Learning to Represent Programs with Code Hierarchies

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Abstract

Graph neural networks have been shown to produce impressive results for a wide range of software engineering tasks. Existing techniques, however, still have two issues: (1) long-term dependency and (2) different code components are treated as equals when they should not be. To address these issues, we propose a method for representing code as a hierarchy (Code Hierarchy), in which different code components are represented separately at various levels of granularity. Then, to process each level of representation, we design a novel network architecture, ECHELON, which combines the strengths of Heterogeneous Graph Transformer Networks and Tree-based Convolutional Neural Networks to learn Abstract Syntax Trees enriched with code dependency information. We also propose a novel pretraining objective called Missing Subtree Prediction to complement our Code Hierarchy. The evaluation results show that our method significantly outperforms other baselines in three tasks: any-code completion, code classification, and code clone detection.

Introduction

Deep Learning (DL) for code has recently received increasing attention in the machine learning research community (Mou et al. 2016; Bui, Yu, and Jiang 2021c; Chen, Liu, and Song 2018; Chakraborty et al. 2020; Allamanis et al. 2018; Hellendoorn et al. 2019; Wang et al. 2020a,b). Various DL-based methods are proposed to process source code, for example, representing the code in a structure, such as Abstract Syntax Trees (ASTs) or graphs, and corresponding neural architectures are designed to process them, such as Tree-based Neural Networks (Mou et al. 2016; Bui, Yu, and Jiang 2021c), or Graph Neural Networks (Allamanis et al. 2018; Li et al. 2016; Hellendoorn et al. 2019; Fernandes, Allamanis, and Brockschmidt 2019). Graph-based models typically outperform tree-based models due to additional inductive biases introduced into the code graph via code dependency analysis (i.e. data-flow, control-flow, etc.) (Allamanis et al. 2018; Wang et al. 2020b) on a wide range of tasks, including bug detection (Allamanis et al. 2018), code summarization (Hellendoorn et al. 2019), and so on.

Understanding graphs in a multiscale perspective is essential for capturing the large-scale structure of source code. However, GNNs constructed by the message passing scheme (Scarselli et al. 2009; Duvenaud et al. 2015; Gilmer et al. 2017), in which each node propagates and aggregates vectorized information (i.e. messages) to and from the neighboring nodes, are inherently flat and unable to capture multiscale and hierarchical structures as suggested by Ying et al. (2018). In the setting of learning representations for source code, we recognize that GNNs have the following two major drawbacks that motivate our novel architecture and pretraining paradigm designed specifically to produce hierarchical representations. First, there is a long-term dependency problem or over-squashing (Alon and Yahav 2021) preventing nodes from effectively transferring messages. Second, code components are represented and processed equally although they should be treated differently. Indeed, almost all state-of-the-art methods adopt AST-based representations; nonetheless, the sizes of ASTs are usually large, which exacerbates the long-term dependency problem. Additionally, an AST is inherently hierarchical, so assuming all elements play the same role does not accurately reflect the relationship between different levels and within a level. Some previous works try to solve the problems above. For example, Bui and Jiang (2018) show that source code can be represented hierarchically, with fine-grained code components combined together to represent coarse-grained ones, e.g., tokens \(\Rightarrow\) statement, statements \(\Rightarrow\) function, and so on. This means that the corresponding code component can be processed according to its properties at each level of the hierarchy. However, Bui and Jiang (2018) only consider a simple hierarchical mechanism by averaging the low-level elements to represent their corresponding higher-level ones, that leads to the loss of structural information in interlevel communication. Yang et al. (2016) also mentions a similar concept of hierarchical structure of document in NLP, e.g., words \(\Rightarrow\) sentence and sentences \(\Rightarrow\) document. Inspired by these observations, we propose a novel framework to represent the source code as a hierarchy and use a combination of different neural network architectures to process each component in the hierarchy. In short, the key ideas of our approach are: (1) A novel hierarchical code representation by breaking the Abstract Syntax Tree into different levels of representation and enriching them with semantic information through edges, called Code Hierarchy. (2) A novel neural network processing such representations by combining the Heterogenous Graph Transformer and Tree-based Con-
volutional Neural Network (TBCNN), called \textit{ECHELON}.

In addition, we also propose a novel pretraining objective for our network. Recent works in large-scale language models of code have shown that pretraining the model over some unsupervised objectives and then fine-tuning it on downstream supervised tasks can improve the performance significantly \cite{Wang2021a,Feng2020,Bui2021b,Phan2021,Lachaux2021,Bui2021a}. In line with our framework, we observe that when splitting the subtree out of the AST, we can perform an objective that \textit{naturally fits with our process}, called \textit{Missing Subtree Prediction (MSP)} task in which we can mask out randomly subtrees and force the model to reconstruct them. Our evaluation results show that this pretraining objective can remarkably boost our model’s performance.

To summarize, our major contributions are as follows. (1) We create a novel code representation called \textit{Code Hierarchy} by breaking the AST into coarse-grained and fine-grained components, and adding semantic edges, e.g., control dependency, data flow, to the coarse-grained components. (2) We develop a novel neural network architecture that combines Heterogenous Graph Transformer and Tree-based CNN to process the \textit{Code Hierarchy}, called \textit{ECHELON}. (3) We propose a novel pretraining objective for our framework, named \textit{Missing Subtree Prediction} task, to predict the missing subtrees. (4) We evaluate or fine-tune our models on three tasks: any-code completion, code classification and clone detection, and conduct extensive evaluations. Experimental results show that our proposed model can outperform other strong baselines with large margins. (5) We demonstrate that \textit{ECHELON} can explain the predictions in a hierarchical fashion to some extent.

\textbf{Related Work}

\textbf{Structural Learning of Code} The \textit{naturalness hypothesis} \cite{Hindle2016}, demonstrates that program source code has properties similar to natural language, allowing us to develop statistical models for reasoning about programs. However, treating source code as a natural language may overlook its various unique properties, leading to a large number of recent works proposing to represent source code in structural representations, such as Abstract Syntax Tree (AST) \cite{Mou2016,Bui2021c,Chen2018,Chakraborty2020,Alamanis2018,Hellendoorn2019,Wang2020}. These models have been shown to be effective on a wide range of software engineering tasks, including code classification and bug prediction \cite{Nix2017,Dahl2013,Pascaru2015,Rastogi2013,LT2013,Li2015,Yang2015,Li2017,Zhou2019,Chen2019,Gu2017,Bui2018,Bui2019b,Nghi2019}, etc.

\textbf{Pretrained Language Models for Code} A large body of recent work employs language models from natural language processing for code \cite{Feng2020,Wang2021b,Guo2020,Ahmad2021,Bui2021a}. They mostly treat code similar to texts and adapt the same pretraining strategies as for natural language. CodeBERT \cite{Feng2020} adapts a Roberta model \cite{Li2019} to pretrain a model of code on multiple programming languages. CuBERT \cite{Kanade2020} pretrains a BERT model for code using a large dataset of curated Python files. GraphCodeBERT \cite{Guo2020} uses a data-flow pretraining strategy. CodeT5 \cite{Wang2021b} extracts unique identifier information from source code to pretrain the T5 \cite{Raffel2019} model for code in a multi-modal style. These models are designed to pretrain on very large-scale datasets in a self-supervised manner, thus they may perform better than structural learning techniques for code. This scaling feature is arguably the main key to make these large pretrained language models outperform smaller models, which have been carefully designed to be aware of syntactic and semantic aspects of code.

We hope to combine the best of both worlds through this framework. Our framework is made up of a new representation (Code Hierarchy) and a new neural architecture (ECHELON) that learns the structural and semantic features of code effectively; we also leverage the power of pretrained on large-scale datasets through a novel Missing Subtree Prediction task.

\textbf{Technical Details}

We give an overview of our approach. There are two stages: (1) Representing code into a novel representation called \textit{Code Hierarchy}; (2) Pretraining the code hierarchy with a novel architecture, \textit{ECHELON} on a novel Missing Subtree Prediction task, and fine-tuning on downstream tasks.

1. The first stage involves parsing a program into AST and extracting a set of subtrees at the statement- and expression-level. Then we transform the AST with the set of subtrees to acquire a novel code representation \textit{Code Hierarchy}. The Code Hierarchy is divided into two layers. The first layer is called \textit{Subtree-level layer} (lower-level layer), which represents statement-level and expression-level code components; each statement/expression is represented as a subtree, and each node in the subtree is the node from the original AST. The second layer is called \textit{AST-level layer} (higher-level layer) which represents code components from the AST which are not identified as subtrees. We enrich the nodes in the \textit{AST-level layer} by connecting them with semantic edges, e.g., control dependency and data flow, to transform the tree into a graph.

2. In the second stage, we design a novel neural architecture \textit{ECHELON} to process the Code Hierarchy. \textit{ECHELON} comprises two main components: The Tree-based Convolutional Neural Network (TBCNN) to process the Subtree-level, and the Heterogeneous Graph Transformer (HGT) to process the AST-level. We pretrain the \textit{ECHELON} first by performing a novel \textit{Missing Subtree Prediction (MSP)} task in which the statement subtrees in the first layer are randomly masked out, and then we use the surrounding context to predict those
missing subtrees. We then fine-tune the model on various downstream tasks after pretraining.

Our novel framework has three advantages. First, because many subtrees have been abstracted into single nodes at the AST-level, the size of the original AST is significantly reduced, making messages passing at the graph level more smoothly. Second, there are many options for processing code components at each layer. Assume that there are more advanced methods for processing the tree or the graph in the future; these can also be integrated into our framework. Third, the framework provides explainability in a hierarchical fashion, e.g., we will know which subtrees or which tokens in a subtree are important.

Representing Code as Hierarchy

We aim to identify and extract a set of subtrees \( S \) from an AST \( T \). Then we abstract each subtree by replacing it with a new node in \( T \) at the root location of the subtree, reducing \( T \) into another tree \( T' \) with a smaller size, where \( \text{Size}(T') < \text{Size}(T) \). We call the new nodes added to \( T \) as subtree nodes to distinguish them from the original AST nodes. The set of subtrees \( S \) is kept separately.

Such subtrees will then be extracted in the first layer of the Code Hierarchy. A subtree will be chosen if its root type is expression or simple statement; the set of subtree types can be looked up in our Supplementary Material. Specifically, a statement that does not contain other statements is considered as simple. The reason is that very large statements, such as for loops, while loops, or if statements, can contain complex code structures. In fact, such large statements may occupy a large portion of the content in some small programs, reducing the effectiveness of our MSP task.

These steps can be done by depth-first preorder traversal of the AST. If the type of a node \( n \) is in \( S \), we replace the whole subtree where \( n \) is the root, and we do not traverse further into lower depths. This procedure is executed recursively until all subtrees are obtained. Once done, we get a new tree \( T' \) and a set of subtrees \( S \). Note that some nodes (subtree nodes) in \( T' \) point to elements in \( S \). This feature is the key to representing the Hierarchy. Figure 1 depicts such a Code Hierarchy where node 5 is a new node in the tree \( T' \), and it represents a specific subtree with three nodes \( b, >, 0 \).

Enriching ASTs with Semantic Edges

Given the tree \( T' \) from the previous step, we enrich \( T' \) with semantic information to make \( T' \) become a graph \( G \). Such information is added to the AST-level by connecting the nodes with different edge types. Through our process, there are four edge types, including AST Edge, Control-Dependence Edge, Data-Flow Edge and Next-Subtree Edge. Each of them is described further below.

1. **AST Edge (AST-E)** \( T' \) consists of a mixture of original AST nodes from \( T \) and new subtree nodes, the AST edges serve as the syntactical representation of code. In Figure 1, AST edges are denoted as green arrows.

2. **Control-Dependence Edge (CD-E)** Control dependency occurs when a program instruction executes if evaluating the preceding instruction permits its execution. In Figure 1, the subtree \( \text{sum} = b \) is control dependent on the subtree \( b > 0 \), so \( b > 0 \) connects with \( \text{sum} = b \) through a control-dependence edge (red dashed arrows in Figure 1). Besides, to keep the order of execution in a function, we connect the root of one statement to the root of the next statement. As in Figure 1, for instance, there is a control-dependence edge connecting node 3 to node 4 where node 3 represents the declaration statement and node 4 is the root of the if statement.

3. **Data-Flow Edge (DF-E)** Data flow indicates how the values of variables change as a program is executed. We use Define-Use chain analysis (Weiser 1984), a well-known data-flow analysis technique to extract such information. For example, the variable \( \text{sum} \) is first defined in line 2, then it is used in line 4 and 6, then the subtree \( \text{sum} = 0 \) connects the two subtrees \( \text{sum} = b \) and \( \text{return sum} \) through data-flow edges (yellow arrows in Figure 1).

4. **Next-Subtree Edge (NS-E)** This edge type represents the textual order of subtrees, not the execution ones. For example, the subtree \( \text{sum} = b \) is written right after \( b > 0 \), but \( \text{sum} = b \) may not be necessarily executed after \( b > 0 \). With that, \( b > 0 \) connects with \( \text{sum} = b \) through a next-subtree edge (blue arrows in Figure 1).

Neural Network Architecture

In this section, we describe our ECHELON to process the Code Hierarchy obtained in the steps above. Our architecture consists of a Tree-based Convolutional Neural Network (Mou et al. 2016) (TBCNN) and a Heterogeneous Graph Transformer (Hu et al. 2020) (HGT). At first, each node in a subtree \( s \in S \) contains two attributes: token and type. The initial representation of a node can be computed by concatenating the embeddings of its token and its type, where such embeddings can be looked up from two embedding matrices (token embedding matrix and type embedding matrix) initialized randomly as the learnable parameters. A token is encoded as the sum of the embeddings of.
its subtokens by a lookup table, while the type embeddings are retrieved by another lookup table. Then, the TBCNN receives each vectorized subtree $s$ in the Subtree-level layer and encodes it into a fixed-size embedding. This embedding will also be used as the initial representation for the corresponding node in the graph at the AST-level layer. The HGT is then used to perform message passing on the nodes to accumulate information.

Tree-based Convolutional Neural Network (TBCNN) TBCNN (Mou et al. 2016) is designed to process tree-structure through the tree-based convolution operator. In a TBCNN, there is at least one tree-based convolutional layer. Each layer is a feature detector and has a fixed-depth convolutional window called the kernel, sliding over the entire tree to extract features. Formally, this procedure can be summarized as: $y = f \left( \sum_{i} W_{\text{conv},i} \cdot x_{i} + b_{\text{conv}} \right)$, where $f$ is an activation function, $W_{\text{conv},i}$ are the weight matrices, $x_{i}$ are the vectors of nodes inside the sliding window, and $b_{\text{conv}}$ is the bias. In summary, at each convolutional step, the feature activation function, $V$ represents a subtree, $E$ are the vectors of nodes inside the sliding window, and $b_{\text{conv}}$ is the bias. In summary, at each convolutional step, the feature of node $i$ is accumulated by its direct children in a sliding window simultaneously. At the end of this step, the fix-sized embedding of a subtree is computed by using a max pooling operator over all of the nodes in such subtree.

Heterogeneous Graph Transformer (HGT) A heterogeneous graph is defined as a directed graph $\mathcal{G} = (V_{t} \cup V_{2}, E, A, \mathcal{R})$ where $V_{t}$ is the node set where a node represents a subtree, $V_{2}$ is a set of non-subtree AST nodes, and $E$ is the edge set. Each node and edge are associated with the types $\tau(n) \in A$ and $\phi(e) \in \mathcal{R}$, respectively. As previously mentioned, the embedding of each node $v_{1} \in V_{t}$ can be computed from the TBCNN step. For each node $v_{2} \in V_{2}$, at first, we compute an initial vector by concatenating the embeddings of its token and its type, which is then fed to a 1-layer nonlinear network, then we annotate this node with the obtained vector. A HGT layer can be decomposed into three components: heterogeneous mutual attention, heterogeneous message passing, and target-specific aggregation. The overall process can be written as:

$$H^{2}[t] \leftarrow \text{Aggregate} \left( \text{Attention}(s, e, t) \cdot \text{Message}(s, e, t) \right)$$

where $N(t)$ is the set of source nodes of node $t$ and $E(s, t)$ denotes all the edges from node $s$ to node $t$. $H^{t}$ is the output of the $t$-th HGT layer, and the next layer receives it as the input. Given a node $t$, Attention(·) computes the score for each source node $s \in N(t)$, Message(·) extracts the message by using the source node $s$, Aggregate(·) is a operation where the node $t$ incorporates the messages of all the source nodes $N(t)$ (details are in our Supplementary Material).

Pre-training as Missing Subtree Prediction (MSP) Because training our model from scratch for each task is costly, we use a pretraining strategy to train a base model before fine-tuning it for downstream tasks. We propose a novel pretraining objective called Missing Subtree Prediction (MSP) which predicts a missing subtree as a sequence of tokens (which represents for that missing subtree) by its surrounding context. For example, if the masked node in the Figure1 is node 6, the model tries to predict the missing subtree as a sequence $\text{sum} = b$. We use the information of the AST-level layer and the other subtrees in the Subtree-level layer to predict a target missing subtree. By doing this, the model learns the relationship between different code components, both syntactically and semantically, i.e., how the other code components are organized structurally to reconstruct the subtrees. We feed all node embeddings from the HGT’s output into a vanilla Transformer decoder to predict the subtree token. Formally, given a set of training samples $D = \{ (n^{(s)}, y^{(s)}) \}_{s=1}^{S}$ where $n^{(s)}$ is the set of nodes after randomly masking one of the subtree nodes in the graph $G^{(s)}$, and $y^{(s)}$ is the token sequence of the masked node with the length $J^{(s)}$, the pretraining objective is to maximize log-likelihood of the training data:

$$\max_{\theta} \mathcal{L}(\theta) = \min_{\theta} \sum_{s=1}^{S} \sum_{j=1}^{J^{(s)}} - \log P \left( y^{(s)}_{j} | n^{(s)}, y^{(s)}_{<j}; \theta \right)$$

Applications

In this section, we describe how our model can be beneficial for different software engineering tasks. First, our pretraining objective naturally fits into a task called any-code completion (Alon et al. 2020). This task is to predict missing parts of a code snippet (statements, expressions, etc.) using existing contexts. Our pretraining goal is to mask a subtree and predict it by the context, which means that our pretraining model could be used directly on this task. Second, we can fine-tune our pretrained model for various downstream tasks. The downstream tasks in this paper are code classification and code clone detection. As such, these three tasks represent three ways to formulate different problems in software engineering: generation-based (any-code completion), classification-based (code-classification), and detection-based (clone detection). Code classification (Mou et al. 2016) is the task of classifying a given code snippet into a given functionality category, which is helpful to understand and extend existing source code. Code clone detection is the task of identifying if two code snippets are semantically equivalent, which is crucial for software maintenance. Note that fine-tuning for these 2 tasks is straightforward, we can apply the max pooling operator through all of the nodes after the HGT step and feed them through a feed-forward layer for classification.1

Empirical Evaluation

Model Pretraining with MSP

It should be noted that our model is language-agnostic. We choose Java and C++ as the two programming languages in our case to pretrain models. These models will then be used for evaluating or fine-tuning in the following sections.

For Java, we choose the Java-small (Alon et al. 2019) dataset, and the Java dataset from CodeSearchNet (Husain et al. 2019) (which is called Java-CSN to distinguish it from Java-small), which have been used for pretraining in previous work (Alon et al. 2020 Wang et al. 2021b Feng et al. 2020). Details of the loss function of these two tasks can be found in the Supplementary Material.
Metrics. We use the top-1 exact match accuracy (Acc@1) to predict the target as a sequence of subtokens. With a special token $<$mask$>$, and then train the network to predict the target as a sequence of subtrees.

From the above three datasets, we pretrain models for our MSP task, yielding three foundation models: ECHELON-Java-small, ECHELON-Java-CSN and ECHELON-C++.

**Any-code completion**

**Datasets.** We choose the test set of Java-small for evaluation including 19165 samples. For each sample, we randomly select one subtree for masking, resulting in 19165 test instances.

| Methods          | Acc@1 | BLEU |
|------------------|-------|------|
| SLM              | 5.31  | 23.96|
| Transformer      | 7.78  | 28.11|
| BiLSTM $\rightarrow$ LSTM | 6.37  | 26.77|
| **ECHELON-Java-small** | **10.02** | **31.51** |

Table 1: Results on any-code completion

**Baselines.** We choose SLM (Alon et al., 2020) as the baseline, which is the state-of-the-art technique for any-code completion task. We follow the steps described in the official artifact[1] to create and process our test instances that fit into the format of SLM for a fair comparison. Then we use the test API provided by SLM to evaluate our test instances. We also choose sequence-to-sequence models, including a vanilla Transformer (Vaswani et al., 2017) and a BiLSTM as other baselines. Given a code snippet, we replace the target with a special token $<$mask$>$, and then train the network to predict the target as a sequence of subtrees.

**Metrics.** We use the top-1 exact match accuracy (Acc@1) and BLEU (Papineni et al., 2002) as the metrics. The Acc@1 is defined as the generated prediction which is identical to the target sentence (ignoring cases and whitespaces).

**Results.** Table 1 shows that ECHELON-Java-small achieves the best results among the baselines in terms of Acc@1 and BLEU. Note that we do not perform any training here, but we use the foundation model ECHELON-Java-small to evaluate on the test instances of Java-Small. This demonstrates the effectiveness of using the Code Hierarchy as the context to predict missing subtrees.

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[1]https://github.com/tech-srl/slm-code-generation

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**Code Classification**

**Datasets.** We choose the POJ-104 (Mou et al., 2016) since it is one of the most well-known benchmarks for code classification. However, POJ-104 is said to be easy to achieve good results, and it is small-scale (52,000 samples for 104 classes). As we aim to perform a large-scale evaluation, we need to have a larger scale dataset. Therefore, we choose the C++1400 and C++1000 datasets from Project CodeNet (Puri et al., 2021), which are on a much larger scale for this task. The C++1400 is made up of many C++ programs that are organized into 1,400 classes. It consists of 267,413/83,562/66,868 samples for training/testing/validation.

**Baselines.** We follow Puri et al. (2021) to choose the baselines: MLP, CNN, C-BERT (Buratti et al., 2020), GCN (Kipf and Welling, 2017) and GIN (Xu et al., 2019) for the C++1000 and C++1400 datasets. For the POJ-104, we refer to Zhang et al. (2019) to choose ASTNN (Zhang et al., 2019), TBCNN (Mou et al., 2016), and PDG+GGNN (Allamanis et al., 2018) as the baselines.

**Results.** Table 2 shows the results of ECHELON. There are two settings, one trained from scratch - ECHELON w/o MSP, and the other is trained from fine-tuning from ECHELON-C++ - ECHELON with MSP. It is shown that we can achieve significant improvement with fine-tuning ($\approx 2\%$) compared to training from scratch for all of the datasets. The ECHELON with MSP is also the best among the baselines for the three datasets.

**Code clone detection**

**Datasets.** We follow Zhang et al. (2019) to create an OJ-clone dataset based on POJ-104 by sampling a subset from all pairs of clones and non-clones. There are 29,989/9,996/9,998 samples for training/validation/testing with 1,957/673/66,868 positive samples, respectively.

| Methods     | Precision | Recall | F1  |
|-------------|-----------|--------|-----|
| CDLH        | 47        | 73     | 57  |
| PDG+GGNN    | 77.3      | 43.6   | 55.8|
| **ASTNN**   | **98.5**  | 88.3   | 93.1|
| **ECHELON-C++** | **97.3**  | **96.3**  | **97.1**|

Table 2: Results on code clone detection

**Baselines.** We refer to the baselines used in ASTNN (Zhang et al., 2019) to evaluate the OJ-clone dataset. The first baseline is the ASTNN (Zhang et al., 2019), which is the SOTA method for clone detection on the OJ-clone. The others are CDLH (Wei and Li, 2017) and GGNN on the Program Dependence Graph (PDG + GGNN).

**Metrics.** We use Precision, Recall and F1 as the metrics.

**Results.** The results for code clone detection are shown in Table 2. Overall, ECHELON-C++ has the best performance in terms of F1. It outperforms the second-best baseline ASTNN by a large margin ($\approx 4\%$). Although ASTNN has higher precision, our approach is better with regard to recall and F1.
**Model Analysis**

**Impact of Different Edge Types**

In this section, we conduct an ablation study to analyze the impact of each edge type on the overall performance of our model. We keep the same neural architecture and change the code representation by removing edge types. Then we train different variants of ECHELON on the same datasets on the any-code completion and code classification. In Table 4 we can see that any of the dependency edges can improve the performance of any-code completion. This implies that the dependency information is useful for our Code Hierarchy. Among the three edge types, DF-E contributes the least to the performance in the any-code completion task while CD-E has the greatest impact. For code classification, NS-E has the strongest impact while DF-E still performs the worst. This implies two points: (1) The impact of each edge type varies depending on the downstream tasks; and (2) Data-flow information does not always perform well, and its impact should be investigated further. This result is consistent with the work of Zhou et al. (2019), as the data-flow edges perform poorly in their graph representation.

**Compare The Embedding’s Quality with Other Pretrained Models**

Despite the fact that different pre-trained models use different pretraining objectives, they all aim for the same result: after pretraining, the model should be able to produce similar vector representations for semantic-equivalent programs, and they should be close in the vector space. We compare the quality of vectors produced by our model with others to see how well ECHELON can perform in general. We choose CodeBERT (Feng et al. 2020) and CodeT5 (Wang et al. 2021) as the competitors since they are two of the most well-known and SOTA methods. These 2 models are pretrained on CodeSearchNet (Husain et al. 2019) with all of the datasets in 6 programming languages (Python, Javascript, Ruby, Go, Java, and PHP). For ECHELON, we choose ECHELON-Java-CSN, which is pretrained only on the Java dataset from CodeSearchNet.

For evaluation, we choose the Java250 from Project Codenet (Puri et al. 2021) that is collected for code classification task. The programs in a class can be seen as the semantically-equivalent ones. We feed the training partition of Java250 through our pretrained ECHELON-Java-CSN model, and we then use a pooling over all the node embeddings of each graph to obtain a representative vector for this graph. As CodeBERT is an encoder-only model, the extracted vectors represent the [CLS] tokens’ final hidden states. CodeT5 is an encoder-decoder model, so the features used are the hidden states of the [EOS] tokens after the last layer in the decoder. Subsequently, we cluster the obtained embedding vectors using K-means with k = 250 which is the number of the classes in Java250. We use Homogeneity Score (HS), Completeness Score (CS), V-measure Score (VMS) (Rosenberg and Hirschberg 2007) and Adjusted Rand Index (ARI) (Yeung and Ruzzo 2001) as the metrics to evaluate the performance of this clustering task. The detailed results in Table 5 demonstrate that ECHELON outperforms the others in terms of the four metrics. This implies that our pretraining goal is superior to the others in which it produces embeddings of semantic-equivalent programs that are closer in the vector space, which results in better performance in term of clustering-based metrics. In addition, we also visualize of the vectors produced by the 3 pretrained models.

### Table 4: Summary of the ablation studies. We use ECHELON-Java-small for any-code completion, and for code classification (Code C), we use ECHELON-C++.

| Methods               | Any-code Completion | Code C |
|-----------------------|---------------------|--------|
|                       | Acc@1               | BLEU   | Acc   |
| AST-E                 | 9.07                | 29.29  | 94.14 |
| AST-E + CD-E          | 9.71                | 30.53  | 94.30 |
| AST-E + DF-E          | 9.17                | 29.40  | 93.42 |
| AST-E + NS-E          | 9.54                | 30.23  | 94.71 |
| ECHELON               | **10.02**           | **31.51** | **94.73** |

### Table 5: Results of the code clustering task

| Methods               | HS     | CS      | VMS    | ARI   |
|-----------------------|--------|---------|--------|-------|
| CodeT5                | 0.2066 | 0.2146  | 0.2105 | 0.0112|
| CodeBERT              | 0.2246 | 0.2295  | 0.2270 | 0.0098|
| ECHELON               | **0.3300** | **0.3382** | **0.3340** | **0.0418** |

### Model Explainability

An interesting aspect of our approach that we want to show is the capability of explaining the prediction. To do this, we use the Contrastive gradient-based saliency maps (Simonyan, Vedaldi, and Zisserman 2014). This method is to differentiate the model output with respect to the input, which can be obtained by back-propagation. The inputs are the nodes in the graph $G$ in our case. This method assumes...
that the norm of a node’s gradient indicates its importance. However, because negative gradients are difficult to explain, the negative values are truncated to zeros to retain only positive values. After computing the scores for all nodes, we use min-max normalization to adjust the scores between 0 and 1. Note that this can be done in both the Subtree-level and the AST-level. We choose the code classification for this analysis. We randomly select a few examples in our C++1400 test set, and here we show one representative sample.

![Figure 2: Visualization on how scores are assigned to nodes](image)

Table 6: Top-10 nodes with corresponding tokens

| Node ID | Token                        |
|---------|------------------------------|
| 1       | using namespace std          |
| 15      | n == 0                       |
| 19      | while                        |
| 20      | n > 0                        |
| 5       | int main()                   |
| 21      | zero = zero + n / 5          |
| 13      | cin >> n                     |
| 22      | n = n / 5                    |
| 16      | break                        |
| 7       | main                         |

Figure 2 shows a visualization of the nodes in the AST-level. Each node is associated with a score, which represents the node’s importance given a prediction. Table 6 shows top-10 most important nodes, which are aligned with specific statements in the original source code. We can also visualize which tokens inside a statement are important.

The results in Figure 2 and Table 6 indicate our model captures the nodes having direct effects on the output; specifically, nodes 21, 13 and 22 are related to the data flow while nodes 15 and 16 are about the control flow. The appearance of node 1 may be due to its token being duplicated in many files, which probably confuses ECHELON. Nodes 19 and 5 are root nodes of the subtrees representing the while loop and the entire program respectively, thus they contain the information of their children apart from their own.

4Due to the page constraint, we only show the visualization at the AST-level, readers are referred to the Supplementary Material for the visualization of the Subtree-level

Discussion & Future Work

Here, we will cover other parts of our framework. By using Code Hierarchy, we modify how code is often represented (as a graph or tree), which somewhat solves the over-squashing issue [Alon and Yahav 2021] in “GNNs for code”. The Code Hierarchy reduces the size of a AST by moving a large number of nodes from the AST-level to the Subtree-level rather than keeping the code as a graph as in earlier work [Allamanis et al. 2018; Wang et al. 2020]. This will make the HGT’s message-passing steps on the AST-level easier. Through our evaluations, we have shown that ECHELON outperforms a few GNNs methods in different tasks. It shows that our model has the potential to address the over-squashing issue of the GNNs model of code. In fact, while in-depth analysis of this problem is not the primary focus of our paper, it is an interesting area for future research. Similar to Alon and Yahav [2021], we plan to perform additional analysis to fully assess our framework, with a focus on the over-squashing issue of GNN models of code on the Code Hierarchy. Moreover, our framework is adaptable, allowing us to pretrain the model using a variety of strategies, such as predicting missing edges (Guo et al. 2020), predicting missing variables (Wang et al. 2021a), predicting natural language descriptions (Wang et al. 2021a), etc. Such pretraining strategies can also be applied to our framework easily. In the future, we hope to create a unified pretraining framework that includes various types of pretraining tasks on top of Code Hierarchy.

For model explainability, in line with our work, there are many previous works that attempt to explain the output of source code models, including AutoFocus (Bui, Yu, and Jiang 2019a) and SIVAND (Rabin et al. 2021). They either use attention scores or simplify programs to remove redundant parts of source code for explainability. However, it is unknown whether such explanations are aligned with how developers understand code, which we believe is critical for the explainability on source code models. Extensive research on human evaluation is required to achieve this, but it is not the primary focus of our work.

Conclusion

In this paper, we present a novel framework for source code modeling. Our framework is comprised of three major components: (1) a novel code representation Code Hierarchy representing different code components at different layers; (2) a novel neural architecture ECHELON to process the Code Hierarchy, where each layer is processed differently with a suitable neural network and the output of the lower-level layer is used as the input for the higher-level layer; and (3) a novel Missing Subtree Prediction pretraining objective to pretrain our model. Our evaluation shows that our framework outperforms the other baselines significantly in three tasks: any-code completion, code classification, and code clone detection. We will target for more downstream tasks in the future.
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