



**KTH Information and
Communication Technology**

Data-Efficient Machine Learning for Multi-Label Classification

Exploration of various models - shallow, deep, tree-structured, and ensembles thereof - for multi-label product classification in multi-modal and transfer learning settings.

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Contents

1	Introduction	1
1.1	Problem	2
1.2	Purpose	2
1.3	Goals	2
1.4	Hypotheses	3
1.5	Ethical Consideration	3
1.6	Sustainability	4
1.7	Delimitations	4
1.8	Outline	4
2	Background	5
2.1	Input Representations	5
2.1.1	Categorical Input	5
2.1.2	Text Input	6
2.1.3	Image Input	7
2.2	Models Considered	7
2.2.1	General Models	7
2.2.2	Text Models	9
2.2.3	Image Models	10
2.2.4	Downstream Models	11
2.3	Unsupervised and Semisupervised Learning	12
2.3.1	Autoencoders & Variational Autoencoders	13
2.3.2	Conditional Variational Autoencoders	14
2.3.3	Generative Adversarial Networks	14
2.4	General Practices in Machine Learning	15
2.5	Combining Models	16
2.6	Active Learning	17
3	Method	19
3.1	Data Preprocessing	19
3.1.1	Category Structure	20
3.1.2	Class and Label Imbalance	21
3.2	System Architecture	22

CONTENTS

3.2.1	Dataflow Pipelines	23
3.3	Experiments	25
3.3.1	Visual Similarity	25
3.3.2	Independent Models	25
3.3.3	Ensembling	25
3.3.4	Active Learning	25
3.4	Evaluation	25
4	Discussion	27
5	Conclusion	29
	References	31
	Declaration	35
	Appendices	35
A	Screenshots	37
A.1	Dataprep Histogram	37

1. Introduction

Machine learning (ML) has recently become a popular research area, and is increasingly applied in industry. A lot of this newfound interest and hype is directed at neural networks and deep learning. This focus is not unfounded - approaches based on deep networks continue to break benchmarks in core machine learning research areas such as computer vision [cite], speech recognition [cite], many natural language processing tasks [cite NMT], and even control and planning tasks [cite].

Artificial neural networks consist of layers of transformations that map multi-dimensional inputs to (usually multidimensional or structured) outputs. A single-layer neural network is a linear transformation of the inputs; each additional layer with a non-linear activation function enables the network to partition the output space and hence approximate more complex functions. Complex models are prone to overfitting and require more training data and heavier regularisation, yet deep models are somewhat unique in that their performance continues to increase with the size of the dataset, while the benefits of more data taper off for other models.

The naive conclusion is to use deep learning only when labeled data is abundant, but the depth of a model is not a binary “deep vs shallow” decision - one can start out with a shallow model and increase model complexity (width and depth) to see the effects on performance and generalisation. Logistic regression might well be the most appropriate approach for a classification problem, but this is often not obvious up front, so it is beneficial to build models in a framework that also supports deep models. In addition to easy experimentation with model architectures, it is easy to do transfer learning with deep models on popular platforms: for example, image or text models pretrained on large datasets can be utilised to increase product classification performance, and representations learned for classification could in turn be used by a downstream product recommender system. Datasets with abundant unlabeled data can benefit from unsupervised and semisupervised learning using deep generative models.

Each project has different requirements on predictive performance, label complexity, interpretability, computational resources and engineering challenges. Neural networks are a good fit for this project due to their amenability to transfer learning and flexibility in handling multi-modal inputs and multi-task objectives. As neural networks are notoriously data-hungry, the question immediately becomes - how to do it without providing many labels.

1.1 Problem

The client company gathers data from various affiliate networks (that in turn get their data from various retailers) and displays it on their website. There are millions of products belonging to roughly 1300 categories, and categories follow the usual nested tree structure. The incoming data is noisy and inconsistent: what kind of data is stored in which column varies across affiliate networks, across retailers within an affiliate network, and the data within a retailer can have lots of missing values, noisy text, missing images, etc. There is currently a rule-based system for assigning products to categories: all products matching a condition (e.g. title contains the word “trousers”) will be assigned to that category, i.e. categories are not mutually exclusive. This way of categorising products works relatively well on some categories, but such a rule-based system has several drawbacks: these rules are cumbersome to define, their evaluation is manual, they fail to match a large fraction of products that in principle should be in a given category, it is hard to trace back the rule that caused a false positive, and such rules are limited to textual data.

The client needs a classification system to replace the old way of categorising products. The predicted outputs can either be a set of independent binary classifications, or the category structure has to be re-organised to ensure classes are mutually exclusive. The system should be able to learn from the output of the old system, and if possible produce models that can be used in downstream tasks such as recommend systems and product similarity models. The highest priority is low label complexity, beating requirements for high accuracy and interpretability. The system should be robust to noisy inputs; data preprocessing should not consider the idiosyncrasies of each affiliate network. There is an additional feature the client requires: given a product image, the visitor should be shown products that are visually similar.

1.2 Purpose

The academic purpose of this work is to (1) assess the relative strengths of different kinds of models and their combinations, and (2) to determine whether an active labelling strategy reduces label complexity on a real-world dataset. Analogously, the commercial purpose is to (1) obtain a model with powerful predictive capabilities, and to (2) reduce costs by using an efficient labelling strategy, and (3) obtain a high-quality product similarity score.

1.3 Goals

The goals of the work, in chronological order, is to:

- Use a pre-trained 2-dimensional convolutional neural network (2D CNN) to extract features for an approximate nearest-neighbour search of visually sim-

1.4. HYPOTHESES

ilar products.

- Build an interface for subjectively evaluating the visual similarity algorithm.
- Train baseline model to reproduce the behaviour of the rule-based system.
- Build an interface for labelling products and obtain small dataset with ground truth labels (further referred to as the “ground truth dataset”).
- Train a number of different models on the rule-based labels. Evaluate these models on the rule-based test set as well as the ground truth dataset.
- Implement the active labelling mechanism defined in [ref] and fine-tune the ensemble (that is pre-trained on rule-based labels) in 10 labelling rounds.
- Document the results as well as the technical architecture and workflow.

1.4 Hypotheses

The following hypotheses were postulated prior to running most experiments¹:

1. Pre-trained 2D CNNs perform reasonably for visual item similarity, but fine-tuning might be needed.
2. Linear models are relatively good at predicting higher-level categories, worse at predicting lower-level categories.
3. Deep models for histogram / TF-IDF inputs do not improve substantially on linear models.
4. Shallow models with embedding inputs generalise better to the ground truth data, and deep models with embedding inputs generalise slightly more.
5. Pre-trained 2D CNN are consistently good predictors of clothing products, yet failed to accurately predict categories such as technology.
6. Fine-tuning CNNs will give little, if any, performance improvement due to inefficient training data.
7. Active learning substantially decreases label complexity. This will be evaluated subjectively, given the difficulties outlined in section [ref].

How these hypotheses were evaluated is described in section 3.4.

1.5 Ethical Consideration

Given how pervasive machine learning is becoming across areas of society, it is good that discussions are happening about safety, transparency and bias in machine learning systems that have the ability to affect lives. The worst case scenario for inaccurate, opaque or biased product classification is embarrassment for the

¹the Wide&Deep baseline model had been trained on rule-based labels

client company, therefore ethical considerations not of much concern for the client company. It is still worth reminding the reader, who might use some of the ideas in this work, that machine learning models always contain some kind of bias: from the data users as input (the way it is gathered, what is gathered), the way the data is processed, and the kinds of models used.

Already at this early stage of machine learning adoption there are cases where blackbox algorithms have been used to decide decisions that severely influence persons life - predicting reoffending probability of convicts to determine whether they are given parole or not - with terrible results. The model that was touted to be an objective substitute to a subjective judge has simply learnt that biases inherent to the data (the prejudices and racism of the judges at the time): it consistently underestimated reoffending rate of white convicts and overestimated the reoffending rate for black convict [cite]. Even though the data did not contain explicit information about race, the algorithm was capable of implicitly detecting race through some other variable that was correlated with race. Most data scientists will never build models with such severe consequences, but even more subtle decisions made autonomously by algorithms can prolong the inequalities of our society by consistently favouring certain characteristics such as race, gender, place of origin, etc. Prime examples are algorithms that determine whether one gets a mortgage or not, what the premium on their insurance would be, whose CV gets shortlisted for a position, and so on.

1.6 Sustainability

The reality of any e-commerce company is that increase revenue almost by definition means more waste and increased carbon released into the atmosphere as a result of production and transport. Efforts to mitigate these unwelcome side effects can be successful at a government level, though the author firmly believes there ought to be stronger intergovernmental regulation to tax carbon emissions and the consumption of materials, as currently there is absolutely no incentive for retailers or consumers to reduce waste, and few incentives to recycle it. The best a data scientist working for a retailer can hope for is poor performance of his models, which would not lead to increased sales.

1.7 Delimitations

our models do not explicitly model the correlation between output variab

1.8 Outline

2. Background

2.1 Input Representations

2.1.1 Categorical Input

The simplest option for representing categorical input is 1-hot encoding, where input has as many dimensions as there are distinct categorical values (vocabulary size); a single dimension is set to 1, with all other dimensions set to 0. This is a straightforward representation: for a simple model such as logistic regression, we can clearly interpret the model parameters and see how the presence or absence of a given category increases or decreases the likelihood of a given output. However, in cases where vocabulary sizes get large, and the number of outputs (the number of units in the next layer in a deep network, or the number of output units in a shallow one) increases, this kind of encoding can really blow up the number of parameters of the model.

An alternative is to use random embeddings: dense, low-dimensional representations of a high-dimensional vectors. It has been shown in compressed sensing literature that if a high-dimensional signal in effect lies on a low-dimensional manifold, then the original signal can be reconstructed from a small number of linear measurements [5]. This has a useful implication for machine learning: categorical variables with large vocabularies of size d can be represented with random embedding vectors of size $M = \log(d)$. This is because it is possible to reconstruct any d -dimensional k -sparse signal using at most $k \log \frac{d}{k}$ dimensional vectors [2], and 1-hot vectors are 1-sparse (only one dimension is nonzero).

An intuitive example is given in [11] about natural images: a 1-million-pixel image could have roughly 20,000 edges¹, i.e. it lies in a roughly 20,000-dimensional manifold from which the original image can be constructed with high fidelity. The 1-million-dimensional image could be projected into a M -dimensional space “by taking M measurements of the image, where each measurement consists of a weighted sum of all the pixel intensities, and allowing the weights themselves to be chosen randomly (for example, drawn independently from a Gaussian distribution)”[11]. The projection is random because the weights for the sum of pixel intensities are

¹technically: wavelet coefficients with a significant power, which roughly corresponds to a superimposition of edges

chosen randomly. Why the projections need to be random is motivated by another intuitive example: when light is shined on a 3-dimensional wireframe, its shadow is a 2-dimensional projection of it. The projection could lose some important information about the regional object if the direction of the light source is chosen poorly, however random directions are likely to result in projections where every link of the wire will have a corresponding nonzero length of shadow.

2.1.2 Text Input

The simplest way to represent text is bag words (**BoW**), which is simply the histogram of word occurrences in the text. BoW representations give equal weight to each of the words in the text, and the model has to learn the relative importance of each of these. A commonly used representation in information retrieval (IR) is **TF-IDF**, which stands for “term frequency - inverse document frequency”. TF-IDF multiplies the term frequency (number of times the word occurred in the text) with its inverse document frequency (the inverse of how often a occurs in all documents). This has the effect of giving lower scores for common words, and higher scores for words which appear often in a document but not too frequently in the whole corpus. Another common representation is bag of n-grams (**BonG**), which is a histogram of character n-grams.

The above representations are sparse, like 1-hot encoding of categorical variables. Text can also be represented as a sequence of **word embeddings**. Word embeddings can either be random vectors or representations learned with word cooccurrence algorithms such as word2vec [28] and GloVe [30]; these representations can remain fixed throughout the learning procedure, or updated as part of the stochastic gradient descent (SGD) when applicable. A simple way to represent text is to average the word embedding contained in it. The average could also be weighted by the TF-IDF score of each word². In [27], paragraph vectors are created in a similar manner to word2vec vectors by relying on these vectors to predict the next word in a sentence.

More complex methods use recurrent neural networks (**RNNs**) to combine a sequence of word embeddings into a fixed length vector (see section 2.2.2). These kinds of models are good at disambiguating the potentially many meanings a word might have. Exactly what gets persisted in the final vector representation of text depends on how the model is trained - two RNNs trained on different tasks (such as sentiment analysis and named entity recognition) would need to store different information in its hidden state to successfully perform their relevant tasks, hence the encoding for the same sentence would be different for either model. Still, an RNN that is trained on one task could provide useful features for another. Encoding text as fixed length vectors using RNNs has been interpreted as compressed sensing [1], with such vectors being “provably at least as powerful on classification tasks, up to small error, as a linear classifier over BonG vectors”.

²the author is unaware whether this has been tried before, but it seems a promising approach

2.2. MODELS CONSIDERED

2.1.3 Image Input

Images can be represented as dense 3-dimensional tensor. A 28x28 RGB image could be represented as a tensor with shape $[28, 28, 3]$, with the final dimension corresponding to the green, red, and blue intensity values at a given x/y coordinate. These intensities are usually in the range 0 ... 255, but are normalised before input to machine learning model. Similarly to RNNs encoding a sequence of words to a vector, 2D convolutional neural networks (2D CNNs) can be used to extract dense feature vectors from raw images (image embedding), further discussed in section 2.2.3.

2.2 Models Considered

The following sections describes a selection of models that could be used for our classification task. This is by no means an exhaustive list, nor is it a selection that is expected to have the highest predictive performance individually. These models will later become part of an ensemble, where diversity matters much more than the performance of any individual model. Engineering considerations and time constraints also influence the selection of models: we did not want to spend time implementing models from scratch, or to use many frameworks for training models. TensorFlow is a widely used machine learning library with a good selection of open source models, in particular a selection of pre-trained models for computer vision and NLP, and has arguably the most mature deployment ecosystem. Therefore models that did not have an open source TensorFlow implementation were automatically excluded.

Section 2.2.1 describes models that can take categorical and text inputs, section 2.2.2 looks at some neural models that take only text inputs, and section 2.2.3 describes 2D CNNs that can classify or extract features from images. In all cases the models are described in terms of how they could be used for solving the problem of multi-label classification.

2.2.1 General Models

Logistic Regression

Logistic regression is a linear, discriminative classifier that is often the baseline model of choice, since it is both interpretable and efficient to train. There are methods that take time linear in the number of non-zeros in the dataset, which is the smallest amount possible, and it can be made to handle non-linear decision boundaries by using kernels [22]. Our case is the binomial logistic regression, with a separate logistic regression model for each output class. This is shown formally in eq 2.1, where x and w correspond to the input and weight vectors, respectively. We follow the notational trick where the first element of x is always 1, and the first element of w corresponds to the bias term. The loss function of this model as well

as how it is optimised is described in section 2.2.1.

$$p(y|x, w) = \text{Ber}(y|\text{sigm}(w^T x)) \quad (2.1)$$

Feedforward Neural Network

Feedforward neural networks (also called deep feedforward networks, multi-layer perceptrons) have been described as function approximator, whose goal is to approximate some functions f^* [12]. We expect some familiarity with neural networks from the reader; for an excellent overview of the various use cases and models of deep learning, refer to. In our case, the input is some representation of categorical and text input: sparse BoW or TF-IDF of text, 1-hot encoded or random embedding vectors of categorical variables, or embedding is extracted from text or images using pre-trained recurrent or convolution on neural networks. The hidden layers of our network are homogenous: they use the same activation function (ReLU, sigmoid, or tanh) and have the same number of units; activation functions and the number of units in hidden layers are determined through hyperparameter tuning. The output layer uses sigmoid activation function and has the same number of units as there are classes.

Wide & Deep

Loss Function and Optimizers

Logistic regression and neural networks are optimised with some variant of gradient descent. For our task the loss function binary cross-entropy between the training data and the model distribution, with the loss value averaged across all classes. This is given in eq. 2.2, where θ corresponds to the model parameters such as the weights and biases of the model, C corresponds to the number of classes, and $P(c = 1|x, \theta)$ gives the predicted probability that the item belongs to class c given the feature vector x .

$$NLL(\theta) = \sum_{c=1}^C \sum_{i=1}^N [c_i \log P(c = 1|x, \theta) + (1 - c_i) \log(P(c = 0|x, \theta))] \quad (2.2)$$

We are minimising the negative log likelihood (NLL) rather than maximising the product of likelihoods. Multiplying large numbers of probabilities could result in numerical underflow and rounding errors, therefore it is pragmatic to work with sums of log probabilities instead. The Adam [24] optimiser works very well with default hyperparameters, and is therefore used for all stochastic gradient descent updates.

2.2. MODELS CONSIDERED

2.2.2 Text Models

1D Convolutional Neural Networks

A simple convolutional architecture for text classification is described in [23]. Pre-trained k -dimensional word vectors are concatenated to represent a sentence, and a filter is $w \in R^{hk}$ is applied to a window of h words at each possible window of words in a sentence; this gives a single variable-length feature vector representing the sentence. Several such filters are learned (each with potentially a different width h), and max-over-time pooling is applied to these feature maps; this gives a vector of the highest activations from each filter, which is then passed to a fully-connected softmax layer for final classification (in the case of multi-class classification). For multi-label classification, the final layer would be a fully-connected layer of sigmoid activations.

This simple architecture should be able to predict output classes reasonably. Each filter can indicate the presence of a sequence of h words; max-pooling discards information about where exactly in the text it appeared, and ensures the output is of a fixed length. The same filter w is used across all possible word windows in the sentence, which can be seen as a form of parameter sharing (and as an infinitely strong prior over the parameters of the model [12]), and enables processing variable-length sequences. The relatively small number of shared parameters requires less training data than an equivalent fully-connected architecture. Using pre-trained word embeddings further simplifies the task, as these already carry some information about the meaning or syntactic role of words.

More sophisticated architectures can be built using 1D CNNs, although not used in our experiments. Most notably, several layers of convolutions (each optionally followed by pooling) can be stacked, where the following layer works on the feature maps output by the previous layer. The model described above uses a stride and dilation of 1, but multi-layer architectures where the higher layers have use exponentially increasing dilation are able to expand the receptive field of the model, and as a result aggregate “contextual information from multiple scales” [42]. Dilated convolutions were beneficial for semantic segmentation of images with 2D CNNs, but this increased receptive field has been useful for sequence-to-sequence models in NLP [41].

Recurrent Neural Networks

Recurrent neural networks (RNNs) are a family of models for processing sequential data. The sequence of inputs $x^{(1)} \dots x^{(t)}$ in our case are vectors of word embeddings, but there are other options for input representations (e.g. sequence of 1-hot encoded tokens, or vectors representing a multivariate time series at a given time step t). Vanilla RNNs maintain a hidden state vector h which contains some information about the sequence it has seen so far, and is calculated from the input at the current

time step t , and the previous hidden state:

$$h^{(t)} = f(h^{(t-1)}, x^{(t)}) \quad (2.3)$$

Vanilla RNNs suffer from the vanishing and exploding gradient problem in long sequences and are notoriously difficult to train. Probably the most widely used variant, the long short-term memory networks (LSTM) [17] overcome this limitation by augmenting the network with a memory cell c ; there is a learned gating mechanism that controls what part of (and the extent to which) the cell is forgotten, what gets persisted in the cell state, and what gets output at a given time step. An intuitive overview of the gating mechanisms is given by [29] and [36] describes well how this helps mitigate vanishing gradients. A simpler gating mechanism is offered by gated recurrent units (GRU) [7], which has fewer parameters and works well on simpler tasks.

We are interested in using RNNs as text encoders, though they are often used for sequence to sequence modelling, or for predicting an output at each time step. In the simplest case, the concatenation of the cell state c and the hidden state h at the last time step could be used as a representation of the sequence.

2.2.3 Image Models

2D CNNs are important historically - excellent results in computer vision revived interest and funding in deep learning - but also applicable to a wide range of problems. Computer vision CNNs tend to be complex models with millions of parameters and dozens (or even hundreds) of layers. It is very compute-intensive and time-consuming to search for new architectures, and the analysis of these is beyond the scope of this work. Our goal is to use a CNN that has a reasonable performance without incurring unreasonable overhead.

The general architecture of a 2D CNN is as follows. Patches of feature extractors are convolved over the x and y axis of the image; these are often small, e.g. $3 \times 3 \times c$ patches that span all the c channels of the image ($c = 3$ for RGB images), and convolution could be strided. Former models used larger patch sizes, but stacking several smaller patches could achieve similar receptive fields while allowing for a larger number of non-linearities for the same number of parameters. One or more layers of convolutions would be followed by a (often max) pooling layer. Computer vision architectures tend to re-use the same sub-structure repeatedly: either the same kinds of convolutions followed by pooling, or the “network in a network” structure popularised by GoogLeNet [37]. After a number of such repeated structures, there are normally a few fully-connected layers followed by a softmax layer. In our case, the final layer would be a fully-connected layer of sigmoid activations.

Transfer learning has shown to be particularly useful in computer vision. Successful computer vision models require a notoriously large training dataset, which would be hard to come by for every distinct computer vision task. Instead, models are often initialised to the values of a model that has been trained on a large dataset such as Imagenet [1], excluding only the last layer(s) of the model that has

2.2. MODELS CONSIDERED

learned features that are specific to the original problem. Representations learned at the lower layers are remarkably universal and useful for other tasks. Therefore pre-trained 2D CNNs can be used as feature extractors for various other tasks, or the models could be fine-tuned to learn representations that are even more useful to the new task.

2.2.4 Downstream Models

Item Similarity

Similarity measures based on tokenised text are easily accessible to e-commerce companies: the popular open source NoSQL database ElasticSearch (which makes use of Lucene, a full-text search engine) provides document similarity metrics that are some combination of normalised TF-IDF vectors between all documents and a query (which could be another document). This gives decent results in many cases, but it does not take advantage of a product image.

Embeddings extracted with a deep network can be viewed as a distributed representation of the original data, which carries semantic meaning [16]. In the contrived examples of distributed representations, each dimension would represent the degree to which a property (e.g. of shape or colour) is present of an object, however the dimensions are not necessarily so nicely disentangled in the representations learned by deep networks³. Still, it is clear that such dense representations help linear models do accurate predictions, and semantically similar data points will have similar embedding vectors.

Therefore we can compare any two embedding vectors (extracted with the same neural network) using standard vector space similarity measures, such as cosine similarity (1 - normalised dot product between the vectors). Such embeddings can be extracted from product images with 2D CNNs pre-trained on another task, 1D CNNs or RNNs on product title and descriptions, or from the joint embeddings described in section 2.5. With large numbers of products, calculating pairwise similarity scores becomes intractable, therefore approximate nearest neighbour methods could be used [3].

Another interesting method of computing similarity scores between documents utilises the full-text search capability of tools such as Lucene, which would be valuable to firms already using such technologies. The embedding vectors of products could be tokenised, by converting each dimension of each embedding vector into tokens that represent the feature with some precision [32]. For example, we could consider two levels of precision and divide the normalised feature into 10 intervals of size 0.1 and 100 intervals of size 0.01; each product would get two tokens per

³The author has not seen strong evidence in literature to support either case, but at least in [18] extra steps had to be taken to *prevent* certain latent variables from encoding properties of the data that were designed to be captured by other latent variables. This implies that by default, each latent variable contains a little bit of information about each aspect of the input, and that the whole pattern of the embedding matters for conveying semantic information

embedding dimension⁴. For example, if the first embedding dimension is 0.46, the inserted tokens would be `d1_0.4` and `d1_0.46`. Full-text search engines would assign higher scores to co-occurrences in the more precise tokens and lower scores to co-occurrences in more coarse token.

Recommender Systems

Several methods have been proposed that use dense embeddings learned by deep models that are used as part of a recommender system. These are briefly described here to motivate our focus on models that obtain dense embeddings of products.

Models that deal exclusively with deep embeddings [9] require huge amounts of user-product feedback pairs, therefore the more interesting solutions are ones which work together with classical methods such as matrix factorisation (MF). MF finds - purely from the implicit or explicit feedback users give to items - vectors of latent factors that represent each user’s preferences and each item’s “qualities”; the inner product between a user’s and item’s latent factors gives a score of compatibility between the two. Deep models can augment the item latent factors by injecting the embeddings learned for another task. The main difference in these methods is how the deep embeddings are merged into MF, and how the deep embeddings are obtained in the first place. In [39], stacked denoising autoencoders are used for unsupervised feature learning of item data, while [14] uses simply visual embeddings extracted from a 2D CNN pre-trained on ImageNet.

2.3 Unsupervised and Semisupervised Learning

This section explores ways in which unsupervised and semi-supervised learning can learn good feature representations and improve sample complexity. Generic semi-supervised methods such as self-training are not considered, as one of our goals is to learn good representations, but also because these methods can reinforce poor predictions or do not make full use of all available unlabelled data.

Some generic methods can still improve the representations learned by our models when applied to models that learn deep embeddings in order to make predictions. Entropy minimisation [13] can be incorporated into models trained with SGD to encourage confident predictions of each class; this encourages the deep model to learn predictions that are strong predictors of some class and avoid producing features that produce mixed predictions. More complex but very performant approach is Mean Teacher [38]. A student that gets a harder task (such as predicting from a noisy/adversarial example), and a teacher that gets an easier task (i.e. the teacher model is an ensemble, which is more accurate). The student is trained on the prediction of the teacher; the teacher’s parameters are an exponential moving average of the student’s, updated after each minibatch. The teacher’s predictions are higher-quality than the student’s (and can be applied on unlabelled data), while

⁴It would be a good idea to also have some wider overlapping intervals as well, e.g. 0 ... 0.5

2.3. UNSUPERVISED AND SEMISUPERVISED LEARNING

the student tries to continuously learn to learn a predictor that is robust to noisy and adversarial examples.

2.3.1 Autoencoders & Variational Autoencoders

Deep autoencoders (AEs) can be used to learn low-dimensional representations of inputs. Many variants exist, but the general pattern is to have an “hourglass-structured” neural network where the first half of the model shrinks the input, and the second half of the network reconstructs the original input. Activations in the middle layer correspond to a dense embedding of the sample; the shrinking layers need to throw away some of the detail in the input, yet persists enough for the expanding layers to be able to reconstruct the original input with some fidelity. The embedding contains information that is mostly unique to the data point, while the parameters of the encoding and decoding layers ensure that the reconstructed input is realistic. It is common to add noise (Gaussian, dropout) to the input or the intermediate layers to increase resilience to noisy inputs and to prevent the autoencoder simply memorising each data point.

If the bottleneck layer is unconstrained, it will use a wide range of values to represent different inputs. We would like embedding for similar inputs to also be similar, which is not always the case for ordinary autoencoders. Variational autoencoders (VAEs) impose a prior distribution on the values of the embedding, often a multivariate Gaussian distribution with a diagonal covariance matrix, and the model is regularised during training to respect this prior. The model is optimised to minimise the reconstruction loss and KL divergence between the model’s distribution z and the prior on it, which can be computed just from μ and σ if the prior is a isotropic standard normal. Enforcing the prior also means that the embeddings z will occupy a smooth, contiguous space, which allows us to draw samples from the prior $\epsilon \sim \mathcal{N}(0, 1)$ and use that as the input to the decoder - this gives us a generative model, which would not be possible with ordinary autoencoders. The output of the VAE is also probabilistic: e.g. for images, the output for a pixel would be a Gaussian distribution, which is sampled the same way as the Gaussians for z .

The VAEs described here are probabilistic models parameterised by neural networks for approximating the true posterior $p(z|x)$, since the exact posterior is intractable. In practice, VAEs add an extra loss term (KL divergence) to AEs, and additional step to determining the embedding z . There are two separate neural network layers from the bottleneck layer of the AE: one for determining μ (the vector of means of the multivariate Gaussian), and one for determining σ (the vector of standard deviations of the multivariate gaussian). Given μ and σ , we can sample the final item embedding $z \sim \mathcal{N}(\mu, \sigma^2)$. Note that sampling of z is a discrete decision that would normally stop gradient from propagating past this step, but we can use the reparametrisation trick introduced by [26] that turns the discrete decision into a deterministic function of $z = \mu + \sigma\epsilon$, where $\epsilon \sim \mathcal{N}(0, 1)$ is a random auxiliary noise parameter.

2.3.2 Conditional Variational Autoencoders

It is easier for linear models to learn from embeddings extracted with AEs, and embeddings from VAEs make the classes even easier to separate. These are unsupervised methods that do not take advantage of labels in the training data. In the semisupervised approach introduced by [25] there are two inference networks: a discriminative classifier that outputs a categorical distribution from the input x , and a class-conditional encoder that takes as input both x and the 1-hot encoded categorical label y ⁵. The model is trained on both labelled and unlabelled data. For labelled examples, the x and y are given as input to the model, which embeds it in z as described earlier, and reconstructs the original x . The value of y is unknown for unlabelled data points; therefore the model is run $|y|$ times, encoding and decoding the data point conditioned on each possible class i ; loss from these runs is averaged, weighted by the discriminator’s estimate of the sample belonging to class i . This approach is acceptable for small numbers of classes, but is impractical for many multi-class problems. A solution uses the reparametrisation trick mentioned above: rather than running the procedure once per class, we take a Gumbel-softmax [20] to get a discrete estimate of y that is still differentiable.

Such class-conditional VAEs can be used in any situation where unlabelled data is abundant but labels are scarce. The discriminator’s loss is optimised as part of the VAE’s loss function, which means adding more unlabelled data can improve the accuracy of the discriminator. The approach was developed and tested on the MNIST dataset, which consists of 28x28 grayscale images - a very simple dataset by today’s standards. Some reports have emerged that fail to reproduce this success on more complex datasets such as CIFAR-10, being outperformed even by PCA [21].

One related approach is offered by [18], where a class-conditional VAE is used to generate synthetic data for a discriminator network, which has reportedly a higher accuracy in semisupervised setting than the approach described just above. They use it for conditional text generation, but this approach of using the class-conditional VAE to synthesise training data to train a discriminator is applicable to any input modality. In fact the general approach to “dreaming up” new training samples in the *sleep phase* and training the classifier in the *wake phase* was introduced already in [15]. The current author has implemented this model and open sourced it⁶.

2.3.3 Generative Adversarial Networks

Generative adversarial networks (GANs) are an interesting approach capable of synthesising realistic data, but also useful for learning good representations of data. GANs have been most successful for image synthesis, but are in fact applicable to any kind of input data including text [] and even mixed data types such as user profiles []. In the GAN setting, there are two networks: a generator that tries to

⁵class-conditional encoder means that the encoder is aware of the class of the data point, i.e. the output distribution z is conditioned on the class y in addition to the original input x

⁶<https://github.com/mattiasarro/seq2seq-cvae-tensorflow>

2.4. GENERAL PRACTICES IN MACHINE LEARNING

produce realistic synthetic samples, and a discriminator whose goal is to distinguish between synthetic and actual samples. Given that the training is stable enough, both the generator’s and the discriminator’s performance improves with time, resulting in more realistic synthetic samples, as opposed to the relative blurry images produced by VAEs. The discriminator needs to learn good representations of the input to accurately distinguish which samples come from the true distribution, and which samples are synthetic; as with many CNNs for computer vision, these representations can be useful for other tasks as well. It has been shown that linear models from the embeddings learned by the discriminator outperform other unsupervised feature learning techniques such as k-means [31]. At the time of writing, variants of Wasserian GANs (WGANs) achieve the best performance by improving training stability and preventing the generator from generating samples from a limited number of modes; this is achieved by minimising the Wasserian distance between the generator’s and real data distributions, as opposed to minimising the JS divergence as was common before. A performant variant of WGAN is CT-GAN, which adds a regularisation term to enforce a Lipschitz continuity condition over the manifold of the real data [40].

2.4 General Practices in Machine Learning

We briefly list some techniques and approaches that could be used for many kinds of machine learning problems. Some of these will be used in our experiments, yet some may not be pragmatic due to long train times and time constraints.

Bootstrap sampling, where data points are sampled from training data with replacement, can be used to repeatedly train the same model, and to observe the variance of its predictions. Bumping can be used to train several models (of the same family) on bootstrap samples to move around in the model space, and will pick the model that best fits the training data. This helps it explore a wider selection of models, but given that the original training data often also included as one of the bootstrap samples, this method can still pick the model original model if it happens to have the best accuracy.

There are some versatile methods that can help regularise a neural network (deep or shallow), or to speed up convergence by improving gradient updates. L2 regularisation should always be used to decrease model complexity and impose prior on the model parameters, which implies that very high and very low values are unlikely. Dropout can mitigate overfitting by preventing neurons from co-adapting, encouraging each to learn representations that are useful independently [35]; this has been interpreted as training an exponential (in the number of parameters) number of models and averaging their predictions.

gradient clipping layer norm Batch normalisation is known to stabilise training and hence speed up convergence by normalising each input to have unit variance and zero mean [19].

2.5 Combining Models

This section introduces common ensembling methods. Some of these (bagging, boosting) are expected to consist of weak learners or models from the same model family, while others (committee methods, BIC, stacked generalisation) or more appropriate for ensembles of strong models.

Bootstrap aggregation (a.k.a bagging) draws several bootstrap samples from the training data, trains a separate model per bootstrap sample, and averages the predictions of these individual models. This reduces the variance of predictions without increasing its bias and generally leads to more accurate predictors [4]. Boosting is another common meta-algorithm that iteratively trains an ensemble of weak models, such that the data points that incurred a higher error on the previous ensemble are weighted more heavily, and each new weak model is added to the ensemble with a weight proportional to the weak learners accuracy. A common boosting algorithm is AdaBoost [10].

We are interested in ways of combining models that are separately trained and combined into a single predictor. Simple solutions are voting or (weighted) averaging, where the weights can be found with k-fold cross-validation. A more appealing approach is stacked generalisation, where a meta-learner is trained on the outputs of the individual models. This meta-learner could be a relatively simple model, such as logistic regression or a decision tree, and the results of the meta-learner could be therefore quite interpretable.

One orthogonal approach to combining models is joint training of model components. All models described here are trained using stochastic gradient descent, so in principle it would be possible to learn the parameters of all components (1D CNN, 2D CNN, RNN, DNN, logistic regression) as part of a single optimisation loop. This would be an engineering challenge due to the different ways these models require their input to be represented and the large size of the model, and optimisation would surely be difficult. In our case this would be clearly an overkill, but it would be an interesting research problem to examine whether joint training has advantages over ensembling in cases where we have different views of the data (in terms of considering different input dimensions or processing the inputs differently). As mentioned in the Wide & Deep paper [6], the wide component of the model has to just handle cases where the deep component falls short, and can therefore be simpler than it would need to be in an ensemble; analogously, jointly training different kinds of models neural networks would allow each component to be simpler.

One of the motivations for picking mostly deep neural networks as our ensemble components was their transfer learning capability: they all produce a dense feature vector (embedding) from which separate logistic regressions predict the class. While it is useful to have separate embeddings for images, text and categorical variables, we would also like to have a compound embedding of each product. A simple concatenation of all individual embeddings could be a useful (albeit a quite high-dimensional) representation to be used in downstream models. Alternatively, we could use this concatenation as an input to a neural network, whose goal is to (1)

2.6. ACTIVE LEARNING

reduce its dimensionality by removing redundant information and (2) predict the output classes from this compressed embedding. The latter case could act as a kind of a (replacement for) the meta-learner, with the difference that it takes the penultimate (as opposed to the final) layer of each individual model as input.

2.6 Active Learning

This section describes the main approaches to active learning; details analysis is beyond the scope of this report.

The goal of active learning is to reduce the number of labels needed to effectively train a machine learning model by being selective about which data points to label. The three general scenarios: membership query synthesis, stream-based selective sampling, and pool-based sampling [33]. In the first scenario, the algorithm synthesises a datapoint and asks a label for it. In stream-based selective sampling, an instance is sampled and the model decides (while having access to the data point's features) whether to acquire a label or not. In pool-based sampling, the model chooses which data point to label from the pool of all unlabelled samples. Our use case is a version of pool-based sampling, where the algorithm picks out a batch of products to be labelled. The rest of the section describes different approaches to picking the data points that are expected to help the model learn.

Uncertainty sampling is the most popular choice: if the model is uncertain about a prediction, obtaining a label for that data point would help it differentiate between different targets. The most common way to quantify uncertainty is by entropy of the model's predictions:

$$x_H^* = \operatorname{argmax}_x - \sum_i P_\theta(y_i|x) \log P_\theta(y_i|x), \quad (2.4)$$

where x_H^* corresponds to the most informative instance according to the entropy (H) measure, and y_i corresponds to each class.

Query by committee uses a number of models trained on the labelled data which all make a prediction on the unlabelled data. Data points with highest disagreement are expected to be most informative, as by definition a larger number of models would have to be wrong in their predictions. The models in the committee do not have to be of different type like in our case, but could be e.g. a set of linear classifiers where each committee member just has different parameter values, yet each member would have to be consistent with the current set of labels (not contradict it with its predictions). Disagreement between committee members can be quantified with vote entropy [8]:

$$x_{VE}^* = \operatorname{argmax}_x - \sum_i \frac{V(y_i)}{C} \log \frac{V(y_i)}{C}, \quad (2.5)$$

where $V(y_i)$ is the number of votes given to class i and C is committee size. Alternatively, KL divergence between each committee member's predictions and

the consensus P_ζ (average prediction of committee members) could be used:

$$x_{KL}^* = \operatorname{argmax}_x \frac{1}{C} \sum_i D(P_{\theta^{(c)}} \parallel P_\zeta) \quad (2.6)$$

$$P_\zeta(y_i|x) = \frac{1}{C} \sum_{c=1}^C P_{\theta^{(c)}}(y_i|x) \quad (2.7)$$

$$D(P_{\theta^{(c)}} \parallel P_\zeta) = \sum_i P_{\theta^{(c)}}(y_i|x) \log \frac{P_{\theta^{(c)}}(y_i|x)}{P_\zeta(y_i|x)} \quad (2.8)$$

Expected model change calculates how much a model would change if we knew its label. In gradient-based learning algorithms it is possible to compute the L2 norm of the gradient vector for each combination of labelings of the unlabelled product [34], which is a direct measure of how much the model would change.

Expected error reduction considers how much the test set error is likely to decrease with the acquisition of a given label. This is done by re-training the model once per each combination of the label values and observing how either the risk or expected log loss of the unlabelled data points decreases. This is not a suitable use case for deep networks, which are trained over several epochs of the data; there is no efficient way to incrementally train the model, and when re-training with a single additional label, the change in the model is probably higher from the stochasticity in the training procedure rather than the additional label. In any case, this method is very expensive computationally.

Variance reduction tries to pick data points which are expected to decrease the variance in predictions. To do that, the Fisher information of the model parameters should be maximised. Unfortunately this involves inverting a $K \times K$ covariance matrix, where K is the number of parameters in the model. This is impractical for deep networks with millions of parameters.

Information density measures consider data points that are not just uncertain but also representative of the underlying distribution. This avoids the problem with many other approaches that ask labels for samples that are controversial, but could otherwise be outliers and not the most useful for good generalisation. In this framework, a base informativeness measure $\phi_A(x)$ such as uncertainty or disagreement is weighted by the average distance of the data point x to other data points in the distribution [?]:

$$x_{ID}^* = \operatorname{argmax}_x \phi_A(x) \times \left(\frac{1}{U} \sum_{u=1}^U \operatorname{sim}(x, x^{(u)}) \right)^\beta, \quad (2.9)$$

where sim is some similarity function and β controls the importance of the density term.

3. Method

Several hypotheses were tested in this work. Section 3.1 gives an overview of how input data was pre-processed. Section 3.2 describes the technical set up required for running all these experiments and deploying the model to production before delving into the specific experiments and their evaluation methods in sections [ref].

The experiments were conducted in four distinct stages:

- Training a baseline model on the rule-based labels to get a sense of the difficulty of this problem. Since there is no fundamental difference in the way this model was trained and evaluated compared to the other classifiers, this is described in section 3.3.2 with the others. After this step, employees of the client company labeled products that would become the ground truth dataset. The visual comparison feature was also subjectively evaluated at this stage.
- Training the independent classifiers to determine best performers (3.3.2).
- Training an ensemble of the independent classifiers (3.3.3).
- Training up to 10 iterations of active learning on the strong predictor (3.3.4).

3.1 Data Preprocessing

There were around a dozen product features that affiliate networks provided. Most of these features were either categorical or textual, with just a single numerical feature (price). Initially, the data was analysed using Dataprep, a Google Cloud Platform (GCP) product for data wrangling, which at the time of use was in beta stage. Dataprep was used to process a sample of 800 000 products; it produced histograms of the values present in each feature column (see appendix A.1).

The histograms revealed that a lot of the input features were mostly empty, but also that many of the inputs that would naturally be considered categorical had much more unique value in them than one might expect. For example, each affiliate gives us the textual representation what they consider to be the category of the product, but rather than containing a small number of unique tokens, these contained all the full category paths along with the category delimiters, which varied retailer by retailer (e.g. it was common to see both “Shoes > Sneakers” and “Shoes // Sneakers”). Representing these as categorical variables would have blown up the

input space, which would have resulted in more parameters, each parameter having fewer examples to learn from. Therefore, many such “categorical” were actually represented as text, which were tokenised and cleaned appropriately, allowing for better generalisation and smaller models.

There was a single numerical field: price. This could have been min-max normalised to the range 0 ... 1, however there was a small number of very high values that would have squash nearly all the other prices. Rather than carefully considering how to mitigate this, the input dimension was dropped, because it is not likely to have much predictive value for product classification. It would be trivial to bring this feature back, for example when building a recommended system, where it would be much more useful.

A trickier question was how many distinct tokens or categorical values to keep per input column. Keeping all of them would not have been sensible: there were still large numbers of tokens that appeared only once, often because there were some unwanted formatting characters, misspellings, or incorrect punctuation that caused a token to be considered a separate entity. There was a single configuration file that dictated which models used which features as input, whether those inputs were represented as textual, categorical, or dense values; it also determined the maximum number of unique values/tokens, and the dimensionality of the embedding. This configuration file was read by Dataflow during pre-processing and by TensorFlow during inference and training, which made experimentation with different types of models and input representations considerably easier.

Below is a list of input features with information about how they were represented; it also lists the dimensionality of embeddings for the models which encoded categorical variables as embedding.

- title - text - max 8000 unique tokens
- brand - categorical - max 5000 unique values - 10 embedding dimensions
- category - categorical - max 950 unique values - 6 embedding dimensions
- rawCategory - text - max 1000 unique tokens
- description - text - max 8000 unique tokens
- gender - categorical - take all unique tokens
- size - categorical - max 100 unique tokens
- image - dense vector of 2048 features extracted with a 2D CNN

3.1.1 Category Structure

At the time of writing, there were roughly 1000 categories defined in the client database. Categories were structured in a way that is typical of e-commerce: categories can have child categories, which in turn can have child categories, etc. In our case, the typical depth of the tree structure was five, i.e. a leaf category often had four parents; naturally, the tree structure was not balanced, so many branches ended at depth three or four.

This structure has to be taken into account when labelling and predicting categories for unseen products. When a product is labelled to belong to a lower level

3.1. DATA PREPROCESSING

category, it should also be labelled to belong to all of its ancestor categories. This does not work the other way around, though: if a product is labelled not to be a Trainer (lower level category), this does not imply it is not a Shoe (ancestor category). Similarly, when the model predicts that a product belongs to a lower level category, it is considered that it also predicted the product to belong to all of its ancestor categories; again, negative predictions at lower levels do not overwrite positive predictions at high levels.

Note that the decision to consider each of the outputs as an independent binary variable in favour of mutually exclusive categories may later change. There are some benefits to this: in some cases categories are inherently ambiguous, and allowing overlapping categories would enable us to use the same model to learn other attributes of products which might be more subjective. For example, we might be able to train a model to distinguish certain styles within a category, which would not have clear boundaries. Predicting binary independent outputs means that when a product is given a label (that it belongs to a category X), this label does not immediately exclude it from other categories; with mutually exclusive categories labelling a product would immediately determine whether or not it belongs to any of the categories.

3.1.2 Class and Label Imbalance

The labels provided by the rule-based system are only positive: some products are labelled to belong to a given category, but many products that ought to belong to a category are not labelled accordingly - but their label still appears to be negative. This (which we call the label imbalance problem) only exacerbates the class imbalance problem (that most products do not belong to most categories). As a result the model trained on rule-based labels will certainly underestimate the likelihood of any product belonging to any category.

Still, most positive labels provided by the rule-based system are correct, which means the model should assign higher likelihoods to products that should actually belong to the given class. Our active learning strategy outlined in section 3.3.4 ensures that products around the decision boundary would receive a label - which during the initial rounds of active labelling would be overwhelmingly positive examples¹. The first rounds of active labelling should therefore counterbalance the underestimating nature of the pre-trained model; as the model starts to make more “optimistic” predictions, the products near the decision boundary should become a more balanced mix of positive and negative examples.

Class imbalance may or may not be an issue after label imbalance has been accounted for. The worst case scenario is that our model continues to underestimate the likelihood of products belonging to classes, particularly if these are rare classes. False negatives are not much of our problem in our setting. There are millions of products that affiliate networks provide, and in any case we can show the average

¹this is confirmed by our experiments, described in section [ref]

user a tiny fraction of those products, so it is okay if some are left out from some categories and their chance to be seen decreases. Conversely, false positives will appear unprofessional and reduce user satisfaction.

3.2 System Architecture

The following technologies were used to build the system which had to interact with existing services at the client company:

- Apache Airflow (AF) - a Python framework for defining workflows of long-running tasks and dependencies between these tasks.
- TensorFlow (TF) - ML framework for Python, capable of defining many kinds of models as a computation graph, and executing this graph locally or in a distributed manner.
- ML Engine (MLE) - a GCP service for running TensorFlow models (training, hyperparameter tuning, inference).
- Apache Beam - a data processing engine akin to Apache Spark and Apache Flink.
- Dataflow - a GCP service for executing Apache Beam workloads.
- Tensorflow Transform - a Python library with a small set of operations for data preprocessing that can run inside a TensorFlow graph as well as an Apache Beam pipeline.
- Google Cloud Storage (GCS) - Google Cloud Platform (GCP) object storage similar to Amazon S3.
- ElasticSearch (ES) - a NoSQL database with powerful full-text search and querying capabilities.
- RabbitMQ - a message queue, used for transferring data among our microservices (using the Logstash adapter, that can read from and write to (among other things) ElasticSearch and RabbitMQ).
- Flask - a simple backend web framework for Python.
- Node.js - a JavaScript backend web framework.
- React.js - a JavaScript front-end framework for JavaScript.
- Redux - a framework for persisting user interface (UI) state and application data in single page applications.
- GraphQL - a query language for building flexible APIs

Figure 3.1 shows the how data is passed between the main services, and how services and technologies interact.

All product data is stored in ElasticSearch (ES): the rule-based labels, the predictions of the ML system, and evaluation metrics from various train runs. ES is

3.2. SYSTEM ARCHITECTURE

accessed from the public web application via GraphQL and the ML administration web UI (further referred to just as web UI²). Data is pulled into the ML pipelines by dumping the results of an ES query to a local file, which is uploaded to GCS. Updates to the ES index are not done directly, since indexing the updated products is computationally expensive; instead, updates are put on a RabbitMQ queue, which is consumed by Logstash, which in turn updates products in ES at a rate that will not overburden the servers.

All ML training and prediction happens in a batch-oriented way, encapsulated as Airflow pipelines. Each pipeline is a directed acyclic graph of tasks, where a task can be a shell command or Python function; a pipeline defines dependencies of task execution, which allows us co-ordinate a series of operations that could be executed locally (inside the Docker container running AF) or remotely (such as in a GCP service). A typical pipeline dumps data locally, uploads it to GCS, schedules a Dataflow job to preprocess data, polls the Dataflow service until the Dataflow job is finished, schedules an ML engine job, polls the MLE service until it has completed, and runs an update process that reads the predictions and evaluation statistics from GCS and sends the updates to the RabbitMQ queue. Reading updates and sending these to RabbitMQ is done in a parallelised manner (using multiprocessing), since the update process is bottlenecked due to network latency as well as computing the appropriate category path for each product (explained in 3.1.1).

3.2.1 Dataflow Pipelines

There are two types of Dataflow pipelines: for preprocessing training data and for calculating product-product visual similarity. Omitting various details, dead-ends and workarounds that were needed due to technical limitations and prior system architecture choices³, the pipelines had the following tasks:

Preprocessing

This pipeline loads the products dumped from ES (as JSON) and preprocesses data according to a configuration file (see section 3.1). All fields are cleaned of obvious noise and superfluous whitespace. Text and categorical fields are tokenised and mapped to integer indices, keeping only the top k values and also computing TF-IDF scores for text fields. This is handled by TensorFlow Transform, which persists this token-to-index mapping in a *transform function* that is saved to GCS at the end of the pipeline. The transform function is used by a TensorFlow model to convert raw text inputs to a sparse inputs; separate pre-processing run will generate a different transform function, with mostly the same tokens mapping to different indices, as the order in which they will be encountered will be different.

²The web UI was initially built with Flask and React by the author as a quick way to get insight about the model, and then re-written as a more feature-rich version by an employee of the client company with Node.js, GraphQL, React and Redux.

³which were completely reasonable at the time, when the ML system was not a consideration

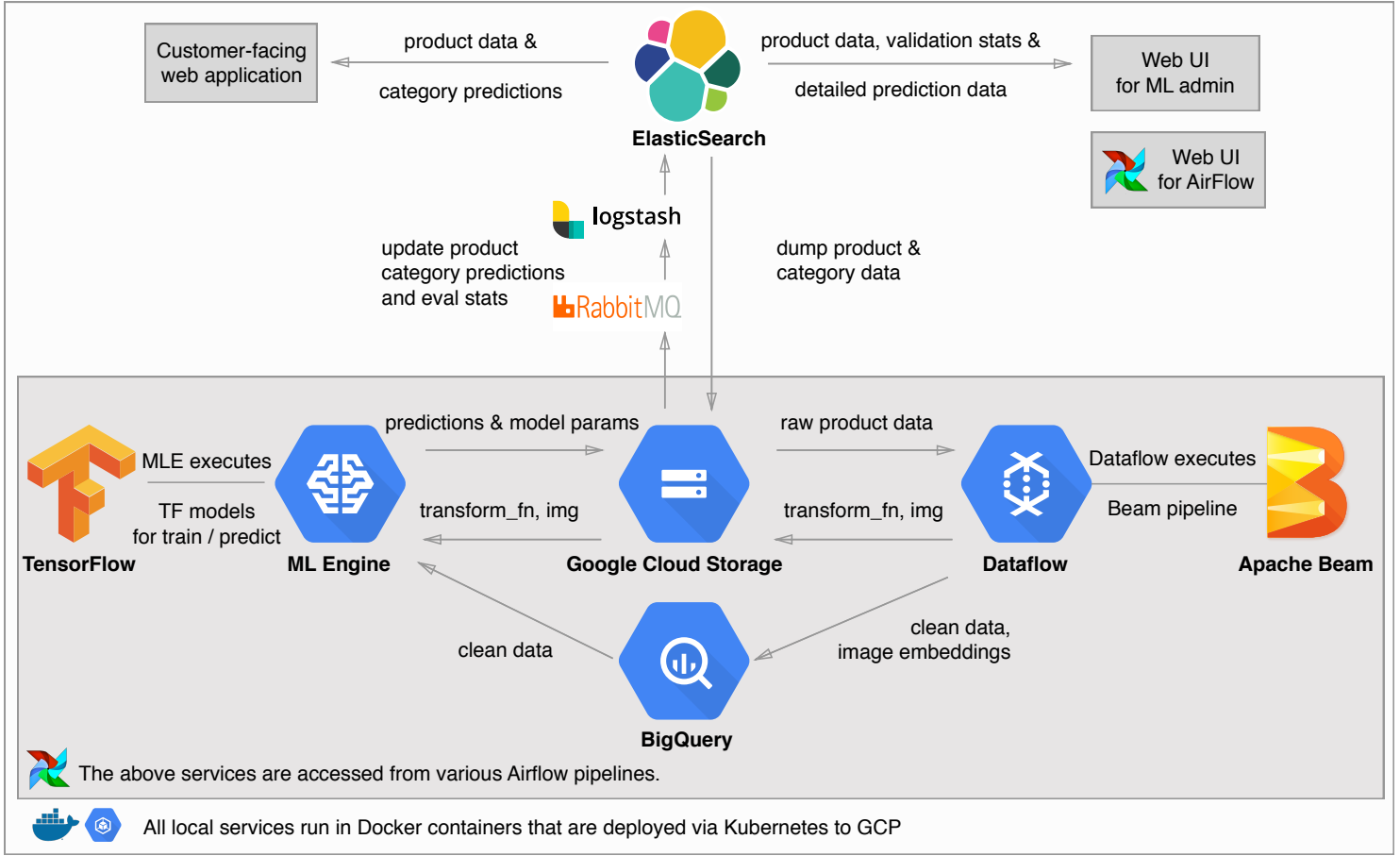


Figure 3.1. High-level system architecture of the ML pipeline

The pipeline is also responsible for downloading product images and using a pre-trained 2D CNN to extract a dense feature vector for each product from the penultimate layer of the CNN.

The clean data and image embeddings are inserted into a new BigQuery table after each run⁴. Note that the data is not inserted in its tokeniser form. Storing tokeniser data would reduce the space it takes marginally, but keeping raw data makes the system easier to debug, and enables the option to do inference on raw data that is not tokenised (e.g. in a streaming banner, when we might not have access to the transform function).

Visual Similarity

This Dataflow pipeline uses the data in BigQuery as input. As explained in section 3.3.1, it needs to find the $k=100$ nearest neighbours of each product based on the

⁴BigQuery is inefficient in updating existing records and limits the number of update per day

3.3. EXPERIMENTS

cosine similarity of their image embeddings. The product-product similarities are computed within products that belong to same second level category, therefore the pipeline only needs to extract the categories previously predicted and image embedding from BigQuery. The resulting predictions (top 100 product UUIDs per product, ordered by similarity) are saved to GCS.

3.3 Experiments

3.3.1 Visual Similarity

ann tfidf-based

3.3.2 Independent Models

3.3.3 Ensembling

3.3.4 Active Learning

3.4 Evaluation

At the beginning of running all these experiments, the dataset was divided into development and test set (90/10%). The development set was used for

we can evaluate the performance of the model on three types of datasets:

- the test or validation set as labelled by the rule-based system (referred to as “rule-based test/validation set”),
- the ground truth dataset gathered before running most experiments,
-

4. Discussion

5. Conclusion

References

- [1] Sanjeev Arora, Mikhail Khodak, Nikunj Saunshi, and Kiran Vodrahalli. A compressed sensing view of unsupervised text embeddings, bag-of-n-grams, and LSTMs. In *International Conference on Learning Representations*, 2018.
- [2] Richard G. Baraniuk. Compressive sensing. In *42nd Annual Conference on Information Sciences and Systems, CISS 2008, Princeton, NJ, USA, 19-21 March 2008*, 2008.
- [3] Leonid Boytsov and Bilegsaikhan Naidan. Engineering efficient and effective non-metric space library. In *Similarity Search and Applications - 6th International Conference, SISAP 2013, A Coruña, Spain, October 2-4, 2013, Proceedings*, pages 280–293, 2013.
- [4] Leo Breiman. Bagging predictors. *Machine learning*, 24(2):123–140, 1996.
- [5] Emmanuel J. Candès, Justin Romberg, and Terence Tao. Robust uncertainty principles: Exact signal reconstruction from highly incomplete frequency information. *Information Theory, IEEE Transactions on*, 52(2):489–509, 2006.
- [6] Heng-Tze Cheng, Levent Koc, Jeremiah Harmsen, Tal Shaked, Tushar Chandra, Hrishikesh Aradhye, Glen Anderson, Greg Corrado, Wei Chai, Mustafa Ispir, Rohan Anil, Zakaria Haque, Lichan Hong, Vihan Jain, Xiaobing Liu, and Hemal Shah. Wide & deep learning for recommender systems. *CoRR*, abs/1606.07792, 2016.
- [7] Kyunghyun Cho, Bart Van Merriënboer, Caglar Gulcehre, Dzmitry Bahdanau, Fethi Bougares, Holger Schwenk, and Yoshua Bengio. Learning phrase representations using rnn encoder-decoder for statistical machine translation. *arXiv preprint arXiv:1406.1078*, 2014.
- [8] Ido Dagan and Sean P Engelson. Committee-based sampling for training probabilistic classifiers. In *Machine Learning Proceedings 1995*, pages 150–157. Elsevier, 1995.
- [9] Ali Mamdouh Elkahky, Yang Song, and Xiaodong He. A multi-view deep learning approach for cross domain user modeling in recommendation systems. In

REFERENCES

- Proceedings of the 24th International Conference on World Wide Web, WWW '15*, pages 278–288, Republic and Canton of Geneva, Switzerland, 2015. International World Wide Web Conferences Steering Committee.
- [10] Yoav Freund and Robert E Schapire. A decision-theoretic generalization of on-line learning and an application to boosting. *Journal of computer and system sciences*, 55(1):119–139, 1997.
 - [11] Surya Ganguli and Haim Sompolinsky. Compressed sensing, sparsity, and dimensionality in neuronal information processing and data analysis. *Annual review of neuroscience*, 35:485–508, 2012.
 - [12] Ian Goodfellow, Yoshua Bengio, Aaron Courville, and Yoshua Bengio. *Deep learning*, volume 1. MIT press Cambridge, 2016.
 - [13] Yves Grandvalet and Yoshua Bengio. Semi-supervised learning by entropy minimization. In L. K. Saul, Y. Weiss, and L. Bottou, editors, *Advances in Neural Information Processing Systems 17*, pages 529–536. MIT Press, 2005.
 - [14] Ruining He and Julian McAuley. Vbpr: Visual bayesian personalized ranking from implicit feedback. In *AAAI*, pages 144–150, 2016.
 - [15] Geoffrey E Hinton, Peter Dayan, Brendan J Frey, and Radford M Neal. The "wake-sleep" algorithm for unsupervised neural networks. *Science*, 268(5214):1158–1161, 1995.
 - [16] Geoffrey E Hinton, James L McClelland, David E Rumelhart, et al. Distributed representations. *Parallel distributed processing: Explorations in the microstructure of cognition*, 1(3):77–109, 1986.
 - [17] Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. *Neural computation*, 9(8):1735–1780, 1997.
 - [18] Zhiting Hu, Zichao Yang, Xiaodan Liang, Ruslan Salakhutdinov, and Eric P. Xing. Toward controlled generation of text. In Doina Precup and Yee Whye Teh, editors, *Proceedings of the 34th International Conference on Machine Learning*, volume 70 of *Proceedings of Machine Learning Research*, pages 1587–1596, International Convention Centre, Sydney, Australia, 06–11 Aug 2017. PMLR.
 - [19] Sergey Ioffe and Christian Szegedy. Batch normalization: Accelerating deep network training by reducing internal covariate shift. *arXiv preprint arXiv:1502.03167*, 2015.
 - [20] Eric Jang, Shixiang Gu, and Ben Poole. Categorical reparameterization with gumbel-softmax. *arXiv preprint arXiv:1611.01144*, 2016.

REFERENCES

- [21] Brian Keng. Semi-supervised Learning with Variational Autoencoders. <http://bjlkeng.github.io/posts/semi-supervised-learning-with-variational-autoencoders/>, 2017. [Online; accessed 1-April-2018].
- [22] Murphy Kevin. Machine learning: a probabilistic perspective, 2012.
- [23] Yoon Kim. Convolutional neural networks for sentence classification. *arXiv preprint arXiv:1408.5882*, 2014.
- [24] Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *arXiv preprint arXiv:1412.6980*, 2014.
- [25] Diederik P Kingma, Shakir Mohamed, Danilo Jimenez Rezende, and Max Welling. Semi-supervised learning with deep generative models. In *Advances in Neural Information Processing Systems*, pages 3581–3589, 2014.
- [26] Diederik P Kingma and Max Welling. Auto-encoding variational bayes. *arXiv preprint arXiv:1312.6114*, 2013.
- [27] Quoc V. Le and Tomas Mikolov. Distributed representations of sentences and documents. *CoRR*, abs/1405.4053, 2014.
- [28] Tomas Mikolov, Kai Chen, Greg Corrado, and Jeffrey Dean. Efficient estimation of word representations in vector space. *CoRR*, abs/1301.3781, 2013.
- [29] Christopher Olah. Understanding LSTM Networks. <http://colah.github.io/posts/2015-08-Understanding-LSTMs/>, 2015. [Online; accessed 30-March-2018].
- [30] Jeffrey Pennington, Richard Socher, and Christopher D. Manning. Glove: Global vectors for word representation. In *Empirical Methods in Natural Language Processing (EMNLP)*, pages 1532–1543, 2014.
- [31] Alec Radford, Luke Metz, and Soumith Chintala. Unsupervised representation learning with deep convolutional generative adversarial networks. *arXiv preprint arXiv:1511.06434*, 2015.
- [32] Jan Rygl, Jan Pomikálek, Radim Rehurek, Michal Ruzicka, Vít Novotný, and Petr Sojka. Semantic vector encoding and similarity search using fulltext search engines. *CoRR*, abs/1706.00957, 2017.
- [33] Burr Settles. Active learning literature survey. Technical report, 2010.
- [34] Burr Settles, Mark Craven, and Soumya Ray. Multiple-instance active learning. In *Advances in neural information processing systems*, pages 1289–1296, 2008.

REFERENCES

- [35] Nitish Srivastava, Geoffrey Hinton, Alex Krizhevsky, Ilya Sutskever, and Ruslan Salakhutdinov. Dropout: A simple way to prevent neural networks from overfitting. *The Journal of Machine Learning Research*, 15(1):1929–1958, 2014.
- [36] Harini Suresh. Vanishing Gradients & LSTMs. <http://harinisuresh.com/2016/10/09/1stms/>, 2016. [Online; accessed 30-March-2018].
- [37] Christian Szegedy, Wei Liu, Yangqing Jia, Pierre Sermanet, Scott E. Reed, Dragomir Anguelov, Dumitru Erhan, Vincent Vanhoucke, and Andrew Rabinovich. Going deeper with convolutions. *CoRR*, abs/1409.4842, 2014.
- [38] Antti Tarvainen and Harri Valpola. Weight-averaged consistency targets improve semi-supervised deep learning results. *CoRR*, abs/1703.01780, 2017.
- [39] Hao Wang, Naiyan Wang, and Dit-Yan Yeung. Collaborative deep learning for recommender systems. In *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 1235–1244. ACM, 2015.
- [40] Xiang Wei, Zixia Liu, Liqiang Wang, and Boqing Gong. Improving the improved training of wasserstein GANs. In *International Conference on Learning Representations*, 2018.
- [41] Zichao Yang, Zhiting Hu, Ruslan Salakhutdinov, and Taylor Berg-Kirkpatrick. Improved variational autoencoders for text modeling using dilated convolutions. *arXiv preprint arXiv:1702.08139*, 2017.
- [42] Fisher Yu and Vladlen Koltun. Multi-scale context aggregation by dilated convolutions. *CoRR*, abs/1511.07122, 2015.

Declaration

I hereby certify that I have written this thesis independently and have only used the specified sources and resources indicated in the bibliography.

London, UK, April 21, 2018

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Mattias Arro

A. Screenshots

A.1 Dataprep Histogram



Figure A.1. Dataprep: the histograms of field values of a subset of fields.