Scalable and interpretable data representation for high-dimensional, complex data

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Abstract

The majority of machine learning research has been focused on building models and inference techniques with sound mathematical properties and cutting edge performance. Little attention has been devoted to the development of data representation that can be used to improve a user's ability to interpret the data and machine learning models to solve real-world problems. In this paper, we quantitatively and qualitatively evaluate an efficient, accurate and scalable feature-compression method using latent Dirichlet allocation for discrete data. This representation can effectively communicate the characteristics of high-dimensional, complex data points. We show that the improvement of a user's interpretability through the use of a topic modeling-based compression technique is statistically significant, according to a number of metrics, when compared with other representations. Also, we find that this representation is scalable — it maintains alignment with human classification accuracy as an increasing number of data points are shown. In addition, the learned topic layer can semantically deliver meaningful information to users that could potentially aid human reasoning about data characteristics in connection with compressed topic space.

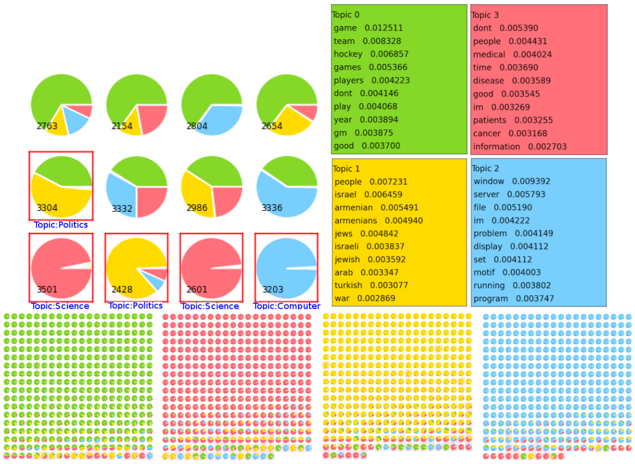

Figure 1: A portion of the analysis report using the data representation studied in this work. Each data point is compressed using topic-based feature compression. Zoomed in (top left), where a pie chart inside of a red square indicates incorrectly classified data points. The document ID number and true labels are also shown as texts. The top 10 words within each color-coded topic are shown at the top right. The bottom shows reports in a bird's-eye view.

Introduction

Machine learning (ML) is a powerful tool that can provide solutions for a number of real-world problems. However, doing so often requires more effort from the user than a simple "plug-and-play" approach. When incorporating machine learning in order to perform data classification tasks, one of the challenges a user may encounter is investigating individual data points and their characteristics, which is often an iterative process. For example, investigating misclassified data points may be necessary to diagnose the reasons for poor performance. This investigation may involve comparing the similarity of the misclassified data point to data points in its true cluster and other clusters and only becomes more challenging when the user is presented with a large, high-dimensional data set (e.g., multiple paged complex legal documents).

Methods to improve a user's ability to interpret, evaluate and debug ML models have received little attention in the ML research community, especially with regard to domains with complex, high-dimensional features. There are domains that are naturally visualizable, such as pictures and videos; however, the majority of domains where ML could be useful do not exhibit this beneficial characteristic. This task becomes more daunting and time consuming at the very least as the number of documents grows. To fully harness the power of ML in the context of real-world problems, we need to provide solutions for this significant hindrance in the use of ML.

This work investigates an efficient, accurate and scalable representation of high-dimensional, complex data points that aid human reasoning when working with ML models. We quantitatively and qualitatively verify a feature compression-based data representation that allows users to efficiently and accurately identify data characteristics, even with an increasing number of data points. This representation accelerates the user's understanding of the complex interaction between ML models and data, and reduces the burden of the iterative debugging process.

The work is part of an effort to provide analysis reports for those who use ML as a problem-solving tool and require an efficient way to interpret, evaluate and debug ML problems. The report provides information about individual data points and their relationships with one another and with class labels, and is presented in a way that allows for quick investigation of the status of classification tasks. Figure 1 presents an example report, where each pie chart represents one document (i.e. one datapoint). The bottom portion of Figure 1 shows reports in a bird's-eye view. A detailed view of a subset of points is shown in the top-left of the report, where misclassified data points are indicated by a red box. The compressed feature space representation allows users to more easily diagnose problems such as incorrect ground truth labels in cases when the misclassified point really resembles other points that belong to the predicted class. In order for such a report to be practical in a real-world setting, the data representation in question should not only be interpretable and scale with the number of data points, but also be capable of working with high-dimensional features.

Here, we compare and analyze several popular feature compression methods, including latent Dirichlet allocation (LDA), principal component analysis (PCA), independent component analysis (ICA), non-negative matrix factorization (NMF) and term frequency-inverse document frequency (Tf-idf), in order to assess how a user's classification accuracy with these methods scales with the number of data points. Through user study, we measure human performance according to both objective and subjective terms: accuracy, efficiency and user confidence and preference. We show that humans' performance of classification tasks when using topic modeling-based compression techniques is improved across various measures, often with statistical significance, compared with traditional techniques.

Related work

A common approach for improving the interpretability of a trained model is to visualize data and it's relationship to classification results. Popular machine learning APIs, such as Weka (Leban et al. 2006), provide basic visualizations for understanding feature distribution and classifications (e.g., bar charts, confusion matrices). Recent work focuses on making some of these basic visualizations interactive (Talbot et al. 2009; Kapoor et al. 2010).

Researchers have also worked on algorithm specific visualizations (Ankerst, Elsen, and Ester 1999; Becker, Kohavi, and Sommerfield 2001). These visualizations link data points and features to the parameters of a model. Algorithm agnostic approaches for visualizing a dataset have also been suggested. For example, one approach helps users find labeling error or opportunities for generating new features by visualizing the relationship between a dataset and the output of multiple learned models (Patel et al. 2011).

Further insight into model performance can be gained by better visualizing the data points themselves. For domains where data points are naturally visualizable (e.g., pictures), simply visualizing the raw data point is sufficient to communicate characteristics of the high dimensional (i.e., many pixels) data point. For example, Fails et al. (Fails and Olsen Jr 2003) present images with translucent highlights indicating how pixels are classified by a learned model.

However, the challenge of efficiently communicating characteristics of data points exists for many other domains where the natural visualization does not exist. One attempt to this challenge is to project data points onto two dimensional space, for example, mapping attribute values to points in a two-dimensional space by selecting the most useful data projections (Leban et al. 2006).

For high-dimensional, complex data points, however, neither projection nor performance metrics are sufficient. It is unclear, for example, how to project complex, 10-page documents, especially when the contents of these documents are also complex. Working with performance metrics is a realistic approach if, and only if, one can completely rule out potential faults within the dataset (e.g., hand-tagged labels with no mistakes). A data representation that can express the characteristics of individual data points to allow for efficient investigation is essential to improve the human reasoning process when working with ML models.

When it comes to representing the features of individual data points, one of the biggest challenges is ensuring the scalability of the representation. This work takes an approach based on feature compression methods, and investigates efficient and scalable data representations. One of the popular ways to compress a large corpus of text documents is to learn an abstract layer called "topics" (e.g., Latent Dirichlet allocation (LDA) (Blei, Ng, and Jordan 2003)), and to map each data point onto the topic space. The majority of data representation work incorporating LDA has been focused on the development of a visualization framework (Chuang et al. 2013) or the design of user interfaces (Chuang et al. 2012).

More recently, Chang et al. (Chang et al. 2009) showed that LDA learns the most human-intuitive topics compared with other topic modeling methods, and the level of abstraction using topics is appropriate for compressing complex documents. This raises the following questions: first, whether there are other feature compression methods that are more intuitive than LDA; and second, whether any of these other feature compression methods are scalable, interpretable and efficient. This work investigates a several feature compression methods (LDA, PCA, NMF and ICA), along with other, more traditional ways to represent data points (Tf-idf, raw documents) in order to answer these questions.

Experiment methodology

Measuring human understanding is a challenging task due to the complexity of human cognition. In order to quantitatively measure human understanding, we must first define the interpretability and scalability of a data representation.

Interpretability An interpretable data representation allows humans to correctly identify data-to-data relationships (e.g., data points that belong to the same cluster share similar

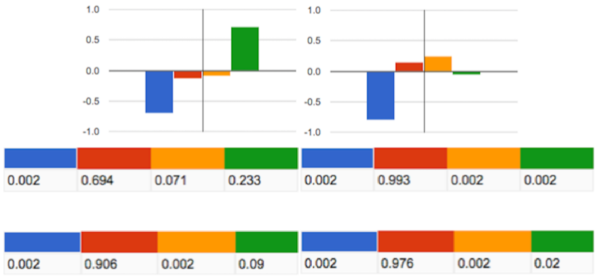

Figure 2: An example of PCA in bar graphs (top, two documents) and LDA in table representations (bottom, four documents) shown to participants during experiments

characteristics).

Scalability A scalable representation maintains a human's ability to efficiently interpret data-to-data relationships as the number of data points increases.

First, we selected a subset of feature compression techniques that are widely used within the ML community. Then, we evaluated them and chose a smaller set of methods to use in an experiment with human subjects, according to their computationally superior metrics (i.e., quality of clustering). We used a dataset of news articles (20 Newsgroups (Lang 1995)), compressed each document using the chosen methods, and projected the data from each document onto identically sized dimensional spaces. Next, we conducted experiments in which human subjects utilized the chosen techniques, and compared the participants' interpretability performance with the different data representations. We also evaluated whether different ways of presenting the same information (e.g., a bar graph vs. a table) impacted human performance. In order to place this study with respect to traditional representations, non-feature-compression-based methods were also evaluated.

Models and corpora

In this section, we briefly present the technical details of four candidate feature compression methods, evaluated according to metrics indicating the quality of clustering: latent Dirichlet allocation (Blei, Ng, and Jordan 2003), principal component analysis (Pearson 1901), independent component analysis (Jutten and Herault 1991), non-negative matrix factorization (Sra and Dhillon 2005) and Tf-idf (Salton 1991). The number of latent topics in LDA and the number of components in PCA, ICA and NMF, K, are set to be identical.

Latent Dirichlet allocation (LDA) LDA is a generative model of documents wherein each document is modeled to be generated from a mixture of topics. Each data point becomes a proportion of low-dimensional topics, a vector of length K (set to 4 in our experiment). We use Gibbs Sampling implementation to perform inference (Phan and Nguyen 2013). The parameter α is set to 0.1, and β is set to 0.1. Additional details for this method can be found at (Blei, Ng, and Jordan 2003).

Principal component analysis (PCA) PCA is a statistical procedure that incorporates an orthogonal transformation to convert a set of observations of potentially correlated variables into a set of values for linearly uncorrelated variables, called "principal components." A data point is compressed into weights of these principal components, a vector of length K (set to 4 in our experiment) (Pearson 1901). PCA provides both positive and negative weights for each component. Figure 2 depicts an example of PCA representation using bar graphs, with each component color-coded.

Independent component analysis (ICA) ICA is a statistical method for transforming an observed multidimensional random vector into components that are as statistically independent from one another as possible (Jutten and Herault 1991). Similar to PCA, ICA provides both positive and negative weights for each component.

Non-negative matrix factorization (NMF) Among other methods, NMF is used for text mining applications (Sra and Dhillon 2005). In this process, a document-term matrix is constructed using the weights of various terms collected from a set of documents. (Typically, such a matrix would consist of weighted word frequency information.) This matrix is then factored into a term-feature and a feature-document matrix. The features are derived from the contents of the documents, and the feature-document matrix describes data clusters of related documents.

Term frequency-inverse document frequency (Tf-idf) Tf-idf is a numerical statistic intended to reflect how important a given word is to a document within a collection or corpus (Salton 1991). It is often used as a weighting factor in information retrieval and text mining. The Tf-idf value increases proportionally with the number of times a word appears in a document, but is offset by the frequency of that word in the corpus, which helps to control for the fact that some words are generally more common than others. In our experiment, we selected the 10 highest-weighted words for each document.

Dataset The 20 Newsgroups dataset includes articles on various topics, along with their true labels. In this paper, we will refer these articles as documents. We first used support vector machine to filter four categories from the initial corpora that consistently performed better than the others (20% test set and train on the remaining 80%). The purpose of limiting categories to a small, fixed number is to maintain a reasonable length of experiment time and limit participant fatigue. The four chosen topics were: sports, politics, medicine and computers. After filtering, the dataset consists of 3,519 documents with a vocabulary of 1,048,576 unique words. The dataset was preprocessed to remove all stop words.

Experiment design

In our experiment, each participant was shown N number of documents ($N \in \{2, 8, 16, 32\}$) and asked whether the documents belonged in the same category as one another. If any of the documents did not belong with the others, participants were instructed to answer "different"; if all documents shared a common category, they were instructed to answer

Per number of documents shown	
Group 1	R - T - BP - TL - TP - BL
Group 2	T - TL - R - BL - BP - TP
Group 3	TL - BL - T - TP - R - BP
Group 4	BL - TP - TL - BP - T - R
Group 5	TP - BP - BL - R - TL - T
Group 6	BP - R - TP - T - BL - TL

Table 1: Design of experiment (R: raw documents, T: Tf-idf, TL: LDA in table, BL: LDA in bar graphs TP: PCA in table, BL: PCA in bar graphs). Participants were randomly assigned to one of the four groups, with four participants per group.

"same." This measures the interpretability of the chosen data representation. The accuracy of participant responses was determined via the ground truth category provided from the dataset. In light of the quantitative results found using convention metrics (shown in the following section), PCA and LDA are chosen as the superior methods to be further evaluated via human experiment. We also provided the top 10 words for each topic, and all topics were color-coded.

To evaluate the scalability of the representation, the number of documents included per question increased from two to eight, sixteen and finally thirty-two. In this paper, we refer to questions depicting the same number of documents as a *batch*. All participants were given *batch2* first, then *batch8*, *batch16* and *batch32* in order to keep the learning effect equivalent across participants.

There were six questions within each batch, and each question depicted documents using four different representations: LDA via bar graph and table representations, PCA via bar graph and table representations, Tf-idf and raw documents. The difference between the table and bar graph representations is that a table depicts the weight of each component in numbers, whereas a bar graph visualizes each weight without the numbers (Figure 2). We include both table and bar representations for two reasons: 1) to understand the effect, if any, of a visual versus textual presentation, and 2) to provide comparable presentation for Tf-idf and raw documents, which do not lend themselves to standard visualizations.

To control learning effects, the order in which representations were shown to a participant was decided by the 6×6 balanced Latin square, as shown in Table 1. There were four subjects in each group. In total, each participant answered 24 questions (four batches of six questions each). For each representation we uniformly at random decide an outcome of "same" or "different" and, based on this, choose documents uniformly at random from one or more categories. In order to maintain roughly equivalent reading times per document and question for the reading of raw documents, we only included documents of 700 ± 200 words in length. All participants took mandatory breaks after every five questions in order to manage fatigue. After each question participants rated their confidence on a five point Likert-scale (e.g., 1: not very confident - 5: very confident). At the end of the study, participants rated their overall preference on a five point Likert-scale.

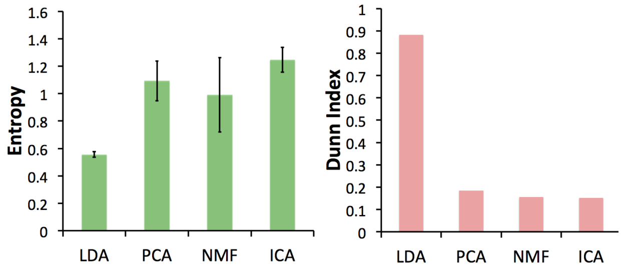

Figure 3: Entropy measure (left) and Dunn Index (right). The entropy measure is calculated for each cluster, then averaged. The error bars represent standard deviation across clusters.

Participants

Twenty-four engineers (seven women and seventeen men) were recruited via email for this experiment. The participants were randomly assigned to one of the groups described above, and performed four batches of tasks. In total, each participant answered 24 questions, and took approximately 40 minutes to finish the task. All participants received a gift card for their role in the experiment.

Results

Through an experiment with human subjects, we verify that the topic modeling-based feature compression method is significantly better than other methods in terms of interpretability and scalability. For the majority of participants, this was true across all evaluated performance measures, including accuracy, speed and confidence, regardless of the batch (i.e., the number of documents shown) or method of display (bar graphs vs. tables).

We first present the pre-experiment evaluation of candidate methods using conventional metrics (entropy and Dunn Index) that measure inter-data relationships. This is followed by the experiment results, and how classification accuracy scaled with increasing data points for each method. We define statistical significance at the $\alpha = 0.05$ level.

Evaluation using conventional metrics

This section presents an evaluation of the candidate methods using standard metrics, Dunn index and entropy, which can be used to measure different aspects of the quality of clusters defined by the true class labels in the compressed feature space induced by each candidate method. Based on these results, a subset of the candidate feature compression methods are evaluated using human experiments. We find that the best method according to these metrics also performs the best according to human performance based metrics.

Dunn index The Dunn index is defined as the ratio between minimum inter-cluster distance and maximum intra-cluster distance. In other words,

$$DI_m = \min_{1\leq i\leq m}\left\{ \min_{1\leq j\leq m, j\neq i}\left\{ \frac{\delta(C_i, C_j)}{\max\limits_{1\leq k\leq m} \Delta_k} \right\}\right\} \qquad (1)$$

where $\Delta_i = \max_{x,y \in C_i} d(x, y)$ and C_i is a cluster of vectors, and x, y are any two n dimensional feature vectors assigned to the same cluster C_i. The inter-cluster distance, $\delta(C_i, C_j)$, is defined as the distance between the centers (mean vector) of cluster i and j. We use the L_2-norm distance to compute Δ_i and $\delta(C_i, C_j)$. Note that clusters here are defined by the ground truth label and distance is measured using the reduced dimensionality space. A larger Dunn index suggests a better clustering, since it implies either a smaller intra-cluster distance or larger inter-cluster distance (or both).

Shannon entropy In information theory, Shannon entropy characterizes uncertainty or disorder within information (Shannon 2001). Formally, the entropy of a discrete random variable X is defined as

$$E = -\sum_{x} p(x) \log p(x), \tag{2}$$

where $p(x)$ is the probability of the event $X = x$. In the case of LDA, the value of each coordinate of the feature vector defines the probability of the instance belonging to a particular topic. Thus, the entropy computed over the topic probabilities describes how concentrated (low-entropy) or how distributed (high-entropy) the weights within the feature vector are. In the case of other methods, such as PCA, we can take the absolute value of each coordinate of the feature vector and normalize in order to induce a probability distribution over feature vector coordinates.

The entropy values in Figure 3 are computed by first averaging together all feature vectors within a class, then normalizing the average feature vector if necessary, and then finally computing the entropy of that aver- aged and normalized vector; the entropy values of all classes are then averaged to produce the final value displayed in the plot.

We note that a low feature vector entropy is not required in order to have a good clustering, e.g. a good Dunn index value, however, may aide in providing an interpretable encoding of the features.

Using these two metrics, we chose LDA and PCA as the superior methods from each of two groups: the compression methods that give *positive only* weights and those that give *positive and negative* weights. Both Dunn index and entropy metrics suggest that LDA is better than NMF for methods that produce *positive only* weights. PCA is better than ICA in terms of both entropy measure and Dunn index.

Although these metrics indicate that LDA may be a promising method, it remains to be verified which of the feature compression methods both scale well with an increasing number of data points and maintain interpretability. We conducted experiments with human subjects in order to answer this question.

Statistically better performance using topic-modeling based feature compression

Our experiment results verified that human performance is better when using the topic modeling-based feature compression method rather than other representations, according to both objective and subjective measures. LDA performed better than PCA with regard to accuracy, speed and the subject's degree of confidence in 23 of 24 cases, with a statistically significant difference in performance in the majority of cases. We used the Wilcoxon signed rank test for paired observation to assess the statistical significance of differences in accuracy, speed and confidence between the methods with a requisite Bonferroni correction of $\frac{\alpha}{N}, N = 2$. Unlike the T-test, the Wilcoxon signed rank test does not assume normal data distribution.

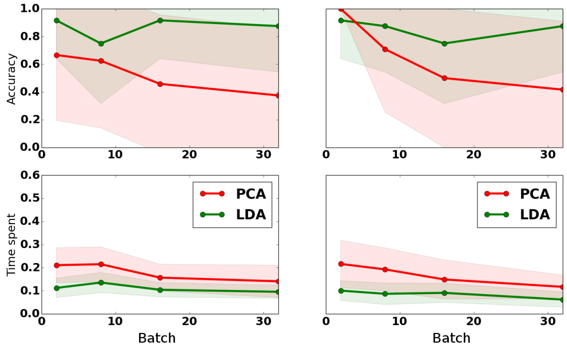

Figure 4: Comparison of accuracy (first row), and the portion of time spent (second row) for LDA and PCA. The performance of the table representation of each method is depicted on the left column, while the bar graph representation is on the right. Note that the large standard deviation is due to the accuracy averaged over binary values (one element for each participant). A smaller time spent (second row) indicates faster speed.

Note that the portion of time spent by each subject is defined as the time spent on a question, normalized by the total time spent on all representations within a batch. For example, the amount of time spent with Tf-idf, raw documents, PCA via table, PCA via bar graph, LDA via table and LDA via bar graph for a given batch add up to 1; a lower amount for a specific method represents faster speed using that method.

Table 2 indicates that the average performance of the human subjects was better when using LDA rather than PCA, in both bar and table representations, especially as the number of documents increased. With regard to accuracy, we observed a statistically significant difference between PCA and LDA with an increasing number of documents, suggesting the superior scalability of LDA compared to PCA. Figure 4 indicates that LDA maintains performance accuracy as the number of documents shown increases, whereas the accuracy of PCA drops with an increasing number of documents. LDA was also superior to PCA with regard to speed and confidence, regardless of the number of documents shown.

Beyond scalability, what is ultimately useful for humans is the semantic meaningfulness of the compressed layer. This is different from interpretability — even if the layer is not semantically meaningful, the user may still be able to identify same or different data points, but may not be able to

	Batch	Accuracy	Speed	Confidence
Bar	2	z = 1.41, p = 0.1	z = 3.54, **p** < **0.05**	z = 6.10, **p** < **0.025**
	8	z = -1.63, p = 0.1	z = 3.34, **p** < **0.05**	z = 6.11, **p** < **0.025**
	16	z = -1.60, p = 0.1	z = 2.60, **p** < **0.05**	z = 6.09, **p** < **0.025**
	32	z = -3.05, **p** < **0.05**	z = 3.57, **p** < **0.05**	z = 6.10, **p** < **0.025**
Table	2	z = -1.90, p = 0.05	z = 3.91, **p** < **0.05**	z = 6.13, **p** < **0.025**
	8	z = -1.00, p = 0.3	z = 3.43, **p** < **0.05**	z = 6.08, **p** < **0.025**
	16	z = -3.32, **p** < **0.05**	z = 3.06, **p** < **0.05**	z = 6.08, **p** < **0.025**
	32	z = -3.21, **p** < **0.05**	z = 3.06, **p** < **0.05**	z = 6.11, **p** < **0.025**

Table 2: Statistical significance test of the performances of LDA and PCA. Statistically significant differences between the two are shown in bold.

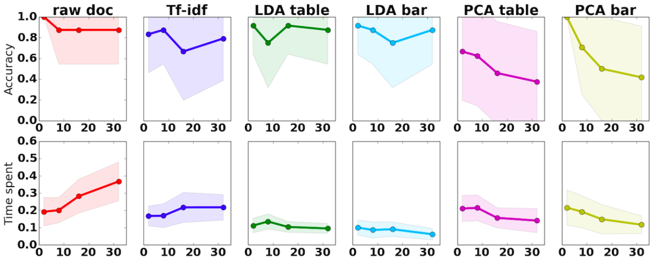

Figure 5: Performance comparison for all representations

draw useful conclusions by determining the meanings of the compressed layer and making connections to the characteristics of data points.

Results from the post-experiment questionnaire indicated that 83% of participants paid attention to the top 10 keywords for topics. In addition, 92% of participants stated their preference for *positive-only* weighted keywords (LDA) over *positive and negative* weighted keywords (PCA). Even though a separate subject experiment is need to evaluate the quality of subjects' understanding of the topic layer, our results suggest that the topic-layer from LDA could be useful beyond interpretability.

Comparison with non-feature compression-based representations

In order to compare this study with more standard representations, we also evaluated participants' performance using traditional data representations: Tf-idf and raw documents.

Figure 5 indicates that the user's accuracy of classification with LDA are similar to those observed for raw documents. The confidence measure also showed a similar trend. Compared with Tf-idf, accuracy and confidence values are higher with LDA, regardless of batch. As indicated in Table 3, the observed differences between the methods in accuracy and confidence are not statistically significant.

	batch	Accuracy	Speed	Confidence
raw document vs. LDA	2	z = 1.41, p = 0.1	z = 3.83, **p** < **0.05**	z = 6.31, p = 0.5
	8	z = 0.00, p = 1.0	z = 3.80, **p** < **0.05**	z = 6.23, p = 0.3
	16	z = 1.13, p = 0.2	z = 4.09, **p** < **0.05**	z = 6.31, **p** < **0.025**
	32	z = 0.00, p = 1.0	z = 4.29, **p** < **0.05**	z = 6.24, p = 1.0
Tf-idf vs. LDA	2	z = -1.41, p = 0.1	z = 3.51, **p** < **0.05**	z = 6.09, **p** < **0.025**
	8	z = 0.00, p = 1.0	z = 3.97, **p** < **0.05**	z = 6.23, p = 0.01
	16	z = -0.82, p = 0.4	z = 3.89, **p** < **0.05**	z = 6.11, p = 0.1
	32	z = -0.71, p = 0.4	z = 4.20, **p** < **0.05**	z = 6.15, p = 0.05

Table 3: Statistical significance test for performance between Tf-idf and LDA, and raw document and LDA. Statistically significant differences between methods are bolded.

However, there was a huge gain in speed when using the LDA representation compared with viewing a raw document. The speed at which participants answered questions using the LDA bar graph representation was significantly greater than that observed when using both raw documents and Tf-idf representations, regardless of the number of documents shown (Table 3). In particular, the speed of LDA with bar graph representation was 4.5 times faster (± 3.5) on average, and at most, 40 times faster than the raw document representation. The speed of LDA with table representation was, on average, 2.8 times faster (±1.6) and, at most, 20 times faster than the raw document representation. When compared with Tf-idf, the speed of LDA with bar graph representation was three times faster (± 1.2) on average, and, at most, 12 times faster, while the speed of LDA with table representation was two times faster on average (± 0.8), and 9.9 times faster at most compared with Tf-idf.

These results suggest that LDA-based representation maintains performance metrics while significantly decreasing the time it takes for humans to investigate data point characteristics.

Post-experiment questionnaire

Despite the superior performance of LDA, results from the post-experiment questionnaire indicated that participants tended to only slightly prefer LDA representations when compared to raw document representations in general. However, these results may differ if the number of documents shown to participants becomes larger by an order of magnitude. Due to time constraints related to experiments involving human subjects, we leave this possibility to be explored in future work.

Conclusion

We quantitatively and qualitatively verified accurate, efficient and scalable data representations for a high-dimensional complex data points. Our findings are supported by both evaluations based on conventional metrics and human subject experiments. The improvement of a user's interpretability throughout the use of a topic modeling-based compression is statistically significant, according to a number of metrics. Furthermore, the compressed layer delivers meaningful informations to users. For the layer to maintain the rich information about the data, the topic modeling-based approach assumes that the features of the input data are interpretable. One method of relaxing this assumption is to add a layer in the LDA model to include domain-specific interpretable representations. This work aims to accelerate the user's understanding of the complex interaction between ML models and data, and reduces the burden of the iterative debugging process.

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