Poster #59

IMPROVED FEATURE SELECTION WITH SIMULATION OPTIMIZATON

Sara Shashaani, Kimia Vahdat
Industrial and Systems Engineering
North Carolina State University

PRESENTER: Sara Shashaani

EDWARD P. FITTS DEPARTMENT OF INDUSTRIAL AND SYSTEMS ENGINEERING

Why not include all features in the model?

- Overfitting
- Computationally expensive
- Less inference or interpretation power

Research Methodology

Given a learning model (linear regression, random forest, *etc.*) we look for the best subset of features

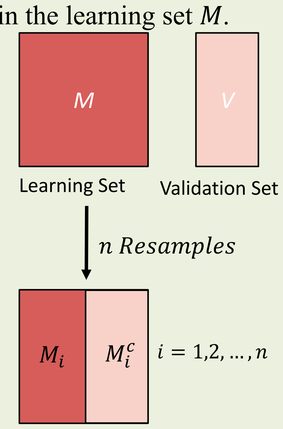
$$S^* = argmin_S \sum_{j \in V} (f_{M,A,S}(x_j) - y_j)^2$$

where $f_{M,A,S}(x_j)$ is the prediction model trained by the subset S of features of the learning set M with the learning algorithm A.

Estimate with its Sample Average Approximation

$$\hat{S}^* = argmin_S \frac{1}{n} \sum_{i=1}^{n} \sum_{j \in M_i^c} (f_{M_i,A,S}(x_j) - y_j)^2$$

where Mi and M_i^c are resampled training and test sets within the learning set M.



Experiment

We compare the performance of Simulation Optimization based Feature Selection SOFS with *Genetic Algorithms* as the optimization method

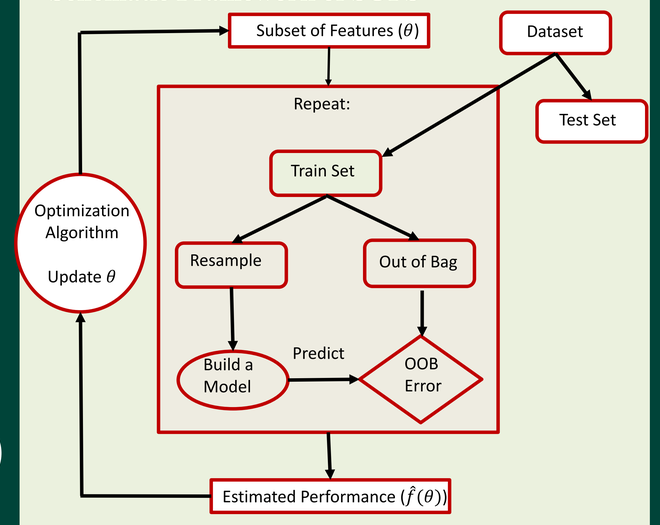
- in terms of mean absolute and squared error;
- with that of *Recursive Feature Elimination (RFE),* the commonly used greedy approach that looks for the best subset size

$$d^* = argmin_d \frac{1}{n} \sum_{i=1}^{n} \sum_{j \in M_i^c} (f_{M_i,A,d}(x_j) - y_j)^2;$$

- on a sample dataset from UCI repository with 55 features and 226 observations;
- on a two learning algorithms: linear regression (LM), and random forest (RF).

When looking in a dataset with many features for the most informative ones, we can develop an **optimization** problem that estimates the predictive accuracy of a prediction model with any subset of features by mimicking a **simulation** of the system under consideration, for which we only have the available data, through resampled datasets.

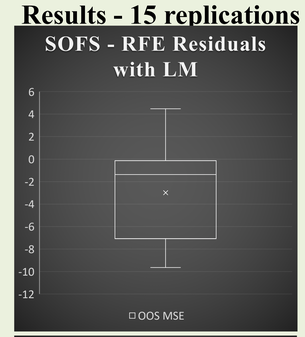
Schematic Framework of SOFS

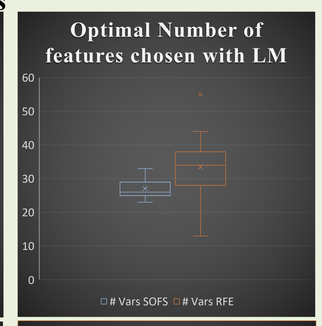


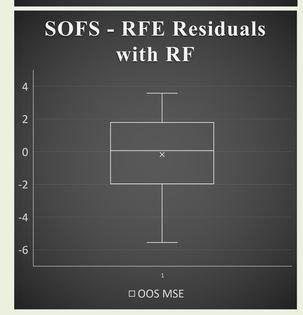
Results - One replication

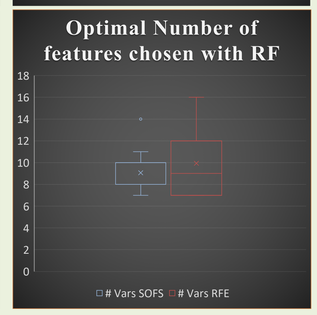
RFE vs. SOFS		# Feat	IS MAE	OS MAE	IS MSE	OS MSE	Time
LM	RFE	33	2.44	3.45	11.92	22.56	.
	GA	27	2.38	3.17	11.62	19.58	.
RF	RFE	10	2.87	3.49	15.15	22.15	0.30
	GA	9	2.79	3.44	14.35	21.98	1015.56

Results - 15 replications









Conclusion

- SOFS gains higher accuracy in predictions and more precision in number of features for both LM and RF.
- The optimization routine GA is only run for a limited budget so in RF it can stop before convergence. More efficient optimization routines are under study.

NC STATE UNIVERSITY

FOPAM
Foundations of Process Analytics and Machine learning
The StateView Hotel — Marriott Autograph Collection
Raleigh, North Carolina — August 6 - 9, 2019

CACHE Computer Aids for Chemical Engineering