Experimental design for bathymetry editing

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Abstract
We describe an application of machine learning to a real-world computer assisted labeling task. Our experimental results expose significant deviations from the IID assumption commonly used in machine learning. These results suggest that the common random split of all data into training and testing can often lead to poor performance.

Keywords: IID assumption, Experimental design, Boosting

1. Introduction
We present results from a large-scale computer assisted labeling problem. We use boosted decision trees as our learning engine, specifically the LightGBM package (Ke et al. (2017)). We use the normalized margin as a measure of prediction confidence (Schapire et al. (1998)).

The standard experimental design for batch learning is to split the data at random into the train and test sets. The main contribution of this paper is to show that in our case, this design leads to poor performance. We show alternative designs that perform better. We argue that this is not an isolated case and that non-standard experimental design are likely to perform better in many situations.

2. Computer assisted bathymetry editing
Bathymetry is the mapping of the topography of the oceans floor (Tozer et al. (2019)). Modern bathymetry drawn on two sources of information: satellite altimeters that have global coverage but poor resolution, and shipboard echo sounders, which provide potentially more accurate data only along the path of the ship. The quality of the data from the echo sounders varies widely. As a consequence, extensive quality assurance is performed on the data after it is collected from the ships and before it is integrated into the map. This process is called “editing” and corresponds to assigning a binary label to each measurement. Measurements labeled “good” are incorporated into the bathymetry map while “bad” measurements are discarded. This process has traditionally been done manually by
domain experts, who analyze the map after a full update (using all measurements), then identify and remove suspicious outliers in the updated map (Figure 1 (a,b)).

Manual editing is labor intensive and the accuracies of the results vary from person to person. The goal of our project is to develop a “computer-assisted editing” method in which the computer assigns a confidence-rated prediction to each measurement. The human editor can then select a large area and instruct the computer to remove all bad measurements within that area (Figure 1 (c,d)).

The learning engine we use is boosted trees, as implemented in LightGBM. Our confidence score is based on the margin theory (Schapire et al. (1998)) and is similar to previous work on boosting-based active learning.

Our initial results were very good, in fact, unbelievably good. It took some work to identify the reasons for this overly optimistic results. Those reasons are the subject of this paper.
3. Bathymetry data

Bathymetry is collected by ships worldwide (Tozer et al. (2019)). Each ship collects data on behalf of one of 17 organizations (the organizations often concentrate on different geographical regions, thus in this paper we use the term “organization” and “region” interchangeably). The combined number of measurements is over 400 millions and growing. The raw data size is 203 GB on disk. The data are not uniformly distributed across the regions. Smaller regions contain about 4 million measurements, while larger regions contain over 100 million measurements.

The quality of data from different regions varies widely due to type of ship, reliability of the ship’s crew, and complexity of the seafloor topography of the measured regions. The fraction of bad measurements per region varies from less than 0.01% to 13.12%. In addition, the quality of the editing process varies significantly among the regions due to the incorrect data labeling by less attentive human editors.

4. Challenges to the IID assumption

In general, the goal of batch learning is to generate classifiers that can accurately classify new test data that was not available at training time. For this to be possible the training data and test data have to be linked in some way. The most common assumption linking the training and testing data is that the examples (in both sets) are Identically and Independently Distributed (IID). This assumption justifies a common experimental design: collect as much data as possible, randomly permute the data, and partition it into a training set and a test set. Use the training set to train the model and use the test set to test it. Under the IID assumption the test error is an unbiased estimate of the true generalization error.

We started our project using the random split design, then we found out several ways that it fails. We describe two failure modes which contradict the IID assumption. The first, which we call sequentiality contradicts the Independence assumption, the second, which we call diversity contradicts the Identical Distribution assumption.

4.1 Data sequentiality

Our first set of experiments followed the standard design: the measurements were partitioned at random between the training set and the test set. The results on both the training set and the test set were spectacular, with an area under the test set ROC of 0.9975. However, the accuracy fell off significantly when the classifier was used on a cruise that was not in the training set.

We discovered that this was a result of the way in which the data was split into a training set and a test set. The standard train/test partitioning places each individual measurement in the training set or the test set respectively. On the other hand, as shown in Figure 2, label sequences produced by humans are likely to have long stretches of good or bad elements. As a result, each test example is likely to be labeled in the same way as its neighboring training examples. In other words the examples are statistically dependent, breaking the independence part of the IID assumption.

Partitioning individual measurements into a train set and a test set results in a situation where it is sufficient for the classifier to learn the boundaries of the bad segments and ignore
the meaningful features. This is possible even if the training set is shuffled because time of day, latitude, or longitude can serve as proxies for the location of the element in the sequence. The resulting classifier has a very high test AUROC, but performs poorly on unseen cruises.

To mitigate this problem we changed the way we partition the data into training and testing. Namely, we divided the data sequences into long sub-sequences and then place each sub-sequence at either the training set or the test set at random. We experimented with two ways of forming sub-sequences. The first way is to take whole cruises as sub-sequences, the second is to take non-overlapping sub-sequences of 100,000 measurements, which correspond to traveling about 2500 kilometers for the multi-beam cruises. Most cruises are shorter than 100,000 and are included as they are, but some are much longer and are split into chunks. Partitioning the sequences in these ways reduces the AUROC significantly, as is shown in Figure 2. However, this performance is a better predictor of the future performance.

4.2 Data diversity

After sequentiality, the main problem we found with the analysis of bathymetry data is that of data diversity. The distribution of measurements, and of errors in measurement, depends on many factors. At the cruise level: The ship and the crew of the ship, whether bathymetry is the main goal of the cruise, sea conditions etc. At the level of region, or the organization to which the ship belongs, there are matters of policy, planning and the resources put towards quality assurance and data editing.

As a result of this diversity, data collected in different regions has significantly different distribution. Each row of the matrix in Figure 3 corresponds to a model (classifier) trained using data from one of the 17 regions, the bottom row correspond to the model trained using all of the data. The columns correspond to the region from which the test set is taken (train and test sets from each region are randomly partitioned over subsequences).
Figure 3: Area under ROC (AUROC) for the models trained using data from one region and tested on the data from another region. Higher values are better.

Table 1: Improvement in terms of AUROC of a model trained on the data sampled from the same region as the test data over the model trained on all of the data.

| Region    | Improvement |
|-----------|-------------|
| AGSO      | 4.29%       |
| NOAA geodas | 3.38%     |
| NGA       | 0.78%       |
| NGA2      | 6.94%       |
| NGDC      | 4.38%       |
| JAMSTEC   | 2.59%       |
| JAMSTEC2  | 5.57%       |
| SIO       | 0.73%       |
| US multi  | 2.95%       |

Figure 4: Comparison of the test performance using the models trained using the data from different sources. The plots show the test performance on the test data sampled from the datasets provided by AGSO (Australia), JAMSTEC (Japan), and NGDC (US-based data center with global data coverage). In all three cases, the optimal models are the one trained on the data sampled from the same origin as the test data. The model trained using all of the data is also included for comparison.

The colors correspond to correspond to the AUROC when the row model is tested on the column test data. First, observe that some pairs, such as model AGSO and test NGA, or JAMSTEC model and test NGDC have a very poor AUROC of 0.5 or smaller. In other words, the distributions corresponding to different regions are very different, which is why we say the data source of the bathymetry dataset is diverse. This contradicts the identically distributed part of the IID assumption.

Further, the highest AUROC in each column corresponds to the the model trained on data from the same region. The second best is usually the classifier trained using all of the
data. However, as shown in Table 1, the classifier using just the data corresponding to the the same region is, in all cases, better than the classifier using all of the data.

We show the full ROC curves of three specific regions in Figure 4. We sampled the test sets from AGSO (Australia-based organization), JAMSTEC (Japan-based research institution), and NGDC (US-based data center). We then used these test sets to evaluate four models: first three are trained using the data from each one of the three regions, and the fourth one trained using all of the data. In all three cases, the best performance (in terms of AUROC) is achieved by the model trained using the data from the same source as the test data, while the performances of the models trained using the data from different sources are significantly worse. Finally, the performance of the model trained using all of the data falls in between.

We conclude that for the bathymetry editing task, combining all data into one large training set is inferior to using only data that is similar to the data in the test set. In other words, maximizing the size of the training set should be balanced against the similarity of the training set to that of the expected test set.

5. Summary

We provide experimental evidence that bathymetry data does not obey the IID assumption usually made in machine learning. We draw two conclusions regarding the experimental design of machine learning. First - data gathered sequentially should be treated in a way that ensures that dependencies between neighboring examples do not bias the generated classifier. Second - when a data source is diverse, it is not enough to collect large amounts of data. One also needs to ensure that the diversity of the training set represents the expected diversity of future test data.

Acknowledgments

We would like to acknowledge support for this project from the National Institutes of Health (NIH grant U19 NS107466) and the Scripps Institution of Oceanography, UC San Diego.

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