Enhancing and Automating University Reporting Of R&D Expenditure Data Using Machine Learning Techniques¹

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Tigher Education Spending on Research and Development

In 2014, U.S. Colleges and Universities reported spending \$67.3 billion on Research & Development (R&D). While this figure constitutes only about 15 percent of the nation's total R&D effort, colleges and universities performed more than half of U.S. basic research.² Most of what we know about R&D performed at the nation's colleges and universities—not only aggregate totals, but also expenditures by field of study and by individual institutions – is derived from data collected by the National Science Foundation's (NSF) National Center for Science and Engineering Statistics (NCSES) as part of its Higher Education R&D (HERD) survey. The HERD survey continued and expanded a data collection effort that was started in 1972 as the Academic R&D Expenditures Survey.

The data collected by the HERD survey are widely used by both university administrators and academic researchers interested in understanding the nation's scientific enterprise. University leadership is interested in tracking total R&D expenditures and rankings of R&D expenditures as an indicator of research prowess. Most universities work to move up in the rankings by increasing their expenditures. Scholars interested in the political economy of federal science funding have used HERD expenditure data to track the expansion of the nation's cadre of research universities and to assess the tendency of the political system to promote more equal distribution of funds across states and regions (Geiger and Feller 1995; Graham and Diamond 1997; Feller 2001). Others have used more disaggregated data on expenditures at the

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discipline level to explore either how funding is related to scientific productivity (Adams and Griliches, Rosenbloom et al 2015) or to uncover factors that influence the allocation of federal R&D funding across institutions (Lanahan et al 2016; Rosenbloom and Ginther forthcoming).

The data collected in the HERD and the earlier Academic R&D Survey are derived from institutional responses to an annual survey distributed by NCSES. Colleges and Universities undoubtedly take different approaches to compiling the necessary data, but at research universities with specialized research administration staff, responsibility for responding to the survey is likely delegated to one or more specialists within the office of sponsored research or institutional research.

The aforementioned method of collecting data on college and university R&D expenditures results in three distinct problems. First, responding to the HERD is costly in terms of the time accurately required to report the requested data. Second, because of the nature of the annual survey and the lead time involved in tabulating responses, the data are available only with a long lag. While the data are useful for retrospective analysis, the lags make them far less valuable for setting institutional strategy or performing real-time analysis of R&D activity. Finally, the effort to classify projects by

their purpose and field of study is inevitably subjective, making it problematic to make comparisons across institutions and introducing spurious variation within institutions when responsibility for data collection shifts from one person to another.³

To address these problems, we have been engaged in an experiment to apply techniques of machine learning to automate project classification. Successful development of classification algorithms would reduce the cost of responding to the HERD survey, allow for essentially real-time tracking of expenditures, and offer the potential to increase the consistency of classification over time and across institutions. As we describe here, our proof of concept investigation suggests that such approaches are potentially feasible, but require further efforts.

Application of Machine Learning to Classify Sponsored Research Projects

With the growth of large data sets and the declining cost of computation, application of machine learning techniques to identify data patterns and make predictions based on these patterns has become increasingly common.⁴ The goal of our project is to develop a classification algorithm that can be used to either supplement or replace human judgement in classifying sponsored research projects. To do so, we begin with a set of sponsored projects awards that have already been classified by Research Administration staff at the University of Kansas. In

³ The survey categorizes projects into 4 different purposes (applied research, basic research, development, and other), and 40 different scientific fields of study (e.g., Bioengineering and Biomedical Engineering, Astronomy and Astrophysics, Political Science and Government, etc.).

⁴ For an overview of machine learning and associated terminology see: <u>https://en.wikipe-</u> <u>dia.org/wiki/Machine_learning</u>

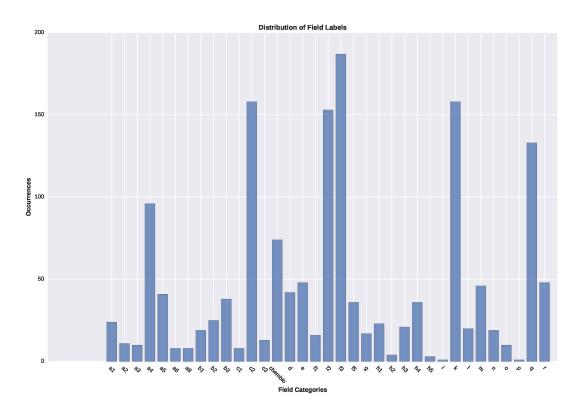
the language of machine learning, this is an example of "supervised learning."

Working with staff in the University of Kansas Office of Research, we obtained a data set of historical sponsored project awards. After dropping awards for which we did not have complete data, we were left with approximately 1,500 projects. For each of these projects, the data included information on the:

- Project sponsor
- Principle Investigator (PI) home unit
- Project abstract describing the project
- Human-assigned classification of the project's purpose and field of study.

Figures 1 and 2 show the distribution of projects across fields of study and purpose based on the human-assigned classification. In addition to the full list of NSF-defined fields of study, our data include KU-specific fields of "Chem-Bio" and "CEBC" (that combines projects across chemistry, chemical engineering and biomedical sciences) that are used for internal institutional purposes.⁵ As Figure 1 illustrates, there are some fields for which we do not have a large number of projects. The distribution of projects by purpose is also somewhat uneven, as illustrated in Figure 2.

Figure 1: Distribution of Projects by Field of Study



⁵ For reporting purposes, expenditures in the Chem-Bio and CEBC categories are split evenly

between the Chemistry and Biological and Biomedical Sciences and Chemistry and Chemical Engineering, respectively.

following codes.	
Field	Code
Computer and Information Sciences	А
Aerospace / Aeronautical / Astronautical Engineering	B1
Bioengineering and Biomedical Engineering	B2
Chemical Engineering	B3
Civil Engineering	B4
Electrical, Electronic, and Communications Engineering	B5
Industrial and Manufacturing Engineering	B6
Mechanical Engineering	B7
Metallurgical & Materials Engineering	B8
Other Engineering	B9
Atmospheric Sciences and Meteorology	C1
Geological and Earth Sciences	C2
Ocean Sciences and Marine Sciences	C3
Other Geosciences, Atmospheric, and Ocean Sciences	C4
Agricultural Sciences	D1
Biological and Biomedical Sciences	D2
Health Sciences	D3
Natural Resources and Conservation	D4
Other Life Sciences	D5
Mathematics and Statistics	E
Astronomy and Astrophysics	F1
Chemistry	F2
Materials Science	F3
Physics	F4
Other Physical Sciences	F5
Psychology	G
Anthropology	H1
Economics	H2
Political Science and Government	H3
Sociology, Demography, and Population Studies	H4
Other Social Sciences	H5
Other Sciences	I
Business Management and Business Administration	К
Communication and Communications Technologies	L
Education	М
Humanities	Ν
Law	0
Social Work	Р
Visual and Performing Arts	Q
Other Non-S&E Fields	R
	IX.

Notes to Figure 1: The University of Kansas Fields of Study are denoted with the following codes.

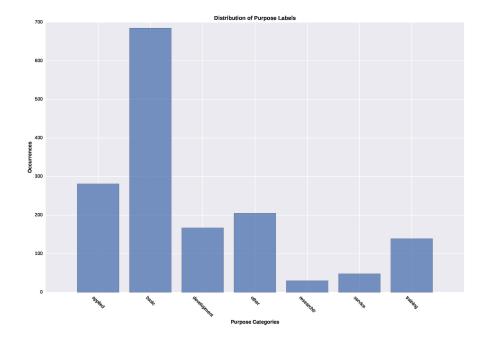


Figure 2: Distribution of Projects by Purpose

The major source of information about each project comes from the proposed statement of work, which is treated as a "bag of words." As a first step, we pre-process the data by standardizing word forms and eliminating "stopwords" (e.g. the, is, to). Individual (or collections of) words are converted to a numerical form based on their frequency of occurrence within and between project abstracts. In machine learning, these numerical representations are referred to as "features." The goal of the machine learning algorithm is to assess which specific combination of features are useful to discriminate between purpose/field categories.

Once the data are processed, we experimented with a selection of commonly used classifiers to identify features that provide predictive power. Following standard practice, we split the data into training and testing samples. The training sample contains approximately 70% of the observations, while the testing sample contains the remaining 30%. The models are trained on the training sample (which is further split into $\cdot \mu^{p\pm\pm}a$ and validation samples) via a cross-validation procedure, which is necessary to prevent the models from over-fitting (i.e. "mem orizing") the data. We estimate the prediction error of the models using the validation samples, and use the testing sample as an assessment of generalization error.

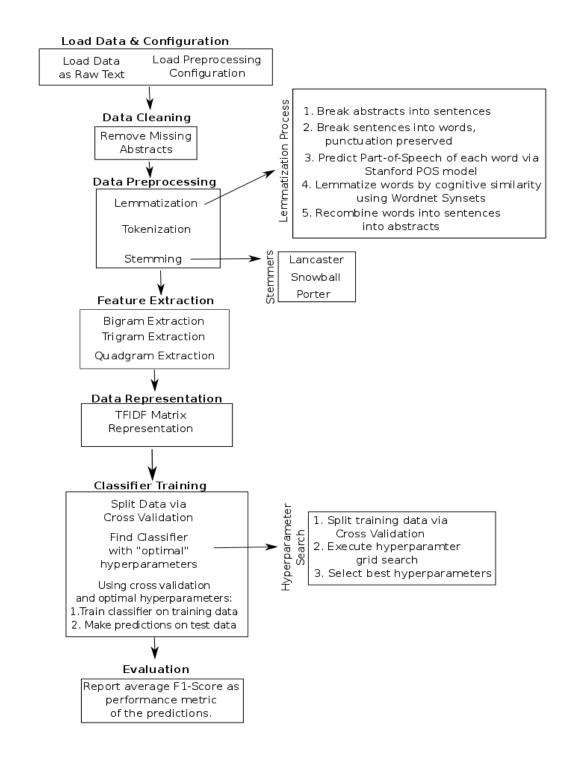


Figure 3: Schematic Representation of Data Analysis Steps

We treat the prediction of purpose and field categories as two separate classification tasks. For each classification problem we tried the following classifiers:

- Decision Tree
- Support Vector Machine
- Logistic Regression
- Random Forest
- Naïve Bayes
- Neural Network

All of these classification schemes are binary: reporting a probability that the project belongs to a particular purpose/field. For each purpose/field, the classifier yields a predicted probability (between 0 and 1) or a categorical determination that the project belongs to that purpose/field. We first find classifiers for each purpose/field by assessing their performance (as described below) and then assign projects to a single purpose/field using the purpose/field with the highest predicted probability across all the classifiers.

The result of our analysis is a prediction of the purpose/field to which each project should be assigned. Comparing the human- and machine-assigned results produces a two-way contingency table depicted in Figure 4. Projects for which the two classifications agree (T1 and T2) are successful predictions, whereas cases where the assignment is different (F1 and F2) are unsuccessful.

Actual Outcome	Predicted Outcome		
	In Field/Purpose	Not in Field/Purpose	
In Field	T1	F1	
Not in Field	F2	T2	

Figure 4: Project Classification Outcome	es
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A number of measures of the performance of machine learning algorithm are possible. The "accuracy" of the predictions is simply the number of correct predictions as a share of all predictions:

(T1+T2)/(T1+T2+F1+F2)

Where the distribution of outcomes is uneven, however, this measure may not be very illuminating. For example, in a binary classification problem where 90% of observations are not in a field, simply guessing that no projects belong to that field would yield an accuracy of 0.9, but would be a thoroughly uninformative classifier.

To correct for this, two other measures of prediction success have been proposed and are routinely used in evaluating the effectiveness of machine learning algorithms. They are:

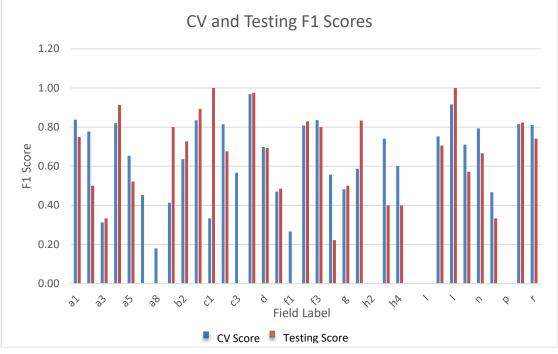
- Precision = T1/(T1+F2), and
- Recall = T1/(T1+F1)

Intuitively, Precision measures the share of all projects belonging to a classification that are correctly identified; Recall measures the share of projects that are predicted to be in the field that are correctly predicted. The F-1 score, which is the harmonic mean of Precision and Recall, is generally viewed as the best single summary of classifier performance.

Results

Among the different machine learning models, we found that the Logistic Regression classifier provides the best overall performance. Figure 5 summarizes the performance of the classifiers for each field of study, and Figure 6 reports performance for the classifiers for project purpose. In each case, we compare F-1 scores from the cross-validation results to those obtained using the testing sample. In cases where the number of projects was too small, we do not have any projects in the testing sample, so we cannot compute an F-1 score.

Figure 5: Comparison of F-1 Scores for Field of Study in Cross-Validation and Testing Samples



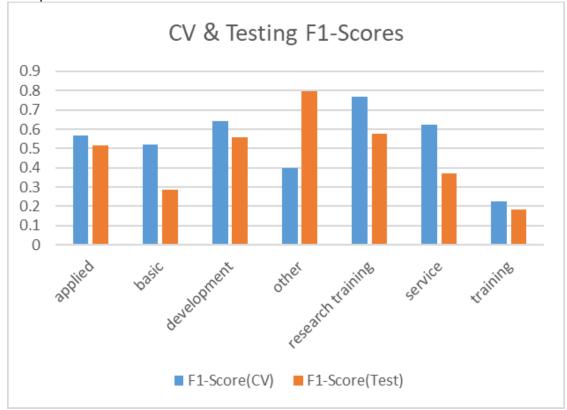


Figure 6: Comparison of F-1 Scores for Purpose in Cross-Validation and Testing Samples

As shown earlier (Figures 1 and 2), the distribution of projects by purpose and field is highly uneven; this difference accounts for much of the variation in classifier performance across the purpose/field categories. Figure 7 plots the relationship between the F-1 score and the number of projects assigned to each field in the training sample. F-1 scores rise sharply as the number of projects increases from 0 to about 40, reaching a range of 0.6-0.9 at this point. For cases with more than 60 projects the F-1 scores are clustered around 0.8.

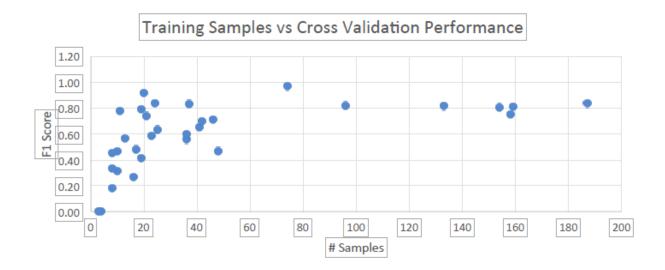


Figure 7: F-1 Scores for Field of Study vs. Number of Projects in Training Sample

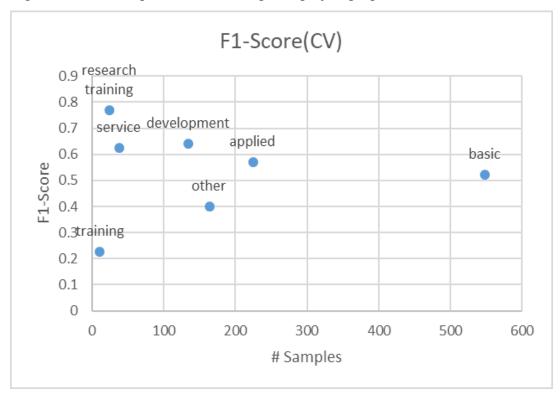
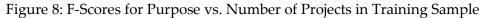


Figure 8 shows comparable relationships for project purpose.



Discussion

We have not yet succeeded in developing a set of classifiers that will precisely reproduce the human judgements underlying the University of Kansas's response to the HERD survey. But it is not clear that this is the appropriate measure of the project's success.

First, while we have relied on human judgements to train the classifiers, it is not entirely obvious that we should regard the human assessments as constituting the ground truth in this case. Furthermore, different individuals at KU have classified projects for the HERD survey over the years; this may have added additional subjectivity or inconsistency in the classification of projects. It may be that the classifiers are more consistent in their judgment than humans. Evaluating this possibility requires more careful examination of the cases in which the two approaches produce different results. Careful analysis of these cases may help clarify the root of the disagreement and yield additional insights.

Second, the end product of the classification process is an aggregated report on expenditures broken down by field of study and purpose. Rather than focusing on the accuracy of the individual project classifications, it may prove more valuable to look at the extent to which aggregated results from the machine classifiers approximate the aggregated results from the human classifiers.

Conclusions

As a proof of concept, we believe that the current project has been successful in demonstrating that it is possible develop reasonably to accurate machine-learning classifiers. We believe that many of the problems encountered so far will be reduced by expanding the training data set to include additional examples.

One initial objective of our project was to bring greater uniformity to HERD reporting across institutions. Future goals for this project include assessing the ability of our classifiers to successfully classify projects at other institutions. Adding additional projects from other institutions to the training data set may also offer opportunities to further refine the classifiers we have developed.

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