Searching Github Python repositories with machine learning

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Chapter 1

Introduction

1.1 Introduction

As of 2021, we observe several years of increased adoption of neural network methods in NLP. There is evidence that language models trained on massive datasets capture various aspects of these datasets. As an evidence for that task one can point to transformer-based neural network models which are able to generate Python code. An example is OpenAI Codex ¹ [5], which is reported to generate programs like simple backend APIs given their descriptions. Even though the models aren't explicitly trained to generate code, the model is able to generate programs, because massive datasets used for training language models contain code.

For example 'gpt-neo-2.7B', a model that is available in opensource hugging-face library, asked to complete prompt:

```
C: def f1(x, y): return x + y
Q: what does this function do
A: addition
###
C: def f2(x, y): return x * y
Q: what does this function do
A:
```

Answers with "multiplication"

¹https://openai.com/blog/openai-codex/

There is increased interest in machine learning models for developer tools. Tools like Kite and Tabnine² use language models for improved autocomplete, which are already available for IDEs and text editors.

In the following we propose a dataset and methods for searching Python machine learning repositories using natural language descriptions.

1.2 Use cases

Github repositories are a standard way to share open-source projects. Software engineers, and to a greater extent data scientists often encounter a situation where for a given novel problem they need to find a solution, possibly for a slightly different problem. This is especially important for a problem that might require machine learning, because this domain is far less standardized than traditional software engineering, and some data science problems might be divided into smaller suproblems which might need less known solutions.

For an example take the task of developing system for reading information from billboards. Whereas some Optical Character Recognition methods are well explored, they are heavily biased towards regular text. If our solution has to read billboards that contain curved text, then we will have to use methods that are far less standardized than reading documents. In this problem, we know that these methods might underperform on curved text. Because of this we might try to search for curved text detection.

"Curved text detection" which the developer might guess as a search query is a phrase that actually occurs in some research papers. In many real world problems we will not have this luxury.

1.3 Searching on github

Github (as of 2021) provides a search interface that can be used to search repository names, its README files, and topics. This functionality is good when we have a good idea for a query, but it suffers from usual problems of bag-of-words model of information retrieval.

Our work can be described as improving Github's topic functionality. Topic labels (which are optionally specified by repository contributors) are very useful for information retrieval. Nonetheless, searching using topics has two problems:

• because they are optional, many projects have few or none topics specified

²https://github.com/codota/TabNine

 topic names are not standardized, so repositories for synonymous topics are not trivial to find

We propose to tackle this information retrieval problem using progressively relaxed assumptions:

- 1. repository is described by paper abstract
- 2. repository has a README file
- 3. repository has none of the above only code is available

Each step of this hierarchy corresponds to growing usefulness of the system. In general we cannot assume that a repository will easily match any paper, and dropping README requirement might be helpful as it might make useful code accessible even before authors decide to summarize their work.

Whereas coming from step 1 and 2 is straightforward, dropping single document representation of a repository poses a hard problem:

- methods need to change, because repository contains multiple code files and there is no single natural way to represent a set of files.
- even though there exist models that potentially can use both code and natural language as input, using pretrained models without finetuning results in poor performance ??

1.4 Papers with Code

Papers with Code is a service for machine learning researchers and practicioners that aims at bringing order to research publications. It extracts paper metadata so that papers for similar tasks may be grouped together, and compared if they provide results for the same problem. For our topic the most important are github implementation links and Papers with Code tasks.

The tasks are short descriptions of problems like Language Modeling or Semantic Segmentation.

In total there are 1625 tasks. PapersWithCode groups them into areas:

area	number of tasks
adversarial	9
audio	28
computer-code	37
computer-vision	500
graphs	49
knowledge-base	22
medical	181
methodology	138
miscellaneous	125
music	16
natural-language-processing	341
playing-games	38
reasoning	15
robots	26
speech	51
time-series	49
total tasks	1625

For example area computer-code contains following tasks:

1.5 Code Search

Programming is like standing on the shoulders of the giants - developers mostly compose previously written libraries instead of writing code from scratch.

Because of this, significant time is spent on finding useful code, either in form of snippets or whole libraries.

In their review paper Chao Liu et al [13] propose several groups of issues ³ faced by code search research . Our problem mostly tries to tackle challenges 3 (model fusion) and and 5 (search tasks) because it is a novel search task. Because it is so novel we cannot use existing models trained on other tasks, so this work also tries to fuse different models or aggregate representations from different models.

1.6 Contributions

In the following we will work on addressing the drawbacks of standard bag-ofwords Github search by leveraging structure of code repositories and NLP techniques for their natural language descriptions.

³section 3.2.0.1 goes into more detail

Table 1.1: Tasks from 'computer code' PapersWithCode area. Missclassifed tasks are highlighted in red

task

code-comment-generation

codesearchnet-java

single-image-portrait-relighting

text-to-sql

annotated-code-search

sparse-subspace-based-clustering

sentinel-1-sar-processing

program-synthesis

sql-synthesis

swapped-operands

api-sequence-recommendation

formalize-foundations-of-universal-algebra-in

wrong-binary-operator

low-rank-compression

variable-misuse

program-induction

code-search

function-docstring-mismatch

fault-localization

semi-supervised-semantic-segmentation

enumerative-search

write-computer-programs-from-specifications

program-repair

type-prediction

code-summarization

webcam-rgb-image-classification

sql-to-text

exception-type

code-generation

learning-to-execute

value-prediction

log-parsing

sql-chatbots

contextual-embedding-for-source-code

git-commit-message-generation

To this end we propose semantic search system on top of features extracted from code.

Specifically we propose a dataset for information retrieval on Github repositories using their natural language descriptions given by PapersWithCode tasks.

Several methods are proposed for feature extraction from code are proposed and evaluated.

These approaches roughly fall into two categories:

- use structural properties of repositories (leveraging node embeddings obtained from Python dependency graph ⁴)
- aggregate lower-level features extracted from code snippets

⁴defined in 4.3.2

Chapter 2

Theoretical background

2.1 Information Retrieval

IR is a sub-branch of Computer Science that investigates systems that enable searching on unstructured data.

In this domain we typically model process of search by assuming that user gives **queries** which are answered by **relevant documents**.

To formalize this, we define **gold standard** results as queries $(q)_{q \in Queryset}$ with their respective relevant document lists $(Rel_q)_{q \in Q}$.

In text retrieval setting for example queries are typically short sequences of words, and the documents come from agreed-upon corpus.

Our problem is akin to multilingual search, and belongs to **multimodal** search, because we match features extracted from natural language for queries, and different features (extracted from code using potentially different model, or from its graph structure) for repositories. Repository representations are aggregated from code features, which are not necessarily extracted the same way as for queries.

In other words we are in the domain of Information Retrieval, but we cannot use classical techniques as-is because of vocabulary mismatch, and semantic gap between natural language and code. Traditional techniques based on inverted index and bag of words work very poorly in this case.

TODO: przykład

2.1.0.1 Evaluating Information Retrieval

2.2 [TODO] Neural Networks

(basic definitions)

2.3 Neural Networks for unsupervised text feature extraction

Although some neural network approaches have long history, with Recurrent Neural Networks being proposed in 80s, it is only the 2010s that witnessed widespread adoption of practical methods.

2.3.0.1 Classical approaches for text data

Pre-neural machine learning methods were mostly based either on linguistical information (part of speech tags, grammatical information) for sequences, or use token or ngram ¹ count data.

One standard method of obtaining text features is the so-called Bag of Words model where documents are treated as sets of characters, words or ngrams. In the following by ngrams we will mean tuples of tokens or words unless it is specified otherwise.

The drawback of manual labeling is that it can't be easily scaled to leverage massive unlabeled text datasets obtained from book corpuses or crawling the web.

Bag-of-words model on the other hand runs into problems with polysemy (the same word might mean different concepts) and synonymy (different tokens define features which are completely unrelated). This approach also poses problems for machine learning methods that suffer from high dimensionality, because for representing reasonably sized corpus one typically needs to use thousands of features. In general optimization problems become harder, and some algorithms, notably tree-based models, fare poorly in such regimes.

2.3.0.2 Language modeling

Language modeling (LM) is a problem of predicting words from their contexts (in the simplest version the problem is to predict next word given preceding text).

Formally the task is to model probability $p(w_t|(w_t')_{t' < t})$

Language Modeling is an old subdomain of artificial intelligence, because for a given corpus one can easily define this probability using word cooccurrences. While this approach was shown to be useful for some tasks like machine translation, it suffers from the same problems as Bag of Words approach. Since it is not possible to estimate probabilities for every accurately using only n-gram counts, generalization capabilities of such models are limited.

 $^{^{1}}n$ gram is a length n subsequence of characters or words from the text

2.3.0.3 Why are neural networks useful for NLP?

Neural models in NLP have several advantages compared to older feature extraction methods. These methods typically contain a part that passess tokens (or their parts) through lower-dimensional representation (this is called **an embedding**). This embedding phase distills linguistic information so that network might generate similar outputs for similar inputs. The exact similarity depends on the method and might encode different aspects - for example Word Embedding methods capture *distributional similarity* as in the phrase "*linguistic items with similar distributions have similar meanings*" One might compare intermediate representation obtained in this way to compression, because it works by encoding information about tokens (which might come from a very big vocabulary, typically thousands of tokens) using fewer parameters (typically several hundred features).

Another advantage compared to older methods is that neural networks are highly composable, which is important for *transfer learning* - for example given a pretrained neural LM one might put classification layer on top, which would turn it into a sequence labeling model.

1. Neural vs count-based Language Models

To compare neural and count-based language models consider the task of estimating probability of a word given previous word, formally p(w|v). In count-based LM we would use p(w|v) = count(w,v)/count(v) (in general left size might be proportional to right size to use smoothing, for example to account for rare words) Note this approach needs to store V0 parameters.

In contrast neural-based method might use $p(w|v) = f_{\theta_0}(g_{\theta_1}(w), h_{\theta_2}(v))$ Where f, g, h are some neural network parametrized by $\theta_0, \theta_1, \theta_2$. Because in each of these networks only input or output depends on |V|, but not both, and the number of parameters is sum of θ sizes, number of parameters is O(|V|).

2.3.0.4 Recurrent Neural Networks

RNN is a neural sequence model that in addition to using current input also contains connections with previous input. This architecture makes it possible to propagate information along the sequence, which in theory can be arbitrarily long.

Concretely one layer of RNN takes two inputs x_t , h_t (called *hidden state*) and provides two outputs y_t , h_{t+1} (we omit bias for notational convenience)

$$y_t = \sigma(W_y h_t)$$

$$h_t = \sigma(W_h h_{t-1} + W_x x_t)$$

Where σ is some kind of nonlinearity.

Because h_t depends on h_{t-1} , output at time t is influenced by hidden states for t' < t. Note that number of parameters for such network does not depend at sequence length at all.

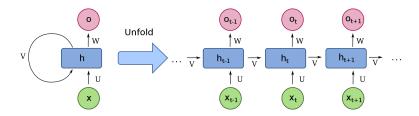


Figure 2.1: folded (left) and unfolded (right) RNN diagram

Procedure for training RNNs is called Backpropagation Through Time and is illustrated in the image above. This works almost like training regular feedforward network, but the parameters of connections for each step are tied.

- 1. [TODO???] Problems with RNNs LSTM and Gated Units
 - ELMO, AWD-LSTM?

2.4 Neural Language Models

First neural LMs were using RNNs where predicted sequence was shifted to the right (at time t, given x_t try to predict x_{t+1})

These models were shown to be useful for various NLP tasks in *Natural Language Processing (Almost) from Scratch* [6] . Authors used the method to work only using text. The obtained results were close to previous state-of-the-art approaches that used hand-crafted features, while using significantly simpler models.

2.4.1 Word embeddings

Training LMs using RNNs requires unrolling which is hard to parallelize. This makes it time-consuming, and sometimes useful word embeddings might be obtained not using information about whole sequences.

image from https://2d3d.ai/index.php/2019/11/11/the-deep-learning-dictionary/

Simpler methods for word embeddings, only making use of fixed-size contexts, were proposed based on *distributional hypothesis*. They obtain word vectors such that vector(w) is similar to vector(w') if w and w' occur in similar contexts, for example "Italy" and "France".

These methods given a sequence $(w_0, w_{t-1}, w_t, w_{t+1}, ..., w_{T-1})$ try to predict w_t by the rest of the context.

$$p(w_t, (w_0, w_{t-1}, w_{t+1}, ..., w_{T-1})) = \prod_{i < T, i \neq t} p(w_t | w_i)$$

1. Word2Vec

This method, proposed in Mikolov et al, 2013 [15] is posed as a standard classification problem and solved using a shallow neural network.

Let us denote by W the matrix of weights such that W(w) is the w's embedding.

Formally
$$p(w_t|w_i) = \frac{e^{W(w_t)^T W(w_i)}}{\sum_k e^{W(w_t)^T W(w_k)}}$$

The model is thus trained to minimize

$$\mathcal{L} = -\mathbb{E}_w[log(p(w_t, (w_0, ..., w_{t-1}, w_{t+1}, ..., w_{T-1})))] =$$

$$= -\mathbb{E}_w[\sum log(p(w_t|w_j)] = \mathbb{E}_w[\sum log(\frac{e^{W(w_t)^T W(w_j)}}{\sum_k e^{W(w_t)^T W(w_k)}})] =$$

$$\mathbb{E}_w[\sum W(w_t)^T W(w_j) - Tlog(\sum_k e^{W(w_t)^T W(w_k)})]$$

The weights between input and hidden layer can be then used as word vectors. Empirically they have been shown that they capture the similarity of words that have similar contexts. In addition to that it also has been shown that geometry of these word embeddings encodes semantic relations, for example

$$vector("king") - vector("man") \approx vector("queen") - vector("woman")$$

The exact formulation has the problem in that would require $W_i^T W_k$ for all i, j. This is unfeasible, as it is $O(|Vocab|^2)$.

In practice this is circumvented either using *hierarchical softmax* or *negative sampling*.

Negative sampling approximates

$$\mathbb{E}_w[\sum W(w_t)^T W(w_j)] \approx \sum_{(w_t, w_j) \in Pos} log \sigma(W(w_t)^T W(w_j))$$

Where $(w_t, w_j) \in Pos$ means these words occur in some context in data and

$$log(\sum_{k} e^{W(w_t)^T W(w_k)}) \approx \sum_{(w_t, w_j) \in Neg} log(\sigma(-W(w_t)^T W(w_j)))$$

where $(w_t, w_i) \in Neg$ are sampled randomly.

2. FastText

One problem of using words as tokens is that they treat them as atomic units, so either tokens need to be stemmed or lemmatized, or they will get treated as unrelated.

A series of papers from starting from Bojanowski et al, 2017 [3] proposed to refine Word2Vec model with subword information. These methods split words into tokens, for example "technical" might be split into "techn*" "*ical", so it will have similar parts with "technician". Although pretrained language models can be used to extract good representations in context, it remains a

In our work FastText is useful for embedding Python function names, as it might figure out that for example "get_http_request" is not an atomic entity.

Although pretrained language models can be used to extract good representations in context, it remains a

2.4.2 [TODO???] Attention and Transformer-based models

2.4.2.1 Sentence embedding models

Although pretrained language models can be used to extract good representations in context, the representations of whole documents they provide are poor because they need a pooling step to represent a document.

Because of this various methods were proposed to finetune

There are two most known ways to finetune pretrained transformers for search:

1. **bi-encoders** (also known as dual encoders).

These models are trained by using pairwise similarity of document features. Typically these features are done by feeding texts into transformer models and pooling, so that each document is represented by fixed-length vector. These vectors are compared using a similarity function like cosine similarity which serves as a relevance score.

2. cross-encoders

In this method a text that is a concatenation of query and relevant document is fed into a transformer model. The model itself outputs relevance score.

In practice cross-encoders tend to give better results. This intuitively makes sense because they can use attention over tokens from query and document.

Unfortunately cross-encoders have serious drawback, as at search time they require running transformer for each document. Thus cross-encoders mostly remain useful for finetuning tasks. Bi-encoders are used widely because they only require extracting feature from each query, and finding matching documents can be used with vector search engines.

2.5 Zero-shot Learning

Because our queries and features come from possibly different modalities (natural language vs code or its representations) we cannot easily use standard ranking methods for information retrieval.

To circumvent this, and also the fact that we cannot use supervised learning (test queries are not seen in training set) we use zero-shot learning.

Zero-shot Learning (ZSL) is a branch of Machine Learning where classes from test set possibly do not occur in training set.

Because it is impossible to transfer between seen to unseen classes using label encoding or one-hot encoding, to sidestep this ZSL assumes that classes are represented by their feature vectors.

These features might be manually constructed as shown in the following image, or they might consist of NLP-extracted features of class names.

To evaluate ZSL a protocol was proposed in [27] that takes into account the fact that accuracy on test set will be lower also because the classes were not seen - the authors propose to use harmonic mean of training/validation and test accuracies.



Figure 2.2: samples from AWA2 dataset showing images and class features

2.5.0.1 TODO - ZSL algorithms

2.6 Graphs in Machine Learning

There exist numerous methods for analyzing graph data that are based on random walks (PageRank, Node2Vec) or graph Laplacian matrix.

Graph Laplacian is defined as

$$L = D - A$$

where D is diagonal matrix where $D_{ii} = degree(v_i)$, and A is adjacency matrix.

Methods that use Laplacian matrix, like spectral clustering, typically work by decomposing L, so they can be used for dimensionality reduction.

It is also worth mentioning that many methods for nonlinear dimensionality reduction like Isomap or tSNE also use graphs. These methods utilize nearest-neighbor graph, in the case of Isomap a distance between points of data manifold is estimated from this graph.

In the following we will focus on Graph Neural Networks (GraphSAGE in particular).

Most older methods for node embeddings are *transductive*, so they assume the same graph structure at training time and test time. This can be problematic, because it means that models embed every vertex separately, which means that these models have O(|V|) parameters. To circumvent this *inductive* models like GraphSAGE were introduced.

2.6.0.1 Graph Neural Networks

Using neural networks for graph-structured data is problematic, because

- node neighborhoods $\mathcal{N}(u)$ may vary in size, and NN layers usually assume fixed-size input
- there is no natural ordering on neighbors

First issue is less severe because we might just sample neighbors so that their number becomes fixed in each iteration. The second one is usually circumvented by explicitly making output layer *permutation invariant* or *equivariant*.

Formally, let us assume that our NN layer f takes A, graph adjacency matrix as input.

Then

$$f(PAP^T) = f(A)$$

means that the layers is permutation invariant, whereas

$$f(PAP^T) = Pf(A)$$

means permutation equivariance.

2.6.0.2 General framework, message passing

The general approach for defining GNNs is called *message passing* and can be interpreted as generalization of convolution to graph data or differentiable graph isomorphism test. The intuition is to incorporate information from neighborhoods so that after each epoch it propagates through graph.

Formally specifying one layer consists of defining node's u embedding $h_u^{(k+1)}$ (superscripts denote layer number).

 $h_u^{(0)}$ are either initialized with some other methods (for example using word embeddings of node names) or by using graph features (node degree et c).

The embeddings of next layer are then

$$m_{neigh}(u) = \operatorname{AGGREGATE}(\{h_v^{(k)}\}_{v \in \mathcal{N}(u)})$$

$$h_u^{(k+1)} = \text{UPDATE}(h_u^{(k)}, m_{neigh})$$

where UPDATE and AGGREGATE are some differentiable functions.

Note that second argument of UPDATE is a set, so this part needs to be permutation invariant. This can be achieved using functions that don't depend on ordering of the input. It is usually achieved using pooling functions like averaging or taking maximum, or by averaging method that is order-sensitive (like LSTM encoder) over sample of permutations.

2.6.0.3 GNN

2.6.0.4 Scalability, GraphSAGE

It is easy to come up with vectorized form of GNN equation that takes the whole graph into account to enable whole batch gradient descent:

$$H^{(k+1)} = \sigma(W_{self}^{(k)}H^{(k)} + AW_{neigh}^{(k)}H^{(k)} + b_k)$$

Where A is graph's adjacency matrix. The problem with this equation is that it is not easy to turn this into minibatch version. This is because the second appearance of $H^{(k)}$ cannot be just replaced by batched version - one would need to take neighbors into account.

Because of this, several approaches for scaling GNNs were proposed.

One such example is GraphSAGE proposed in Hamilton et al, 2017 [10] It creates minibatches by sampling nodes, and creating fixed size contexts from their neighbors.

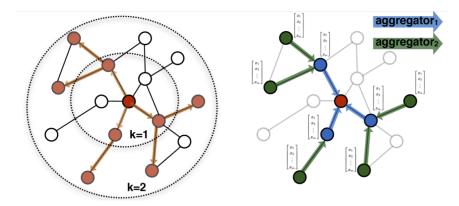


Figure 2.3: GraphSAGE: SAmple and AggregatE

Formally, for each minibatch B, K -layer GraphSAGE fetches embeddings of nodes sampled from K -hop neighborhoods of each $u \in B$.

This is achieved by the following algorithm:

2.6.0.5 [TODO???] Deep Graph Infomax

Method related to Masked Language Models

image from http://snap.stanford.edu/graphsage/

```
Algorithm 1: name embedding generation (i.e., forward propagation) algorithm
```

```
Input: Graph \mathcal{G}(\mathcal{V}, \mathcal{E}); input features \{\mathbf{x}_v, \forall v \in \mathcal{V}\}; depth K; weight matrices \mathbf{W}^k, \forall k \in \{1, ..., K\}; non-linearity \sigma; differentiable aggregator functions AGGREGATE_k, \forall k \in \{1, ..., K\}; neighborhood function \mathcal{N}: v \to 2^{\mathcal{V}}

Output: Vector representations \mathbf{z}_v for all v \in \mathcal{V}

1 \mathbf{h}_v^0 \leftarrow \mathbf{x}_v, \forall v \in \mathcal{V};
2 for k = 1...K do
3 | for v \in \mathcal{V} do
4 | \mathbf{h}_{\mathcal{N}(v)}^k \leftarrow \mathsf{AGGREGATE}_k(\{\mathbf{h}_u^{k-1}, \forall u \in \mathcal{N}(v)\});
5 | \mathbf{h}_v^k \leftarrow \sigma\left(\mathbf{W}^k \cdot \mathsf{CONCAT}(\mathbf{h}_v^{k-1}, \mathbf{h}_{\mathcal{N}(v)}^k)\right)
6 end
7 | \mathbf{h}_v^k \leftarrow \mathbf{h}_v^k / \|\mathbf{h}_v^k\|_2, \forall v \in \mathcal{V}
8 end
9 \mathbf{z}_v \leftarrow \mathbf{h}_v^K, \forall v \in \mathcal{V}
```

Chapter 3

Related work

3.1 Mining Software Repositories conference

Using NLP and more generally machine learning for analyzing code has long history. Mining Software Repositories (MSR) [1] is an example conference on this topic, existing from 2004.

Papers submitted to MSR typically focus on several tasks:

- software error detection and correction
- mining software QA sites
- mining metadata (commit history et c) of sotware projects
- NLP in software engineering

Another research track relevant to our work is using neural networks for feature extraction from code. These features are then used for code classification, generation or search.

3.2 Programming languages as machine learning data

3.2.0.1 Code Search

Code search which is one of the most significant programming activities is not well researched topic. Chao Liu et al [13] review papers that try to tackle this problem, and they identify several issues that might explain this relative obscurity. The authors hypothesize that due to lack of standardization and big, clean datasets it is hard to talk about progress in this area. They identify several issues with code search that are typically solved by the papers:

- 1. benchmarks providing datasets for relevant problems
- 2. learning models coming up with learning metrics, representation methods and new models
- 3. model fusion combining different kinds of models like classical information retrieval and deep learning
- 4. cross-language search building multi-language tools
- 5. search tasks solving novel search-related problems like searching code from programming video tutorials

3.2.1 Tasks

Code search tasks may be split into categories according to scale of expected results

type	microscopic	mesoscopic	macroscopic
expected re-	code snippet or method	file or bigger code	whole project
sults		fragment	
example	text-based code snippet	clone detection	find library or project (our
tasks	search	UI search	problem)
	IO based search	API search	

3.2.2 Performance metrics

3.2.3 Models

3.2.3.1 Code2Vec

3.2.3.2 CodeSearchNet

Husain et al 2019 [11] propose a dataset for semantic search of code snippets. They use pretrained CodeBert model Feng et al, 2020 [7] which is then trained for matching of function comments with code. This can be considered as microscopic version of our problem, as we propose to match **repositories** with descriptions.

3.2.3.3 Import2Vec

Theeten et al, 2019 [23] explore using Word2Vec model for extracting features of modules. Import2Vec is an unsupervised model which tries to classify whether two modules cooccur in some context. The approach proposed in this paper is most

relevant to our work, as it is the only approach that provides features for higher-level software objects. Whereas most work focuses on extracting features for code snippets or functions, Import2Vec provides features that can be directly used to featurize repositories.

3.2.4 Attention models

- 1. CodeSearchNet
- 2. CodeBERT
- 3. CodeT5

3.2.5 Auxillary techniques

3.2.6 Challenges

3.3 Programming language-specific feature extraction

In the following we list topics related to our problem and summarize important papers. The two approaches most relevant for our work are Language Models for code search and Import2Vec.

3.4 Hierarchical structure

Because repository code consists of files, which in turn consist of classes and methods defined in them, a natural question is:

RQ1: can we leverage this hierarchy to obtain better features?

The following work evaluates following approaches to use hierarchical structure of repositories:

- use definition dependencies (file contains functions, functions contain other subfunctions called in them etc) to create a graph that can be used to extract features
- summarize repositories using clustering methods
- 1. Hyperbolic geometry for exploiting hierarchical graph structure Embeddings of graphs, and more general, finite metric spaces into Euclidean spaces is a well-studied topic. An example fact about such embeddings is Johnson-Lindenstrauss Lemma.

A known fact about such embeddings is that they have large distortion for some classes of graphs. For example, there doesn't exist an isometric embedding of ternary tree into Euclidean space.

In contrast to this, for each tree there exists an embedding into 2-dimensional hyperbolic space with low distortion, as proved in Sarkar 2011 [21].

This fact justifies calling hyperbolic spaces continuous analogs of trees.

(a) Hyperbolic graph embeddings

Embeddings into hyperbolic spaces were first proposed in Poincaré Embeddings for Learning Hierarchical Representations [16].

Because of numerical issues with Poincare model (in this model hyperbolic space is represented by unit disk, where distances between points near the unit circle are unbounded) there have been proposals for improving this model using hyperboloid (Lorentz) model.

One of these is Hyperbolic Multidimensional Scaling proposed in Representation Tradeoffs for Hyperbolic Embeddings [20].

Comparing these methods is challenging, especially for larger networks, as some of them use distance matrices.

RQ: are embeddings into hyperbolic spaces feasible for big graphs?

Chapter 4

Data

4.1 Dataset

4.1.1 Sources

- 1. Project README
- 2. Python function call graph

4.1.2 Train-test split

Test queries were selected as 20% from each PapersWithCode area.

4.2 Data Sources

4.2.1 Raw Data

4.2.1.1 Papers

We use publicly available Papers with Code dataset

It contains paper title, abstract, and links to both arxiv pdf and github repository.

Dataset contains information about over 50 thousands papers and implementations.

Using this data we can extract paper tasks. Tasks were filtered to remove rare ones that had less than 10 papers. Papers without any task that occured 10 times or more were dropped.

 $^{1\,\}verb|https://github.com/paperswithcode/paperswithcode-data|\\$

There are TODO **tasks** that are used for queries. PapersWithCode groups them into areas:

area	number of tasks
computer-vision	107
miscellaneous	104
natural-language-processing	77
methodology	64
graphs	15
medical	14
speech	13
time-series	10
playing-games	9
robots	8
audio	6
knowledge-base	5
music	5
reasoning	3
computer-code	3
adversarial	3

4.2.2 Text corpora

- paper abstracts (only used in topline)
- Python code
- README files

4.3 Extracted datasets

4.3.1 Python functions

Using 'ast' Python files were parsed and then used to extract class and function definitions.

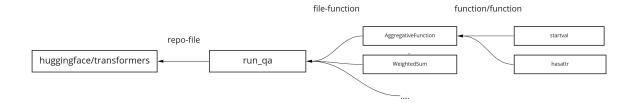


Figure 4.1: example subgraph

4.3.2 Python Dependency graph

We define a directed graph (V, E) where

 V_{repo} - repository edges

 V_{file} - files from repositorires

 V_{df} - functions defined in repositories

 V_{cf} - functions called in functions defined in repositories

 $V = \{ROOT\} \cup V_{repo} \cup V_{file} \cup V_{df} \cup V_{cf}$

Vertices from V form dependency hierarchy, where next level contains elements dependent on previous level elements.

This gives a natural definition of (directed) edges:

 $(v, w) \in E$ if w is defined/contained in v, where v is from one level higher (root-repo, repo-file, file-function, function-called function)

Chapter 5

Approach

5.1 Introduction

As a proxy for retrieval by natural language queries we evaluate retrieval of arXiv paper's Python repository given its PapersWithCode **task**.

Table 5.1: Gold standard results for 'anomaly detection' task

paper title	repository name	
PyOD: A Python Toolbox for Scalable	winstonll/SynC	
Outlier Detection		
Anomalous Sound Detection as a Sim-	OptimusPrimus/dcase2020_workshop	
ple Binary Classification Problem with		
Careful Selection of Proxy Outlier Ex-		
amples		
Learning Generalized Spoof Cues for	Podidiving/lgsc-for-fas-pytorch	
Face Anti-spoofing		
Combining Machine Learning Models	yzhao062/combo	
using combo Library		
Detecting Regions of Maximal Diver-	cvjena/libmaxdiv	
gence for Spatio-Temporal Anomaly		
Detection		

5.2 General ideas

5.2.1 Classical information retrieval

5.2.2 Feature extraction for documents and queries using NLP models

We experimented with information retrieval using the same model for queries and documents. These models can be trained to achieve reasonable effectiveness for abstracts/READMEs, for example learning pooled embeddings from transformer models [18].

These approaches fail to scale to whole repositories in a straightforward fashion. Bi- and cross-encoders were trained for similarity search using (task, representation) pairs for using representations of functions from a given repository.

Experiment results show that both using sentence-transformers on raw function code and summaries from sequence2sequence models perform poorly for retrieval using tasks.

- functions have lower abstraction level than paperswithcode tasks. The same exact function for image processing might be used either in image classification or image captioning repository.
- straightforward aggregation of task-function scores with max/mean fails to take into account the fact the degree function importances with respect to task.

Below we show distribution of task-representation scores produced by cross-encoder model, where representation is either function's Python code or its summary using T5 model finetuned on code.

TODO: show results and describe why they look like essentially random

5.2.3 Seq2Seq models

5.2.3.1 Summarization

We experimented with summarization models to predict tasks given Python file.

TODO: semantic IDs

Because code dataset is naturally hierarchicaly structured, we try to use file paths analogously to semantic document IDs from [22]. **pegasus <REPO SEP> pegasus/models/transformer.py**

5.2.4 Feature extraction and zero-shot learning

5.2.4.1 TODO schematic

Our system can be decomposed into two separate parts:

- 1. Repository feature extraction
- 2. Matching repository features with query features

5.2.4.2 Matching queries with repositories

We use Zero-shot learning (ZSL) methods because there is a need to match representations from different domains,

for example FastText vectors for query and graph-based representation of repository.

Existing Zero-shot learning methods typically model similarity between entities that use different representations.

This naturally fits our problem as most information retrieval models use query-document similarities to find most relevant documents.

5.2.4.3 Query features

Because ZSL needs class features, we evaluate several methods for extracting representations from PapersWithCode task names:

- pretrained word embeddings available in Gensim [17]
- word embeddings (FastText and Word2Vec) trained on Python file corpus

5.2.4.4 Repository features

Due to explosion of interest in transformer-based models in NLP there exist several methods enabling search beyond bag-of-words model.

This kind of functionality is very useful for cases where given specific query we want to find text fragment related to query, like in question answering models

Unfortunately this cannot be used as-is for repository search, because repositories contain multitude of such fragments.

This means that for repository search we would need to find method for extracting features from parts into more global features.

We use several methods to extract repository features

• text features extracted from README. These use either FastText or Word2Vec.

- Import2Vec features
- graph Node Embedding features (these methods are inductive, so the main point of using them is to compare their results to GNN features)
- GNN features extracted using GraphSAGE

5.2.5 Proxy ZSL problem

Zero-shot learning algorithms are used for matching task $\phi(t)$ features with repository $\psi(r)$ features. Using these features ZSL model comes up with a scoring function F(t,r) that measures how well repository r matches task t.

For simplicity we only use single-label Zero-Shot learning methods. For this we needed to extract single task that best describes the repository. One way to do this is to select **least common task**.

Using F(t,r) learned with ZSL methods we score task-repository similarities and for a given repository retrieve top k matched tasks.

5.2.6 Sentence embeddings

Using sentence transformers we can finetune models that are trained for various tasks like comment generation or summarization to extract features for whole texts.

5.2.6.0.1 Used datasets

5.3 Representation

- 1. Text data:
 - (a) Word2Vec
 - (b) FastText
 - (c) Transformer-based features
 - (d) Import2Vec
- 2. Dependency graph:
 - (a) Node embeddings
 - (b) GraphSAGE

Graph-based features are extracted for nodes in dependency graph, so for each repository we need to aggregate them from its constituents.

To do this we fetch file name node embeddings, and their average is taken to represent a project.

For transductive models like GraphSAGE we initialize node embeddings with text features (extracted from file names, functions et c).

These representations use either FastText trained on Python code corpus or embeddings CodeBERT model.

Chapter 6

Evaluation

6.1 Metrics

We envision two search scenarios:

- 1. Looking for a single or a few relevant projects from a given domain
- 2. Browsing projects.

In 1st scenario user is interested to retrieve at least one relevant project. Thus accuracy @ k is appropriate metric.

The 2nd case developer will be interested in having as many relevant projects as high as possible in result list. This can be captured using MAP (mean average precision).

6.2 Topline

Topline was established by matching queries (tasks) with paper abstracts.

6.3 Results

Repository	Query	Repository	Top-10
representation	embedding	embedding	accuracy
	model	model	
Abstract (topline)	Word2Vec	Word2Vec	0.828
README	Word2Vec	Word2Vec	0.687
README	Word2Vec	FastText	0.466
Imports	Word2Vec	Import2Vec	0.206
Graph	Word2Vec	ProNE	0.100
Graph	Word2Vec	GraphSAGE	0.244

6.4 Detailed results

More detailed results are shown that take into account not only literal task match, but also how many papers from related tasks (tasks from the same area as query) were retrieved. We also provide information about relative positions of recalled papers.

recalled mean		num_recalled mean	area_recalled mean	num_area_recalled mean	area_recalled_position median	count
area	mean	meun	incui	mean	median	
miscellaneou 3.45		1.17	0.91	0.91	3.0	133
computer-	0.48	1.46	0.97	0.97	0.0	123
vision						
methodolog	y0.56	1.26	1.00	1.00	1.0	77
natural-	0.31	0.81	0.92	0.92	3.0	74
language-						
processing						
graphs	0.47	1.59	0.82	0.82	1.0	17
medical	0.41	0.82	0.88	0.88	2.0	17
playing-	0.44	1.19	0.81	0.81	2.5	16
games						
speech	0.75	1.25	0.92	0.92	4.0	12
time-	0.45	1.09	0.82	0.82	6.0	11
series						
robots	0.30	0.70	0.50	0.50	inf	10
audio	0.33	0.50	0.67	0.67	0.0	6
computer-	0.25	0.25	0.25	0.25	inf	4
code						
knowledge-	1.00	2.00	1.00	1.00	2.0	4
base						
music	0.50	0.50	0.50	0.50	inf	4
adversarial	1.00	2.33	1.00	1.00	0.0	3
reasoning	0.00	0.00	0.00	0.00	inf	2

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