ 9	135 $\pm$ 12
UCSD.	0.68	0.68 $\ominus$	0.67 $\ominus$	487 $\pm$ 16	417 $\pm$ 19 $\Diamond$	476 $\pm$ 17

Summary

- The DMO framework for designing new FMS algorithms
- The GPS algorithm for FMS
- Speeding up GPS with the perfect-binary-tree structure

A GUI for FMS

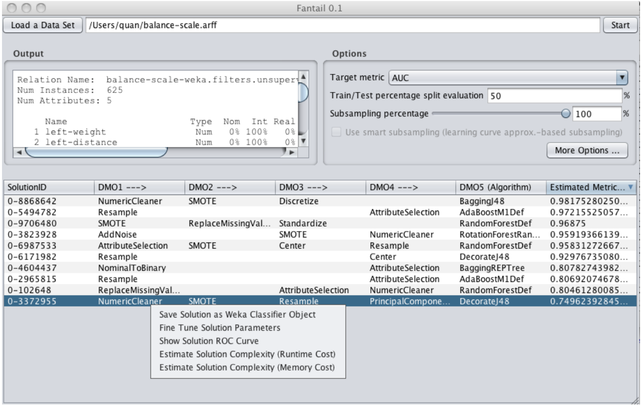


Figure: A proof-of-concept system based on the DMO framework using the GPS algorithm as the optimisation engine.

Questions

Thank you :-)